



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:08 AM EDT

PDB ID : 2Z8Y / pdb_00002z8y
Title : Xenon-bound structure of bifunctional carbon monoxide dehydrogenase/acet
yl-CoA synthase(CODH/ACS) from Moorella thermoacetica
Authors : Doukov, T.I.; Blasiak, L.C.; Drennan, C.L.
Deposited on : 2007-09-12
Resolution : 2.51 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

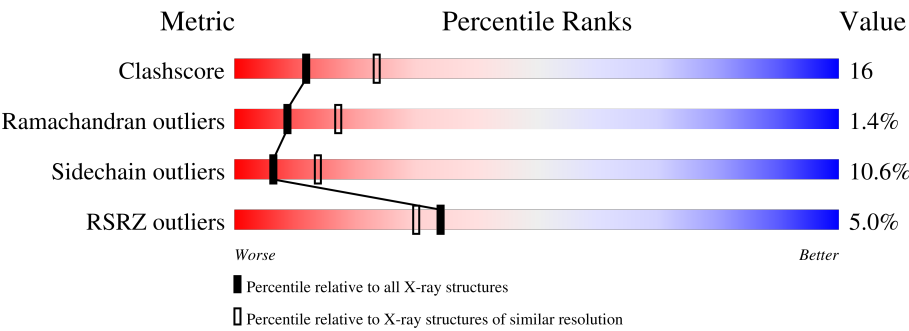
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	674	70%26%.
1	B	674	70%25%.
1	C	674	70%25%.
1	D	674	64%32%.
2	M	729	%70%24%5%.
2	N	729	68%27%. .
2	O	729	24% 41%41%16%. .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	P	729	

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	SF4	O	900	-	-	X	-
4	XCC	A	800	-	-	X	-
4	XCC	B	800	-	-	X	-
4	XCC	C	800	-	-	X	-
5	XE	A	1001	-	-	X	-
5	XE	A	1003[A]	-	-	X	-
5	XE	A	1003[B]	-	-	X	-
5	XE	A	1004	-	-	X	-
5	XE	B	1001	-	-	X	-
5	XE	B	1003[B]	-	-	X	-
5	XE	B	1004	-	-	X	-
5	XE	C	1003[B]	-	-	X	-
5	XE	C	1004	-	-	X	-
5	XE	D	1003[B]	-	-	X	-
5	XE	M	1006	-	-	X	-
5	XE	N	1006	-	-	X	-
5	XE	N	1009	-	-	X	-
5	XE	O	1006	-	-	X	-
5	XE	O	1009	-	-	X	-
5	XE	P	1008	-	-	X	-
6	GOL	A	862	-	-	X	-
6	GOL	D	863	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 44706 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.

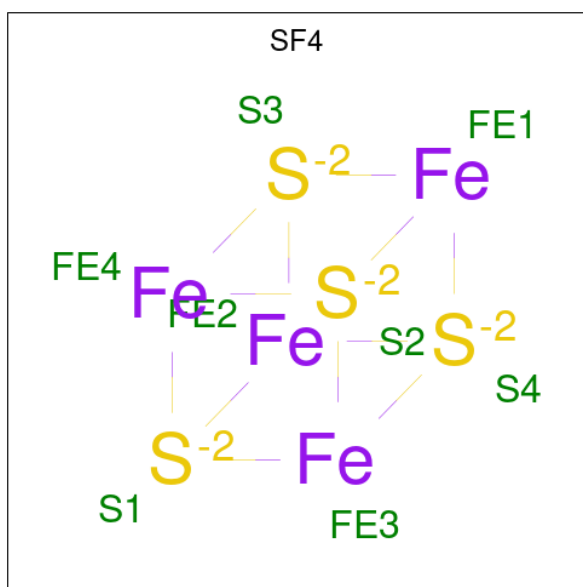
- Molecule 1 is a protein called Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	2	0
			5094	3202	891	959	42			
1	B	673	Total	C	N	O	S	0	7	0
			5094	3202	891	959	42			
1	C	673	Total	C	N	O	S	0	4	0
			5094	3202	891	959	42			
1	D	673	Total	C	N	O	S	0	2	0
			5094	3202	891	959	42			

- Molecule 2 is a protein called Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha.

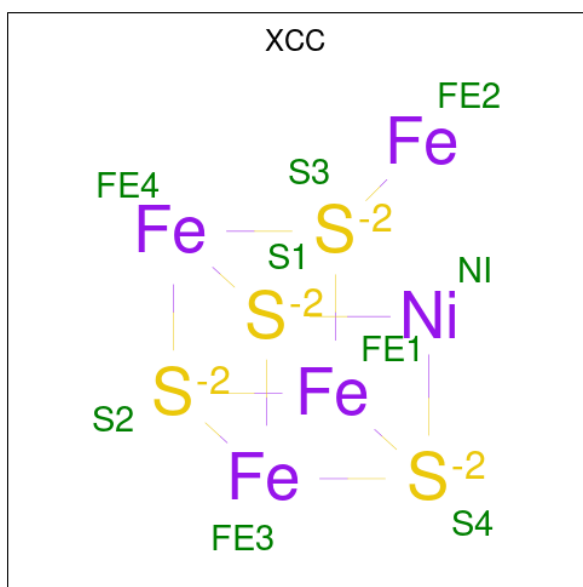
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	4	0
			5740	3681	956	1068	35			
2	N	728	Total	C	N	O	S	0	3	0
			5740	3681	956	1068	35			
2	O	727	Total	C	N	O	S	0	1	0
			5725	3673	952	1066	34			
2	P	728	Total	C	N	O	S	0	3	0
			5740	3681	956	1068	35			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	N	1	Total	Fe	S	0	0
			8	4	4		
3	O	1	Total	Fe	S	0	0
			8	4	4		
3	P	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe₄NiS₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 5 is XENON (CCD ID: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	Xe	0	1
			7	7		
5	B	6	Total	Xe	0	1
			7	7		
5	C	6	Total	Xe	0	1
			7	7		
5	D	6	Total	Xe	0	1
			7	7		
5	M	3	Total	Xe	0	0
			3	3		
5	N	4	Total	Xe	0	0
			4	4		
5	O	3	Total	Xe	0	0
			3	3		
5	P	4	Total	Xe	0	0
			4	4		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

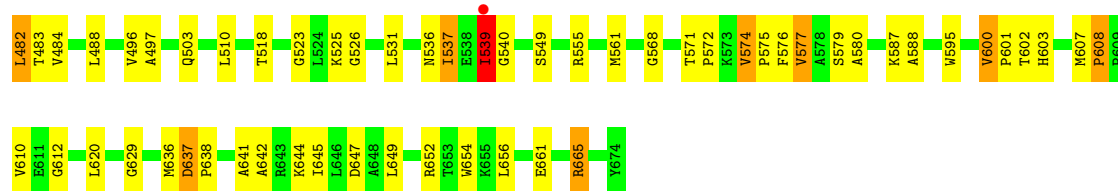
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total Cu 1 1	0	0
7	N	1	Total Cu 1 1	0	0
7	O	1	Total Cu 1 1	0	0
7	P	1	Total Cu 1 1	0	0

- Molecule 8 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total Ni 1 1	0	0
8	N	1	Total Ni 1 1	0	0
8	O	1	Total Ni 1 1	0	0
8	P	1	Total Ni 1 1	0	0

