



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:57 AM EDT

PDB ID : 1JRO / pdb_00001jro
Title : Crystal Structure of Xanthine Dehydrogenase from Rhodobacter capsulatus
Authors : Truglio, J.J.; Theis, K.; Leimkuhler, S.; Rappa, R.; Rajagopalan, K.V.; Kisker, C.
Deposited on : 2001-08-14
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

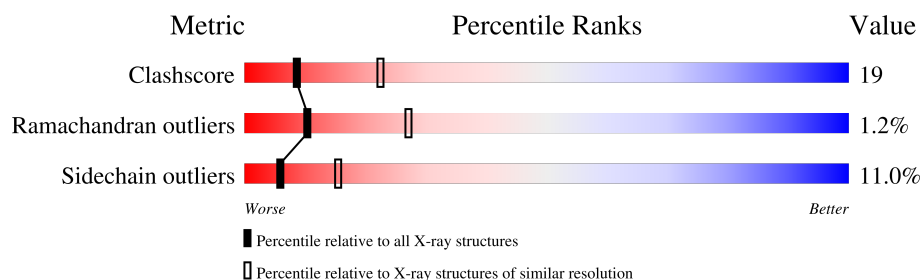
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	462	61% 29% 7% .
1	C	462	64% 26% 6% .
1	E	462	48% 38% 11% ..
1	G	462	47% 40% 9% ..
2	B	777	60% 31% 7% .
2	D	777	61% 30% 6% ..
2	F	777	56% 34% 7% ..
2	H	777	54% 34% 8% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	G	3001	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 36831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called xanthine dehydrogenase, chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	C	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	E	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	G	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			

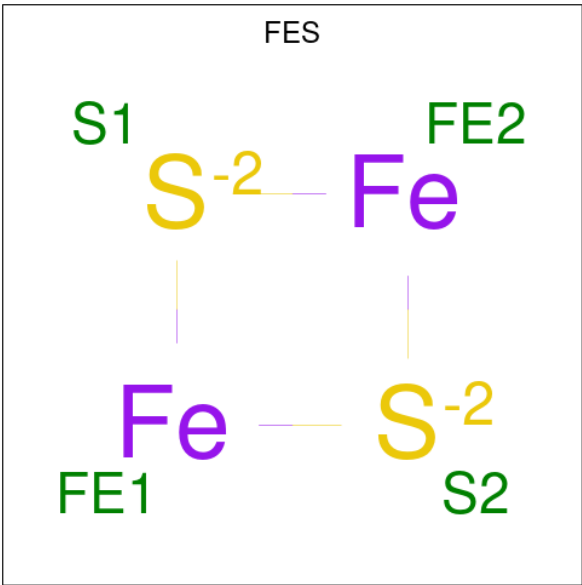
- Molecule 2 is a protein called xanthine dehydrogenase, chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	D	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	F	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	H	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			

There are 4 discrepancies between the modelled and reference sequences:

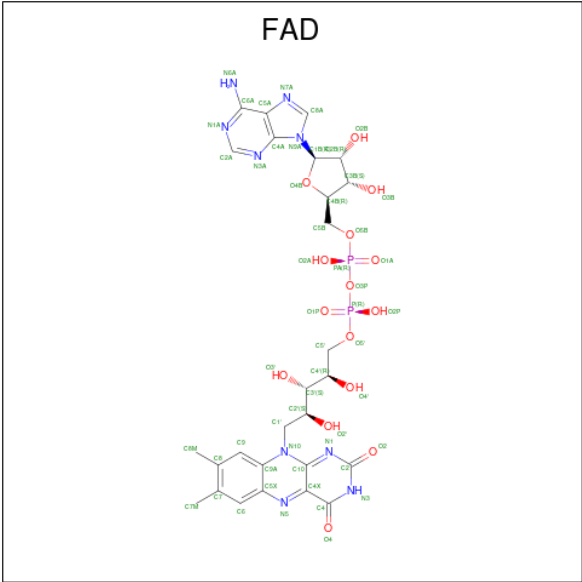
Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	conflict	EMBL 13397863
D	772	ARG	GLY	conflict	EMBL 13397863
F	772	ARG	GLY	conflict	EMBL 13397863
H	772	ARG	GLY	conflict	EMBL 13397863

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		

- Molecule 6 is Molybdopterin dihydroxy-thioxo-molybdenum (CCD ID: HOH) (formula: H₂O).

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	B	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	D	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
6	F	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
6	H	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		

- Molecule 7 is water.

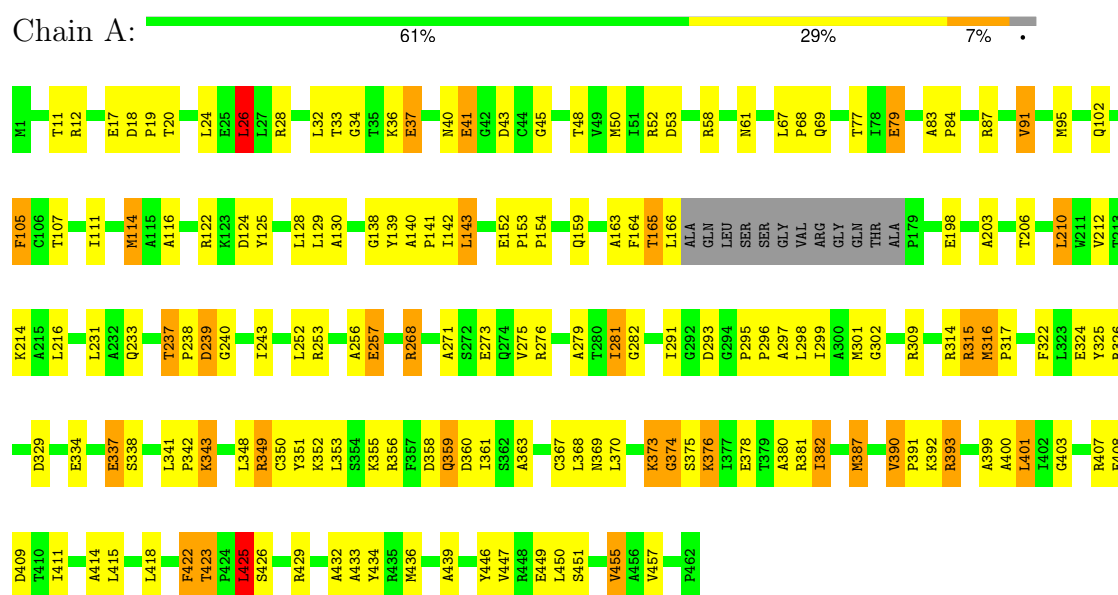
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	11	Total	O	0	0
			11	11		
7	B	26	Total	O	0	0
			26	26		
7	C	7	Total	O	0	0
			7	7		
7	D	25	Total	O	0	0
			25	25		
7	E	7	Total	O	0	0
			7	7		
7	F	20	Total	O	0	0
			20	20		
7	G	6	Total	O	0	0
			6	6		
7	H	21	Total	O	0	0
			21	21		

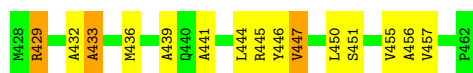
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

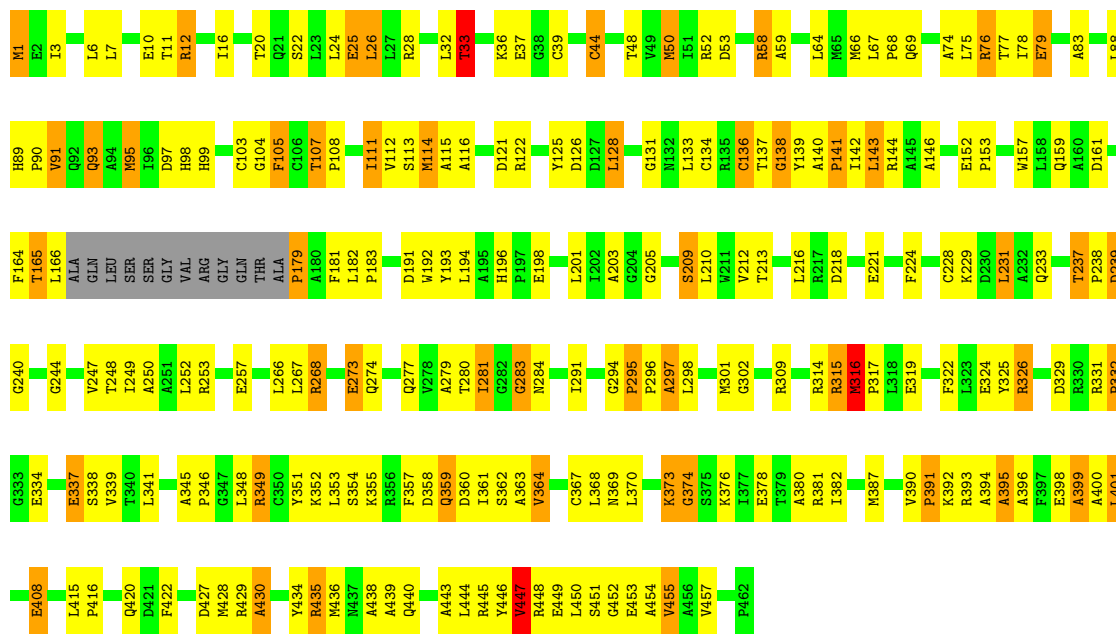
• Molecule 1: xanthine dehydrogenase, chain A





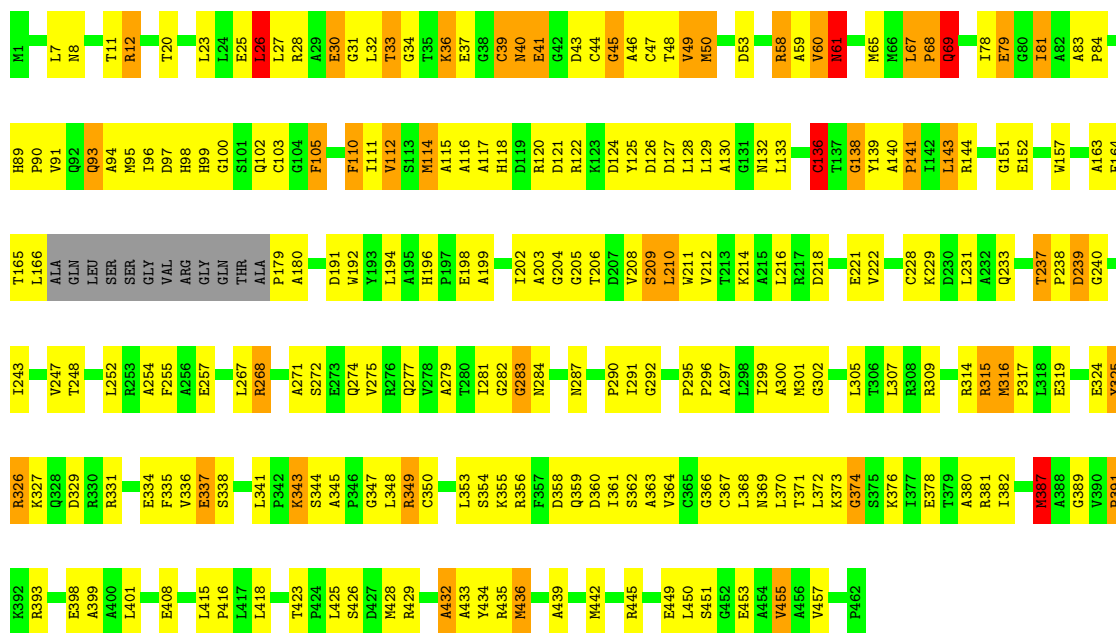
• Molecule 1: xanthine dehydrogenase, chain A

Chain E: 48% 38% 11% ..



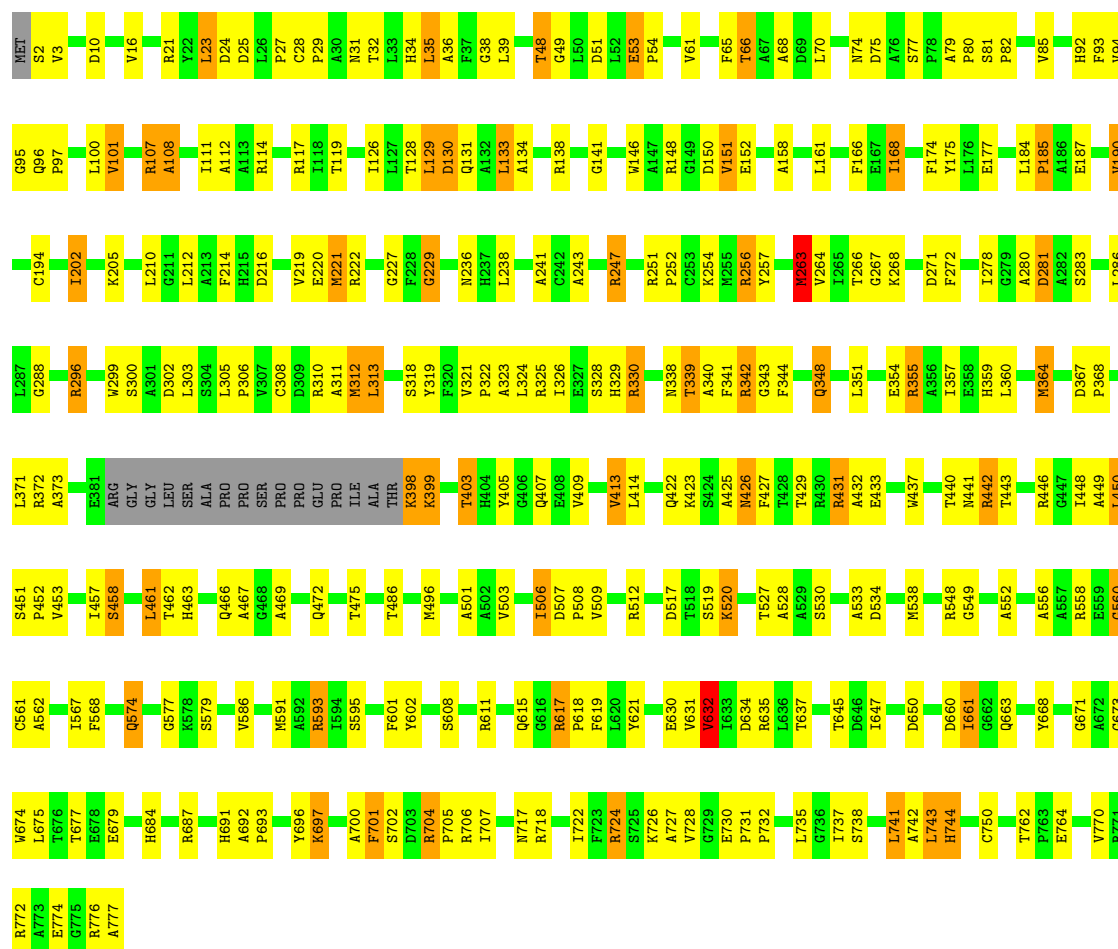
• Molecule 1: xanthine dehydrogenase, chain A

Chain G: 47% 40% 9% ..



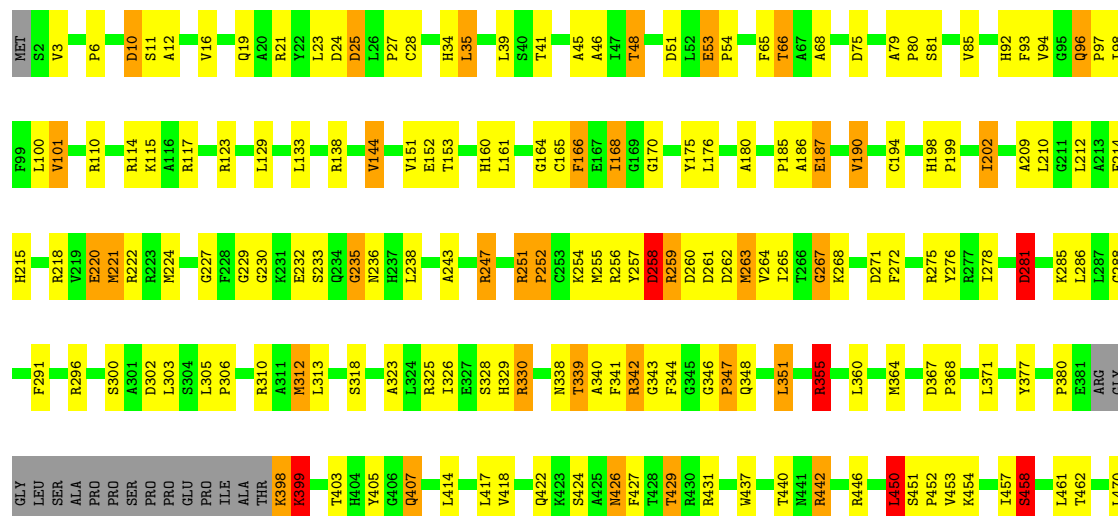
• Molecule 2: xanthine dehydrogenase, chain B

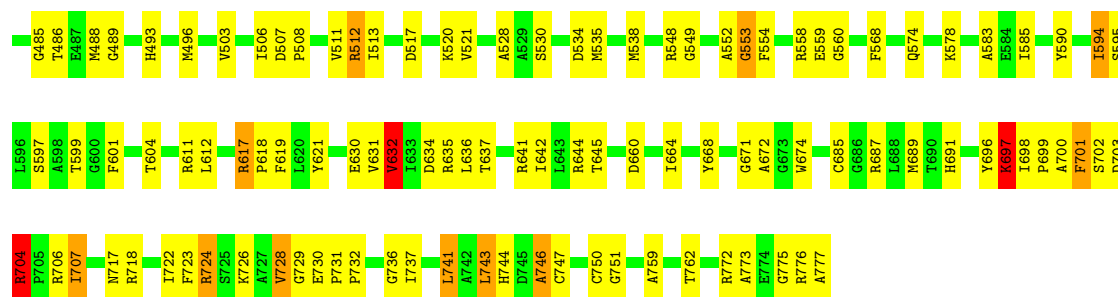
Chain B:



- Molecule 2: xanthine dehydrogenase, chain B

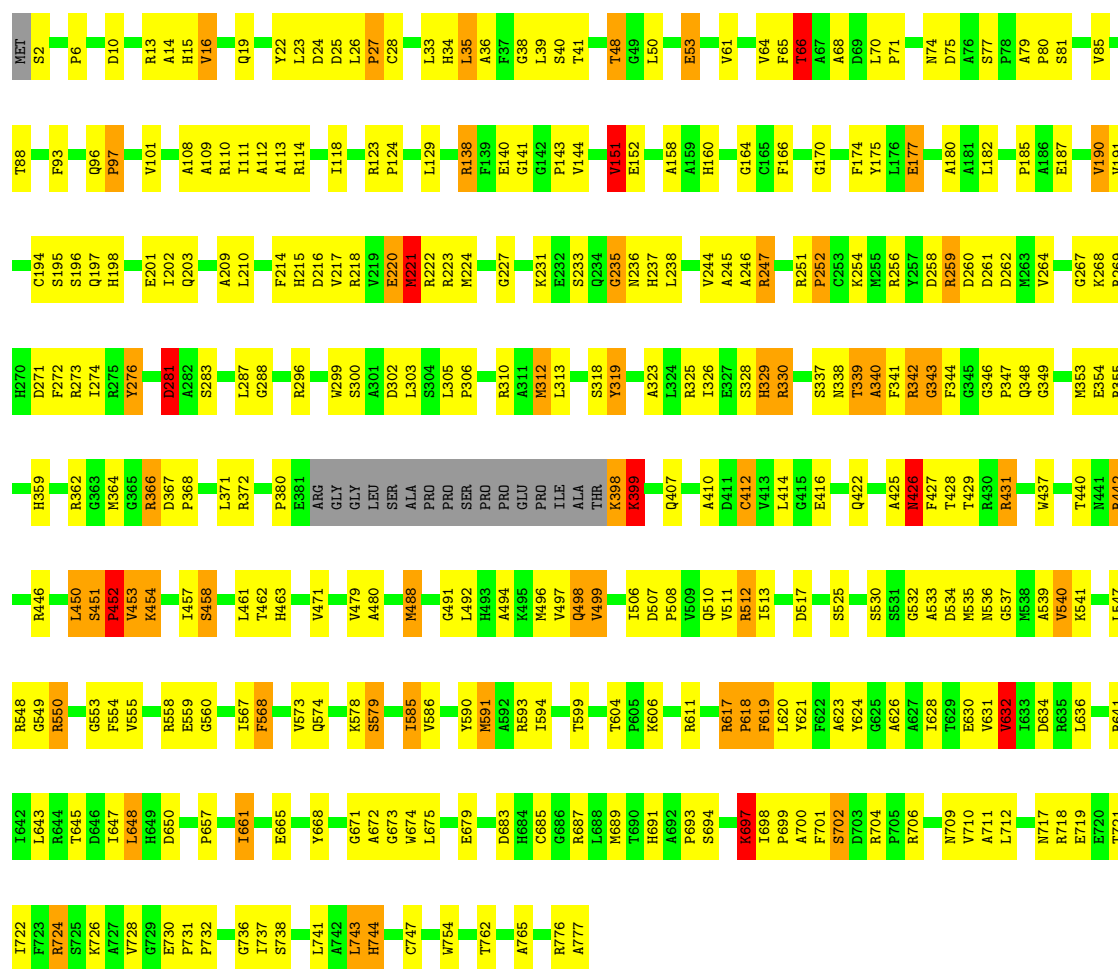
Chain D:





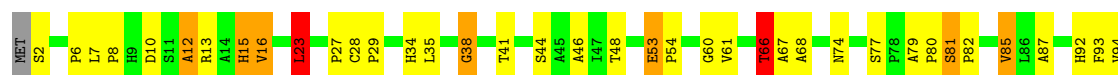
• Molecule 2: xanthine dehydrogenase, chain B

Chain F: 56% 34% 7% ..



• Molecule 2: xanthine dehydrogenase, chain B

Chain H: 54% 34% 8% ..



R724	D634	D517	F427	Q348	D262	A186	Q95
S725	G638	T518	T428	G349	M263	Q96	Q96
A726	E639	S519	T429	E354	V264	P97	P97
A727	N640	K520	R431	R355	T265	I98	I98
G729	L643	V521	T440	A356	T267	F99	F99
E730	L648	A526	M441	I357	K268	L100	L100
F731	L653	T527	T442	E358	R269	V101	V101
F732	A653	A528	T443	H359	H270	A102	A102
F733	L655	A529	R446	L360	D271	A103	A103
G736	L656	S530	G447	M364	F272	S105	S105
I737	N657	S531	I448	G365	Y276	H106	H106
S738	G657	G537	A449	R366	A280	R107	R107
L741	A658	L551	S451	D367	D281	A108	A108
A742	L659	K541	V452	P368	L287	A112	A112
L743	D660	R548	W453	R372	G288	A113	A113
H744	G662	G549	K454	A373	V292	R114	R114
B745	Q663	R550	S458	Y377	R296	R123	R123
C747	E665	L551	L461	P380	C297	P124	P124
F752	Y668	V555	T462	E381	G298	A125	A125
H753	V669	R558	H463	GLY	V217	I126	I126
W754	G670	E559	Q466	GLY	D216	T127	T127
A761	A671	G560	Q472	LEU	R218	L129	L129
T762	A672	C561	V471	SER	V219	D130	D130
F763	G673	A562	Q476	ALA	E220	Q131	Q131
E764	W674	A563	S478	PRO	M221	A132	A132
V770	L675	R564	T475	PRO	R222	L133	L133
R771	E678	D565	D476	SER	R223	R138	R138
R772	D683	Q574	G477	PRO	M224	F139	F139
G776	R687	M591	S479	GLU	G227	E140	E140
R776	P693	A592	A480	PRO	F228	G141	G141
A777	Y696	R593	L481	PRO	G229	G142	G142
	K697	T599	H483	ILE	G230	P143	P143
	I698	T604	T486	ALA	G235	V144	V144
	A700	R611	Q489	THR	N236	I145	I145
	F701	G616	Q490	K398	H237	W146	W146
	S702	G617	L492	K399	L238	V151	V151
	B703	R618	H493	V413	A239	E152	E152
	R704	F619	A494	L414	I240	A158	A158
	R705	L620	M496	E416	A243	L161	L161
	R706	Y621	I506	L417	R247	G164	G164
	A711	Y624	D507	V418	P252	C165	C165
	L712	E630	P508	T419	C253	F166	F166
	W713	V631	R512	R420	K254	G170	G170
	T721	I722	I513	L421	M255	H173	H173
	F723	F632		G343	R256	F174	F174
				Q422	Y257	X175	X175
				K423	D258	L176	L176
					R259	D260	D260
					D261	P185	P185

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.88Å 141.05Å 158.11Å 109.53° 105.83° 101.33°	Depositor
Resolution (Å)	50.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.2 (50.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.213 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36831	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, ZW9, CA, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.25	10/3431 (0.3%)	1.39	19/4647 (0.4%)
1	C	1.58	27/3431 (0.8%)	1.49	34/4647 (0.7%)
1	E	1.31	17/3431 (0.5%)	1.49	35/4647 (0.8%)
1	G	1.23	10/3431 (0.3%)	1.49	32/4647 (0.7%)
2	B	1.52	38/5845 (0.7%)	1.54	46/7942 (0.6%)
2	D	1.67	52/5845 (0.9%)	1.57	52/7942 (0.7%)
2	F	1.55	45/5845 (0.8%)	1.58	70/7942 (0.9%)
2	H	1.46	30/5845 (0.5%)	1.55	63/7942 (0.8%)
All	All	1.48	229/37104 (0.6%)	1.53	351/50356 (0.7%)