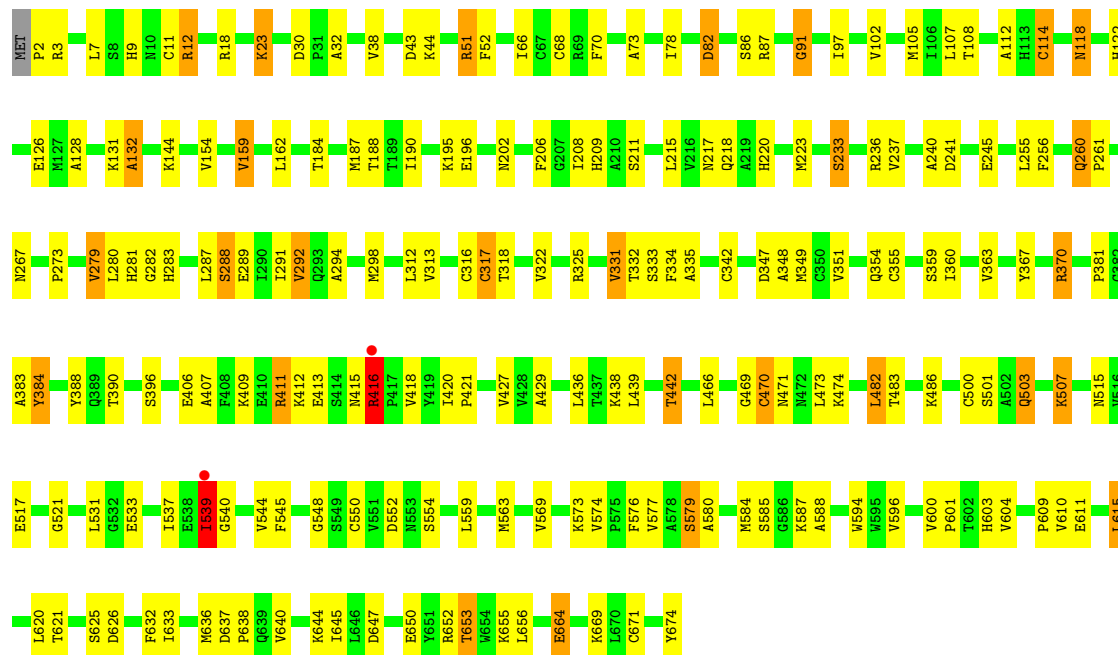
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	168	Total O 168 168	0	0
9	B	220	Total O 220 220	0	0
9	C	130	Total O 130 130	0	0
9	D	105	Total O 105 105	0	0
9	M	201	Total O 201 201	0	0
9	N	222	Total O 222 222	0	0
9	O	27	Total O 27 27	0	0
9	P	80	Total O 80 80	0	0



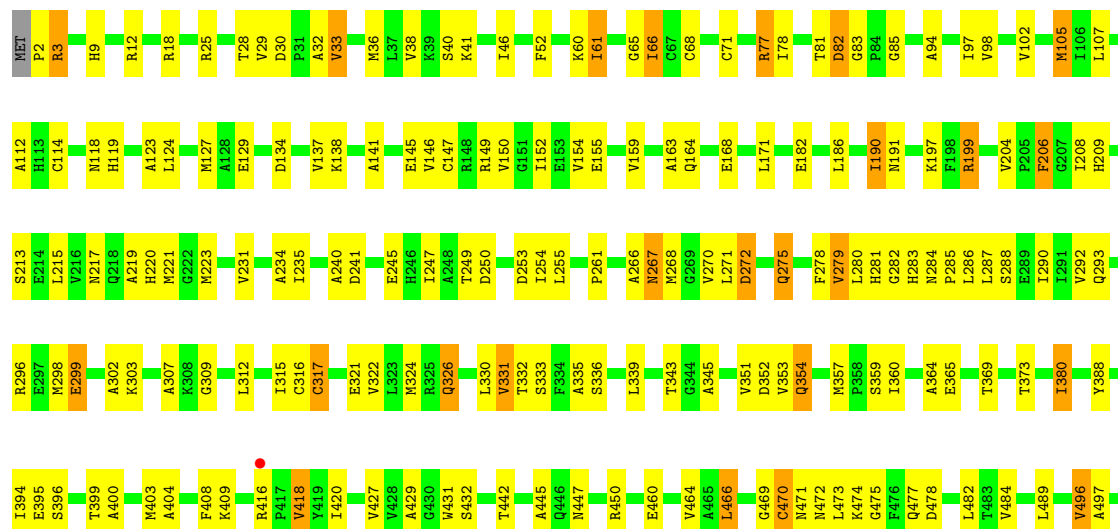
● Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta

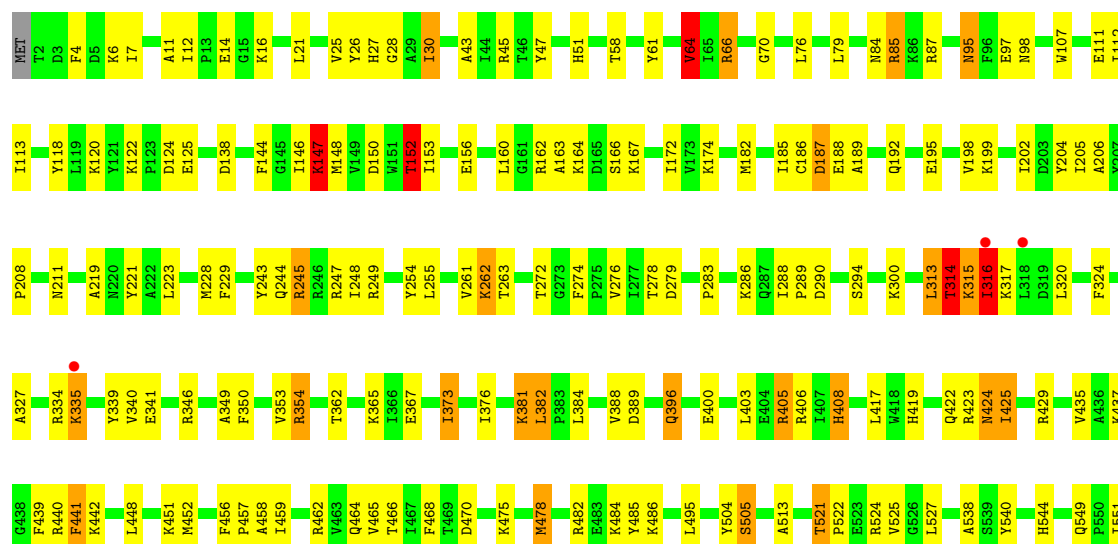
Chain C: 70% 25% .

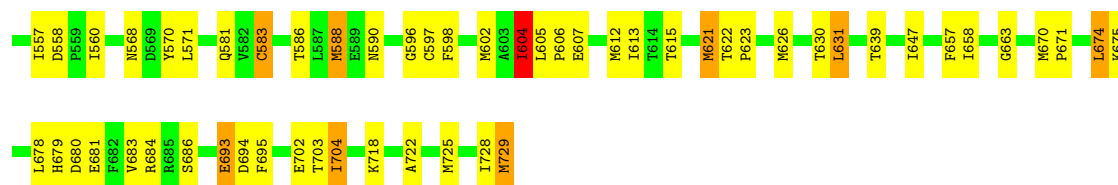


● Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta

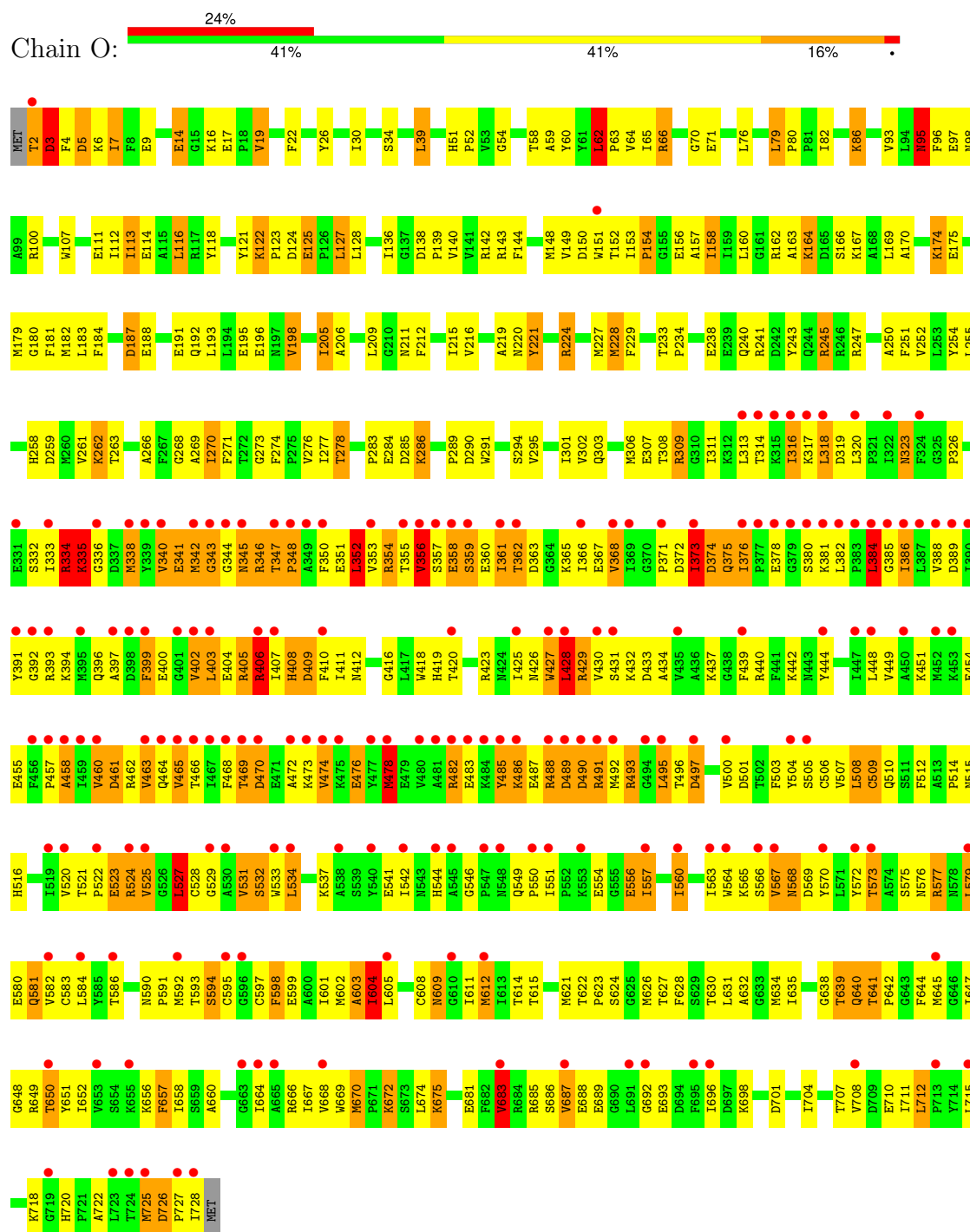
Chain D: 64% 32% .



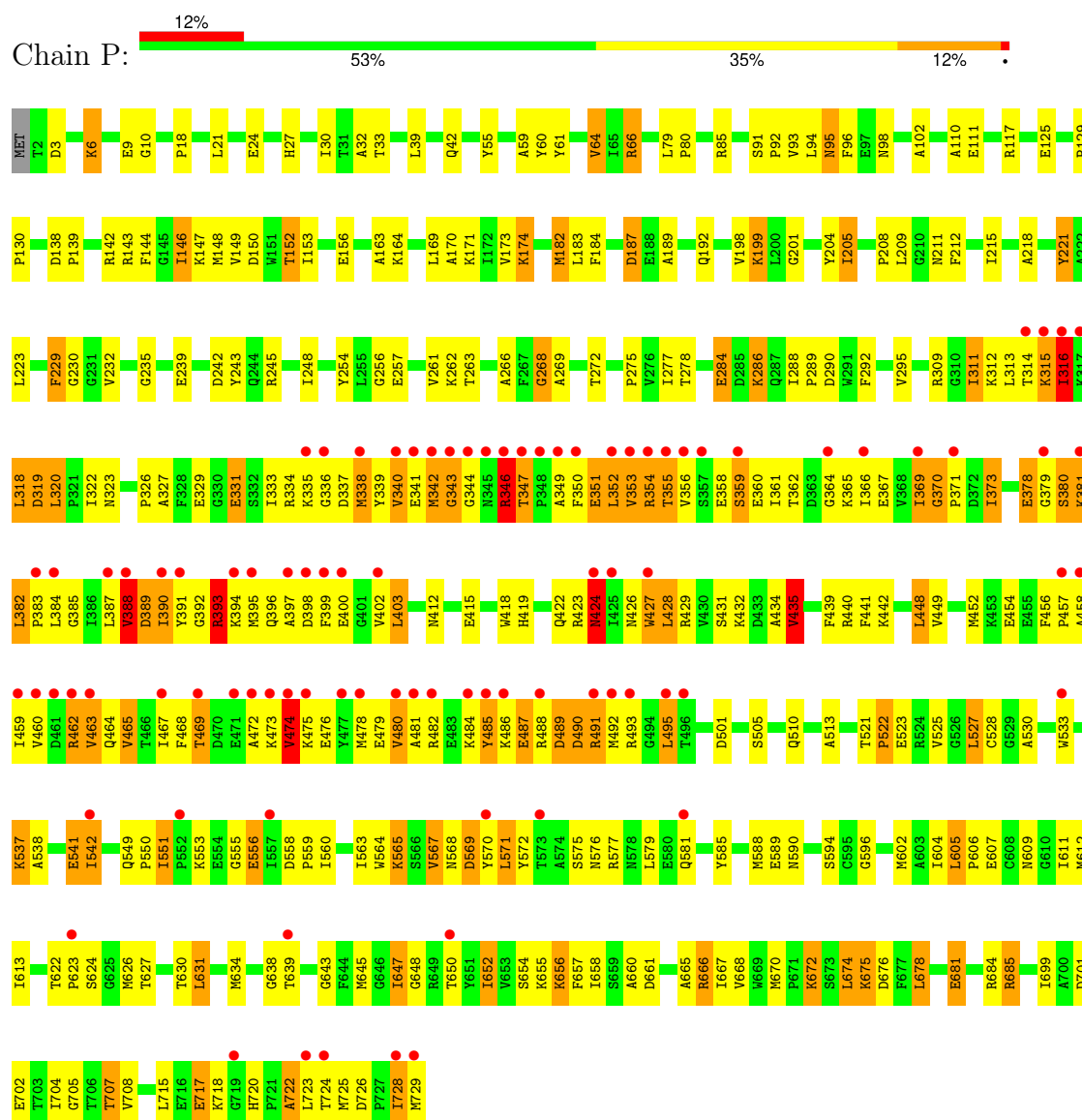




• Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha



• Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.54Å 136.60Å 141.75Å 101.29° 109.22° 103.91°	Depositor
Resolution (Å)	49.00 – 2.51 49.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.00-2.51) 96.1 (49.00-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.178 , 0.250 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	44706	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XCC, SF4, NI, XE, GOL, CU1

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	1.58	29/5187 (0.6%)	1.44	30/7028 (0.4%)
1	B	1.60	34/5187 (0.7%)	1.43	35/7028 (0.5%)
1	C	1.54	19/5187 (0.4%)	1.44	32/7028 (0.5%)
1	D	1.47	15/5187 (0.3%)	1.44	49/7028 (0.7%)
2	M	1.49	24/5874 (0.4%)	1.36	39/7954 (0.5%)
2	N	1.51	27/5874 (0.5%)	1.41	48/7954 (0.6%)
2	O	1.40	15/5859 (0.3%)	1.36	42/7937 (0.5%)
2	P	1.39	16/5874 (0.3%)	1.36	43/7954 (0.5%)
All	All	1.50	179/44229 (0.4%)	1.41	318/59911 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
2	N	0	1
2	P	0	2
All	All	0	8