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	312	MET	SD-CE	-14.76	1.42	1.79
2	H	521	VAL	CA-CB	-14.02	1.36	1.54
2	B	312	MET	SD-CE	-12.82	1.47	1.79
1	C	114	MET	SD-CE	-11.94	1.49	1.79
2	D	521	VAL	CA-CB	-11.90	1.43	1.54
1	E	316	MET	SD-CE	11.10	2.07	1.79
2	F	312	MET	SD-CE	-9.44	1.55	1.79
1	C	140	ALA	CA-CB	-9.17	1.45	1.54
1	C	251	ALA	CA-CB	-9.11	1.38	1.53
1	E	111	ILE	CA-CB	-9.10	1.43	1.54
2	F	245	ALA	CA-CB	-8.86	1.39	1.53
2	H	243	ALA	CA-CB	-8.69	1.39	1.53
1	C	50	MET	SD-CE	-8.68	1.57	1.79
1	A	107	THR	CA-CB	-8.60	1.42	1.53
2	D	258	ASP	CA-C	-8.35	1.41	1.52
1	C	456	ALA	CA-CB	-8.18	1.42	1.53
2	H	471	VAL	CA-CB	-7.94	1.44	1.54
2	B	263	MET	SD-CE	-7.89	1.59	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	258	ASP	CB-CG	-7.87	1.32	1.52
2	D	594	ILE	C-O	-7.73	1.15	1.24
2	D	511	VAL	C-O	-7.73	1.15	1.24
2	B	219	VAL	C-O	-7.70	1.15	1.24
2	D	689	MET	SD-CE	7.66	1.98	1.79
2	F	353	MET	SD-CE	-7.60	1.60	1.79
2	H	16	VAL	CA-CB	-7.59	1.44	1.54
2	B	409	VAL	CA-CB	-7.52	1.44	1.53
1	A	91	VAL	CA-CB	-7.28	1.45	1.54
1	G	60	VAL	CA-CB	-7.21	1.42	1.55
2	D	759	ALA	CA-CB	-7.18	1.42	1.53
2	H	220	GLU	CA-C	-7.16	1.43	1.52
1	C	37	GLU	C-O	-7.13	1.15	1.24
2	B	707	ILE	CA-CB	-6.97	1.45	1.54
2	H	85	VAL	C-O	-6.90	1.16	1.24
1	E	50	MET	SD-CE	-6.77	1.62	1.79
1	E	91	VAL	CA-CB	-6.74	1.46	1.54
2	F	64	VAL	CA-CB	-6.68	1.46	1.54
2	B	32	THR	CA-CB	6.65	1.63	1.53
2	H	126	ILE	CA-CB	-6.62	1.46	1.53
2	F	479	VAL	C-O	6.61	1.30	1.24
2	F	511	VAL	C-O	-6.60	1.17	1.24
2	B	61	VAL	CA-CB	-6.57	1.46	1.54
1	E	59	ALA	CA-CB	-6.53	1.44	1.53
1	A	299	ILE	CA-CB	-6.52	1.46	1.54
2	D	672	ALA	CA-CB	-6.51	1.43	1.53
2	H	664	ILE	CA-CB	-6.49	1.46	1.54
1	G	39	CYS	CA-C	-6.49	1.44	1.52
1	C	295	PRO	C-O	-6.49	1.17	1.24
1	E	281	ILE	CA-CB	-6.47	1.46	1.54
2	F	499	VAL	CA-CB	-6.40	1.47	1.54
2	D	599	THR	C-O	-6.38	1.15	1.23
2	D	746	ALA	CA-CB	-6.37	1.43	1.53
1	E	280	THR	CA-C	-6.37	1.44	1.52
2	F	672	ALA	CA-CB	-6.37	1.42	1.53
2	H	108	ALA	CA-CB	-6.36	1.43	1.53
1	E	48	THR	CA-CB	-6.35	1.43	1.53
1	E	134	CYS	C-O	-6.35	1.16	1.23
2	F	535	MET	SD-CE	6.35	1.95	1.79
2	B	111	ILE	CA-CB	-6.33	1.47	1.54
2	F	555	VAL	CA-CB	-6.32	1.45	1.54
2	F	591	MET	SD-CE	6.29	1.95	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	212	LEU	C-O	-6.29	1.16	1.23
2	B	722	ILE	CA-CB	6.27	1.62	1.54
1	E	436	MET	SD-CE	-6.26	1.63	1.79
2	F	36	ALA	CA-CB	-6.25	1.42	1.53
2	B	35	LEU	C-O	-6.23	1.15	1.23
1	C	107	THR	C-O	-6.22	1.18	1.24
1	G	96	ILE	CA-CB	-6.21	1.47	1.54
2	B	220	GLU	CA-C	-6.19	1.45	1.52
2	H	146	TRP	CA-C	-6.19	1.45	1.52
2	F	525	SER	CA-C	-6.16	1.45	1.52
2	B	538	MET	SD-CE	6.16	1.95	1.79
2	B	364	MET	SD-CE	-6.16	1.64	1.79
1	A	37	GLU	C-O	-6.15	1.16	1.24
1	A	116	ALA	CA-CB	-6.13	1.43	1.53
2	D	168	ILE	CA-CB	-6.13	1.46	1.54
1	C	349	ARG	C-O	-6.11	1.16	1.23
2	F	191	VAL	N-CA	-6.11	1.39	1.46
2	H	762	THR	CA-CB	-6.11	1.44	1.53
2	F	648	LEU	N-CA	-6.11	1.38	1.46
2	D	243	ALA	CA-CB	-6.10	1.43	1.53
2	F	40	SER	CA-C	-6.09	1.44	1.52
1	C	271	ALA	CA-CB	-6.09	1.43	1.53
2	F	220	GLU	CA-C	-6.08	1.45	1.52
2	D	10	ASP	C-O	-6.08	1.16	1.24
2	B	311	ALA	CA-CB	-6.07	1.43	1.53
2	D	583	ALA	CA-CB	-6.06	1.43	1.53
1	A	382	ILE	CA-CB	-6.05	1.46	1.54
2	D	180	ALA	CA-CB	-6.04	1.44	1.53
2	H	44	SER	CA-C	-6.04	1.44	1.52
2	B	568	PHE	CA-C	-6.01	1.45	1.52
2	H	722	ILE	CA-CB	-6.00	1.46	1.54
2	D	642	ILE	C-O	-5.99	1.17	1.24
1	C	362	SER	CA-C	-5.98	1.45	1.52
2	F	494	ALA	CA-CB	-5.96	1.44	1.53
2	B	112	ALA	CA-CB	-5.95	1.43	1.53
1	C	297	ALA	CA-CB	-5.95	1.44	1.53
2	B	469	ALA	CA-CB	-5.95	1.43	1.53
2	F	177	GLU	CA-C	5.91	1.59	1.52
1	G	50	MET	SD-CE	-5.89	1.64	1.79
2	B	467	ALA	CA-CB	-5.87	1.44	1.53
2	D	707	ILE	CA-CB	-5.86	1.47	1.54
1	C	436	MET	SD-CE	-5.86	1.64	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	728	VAL	C-O	-5.85	1.17	1.24
1	C	103	CYS	C-O	-5.84	1.16	1.24
1	E	1	MET	SD-CE	-5.83	1.65	1.79
1	C	441	ALA	CA-CB	-5.82	1.43	1.53
2	F	540	VAL	N-CA	-5.82	1.39	1.46
2	D	257	TYR	C-O	-5.81	1.16	1.23
2	H	727	ALA	CA-CB	-5.80	1.43	1.53
2	F	689	MET	SD-CE	5.80	1.94	1.79
2	D	263	MET	SD-CE	-5.79	1.65	1.79
2	B	36	ALA	CA-CB	-5.76	1.43	1.53
2	D	176	LEU	C-O	-5.76	1.17	1.24
2	F	337	SER	CA-CB	-5.76	1.45	1.53
2	F	28	CYS	N-CA	5.75	1.51	1.45
2	F	48	THR	CA-C	-5.74	1.44	1.52
2	B	348	GLN	C-O	-5.74	1.17	1.24
1	C	362	SER	C-O	-5.73	1.16	1.23
2	F	765	ALA	CA-CB	-5.70	1.43	1.53
2	B	126	ILE	CA-CB	-5.70	1.47	1.53
2	D	339	THR	C-O	-5.70	1.18	1.24
1	C	67	LEU	C-O	-5.70	1.19	1.24
2	F	626	ALA	CA-CB	-5.68	1.44	1.53
2	F	555	VAL	N-CA	-5.67	1.39	1.46
2	D	98	ILE	CA-C	-5.64	1.45	1.52
2	D	632	VAL	CA-C	-5.63	1.46	1.52
2	H	6	PRO	CA-C	-5.63	1.47	1.52
2	B	727	ALA	C-O	-5.62	1.17	1.23
2	D	597	SER	N-CA	-5.61	1.39	1.46
2	H	263	MET	SD-CE	-5.61	1.65	1.79
2	B	556	ALA	CA-CB	-5.61	1.44	1.53
2	D	267	GLY	C-O	-5.60	1.16	1.23
2	H	112	ALA	CA-CB	-5.59	1.44	1.53
1	E	105	PHE	C-O	-5.58	1.17	1.24
2	D	291	PHE	CA-C	-5.58	1.45	1.52
2	D	470	LEU	CA-C	-5.58	1.46	1.52
1	C	202	ILE	C-O	-5.56	1.18	1.24
2	F	488	MET	N-CA	-5.55	1.40	1.46
2	H	12	ALA	CA-C	5.55	1.60	1.52
1	E	392	LYS	CA-C	5.54	1.59	1.52
2	H	253	CYS	CA-C	-5.54	1.45	1.52
2	D	3	VAL	CA-CB	-5.53	1.48	1.54
2	D	96	GLN	C-O	-5.53	1.17	1.24
1	C	107	THR	N-CA	-5.51	1.42	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	PHE	N-CA	-5.50	1.39	1.46
2	F	453	VAL	CA-CB	-5.50	1.47	1.54
2	B	257	TYR	C-O	-5.48	1.17	1.23
2	D	220	GLU	CA-C	-5.48	1.46	1.52
2	F	480	ALA	C-O	5.47	1.30	1.24
2	B	321	VAL	C-O	-5.47	1.17	1.24
2	B	475	THR	C-O	-5.46	1.17	1.24
1	C	402	ILE	CA-CB	-5.46	1.48	1.54
2	F	326	ILE	CA-CB	-5.46	1.47	1.54
2	D	590	TYR	N-CA	-5.45	1.40	1.46
1	E	114	MET	SD-CE	-5.44	1.66	1.79
2	F	339	THR	C-O	-5.44	1.18	1.24
2	B	727	ALA	CA-C	-5.43	1.46	1.52
1	G	81	ILE	CA-CB	-5.43	1.48	1.54
1	C	107	THR	CA-CB	-5.42	1.46	1.53
2	D	403	THR	CA-CB	5.42	1.61	1.53
2	D	418	VAL	CA-CB	-5.41	1.48	1.54
2	F	709	ASN	CA-C	-5.41	1.46	1.52
2	D	450	LEU	C-O	-5.39	1.17	1.24
2	F	471	VAL	CA-CB	5.39	1.64	1.55
2	H	330	ARG	CA-C	-5.39	1.46	1.52
1	E	107	THR	CA-CB	-5.37	1.47	1.53
2	H	356	ALA	CA-CB	-5.36	1.45	1.53
2	D	25	ASP	C-O	-5.36	1.17	1.24
2	H	712	LEU	CA-C	-5.35	1.46	1.52
2	F	585	ILE	CA-CB	-5.34	1.47	1.54
1	C	135	ARG	C-O	-5.34	1.17	1.24
2	H	479	VAL	CA-CB	-5.31	1.47	1.54
2	H	364	MET	SD-CE	-5.31	1.66	1.79
2	D	209	ALA	C-O	-5.30	1.17	1.24
2	B	506	ILE	CA-C	-5.30	1.46	1.52
2	H	192	ILE	CA-CB	5.30	1.60	1.54
1	G	61	ASN	C-O	-5.28	1.18	1.24
2	F	246	ALA	CA-CB	-5.27	1.44	1.53
2	D	450	LEU	CA-C	-5.27	1.46	1.52
2	H	312	MET	SD-CE	-5.26	1.66	1.79
2	B	25	ASP	C-O	-5.26	1.17	1.24
1	A	61	ASN	C-O	-5.26	1.17	1.24
1	E	76	ARG	CA-C	5.25	1.58	1.52
2	F	209	ALA	CA-CB	-5.25	1.44	1.53
1	C	74	ALA	CA-CB	-5.25	1.46	1.53
2	B	3	VAL	CA-CB	-5.24	1.48	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	112	VAL	CA-CB	-5.24	1.48	1.54
1	G	361	ILE	CA-CB	-5.23	1.48	1.54
2	D	762	THR	CA-CB	-5.22	1.45	1.53
2	D	232	GLU	C-O	-5.21	1.17	1.24
2	F	568	PHE	CA-C	-5.21	1.46	1.52
1	A	114	MET	SD-CE	-5.20	1.66	1.79
2	F	221	MET	SD-CE	5.20	1.92	1.79
1	C	276	ARG	CZ-NH1	-5.19	1.25	1.32
2	F	623	ALA	CA-C	-5.18	1.46	1.52
1	C	48	THR	C-O	-5.15	1.17	1.23
2	F	113	ALA	CA-CB	-5.15	1.44	1.53
2	H	61	VAL	CA-CB	-5.15	1.47	1.54
2	D	355	ARG	C-O	-5.14	1.18	1.24
2	D	568	PHE	CA-C	-5.13	1.46	1.52
2	D	19	GLN	C-O	-5.12	1.17	1.24
2	D	664	ILE	C-O	-5.12	1.18	1.24
1	G	49	VAL	CA-CB	-5.12	1.46	1.54
2	H	711	ALA	CA-CB	-5.12	1.43	1.54
2	B	241	ALA	CA-CB	-5.11	1.45	1.53
1	A	281	ILE	CA-CB	-5.11	1.48	1.54
2	B	593	ARG	NE-CZ	-5.10	1.27	1.33
2	D	255	MET	CA-C	-5.08	1.46	1.52
2	B	520	LYS	CA-C	5.08	1.57	1.52
2	H	599	THR	CA-CB	-5.08	1.45	1.53
1	C	155	ALA	CA-CB	-5.07	1.45	1.53
2	B	449	ALA	CA-CB	-5.07	1.45	1.53
2	F	647	ILE	C-O	-5.06	1.19	1.24
1	E	382	ILE	CA-CB	-5.06	1.47	1.54
2	F	61	VAL	CA-CB	-5.06	1.48	1.54
1	A	50	MET	SD-CE	-5.05	1.67	1.79
2	B	243	ALA	C-O	-5.05	1.18	1.24
2	D	503	VAL	CA-CB	-5.05	1.47	1.54
1	G	114	MET	SD-CE	-5.04	1.67	1.79
2	D	180	ALA	C-O	5.04	1.30	1.23
2	B	168	ILE	CA-CB	-5.04	1.47	1.54
2	B	533	ALA	CA-CB	-5.04	1.45	1.53
2	F	412	CYS	CA-C	5.04	1.59	1.52
2	H	480	ALA	CA-CB	-5.03	1.46	1.53
2	B	762	THR	CA-CB	-5.03	1.45	1.53
2	D	424	SER	C-O	-5.02	1.17	1.24
2	F	274	ILE	C-O	-5.02	1.18	1.24
2	D	458	SER	C-O	-5.02	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	LYS	CA-C	-5.01	1.46	1.52

All (351) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	VAL	CB-CA-C	-10.65	92.29	110.30
2	D	632	VAL	CB-CA-C	-10.21	92.43	110.71
2	F	632	VAL	CB-CA-C	-10.08	94.97	110.50
1	C	125	TYR	N-CA-C	9.66	121.41	111.07
2	B	185	PRO	CB-CA-C	-9.56	99.42	111.56
2	D	185	PRO	CB-CA-C	-8.92	100.31	111.64
2	H	190	VAL	CB-CA-C	-8.78	95.46	110.30
2	B	202	ILE	N-CA-C	-8.77	101.87	110.72
2	H	229	GLY	N-CA-C	-8.68	104.29	113.58
2	D	85	VAL	N-CA-C	-8.62	103.48	111.67
2	B	85	VAL	N-CA-C	-8.58	103.47	111.45
1	C	391	PRO	CA-C-O	-8.47	111.37	121.03
2	B	661	ILE	N-CA-C	-8.42	102.03	110.62
2	D	190	VAL	CB-CA-C	-8.37	96.16	110.30
2	B	632	VAL	CB-CA-C	-8.31	95.83	110.71
1	A	447	VAL	CB-CA-C	-8.11	101.59	111.97
2	B	462	THR	N-CA-C	8.05	124.65	111.37
2	D	685	CYS	CB-CA-C	-7.97	95.62	110.36
2	F	553	GLY	N-CA-C	-7.86	103.29	112.73
2	B	151	VAL	N-CA-C	7.78	118.32	110.23
2	H	202	ILE	N-CA-C	-7.77	102.69	110.62
2	B	151	VAL	CB-CA-C	-7.75	101.78	111.70
2	F	685	CYS	CB-CA-C	-7.67	96.20	110.01
1	C	30	GLU	N-CA-C	-7.64	103.69	113.16
1	G	141	PRO	N-CA-C	-7.58	103.64	113.57
1	C	447	VAL	CB-CA-C	-7.55	102.30	111.97
2	B	281	ASP	N-CA-CB	-7.53	100.05	110.29
2	F	462	THR	N-CA-C	7.47	123.69	111.37
2	B	338	ASN	N-CA-C	7.35	120.05	110.43
2	F	190	VAL	CB-CA-C	-7.34	99.00	110.52
1	G	45	GLY	N-CA-C	-7.33	105.39	114.92
2	B	567	ILE	N-CA-C	7.30	118.39	108.17
2	B	534	ASP	N-CA-C	-7.28	103.28	111.14
2	D	405	TYR	N-CA-C	-7.27	102.69	112.94
2	H	673	GLY	N-CA-C	-7.20	105.45	114.16
1	G	271	ALA	CB-CA-C	-7.16	108.32	116.63
2	H	658	ALA	N-CA-C	-7.11	103.47	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	251	ARG	N-CA-C	7.09	121.43	109.09
2	F	673	GLY	N-CA-C	-7.01	103.80	112.77
1	G	28	ARG	N-CA-C	-6.98	103.72	111.82
2	D	39	LEU	N-CA-C	6.94	120.90	110.14
2	D	23	LEU	N-CA-C	6.92	119.42	111.11
1	G	105	PHE	N-CA-C	6.85	118.75	111.28
2	B	586	VAL	N-CA-C	6.79	116.94	110.42
2	H	494	ALA	N-CA-C	-6.78	103.95	111.82
2	D	338	ASN	N-CA-C	6.76	119.29	110.43
1	E	136	CYS	N-CA-C	6.74	119.98	111.69
2	F	329	HIS	CA-C-N	-6.73	114.09	122.84
2	F	329	HIS	C-N-CA	-6.73	114.09	122.84
1	E	26	LEU	N-CA-CB	6.72	119.75	110.01
1	A	26	LEU	N-CA-C	-6.68	104.00	111.28
2	B	677	THR	CA-C-N	-6.66	112.06	121.72
2	B	677	THR	C-N-CA	-6.66	112.06	121.72
2	B	552	ALA	N-CA-C	-6.65	103.51	111.69
2	H	632	VAL	CB-CA-C	-6.62	100.30	110.50
2	H	38	GLY	N-CA-C	-6.61	99.45	110.95
1	E	364	VAL	CB-CA-C	-6.58	100.49	111.29
1	C	44	CYS	N-CA-C	6.58	121.60	113.50
2	F	359	HIS	N-CA-C	-6.58	103.80	110.97
2	F	412	CYS	N-CA-C	6.57	118.85	108.67
2	F	549	GLY	N-CA-C	-6.52	104.42	112.77
2	H	329	HIS	CA-C-N	-6.52	113.85	123.11
2	H	329	HIS	C-N-CA	-6.52	113.85	123.11
1	A	271	ALA	CB-CA-C	-6.51	109.05	116.54
1	A	91	VAL	CB-CA-C	-6.49	103.26	112.22
1	C	43	ASP	N-CA-C	6.49	119.35	111.82
1	C	137	THR	CB-CA-C	-6.49	98.36	109.65
1	A	43	ASP	N-CA-C	6.46	120.90	112.89
1	E	64	LEU	CA-C-N	-6.45	113.90	122.99
1	E	64	LEU	C-N-CA	-6.45	113.90	122.99
2	H	409	VAL	CB-CA-C	-6.42	104.14	111.59
2	D	252	PRO	CA-C-O	-6.41	114.12	121.56
2	H	46	ALA	N-CA-C	-6.35	99.94	110.17
2	B	101	VAL	CB-CA-C	-6.34	101.17	110.81
2	F	281	ASP	N-CA-CB	-6.34	99.78	110.49
2	F	287	LEU	N-CA-C	-6.33	106.19	114.04
2	F	77	SER	N-CA-C	6.32	116.87	109.60
2	H	281	ASP	N-CA-CB	-6.31	99.83	110.49
2	F	252	PRO	CA-C-O	-6.25	114.30	121.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	136	CYS	N-CA-C	6.22	121.00	112.04
2	B	403	THR	N-CA-C	-6.21	101.27	110.46
2	F	536	ASN	N-CA-C	-6.20	104.41	112.23
2	H	15	HIS	N-CA-C	-6.20	104.15	111.03
1	E	363	ALA	N-CA-C	-6.18	104.44	112.23
2	D	281	ASP	N-CA-CB	-6.18	100.05	110.49
2	H	481	LEU	CB-CG-CD1	-6.18	92.17	110.70
2	H	175	TYR	N-CA-C	-6.17	100.44	110.20
2	B	38	GLY	N-CA-C	-6.16	100.24	110.95
1	E	146	ALA	N-CA-C	-6.16	104.65	111.36
2	F	39	LEU	N-CA-C	6.15	119.55	109.72
1	E	137	THR	CB-CA-C	-6.13	98.12	109.29
1	C	33	THR	N-CA-CB	-6.13	99.66	110.39
2	D	703	ASP	N-CA-C	-6.13	105.85	113.15
1	G	110	PHE	N-CA-C	-6.13	104.51	111.07
1	A	363	ALA	N-CA-C	-6.13	104.15	111.69
2	F	97	PRO	CA-C-O	-6.12	113.96	121.31
2	D	549	GLY	N-CA-C	-6.12	105.09	112.49
1	E	44	CYS	N-CA-C	6.11	119.92	112.23
2	H	297	CYS	N-CA-C	6.09	120.71	113.28
2	H	661	ILE	N-CA-C	-6.09	104.41	110.62
1	G	363	ALA	N-CA-C	-6.09	104.56	112.23
2	F	747	CYS	N-CA-C	-6.08	104.73	111.36
2	H	287	LEU	N-CA-C	-6.07	106.51	114.04
2	H	668	TYR	N-CA-C	-6.06	104.36	110.97
1	C	26	LEU	N-CA-C	-6.06	104.67	111.28
1	C	110	PHE	N-CA-C	-6.04	104.77	111.36
1	C	439	ALA	N-CA-C	-6.02	104.71	111.28
2	H	476	ASP	N-CA-C	-6.01	105.80	113.02
1	A	422	PHE	N-CA-C	6.01	118.84	109.52
2	H	665	GLU	N-CA-C	-6.01	104.36	111.03
2	F	661	ILE	N-CA-C	-6.00	104.50	110.62
1	G	96	ILE	CB-CA-C	-6.00	104.30	111.97
1	C	240	GLY	N-CA-C	5.99	120.73	112.52
2	F	273	ARG	N-CA-C	-5.97	98.67	108.76
1	G	43	ASP	CA-C-N	-5.96	112.11	122.36
1	G	43	ASP	C-N-CA	-5.96	112.11	122.36
1	E	193	TYR	N-CA-C	-5.94	104.89	111.36
2	D	453	VAL	CB-CA-C	-5.93	100.45	110.71
2	D	729	GLY	N-CA-C	5.92	119.66	112.49
2	D	166	PHE	N-CA-C	5.92	117.40	108.46
2	F	16	VAL	N-CA-C	5.92	118.45	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	436	MET	N-CA-C	-5.92	104.52	110.97
1	C	363	ALA	N-CA-C	-5.90	104.44	111.69
1	C	204	GLY	N-CA-C	-5.89	105.23	112.77
2	F	101	VAL	CB-CA-C	-5.89	102.67	110.98
2	F	235	GLY	N-CA-C	-5.88	107.36	114.66
1	A	125	TYR	N-CA-C	5.87	117.35	111.07
1	E	420	GLN	N-CA-C	-5.87	106.25	113.41
2	F	138	ARG	N-CA-C	5.87	117.17	108.60
2	B	772	ARG	N-CA-C	-5.86	105.03	111.82
2	D	697	LYS	N-CA-C	5.86	119.16	107.62
1	E	111	ILE	CB-CA-C	-5.86	104.37	112.04
2	D	462	THR	N-CA-C	5.84	123.24	110.80
2	H	85	VAL	N-CA-C	-5.84	105.15	110.82
1	G	287	ASN	N-CA-C	-5.82	104.89	112.23
2	D	75	ASP	N-CA-C	5.81	117.72	107.61
2	B	280	ALA	CA-C-N	5.80	131.28	120.95
2	B	280	ALA	C-N-CA	5.80	131.28	120.95
1	E	361	ILE	N-CA-C	-5.80	100.07	108.71
1	C	106	CYS	N-CA-C	-5.79	105.87	113.17
2	F	185	PRO	CB-CA-C	-5.78	104.01	111.46
2	H	151	VAL	CB-CA-C	-5.78	104.31	111.70
1	C	433	ALA	N-CA-C	-5.77	104.90	111.07
2	F	343	GLY	N-CA-C	-5.77	107.41	113.58
1	G	391	PRO	CA-C-O	-5.75	115.08	121.23
1	C	179	PRO	CA-C-N	5.75	132.52	121.54
1	C	179	PRO	C-N-CA	5.75	132.52	121.54
2	H	359	HIS	N-CA-C	-5.75	104.92	111.07
1	E	392	LYS	N-CA-C	5.74	118.12	109.23
2	F	217	VAL	CB-CA-C	-5.74	102.68	110.42
2	B	107	ARG	NE-CZ-NH1	-5.72	115.78	121.50
2	F	158	ALA	N-CA-C	5.71	118.94	109.46
2	F	191	VAL	CA-C-N	-5.70	115.68	123.14
2	F	191	VAL	C-N-CA	-5.70	115.68	123.14
1	E	95	MET	CA-C-N	-5.69	113.27	120.56
1	E	95	MET	C-N-CA	-5.69	113.27	120.56
2	H	492	LEU	N-CA-C	-5.69	104.98	111.07
2	D	21	ARG	CB-CA-C	-5.69	100.15	109.53
2	D	101	VAL	CB-CA-C	-5.68	102.18	110.81
2	B	774	GLU	N-CA-C	-5.67	106.31	113.18
2	B	673	GLY	N-CA-C	-5.67	105.92	112.50
2	H	462	THR	N-CA-C	5.67	122.88	110.80
2	H	616	GLY	N-CA-C	5.67	118.08	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	359	HIS	N-CA-C	-5.67	105.11	111.28
1	C	69	GLN	CA-C-N	-5.66	114.24	122.28
1	C	69	GLN	C-N-CA	-5.66	114.24	122.28
2	H	230	GLY	CA-C-N	-5.66	113.77	122.60
2	H	230	GLY	C-N-CA	-5.66	113.77	122.60
1	C	207	ASP	N-CA-C	-5.66	106.05	113.12
1	C	326	ARG	CB-CA-C	-5.65	102.63	111.39
2	F	88	THR	OG1-CB-CG2	-5.63	98.03	109.30
2	D	347	PRO	N-CD-CG	-5.63	94.75	103.20
2	F	641	ARG	N-CA-C	5.63	117.41	108.79
2	D	453	VAL	N-CA-C	5.63	116.78	108.45
2	F	697	LYS	N-CA-C	5.63	118.49	107.57
2	H	653	ALA	N-CA-C	-5.62	99.95	108.67
2	H	265	ILE	N-CA-C	5.62	117.54	111.58
2	B	126	ILE	N-CA-C	5.61	115.72	107.15
1	G	43	ASP	N-CA-C	5.58	119.94	113.18
2	H	66	THR	N-CA-CB	-5.57	102.00	111.69
2	F	697	LYS	CB-CA-C	-5.57	102.39	111.68
1	E	138	GLY	N-CA-C	-5.55	107.66	115.32
1	G	283	GLY	CA-C-N	-5.55	112.84	120.28
1	G	283	GLY	C-N-CA	-5.55	112.84	120.28
2	F	319	TYR	N-CA-C	5.55	118.59	109.72
2	B	21	ARG	N-CA-C	5.54	119.28	109.96
2	H	27	PRO	CA-C-O	-5.53	114.68	121.31
2	F	276	TYR	N-CA-C	5.52	117.58	109.24
2	F	585	ILE	N-CA-C	-5.52	105.14	110.72
1	E	391	PRO	CA-C-O	-5.52	114.01	120.85
2	D	704	ARG	NE-CZ-NH1	-5.50	116.00	121.50
2	F	498	GLN	CA-C-N	-5.50	113.50	120.60
2	F	498	GLN	C-N-CA	-5.50	113.50	120.60
2	B	339	THR	N-CA-C	5.49	115.81	108.23
2	B	705	PRO	CA-C-O	-5.49	115.08	121.34
1	E	112	VAL	N-CA-C	-5.48	105.38	110.53
2	D	697	LYS	CB-CA-C	-5.48	101.79	111.22
2	D	538	MET	N-CA-C	-5.48	105.22	111.14
2	B	27	PRO	CB-CA-C	-5.48	103.93	111.21
2	H	693	PRO	N-CA-C	-5.47	106.27	113.65
1	C	349	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	E	357	PHE	N-CA-C	5.46	117.03	111.14
2	H	672	ALA	N-CA-C	-5.45	105.34	111.28
1	C	429	ARG	NE-CZ-NH2	-5.45	114.30	119.20
2	H	23	LEU	N-CA-C	5.45	120.31	111.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	ASP	CA-C-N	-5.45	112.49	121.92
1	C	43	ASP	C-N-CA	-5.45	112.49	121.92
2	B	549	GLY	N-CA-C	-5.45	106.20	112.73
1	G	208	VAL	N-CA-C	5.45	116.22	110.72
2	F	19	GLN	CA-C-N	-5.44	113.64	121.42
2	F	19	GLN	C-N-CA	-5.44	113.64	121.42
2	F	452	PRO	CB-CA-C	-5.44	102.58	111.56
2	H	453	VAL	CB-CA-C	-5.44	100.98	110.71
2	D	115	LYS	N-CA-C	5.44	119.54	113.02
2	H	77	SER	N-CA-C	5.42	116.72	109.83
2	B	409	VAL	CB-CA-C	-5.41	104.40	111.81
1	G	372	LEU	N-CA-C	5.40	118.36	109.72
2	F	66	THR	N-CA-CB	-5.39	102.86	111.43
2	D	696	TYR	N-CA-C	-5.39	99.73	108.52
1	G	344	SER	N-CA-C	5.39	117.26	109.07
2	B	701	PHE	CA-C-N	-5.38	110.52	121.18
2	B	701	PHE	C-N-CA	-5.38	110.52	121.18
2	D	351	LEU	N-CA-C	-5.38	105.50	111.36
1	E	131	GLY	CA-C-N	-5.37	115.43	123.00
1	E	131	GLY	C-N-CA	-5.37	115.43	123.00
1	E	105	PHE	N-CA-C	5.36	118.61	111.75
2	B	413	VAL	N-CA-C	-5.35	107.77	112.90
2	F	650	ASP	N-CA-C	5.35	117.41	107.99
2	B	107	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	C	300	ALA	CA-C-N	-5.34	113.72	122.54
1	C	300	ALA	C-N-CA	-5.34	113.72	122.54
1	A	350	CYS	N-CA-C	5.34	117.61	108.90
2	D	27	PRO	CA-C-O	-5.34	114.90	121.31
2	F	151	VAL	N-CA-C	5.34	116.11	110.72
2	B	31	ASN	N-CA-C	5.34	119.35	113.21
1	C	164	PHE	N-CA-C	5.34	118.76	110.17
2	H	475	THR	N-CA-C	5.33	119.41	113.01
1	E	125	TYR	N-CA-C	5.33	117.51	111.11
2	D	258	ASP	CB-CG-OD1	-5.33	106.15	118.40
1	C	387	MET	N-CA-C	-5.33	106.16	113.30
2	D	772	ARG	N-CA-C	-5.33	105.55	111.36
2	F	152	GLU	N-CA-C	-5.32	105.38	111.07
2	B	453	VAL	CB-CA-C	-5.32	101.46	111.30
1	A	69	GLN	CA-C-N	-5.32	114.73	122.28
1	A	69	GLN	C-N-CA	-5.32	114.73	122.28
2	F	349	GLY	CA-C-N	-5.31	112.75	120.29
2	F	349	GLY	C-N-CA	-5.31	112.75	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	713	TRP	N-CA-C	-5.29	100.54	108.96
2	D	265	ILE	CB-CA-C	-5.29	103.54	112.16
1	E	33	THR	N-CA-CB	-5.29	101.56	110.49
2	F	362	ARG	N-CA-C	-5.28	105.69	111.82
2	F	237	HIS	N-CA-C	5.27	117.03	111.28
1	E	39	CYS	N-CA-C	-5.27	108.61	114.62
1	G	30	GLU	N-CA-C	-5.27	106.85	113.28
2	H	185	PRO	CB-CA-C	-5.26	105.01	111.64
2	F	27	PRO	CA-C-O	-5.26	115.17	121.48
1	A	26	LEU	N-CA-CB	5.25	117.83	110.12
2	D	641	ARG	N-CA-C	5.24	116.25	108.60
2	H	197	GLN	CA-C-N	-5.24	117.49	122.37
2	H	197	GLN	C-N-CA	-5.24	117.49	122.37
2	D	194	CYS	CA-CB-SG	-5.24	102.35	114.40
1	A	28	ARG	N-CA-C	-5.24	105.75	111.82
2	D	230	GLY	CA-C-N	-5.22	113.42	122.14
2	D	230	GLY	C-N-CA	-5.22	113.42	122.14
2	D	403	THR	N-CA-C	-5.22	102.29	110.17
1	C	420	GLN	N-CA-C	-5.22	107.05	113.41
2	F	75	ASP	N-CA-C	5.21	116.06	107.20
2	B	229	GLY	N-CA-C	-5.21	108.49	114.69
2	D	202	ILE	N-CA-C	-5.21	105.30	110.62
2	F	619	PHE	N-CA-C	5.21	117.89	109.40
2	D	235	GLY	N-CA-C	-5.20	106.05	113.86
2	F	599	THR	CB-CA-C	-5.20	101.22	109.80
2	D	21	ARG	N-CA-C	5.18	118.67	109.96
1	E	283	GLY	CA-C-N	-5.18	113.34	120.28
1	E	283	GLY	C-N-CA	-5.18	113.34	120.28
2	H	107	ARG	NE-CZ-NH1	-5.18	116.32	121.50
2	D	6	PRO	CB-CA-C	-5.18	106.05	113.09
1	E	422	PHE	N-CA-C	5.17	117.24	109.23
2	F	259	ARG	N-CA-C	5.17	117.32	111.11
2	H	6	PRO	CB-CA-C	-5.17	106.06	113.09
1	C	283	GLY	N-CA-C	5.17	118.93	112.73
1	E	141	PRO	N-CA-C	-5.17	106.80	113.57
2	F	41	THR	N-CA-C	-5.17	106.22	112.88
1	G	211	TRP	N-CA-C	-5.16	105.73	112.23
2	H	265	ILE	CB-CA-C	-5.16	105.44	111.94
2	F	497	VAL	N-CA-C	-5.16	105.47	110.42
1	C	105	PHE	N-CA-C	5.16	117.80	111.82
2	D	251	ARG	CA-CB-CG	5.16	124.41	114.10
2	B	75	ASP	N-CA-C	5.15	115.95	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLU	N-CA-C	-5.14	107.66	114.04
1	A	91	VAL	N-CA-C	5.14	115.92	110.72
1	G	69	GLN	CA-C-N	-5.14	114.68	122.76
1	G	69	GLN	C-N-CA	-5.14	114.68	122.76
1	G	26	LEU	N-CA-CB	5.14	117.77	110.06
2	H	228	PHE	CA-C-N	-5.14	117.85	123.30
2	H	228	PHE	C-N-CA	-5.14	117.85	123.30
2	H	655	LEU	N-CA-C	-5.13	106.86	113.23
1	G	204	GLY	N-CA-C	-5.13	106.28	112.49
2	D	380	PRO	CA-C-O	-5.13	115.82	122.13
2	H	158	ALA	N-CA-C	5.13	117.60	109.24
2	F	38	GLY	N-CA-C	-5.12	102.08	111.25
2	D	258	ASP	CB-CG-OD2	5.12	130.17	118.40
1	E	28	ARG	N-CA-C	-5.12	105.88	111.82
1	A	425	LEU	N-CA-CB	-5.11	102.65	110.42
1	E	373	LYS	N-CA-C	-5.11	101.34	108.54
2	B	158	ALA	N-CA-C	5.11	117.29	109.07
2	D	46	ALA	N-CA-C	-5.11	102.20	110.32
1	G	387	MET	N-CA-C	-5.10	106.75	113.17
2	D	535	MET	CA-C-N	-5.10	112.56	120.31
2	D	535	MET	C-N-CA	-5.10	112.56	120.31
1	G	60	VAL	N-CA-C	5.09	117.36	108.90
2	D	144	VAL	CB-CA-C	-5.09	103.09	110.63
2	H	257	TYR	CB-CA-C	-5.09	101.45	109.80
1	A	105	PHE	N-CA-C	5.09	117.56	111.71
2	D	417	LEU	N-CA-C	5.08	116.51	111.07
2	F	510	GLN	CA-C-N	-5.08	116.34	123.10
2	F	510	GLN	C-N-CA	-5.08	116.34	123.10
2	H	752	PRO	N-CD-CG	-5.08	95.58	103.20
2	H	727	ALA	CA-C-N	-5.08	112.83	121.97
2	H	727	ALA	C-N-CA	-5.08	112.83	121.97
1	A	387	MET	N-CA-C	-5.07	107.14	113.38
1	C	284	ASN	N-CA-C	-5.07	105.83	111.36
1	G	23	LEU	N-CA-C	-5.07	105.64	111.07
2	B	266	THR	N-CA-C	5.07	117.07	110.53
2	D	553	GLY	N-CA-C	-5.07	106.64	112.83
2	H	706	ARG	CA-C-N	-5.07	116.36	123.10
2	H	706	ARG	C-N-CA	-5.07	116.36	123.10
2	H	663	GLN	N-CA-C	-5.07	105.41	112.45
1	G	432	ALA	CA-C-N	-5.06	113.70	120.54
1	G	432	ALA	C-N-CA	-5.06	113.70	120.54
2	F	338	ASN	N-CA-C	5.06	117.06	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	ALA	CA-C-N	-5.06	113.11	120.29
2	B	108	ALA	C-N-CA	-5.06	113.11	120.29
2	F	108	ALA	N-CA-C	-5.06	105.77	111.28
2	F	550	ARG	N-CA-C	-5.05	105.85	111.36
2	F	166	PHE	N-CA-C	5.04	116.73	108.76
2	H	308	CYS	CA-CB-SG	-5.04	102.80	114.40
2	F	198	HIS	N-CA-C	5.04	116.81	109.30
2	F	6	PRO	CB-CA-C	-5.04	105.44	112.64
2	F	537	GLY	CA-C-N	-5.04	113.53	120.28
2	F	537	GLY	C-N-CA	-5.04	113.53	120.28
1	E	111	ILE	CA-C-N	-5.04	114.11	120.56
1	E	111	ILE	C-N-CA	-5.04	114.11	120.56
2	H	292	VAL	N-CA-C	-5.04	100.82	108.17
1	G	138	GLY	N-CA-C	-5.03	108.34	115.43
2	H	280	ALA	CA-C-N	5.03	131.14	121.54
2	H	280	ALA	C-N-CA	5.03	131.14	121.54
2	F	340	ALA	N-CA-C	5.03	117.19	110.35
1	A	373	LYS	N-CA-C	-5.02	101.46	108.54
1	E	273	GLU	N-CA-C	-5.01	104.91	111.02
2	D	133	LEU	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3370	0	3368	134	0
1	C	3370	0	3368	91	0
1	E	3370	0	3368	187	0
1	G	3370	0	3370	211	0
2	B	5717	0	5630	179	0
2	D	5717	0	5631	173	0
2	F	5717	0	5631	206	0
2	H	5717	0	5630	239	0
3	A	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	0	0	0
3	E	8	0	0	2	0
3	G	8	0	0	4	0
4	A	53	0	31	6	0
4	C	53	0	30	3	0
4	E	53	0	31	6	0
4	G	53	0	31	11	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	B	28	0	0	0	0
6	D	28	0	0	0	0
6	F	28	0	0	0	0
6	H	28	0	0	0	0
7	A	11	0	0	1	0
7	B	26	0	0	6	0
7	C	7	0	0	0	0
7	D	25	0	0	8	0
7	E	7	0	0	0	0
7	F	20	0	0	3	0
7	G	6	0	0	6	0
7	H	21	0	0	9	0
All	All	36831	0	36119	1372	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:MET:SD	1:E:316:MET:CE	2.07	1.42
1:G:325:TYR:CE1	1:G:326:ARG:HG2	1.64	1.33
1:E:325:TYR:O	1:E:326:ARG:HB2	1.41	1.18
2:F:621:TYR:CE1	2:F:726:LYS:HG2	1.84	1.11
1:G:325:TYR:CD1	1:G:326:ARG:HG2	1.85	1.11
1:G:325:TYR:CE1	1:G:326:ARG:CG	2.33	1.10
1:E:95:MET:SD	1:E:114:MET:HE1	1.94	1.07
1:E:381:ARG:HH21	1:E:393:ARG:NH2	1.56	1.04
2:H:66:THR:HG22	2:H:68:ALA:H	1.23	1.03
2:F:446:ARG:NH1	2:F:630:GLU:OE2	1.92	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ARG:HH11	2:B:247:ARG:HG2	1.22	1.00
1:A:358:ASP:OD2	2:B:702:SER:OG	1.80	1.00
1:A:425:LEU:HD12	2:F:579:SER:HB3	1.42	0.99
1:E:381:ARG:HH21	1:E:393:ARG:CZ	1.80	0.95
1:E:445:ARG:NH2	2:F:634:ASP:OD2	2.00	0.94
1:A:348:LEU:HD12	1:A:349:ARG:H	1.27	0.94
2:D:247:ARG:HG2	2:D:247:ARG:HH11	1.30	0.94
2:H:312:MET:HE2	2:H:330:ARG:HH12	1.32	0.94
1:E:301:MET:HE2	1:E:341:LEU:HD22	1.49	0.93
2:F:559:GLU:OE1	2:F:578:LYS:NZ	2.02	0.90
1:G:325:TYR:O	1:G:326:ARG:HB2	1.69	0.90
2:D:507:ASP:OD1	2:D:508:PRO:HD2	1.69	0.90
4:G:3005:FAD:H51A	4:G:3005:FAD:H8A	1.53	0.90
2:F:621:TYR:HE1	2:F:726:LYS:HG2	1.26	0.88
2:F:216:ASP:OD1	2:H:512:ARG:HD2	1.73	0.88
1:G:387:MET:HE2	1:G:439:ALA:HB2	1.55	0.87
1:A:348:LEU:HD12	1:A:349:ARG:N	1.89	0.87
2:B:66:THR:HG22	2:B:68:ALA:H	1.38	0.87
2:H:87:ALA:O	7:H:3009:HOH:O	1.92	0.87
1:C:390:VAL:HG22	1:C:391:PRO:HD2	1.55	0.86
4:G:3005:FAD:H51A	4:G:3005:FAD:C8A	2.06	0.86
2:H:671:GLY:O	2:H:674:TRP:HB3	1.75	0.86
2:H:621:TYR:CE1	2:H:726:LYS:HG2	2.12	0.85
2:F:24:ASP:OD2	2:F:254:LYS:NZ	2.09	0.85
1:A:373:LYS:HB2	1:A:378:GLU:HG2	1.58	0.85
2:H:446:ARG:HG2	2:H:632:VAL:HG12	1.57	0.85
1:A:325:TYR:O	1:A:326:ARG:HB2	1.75	0.84
2:H:247:ARG:HG2	2:H:247:ARG:HH11	1.39	0.84
2:D:229:GLY:HA2	7:D:3007:ZW9:S	2.18	0.84
2:D:360:LEU:HG	2:D:364:MET:HE3	1.60	0.83
2:F:34:HIS:C	2:F:35:LEU:HD23	2.03	0.83
1:A:138:GLY:O	1:A:139:TYR:HB2	1.79	0.83
2:B:247:ARG:HG2	2:B:247:ARG:NH1	1.90	0.83
1:E:337:GLU:O	1:E:338:SER:HB3	1.79	0.83
2:D:621:TYR:HE1	2:D:726:LYS:HG2	1.42	0.83
1:A:408:GLU:OE1	2:B:442:ARG:NH2	2.11	0.82
2:F:247:ARG:HG2	2:F:247:ARG:HH11	1.42	0.82
2:D:559:GLU:OE1	2:D:578:LYS:NZ	2.11	0.81
4:G:3005:FAD:H8A	4:G:3005:FAD:C5B	2.11	0.81
2:D:621:TYR:CE1	2:D:726:LYS:HG2	2.16	0.81
1:G:301:MET:HE2	1:G:341:LEU:HD22	1.60	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:LYS:HE3	1:E:362:SER:OG	1.80	0.81
1:G:373:LYS:HB2	1:G:378:GLU:HG2	1.63	0.81
2:F:35:LEU:HD23	2:F:35:LEU:N	1.95	0.80
2:H:446:ARG:HG2	2:H:632:VAL:CG1	2.11	0.80
1:G:237:THR:OG1	1:G:238:PRO:HD2	1.82	0.80
2:H:730:GLU:C	2:H:732:PRO:HD2	2.07	0.80
1:G:301:MET:CE	1:G:341:LEU:HB3	2.13	0.79
2:D:446:ARG:HG2	2:D:632:VAL:HG13	1.65	0.79
1:E:77:THR:OG1	1:E:79:GLU:HG2	1.83	0.78
1:E:360:ASP:OD1	2:F:697:LYS:HE3	1.83	0.78
1:E:381:ARG:NH2	1:E:393:ARG:CZ	2.45	0.78
2:H:138:ARG:NH2	2:H:329:HIS:ND1	2.30	0.78
2:B:446:ARG:HG2	2:B:632:VAL:HG13	1.64	0.78
2:H:360:LEU:HG	2:H:364:MET:HE3	1.65	0.78
1:C:322:PHE:HB3	1:C:390:VAL:CG2	2.14	0.78
2:D:267:GLY:C	2:D:268:LYS:HG3	2.07	0.78
2:F:590:TYR:CE1	2:H:466:GLN:NE2	2.51	0.77
2:F:70:LEU:HD12	2:F:74:ASN:HB2	1.65	0.77
2:B:360:LEU:HG	2:B:364:MET:HE3	1.66	0.77
1:G:359:GLN:O	1:G:359:GLN:HG3	1.81	0.77
1:G:295:PRO:HB2	1:G:296:PRO:HD3	1.64	0.77
7:H:3007:ZW9:S1'	7:H:3007:ZW9:S	2.82	0.77
1:C:337:GLU:O	1:C:338:SER:HB3	1.84	0.77
1:A:301:MET:HE2	1:A:341:LEU:HD22	1.66	0.77
2:H:66:THR:HG22	2:H:68:ALA:N	2.00	0.77
1:E:12:ARG:HG3	1:E:12:ARG:HH11	1.48	0.76
1:G:367:CYS:C	1:G:368:LEU:HD12	2.10	0.76
1:A:237:THR:OG1	1:A:238:PRO:HD2	1.85	0.75
1:G:136:CYS:SG	3:G:3001:FES:FE1	1.79	0.75
1:C:325:TYR:O	1:C:326:ARG:HB2	1.87	0.75
2:B:138:ARG:NH2	2:B:329:HIS:ND1	2.35	0.74
2:F:138:ARG:NH2	2:F:329:HIS:ND1	2.34	0.74
1:G:252:LEU:CD2	1:G:281:ILE:HD12	2.17	0.74
1:E:355:LYS:HE2	2:F:679:GLU:OE1	1.87	0.74
1:G:50:MET:HE3	1:G:116:ALA:HB2	1.68	0.74
1:C:237:THR:OG1	1:C:238:PRO:HD2	1.87	0.74
1:E:302:GLY:HA2	1:E:381:ARG:HH11	1.52	0.74
2:D:260:ASP:OD1	2:D:691:HIS:CD2	2.40	0.74
1:G:136:CYS:HG	3:G:3001:FES:FE1	1.01	0.74
1:G:237:THR:HG23	1:G:239:ASP:H	1.52	0.74
1:G:393:ARG:HD2	1:G:398:GLU:OE1	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLN:HG3	1:A:359:GLN:O	1.87	0.73
2:H:507:ASP:OD1	2:H:508:PRO:HD2	1.88	0.73
2:D:138:ARG:NH2	2:D:329:HIS:ND1	2.35	0.73
4:A:3005:FAD:H8A	4:A:3005:FAD:H51A	1.69	0.73
2:D:631:VAL:HG21	2:D:743:LEU:HD13	1.68	0.73
4:A:3005:FAD:H51A	4:A:3005:FAD:C8A	2.19	0.73
2:B:247:ARG:HH11	2:B:247:ARG:CG	2.02	0.73
2:H:303:LEU:O	2:H:306:PRO:HD2	1.89	0.73
2:B:446:ARG:HG2	2:B:632:VAL:CG1	2.18	0.73
1:E:368:LEU:N	1:E:368:LEU:HD12	2.04	0.73
1:E:50:MET:HE3	1:E:116:ALA:HA	1.71	0.72
2:F:507:ASP:OD1	2:F:508:PRO:HD2	1.89	0.72
2:D:305:LEU:HB3	2:D:306:PRO:HD3	1.71	0.72
1:A:24:LEU:HD21	1:A:37:GLU:HB2	1.70	0.72
1:G:368:LEU:HD12	1:G:368:LEU:N	2.03	0.72
1:E:89:HIS:ND1	1:E:90:PRO:HD2	2.05	0.72
1:G:325:TYR:CE1	1:G:326:ARG:HG3	2.24	0.72
2:B:34:HIS:C	2:B:35:LEU:HD23	2.14	0.72
7:D:3007:ZW9:S	7:D:3007:ZW9:MO	2.00	0.72
1:G:138:GLY:O	1:G:139:TYR:HB2	1.89	0.72
1:E:358:ASP:OD2	2:F:702:SER:HB3	1.89	0.72
1:G:50:MET:CE	1:G:116:ALA:HA	2.20	0.72
2:B:776:ARG:O	2:B:777:ALA:HB3	1.89	0.72
2:D:507:ASP:OD1	2:D:508:PRO:CD	2.37	0.72
2:F:451:SER:HB3	2:F:738:SER:HB3	1.69	0.72
1:G:33:THR:O	1:G:36:LYS:NZ	2.16	0.72
2:B:398:LYS:HE3	2:B:398:LYS:N	2.04	0.72
2:H:561:CYS:SG	2:H:562:ALA:N	2.62	0.72
2:D:310:ARG:HD2	2:D:344:PHE:O	1.90	0.71
2:H:247:ARG:HG2	2:H:247:ARG:NH1	2.05	0.71
1:A:423:THR:HG22	1:A:423:THR:O	1.88	0.71
2:D:24:ASP:OD2	2:D:254:LYS:NZ	2.23	0.71
1:E:279:ALA:HB1	4:E:3005:FAD:H4'	1.71	0.71
2:H:673:GLY:O	2:H:678:GLU:HB2	1.90	0.71
2:H:66:THR:CG2	2:H:68:ALA:H	2.03	0.71
1:G:325:TYR:O	1:G:326:ARG:CB	2.38	0.71
2:H:35:LEU:HB2	2:H:255:MET:HG3	1.73	0.71
1:A:455:VAL:HG22	2:B:443:THR:HG21	1.72	0.71
2:F:305:LEU:HB3	2:F:306:PRO:HD3	1.71	0.71
7:F:3007:ZW9:S	7:F:3007:ZW9:MO	2.02	0.71
1:G:252:LEU:HD22	1:G:281:ILE:HD12	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:301:MET:HE3	1:G:341:LEU:HB3	1.74	0.70
1:E:24:LEU:HD21	1:E:37:GLU:HB2	1.72	0.70
2:F:218:ARG:NE	2:F:220:GLU:OE2	2.24	0.70
2:F:593:ARG:NH1	2:H:604:THR:O	2.20	0.70
2:D:247:ARG:HG2	2:D:247:ARG:NH1	1.98	0.70
1:E:3:ILE:HD13	1:E:16:ILE:HD11	1.73	0.70
1:G:37:GLU:CD	2:H:256:ARG:HH21	2.00	0.70
1:A:360:ASP:OD1	2:B:697:LYS:HE3	1.91	0.70
1:G:37:GLU:CD	2:H:256:ARG:NH2	2.50	0.70
1:G:353:LEU:HD21	1:G:434:TYR:OH	1.92	0.70
1:A:390:VAL:HG22	1:A:391:PRO:HD2	1.73	0.70
2:D:398:LYS:HE3	2:D:398:LYS:N	2.07	0.69
2:H:296:ARG:NH1	2:H:296:ARG:HG3	2.06	0.69
1:A:95:MET:HG3	1:A:111:ILE:HD11	1.71	0.69
2:F:425:ALA:O	2:F:426:ASN:HB2	1.92	0.69
1:A:301:MET:CE	1:A:341:LEU:HB3	2.22	0.69
2:H:450:LEU:HG	2:H:451:SER:N	1.99	0.69
1:E:88:LEU:HD21	2:F:13:ARG:NH2	2.08	0.69
2:F:512:ARG:HD2	2:H:216:ASP:OD1	1.93	0.69
1:G:44:CYS:N	3:G:3002:FES:S1	2.63	0.69
2:H:496:MET:HE2	2:H:496:MET:HA	1.75	0.69
2:H:776:ARG:O	2:H:777:ALA:HB3	1.91	0.69
1:E:115:ALA:O	1:E:116:ALA:C	2.36	0.68
1:E:314:ARG:HD3	1:E:334:GLU:OE1	1.93	0.68
2:H:731:PRO:N	2:H:732:PRO:HD2	2.07	0.68
2:F:247:ARG:HG2	2:F:247:ARG:NH1	2.02	0.68
2:H:12:ALA:O	2:H:13:ARG:C	2.35	0.68
4:C:3005:FAD:N1	4:C:3005:FAD:H2'	2.08	0.68
2:H:531:SER:OG	7:H:3027:HOH:O	2.11	0.68
1:G:445:ARG:NH2	2:H:634:ASP:OD2	2.27	0.68
2:H:269:ARG:NH2	2:H:341:PHE:CD2	2.62	0.68
1:A:361:ILE:HD12	1:A:429:ARG:NH2	2.08	0.68
1:E:301:MET:CE	1:E:341:LEU:HB3	2.24	0.68
1:E:319:GLU:N	1:E:319:GLU:OE2	2.22	0.68
1:E:322:PHE:HB3	1:E:390:VAL:HG23	1.75	0.68
1:E:415:LEU:HB3	1:E:440:GLN:HG2	1.76	0.68
1:C:32:LEU:HD22	1:C:79:GLU:HG3	1.75	0.67
2:D:66:THR:HG22	2:D:68:ALA:H	1.59	0.67
1:C:53:ASP:OD2	1:C:58:ARG:NH2	2.27	0.67
2:H:296:ARG:HG3	2:H:296:ARG:HH11	1.57	0.67
2:H:372:ARG:O	2:H:373:ALA:C	2.37	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:LEU:HD12	2:B:238:LEU:H	1.59	0.67
2:H:527:THR:OG1	7:H:3021:HOH:O	2.12	0.67
2:F:498:GLN:O	2:F:499:VAL:C	2.33	0.67
1:C:359:GLN:O	1:C:359:GLN:HG2	1.94	0.67
2:H:737:ILE:HG22	2:H:741:LEU:CD2	2.24	0.67
2:F:196:SER:O	2:F:224:MET:HE2	1.94	0.67
2:F:657:PRO:O	2:F:661:ILE:HG12	1.95	0.67
1:E:12:ARG:HH11	1:E:12:ARG:CG	2.08	0.67
1:E:301:MET:HE3	1:E:341:LEU:HB3	1.75	0.67
7:B:3007:ZW9:S	7:B:3007:ZW9:MO	2.06	0.67
1:E:325:TYR:O	1:E:326:ARG:CB	2.26	0.67
2:B:776:ARG:O	2:B:777:ALA:CB	2.43	0.66
2:F:496:MET:HE2	2:F:496:MET:HA	1.76	0.66
2:F:23:LEU:HD13	2:F:194:CYS:HA	1.77	0.66
1:G:366:GLY:HA3	1:G:442:MET:SD	2.35	0.66
1:E:192:TRP:O	1:E:196:HIS:HD2	1.78	0.66
1:E:58:ARG:HD3	1:E:277:GLN:OE1	1.96	0.66
1:E:237:THR:HG23	1:E:238:PRO:CD	2.24	0.66
1:E:295:PRO:HB2	1:E:296:PRO:HD3	1.77	0.66
2:H:310:ARG:HD2	2:H:344:PHE:O	1.96	0.66
2:B:631:VAL:HG21	2:B:743:LEU:HD13	1.77	0.66
2:D:303:LEU:O	2:D:306:PRO:HD2	1.95	0.66
2:F:260:ASP:OD1	2:F:691:HIS:CD2	2.48	0.66
4:G:3005:FAD:C8A	4:G:3005:FAD:C5B	2.71	0.66
2:B:440:THR:O	2:B:440:THR:HG22	1.95	0.66
1:E:252:LEU:HD12	1:E:252:LEU:O	1.96	0.66
2:F:425:ALA:O	2:F:426:ASN:CB	2.44	0.66
7:H:3007:ZW9:S	7:H:3007:ZW9:MO	2.07	0.66
2:D:377:TYR:CE1	2:D:454:LYS:HE3	2.31	0.66
2:D:660:ASP:OD1	2:D:728:VAL:HG11	1.96	0.66
1:E:322:PHE:HB3	1:E:390:VAL:CG2	2.26	0.66
2:D:440:THR:HG22	2:D:440:THR:O	1.97	0.65
2:H:272:PHE:CD2	2:H:348:GLN:HG2	2.31	0.65
1:E:7:LEU:HD12	1:E:75:LEU:HD23	1.78	0.65
1:E:399:ALA:O	1:E:401:LEU:N	2.29	0.65
1:G:95:MET:HG3	1:G:111:ILE:HD11	1.78	0.65
1:A:32:LEU:HD22	1:A:79:GLU:HG3	1.79	0.65
1:E:316:MET:HB2	1:E:317:PRO:HD2	1.79	0.65
1:G:381:ARG:NH1	7:G:3010:HOH:O	2.29	0.65
1:G:408:GLU:OE1	2:H:442:ARG:NH2	2.26	0.65
1:A:122:ARG:NH2	1:A:124:ASP:OD2	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:ARG:HD2	2:B:344:PHE:O	1.97	0.65
1:E:138:GLY:O	1:E:139:TYR:HB2	1.97	0.65
1:G:37:GLU:OE2	2:H:256:ARG:NH2	2.29	0.65
1:G:44:CYS:C	7:G:3007:HOH:O	2.40	0.65
2:H:267:GLY:O	2:H:268:LYS:HG3	1.96	0.65
1:E:237:THR:HG23	1:E:239:ASP:H	1.60	0.65
2:D:251:ARG:HB3	2:D:252:PRO:HD2	1.78	0.64
2:D:704:ARG:HH11	2:D:704:ARG:HG2	1.62	0.64
1:C:252:LEU:CD2	1:C:281:ILE:HD12	2.28	0.64
1:E:111:ILE:HD13	1:E:114:MET:HE3	1.80	0.64
1:A:337:GLU:O	1:A:337:GLU:HG3	1.98	0.64
2:B:251:ARG:HB3	2:B:252:PRO:HD2	1.78	0.64
2:D:704:ARG:HH11	2:D:704:ARG:CG	2.10	0.64
2:B:296:ARG:HG3	2:B:296:ARG:NH1	2.11	0.64
2:B:367:ASP:OD1	2:B:368:PRO:HD2	1.98	0.64
1:E:233:GLN:HA	1:E:233:GLN:OE1	1.97	0.64
1:G:348:LEU:HD12	1:G:349:ARG:H	1.62	0.64
2:H:440:THR:HG22	2:H:440:THR:O	1.96	0.64
2:D:202:ILE:HD13	2:D:236:ASN:HD22	1.63	0.64
2:F:281:ASP:OD1	2:F:283:SER:OG	2.07	0.64
1:A:237:THR:HG23	1:A:239:ASP:H	1.62	0.64
1:G:58:ARG:HD3	1:G:277:GLN:OE1	1.97	0.64
2:B:617:ARG:HD3	2:B:619:PHE:O	1.98	0.64
1:E:373:LYS:HB2	1:E:378:GLU:HG2	1.79	0.64
2:F:451:SER:HB3	2:F:738:SER:CB	2.28	0.64
2:F:532:GLY:N	7:F:3007:ZW9:O3P	2.29	0.64
1:G:91:VAL:HG12	1:G:111:ILE:HD12	1.79	0.64
1:A:425:LEU:CD1	2:F:579:SER:HB3	2.24	0.63
2:D:496:MET:HA	2:D:496:MET:HE2	1.79	0.63
1:G:41:GLU:HG3	1:G:214:LYS:HE3	1.79	0.63
1:G:44:CYS:O	7:G:3007:HOH:O	2.15	0.63
7:H:3007:ZW9:MO	7:H:3007:ZW9:O2	1.70	0.63
2:B:24:ASP:OD2	2:B:254:LYS:NZ	2.30	0.63
2:F:422:GLN:HG2	2:F:427:PHE:CD2	2.33	0.63
1:E:1:MET:HE3	1:E:179:PRO:HA	1.80	0.63
2:H:35:LEU:HA	2:H:101:VAL:O	1.98	0.63
2:D:644:ARG:HG3	2:D:707:ILE:HB	1.79	0.63
2:D:728:VAL:HG22	2:D:728:VAL:O	1.97	0.63
7:D:3007:ZW9:MO	7:D:3007:ZW9:O2	1.70	0.63
1:E:354:SER:HB2	1:E:360:ASP:OD2	1.99	0.63
1:A:122:ARG:HH21	1:A:124:ASP:CG	2.06	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLY:HA2	7:A:3012:HOH:O	1.98	0.62
1:C:50:MET:HE3	1:C:116:ALA:HA	1.81	0.62
4:E:3005:FAD:N1	4:E:3005:FAD:H2'	2.13	0.62
2:D:730:GLU:N	2:D:731:PRO:CD	2.62	0.62
2:H:341:PHE:O	2:H:342:ARG:C	2.41	0.62
2:H:446:ARG:NH1	2:H:630:GLU:OE2	2.28	0.62
1:C:360:ASP:OD1	2:D:697:LYS:HE3	2.00	0.62
1:E:302:GLY:HA2	1:E:381:ARG:NH1	2.15	0.62
1:G:34:GLY:HA2	1:G:36:LYS:NZ	2.15	0.62
2:H:339:THR:OG1	2:H:340:ALA:N	2.28	0.62
4:A:3005:FAD:H2'	4:A:3005:FAD:N1	2.14	0.62
2:F:66:THR:CG2	2:F:68:ALA:H	2.12	0.62
2:F:238:LEU:HD12	2:F:238:LEU:H	1.63	0.62
2:F:367:ASP:OD1	2:F:368:PRO:HD2	2.00	0.62
2:B:296:ARG:HG3	2:B:296:ARG:HH11	1.65	0.62
1:C:165:THR:O	1:C:166:LEU:HD23	1.98	0.62
1:E:381:ARG:NH2	1:E:393:ARG:NH2	2.38	0.62
1:C:301:MET:HE2	1:C:341:LEU:HD22	1.81	0.62
1:E:201:LEU:O	4:E:3005:FAD:O2B	2.11	0.62
1:E:387:MET:HE2	1:E:439:ALA:HB2	1.81	0.62
2:F:310:ARG:HD2	2:F:344:PHE:O	2.00	0.62
1:C:60:VAL:HG21	1:C:65:MET:HE1	1.82	0.62
2:F:440:THR:HG22	2:F:440:THR:O	2.00	0.62
2:H:305:LEU:HB3	2:H:306:PRO:HD3	1.80	0.62
2:H:559:GLU:O	2:H:560:GLY:O	2.18	0.62
1:E:367:CYS:C	1:E:368:LEU:HD12	2.24	0.61
1:E:399:ALA:C	1:E:401:LEU:H	2.08	0.61
2:D:339:THR:OG1	2:D:340:ALA:N	2.32	0.61
2:D:446:ARG:NH1	2:D:630:GLU:OE2	2.31	0.61
1:G:81:ILE:HG22	1:G:81:ILE:O	2.01	0.61
2:H:592:ALA:O	2:H:593:ARG:HB2	1.98	0.61
2:F:512:ARG:NH1	2:H:216:ASP:OD2	2.33	0.61
1:G:127:ASP:OD1	1:G:268:ARG:HD2	2.01	0.61
1:G:314:ARG:HH22	1:G:329:ASP:CG	2.09	0.61
2:B:221:MET:O	2:B:221:MET:HG3	2.00	0.61
2:D:776:ARG:O	2:D:777:ALA:HB3	2.00	0.61
2:H:457:ILE:O	2:H:458:SER:HB2	1.99	0.61
2:H:621:TYR:HE1	2:H:726:LYS:HG2	1.65	0.61
1:G:50:MET:HE1	1:G:116:ALA:HA	1.81	0.61
1:E:314:ARG:HH22	1:E:329:ASP:CG	2.09	0.60
1:A:337:GLU:O	1:A:338:SER:HB3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:ARG:NE	2:D:258:ASP:OD2	2.34	0.60
1:A:407:ARG:NH1	1:A:409:ASP:OD2	2.34	0.60
2:H:457:ILE:O	2:H:458:SER:CB	2.49	0.60
2:D:422:GLN:HG2	2:D:427:PHE:CD2	2.36	0.60
1:E:6:LEU:HD12	1:E:10:GLU:C	2.27	0.60
1:E:33:THR:CG2	2:F:25:ASP:HB3	2.31	0.60
1:G:53:ASP:C	1:G:53:ASP:OD1	2.43	0.60
1:A:369:ASN:HB3	1:A:381:ARG:HB2	1.84	0.60
1:C:301:MET:CE	1:C:341:LEU:HB3	2.32	0.60
2:D:731:PRO:N	2:D:732:PRO:HD2	2.17	0.60
2:F:215:HIS:ND1	2:H:478:SER:HB2	2.16	0.60
1:G:297:ALA:HA	1:G:367:CYS:SG	2.42	0.60
1:C:322:PHE:HB3	1:C:390:VAL:HG21	1.84	0.60
2:F:339:THR:OG1	2:F:340:ALA:N	2.34	0.60
2:F:507:ASP:OD1	2:F:508:PRO:CD	2.49	0.60
1:G:373:LYS:O	1:G:374:GLY:O	2.20	0.60
1:G:428:MET:SD	1:G:428:MET:N	2.74	0.60
2:H:482:ASN:C	2:H:482:ASN:OD1	2.44	0.60
7:B:3007:ZW9:MO	7:B:3007:ZW9:O2	1.71	0.59
1:E:291:ILE:O	1:E:291:ILE:HG22	2.01	0.59
2:F:218:ARG:NH2	2:F:517:ASP:OD1	2.35	0.59
1:E:370:LEU:HD22	1:E:380:ALA:HA	1.83	0.59
1:G:281:ILE:HG23	1:G:282:GLY:N	2.17	0.59
1:G:325:TYR:CD1	1:G:325:TYR:C	2.76	0.59
2:H:736:GLY:O	2:H:737:ILE:C	2.45	0.59
2:B:77:SER:O	2:B:205:LYS:NZ	2.29	0.59
2:B:267:GLY:C	2:B:268:LYS:HG3	2.27	0.59
2:B:328:SER:OG	2:B:330:ARG:NH1	2.34	0.59
2:D:367:ASP:OD1	2:D:368:PRO:HD2	2.02	0.59
1:E:349:ARG:NH1	1:E:450:LEU:HD21	2.16	0.59
2:B:271:ASP:OD2	2:B:296:ARG:NH1	2.35	0.59
1:C:390:VAL:CG2	1:C:391:PRO:HD2	2.30	0.59
1:E:95:MET:HG3	1:E:111:ILE:HD11	1.84	0.59
2:F:305:LEU:HB3	2:F:306:PRO:CD	2.33	0.59
2:H:776:ARG:O	2:H:777:ALA:CB	2.50	0.59
1:A:165:THR:O	1:A:166:LEU:HD23	2.02	0.59
1:E:348:LEU:HD12	1:E:349:ARG:H	1.67	0.59
1:G:359:GLN:O	1:G:359:GLN:CG	2.49	0.59
2:B:704:ARG:HG2	2:B:704:ARG:HH11	1.66	0.59
1:E:447:VAL:O	1:E:448:ARG:C	2.46	0.59
2:F:66:THR:HG22	2:F:68:ALA:H	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:450:LEU:HG	2:F:451:SER:N	2.18	0.59
2:F:617:ARG:HD3	2:F:619:PHE:O	2.02	0.59
1:G:165:THR:O	1:G:165:THR:HG23	2.03	0.59
2:H:730:GLU:O	2:H:731:PRO:C	2.45	0.59
7:D:3007:ZW9:O2	7:D:3007:ZW9:S1'	2.61	0.59
2:H:668:TYR:O	2:H:669:VAL:C	2.45	0.59
1:A:351:TYR:OH	1:A:449:GLU:OE1	2.13	0.59
1:E:205:GLY:O	1:E:209:SER:OG	2.20	0.59
1:E:301:MET:HE1	1:E:341:LEU:HD13	1.83	0.59
2:H:306:PRO:HB2	2:H:344:PHE:CE2	2.38	0.59
2:H:507:ASP:OD1	2:H:508:PRO:CD	2.51	0.58
1:E:302:GLY:CA	1:E:381:ARG:HH11	2.16	0.58
2:H:671:GLY:O	2:H:674:TRP:N	2.34	0.58
1:C:3:ILE:HG23	1:C:16:ILE:HD12	1.84	0.58
2:F:632:VAL:HG22	2:F:643:LEU:HD11	1.85	0.58
1:C:301:MET:CE	1:C:341:LEU:HD13	2.34	0.58
1:C:192:TRP:O	1:C:196:HIS:HD2	1.87	0.58
1:E:349:ARG:HD3	1:E:449:GLU:OE2	2.03	0.58
2:H:247:ARG:HH11	2:H:247:ARG:CG	2.15	0.58
1:A:233:GLN:HA	1:A:233:GLN:OE1	2.03	0.58
2:B:229:GLY:HA2	7:B:3007:ZW9:S	2.44	0.58
1:C:164:PHE:O	1:C:166:LEU:HG	2.04	0.58
1:A:322:PHE:HB3	1:A:390:VAL:CG2	2.33	0.58
2:B:730:GLU:N	2:B:731:PRO:CD	2.66	0.58
2:D:631:VAL:HG21	2:D:743:LEU:CD1	2.34	0.58
1:E:152:GLU:OE1	1:E:153:PRO:HD2	2.03	0.58
1:E:183:PRO:O	1:E:228:CYS:SG	2.62	0.58
1:E:237:THR:CG2	1:E:239:ASP:H	2.16	0.58
2:F:730:GLU:OE2	7:F:3007:ZW9:O1	2.21	0.58
1:A:41:GLU:HG3	1:A:214:LYS:HE3	1.85	0.57
1:A:143:LEU:HD23	1:A:143:LEU:O	2.03	0.57
1:A:105:PHE:CD1	2:B:177:GLU:HB2	2.39	0.57
2:B:341:PHE:O	2:B:342:ARG:C	2.47	0.57
2:F:160:HIS:CB	2:F:364:MET:HE2	2.34	0.57
2:F:776:ARG:O	2:F:777:ALA:HB3	2.04	0.57
1:G:50:MET:HE3	1:G:116:ALA:CB	2.34	0.57
1:A:390:VAL:HG22	1:A:391:PRO:CD	2.35	0.57
1:G:116:ALA:O	1:G:117:ALA:C	2.46	0.57
1:A:18:ASP:OD2	1:A:19:PRO:HD2	2.04	0.57
1:C:279:ALA:HB1	4:C:3005:FAD:H4'	1.86	0.57
2:F:496:MET:HE2	2:F:496:MET:CA	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:ILE:HD13	1:G:114:MET:CE	2.34	0.57
1:A:301:MET:HE3	1:A:341:LEU:HB3	1.87	0.57
1:C:252:LEU:HD22	1:C:281:ILE:HD12	1.86	0.57
2:F:174:PHE:CZ	2:F:693:PRO:HG3	2.39	0.57
2:F:661:ILE:HD11	2:F:712:LEU:HG	1.87	0.57
2:D:367:ASP:OD1	2:D:367:ASP:C	2.47	0.57
2:F:267:GLY:C	2:F:268:LYS:HG3	2.29	0.57
1:G:81:ILE:O	1:G:81:ILE:CG2	2.53	0.57
2:H:94:VAL:HG11	2:H:687:ARG:HG2	1.86	0.57
2:H:205:LYS:HB3	2:H:240:ILE:HD11	1.85	0.57
2:B:134:ALA:HB1	2:F:724:ARG:HH11	1.70	0.57
1:G:432:ALA:O	1:G:433:ALA:C	2.45	0.57
2:H:355:ARG:O	2:H:356:ALA:C	2.46	0.57
1:A:95:MET:HG3	1:A:111:ILE:CD1	2.35	0.57
2:B:281:ASP:OD1	2:B:283:SER:N	2.33	0.57
2:F:457:ILE:O	2:F:458:SER:CB	2.53	0.57
1:G:358:ASP:OD2	2:H:702:SER:OG	2.19	0.57
1:G:455:VAL:HG22	2:H:443:THR:HG21	1.87	0.57
1:A:297:ALA:HA	1:A:367:CYS:SG	2.45	0.57
1:C:314:ARG:O	1:C:315:ARG:HB2	2.05	0.57
1:E:429:ARG:O	1:E:430:ALA:HB2	2.05	0.57
1:E:395:ALA:O	1:E:396:ALA:C	2.48	0.56
2:F:491:GLY:O	2:F:492:LEU:C	2.45	0.56
1:G:302:GLY:HA2	7:G:3010:HOH:O	2.05	0.56
2:H:214:PHE:CD1	2:H:214:PHE:N	2.73	0.56
1:A:399:ALA:O	1:A:401:LEU:N	2.38	0.56
2:B:305:LEU:HB3	2:B:306:PRO:HD3	1.86	0.56
1:C:373:LYS:HB2	1:C:378:GLU:HG2	1.87	0.56
2:D:238:LEU:HD12	2:D:238:LEU:H	1.69	0.56
2:B:305:LEU:HD23	2:B:305:LEU:C	2.30	0.56
2:H:38:GLY:HA3	2:H:99:PHE:CE2	2.40	0.56
2:H:144:VAL:HG11	2:H:312:MET:HE1	1.88	0.56
2:H:229:GLY:HA2	7:H:3007:ZW9:S	2.46	0.56
2:H:683:ASP:OD1	2:H:683:ASP:C	2.48	0.56
2:F:174:PHE:HZ	2:F:693:PRO:HG3	1.70	0.56
2:H:453:VAL:HG12	2:H:454:LYS:N	2.20	0.56
4:E:3005:FAD:H51A	4:E:3005:FAD:H8A	1.88	0.56
1:G:301:MET:HB3	1:G:348:LEU:HD22	1.88	0.56
2:D:214:PHE:CD1	2:D:214:PHE:N	2.74	0.56
1:G:295:PRO:HB2	1:G:296:PRO:CD	2.36	0.56
2:H:412:CYS:HA	2:H:624:TYR:CZ	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ASP:O	1:C:128:LEU:HD22	2.06	0.56
2:B:216:ASP:OD1	2:D:512:ARG:HD2	2.06	0.56
1:C:237:THR:HG23	1:C:239:ASP:H	1.71	0.56
1:E:281:ILE:HD11	1:E:298:LEU:HD11	1.87	0.56
1:A:295:PRO:HB2	1:A:296:PRO:HD3	1.87	0.56
1:E:415:LEU:N	1:E:416:PRO:CD	2.69	0.56
1:E:427:ASP:OD1	1:E:435:ARG:NH2	2.39	0.56
2:F:251:ARG:HB3	2:F:252:PRO:HD2	1.86	0.56
2:H:173:HIS:HA	2:H:341:PHE:CE1	2.39	0.56
2:H:267:GLY:C	2:H:268:LYS:HG3	2.31	0.56
2:B:66:THR:HG22	2:B:68:ALA:N	2.15	0.55
2:B:166:PHE:CZ	2:B:355:ARG:HG3	2.40	0.55
1:E:83:ALA:HB2	1:E:157:TRP:CZ3	2.40	0.55
2:F:328:SER:OG	2:F:330:ARG:NH1	2.36	0.55
1:G:34:GLY:HA2	1:G:36:LYS:HZ2	1.71	0.55
1:A:105:PHE:CE1	2:B:177:GLU:HB2	2.41	0.55
1:A:279:ALA:HB1	4:A:3005:FAD:H4'	1.87	0.55
1:C:316:MET:HB2	1:C:317:PRO:HD2	1.89	0.55
1:E:89:HIS:CE1	1:E:90:PRO:HD2	2.41	0.55
1:E:316:MET:HB2	1:E:317:PRO:CD	2.36	0.55
2:F:621:TYR:CE1	2:F:726:LYS:CG	2.76	0.55
2:H:528:ALA:O	2:H:529:ALA:HB3	2.06	0.55
1:A:301:MET:HB3	1:A:348:LEU:HD22	1.88	0.55
2:D:704:ARG:CG	2:D:704:ARG:NH1	2.68	0.55
1:E:237:THR:HG23	1:E:238:PRO:HD2	1.88	0.55
2:F:197:GLN:HA	2:F:224:MET:HE1	1.88	0.55
1:G:133:LEU:HD13	2:H:698:ILE:HD11	1.88	0.55
2:D:110:ARG:CZ	2:D:258:ASP:OD2	2.54	0.55
2:F:398:LYS:C	2:F:399:LYS:HD2	2.31	0.55
1:G:423:THR:HG22	1:G:423:THR:O	2.05	0.55
1:A:53:ASP:OD1	1:A:53:ASP:C	2.48	0.55
1:C:60:VAL:HG21	1:C:65:MET:CE	2.36	0.55
1:E:450:LEU:C	1:E:452:GLY:H	2.14	0.55
2:B:660:ASP:OD1	2:B:728:VAL:HG11	2.07	0.55
1:E:297:ALA:HA	1:E:367:CYS:SG	2.47	0.55
2:F:463:HIS:CE1	2:H:591:MET:HE1	2.41	0.55
1:G:46:ALA:N	7:G:3007:HOH:O	2.39	0.55
1:A:399:ALA:C	1:A:401:LEU:H	2.15	0.55
1:C:390:VAL:HG22	1:C:391:PRO:CD	2.31	0.55
2:B:92:HIS:O	2:B:93:PHE:HB3	2.07	0.55
1:E:390:VAL:HG22	1:E:391:PRO:HD2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:TYR:O	1:A:326:ARG:CB	2.52	0.54
1:G:348:LEU:HD12	1:G:349:ARG:N	2.23	0.54
1:G:418:LEU:HB3	1:G:436:MET:HE1	1.88	0.54
2:B:737:ILE:HG22	2:B:741:LEU:HD22	1.89	0.54
1:C:301:MET:HE1	1:C:341:LEU:HD13	1.89	0.54
2:D:731:PRO:HB2	2:D:732:PRO:HD3	1.88	0.54
2:D:737:ILE:HG22	2:D:741:LEU:HD22	1.89	0.54
1:A:446:TYR:CE2	1:A:450:LEU:HD12	2.42	0.54
2:F:573:VAL:HG21	2:F:585:ILE:HG13	1.90	0.54
1:C:53:ASP:C	1:C:53:ASP:OD1	2.51	0.54
1:G:299:ILE:O	1:G:300:ALA:C	2.49	0.54
2:H:448:ILE:HG23	2:H:448:ILE:O	2.07	0.54
1:A:26:LEU:HD13	1:A:67:LEU:HD11	1.89	0.54
2:D:94:VAL:HG11	2:D:687:ARG:HG2	1.90	0.54
1:E:301:MET:CE	1:E:341:LEU:HD13	2.37	0.54
2:B:407:GLN:OE1	2:B:618:PRO:HD2	2.08	0.54
2:F:704:ARG:HG3	2:F:704:ARG:O	2.07	0.54
1:G:237:THR:HG23	1:G:238:PRO:CD	2.38	0.54
1:G:240:GLY:HA2	1:G:343:LYS:HG2	1.88	0.54
2:F:631:VAL:HG21	2:F:743:LEU:HD13	1.89	0.54
1:G:143:LEU:O	1:G:144:ARG:C	2.51	0.54
1:G:206:THR:HG21	1:G:275:VAL:HG13	1.90	0.54
1:A:418:LEU:HB3	1:A:436:MET:HE1	1.90	0.54
2:B:730:GLU:H	2:B:731:PRO:CD	2.21	0.54
1:E:399:ALA:C	1:E:401:LEU:N	2.65	0.54
2:F:604:THR:O	2:H:593:ARG:NH1	2.40	0.54
2:H:491:GLY:O	2:H:495:LYS:HG3	2.07	0.54
2:D:218:ARG:NE	2:D:220:GLU:OE2	2.40	0.53
2:D:731:PRO:HB2	2:D:732:PRO:CD	2.38	0.53
1:E:218:ASP:OD1	1:E:218:ASP:C	2.50	0.53
2:B:730:GLU:C	2:B:732:PRO:HD2	2.33	0.53
2:D:328:SER:OG	2:D:330:ARG:NH1	2.37	0.53
1:G:356:ARG:NH2	1:G:359:GLN:O	2.40	0.53
2:H:398:LYS:N	2:H:398:LYS:HE3	2.23	0.53
2:H:631:VAL:HG21	2:H:743:LEU:HD13	1.90	0.53
2:H:731:PRO:N	2:H:732:PRO:CD	2.71	0.53
1:A:423:THR:O	1:A:423:THR:CG2	2.56	0.53
2:D:229:GLY:CA	7:D:3007:ZW9:S	2.94	0.53
1:E:7:LEU:CD1	1:E:75:LEU:HD23	2.38	0.53
1:E:249:ILE:O	1:E:250:ALA:C	2.48	0.53
2:F:210:LEU:HD22	2:F:247:ARG:HD3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:PRO:HG2	1:E:224:PHE:CE1	2.43	0.53
1:E:359:GLN:O	1:E:359:GLN:HG3	2.08	0.53
1:E:445:ARG:HG3	1:E:455:VAL:HG11	1.89	0.53
2:F:164:GLY:HA3	2:F:276:TYR:CZ	2.43	0.53
2:H:34:HIS:C	2:H:35:LEU:HD23	2.34	0.53
1:A:165:THR:O	1:A:165:THR:HG23	2.08	0.53
1:C:37:GLU:CD	2:D:256:ARG:HH21	2.17	0.53
2:H:346:GLY:N	2:H:347:PRO:CD	2.72	0.53
2:B:272:PHE:CD2	2:B:348:GLN:HG2	2.44	0.53
2:B:457:ILE:O	2:B:458:SER:CB	2.56	0.53
1:C:95:MET:HE2	1:C:114:MET:HE1	1.91	0.53
2:H:671:GLY:O	2:H:674:TRP:CB	2.51	0.53
2:B:325:ARG:C	2:B:326:ILE:HG13	2.33	0.53
2:D:407:GLN:OE1	2:D:618:PRO:HD2	2.07	0.53
4:E:3005:FAD:H51A	4:E:3005:FAD:C8A	2.38	0.53
2:F:216:ASP:CG	2:H:512:ARG:HH11	2.16	0.53
2:F:728:VAL:O	2:F:728:VAL:HG22	2.09	0.53
2:H:210:LEU:HD22	2:H:247:ARG:HD3	1.89	0.53
2:D:34:HIS:C	2:D:35:LEU:HD23	2.34	0.53
1:E:133:LEU:HD13	2:F:698:ILE:HD11	1.89	0.53
1:G:237:THR:CB	1:G:238:PRO:HD2	2.39	0.53
2:H:306:PRO:HB2	2:H:344:PHE:HE2	1.73	0.53
1:A:273:GLU:OE1	1:A:276:ARG:NH1	2.42	0.53
1:A:367:CYS:C	1:A:368:LEU:HD12	2.34	0.53
2:B:601:PHE:CG	2:D:595:SER:HB2	2.44	0.53
2:F:698:ILE:HB	2:F:699:PRO:CD	2.38	0.53
2:H:701:PHE:O	2:H:704:ARG:HG2	2.09	0.53
1:C:314:ARG:HD3	1:C:334:GLU:OE1	2.09	0.53
1:E:53:ASP:C	1:E:53:ASP:OD1	2.52	0.53
1:E:370:LEU:CD2	1:E:380:ALA:HA	2.39	0.53
1:G:369:ASN:HB3	1:G:381:ARG:HB2	1.90	0.53
1:A:138:GLY:O	1:A:139:TYR:CB	2.52	0.52
2:B:450:LEU:HG	2:B:451:SER:N	2.14	0.52
1:E:253:ARG:NH2	1:E:268:ARG:HG3	2.23	0.52
2:F:23:LEU:HD22	2:F:180:ALA:HB1	1.91	0.52
2:F:195:SER:O	2:F:231:LYS:HD3	2.09	0.52
1:G:50:MET:CE	1:G:116:ALA:CA	2.87	0.52
1:G:360:ASP:OD1	2:H:697:LYS:HE3	2.09	0.52
1:G:451:SER:O	1:G:451:SER:OG	2.22	0.52
2:H:453:VAL:CG1	2:H:454:LYS:N	2.70	0.52
2:H:730:GLU:N	2:H:731:PRO:CD	2.71	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:N	1:A:210:LEU:HD23	2.23	0.52
2:B:621:TYR:CE1	2:B:726:LYS:HG2	2.45	0.52
2:D:723:PHE:O	2:D:724:ARG:HB2	2.09	0.52
1:E:33:THR:HG21	2:F:25:ASP:HB3	1.92	0.52
1:E:337:GLU:O	1:E:338:SER:CB	2.52	0.52
2:F:367:ASP:OD2	2:F:431:ARG:NH1	2.32	0.52
2:D:450:LEU:HG	2:D:451:SER:N	2.17	0.52
2:D:617:ARG:HD3	2:D:619:PHE:O	2.09	0.52
1:E:12:ARG:CG	1:E:12:ARG:NH1	2.68	0.52
1:E:237:THR:HG23	1:E:238:PRO:N	2.24	0.52
2:F:272:PHE:CD2	2:F:348:GLN:HG2	2.44	0.52
1:G:89:HIS:O	1:G:90:PRO:C	2.53	0.52
2:H:730:GLU:H	2:H:731:PRO:CD	2.22	0.52
2:B:174:PHE:HZ	2:B:693:PRO:HG3	1.75	0.52
2:D:258:ASP:O	2:D:259:ARG:C	2.51	0.52
1:G:110:PHE:O	1:G:111:ILE:C	2.50	0.52
1:G:359:GLN:NE2	4:G:3005:FAD:H6	2.25	0.52
1:C:37:GLU:CD	2:D:256:ARG:NH2	2.68	0.52
2:D:306:PRO:HB2	2:D:344:PHE:CE2	2.45	0.52
2:D:312:MET:HE2	2:D:330:ARG:HH12	1.74	0.52
1:G:136:CYS:SG	3:G:3001:FES:S1	3.05	0.52
2:H:79:ALA:HB1	2:H:80:PRO:HD2	1.91	0.52
2:D:210:LEU:HD22	2:D:247:ARG:HD3	1.91	0.52
2:D:341:PHE:O	2:D:342:ARG:C	2.53	0.52
1:E:216:LEU:HD12	2:F:114:ARG:HD2	1.91	0.52
1:E:324:GLU:O	1:E:325:TYR:C	2.53	0.52
2:H:737:ILE:HG22	2:H:741:LEU:HD22	1.92	0.52
1:A:301:MET:HE1	1:A:341:LEU:HD13	1.92	0.52
1:E:67:LEU:O	1:E:68:PRO:C	2.52	0.52
1:E:250:ALA:O	1:E:253:ARG:N	2.40	0.52
2:H:328:SER:OG	2:H:330:ARG:NH1	2.39	0.52
2:B:210:LEU:HD22	2:B:247:ARG:HD3	1.92	0.52
2:B:634:ASP:OD2	2:B:637:THR:OG1	2.11	0.52
1:C:102:GLN:HB3	2:D:489:GLY:O	2.10	0.52
2:H:28:CYS:HB2	2:H:29:PRO:HD2	1.92	0.52
2:H:238:LEU:H	2:H:238:LEU:HD12	1.74	0.52
2:H:239:ALA:O	2:H:240:ILE:C	2.53	0.52
2:B:48:THR:HG22	2:B:119:THR:OG1	2.10	0.52
2:H:496:MET:HE2	2:H:496:MET:CA	2.39	0.52
1:C:165:THR:O	1:C:165:THR:HG23	2.10	0.51
2:D:552:ALA:O	2:D:553:GLY:C	2.53	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:446:TYR:O	1:E:447:VAL:C	2.51	0.51
1:G:281:ILE:CG2	1:G:282:GLY:N	2.73	0.51
1:G:337:GLU:HG3	1:G:337:GLU:O	2.08	0.51
2:F:721:THR:O	2:F:722:ILE:C	2.51	0.51
2:B:354:GLU:O	2:B:357:ILE:HG22	2.10	0.51
1:G:105:PHE:HD2	2:H:176:LEU:HB3	1.75	0.51
1:G:325:TYR:CZ	1:G:326:ARG:HG3	2.45	0.51
2:H:276:TYR:OH	2:H:359:HIS:HD2	1.94	0.51
4:E:3005:FAD:N1	4:E:3005:FAD:C2'	2.72	0.51
2:H:299:TRP:CD1	2:H:299:TRP:H	2.29	0.51
2:H:536:ASN:O	2:H:537:GLY:C	2.51	0.51
2:H:559:GLU:O	2:H:560:GLY:C	2.53	0.51
1:A:37:GLU:CD	2:B:256:ARG:NH2	2.68	0.51
2:D:53:GLU:OE1	2:D:53:GLU:HA	2.09	0.51
2:D:325:ARG:C	2:D:326:ILE:HG13	2.34	0.51
2:F:717:ASN:O	2:F:724:ARG:HD3	2.11	0.51
1:C:139:TYR:O	1:C:140:ALA:C	2.52	0.51
2:F:721:THR:O	2:F:724:ARG:N	2.35	0.51
1:G:102:GLN:HB3	2:H:489:GLY:O	2.11	0.51
1:G:67:LEU:O	1:G:68:PRO:C	2.52	0.51
2:H:517:ASP:OD2	2:H:517:ASP:C	2.53	0.51
1:A:206:THR:HG21	1:A:275:VAL:HG13	1.92	0.51
2:D:635:ARG:HD3	2:D:750:CYS:SG	2.51	0.51
1:E:349:ARG:NH1	1:E:450:LEU:CD2	2.74	0.51
1:G:164:PHE:O	1:G:166:LEU:HG	2.11	0.51
2:H:482:ASN:OD1	2:H:483:HIS:N	2.43	0.51
1:A:353:LEU:HD21	1:A:434:TYR:OH	2.11	0.51
1:C:83:ALA:HB1	1:C:84:PRO:HD2	1.93	0.51
1:C:165:THR:C	1:C:166:LEU:HD23	2.35	0.51
2:D:164:GLY:HA3	2:D:276:TYR:CZ	2.46	0.51
2:F:700:ALA:O	2:F:701:PHE:C	2.52	0.51
2:H:529:ALA:O	2:H:530:SER:C	2.52	0.51
2:D:53:GLU:HB3	2:D:54:PRO:HD3	1.93	0.51
2:D:79:ALA:HB1	2:D:80:PRO:CD	2.41	0.51
2:D:281:ASP:HB2	2:D:285:LYS:O	2.10	0.51
1:E:126:ASP:OD1	2:F:704:ARG:NH1	2.33	0.51
1:E:237:THR:OG1	1:E:238:PRO:HD2	2.11	0.51
1:E:314:ARG:O	1:E:315:ARG:HB2	2.11	0.51
2:H:128:THR:O	2:H:129:LEU:C	2.52	0.51
2:H:302:ASP:OD1	2:H:303:LEU:N	2.44	0.51
2:H:398:LYS:O	2:H:399:LYS:O	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:HB2	1:A:317:PRO:CD	2.41	0.50
2:F:697:LYS:HD2	2:F:697:LYS:N	2.26	0.50
1:G:103:CYS:SG	1:G:136:CYS:SG	3.10	0.50
1:G:111:ILE:HD13	1:G:114:MET:HE3	1.93	0.50
2:B:574:GLN:HG3	2:B:579:SER:HB2	1.92	0.50
1:C:314:ARG:HH22	1:C:329:ASP:CG	2.19	0.50
2:F:312:MET:HE2	2:F:330:ARG:HH12	1.75	0.50
2:F:730:GLU:N	2:F:731:PRO:CD	2.74	0.50
2:H:23:LEU:HD13	2:H:194:CYS:HA	1.93	0.50
2:B:214:PHE:CD1	2:B:214:PHE:N	2.77	0.50
1:E:139:TYR:C	1:E:141:PRO:HD2	2.35	0.50
1:E:380:ALA:O	1:E:398:GLU:HG2	2.12	0.50
1:G:39:CYS:SG	1:G:40:ASN:N	2.84	0.50
2:H:517:ASP:OD2	2:H:519:SER:N	2.33	0.50
1:A:414:ALA:O	1:A:415:LEU:C	2.53	0.50
2:D:272:PHE:CD2	2:D:348:GLN:HG2	2.46	0.50
2:F:144:VAL:HG11	2:F:312:MET:HE1	1.93	0.50
1:G:140:ALA:N	1:G:141:PRO:HD2	2.26	0.50
1:G:337:GLU:O	1:G:338:SER:HB3	2.12	0.50
2:H:79:ALA:HB1	2:H:80:PRO:CD	2.41	0.50
2:H:261:ASP:O	2:H:262:ASP:C	2.51	0.50
2:H:251:ARG:CB	2:H:252:PRO:CD	2.90	0.50
2:H:440:THR:O	2:H:440:THR:CG2	2.60	0.50
1:A:237:THR:CB	1:A:238:PRO:HD2	2.42	0.50
1:E:369:ASN:C	1:E:370:LEU:HD23	2.37	0.50
2:F:731:PRO:N	2:F:732:PRO:HD2	2.26	0.50
1:G:295:PRO:CB	1:G:296:PRO:HD3	2.37	0.50
1:C:95:MET:SD	1:C:114:MET:HE1	2.52	0.50
2:F:512:ARG:HH11	2:H:216:ASP:CG	2.19	0.50
1:G:248:THR:HA	1:G:279:ALA:O	2.12	0.50
2:H:92:HIS:O	2:H:93:PHE:HB3	2.11	0.50
1:E:181:PHE:C	1:E:182:LEU:HD12	2.37	0.50
4:G:3005:FAD:H8A	4:G:3005:FAD:H52A	1.93	0.50
2:H:196:SER:O	2:H:224:MET:HE2	2.12	0.50
2:H:639:GLU:O	2:H:640:ASN:HB3	2.11	0.50
2:B:674:TRP:CE3	2:B:675:LEU:HD21	2.47	0.50
1:C:324:GLU:O	1:C:325:TYR:C	2.54	0.50
2:F:554:PHE:HB2	2:F:594:ILE:CD1	2.42	0.50
1:G:210:LEU:HD23	1:G:210:LEU:N	2.27	0.50
1:G:314:ARG:HD3	1:G:334:GLU:OE1	2.12	0.50
2:H:74:ASN:OD1	2:H:85:VAL:N	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:HE2	1:A:114:MET:HE1	1.94	0.49
1:A:291:ILE:HG22	1:A:291:ILE:O	2.12	0.49
2:B:448:ILE:HG13	2:B:630:GLU:HB2	1.94	0.49
1:E:331:ARG:O	1:E:332:PRO:C	2.55	0.49
2:F:683:ASP:OD1	2:F:683:ASP:C	2.53	0.49
1:G:59:ALA:C	1:G:60:VAL:HG13	2.35	0.49
1:A:355:LYS:HE2	2:B:679:GLU:OE1	2.12	0.49
2:B:645:THR:HG21	2:B:668:TYR:CZ	2.47	0.49
1:E:33:THR:HG23	2:F:25:ASP:HB3	1.94	0.49
1:G:233:GLN:OE1	1:G:233:GLN:HA	2.11	0.49
2:H:296:ARG:HH11	2:H:296:ARG:CG	2.24	0.49
2:F:23:LEU:HD22	2:F:180:ALA:CB	2.42	0.49
1:G:369:ASN:O	1:G:370:LEU:HD23	2.11	0.49
2:B:348:GLN:N	2:B:348:GLN:OE1	2.44	0.49
1:C:337:GLU:O	1:C:337:GLU:HG3	2.11	0.49
2:F:70:LEU:HD12	2:F:74:ASN:CB	2.39	0.49
2:F:407:GLN:CD	2:F:617:ARG:HG2	2.36	0.49
2:H:166:PHE:CZ	2:H:355:ARG:HG3	2.47	0.49
1:A:368:LEU:HD12	1:A:368:LEU:N	2.27	0.49
2:B:302:ASP:OD1	2:B:303:LEU:N	2.44	0.49
2:B:503:VAL:O	2:B:503:VAL:HG12	2.12	0.49
1:E:103:CYS:N	3:E:3001:FES:S1	2.85	0.49
1:G:349:ARG:HD3	1:G:449:GLU:OE2	2.12	0.49
2:H:555:VAL:O	2:H:555:VAL:HG12	2.11	0.49
1:A:399:ALA:C	1:A:401:LEU:N	2.71	0.49
2:B:128:THR:O	2:B:129:LEU:C	2.53	0.49
1:C:138:GLY:O	1:C:139:TYR:HB2	2.13	0.49
1:E:143:LEU:O	1:E:144:ARG:C	2.55	0.49
2:F:346:GLY:N	2:F:347:PRO:CD	2.74	0.49
1:G:93:GLN:NE2	1:G:97:ASP:OD1	2.45	0.49
1:G:98:HIS:O	1:G:99:HIS:HB2	2.12	0.49
2:D:700:ALA:O	2:D:701:PHE:C	2.56	0.49
1:E:50:MET:CE	1:E:116:ALA:HA	2.43	0.49
1:E:369:ASN:O	1:E:370:LEU:HD23	2.13	0.49
2:F:256:ARG:O	2:F:256:ARG:HG3	2.12	0.49
2:B:731:PRO:N	2:B:732:PRO:CD	2.76	0.49
1:C:237:THR:HG23	1:C:238:PRO:CD	2.43	0.49
1:C:346:PRO:O	1:C:349:ARG:NH2	2.46	0.49
2:D:367:ASP:OD1	2:D:368:PRO:CD	2.60	0.49
2:F:457:ILE:O	2:F:458:SER:OG	2.30	0.49
1:A:324:GLU:O	1:A:325:TYR:C	2.55	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:PHE:CZ	2:B:693:PRO:HG3	2.47	0.49
2:B:577:GLY:O	7:B:3011:HOH:O	2.19	0.49
1:C:427:ASP:C	1:C:427:ASP:OD1	2.56	0.49
2:F:74:ASN:OD1	2:F:85:VAL:N	2.42	0.49
2:F:440:THR:O	2:F:440:THR:CG2	2.60	0.49
2:F:617:ARG:NH1	2:F:620:LEU:O	2.46	0.49
1:G:59:ALA:C	1:G:60:VAL:CG1	2.84	0.49
1:G:122:ARG:NH2	1:G:124:ASP:OD2	2.46	0.49
1:A:281:ILE:HD11	1:A:298:LEU:HD11	1.94	0.49
1:E:69:GLN:NE2	1:E:203:ALA:O	2.46	0.49
2:F:33:LEU:HD21	2:F:251:ARG:NH1	2.27	0.49
2:B:730:GLU:O	2:B:731:PRO:C	2.54	0.48
2:D:776:ARG:O	2:D:777:ALA:CB	2.61	0.48
2:F:736:GLY:O	2:F:737:ILE:C	2.56	0.48
1:G:61:ASN:ND2	1:G:274:GLN:HB3	2.28	0.48
2:H:730:GLU:C	2:H:732:PRO:CD	2.85	0.48
1:A:216:LEU:HD12	2:B:114:ARG:HD2	1.95	0.48
2:D:343:GLY:O	2:D:344:PHE:C	2.52	0.48
2:D:426:ASN:HD22	2:D:429:THR:HB	1.78	0.48
1:E:88:LEU:HD21	2:F:13:ARG:CZ	2.43	0.48
1:G:237:THR:HG23	1:G:238:PRO:N	2.26	0.48
1:G:399:ALA:C	1:G:401:LEU:H	2.21	0.48
1:A:252:LEU:CD2	1:A:281:ILE:HD12	2.43	0.48
2:B:166:PHE:CE1	2:B:355:ARG:HG3	2.49	0.48
2:B:635:ARG:HD3	2:B:750:CYS:SG	2.53	0.48
1:C:33:THR:CG2	2:D:25:ASP:HB3	2.44	0.48
1:C:316:MET:HB2	1:C:317:PRO:CD	2.42	0.48
2:F:221:MET:HE1	2:F:224:MET:HG3	1.94	0.48
2:F:648:LEU:HA	2:F:711:ALA:O	2.13	0.48
1:G:252:LEU:HD22	1:G:281:ILE:CD1	2.42	0.48
2:B:28:CYS:HB2	2:B:29:PRO:HD2	1.94	0.48
2:D:731:PRO:N	2:D:732:PRO:CD	2.77	0.48
1:E:337:GLU:O	1:E:337:GLU:HG3	2.13	0.48
2:F:398:LYS:N	2:F:398:LYS:HE3	2.27	0.48
1:G:325:TYR:HB2	1:G:389:GLY:CA	2.43	0.48
2:H:471:VAL:HG12	2:H:472:GLN:N	2.27	0.48
1:A:322:PHE:HB3	1:A:390:VAL:HG22	1.96	0.48
2:F:590:TYR:HE1	2:H:466:GLN:NE2	2.09	0.48
2:H:730:GLU:H	2:H:731:PRO:HD2	1.78	0.48
2:B:601:PHE:CD1	2:D:595:SER:HB2	2.49	0.48
1:E:7:LEU:HD21	1:E:32:LEU:HD11	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:THR:HG23	1:E:165:THR:O	2.13	0.48
2:F:671:GLY:O	2:F:674:TRP:HB3	2.14	0.48
1:G:203:ALA:HB3	4:G:3005:FAD:O1P	2.14	0.48
2:H:221:MET:HE2	2:H:224:MET:HE2	1.95	0.48
7:B:3007:ZW9:S	7:B:3007:ZW9:O2	2.71	0.48
2:H:201:GLU:O	2:H:202:ILE:C	2.57	0.48
2:H:409:VAL:O	2:H:409:VAL:HG12	2.13	0.48
2:B:595:SER:HB2	2:D:601:PHE:CG	2.49	0.48
1:C:240:GLY:HA2	1:C:343:LYS:HG2	1.96	0.48
2:F:319:TYR:OH	2:F:372:ARG:HD3	2.12	0.48
1:G:115:ALA:O	1:G:116:ALA:C	2.57	0.48
2:H:105:SER:O	2:H:106:HIS:C	2.53	0.48
2:H:298:GLY:HA3	2:H:337:SER:HA	1.96	0.48
2:B:35:LEU:HA	2:B:101:VAL:O	2.14	0.48
2:D:175:TYR:O	2:D:259:ARG:NH2	2.42	0.48
2:D:218:ARG:NH2	2:D:517:ASP:OD1	2.46	0.48
1:E:77:THR:O	1:E:78:ILE:C	2.53	0.48
1:E:394:ALA:O	1:E:395:ALA:C	2.56	0.48
2:F:606:LYS:NZ	2:F:719:GLU:OE1	2.36	0.48
2:H:60:GLY:O	2:H:103:ALA:HB1	2.14	0.48
2:B:288:GLY:HA2	2:B:323:ALA:O	2.13	0.47
1:A:314:ARG:HH22	1:A:329:ASP:CG	2.22	0.47
1:A:356:ARG:NH2	1:A:359:GLN:O	2.46	0.47
1:C:129:LEU:O	1:C:130:ALA:C	2.56	0.47
2:F:201:GLU:O	2:F:202:ILE:C	2.58	0.47
2:F:299:TRP:CD1	2:F:299:TRP:H	2.32	0.47
1:G:7:LEU:O	1:G:8:ASN:C	2.57	0.47
1:G:151:GLY:O	1:G:152:GLU:HG2	2.14	0.47
2:H:414:LEU:O	2:H:415:GLY:C	2.58	0.47
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.68	0.47
2:B:107:ARG:O	2:B:108:ALA:C	2.56	0.47
2:B:148:ARG:HD3	2:B:322:PRO:O	2.14	0.47
1:C:237:THR:CB	1:C:238:PRO:HD2	2.44	0.47
1:C:432:ALA:O	1:C:433:ALA:C	2.56	0.47
1:G:31:GLY:O	1:G:33:THR:N	2.40	0.47
1:G:325:TYR:CZ	1:G:326:ARG:CG	2.93	0.47
2:H:380:PRO:HB3	2:H:410:ALA:O	2.14	0.47
1:A:281:ILE:HG23	1:A:282:GLY:N	2.28	0.47
2:B:560:GLY:O	2:B:561:CYS:HB3	2.15	0.47
2:B:168:ILE:HD13	2:B:351:LEU:HD23	1.97	0.47
1:E:322:PHE:CB	1:E:390:VAL:CG2	2.93	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HD21	1:A:434:TYR:CZ	2.50	0.47
2:B:730:GLU:N	2:B:731:PRO:HD2	2.30	0.47
1:C:25:GLU:H	1:C:25:GLU:HG2	1.57	0.47
1:E:68:PRO:HB2	1:E:224:PHE:CE1	2.49	0.47
1:E:373:LYS:O	1:E:374:GLY:O	2.33	0.47
1:A:432:ALA:O	1:A:433:ALA:C	2.54	0.47
2:B:251:ARG:CB	2:B:252:PRO:HD2	2.44	0.47
2:B:496:MET:HE2	2:B:496:MET:HA	1.95	0.47
2:B:731:PRO:HB2	2:B:732:PRO:HD3	1.97	0.47
4:C:3005:FAD:N1	4:C:3005:FAD:C2'	2.72	0.47
2:D:251:ARG:HB3	2:D:252:PRO:CD	2.44	0.47
2:D:288:GLY:HA2	2:D:323:ALA:O	2.13	0.47
2:D:621:TYR:CE1	2:D:726:LYS:CG	2.95	0.47
1:E:103:CYS:HB3	1:E:136:CYS:SG	2.55	0.47
1:G:67:LEU:HD23	1:G:67:LEU:HA	1.45	0.47
2:H:53:GLU:N	2:H:54:PRO:CD	2.77	0.47
2:H:93:PHE:HD1	2:H:94:VAL:O	1.98	0.47
2:H:493:HIS:CG	2:H:513:ILE:HG12	2.50	0.47
2:H:550:ARG:O	2:H:551:LEU:C	2.51	0.47
2:B:28:CYS:HB2	2:B:29:PRO:CD	2.45	0.47
2:F:380:PRO:HB3	2:F:410:ALA:O	2.14	0.47
1:A:45:GLY:O	1:A:48:THR:OG1	2.32	0.47
1:C:427:ASP:OD1	1:C:429:ARG:N	2.31	0.47
2:D:160:HIS:CB	2:D:364:MET:HE2	2.44	0.47
2:D:360:LEU:CG	2:D:364:MET:HE3	2.37	0.47
2:F:160:HIS:CG	2:F:364:MET:HE2	2.49	0.47
2:F:371:LEU:HD12	2:F:371:LEU:HA	1.76	0.47
2:F:452:PRO:O	2:F:452:PRO:HG2	2.14	0.47
1:G:350:CYS:HG	1:G:367:CYS:HG	1.61	0.47
2:H:227:GLY:O	2:H:229:GLY:N	2.48	0.47
2:H:343:GLY:O	2:H:344:PHE:C	2.58	0.47
2:B:202:ILE:HD13	2:B:236:ASN:HD22	1.80	0.47
2:D:221:MET:O	2:D:221:MET:HG3	2.15	0.47
2:D:310:ARG:HD2	2:D:344:PHE:HB3	1.97	0.47
2:D:346:GLY:N	2:D:347:PRO:CD	2.78	0.47
1:G:218:ASP:OD1	1:G:218:ASP:C	2.58	0.47
2:B:422:GLN:HG2	2:B:427:PHE:CD2	2.50	0.46
1:C:373:LYS:O	1:C:374:GLY:O	2.33	0.46
2:F:568:PHE:CD2	2:F:573:VAL:HG22	2.49	0.46
1:G:103:CYS:HG	1:G:136:CYS:HG	1.54	0.46
1:A:401:LEU:HD11	1:A:411:ILE:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:744:HIS:C	2:B:744:HIS:CD2	2.91	0.46
1:E:453:GLU:HG2	1:E:454:ALA:N	2.31	0.46
2:F:354:GLU:OE1	2:F:372:ARG:NE	2.42	0.46
1:G:83:ALA:HB2	1:G:157:TRP:CD2	2.49	0.46
1:A:153:PRO:HA	1:A:154:PRO:HD3	1.82	0.46
2:B:96:GLN:HA	2:B:97:PRO:HD3	1.86	0.46
1:E:283:GLY:O	1:E:284:ASN:C	2.55	0.46
1:G:192:TRP:O	1:G:196:HIS:HD2	1.98	0.46
2:H:7:LEU:HB3	2:H:8:PRO:HD2	1.96	0.46
2:H:418:VAL:O	2:H:421:LEU:N	2.47	0.46
2:B:671:GLY:O	2:B:674:TRP:HB3	2.16	0.46
2:D:517:ASP:OD2	2:D:517:ASP:C	2.58	0.46
1:E:68:PRO:CB	1:E:224:PHE:CE1	2.98	0.46
1:E:248:THR:HA	1:E:279:ALA:O	2.15	0.46
2:F:547:LEU:O	2:F:550:ARG:N	2.49	0.46
1:G:125:TYR:O	1:G:126:ASP:C	2.58	0.46
1:G:325:TYR:O	1:G:325:TYR:CG	2.62	0.46
1:G:348:LEU:HD12	1:G:348:LEU:HA	1.58	0.46
1:G:364:VAL:HG12	1:G:442:MET:HE1	1.97	0.46
2:H:348:GLN:O	2:H:349:GLY:C	2.54	0.46
1:A:237:THR:HG23	1:A:238:PRO:CD	2.46	0.46
1:A:314:ARG:HD3	1:A:334:GLU:OE1	2.16	0.46
2:B:324:LEU:HD21	2:B:326:ILE:HD11	1.98	0.46
2:D:302:ASP:OD1	2:D:303:LEU:N	2.49	0.46
2:F:247:ARG:HH11	2:F:247:ARG:CG	2.19	0.46
2:F:341:PHE:O	2:F:342:ARG:C	2.57	0.46
2:H:656:ASN:C	2:H:656:ASN:OD1	2.57	0.46
1:A:141:PRO:HG2	1:A:142:ILE:N	2.31	0.46
2:B:507:ASP:OD1	2:B:508:PRO:HD2	2.16	0.46
1:C:237:THR:HG23	1:C:238:PRO:N	2.31	0.46
1:C:281:ILE:HD11	1:C:298:LEU:HD11	1.96	0.46
1:E:44:CYS:N	3:E:3002:FES:S1	2.88	0.46
1:G:370:LEU:CD2	1:G:380:ALA:HA	2.46	0.46
2:H:701:PHE:HE2	2:H:704:ARG:NH1	2.14	0.46
1:A:376:LYS:HD3	1:A:403:GLY:O	2.14	0.46
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.76	0.46
2:D:51:ASP:HB3	2:D:117:ARG:HB2	1.97	0.46
2:D:645:THR:HG21	2:D:668:TYR:CZ	2.51	0.46
2:F:744:HIS:HE1	2:F:754:TRP:CZ3	2.34	0.46
1:G:48:THR:C	1:G:49:VAL:HG13	2.38	0.46
2:H:133:LEU:HD12	2:H:133:LEU:HA	1.75	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:367:ASP:CG	2:H:431:ARG:HH12	2.19	0.46
2:H:730:GLU:N	2:H:731:PRO:HD2	2.31	0.46
2:B:51:ASP:HB3	2:B:117:ARG:HB2	1.98	0.46
2:B:308:CYS:O	2:B:312:MET:HG3	2.15	0.46
2:D:278:ILE:HD11	2:D:286:LEU:HD22	1.98	0.46
1:E:89:HIS:ND1	1:E:90:PRO:CD	2.78	0.46
4:G:3005:FAD:H2'	4:G:3005:FAD:N1	2.30	0.46
2:H:144:VAL:CG1	2:H:312:MET:HE1	2.46	0.46
2:H:228:PHE:O	2:H:341:PHE:HA	2.16	0.46
2:H:617:ARG:HD3	2:H:619:PHE:O	2.16	0.46
1:C:67:LEU:HD23	1:C:67:LEU:HA	1.55	0.46
2:D:457:ILE:O	2:D:458:SER:CB	2.64	0.46
1:E:316:MET:CE	1:E:316:MET:CG	2.92	0.46
2:F:450:LEU:HD12	2:F:628:ILE:CG1	2.46	0.46
1:G:202:ILE:HD12	1:G:222:VAL:HG13	1.97	0.46
1:G:216:LEU:HD12	2:H:114:ARG:HD2	1.97	0.46
1:G:283:GLY:O	1:G:284:ASN:C	2.56	0.46
1:G:301:MET:HE1	1:G:341:LEU:HD13	1.97	0.46
1:G:382:ILE:O	1:G:393:ARG:HA	2.16	0.46
2:H:632:VAL:HG13	2:H:643:LEU:HD11	1.97	0.46
1:A:37:GLU:CD	2:B:256:ARG:HH22	2.24	0.46
2:D:79:ALA:HB1	2:D:80:PRO:HD2	1.98	0.46
1:E:390:VAL:HG22	1:E:391:PRO:CD	2.46	0.46
2:F:343:GLY:O	2:F:344:PHE:C	2.58	0.46
1:A:91:VAL:O	1:A:91:VAL:CG1	2.55	0.45
1:A:293:ASP:OD2	1:A:352:LYS:NZ	2.46	0.45
1:A:316:MET:HB2	1:A:317:PRO:HD2	1.98	0.45
2:D:221:MET:HE2	2:D:486:THR:HB	1.97	0.45
2:F:143:PRO:HB3	2:F:329:HIS:CE1	2.52	0.45
1:G:151:GLY:C	1:G:152:GLU:HG2	2.40	0.45
1:A:32:LEU:HA	1:A:32:LEU:HD23	1.67	0.45
1:A:349:ARG:HD3	1:A:449:GLU:OE2	2.15	0.45
1:A:370:LEU:HD23	1:A:380:ALA:HA	1.98	0.45
1:C:3:ILE:HG23	1:C:16:ILE:CD1	2.45	0.45
2:D:48:THR:O	2:D:48:THR:HG23	2.16	0.45
2:D:717:ASN:O	2:D:724:ARG:HD3	2.16	0.45
1:E:164:PHE:CG	1:E:165:THR:N	2.84	0.45
2:F:722:ILE:HD12	2:F:722:ILE:HA	1.78	0.45
1:G:50:MET:HE3	1:G:116:ALA:CA	2.47	0.45
1:G:335:PHE:HD1	1:G:336:VAL:O	1.98	0.45
2:H:66:THR:CG2	2:H:67:ALA:N	2.77	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:CZ	2:B:697:LYS:NZ	2.80	0.45
2:B:437:TRP:CZ3	2:B:446:ARG:HG3	2.51	0.45
2:B:466:GLN:HA	2:B:602:TYR:O	2.16	0.45
2:B:704:ARG:HH11	2:B:704:ARG:CG	2.30	0.45
2:B:728:VAL:HG22	2:B:728:VAL:O	2.16	0.45
2:B:742:ALA:O	2:B:743:LEU:C	2.59	0.45
2:F:513:ILE:O	2:F:513:ILE:HG23	2.16	0.45
1:G:291:ILE:O	1:G:291:ILE:HG22	2.14	0.45
2:H:35:LEU:HD13	2:H:100:LEU:HD11	1.98	0.45
2:D:634:ASP:OD2	2:D:637:THR:OG1	2.25	0.45
1:E:237:THR:CB	1:E:238:PRO:HD2	2.46	0.45
2:F:450:LEU:HD12	2:F:628:ILE:HG13	1.98	0.45
1:G:418:LEU:HD23	1:G:418:LEU:HA	1.73	0.45
7:H:3007:ZW9:S1'	7:H:3007:ZW9:O2	2.75	0.45
2:B:324:LEU:CD2	2:B:326:ILE:HD11	2.46	0.45
1:E:76:ARG:HH11	1:E:161:ASP:CG	2.19	0.45
1:G:83:ALA:HB2	1:G:157:TRP:CE3	2.52	0.45
1:G:237:THR:CG2	1:G:239:ASP:H	2.24	0.45
2:H:702:SER:O	2:H:706:ARG:NH2	2.46	0.45
1:A:203:ALA:HB3	4:A:3005:FAD:O1P	2.17	0.45
1:A:434:TYR:CE1	2:B:764:GLU:HA	2.51	0.45
2:B:697:LYS:N	2:B:697:LYS:HD2	2.31	0.45
2:D:261:ASP:O	2:D:262:ASP:C	2.59	0.45
2:D:702:SER:HB2	2:D:706:ARG:HH22	1.81	0.45
1:E:164:PHE:O	1:E:166:LEU:HG	2.16	0.45
1:E:228:CYS:O	1:E:229:LYS:C	2.59	0.45
2:F:288:GLY:HA2	2:F:323:ALA:O	2.17	0.45
2:F:533:ALA:O	2:F:534:ASP:C	2.56	0.45
1:A:129:LEU:O	1:A:130:ALA:C	2.55	0.45
1:A:314:ARG:O	1:A:315:ARG:HB2	2.16	0.45
2:D:263:MET:HE3	2:D:691:HIS:C	2.42	0.45
2:D:554:PHE:HB2	2:D:594:ILE:CD1	2.47	0.45
1:G:26:LEU:O	1:G:26:LEU:HG	2.17	0.45
2:H:174:PHE:HZ	2:H:693:PRO:HG3	1.80	0.45
2:H:446:ARG:HG2	2:H:632:VAL:HG13	1.96	0.45
2:H:674:TRP:CE3	2:H:675:LEU:HD21	2.51	0.45
1:E:91:VAL:HG11	1:E:114:MET:HB3	1.99	0.45
2:F:446:ARG:HG2	2:F:632:VAL:HG13	1.99	0.45
1:G:122:ARG:HH21	1:G:124:ASP:CG	2.23	0.45
1:G:228:CYS:O	1:G:229:LYS:C	2.60	0.45
1:A:392:LYS:HG3	1:A:422:PHE:HE2	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:730:GLU:HB2	2:B:731:PRO:HD3	1.98	0.45
2:D:367:ASP:OD1	2:D:368:PRO:N	2.50	0.45
1:E:358:ASP:OD2	2:F:702:SER:CB	2.63	0.45
2:F:744:HIS:CD2	2:F:744:HIS:C	2.94	0.45
1:G:45:GLY:O	1:G:48:THR:OG1	2.33	0.45
1:G:354:SER:HB2	1:G:360:ASP:OD2	2.17	0.45
1:E:316:MET:CB	1:E:317:PRO:CD	2.95	0.45
2:F:93:PHE:CE2	2:F:299:TRP:NE1	2.85	0.45
2:F:214:PHE:N	2:F:214:PHE:CD1	2.84	0.45
2:F:776:ARG:O	2:F:777:ALA:CB	2.65	0.45
1:G:353:LEU:HD21	1:G:434:TYR:CZ	2.51	0.45
2:H:551:LEU:HA	2:H:551:LEU:HD23	1.65	0.45
2:B:561:CYS:SG	2:B:562:ALA:N	2.90	0.44
1:C:374:GLY:C	1:C:376:LYS:H	2.24	0.44
2:D:233:SER:C	2:D:235:GLY:H	2.25	0.44
2:D:247:ARG:HH11	2:D:247:ARG:CG	2.14	0.44
2:D:698:ILE:HB	2:D:699:PRO:CD	2.47	0.44
1:E:83:ALA:HB2	1:E:157:TRP:CH2	2.52	0.44
2:F:645:THR:HG21	2:F:668:TYR:CZ	2.52	0.44
1:G:434:TYR:CE1	2:H:764:GLU:HA	2.52	0.44
2:B:717:ASN:O	2:B:724:ARG:HD3	2.17	0.44
2:F:140:GLU:O	2:F:141:GLY:C	2.60	0.44
1:G:129:LEU:O	1:G:130:ALA:C	2.59	0.44
2:B:595:SER:HB2	2:D:601:PHE:CD1	2.52	0.44
1:C:407:ARG:NH1	1:C:409:ASP:OD2	2.50	0.44
1:E:32:LEU:HD23	1:E:32:LEU:HA	1.83	0.44
2:F:306:PRO:HB2	2:F:344:PHE:CE2	2.52	0.44
1:G:89:HIS:C	1:G:91:VAL:N	2.74	0.44
2:H:743:LEU:HD12	2:H:743:LEU:HA	1.65	0.44
2:B:405:TYR:O	2:B:615:GLN:HA	2.18	0.44
1:C:33:THR:HG23	2:D:25:ASP:HB3	1.99	0.44
1:C:281:ILE:HG23	1:C:282:GLY:N	2.31	0.44
2:D:214:PHE:N	2:D:214:PHE:HD1	2.13	0.44
2:D:730:GLU:C	2:D:732:PRO:HD2	2.41	0.44
2:F:196:SER:C	2:F:224:MET:HE2	2.43	0.44
2:F:202:ILE:O	2:F:203:GLN:C	2.60	0.44
1:G:61:ASN:ND2	1:G:61:ASN:H	2.15	0.44
2:H:107:ARG:O	2:H:108:ALA:C	2.58	0.44
2:H:143:PRO:HB3	2:H:329:HIS:CE1	2.53	0.44
2:H:288:GLY:HA2	2:H:323:ALA:O	2.17	0.44
1:A:301:MET:CE	1:A:341:LEU:HD13	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:TYR:CZ	1:C:450:LEU:HD11	2.53	0.44
2:D:160:HIS:HB3	2:D:364:MET:HE2	2.00	0.44
2:F:283:SER:C	2:F:366:ARG:HH22	2.25	0.44
2:F:454:LYS:O	2:F:454:LYS:CG	2.63	0.44
1:G:27:LEU:HD22	1:G:32:LEU:HD12	1.99	0.44
1:G:316:MET:HB2	1:G:317:PRO:HD2	1.99	0.44
2:H:146:TRP:CZ3	2:H:313:LEU:HD13	2.53	0.44
2:H:721:THR:O	2:H:722:ILE:C	2.57	0.44
1:E:67:LEU:O	1:E:69:GLN:N	2.50	0.44
2:F:66:THR:HG22	2:F:68:ALA:N	2.30	0.44
1:G:48:THR:C	1:G:49:VAL:CG1	2.90	0.44
1:G:254:ALA:O	1:G:255:PHE:C	2.61	0.44
2:H:448:ILE:O	2:H:448:ILE:CG2	2.62	0.44
1:A:83:ALA:HB1	1:A:84:PRO:HD2	2.00	0.44
2:B:343:GLY:O	2:B:344:PHE:C	2.56	0.44
2:B:440:THR:O	2:B:440:THR:CG2	2.63	0.44
1:E:368:LEU:N	1:E:368:LEU:CD1	2.78	0.44
1:E:438:ALA:O	1:E:439:ALA:C	2.61	0.44
2:F:79:ALA:HB1	2:F:80:PRO:HD2	2.00	0.44
2:F:453:VAL:HG12	2:F:454:LYS:N	2.32	0.44
1:G:49:VAL:HA	1:G:112:VAL:HG11	1.98	0.44
1:G:65:MET:HE3	1:G:65:MET:HB2	1.85	0.44
1:G:78:ILE:HG23	1:G:79:GLU:N	2.33	0.44
1:A:348:LEU:CD1	1:A:349:ARG:N	2.74	0.44
1:A:382:ILE:O	1:A:393:ARG:HA	2.16	0.44
2:B:501:ALA:HB1	2:B:506:ILE:O	2.17	0.44
2:B:647:ILE:HD13	2:B:735:LEU:HD13	1.99	0.44
2:D:251:ARG:CB	2:D:252:PRO:CD	2.96	0.44
2:D:730:GLU:N	2:D:731:PRO:HD2	2.31	0.44
2:H:319:TYR:OH	2:H:372:ARG:HD3	2.17	0.44
2:B:319:TYR:OH	2:B:372:ARG:HD3	2.18	0.44
2:D:144:VAL:HG11	2:D:312:MET:HE1	1.99	0.44
2:D:215:HIS:CD2	2:D:215:HIS:C	2.96	0.44
1:E:140:ALA:N	1:E:141:PRO:CD	2.81	0.44
1:E:266:LEU:O	1:E:268:ARG:N	2.51	0.44
1:G:453:GLU:OE1	2:H:442:ARG:NH1	2.51	0.44
2:H:218:ARG:NH2	2:H:517:ASP:OD1	2.51	0.44
2:H:354:GLU:O	2:H:357:ILE:HG22	2.18	0.44
2:B:414:LEU:HD23	2:B:414:LEU:HA	1.83	0.43
2:B:432:ALA:O	2:B:433:GLU:C	2.59	0.43
2:D:66:THR:HG22	2:D:68:ALA:N	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:485:GLY:HA2	7:D:3021:HOH:O	2.18	0.43
2:D:528:ALA:HA	7:D:3007:ZW9:S2'	2.57	0.43
2:D:671:GLY:O	2:D:674:TRP:HB3	2.19	0.43
1:E:443:ALA:O	1:E:444:LEU:C	2.60	0.43
2:F:96:GLN:HA	2:F:97:PRO:HD3	1.84	0.43
2:F:591:MET:HE1	2:H:463:HIS:CE1	2.52	0.43
2:F:618:PRO:HG2	2:F:619:PHE:CD1	2.52	0.43
1:G:373:LYS:O	1:G:374:GLY:C	2.59	0.43
1:G:67:LEU:O	1:G:69:GLN:N	2.52	0.43
1:C:22:SER:OG	1:C:25:GLU:HG2	2.17	0.43
1:C:301:MET:HE2	1:C:341:LEU:HD13	2.00	0.43
1:C:445:ARG:NH2	2:D:634:ASP:OD2	2.52	0.43
1:E:139:TYR:O	1:E:140:ALA:C	2.61	0.43
1:G:111:ILE:HD13	1:G:114:MET:HE1	2.00	0.43
1:G:111:ILE:HA	1:G:114:MET:HE3	2.00	0.43
1:G:325:TYR:HA	1:G:389:GLY:O	2.17	0.43
2:B:35:LEU:HD23	2:B:35:LEU:N	2.32	0.43
2:B:691:HIS:O	2:B:692:ALA:HB2	2.18	0.43
1:A:77:THR:OG1	1:A:79:GLU:HG2	2.19	0.43
4:A:3005:FAD:HM83	4:A:3005:FAD:HM71	1.83	0.43
2:B:79:ALA:HB1	2:B:80:PRO:CD	2.48	0.43
2:B:461:LEU:HD12	2:B:463:HIS:CE1	2.54	0.43
1:C:216:LEU:HD12	2:D:114:ARG:NH1	2.33	0.43
1:E:209:SER:O	1:E:213:THR:HG23	2.18	0.43
1:E:297:ALA:O	1:E:298:LEU:C	2.61	0.43
2:F:26:LEU:HA	2:F:27:PRO:HD3	1.90	0.43
2:F:706:ARG:HA	2:F:706:ARG:HD3	1.78	0.43
1:G:12:ARG:HH11	1:G:12:ARG:CG	2.31	0.43
1:G:279:ALA:HB1	4:G:3005:FAD:H4'	1.99	0.43
2:H:775:GLY:C	2:H:777:ALA:H	2.25	0.43
1:A:143:LEU:C	1:A:143:LEU:CD2	2.91	0.43
2:B:517:ASP:OD2	2:B:519:SER:OG	2.22	0.43
1:C:399:ALA:C	1:C:401:LEU:H	2.27	0.43
4:G:3005:FAD:H1'2	4:G:3005:FAD:H9	1.71	0.43
2:H:214:PHE:N	2:H:214:PHE:HD1	2.14	0.43
2:B:70:LEU:HD12	2:B:74:ASN:HB2	2.01	0.43
2:D:371:LEU:HD12	2:D:371:LEU:HA	1.79	0.43
1:E:139:TYR:O	1:E:142:ILE:N	2.51	0.43
1:E:294:GLY:O	1:E:295:PRO:C	2.61	0.43
2:F:170:GLY:N	2:F:271:ASP:HB3	2.33	0.43
2:F:310:ARG:HD2	2:F:344:PHE:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:683:ASP:OD2	2:F:687:ARG:NE	2.47	0.43
1:G:415:LEU:HB2	1:G:416:PRO:HD3	2.00	0.43
1:A:152:GLU:OE1	1:A:153:PRO:HD2	2.19	0.43
1:A:291:ILE:HG21	1:A:291:ILE:HD13	1.71	0.43
1:A:301:MET:HE3	1:A:342:PRO:HD2	2.01	0.43
1:A:450:LEU:HD23	1:A:450:LEU:HA	1.38	0.43
2:D:198:HIS:N	2:D:199:PRO:HD3	2.33	0.43
2:D:507:ASP:HA	2:D:508:PRO:HD3	1.87	0.43
1:E:122:ARG:HB3	1:E:128:LEU:HD21	2.00	0.43
1:E:408:GLU:CD	2:F:442:ARG:HH22	2.26	0.43
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.19	0.43
1:G:205:GLY:O	1:G:209:SER:OG	2.35	0.43
1:G:319:GLU:N	1:G:319:GLU:OE2	2.48	0.43
1:G:428:MET:SD	1:G:429:ARG:N	2.92	0.43
2:H:174:PHE:CD2	2:H:698:ILE:HD13	2.53	0.43
1:A:102:GLN:OE1	2:B:663:GLN:NE2	2.52	0.43
1:A:253:ARG:NH2	1:A:268:ARG:HG3	2.34	0.43
2:B:367:ASP:OD1	2:B:368:PRO:CD	2.67	0.43
2:B:403:THR:HG23	2:B:407:GLN:O	2.18	0.43
2:B:737:ILE:O	2:B:738:SER:C	2.60	0.43
1:E:348:LEU:HD12	1:E:348:LEU:HA	1.59	0.43
2:F:367:ASP:OD1	2:F:368:PRO:CD	2.66	0.43
1:G:305:LEU:HD21	1:G:307:LEU:HD21	2.01	0.43
1:A:374:GLY:O	1:A:375:SER:HB3	2.19	0.43
2:B:407:GLN:CD	2:B:617:ARG:HG2	2.44	0.43
2:D:398:LYS:C	2:D:399:LYS:HD2	2.43	0.43
2:D:414:LEU:HD23	2:D:414:LEU:HA	1.86	0.43
2:D:743:LEU:HD12	2:D:743:LEU:HA	1.80	0.43
1:E:98:HIS:O	1:E:99:HIS:HB2	2.19	0.43
1:G:122:ARG:NH2	1:G:124:ASP:OD1	2.52	0.43
1:G:355:LYS:N	1:G:360:ASP:OD2	2.52	0.43
1:A:67:LEU:N	1:A:68:PRO:HD2	2.34	0.42
1:A:140:ALA:HB3	1:A:141:PRO:CD	2.48	0.42
2:D:11:SER:O	2:D:12:ALA:C	2.62	0.42
1:E:364:VAL:CG2	1:E:435:ARG:HG2	2.49	0.42
1:G:281:ILE:O	1:G:282:GLY:C	2.57	0.42
4:G:3005:FAD:H51A	4:G:3005:FAD:H2B	1.39	0.42
2:H:367:ASP:OD2	2:H:431:ARG:NH1	2.33	0.42
1:A:295:PRO:O	1:A:296:PRO:C	2.62	0.42
2:D:45:ALA:HA	2:D:123:ARG:HG3	1.99	0.42
2:D:260:ASP:OD1	2:D:691:HIS:HD2	1.96	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:440:THR:O	2:D:440:THR:CG2	2.66	0.42
2:F:70:LEU:HA	2:F:71:PRO:HD3	1.94	0.42
2:F:79:ALA:HB1	2:F:80:PRO:CD	2.49	0.42
2:F:221:MET:HE1	2:F:223:ARG:C	2.44	0.42
1:G:89:HIS:CE1	1:G:91:VAL:HG23	2.54	0.42
1:G:102:GLN:O	2:H:15:HIS:CE1	2.71	0.42
2:H:93:PHE:CE2	2:H:299:TRP:NE1	2.87	0.42
2:H:123:ARG:HB3	2:H:124:PRO:HD2	2.00	0.42
2:B:367:ASP:OD2	2:B:431:ARG:NH1	2.43	0.42
1:C:95:MET:HG3	1:C:111:ILE:HD11	2.01	0.42
1:C:444:LEU:HD23	1:C:444:LEU:HA	1.87	0.42
2:D:152:GLU:O	2:D:153:THR:C	2.61	0.42
1:E:301:MET:HE2	1:E:341:LEU:CD2	2.36	0.42
2:B:425:ALA:O	2:B:426:ASN:CB	2.68	0.42
2:D:96:GLN:HA	2:D:97:PRO:HD3	1.89	0.42
2:F:151:VAL:HG21	2:F:325:ARG:HB2	2.01	0.42
2:F:233:SER:C	2:F:235:GLY:H	2.26	0.42
1:G:83:ALA:HB1	1:G:84:PRO:HD2	2.00	0.42
2:H:746:ALA:O	2:H:747:CYS:C	2.60	0.42
2:B:39:LEU:HD22	2:B:95:GLY:O	2.20	0.42
2:B:150:ASP:OD1	2:B:150:ASP:C	2.62	0.42
2:B:184:LEU:HA	2:B:185:PRO:HD2	1.81	0.42
1:C:319:GLU:OE2	1:C:319:GLU:N	2.42	0.42
2:D:697:LYS:N	2:D:697:LYS:CD	2.82	0.42
1:E:353:LEU:HD21	1:E:434:TYR:OH	2.19	0.42
1:E:401:LEU:HD12	1:E:401:LEU:HA	1.57	0.42
2:F:50:LEU:CD1	2:F:118:ILE:HG12	2.50	0.42
2:F:341:PHE:HD2	2:F:342:ARG:N	2.17	0.42
2:H:213:ALA:O	2:H:214:PHE:C	2.62	0.42
2:B:23:LEU:O	2:B:23:LEU:HG	2.17	0.42
2:B:696:TYR:C	2:B:697:LYS:HD2	2.44	0.42
2:D:585:ILE:HD13	2:D:585:ILE:HA	1.81	0.42
2:D:730:GLU:H	2:D:731:PRO:CD	2.33	0.42
1:E:133:LEU:HD22	2:F:698:ILE:HD11	2.02	0.42
2:F:261:ASP:O	2:F:262:ASP:C	2.63	0.42
2:F:269:ARG:NH2	2:F:341:PHE:CD2	2.87	0.42
2:H:106:HIS:O	2:H:107:ARG:C	2.61	0.42
2:H:348:GLN:OE1	2:H:348:GLN:N	2.37	0.42
2:B:34:HIS:O	2:B:35:LEU:HD23	2.20	0.42
1:C:237:THR:HG23	1:C:238:PRO:HD2	2.00	0.42
2:D:65:PHE:HB2	2:D:100:LEU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:224:MET:HE3	2:D:488:MET:HB3	2.02	0.42
2:F:111:ILE:O	2:F:112:ALA:C	2.59	0.42
2:F:437:TRP:CZ3	2:F:446:ARG:HG3	2.54	0.42
2:H:170:GLY:N	2:H:271:ASP:HB3	2.34	0.42
2:B:305:LEU:HB3	2:B:306:PRO:CD	2.48	0.42
1:C:228:CYS:HB2	1:C:231:LEU:HB2	2.01	0.42
2:D:493:HIS:CG	2:D:513:ILE:HG12	2.55	0.42
1:E:22:SER:OG	1:E:25:GLU:HG2	2.19	0.42
1:E:89:HIS:O	1:E:90:PRO:C	2.62	0.42
1:E:301:MET:HB3	1:E:348:LEU:HD22	2.01	0.42
2:F:302:ASP:OD1	2:F:303:LEU:N	2.51	0.42
1:G:325:TYR:HB2	1:G:389:GLY:HA3	2.01	0.42
2:H:744:HIS:HE1	2:H:754:TRP:CZ3	2.38	0.42
1:A:140:ALA:N	1:A:141:PRO:HD2	2.35	0.42
1:A:237:THR:HG23	1:A:238:PRO:N	2.34	0.42
1:A:387:MET:HE2	1:A:439:ALA:HB2	2.01	0.42
2:B:133:LEU:O	2:B:134:ALA:C	2.60	0.42
2:B:367:ASP:CG	2:B:431:ARG:HH12	2.27	0.42
2:B:591:MET:HE3	2:B:591:MET:HB3	1.99	0.42
1:C:382:ILE:O	1:C:393:ARG:HA	2.18	0.42
2:D:92:HIS:O	2:D:93:PHE:HB3	2.19	0.42
2:D:318:SER:HB3	2:D:414:LEU:CD1	2.49	0.42
2:D:736:GLY:O	2:D:737:ILE:C	2.63	0.42
1:E:105:PHE:CD1	2:F:177:GLU:HB2	2.55	0.42
2:F:547:LEU:O	2:F:548:ARG:C	2.60	0.42
2:H:112:ALA:C	2:H:114:ARG:N	2.75	0.42
2:H:418:VAL:O	2:H:419:THR:C	2.62	0.42
1:A:243:ILE:HD12	1:A:341:LEU:HG	2.02	0.42
1:A:281:ILE:CG2	1:A:282:GLY:N	2.82	0.42
2:B:65:PHE:N	2:B:100:LEU:O	2.47	0.42
1:C:408:GLU:CD	2:D:442:ARG:HH22	2.27	0.42
1:E:237:THR:HG22	1:E:240:GLY:O	2.20	0.42
2:F:233:SER:C	2:F:235:GLY:N	2.78	0.42
2:F:636:LEU:HA	2:F:636:LEU:HD23	1.82	0.42
1:G:44:CYS:O	1:G:132:ASN:HA	2.20	0.42
2:H:81:SER:HA	2:H:82:PRO:HD3	1.81	0.42
2:H:175:TYR:OH	2:H:262:ASP:OD2	2.33	0.42
2:H:367:ASP:O	2:H:368:PRO:C	2.63	0.42
1:A:41:GLU:HG2	1:A:210:LEU:HD13	2.02	0.41
2:B:413:VAL:O	2:B:414:LEU:C	2.62	0.41
1:C:268:ARG:HH11	1:C:268:ARG:HD2	1.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:PRO:HB2	1:C:296:PRO:HD3	2.02	0.41
2:D:202:ILE:HD13	2:D:236:ASN:ND2	2.31	0.41
2:D:233:SER:C	2:D:235:GLY:N	2.76	0.41
1:E:191:ASP:O	1:E:194:LEU:HB3	2.19	0.41
1:E:349:ARG:HG2	1:E:351:TYR:OH	2.20	0.41
2:F:65:PHE:CD1	2:F:65:PHE:N	2.88	0.41
2:F:251:ARG:HB3	2:F:252:PRO:CD	2.50	0.41
2:F:412:CYS:HA	2:F:624:TYR:CZ	2.54	0.41
2:F:701:PHE:O	2:F:704:ARG:HG2	2.19	0.41
1:G:191:ASP:O	1:G:194:LEU:HB3	2.20	0.41
2:H:643:LEU:HD23	2:H:643:LEU:HA	1.89	0.41
2:H:696:TYR:HA	7:H:3020:HOH:O	2.19	0.41
1:A:52:ARG:HG2	1:A:53:ASP:N	2.34	0.41
2:D:166:PHE:CZ	2:D:355:ARG:HG3	2.55	0.41
2:D:186:ALA:O	2:D:187:GLU:C	2.63	0.41
2:F:66:THR:HG23	2:F:68:ALA:H	1.84	0.41
2:F:367:ASP:OD1	2:F:367:ASP:C	2.63	0.41
1:G:290:PRO:HA	1:G:391:PRO:HD3	2.01	0.41
2:H:563:ALA:C	2:H:565:ASP:H	2.28	0.41
2:B:81:SER:HA	2:B:82:PRO:HD3	1.79	0.41
2:B:650:ASP:OD2	2:B:726:LYS:NZ	2.40	0.41
1:C:95:MET:CE	1:C:114:MET:HE1	2.50	0.41
2:D:35:LEU:HA	2:D:101:VAL:O	2.20	0.41
2:D:367:ASP:CG	2:D:431:ARG:HH12	2.27	0.41
2:D:698:ILE:HG21	2:D:698:ILE:HD13	1.70	0.41
1:E:237:THR:CG2	1:E:238:PRO:N	2.84	0.41
1:G:299:ILE:HA	7:G:3010:HOH:O	2.20	0.41
1:G:314:ARG:O	1:G:315:ARG:HB2	2.20	0.41
1:G:418:LEU:HB3	1:G:436:MET:CE	2.49	0.41
2:H:310:ARG:HB3	2:H:344:PHE:O	2.19	0.41
2:B:503:VAL:O	2:B:503:VAL:CG1	2.66	0.41
2:B:593:ARG:NH1	2:D:604:THR:O	2.44	0.41
1:C:450:LEU:HA	1:C:450:LEU:HD23	1.74	0.41
1:E:140:ALA:N	1:E:141:PRO:HD2	2.35	0.41
1:G:27:LEU:O	1:G:30:GLU:HB2	2.20	0.41
1:G:324:GLU:O	1:G:325:TYR:C	2.63	0.41
2:H:140:GLU:O	2:H:141:GLY:C	2.64	0.41
1:A:356:ARG:NH2	2:B:697:LYS:NZ	2.67	0.41
2:B:660:ASP:O	2:B:661:ILE:C	2.63	0.41
1:C:361:ILE:HD12	1:C:429:ARG:NH2	2.36	0.41
2:D:731:PRO:CB	2:D:732:PRO:CD	2.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:LEU:O	1:E:244:GLY:HA3	2.20	0.41
1:E:273:GLU:O	1:E:274:GLN:C	2.62	0.41
2:H:276:TYR:OH	2:H:359:HIS:CD2	2.71	0.41
2:B:53:GLU:N	2:B:54:PRO:CD	2.83	0.41
2:B:281:ASP:OD1	2:B:283:SER:OG	2.27	0.41
2:B:700:ALA:O	2:B:701:PHE:C	2.62	0.41
1:C:102:GLN:OE1	7:D:3007:ZW9:N2	2.53	0.41
2:D:398:LYS:O	2:D:399:LYS:HD2	2.21	0.41
1:E:104:GLY:HA3	2:F:22:TYR:OH	2.21	0.41
1:E:267:LEU:HD23	1:E:267:LEU:HA	1.83	0.41
1:G:291:ILE:O	1:G:292:GLY:C	2.61	0.41
2:H:96:GLN:HA	2:H:97:PRO:HD3	1.88	0.41
2:H:202:ILE:HD13	2:H:236:ASN:HD22	1.85	0.41
2:H:563:ALA:C	2:H:565:ASP:N	2.79	0.41
2:B:299:TRP:H	2:B:299:TRP:CD1	2.37	0.41
2:B:527:THR:O	2:B:528:ALA:HB2	2.21	0.41
2:B:706:ARG:HD3	2:B:706:ARG:HA	1.63	0.41
1:E:381:ARG:NH2	1:E:393:ARG:NE	2.68	0.41
2:F:123:ARG:HB3	2:F:124:PRO:HD2	2.03	0.41
1:G:387:MET:HE2	1:G:439:ALA:CB	2.38	0.41
2:H:737:ILE:O	2:H:738:SER:C	2.64	0.41
1:A:252:LEU:HD22	1:A:281:ILE:HD12	2.02	0.41
2:B:743:LEU:HD12	2:B:743:LEU:HA	1.71	0.41
1:C:256:ALA:O	1:C:257:GLU:C	2.60	0.41
2:D:496:MET:HE2	2:D:496:MET:CA	2.49	0.41
2:D:775:GLY:C	2:D:777:ALA:H	2.29	0.41
1:E:52:ARG:N	1:E:74:ALA:O	2.52	0.41
2:F:238:LEU:HD12	2:F:238:LEU:N	2.32	0.41
2:F:665:GLU:HG2	2:F:710:VAL:HG21	2.03	0.41
1:G:39:CYS:O	1:G:40:ASN:CB	2.68	0.41
1:G:94:ALA:O	1:G:98:HIS:HB2	2.20	0.41
2:H:164:GLY:HA3	2:H:276:TYR:CZ	2.56	0.41
2:H:235:GLY:O	2:H:236:ASN:C	2.64	0.41
2:H:555:VAL:O	2:H:555:VAL:CG1	2.64	0.41
1:A:32:LEU:HD22	1:A:79:GLU:CG	2.48	0.41
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.91	0.41
1:A:353:LEU:HD21	1:A:434:TYR:CE2	2.55	0.41
2:B:210:LEU:CD1	2:B:212:LEU:HD12	2.51	0.41
2:B:263:MET:HE3	2:B:692:ALA:N	2.35	0.41
2:B:278:ILE:HD11	2:B:286:LEU:HD22	2.03	0.41
2:B:704:ARG:CG	2:B:704:ARG:NH1	2.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LEU:HD23	1:C:158:LEU:HA	1.81	0.41
1:C:233:GLN:HA	1:C:233:GLN:OE1	2.21	0.41
2:D:636:LEU:HA	2:D:636:LEU:HD23	1.86	0.41
2:D:751:GLY:HA3	2:D:773:ALA:O	2.21	0.41
2:F:202:ILE:HD13	2:F:236:ASN:HD22	1.86	0.41
2:F:318:SER:HB3	2:F:414:LEU:HD13	2.03	0.41
2:F:762:THR:H	2:F:762:THR:HG23	1.68	0.41
1:G:126:ASP:OD1	2:H:704:ARG:NH1	2.44	0.41
1:G:139:TYR:O	1:G:140:ALA:C	2.64	0.41
1:G:272:SER:O	1:G:275:VAL:N	2.53	0.41
2:H:93:PHE:CD1	2:H:93:PHE:C	2.99	0.41
2:H:98:ILE:HD13	2:H:98:ILE:HG21	1.77	0.41
2:H:186:ALA:O	2:H:187:GLU:C	2.64	0.41
2:H:227:GLY:C	2:H:229:GLY:H	2.29	0.41
2:B:318:SER:HB3	2:B:414:LEU:CD1	2.51	0.41
2:B:684:HIS:CE1	2:F:567:ILE:HD11	2.55	0.41
2:D:170:GLY:N	2:D:271:ASP:HB3	2.36	0.41
1:E:345:ALA:N	1:E:346:PRO:HD3	2.36	0.41
2:F:23:LEU:HD13	2:F:194:CYS:CA	2.48	0.41
2:F:258:ASP:O	2:F:259:ARG:C	2.62	0.41
1:G:243:ILE:CD1	1:G:341:LEU:HD11	2.51	0.41
1:G:326:ARG:HA	1:G:326:ARG:HD3	1.89	0.41
2:H:66:THR:O	2:H:67:ALA:C	2.63	0.41
2:H:422:GLN:HG2	2:H:427:PHE:CD2	2.56	0.41
2:H:656:ASN:HA	2:H:657:PRO:HD3	1.90	0.41
2:H:674:TRP:CD2	2:H:675:LEU:HD21	2.56	0.41
1:A:139:TYR:O	1:A:140:ALA:C	2.63	0.40
1:A:256:ALA:O	1:A:257:GLU:C	2.62	0.40
2:B:146:TRP:CZ3	2:B:313:LEU:HD13	2.56	0.40
2:B:451:SER:HA	2:B:452:PRO:HD3	1.97	0.40
2:D:168:ILE:HD13	2:D:351:LEU:HD23	2.03	0.40
2:D:612:LEU:HD23	2:D:612:LEU:HA	1.80	0.40
1:E:93:GLN:NE2	1:E:97:ASP:OD1	2.55	0.40
1:E:266:LEU:C	1:E:268:ARG:H	2.29	0.40
1:E:374:GLY:C	1:E:376:LYS:H	2.29	0.40
1:G:120:ARG:O	1:G:121:ASP:C	2.64	0.40
1:G:216:LEU:HD23	1:G:216:LEU:HA	1.92	0.40
1:G:237:THR:HG23	1:G:238:PRO:HD2	2.03	0.40
1:G:237:THR:HG1	1:G:238:PRO:HD2	1.82	0.40
1:G:267:LEU:O	1:G:268:ARG:C	2.62	0.40
1:G:302:GLY:HA2	1:G:381:ARG:NH1	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:701:PHE:CE2	2:H:704:ARG:NH1	2.89	0.40
1:A:164:PHE:O	1:A:166:LEU:HG	2.22	0.40
2:B:372:ARG:O	2:B:373:ALA:C	2.63	0.40
1:C:32:LEU:HD22	1:C:79:GLU:CG	2.47	0.40
2:F:22:TYR:CE2	2:F:223:ARG:HD3	2.56	0.40
1:G:12:ARG:CG	1:G:12:ARG:NH1	2.82	0.40
2:H:733:PHE:CD2	2:H:733:PHE:C	2.98	0.40
2:H:753:HIS:HB2	2:H:772:ARG:O	2.21	0.40
2:B:94:VAL:HG11	2:B:687:ARG:HG2	2.03	0.40
2:B:130:ASP:O	2:B:131:GLN:C	2.61	0.40
2:B:214:PHE:N	2:B:214:PHE:HD1	2.17	0.40
2:B:371:LEU:HD12	2:B:371:LEU:HA	1.91	0.40
7:B:3007:ZW9:S	7:B:3007:ZW9:S1'	3.19	0.40
1:C:228:CYS:O	1:C:229:LYS:C	2.61	0.40
2:D:437:TRP:CZ3	2:D:446:ARG:HG3	2.57	0.40
2:D:746:ALA:O	2:D:747:CYS:C	2.64	0.40
1:G:345:ALA:C	1:G:347:GLY:H	2.30	0.40
2:H:130:ASP:O	2:H:131:GLN:C	2.64	0.40
2:H:175:TYR:O	2:H:259:ARG:NH2	2.47	0.40
2:H:198:HIS:ND1	2:H:526:ALA:HB2	2.35	0.40
2:H:258:ASP:O	2:H:259:ARG:C	2.63	0.40
2:H:377:TYR:CE1	2:H:454:LYS:HE3	2.57	0.40
2:H:481:LEU:HD12	2:H:482:ASN:N	2.36	0.40
2:H:660:ASP:O	2:H:661:ILE:C	2.64	0.40
2:H:704:ARG:O	2:H:704:ARG:HG3	2.20	0.40
1:A:240:GLY:HA2	1:A:343:LYS:HG2	2.02	0.40
2:B:724:ARG:HH11	2:B:724:ARG:HD2	1.74	0.40
2:D:165:CYS:O	2:D:166:PHE:HB3	2.20	0.40
2:D:507:ASP:OD1	2:D:508:PRO:N	2.54	0.40
1:E:348:LEU:HD12	1:E:349:ARG:N	2.33	0.40
2:F:539:ALA:O	2:F:540:VAL:C	2.61	0.40
1:G:47:CYS:O	1:G:49:VAL:HG13	2.21	0.40
1:G:117:ALA:O	1:G:118:HIS:C	2.65	0.40
1:G:399:ALA:C	1:G:401:LEU:N	2.79	0.40
2:H:507:ASP:OD1	2:H:508:PRO:N	2.54	0.40
2:H:638:GLY:O	2:H:639:GLU:C	2.64	0.40
2:H:648:LEU:HD12	2:H:711:ALA:O	2.21	0.40
1:A:34:GLY:O	1:A:36:LYS:HE2	2.21	0.40
2:B:23:LEU:HD13	2:B:194:CYS:HA	2.03	0.40
2:B:48:THR:HG22	2:B:49:GLY:N	2.36	0.40
2:B:339:THR:OG1	2:B:340:ALA:N	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:706:ARG:HD3	2:D:706:ARG:HA	1.82	0.40
1:E:107:THR:HB	1:E:108:PRO:HD3	2.03	0.40
2:F:14:ALA:O	2:F:15:HIS:C	2.62	0.40
2:F:109:ALA:O	2:F:110:ARG:C	2.64	0.40
2:F:507:ASP:OD1	2:F:507:ASP:C	2.64	0.40
2:F:717:ASN:ND2	2:F:726:LYS:HG3	2.36	0.40
1:G:34:GLY:CA	1:G:36:LYS:NZ	2.84	0.40
2:H:722:ILE:HD12	2:H:722:ILE:HA	1.89	0.40
2:H:762:THR:HB	2:H:763:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/462 (96%)	401 (90%)	41 (9%)	4 (1%)	14	35
1	C	446/462 (96%)	415 (93%)	27 (6%)	4 (1%)	14	35
1	E	446/462 (96%)	383 (86%)	53 (12%)	10 (2%)	5	14
1	G	446/462 (96%)	395 (89%)	44 (10%)	7 (2%)	7	20
2	B	756/777 (97%)	708 (94%)	40 (5%)	8 (1%)	11	29
2	D	756/777 (97%)	718 (95%)	31 (4%)	7 (1%)	14	35
2	F	756/777 (97%)	709 (94%)	39 (5%)	8 (1%)	11	29
2	H	756/777 (97%)	700 (93%)	47 (6%)	9 (1%)	10	27
All	All	4808/4956 (97%)	4429 (92%)	322 (7%)	57 (1%)	10	27