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	383	ALA	CA-CB	-9.21	1.37	1.53
1	A	397	ALA	CA-CB	-9.02	1.39	1.53
1	C	363	VAL	CA-CB	-8.55	1.45	1.54
2	P	208	PRO	C-O	8.10	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3	ARG	CA-C	7.96	1.62	1.52
1	D	484	VAL	CA-CB	7.93	1.62	1.54
2	M	504	TYR	CA-C	-7.86	1.43	1.52
1	A	168	GLU	CG-CD	7.48	1.70	1.52
1	B	113	HIS	CA-C	-7.47	1.42	1.52
2	O	683	VAL	CA-CB	7.37	1.62	1.54
2	M	269	ALA	CA-CB	7.35	1.64	1.53
2	N	538	ALA	CA-CB	-7.16	1.42	1.53
2	N	324	PHE	CA-C	-7.15	1.44	1.52
2	N	521	THR	CA-CB	7.09	1.62	1.54
2	O	113	ILE	CA-CB	-6.98	1.46	1.54
1	C	132	ALA	CA-CB	-6.90	1.45	1.53
1	A	591	ILE	CA-CB	-6.87	1.45	1.54
1	B	305	ALA	CA-CB	-6.85	1.42	1.53
1	A	578	ALA	CA-CB	-6.84	1.41	1.53
1	B	92	ALA	CA-CB	-6.79	1.42	1.53
1	D	231	VAL	CA-CB	-6.77	1.46	1.54
2	N	97	GLU	N-CA	-6.75	1.38	1.46
2	M	61	TYR	C-O	-6.73	1.17	1.24
2	P	129	PRO	CA-C	-6.69	1.46	1.52
2	M	329	GLU	C-O	-6.63	1.16	1.24
1	C	288	SER	N-CA	-6.62	1.37	1.46
2	N	320	LEU	N-CA	-6.58	1.41	1.46
2	N	294	SER	N-CA	-6.57	1.38	1.46
1	B	214	GLU	CA-C	6.56	1.61	1.52
2	M	590	ASN	C-O	-6.56	1.20	1.23
1	A	542	PRO	C-O	-6.52	1.17	1.24
2	N	279	ASP	C-O	-6.49	1.15	1.24
2	P	232	VAL	CA-CB	-6.49	1.47	1.54
1	B	539	ILE	CA-CB	6.42	1.63	1.54
2	O	520	VAL	CA-CB	6.42	1.61	1.53
1	A	407	ALA	CA-CB	-6.38	1.42	1.53
1	D	33	VAL	CA-CB	6.35	1.63	1.54
1	D	78	ILE	CA-C	-6.34	1.45	1.52
1	B	378	ALA	CA-CB	6.32	1.61	1.52
1	C	548	GLY	C-O	-6.31	1.19	1.24
1	D	641	ALA	CA-CB	-6.30	1.43	1.53
2	O	542	ILE	CA-CB	6.29	1.61	1.54
1	A	379	LYS	C-O	6.25	1.31	1.23
2	P	622	THR	CA-CB	6.25	1.63	1.54
2	O	687	VAL	CA-CB	6.21	1.62	1.54
1	A	401	ILE	CA-CB	-6.18	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	267	ASN	CA-C	-6.17	1.44	1.52
1	C	388	TYR	C-O	-6.14	1.16	1.24
1	C	580	ALA	CA-CB	-6.13	1.45	1.53
2	N	316	ILE	CA-CB	6.13	1.62	1.54
1	A	164	GLN	C-O	-6.12	1.17	1.24
1	A	258	THR	CA-C	-6.12	1.45	1.52
2	P	93	VAL	CA-C	-6.12	1.45	1.52
2	P	263	THR	CA-CB	-6.06	1.43	1.53
1	B	349	MET	N-CA	-6.06	1.38	1.46
2	N	276	VAL	CA-CB	6.01	1.61	1.54
2	M	206	ALA	CA-CB	-5.98	1.43	1.53
2	M	246	ARG	C-O	-5.97	1.17	1.24
2	N	186	CYS	N-CA	-5.96	1.38	1.46
2	N	465	VAL	CA-CB	5.96	1.62	1.54
2	M	138	ASP	CA-C	5.95	1.60	1.52
2	N	113	ILE	CA-CB	-5.94	1.47	1.54
1	B	447	ASN	C-O	5.94	1.30	1.24
2	N	25	VAL	CA-CB	-5.93	1.47	1.54
2	O	311	ILE	CA-CB	5.92	1.59	1.53
2	N	604	ILE	CA-CB	5.91	1.60	1.54
1	A	305	ALA	CA-CB	-5.89	1.43	1.53
1	A	63	TYR	C-O	-5.88	1.17	1.24
2	M	53	VAL	CA-CB	5.83	1.63	1.54
1	B	196	GLU	CG-CD	5.82	1.66	1.52
2	P	94	LEU	C-O	-5.78	1.17	1.24
2	N	683	VAL	CA-CB	5.78	1.61	1.54
1	D	546	HIS	N-CA	-5.77	1.39	1.46
2	P	311	ILE	CA-CB	5.76	1.61	1.54
1	B	21	GLU	N-CA	5.76	1.50	1.46
1	B	188	THR	CA-CB	5.75	1.63	1.53
1	D	254	ILE	CA-CB	-5.75	1.47	1.54
2	P	316	ILE	CA-CB	5.74	1.62	1.54
1	A	353	VAL	C-O	-5.74	1.18	1.24
1	B	539	ILE	CA-C	5.73	1.60	1.52
2	N	525	VAL	CA-CB	5.70	1.59	1.54
1	B	568	GLY	CA-C	5.69	1.57	1.51
1	B	225	ASN	N-CA	-5.68	1.40	1.46
2	O	356	VAL	CA-CB	5.66	1.62	1.54
2	M	465	VAL	CA-CB	5.66	1.61	1.54
1	B	38	VAL	CA-CB	5.64	1.61	1.54
1	B	32	ALA	CA-CB	-5.64	1.44	1.53
2	O	508	LEU	C-O	5.63	1.28	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	404	GLU	CA-C	-5.62	1.45	1.52
2	P	218	ALA	CA-CB	-5.60	1.44	1.53
1	B	21	GLU	C-O	-5.60	1.21	1.23
2	P	173	VAL	CA-CB	-5.59	1.47	1.54
1	A	3	ARG	C-O	-5.58	1.17	1.24
2	N	120	LYS	CE-NZ	5.58	1.66	1.49
1	A	90	CYS	N-CA	5.57	1.53	1.46
2	N	172	ILE	CA-CB	-5.56	1.47	1.54
1	C	610	VAL	CA-CB	-5.55	1.48	1.54
2	M	288	ILE	N-CA	-5.55	1.39	1.46
2	M	524	ARG	C-O	5.54	1.30	1.24
1	C	128	ALA	C-O	-5.51	1.17	1.24
1	A	61	ILE	C-O	-5.50	1.18	1.24
1	B	210	ALA	CA-C	5.50	1.60	1.52
1	C	279	VAL	CA-CB	-5.48	1.47	1.54
1	B	577	VAL	CA-CB	5.48	1.64	1.55
1	A	314	GLY	N-CA	5.47	1.50	1.44
1	B	362	ALA	CA-CB	-5.46	1.44	1.53
1	A	243	THR	CA-CB	-5.46	1.44	1.53
2	O	355	THR	CA-C	5.46	1.59	1.53
1	B	229	ASN	C-O	-5.45	1.17	1.24
1	D	163	ALA	N-CA	-5.45	1.39	1.46
1	A	383	ALA	CA-CB	-5.44	1.41	1.53
2	O	557	ILE	CA-CB	5.44	1.61	1.54
2	N	202	ILE	C-O	-5.43	1.18	1.24
2	P	724	THR	CA-CB	5.42	1.62	1.53
2	O	507	VAL	C-O	5.39	1.30	1.24
1	B	482	LEU	C-O	-5.39	1.17	1.24
1	B	523	GLY	C-O	5.38	1.30	1.23
2	M	315	LYS	N-CA	5.36	1.53	1.46
1	D	119	HIS	CA-C	5.34	1.59	1.52
1	A	163	ALA	N-CA	-5.33	1.39	1.46
2	M	19	VAL	C-O	-5.33	1.18	1.24
1	B	272	ASP	CA-C	5.32	1.57	1.52
1	B	287	LEU	CG-CD1	5.30	1.70	1.52
1	B	418	VAL	C-O	-5.30	1.18	1.24
1	B	112	ALA	CA-CB	5.28	1.61	1.53
1	C	255	LEU	N-CA	5.28	1.53	1.46
1	D	571	THR	CA-C	5.28	1.59	1.52
2	P	32	ALA	CA-C	5.26	1.59	1.52
2	M	303	GLN	N-CA	-5.23	1.40	1.46
1	B	384	TYR	CA-C	-5.23	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	347	ASP	CA-CB	-5.23	1.44	1.53
2	O	270	ILE	CA-CB	-5.22	1.48	1.54
1	A	82	ASP	CB-CG	-5.21	1.39	1.52
1	A	77	ARG	C-O	-5.20	1.17	1.23
2	M	286	LYS	CA-C	5.20	1.59	1.52
1	C	473	LEU	CA-C	5.20	1.59	1.52
2	N	504	TYR	CA-C	-5.20	1.46	1.52
1	A	226	ASP	C-O	-5.19	1.18	1.24
1	A	202	ASN	CA-C	-5.19	1.46	1.53
2	O	650	THR	CA-CB	5.18	1.62	1.53
2	N	30	ILE	CA-CB	-5.17	1.48	1.54
2	O	39	LEU	CA-C	-5.17	1.46	1.52
2	N	583	CYS	N-CA	-5.17	1.39	1.46
2	N	524	ARG	CZ-NH2	5.16	1.40	1.33
2	N	702	GLU	CB-CG	-5.15	1.36	1.52
1	B	574	VAL	C-O	-5.15	1.18	1.24
2	M	210	GLY	C-O	5.15	1.27	1.24
2	N	28	GLY	C-O	-5.13	1.17	1.23
1	C	32	ALA	CA-CB	-5.12	1.45	1.53
1	D	77	ARG	CA-C	-5.12	1.46	1.52
1	D	247	ILE	C-O	-5.11	1.18	1.24
1	A	548	GLY	N-CA	5.11	1.50	1.45
2	M	595	CYS	C-O	-5.11	1.19	1.23
1	B	247	ILE	CB-CG2	5.11	1.69	1.52
1	C	184	THR	CA-CB	-5.10	1.45	1.53
2	M	54	GLY	N-CA	5.09	1.49	1.45
2	N	263	THR	N-CA	-5.09	1.40	1.46
1	A	116	HIS	C-O	-5.08	1.17	1.24
2	P	292	PHE	CA-C	-5.08	1.47	1.53
2	M	550	PRO	CA-C	-5.07	1.47	1.52
1	C	292	VAL	CA-CB	-5.07	1.48	1.54
1	B	406	GLU	CA-C	-5.07	1.46	1.52
1	D	627	VAL	N-CA	-5.07	1.40	1.46
1	A	209	HIS	C-O	5.06	1.30	1.24
2	P	32	ALA	CA-CB	-5.05	1.45	1.53
2	M	113	ILE	C-O	-5.05	1.18	1.24
2	M	639	THR	CA-C	5.04	1.59	1.52
1	D	464	VAL	C-O	-5.04	1.19	1.24
2	N	11	ALA	CA-CB	-5.04	1.45	1.53
1	B	415	ASN	CA-C	5.04	1.60	1.53
1	B	610	VAL	CB-CG2	5.04	1.69	1.52
1	B	246	HIS	N-CA	-5.04	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	VAL	C-N	5.03	1.39	1.33
1	C	580	ALA	CA-C	-5.03	1.47	1.52
1	C	237	VAL	CA-CB	-5.03	1.48	1.54
1	A	216	VAL	N-CA	-5.02	1.40	1.46
2	P	55	TYR	CA-C	-5.02	1.46	1.52
2	O	532	SER	C-O	5.01	1.30	1.23
2	M	288	ILE	CA-CB	-5.01	1.47	1.54