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	399	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	458	SER
1	C	180	ALA
1	C	374	GLY
2	D	281	ASP
2	D	399	LYS
2	D	458	SER
1	E	374	GLY
2	F	399	LYS
2	F	458	SER
1	G	374	GLY
2	H	399	LYS
2	H	458	SER
1	A	315	ARG
1	A	374	GLY
1	A	400	ALA
2	B	187	GLU
2	B	342	ARG
2	B	560	GLY
2	B	608	SER
2	D	187	GLU
2	D	342	ARG
1	E	395	ALA
1	E	400	ALA
2	F	342	ARG
2	H	187	GLU
2	H	342	ARG
2	H	560	GLY
2	H	761	ALA
1	A	163	ALA
1	E	315	ARG
1	E	326	ARG
1	E	399	ALA
2	F	187	GLU
2	F	426	ASN
1	G	180	ALA
1	G	315	ARG
1	G	326	ARG
2	H	227	GLY
2	H	561	CYS
2	H	639	GLU
1	C	315	ARG
1	E	297	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	447	VAL
1	G	199	ALA
1	C	163	ALA
2	D	227	GLY
2	F	281	ASP
2	F	560	GLY
1	G	163	ALA
2	B	227	GLY
1	E	430	ALA
2	D	560	GLY
2	F	227	GLY
2	B	141	GLY
1	G	100	GLY
1	E	332	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/347 (98%)	301 (89%)	38 (11%)	6	15
1	C	339/347 (98%)	302 (89%)	37 (11%)	6	16
1	E	339/347 (98%)	295 (87%)	44 (13%)	4	10
1	G	339/347 (98%)	290 (86%)	49 (14%)	3	8
2	B	571/584 (98%)	515 (90%)	56 (10%)	7	19
2	D	571/584 (98%)	518 (91%)	53 (9%)	8	21
2	F	571/584 (98%)	512 (90%)	59 (10%)	7	18
2	H	571/584 (98%)	508 (89%)	63 (11%)	6	15
All	All	3640/3724 (98%)	3241 (89%)	399 (11%)	6	15

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	12	ARG
1	A	20	THR
1	A	26	LEU
1	A	33	THR
1	A	40	ASN
1	A	41	GLU
1	A	58	ARG
1	A	79	GLU
1	A	87	ARG
1	A	128	LEU
1	A	143	LEU
1	A	159	GLN
1	A	165	THR
1	A	198	GLU
1	A	210	LEU
1	A	212	VAL
1	A	231	LEU
1	A	237	THR
1	A	239	ASP
1	A	257	GLU
1	A	268	ARG
1	A	309	ARG
1	A	316	MET
1	A	337	GLU
1	A	343	LYS
1	A	349	ARG
1	A	359	GLN
1	A	376	LYS
1	A	390	VAL
1	A	393	ARG
1	A	401	LEU
1	A	423	THR
1	A	425	LEU
1	A	426	SER
1	A	451	SER
1	A	455	VAL
1	A	457	VAL
2	B	2	SER
2	B	10	ASP
2	B	16	VAL
2	B	23	LEU
2	B	48	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	53	GLU
2	B	66	THR
2	B	129	LEU
2	B	130	ASP
2	B	133	LEU
2	B	151	VAL
2	B	152	GLU
2	B	161	LEU
2	B	175	TYR
2	B	190	VAL
2	B	221	MET
2	B	222	ARG
2	B	247	ARG
2	B	256	ARG
2	B	263	MET
2	B	264	VAL
2	B	296	ARG
2	B	300	SER
2	B	313	LEU
2	B	330	ARG
2	B	355	ARG
2	B	398	LYS
2	B	399	LYS
2	B	423	LYS
2	B	426	ASN
2	B	429	THR
2	B	431	ARG
2	B	441	ASN
2	B	442	ARG
2	B	450	LEU
2	B	461	LEU
2	B	472	GLN
2	B	486	THR
2	B	509	VAL
2	B	512	ARG
2	B	520	LYS
2	B	530	SER
2	B	548	ARG
2	B	558	ARG
2	B	574	GLN
2	B	611	ARG
2	B	617	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	632	VAL
2	B	697	LYS
2	B	704	ARG
2	B	718	ARG
2	B	724	ARG
2	B	741	LEU
2	B	743	LEU
2	B	744	HIS
2	B	770	VAL
1	C	11	THR
1	C	20	THR
1	C	25	GLU
1	C	26	LEU
1	C	33	THR
1	C	40	ASN
1	C	79	GLU
1	C	87	ARG
1	C	91	VAL
1	C	128	LEU
1	C	143	LEU
1	C	165	THR
1	C	198	GLU
1	C	209	SER
1	C	210	LEU
1	C	212	VAL
1	C	221	GLU
1	C	226	SER
1	C	231	LEU
1	C	237	THR
1	C	239	ASP
1	C	257	GLU
1	C	268	ARG
1	C	309	ARG
1	C	316	MET
1	C	337	GLU
1	C	349	ARG
1	C	354	SER
1	C	355	LYS
1	C	376	LYS
1	C	379	THR
1	C	393	ARG
1	C	401	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	447	VAL
1	C	451	SER
1	C	455	VAL
1	C	457	VAL
2	D	10	ASP
2	D	16	VAL
2	D	28	CYS
2	D	35	LEU
2	D	41	THR
2	D	48	THR
2	D	53	GLU
2	D	66	THR
2	D	81	SER
2	D	129	LEU
2	D	151	VAL
2	D	161	LEU
2	D	190	VAL
2	D	221	MET
2	D	222	ARG
2	D	247	ARG
2	D	258	ASP
2	D	259	ARG
2	D	264	VAL
2	D	275	ARG
2	D	296	ARG
2	D	300	SER
2	D	313	LEU
2	D	330	ARG
2	D	355	ARG
2	D	398	LYS
2	D	399	LYS
2	D	407	GLN
2	D	426	ASN
2	D	429	THR
2	D	442	ARG
2	D	450	LEU
2	D	452	PRO
2	D	461	LEU
2	D	506	ILE
2	D	512	ARG
2	D	520	LYS
2	D	530	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	534	ASP
2	D	548	ARG
2	D	558	ARG
2	D	574	GLN
2	D	611	ARG
2	D	617	ARG
2	D	632	VAL
2	D	697	LYS
2	D	704	ARG
2	D	718	ARG
2	D	722	ILE
2	D	724	ARG
2	D	741	LEU
2	D	743	LEU
2	D	744	HIS
1	E	11	THR
1	E	12	ARG
1	E	20	THR
1	E	25	GLU
1	E	26	LEU
1	E	33	THR
1	E	36	LYS
1	E	58	ARG
1	E	66	MET
1	E	79	GLU
1	E	93	GLN
1	E	113	SER
1	E	121	ASP
1	E	128	LEU
1	E	143	LEU
1	E	159	GLN
1	E	165	THR
1	E	179	PRO
1	E	198	GLU
1	E	209	SER
1	E	210	LEU
1	E	212	VAL
1	E	221	GLU
1	E	231	LEU
1	E	237	THR
1	E	239	ASP
1	E	247	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	257	GLU
1	E	268	ARG
1	E	295	PRO
1	E	309	ARG
1	E	316	MET
1	E	337	GLU
1	E	339	VAL
1	E	349	ARG
1	E	359	GLN
1	E	401	LEU
1	E	408	GLU
1	E	428	MET
1	E	435	ARG
1	E	447	VAL
1	E	451	SER
1	E	455	VAL
1	E	457	VAL
2	F	2	SER
2	F	10	ASP
2	F	16	VAL
2	F	35	LEU
2	F	48	THR
2	F	53	GLU
2	F	66	THR
2	F	81	SER
2	F	129	LEU
2	F	151	VAL
2	F	175	TYR
2	F	182	LEU
2	F	190	VAL
2	F	221	MET
2	F	222	ARG
2	F	244	VAL
2	F	247	ARG
2	F	264	VAL
2	F	296	ARG
2	F	300	SER
2	F	313	LEU
2	F	330	ARG
2	F	355	ARG
2	F	366	ARG
2	F	398	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	399	LYS
2	F	416	GLU
2	F	426	ASN
2	F	428	THR
2	F	429	THR
2	F	431	ARG
2	F	442	ARG
2	F	450	LEU
2	F	451	SER
2	F	452	PRO
2	F	454	LYS
2	F	461	LEU
2	F	488	MET
2	F	506	ILE
2	F	512	ARG
2	F	530	SER
2	F	541	LYS
2	F	558	ARG
2	F	574	GLN
2	F	579	SER
2	F	586	VAL
2	F	611	ARG
2	F	617	ARG
2	F	618	PRO
2	F	632	VAL
2	F	675	LEU
2	F	694	SER
2	F	697	LYS
2	F	702	SER
2	F	718	ARG
2	F	724	ARG
2	F	741	LEU
2	F	743	LEU
2	F	744	HIS
1	G	11	THR
1	G	12	ARG
1	G	20	THR
1	G	25	GLU
1	G	26	LEU
1	G	33	THR
1	G	36	LYS
1	G	40	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	41	GLU
1	G	58	ARG
1	G	61	ASN
1	G	67	LEU
1	G	68	PRO
1	G	69	GLN
1	G	79	GLU
1	G	93	GLN
1	G	128	LEU
1	G	136	CYS
1	G	143	LEU
1	G	179	PRO
1	G	198	GLU
1	G	209	SER
1	G	210	LEU
1	G	212	VAL
1	G	221	GLU
1	G	231	LEU
1	G	237	THR
1	G	239	ASP
1	G	247	VAL
1	G	257	GLU
1	G	268	ARG
1	G	309	ARG
1	G	316	MET
1	G	325	TYR
1	G	327	LYS
1	G	331	ARG
1	G	337	GLU
1	G	343	LYS
1	G	349	ARG
1	G	362	SER
1	G	371	THR
1	G	376	LYS
1	G	387	MET
1	G	425	LEU
1	G	426	SER
1	G	435	ARG
1	G	450	LEU
1	G	455	VAL
1	G	457	VAL
2	H	2	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	10	ASP
2	H	16	VAL
2	H	23	LEU
2	H	41	THR
2	H	48	THR
2	H	53	GLU
2	H	66	THR
2	H	81	SER
2	H	123	ARG
2	H	129	LEU
2	H	133	LEU
2	H	151	VAL
2	H	152	GLU
2	H	161	LEU
2	H	165	CYS
2	H	175	TYR
2	H	190	VAL
2	H	210	LEU
2	H	221	MET
2	H	222	ARG
2	H	247	ARG
2	H	251	ARG
2	H	259	ARG
2	H	264	VAL
2	H	296	ARG
2	H	300	SER
2	H	313	LEU
2	H	330	ARG
2	H	366	ARG
2	H	398	LYS
2	H	399	LYS
2	H	416	GLU
2	H	423	LYS
2	H	426	ASN
2	H	429	THR
2	H	431	ARG
2	H	442	ARG
2	H	451	SER
2	H	461	LEU
2	H	472	GLN
2	H	481	LEU
2	H	486	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	496	MET
2	H	506	ILE
2	H	512	ARG
2	H	530	SER
2	H	541	LYS
2	H	548	ARG
2	H	558	ARG
2	H	574	GLN
2	H	611	ARG
2	H	617	ARG
2	H	632	VAL
2	H	697	LYS
2	H	699	PRO
2	H	706	ARG
2	H	724	ARG
2	H	728	VAL
2	H	741	LEU
2	H	743	LEU
2	H	744	HIS
2	H	770	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	118	HIS
1	A	196	HIS
1	A	328	GLN
1	A	437	ASN
2	B	160	HIS
2	B	193	HIS
2	B	204	HIS
2	B	208	HIS
2	B	236	ASN
2	B	359	HIS
2	B	426	ASN
2	B	463	HIS
2	B	574	GLN
2	B	744	HIS
1	C	40	ASN
1	C	98	HIS
1	C	196	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	359	GLN
1	C	420	GLN
1	C	437	ASN
2	D	15	HIS
2	D	234	GLN
2	D	236	ASN
2	D	359	HIS
2	D	426	ASN
2	D	441	ASN
2	D	482	ASN
2	D	536	ASN
2	D	691	HIS
2	D	744	HIS
1	E	40	ASN
1	E	196	HIS
1	E	284	ASN
1	E	437	ASN
2	F	208	HIS
2	F	236	ASN
2	F	359	HIS
2	F	463	HIS
2	F	482	ASN
2	F	536	ASN
2	F	744	HIS
1	G	40	ASN
1	G	61	ASN
1	G	93	GLN
1	G	98	HIS
1	G	159	GLN
1	G	196	HIS
1	G	328	GLN
2	H	15	HIS
2	H	31	ASN
2	H	160	HIS
2	H	208	HIS
2	H	236	ASN
2	H	359	HIS
2	H	463	HIS
2	H	744	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ZW9	H	3007	2	21,31,31	5.58	10 (47%)	22,52,52	6.54	15 (68%)
3	FES	C	3002	1	0,4,4	-	-	-		
3	FES	E	3002	1	0,4,4	-	-	-		
3	FES	A	3002	1	0,4,4	-	-	-		
4	FAD	G	3005	-	58,58,58	1.32	8 (13%)	85,89,89	2.23	34 (40%)
3	FES	G	3001	1	0,4,4	-	-	-		
7	ZW9	F	3007	2	21,31,31	5.61	10 (47%)	22,52,52	6.87	14 (63%)
3	FES	A	3001	1	0,4,4	-	-	-		
3	FES	C	3001	1	0,4,4	-	-	-		
7	ZW9	D	3007	2	21,31,31	4.79	11 (52%)	22,52,52	7.64	13 (59%)
3	FES	E	3001	1	0,4,4	-	-	-		
7	ZW9	B	3007	2	21,31,31	5.53	10 (47%)	22,52,52	5.86	13 (59%)
4	FAD	A	3005	-	58,58,58	1.34	8 (13%)	85,89,89	2.14	31 (36%)
4	FAD	C	3005	-	58,58,58	1.66	9 (15%)	85,89,89	2.54	38 (44%)
3	FES	G	3002	1	0,4,4	-	-	-		
4	FAD	E	3005	-	58,58,58	1.62	9 (15%)	85,89,89	2.10	29 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ZW9	H	3007	2	-	1/6/46/46	0/4/4/4
3	FES	G	3002	1	-	-	0/1/1/1
3	FES	C	3002	1	-	-	0/1/1/1
4	FAD	G	3005	-	-	9/34/50/50	0/6/6/6
7	ZW9	F	3007	2	-	4/6/46/46	0/4/4/4
3	FES	A	3002	1	-	-	0/1/1/1
3	FES	E	3002	1	-	-	0/1/1/1
3	FES	G	3001	1	-	-	0/1/1/1
3	FES	A	3001	1	-	-	0/1/1/1
3	FES	C	3001	1	-	-	0/1/1/1
7	ZW9	D	3007	2	-	3/6/46/46	0/4/4/4
3	FES	E	3001	1	-	-	0/1/1/1
7	ZW9	B	3007	2	-	0/6/46/46	0/4/4/4
4	FAD	C	3005	-	-	10/34/50/50	0/6/6/6
4	FAD	A	3005	-	-	14/34/50/50	0/6/6/6
4	FAD	E	3005	-	-	12/34/50/50	0/6/6/6