All (318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	416	ARG	CA-C-N	-16.11	104.52	120.31
1	C	416	ARG	C-N-CA	-16.11	104.52	120.31
1	D	38	VAL	N-CA-C	-11.73	99.44	110.82
1	A	331	VAL	CB-CA-C	-10.49	98.18	111.92
2	O	347	THR	CA-C-N	10.18	132.57	119.84
2	O	347	THR	C-N-CA	10.18	132.57	119.84
1	C	331	VAL	CB-CA-C	-10.03	98.90	112.04
2	O	546	GLY	CA-C-N	9.53	130.70	120.12
2	O	546	GLY	C-N-CA	9.53	130.70	120.12
1	C	539[A]	ILE	N-CA-C	9.47	120.29	110.72
2	P	675	LYS	N-CA-C	-9.38	100.61	111.03
1	D	272	ASP	CA-C-N	-8.94	110.58	119.87
1	D	272	ASP	C-N-CA	-8.94	110.58	119.87
1	D	365	GLU	N-CA-C	-8.90	102.20	113.23
2	O	343	GLY	N-CA-C	8.83	122.36	110.43
1	A	395	GLU	N-CA-C	8.78	120.85	111.28
1	A	471	ASN	N-CA-C	-8.70	96.66	110.14
2	P	102	ALA	N-CA-C	-8.69	102.11	112.89
1	C	521	GLY	N-CA-C	-8.46	100.91	112.25
2	P	30	ILE	N-CA-C	-8.45	102.31	110.42
2	N	456	PHE	CA-C-N	-8.39	111.38	119.85
2	N	456	PHE	C-N-CA	-8.39	111.38	119.85
1	A	380	ILE	CA-C-N	-8.33	111.39	119.89
1	A	380	ILE	C-N-CA	-8.33	111.39	119.89
2	O	79	LEU	CA-C-N	-8.28	111.85	120.38
2	O	79	LEU	C-N-CA	-8.28	111.85	120.38
1	D	284	ASN	CA-C-N	-7.84	111.75	120.45
1	D	284	ASN	C-N-CA	-7.84	111.75	120.45
1	D	475	GLY	N-CA-C	-7.83	99.12	111.18
1	C	349	MET	N-CA-C	-7.82	96.15	108.90
2	O	309	ARG	N-CA-C	-7.81	102.72	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	615	LEU	N-CA-C	-7.71	102.82	111.14
1	D	141	ALA	N-CA-C	-7.64	103.03	111.36
2	O	59	ALA	N-CA-C	-7.58	101.91	113.89
2	N	703	THR	CA-C-N	-7.55	115.33	122.66
2	N	703	THR	C-N-CA	-7.55	115.33	122.66
2	N	376	ILE	CA-C-N	-7.53	112.93	120.31
2	N	376	ILE	C-N-CA	-7.53	112.93	120.31
2	N	621	MET	CG-SD-CE	-7.53	84.33	100.90
2	M	376	ILE	CA-C-N	-7.52	111.64	120.13
2	M	376	ILE	C-N-CA	-7.52	111.64	120.13
2	N	382	LEU	CA-C-N	-7.50	112.97	120.31
2	N	382	LEU	C-N-CA	-7.50	112.97	120.31
1	B	230	LEU	N-CA-C	7.37	119.31	111.28
2	M	697	ASP	N-CA-C	-7.36	104.45	113.50
1	C	664	GLU	N-CA-C	-7.34	102.45	111.40
1	C	51	ARG	N-CA-C	-7.26	103.40	111.82
1	D	331	VAL	CB-CA-C	-7.24	102.54	112.02
1	D	331	VAL	N-CA-C	7.23	117.33	110.53
1	B	537	ILE	CB-CA-C	7.22	119.45	111.80
2	N	702	GLU	CB-CA-C	-7.21	96.47	110.46
2	N	147	LYS	N-CA-C	-7.18	104.78	113.97
2	N	631	LEU	N-CA-C	-7.16	103.55	111.36
2	O	573	THR	N-CA-C	7.16	119.16	111.36
1	D	629	GLY	N-CA-C	-7.11	106.62	115.08
2	M	687	VAL	N-CA-C	-7.08	103.43	110.30
2	O	352	LEU	N-CA-C	7.04	119.56	108.79
1	B	163	ALA	N-CA-C	-7.03	103.61	111.28
2	N	704	ILE	CB-CA-C	7.03	118.05	111.30
1	B	344	GLY	N-CA-C	-7.02	106.09	115.21
1	D	548	GLY	N-CA-C	7.00	118.63	111.56
2	M	728	ILE	N-CA-C	-6.97	102.10	111.44
1	C	38	VAL	N-CA-C	-6.96	103.99	110.53
1	D	394	ILE	N-CA-C	6.88	117.03	110.42
2	N	670	MET	CA-C-N	-6.87	112.91	119.85
2	N	670	MET	C-N-CA	-6.87	112.91	119.85
1	D	81	THR	N-CA-C	-6.86	105.06	113.50
1	B	66	ILE	N-CA-C	6.85	118.73	112.29
1	B	29	VAL	N-CA-C	-6.83	105.68	112.17
1	C	70	PHE	N-CA-C	6.82	121.19	113.01
1	A	38	VAL	N-CA-C	-6.82	104.12	110.53
2	P	153	ILE	N-CA-C	-6.81	100.81	107.55
1	D	442	THR	N-CA-C	-6.74	104.32	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	MET	CG-SD-CE	-6.74	86.08	100.90
2	O	384	LEU	N-CA-C	6.69	120.37	109.59
2	P	59	ALA	N-CA-C	-6.68	103.52	112.94
1	A	291	ILE	N-CA-C	-6.65	103.84	110.62
1	B	642	ALA	N-CA-C	-6.60	104.16	111.82
2	N	459	ILE	N-CA-C	-6.60	102.84	111.09
1	B	115	GLU	N-CA-C	-6.58	104.10	111.28
1	C	240	ALA	N-CA-C	-6.55	104.22	111.36
1	B	110	ALA	N-CA-C	-6.55	104.06	111.07
2	P	91	SER	CA-C-N	-6.53	114.17	120.83
2	P	91	SER	C-N-CA	-6.53	114.17	120.83
2	P	268	GLY	N-CA-C	-6.51	104.64	113.37
1	A	623	ILE	N-CA-C	6.51	117.26	110.62
2	M	459	ILE	N-CA-C	-6.49	102.74	111.44
1	C	355	CYS	CA-C-N	-6.46	114.63	122.90
1	C	355	CYS	C-N-CA	-6.46	114.63	122.90
1	B	236	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	D	206	PHE	N-CA-C	-6.46	101.68	111.56
1	D	240	ALA	N-CA-C	-6.44	104.34	111.36
2	N	70	GLY	N-CA-C	6.44	122.74	115.08
1	A	388	TYR	N-CA-C	6.43	119.55	109.96
1	C	82	ASP	N-CA-C	6.43	117.93	108.86
1	A	438	LYS	N-CA-C	-6.42	103.40	111.11
2	N	513	ALA	CA-C-N	6.40	126.08	119.56
2	N	513	ALA	C-N-CA	6.40	126.08	119.56
1	B	357	MET	CA-C-N	-6.38	113.23	119.87
1	B	357	MET	C-N-CA	-6.38	113.23	119.87
2	O	221	TYR	N-CA-C	-6.38	103.95	111.03
2	O	70	GLY	CA-C-N	-6.36	112.68	122.09
2	O	70	GLY	C-N-CA	-6.36	112.68	122.09
2	O	3	ASP	N-CA-C	-6.34	105.37	113.23
1	A	307	ALA	N-CA-C	-6.33	101.57	110.50