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	3007	ZW9	C7-C6	14.92	1.65	1.53
7	B	3007	ZW9	C7-C6	14.34	1.65	1.53
7	H	3007	ZW9	C7-C6	12.73	1.63	1.53
7	F	3007	ZW9	C9-C10	12.48	1.59	1.38
7	H	3007	ZW9	C9-C10	12.43	1.59	1.38
7	B	3007	ZW9	C9-C10	12.41	1.59	1.38
7	D	3007	ZW9	C9-C10	11.50	1.58	1.38
7	H	3007	ZW9	C6-N5	10.31	1.58	1.46
7	D	3007	ZW9	C7-C6	10.22	1.61	1.53
7	F	3007	ZW9	C4'-C3'	-9.03	1.39	1.51
7	H	3007	ZW9	C4'-C3'	-8.67	1.39	1.51
7	B	3007	ZW9	P-O4'	-8.27	1.34	1.60
7	F	3007	ZW9	C6-N5	8.01	1.55	1.46
7	B	3007	ZW9	C6-N5	7.81	1.55	1.46
7	B	3007	ZW9	C4'-C3'	-7.75	1.41	1.51
7	D	3007	ZW9	C6-N5	7.33	1.54	1.46
7	H	3007	ZW9	P-O4'	-7.13	1.37	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	3007	ZW9	C4'-C3'	-7.02	1.42	1.51
7	D	3007	ZW9	P-O4'	-6.63	1.39	1.60
7	F	3007	ZW9	P-O4'	-6.41	1.40	1.60
7	H	3007	ZW9	P-O1P	-5.42	1.34	1.54
7	B	3007	ZW9	C9-N5	5.40	1.50	1.37
4	E	3005	FAD	P-O3P	5.39	1.65	1.59
7	B	3007	ZW9	P-O1P	-5.32	1.35	1.54
7	D	3007	ZW9	P-O1P	-5.29	1.35	1.54
7	F	3007	ZW9	O4-C4	5.22	1.33	1.23
7	H	3007	ZW9	C9-N5	5.18	1.50	1.37
4	C	3005	FAD	C2'-C3'	-5.16	1.44	1.53
7	H	3007	ZW9	O4-C4	5.00	1.33	1.23
7	F	3007	ZW9	P-O1P	-4.72	1.37	1.54
7	F	3007	ZW9	C9-N5	4.44	1.48	1.37
7	D	3007	ZW9	O4-C4	4.41	1.31	1.23
7	D	3007	ZW9	C9-N5	4.18	1.47	1.37
4	C	3005	FAD	C4X-N5	4.17	1.39	1.30
4	A	3005	FAD	C4X-N5	4.11	1.39	1.30
4	G	3005	FAD	C4X-N5	3.79	1.38	1.30
4	E	3005	FAD	C2'-C3'	-3.47	1.47	1.53
4	E	3005	FAD	C4X-N5	3.45	1.38	1.30
4	E	3005	FAD	PA-O3P	3.39	1.63	1.59
4	E	3005	FAD	C2A-N1A	3.33	1.39	1.33
4	C	3005	FAD	C1'-C2'	3.29	1.57	1.52
7	D	3007	ZW9	C2-N1	3.27	1.41	1.33
4	C	3005	FAD	O2B-C2B	-3.08	1.35	1.43
4	E	3005	FAD	C6-C7	-3.05	1.35	1.39
4	C	3005	FAD	C9A-C5X	-3.02	1.36	1.41
7	D	3007	ZW9	C2-N3	-2.99	1.30	1.37
4	E	3005	FAD	C2A-N3A	2.95	1.39	1.33
7	B	3007	ZW9	O4-C4	2.91	1.29	1.23
7	B	3007	ZW9	C2-N1	2.87	1.40	1.33
4	A	3005	FAD	C4'-C3'	2.76	1.58	1.53
4	E	3005	FAD	C9A-C5X	-2.72	1.36	1.41
4	C	3005	FAD	O4B-C4B	-2.70	1.39	1.45
4	G	3005	FAD	O4'-C4'	-2.69	1.37	1.43
7	F	3007	ZW9	C10-N8	2.68	1.38	1.35
4	C	3005	FAD	C2B-C1B	-2.58	1.45	1.53
4	C	3005	FAD	C10-N1	2.58	1.38	1.33
4	A	3005	FAD	O4B-C4B	-2.56	1.39	1.45
4	A	3005	FAD	C5A-N7A	-2.55	1.34	1.39
7	H	3007	ZW9	C2-N3	-2.50	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3005	FAD	C5'-C4'	-2.38	1.48	1.51
4	A	3005	FAD	C10-N1	2.36	1.38	1.33
4	G	3005	FAD	O4B-C4B	-2.28	1.39	1.45
7	D	3007	ZW9	C9-C4	2.28	1.48	1.41
4	A	3005	FAD	C1'-C2'	2.27	1.55	1.52
4	C	3005	FAD	C8-C7	-2.26	1.35	1.40
7	B	3007	ZW9	C9-C4	2.25	1.48	1.41
4	E	3005	FAD	C10-N1	2.25	1.37	1.33
4	G	3005	FAD	C2A-N1A	2.24	1.37	1.33
4	A	3005	FAD	C2A-N1A	2.14	1.37	1.33
7	H	3007	ZW9	C7-N8	-2.12	1.41	1.45
4	G	3005	FAD	O5B-C5B	-2.11	1.36	1.44
7	F	3007	ZW9	C7-N8	-2.05	1.41	1.45
4	A	3005	FAD	C8A-N9A	-2.05	1.34	1.37
4	G	3005	FAD	C10-N1	2.04	1.37	1.33
4	G	3005	FAD	C4'-C3'	2.03	1.57	1.53

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	3007	ZW9	C1'-C2'-S2'	-25.51	105.67	120.15
7	B	3007	ZW9	C1'-C2'-S2'	-21.61	107.89	120.15
7	F	3007	ZW9	C1'-C2'-S2'	-20.85	108.32	120.15
7	D	3007	ZW9	O3'-C7-C6	-19.89	95.70	108.96
7	F	3007	ZW9	O3'-C7-C6	-16.03	98.27	108.96
7	H	3007	ZW9	C1'-C2'-S2'	-15.64	111.27	120.15
7	H	3007	ZW9	O3'-C7-C6	-15.63	98.54	108.96
7	H	3007	ZW9	C2'-C1'-S1'	13.90	128.04	120.15
7	F	3007	ZW9	C2'-C1'-S1'	9.16	125.35	120.15
7	F	3007	ZW9	C2-N1-C10	8.72	128.76	113.36
7	D	3007	ZW9	C2-N1-C10	8.53	128.42	113.36
4	C	3005	FAD	O2'-C2'-C3'	-8.19	90.07	109.25
7	B	3007	ZW9	C2-N1-C10	8.12	127.69	113.36
7	H	3007	ZW9	C2-N1-C10	7.93	127.36	113.36
7	H	3007	ZW9	O3'-C7-N8	-7.61	101.70	108.61
7	F	3007	ZW9	O4-C4-C9	-6.80	110.86	127.26
4	C	3005	FAD	C1'-C2'-C3'	-6.75	91.36	109.66
7	D	3007	ZW9	O3'-C3'-C2'	-6.62	99.75	109.09
4	C	3005	FAD	O3'-C3'-C4'	6.54	123.79	108.93
7	B	3007	ZW9	O4-C4-C9	-6.52	111.54	127.26
7	B	3007	ZW9	C2'-C1'-S1'	6.51	123.84	120.15
7	F	3007	ZW9	O3'-C7-N8	-6.22	102.96	108.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3005	FAD	N3A-C2A-N1A	-6.11	119.33	128.58
7	D	3007	ZW9	O3'-C7-N8	-6.05	103.12	108.61
4	E	3005	FAD	N3A-C2A-N1A	-6.03	119.46	128.58
4	A	3005	FAD	C5X-C9A-N10	5.58	123.01	117.97
4	A	3005	FAD	O2'-C2'-C3'	-5.51	96.36	109.25
4	C	3005	FAD	O5'-C5'-C4'	-5.50	94.68	109.36
7	B	3007	ZW9	O3'-C7-N8	-5.48	103.63	108.61
7	F	3007	ZW9	O4-C4-N3	5.40	130.26	120.11
4	G	3005	FAD	C5X-C9A-N10	5.32	122.77	117.97
4	C	3005	FAD	N3A-C2A-N1A	-5.26	120.62	128.58
4	A	3005	FAD	N3A-C2A-N1A	-4.99	121.03	128.58
4	C	3005	FAD	O3'-C3'-C2'	-4.91	97.77	108.93
4	A	3005	FAD	C5A-C4A-N3A	-4.87	120.01	126.72
4	A	3005	FAD	O5'-C5'-C4'	-4.75	96.67	109.36
7	H	3007	ZW9	C7-C6-N5	4.75	112.53	107.87
7	B	3007	ZW9	C7-C6-N5	4.62	112.41	107.87
4	G	3005	FAD	O4'-C4'-C5'	-4.61	99.82	109.99
7	H	3007	ZW9	O4-C4-C9	-4.61	116.15	127.26
7	F	3007	ZW9	N2-C2-N3	4.58	126.42	116.76
7	H	3007	ZW9	N2-C2-N3	4.52	126.31	116.76
4	G	3005	FAD	O2A-PA-O3P	4.41	119.19	107.27
7	H	3007	ZW9	O2P-P-O4'	4.40	118.14	106.67
4	G	3005	FAD	C9A-C5X-N5	-4.19	118.01	122.45
4	E	3005	FAD	C2B-C1B-N9A	-4.14	103.02	113.30
7	D	3007	ZW9	C4-C9-N5	4.09	127.42	116.27
4	G	3005	FAD	O5'-C5'-C4'	-4.08	98.48	109.36
4	A	3005	FAD	C5A-N7A-C8A	4.03	109.78	103.45
4	A	3005	FAD	C4A-C5A-N7A	-4.01	106.00	110.58
4	E	3005	FAD	C5X-C9A-N10	4.00	121.58	117.97
7	D	3007	ZW9	O4-C4-C9	-3.99	117.64	127.26
4	C	3005	FAD	C8M-C8-C9	3.96	126.55	119.57
4	G	3005	FAD	C5A-C4A-N3A	-3.91	121.33	126.72
7	H	3007	ZW9	C4-C9-N5	3.89	126.86	116.27
4	E	3005	FAD	C5'-C4'-C3'	-3.84	104.98	112.22
7	D	3007	ZW9	O1P-P-O4'	3.81	116.61	106.67
4	G	3005	FAD	O4B-C4B-C3B	-3.78	97.64	105.15
7	B	3007	ZW9	C4-C9-N5	3.78	126.58	116.27
4	G	3005	FAD	O4-C4-C4X	-3.75	116.64	126.53
7	F	3007	ZW9	O1P-P-O4'	3.73	116.38	106.67
4	E	3005	FAD	C5A-C4A-N3A	-3.72	121.59	126.72
4	G	3005	FAD	C5B-C4B-C3B	-3.69	101.92	115.21
7	H	3007	ZW9	O3'-C3'-C2'	-3.68	103.90	109.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3005	FAD	O4B-C1B-N9A	3.62	115.05	108.09
4	E	3005	FAD	O3'-C3'-C2'	-3.62	100.71	108.93
4	E	3005	FAD	O3B-C3B-C2B	-3.61	100.24	111.82
4	G	3005	FAD	O3'-C3'-C4'	3.59	117.08	108.93
4	C	3005	FAD	C5A-C4A-N3A	-3.57	121.80	126.72
7	B	3007	ZW9	C9-C4-N3	3.57	121.94	112.13
4	C	3005	FAD	C5X-C9A-N10	3.53	121.16	117.97
4	A	3005	FAD	N9A-C8A-N7A	-3.49	108.98	113.94
4	E	3005	FAD	N3A-C4A-N9A	3.49	133.10	127.17
4	G	3005	FAD	N9A-C8A-N7A	-3.48	108.99	113.94
7	B	3007	ZW9	N2-C2-N3	3.47	124.09	116.76
4	C	3005	FAD	C7M-C7-C6	3.43	125.62	119.57
4	G	3005	FAD	C4-N3-C2	-3.42	119.57	125.64
4	C	3005	FAD	O4'-C4'-C3'	3.39	117.18	109.25
4	C	3005	FAD	O2'-C2'-C1'	3.38	124.11	110.20
7	B	3007	ZW9	O4-C4-N3	3.33	126.38	120.11
4	E	3005	FAD	O2A-PA-O5B	3.29	122.48	107.57
4	C	3005	FAD	C8M-C8-C7	-3.29	114.04	120.76
4	C	3005	FAD	N9A-C8A-N7A	-3.28	109.28	113.94
4	E	3005	FAD	C5A-C6A-N6A	-3.27	115.20	123.29
4	A	3005	FAD	O3'-C3'-C4'	3.23	116.27	108.93
4	E	3005	FAD	C1'-C2'-C3'	-3.23	100.90	109.66
4	C	3005	FAD	C9A-C5X-N5	-3.23	119.03	122.45
4	A	3005	FAD	O4'-C4'-C3'	3.21	116.77	109.25
4	E	3005	FAD	C2A-N3A-C4A	3.18	119.59	111.83
4	G	3005	FAD	C2A-N3A-C4A	3.12	119.44	111.83
4	C	3005	FAD	C9-C9A-C5X	-3.10	114.54	120.03
4	A	3005	FAD	C2A-N3A-C4A	3.10	119.41	111.83
4	G	3005	FAD	C5A-N7A-C8A	3.10	108.32	103.45
4	C	3005	FAD	C4A-C5A-N7A	-3.09	107.05	110.58
4	E	3005	FAD	O3'-C3'-C4'	3.07	115.92	108.93
4	C	3005	FAD	C5A-N7A-C8A	3.05	108.24	103.45
7	B	3007	ZW9	O3'-C7-C6	-3.05	106.93	108.96
4	E	3005	FAD	N6A-C6A-N1A	3.04	125.15	118.38
4	C	3005	FAD	C6-C5X-C9A	3.04	123.22	119.05
4	G	3005	FAD	O4B-C4B-C5B	-3.01	99.69	109.33
4	A	3005	FAD	O4B-C4B-C3B	-3.00	99.20	105.15
7	D	3007	ZW9	N3-C2-N1	-2.99	117.85	123.32
4	A	3005	FAD	C9A-N10-C10	-2.94	116.27	120.75
4	C	3005	FAD	C4-N3-C2	-2.92	120.46	125.64
4	A	3005	FAD	C6A-C5A-C4A	2.91	121.16	117.18
4	G	3005	FAD	C5A-C6A-N6A	-2.90	116.11	123.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3005	FAD	O2A-PA-O1A	-2.88	99.05	112.44
4	G	3005	FAD	C2A-N1A-C6A	2.87	123.45	118.73
4	C	3005	FAD	O3B-C3B-C2B	-2.84	102.72	111.82
4	A	3005	FAD	O4B-C4B-C5B	-2.81	100.32	109.33
7	H	3007	ZW9	N2-C2-N1	-2.80	114.20	119.67
4	E	3005	FAD	C2B-C3B-C4B	-2.73	97.34	102.61
4	E	3005	FAD	C4'-C3'-C2'	-2.72	109.05	113.57
4	G	3005	FAD	C9-C9A-N10	-2.71	118.20	121.85
4	E	3005	FAD	C9A-C5X-N5	-2.70	119.59	122.45
4	A	3005	FAD	C9-C9A-C5X	-2.69	115.28	120.03
4	G	3005	FAD	C5'-C4'-C3'	2.68	117.28	112.22
4	C	3005	FAD	C4'-C3'-C2'	-2.67	109.12	113.57
4	E	3005	FAD	O2'-C2'-C3'	-2.66	103.02	109.25
4	C	3005	FAD	C2A-N3A-C4A	2.66	118.33	111.83
7	D	3007	ZW9	C9-C4-N3	2.66	119.43	112.13
4	C	3005	FAD	C7M-C7-C8	-2.64	115.37	120.76
4	A	3005	FAD	O3'-C3'-C2'	-2.64	102.94	108.93
7	F	3007	ZW9	C4-C9-N5	2.61	123.37	116.27
4	G	3005	FAD	O5B-PA-O1A	-2.60	98.62	108.94
4	E	3005	FAD	O2'-C2'-C1'	2.60	120.87	110.20
4	A	3005	FAD	O2'-C2'-C1'	2.59	120.85	110.20
4	A	3005	FAD	C1'-N10-C9A	2.59	125.66	120.63
7	B	3007	ZW9	C2-N3-C4	-2.58	120.43	125.11
4	G	3005	FAD	N3A-C4A-N9A	2.58	131.56	127.17
4	G	3005	FAD	O3B-C3B-C4B	-2.58	103.67	111.08
7	H	3007	ZW9	C9-C4-N3	2.58	119.20	112.13
4	A	3005	FAD	O2A-PA-O3P	2.56	114.20	107.27
4	A	3005	FAD	C4X-C10-N10	2.56	120.15	116.48
4	A	3005	FAD	C5A-C4A-N9A	2.56	108.60	105.81
4	G	3005	FAD	C4-C4X-C10	2.56	121.32	116.93
7	F	3007	ZW9	N2-C2-N1	-2.54	114.70	119.67
4	C	3005	FAD	C2A-N1A-C6A	2.54	122.91	118.73
4	E	3005	FAD	C6-C7-C8	-2.53	115.97	119.69
4	C	3005	FAD	O2P-P-O3P	2.51	114.05	107.27
4	A	3005	FAD	N3A-C4A-N9A	2.48	131.39	127.17
4	A	3005	FAD	C9A-C9-C8	2.48	124.21	119.22
4	E	3005	FAD	C4X-C10-N10	2.48	120.03	116.48
4	C	3005	FAD	C4X-C4-N3	2.46	119.52	113.25
7	F	3007	ZW9	C9-C4-N3	2.46	118.88	112.13
4	E	3005	FAD	C10-C4X-N5	-2.45	119.81	124.81
4	G	3005	FAD	O4-C4-N3	2.44	124.71	120.11
7	F	3007	ZW9	N3-C2-N1	-2.43	118.86	123.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	3007	ZW9	C7-C6-N5	2.41	110.24	107.87
7	D	3007	ZW9	N2-C2-N3	2.41	121.84	116.76
4	C	3005	FAD	O4B-C1B-C2B	-2.40	101.47	106.62
7	H	3007	ZW9	O4-C4-N3	2.40	124.62	120.11
4	G	3005	FAD	C6A-C5A-C4A	2.38	120.43	117.18
7	B	3007	ZW9	N2-C2-N1	-2.38	115.03	119.67
4	C	3005	FAD	O4'-C4'-C5'	-2.38	104.74	109.99
4	E	3005	FAD	C4-N3-C2	-2.37	121.43	125.64
4	G	3005	FAD	O2-C2-N1	-2.36	117.88	121.80
4	A	3005	FAD	C9A-C5X-N5	-2.35	119.96	122.45
7	D	3007	ZW9	O1P-P-O2P	-2.34	99.05	107.80
4	A	3005	FAD	C5'-C4'-C3'	2.32	116.60	112.22
4	A	3005	FAD	C4'-C3'-C2'	-2.32	109.71	113.57
4	G	3005	FAD	C4A-C5A-N7A	-2.32	107.93	110.58
4	E	3005	FAD	O2P-P-O5'	2.31	118.02	107.57
4	G	3005	FAD	C4X-C10-N10	2.30	119.77	116.48
4	G	3005	FAD	O5'-P-O1P	2.29	118.00	108.94
4	C	3005	FAD	O2-C2-N3	-2.29	114.20	118.58
4	A	3005	FAD	C7M-C7-C6	2.26	123.55	119.57
4	C	3005	FAD	O4B-C1B-N9A	-2.25	103.76	108.09
4	E	3005	FAD	N9A-C8A-N7A	-2.20	110.82	113.94
4	G	3005	FAD	C7M-C7-C8	-2.20	116.28	120.76
4	C	3005	FAD	C4-C4X-C10	2.18	120.67	116.93
4	C	3005	FAD	C4X-C10-N1	-2.14	119.33	124.59
4	E	3005	FAD	O2A-PA-O3P	2.14	113.05	107.27
4	G	3005	FAD	C7M-C7-C6	2.13	123.33	119.57
7	H	3007	ZW9	N3-C2-N1	-2.13	119.43	123.32
4	C	3005	FAD	O2B-C2B-C1B	-2.11	102.84	110.10
4	G	3005	FAD	O4B-C1B-N9A	2.11	112.14	108.09
7	D	3007	ZW9	O2P-P-O3P	2.09	118.99	110.83
4	C	3005	FAD	C10-C4X-N5	-2.09	120.55	124.81
4	C	3005	FAD	C9A-C9-C8	2.08	123.41	119.22
4	E	3005	FAD	C9-C9A-C5X	-2.08	116.35	120.03
4	A	3005	FAD	O4-C4-C4X	-2.08	121.05	126.53
4	G	3005	FAD	C4X-C4-N3	2.05	118.47	113.25
4	A	3005	FAD	O4B-C1B-N9A	2.04	112.02	108.09
4	C	3005	FAD	N3A-C4A-N9A	2.04	130.64	127.17
4	C	3005	FAD	C5X-N5-C4X	2.03	121.37	118.09
4	A	3005	FAD	C6-C5X-C9A	2.00	121.80	119.05

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3005	FAD	C5B-O5B-PA-O2A
4	A	3005	FAD	C5B-O5B-PA-O3P
4	A	3005	FAD	C2'-C1'-N10-C10
4	A	3005	FAD	N10-C1'-C2'-O2'
4	A	3005	FAD	N10-C1'-C2'-C3'
4	A	3005	FAD	C2'-C3'-C4'-C5'
4	A	3005	FAD	C3'-C4'-C5'-O5'
4	A	3005	FAD	C5'-O5'-P-O3P
4	C	3005	FAD	C5B-O5B-PA-O1A
4	C	3005	FAD	C2'-C1'-N10-C10
4	C	3005	FAD	N10-C1'-C2'-O2'
4	C	3005	FAD	N10-C1'-C2'-C3'
4	C	3005	FAD	C2'-C3'-C4'-O4'
4	C	3005	FAD	O3'-C3'-C4'-O4'
4	C	3005	FAD	O3'-C3'-C4'-C5'
4	E	3005	FAD	C5B-O5B-PA-O2A
4	E	3005	FAD	C5B-O5B-PA-O3P
4	E	3005	FAD	N10-C1'-C2'-O2'
4	E	3005	FAD	N10-C1'-C2'-C3'
4	E	3005	FAD	C2'-C3'-C4'-O4'
4	E	3005	FAD	O3'-C3'-C4'-O4'
4	E	3005	FAD	O3'-C3'-C4'-C5'
4	G	3005	FAD	N10-C1'-C2'-O2'
4	G	3005	FAD	N10-C1'-C2'-C3'
4	G	3005	FAD	C2'-C3'-C4'-O4'
4	G	3005	FAD	C2'-C3'-C4'-C5'
4	G	3005	FAD	O3'-C3'-C4'-O4'
4	G	3005	FAD	C3'-C4'-C5'-O5'
4	G	3005	FAD	O4'-C4'-C5'-O5'
4	G	3005	FAD	C5'-O5'-P-O3P
7	F	3007	ZW9	C2'-C3'-C4'-O4'
4	A	3005	FAD	C2'-C3'-C4'-O4'
4	A	3005	FAD	O3'-C3'-C4'-C5'
4	G	3005	FAD	O3'-C3'-C4'-C5'
4	C	3005	FAD	C2'-C3'-C4'-C5'
4	E	3005	FAD	C2'-C3'-C4'-C5'
4	A	3005	FAD	O3'-C3'-C4'-O4'
4	A	3005	FAD	O4'-C4'-C5'-O5'
4	C	3005	FAD	O4'-C4'-C5'-O5'
4	A	3005	FAD	O4B-C4B-C5B-O5B
4	E	3005	FAD	O4B-C4B-C5B-O5B
4	C	3005	FAD	C3'-C4'-C5'-O5'
7	F	3007	ZW9	C4'-O4'-P-O3P

Continued on next page...