1	B	665[A]	ARG	N-CA-C	-6.32	103.92	111.69
2	O	465	VAL	N-CA-C	6.31	117.86	108.46
1	C	406	GLU	N-CA-C	-6.30	104.41	111.28
2	O	568	ASN	N-CA-C	6.29	118.14	111.28
1	D	359	SER	CA-CB-OG	-6.27	98.56	111.10
2	P	551	ILE	CA-C-N	-6.25	113.52	120.14
2	P	551	ILE	C-N-CA	-6.25	113.52	120.14
2	O	95	ASN	N-CA-C	6.24	116.31	108.45
2	O	62	LEU	CA-C-N	6.23	125.96	119.05
2	O	62	LEU	C-N-CA	6.23	125.96	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	278	THR	N-CA-C	6.22	118.87	109.23
2	N	248	ILE	CA-C-N	-6.21	112.86	122.05
2	N	248	ILE	C-N-CA	-6.21	112.86	122.05
2	M	119	LEU	N-CA-C	-6.17	105.01	112.54
1	D	29	VAL	N-CA-C	-6.15	106.78	112.43
1	B	540	GLY	N-CA-C	-6.14	103.45	111.37
1	D	521	GLY	N-CA-C	-6.14	103.11	112.51
1	B	608	PRO	N-CA-C	-6.14	103.21	110.70
1	B	43	ASP	N-CA-C	-6.12	105.80	113.20
2	O	647	ILE	N-CA-C	6.11	117.50	108.45
1	A	530	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	B	151	GLY	N-CA-C	-6.03	106.77	115.27
1	C	604	VAL	N-CA-C	-6.02	99.38	108.17
2	O	605	LEU	CA-C-N	6.00	126.11	119.87
2	O	605	LEU	C-N-CA	6.00	126.11	119.87
2	P	284	GLU	N-CA-C	-6.00	105.44	112.89
1	D	123	ALA	N-CA-C	6.00	117.82	111.28
1	D	317	CYS	N-CA-C	5.99	117.89	111.36
2	M	526	GLY	N-CA-C	-5.94	104.41	111.36
2	O	531	VAL	N-CA-C	5.93	116.72	108.89
1	D	445	ALA	N-CA-C	-5.92	106.10	113.38
2	M	587	LEU	N-CA-C	-5.91	106.03	113.72
2	N	590	ASN	CA-C-N	-5.91	114.18	120.03
2	N	590	ASN	C-N-CA	-5.91	114.18	120.03
2	P	388	VAL	N-CA-C	5.91	116.61	107.99
2	M	26	TYR	N-CA-C	-5.88	104.95	111.36
2	P	92	PRO	N-CA-C	-5.88	108.57	114.68
2	P	33	THR	N-CA-C	-5.87	105.22	112.90
1	C	442	THR	N-CA-C	-5.84	105.65	112.89
2	M	64	VAL	N-CA-CB	5.84	119.34	110.58
2	P	42	GLN	N-CA-C	-5.84	104.87	112.23
1	A	163	ALA	N-CA-C	-5.84	105.00	111.36
1	B	48	ALA	N-CA-C	5.84	118.39	111.33
1	A	244	GLY	N-CA-C	-5.82	105.32	112.77
1	D	592	GLY	N-CA-C	-5.79	105.36	112.77
2	O	273	GLY	N-CA-C	5.79	123.59	115.43
2	N	85	ARG	CG-CD-NE	-5.79	99.26	112.00
2	P	521	THR	CA-C-N	5.77	127.05	119.84
2	P	521	THR	C-N-CA	5.77	127.05	119.84
2	P	530	ALA	N-CA-C	5.75	117.63	111.36
1	B	612	GLY	CA-C-N	-5.75	114.70	122.86
1	B	612	GLY	C-N-CA	-5.75	114.70	122.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	557	ILE	N-CA-C	-5.74	107.30	112.12
2	P	381	LYS	N-CA-C	-5.74	100.82	108.34
2	N	118	TYR	N-CA-C	-5.74	106.04	113.16
2	P	229	PHE	N-CA-C	-5.74	105.05	112.68
1	D	404	ALA	N-CA-C	-5.74	104.64	111.69
1	A	66	ILE	N-CA-C	5.70	117.70	111.77
1	B	225	ASN	N-CA-C	-5.70	104.55	112.30
1	B	600	VAL	N-CA-CB	-5.70	106.33	112.37
1	A	423	ILE	N-CA-C	5.69	116.05	107.75
2	O	241	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	D	60	LYS	N-CA-C	-5.67	105.08	112.23
2	P	235	GLY	N-CA-C	-5.67	107.94	114.69
2	O	140	VAL	N-CA-C	-5.67	104.36	112.35
1	D	542	PRO	CA-C-N	-5.66	113.19	119.19
1	D	542	PRO	C-N-CA	-5.66	113.19	119.19
1	D	339	LEU	CA-CB-CG	-5.65	96.52	116.30
2	N	152	THR	N-CA-CB	5.65	118.92	110.22
2	M	604	ILE	CB-CA-C	-5.64	103.85	111.63
2	O	116	LEU	N-CA-C	5.63	117.09	111.07
2	O	455	GLU	N-CA-C	5.63	120.14	113.16
2	N	12	ILE	CA-C-N	5.61	125.52	119.85
2	N	12	ILE	C-N-CA	5.61	125.52	119.85
2	N	505	SER	N-CA-C	-5.59	102.25	110.52
1	A	488	LEU	N-CA-C	-5.58	105.27	111.36
2	N	441	PHE	N-CA-C	5.57	118.12	111.71
1	D	489	LEU	N-CA-C	-5.57	105.21	111.28
2	M	122	LYS	CA-C-N	5.57	125.67	119.32
2	M	122	LYS	C-N-CA	5.57	125.67	119.32
1	A	104	LEU	N-CA-C	-5.56	105.30	111.36
2	N	64	VAL	N-CA-CB	5.55	118.09	110.54
2	N	245	ARG	CB-CG-CD	5.55	124.06	111.30
1	D	380	ILE	CA-C-N	5.51	125.41	119.85
1	D	380	ILE	C-N-CA	5.51	125.41	119.85
2	P	705	GLY	N-CA-C	5.50	118.77	110.18
2	N	406	ARG	N-CA-C	5.49	119.98	113.28
2	P	352	LEU	N-CA-C	5.49	118.39	109.06
1	C	594	TRP	CA-CB-CG	5.49	124.03	113.60
1	A	126	GLU	N-CA-C	-5.49	105.30	111.28
2	M	651	TYR	N-CA-C	-5.48	105.41	111.71
2	O	54	GLY	N-CA-C	5.48	118.01	110.56
1	D	497	ALA	N-CA-C	5.48	117.59	108.99
2	P	85	ARG	CG-CD-NE	-5.47	99.97	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	314	THR	N-CA-C	-5.46	105.41	112.68
2	O	603	ALA	N-CA-C	5.46	117.52	108.13
2	P	316	ILE	N-CA-C	5.45	120.68	109.34
1	B	226	ASP	CA-C-N	-5.44	113.42	119.19
1	B	226	ASP	C-N-CA	-5.44	113.42	119.19
2	M	128	LEU	CA-C-N	-5.44	114.77	120.38
2	M	128	LEU	C-N-CA	-5.44	114.77	120.38
2	N	604	ILE	CB-CA-C	-5.43	103.10	111.08
1	A	420	ILE	N-CA-C	5.42	113.40	107.60
2	N	346	ARG	N-CA-C	-5.42	103.27	111.56
1	D	661	GLU	CB-CA-C	-5.41	102.39	110.88
1	D	253	ASP	N-CA-C	-5.40	105.48	111.36