Continued from previous page...

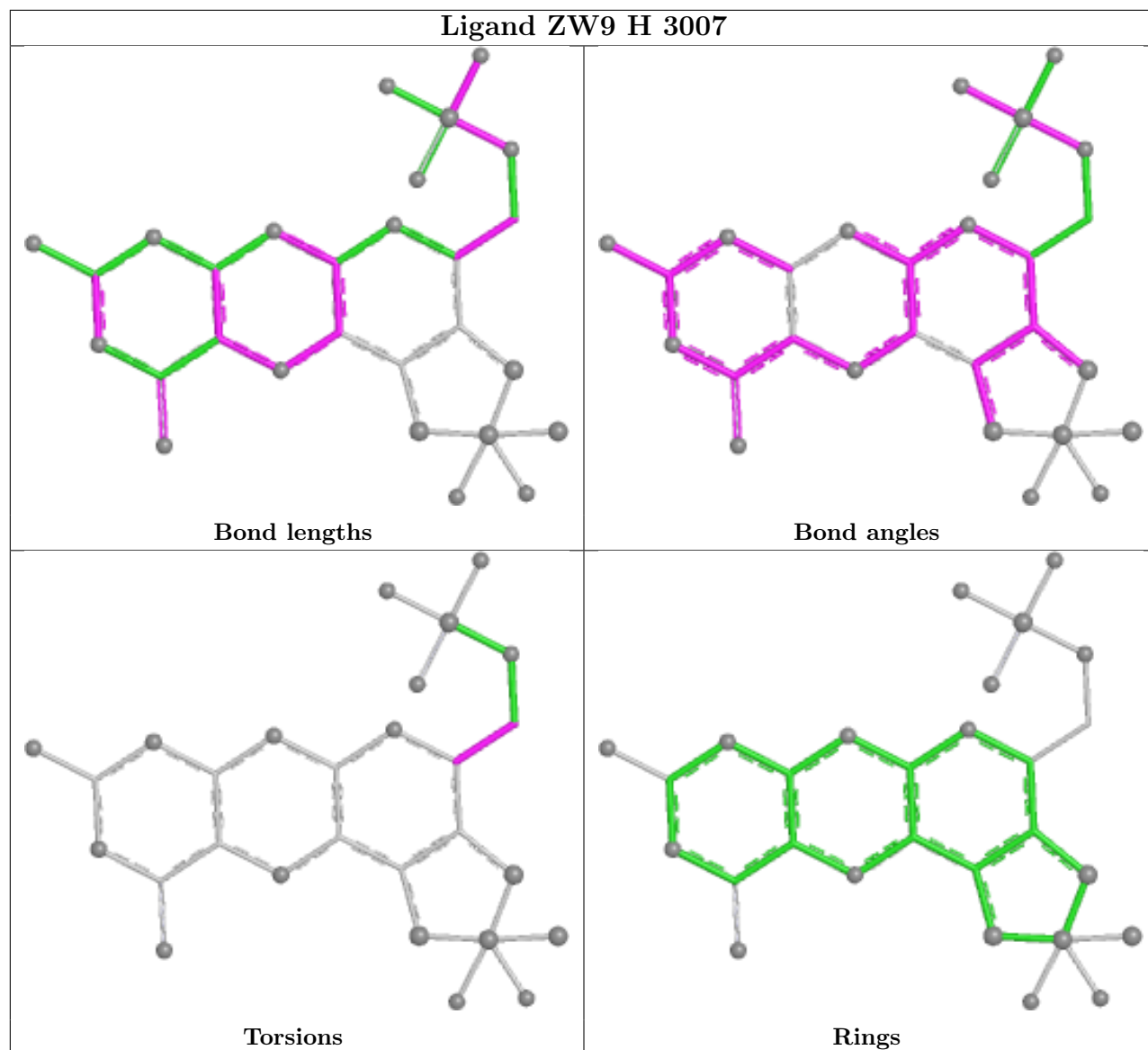
Mol	Chain	Res	Type	Atoms
7	D	3007	ZW9	C4'-O4'-P-O2P
4	E	3005	FAD	C3'-C4'-C5'-O5'
4	A	3005	FAD	C5B-O5B-PA-O1A
4	E	3005	FAD	C2'-C1'-N10-C10
4	E	3005	FAD	C2B-C1B-N9A-C8A
7	D	3007	ZW9	O3'-C3'-C4'-O4'
7	F	3007	ZW9	O3'-C3'-C4'-O4'
7	H	3007	ZW9	O3'-C3'-C4'-O4'
7	F	3007	ZW9	C4'-O4'-P-O2P
7	D	3007	ZW9	C2'-C3'-C4'-O4'

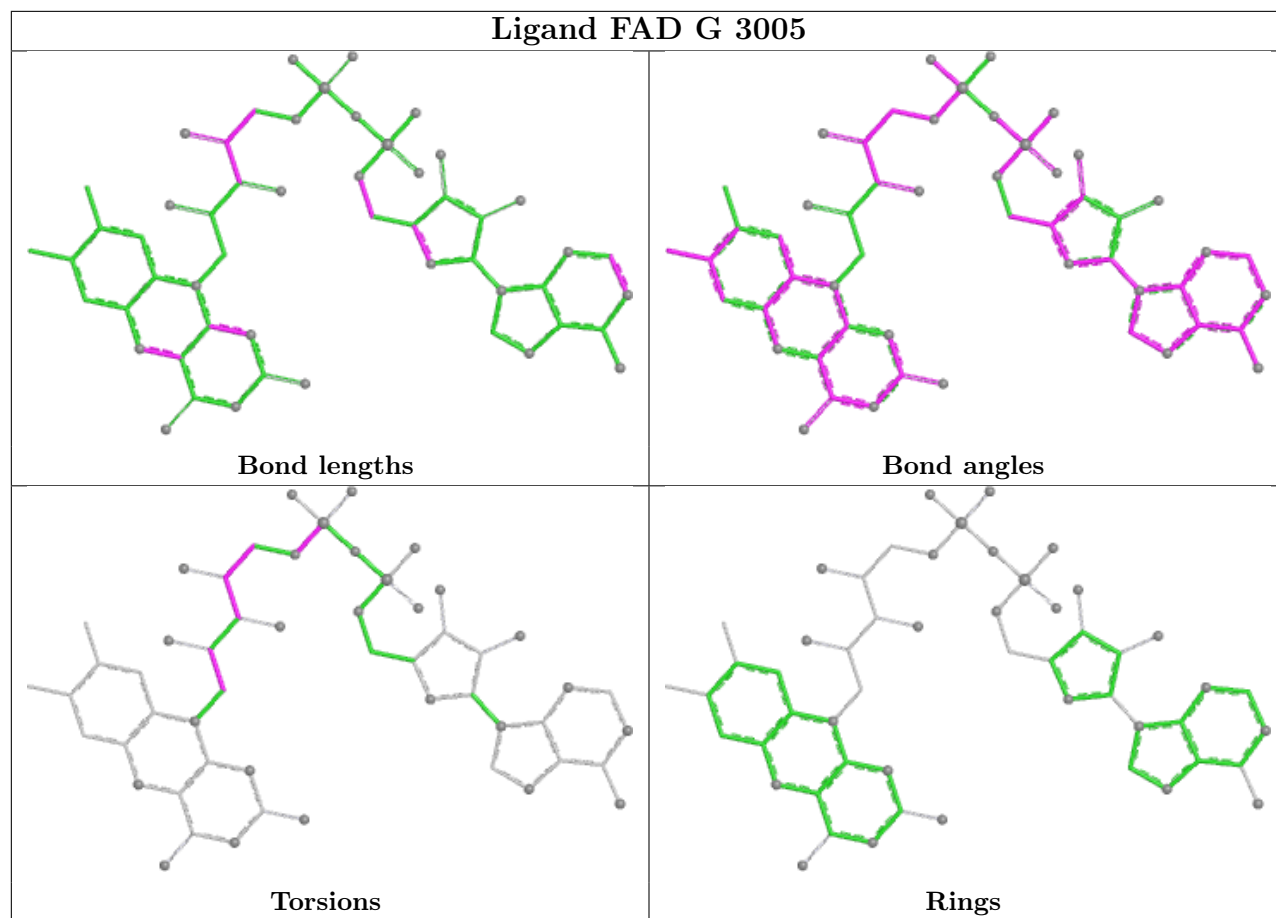
There are no ring outliers.

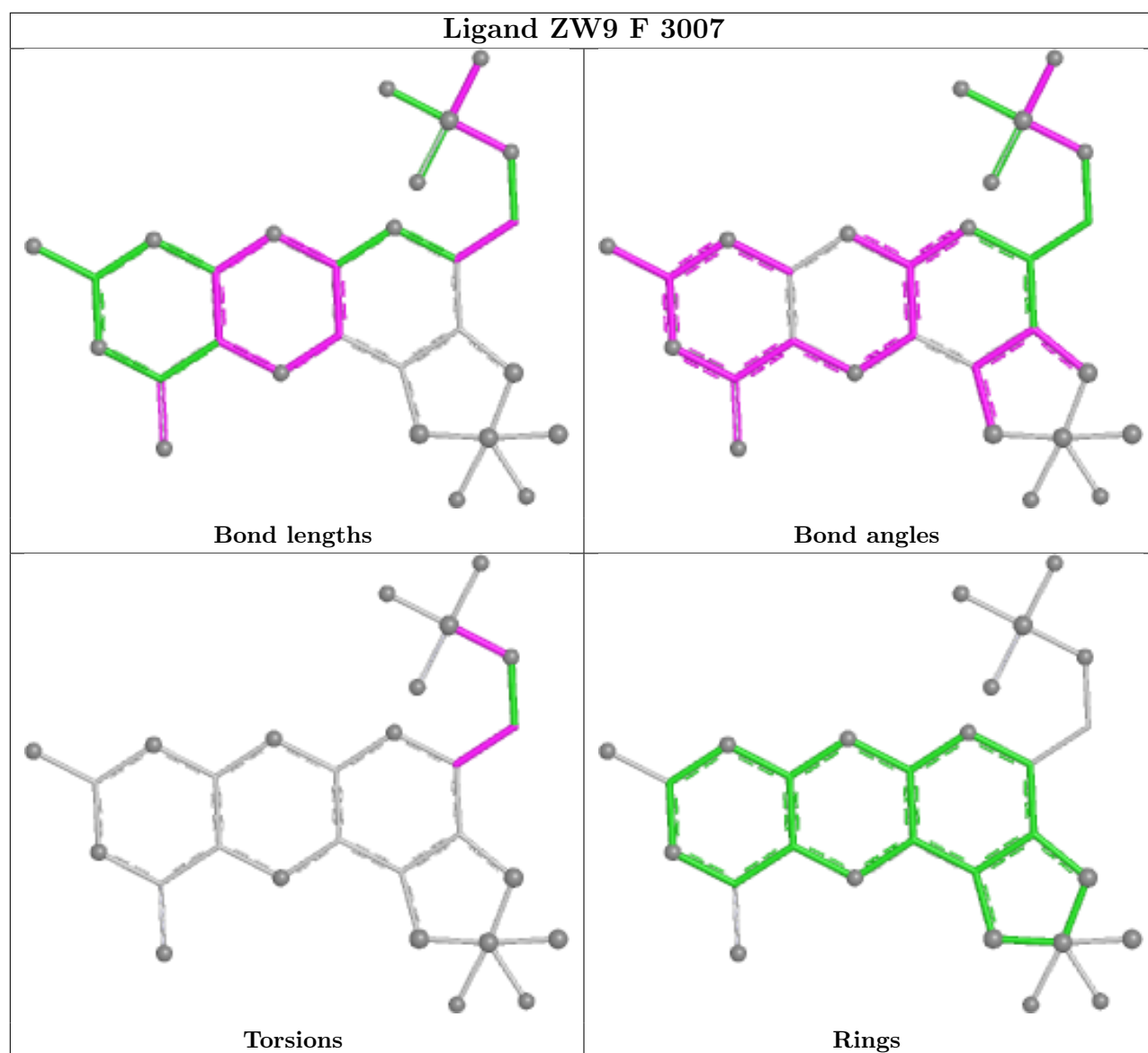
12 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	3007	ZW9	5	0
3	E	3002	FES	1	0
4	G	3005	FAD	11	0
3	G	3001	FES	3	0
7	F	3007	ZW9	3	0
7	D	3007	ZW9	7	0
3	E	3001	FES	1	0
7	B	3007	ZW9	5	0
4	A	3005	FAD	6	0
4	C	3005	FAD	3	0
3	G	3002	FES	1	0
4	E	3005	FAD	6	0

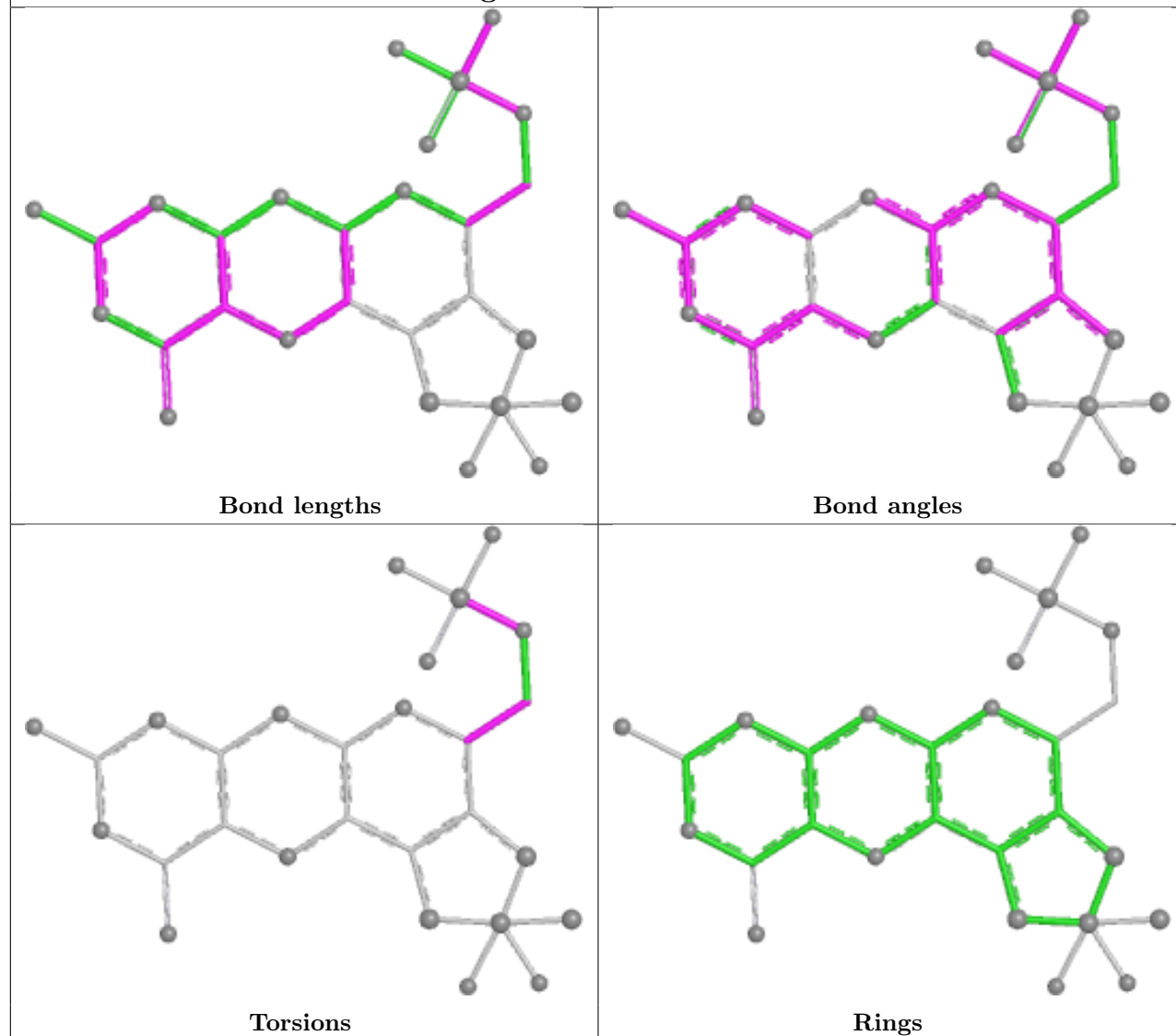
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

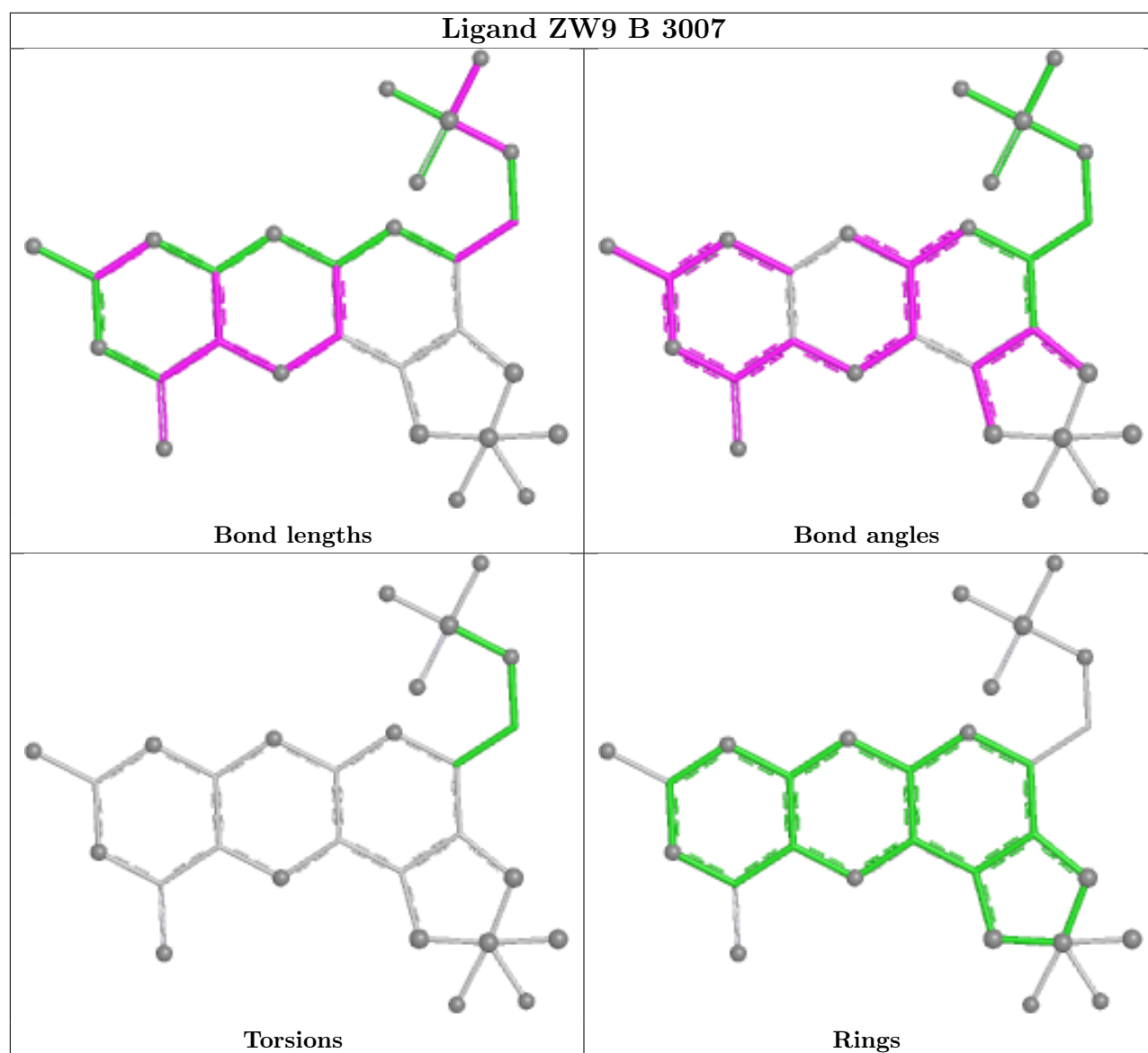


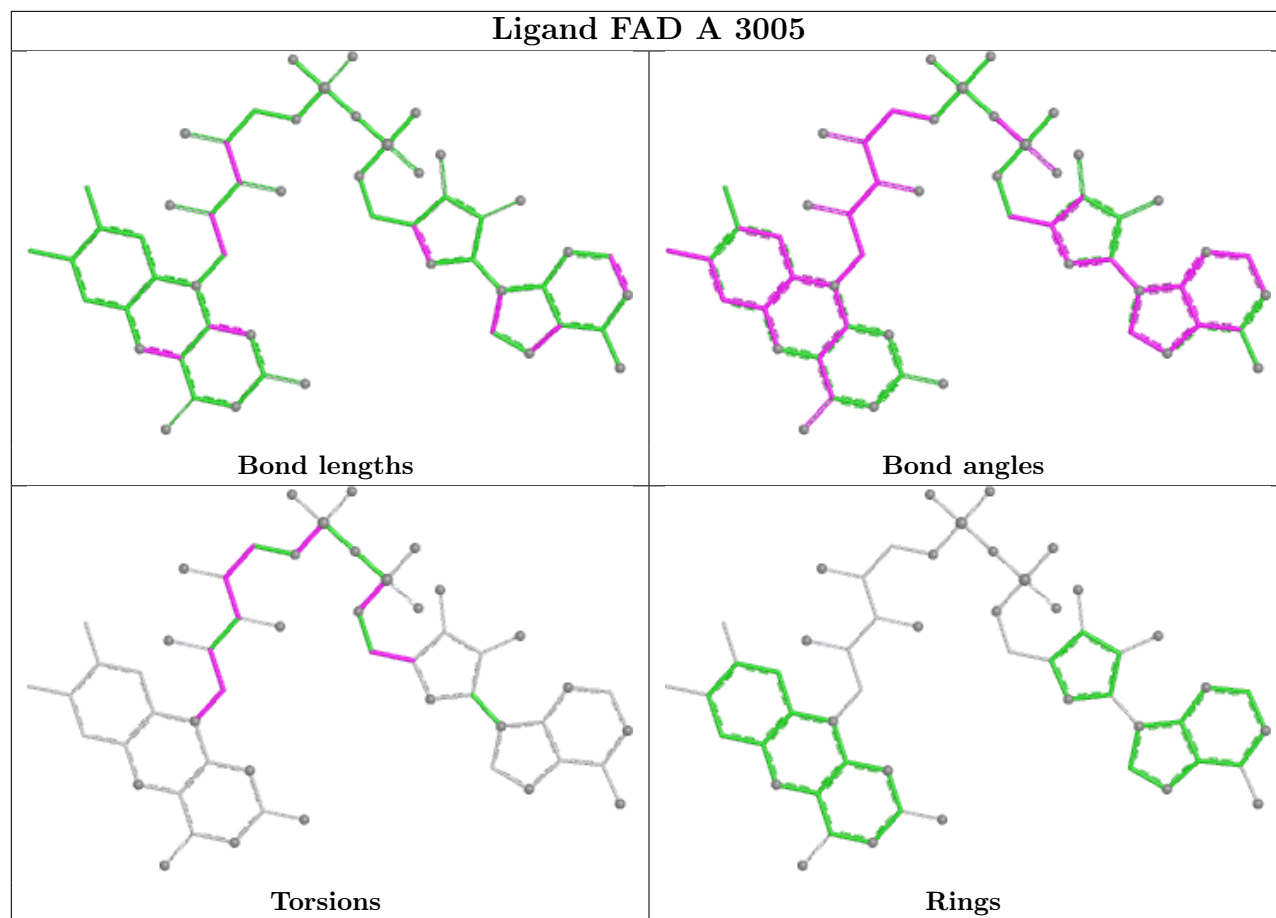


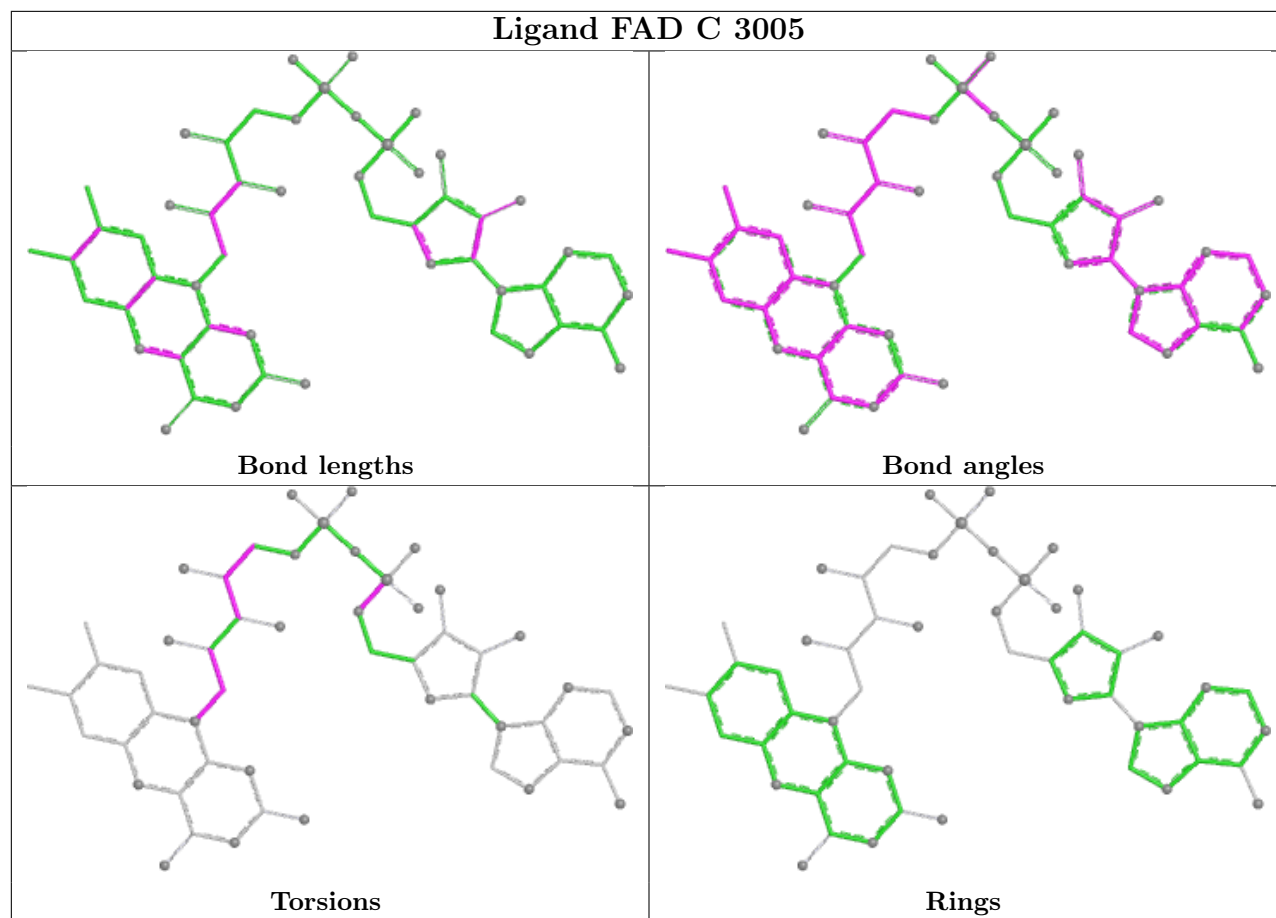


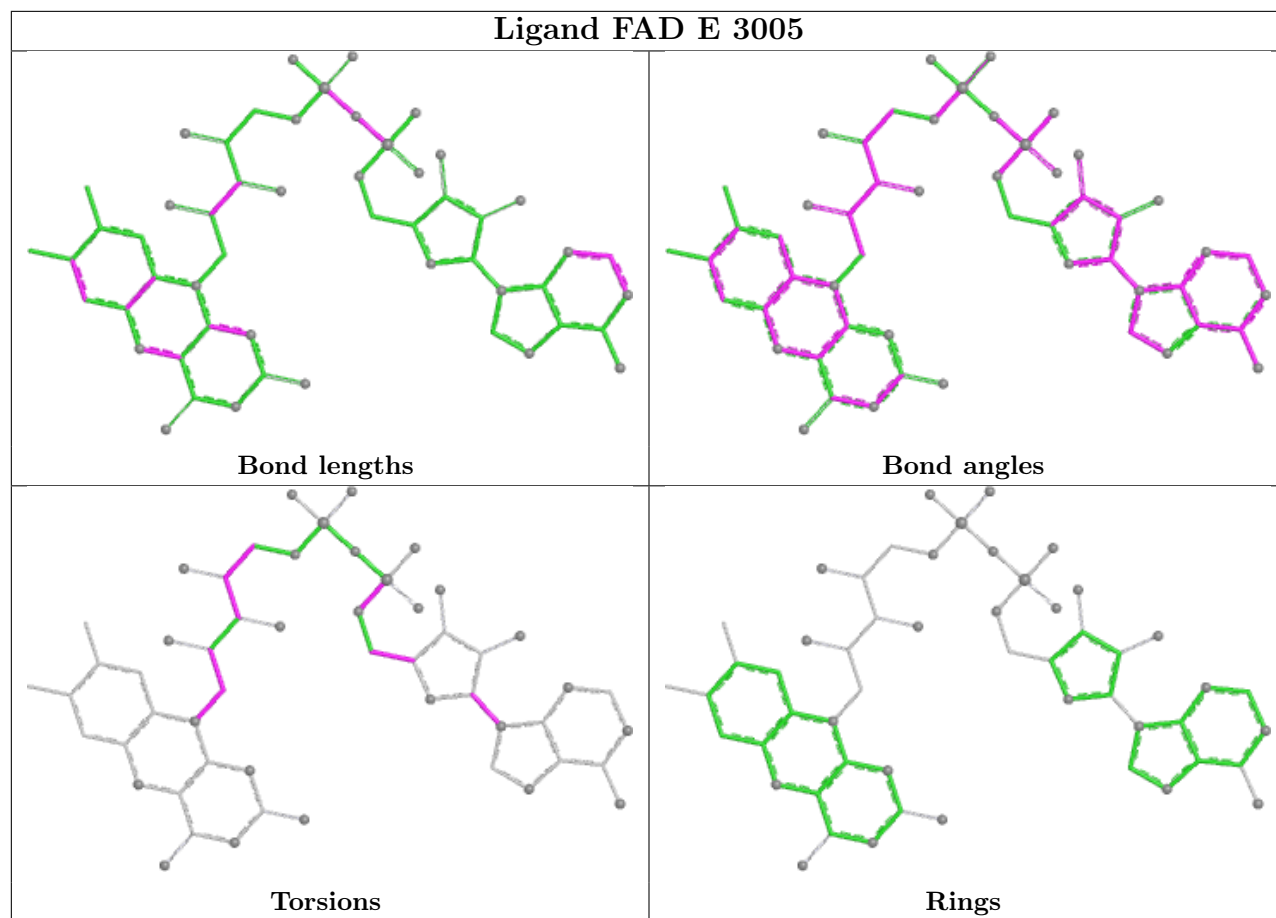
Ligand ZW9 D 3007











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.