2	M	151	TRP	CA-C-N	-5.40	112.62	120.29
2	M	151	TRP	C-N-CA	-5.40	112.62	120.29
1	A	194	ARG	NE-CZ-NH2	5.39	124.06	119.20
2	M	167	LYS	N-CA-C	-5.39	105.06	111.69
2	N	597	CYS	CA-CB-SG	-5.39	102.00	114.40
1	D	316	CYS	CB-CA-C	-5.39	109.37	115.79
1	C	517	GLU	CA-C-N	5.39	127.50	120.28
1	C	517	GLU	C-N-CA	5.39	127.50	120.28
1	C	211	SER	N-CA-C	-5.38	105.58	111.82
2	P	428	LEU	N-CA-C	5.37	117.38	108.20
2	N	166	SER	N-CA-C	5.36	117.54	111.11
2	O	604	ILE	N-CA-CB	5.35	117.11	110.05
2	P	722	ALA	N-CA-C	-5.33	105.64	111.82
1	B	343	THR	N-CA-C	-5.32	106.29	112.89
2	M	677	PHE	N-CA-C	-5.32	105.15	111.69
2	N	408	HIS	CA-C-N	5.32	127.72	120.54
2	N	408	HIS	C-N-CA	5.32	127.72	120.54
2	M	57	ASP	CB-CA-C	-5.31	104.74	111.86
1	A	433	LEU	N-CA-C	-5.31	105.61	111.71
1	C	317	CYS	N-CA-C	5.30	117.06	111.28
1	D	637	ASP	CA-C-N	5.30	125.11	119.28
1	D	637	ASP	C-N-CA	5.30	125.11	119.28
2	M	532	SER	N-CA-C	-5.30	102.35	110.14
1	D	539	ILE	N-CA-C	5.29	116.19	111.90
1	A	553	ASN	N-CA-C	-5.29	105.63	111.71
2	M	693	GLU	CA-C-N	-5.28	114.23	122.37
2	M	693	GLU	C-N-CA	-5.28	114.23	122.37
2	P	242	ASP	N-CA-C	5.28	117.45	111.11
1	B	588	ALA	N-CA-C	-5.27	105.59	112.23
2	N	400	GLU	N-CA-C	-5.24	105.48	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	397	ALA	N-CA-C	-5.23	106.20	112.59
2	M	237	ARG	N-CA-C	5.23	117.39	111.11
2	P	239	GLU	N-CA-C	-5.23	106.16	112.54
2	M	363	ASP	N-CA-C	5.23	117.81	110.23
1	C	188	THR	CA-C-N	-5.22	114.29	122.49
1	C	188	THR	C-N-CA	-5.22	114.29	122.49
2	M	726	ASP	CA-C-N	-5.22	114.24	120.13
2	M	726	ASP	C-N-CA	-5.22	114.24	120.13
1	D	279	VAL	CB-CA-C	-5.21	104.37	111.15
2	M	51	HIS	CA-C-N	-5.21	114.58	119.90
2	M	51	HIS	C-N-CA	-5.21	114.58	119.90
2	M	194	LEU	N-CA-C	5.21	117.04	111.36
1	B	453	ASN	N-CA-C	5.21	117.63	111.33
2	M	449	VAL	CB-CA-C	-5.21	105.03	111.70
2	P	465	VAL	N-CA-C	5.21	116.16	108.45
2	O	460	VAL	CA-C-N	5.20	127.67	120.29
2	O	460	VAL	C-N-CA	5.20	127.67	120.29
2	M	30	ILE	N-CA-C	-5.19	105.44	110.42
2	P	435	VAL	N-CA-C	-5.19	105.48	110.72
1	A	341	ILE	N-CA-C	-5.18	104.61	111.09
1	B	571	THR	CA-C-N	-5.18	114.74	119.82
1	B	571	THR	C-N-CA	-5.18	114.74	119.82
1	C	236	ARG	NE-CZ-NH2	-5.18	114.53	119.20
2	M	691	LEU	N-CA-C	-5.18	105.84	113.61
1	D	85	GLY	CA-C-N	-5.18	113.65	122.56
1	D	85	GLY	C-N-CA	-5.18	113.65	122.56
1	B	471	ASN	N-CA-C	-5.18	101.72	109.95
2	O	334	ARG	N-CA-C	5.17	118.05	109.46
2	P	292	PHE	CA-C-N	-5.17	113.51	122.10
2	P	292	PHE	C-N-CA	-5.17	113.51	122.10
1	C	91	GLY	N-CA-C	5.17	122.46	115.32
2	P	331	GLU	N-CA-C	-5.17	101.45	109.72
2	N	255	LEU	N-CA-C	5.16	117.90	109.59
2	N	152	THR	CA-C-N	-5.14	116.99	122.85
2	N	152	THR	C-N-CA	-5.14	116.99	122.85
2	P	367	GLU	N-CA-C	5.14	117.44	108.76
2	P	221	TYR	N-CA-C	-5.13	105.14	111.40
1	D	94	ALA	N-CA-C	-5.13	105.69	111.28
2	O	403	LEU	N-CA-C	-5.13	106.72	112.87
1	A	58	GLN	N-CA-C	-5.12	101.92	110.17
1	B	637	ASP	CA-C-N	5.12	125.16	119.32
1	B	637	ASP	C-N-CA	5.12	125.16	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	THR	N-CA-C	-5.12	105.78	111.36
1	B	415	ASN	N-CA-C	5.12	118.65	111.90
2	O	227	MET	N-CA-C	-5.12	106.20	112.90
1	D	595	TRP	N-CA-C	-5.10	105.61	111.07
2	M	166	SER	CB-CA-C	-5.10	102.32	110.79
2	O	341	GLU	N-CA-C	-5.10	102.23	110.14
2	P	666	ARG	N-CA-C	5.10	118.76	112.54
2	P	110	ALA	N-CA-C	-5.10	105.80	111.36
1	B	561	MET	N-CA-C	-5.09	105.81	112.23
1	A	603	HIS	CA-C-N	-5.09	116.33	123.10
1	A	603	HIS	C-N-CA	-5.09	116.33	123.10
1	D	154	VAL	CA-C-O	5.09	123.57	119.29
1	D	137	VAL	CB-CA-C	-5.09	106.41	111.80
1	A	608	PRO	N-CA-C	-5.09	104.49	110.70
1	C	544	VAL	CA-C-N	-5.08	116.23	122.84
1	C	544	VAL	C-N-CA	-5.08	116.23	122.84
2	O	158	ILE	CB-CA-C	5.08	117.60	110.99
2	P	594	SER	N-CA-C	5.06	117.56	109.81
2	P	60	TYR	N-CA-C	5.06	118.94	112.26
2	N	274	PHE	CA-C-N	-5.05	115.36	120.31
2	N	274	PHE	C-N-CA	-5.05	115.36	120.31
1	D	171	LEU	N-CA-C	-5.05	105.90	111.71
2	P	647	ILE	N-CA-C	5.05	117.28	108.90
1	D	345	ALA	N-CA-C	5.04	119.52	113.17
2	M	704	ILE	N-CA-C	5.04	116.14	111.81
1	B	539	ILE	CB-CA-C	5.03	119.54	111.29
2	N	422[A]	GLN	N-CA-C	-5.03	101.10	108.79
2	P	343	GLY	N-CA-C	5.02	120.24	112.81
1	C	334	PHE	N-CA-C	5.02	116.44	110.97
1	D	197	LYS	N-CA-C	-5.02	105.70	111.07
2	O	93	VAL	N-CA-CB	5.02	116.72	111.00
1	C	407	ALA	N-CA-C	-5.01	106.01	111.82
1	A	363	VAL	N-CA-C	-5.00	105.72	110.42
2	M	221	TYR	N-CA-C	-5.00	104.78	111.24
2	M	441	PHE	N-CA-C	5.00	118.16	111.75

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	SER	Peptide
1	B	469	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	415	ASN	Peptide
1	C	469	GLY	Peptide
1	D	469	GLY	Peptide
2	N	313	LEU	Peptide
2	P	315[A]	LYS	Peptide
2	P	389	ASP	Peptide

5.2 Too-close contacts [i](#)

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	5094	0	5088	124	0
1	B	5094	0	5082	142	0
1	C	5094	0	5086	144	0
1	D	5094	0	5093	162	0
2	M	5740	0	5693	116	0
2	N	5740	0	5695	136	0
2	O	5725	0	5680	329	0
2	P	5740	0	5693	259	0
3	A	16	0	0	0	0
3	B	8	0	0	1	0
3	C	16	0	0	0	0
3	D	8	0	0	0	0
3	M	8	0	0	0	0
3	N	8	0	0	0	0
3	O	8	0	0	5	0
3	P	8	0	0	1	0
4	A	9	0	0	2	0
4	B	9	0	0	3	0
4	C	9	0	0	4	0
4	D	9	0	0	1	0
5	A	7	0	0	11	0
5	B	7	0	0	12	0
5	C	7	0	0	7	0
5	D	7	0	0	6	0
5	M	3	0	0	2	0
5	N	4	0	0	5	0
5	O	3	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	4	0	0	4	0
6	A	24	0	32	5	0
6	B	18	0	24	5	0
6	C	12	0	16	1	0
6	D	12	0	16	7	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	1	0
7	P	1	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
9	A	168	0	0	5	0
9	B	220	0	0	13	0
9	C	130	0	0	14	0
9	D	105	0	0	12	0
9	M	201	0	0	9	0
9	N	222	0	0	20	0
9	O	27	0	0	5	0
9	P	80	0	0	8	0
All	All	44706	0	43198	1374	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 16.

All (1374) 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:B:114[A]:CYS:HB2	9:B:1217:HOH:O	1.29	1.28
2:O:373:ILE:HG22	2:O:440:ARG:HG3	1.28	1.09
2:P:602:MET:HE1	2:P:645:MET:HE2	1.32	1.09
1:B:148[A]:ARG:NH1	9:B:1185:HOH:O	1.78	1.08
1:D:114:CYS:HB2	9:D:1050:HOH:O	1.50	1.08
1:D:279:VAL:HG11	1:D:315:ILE:HD12	1.34	1.07
1:D:105:MET:CE	1:D:609:PRO:HD3	1.84	1.06
1:D:525:LYS:HE2	9:D:1094:HOH:O	1.57	1.04
1:D:105:MET:HE2	1:D:609:PRO:CD	1.93	0.99
1:A:577:VAL:HG21	1:A:645:ILE:HG23	1.41	0.98
2:O:144:PHE:O	2:O:148:MET:HG3	1.64	0.98
6:A:862:GOL:H31	2:M:259:ASP:HB3	1.44	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:698:LYS:HA	2:O:718:LYS:HG2	1.46	0.96
2:M:602:MET:HE2	2:M:647:ILE:HD13	1.48	0.96
2:O:670:MET:HG2	2:O:674:LEU:HD23	1.48	0.95
2:N:588:MET:HE1	2:N:604:ILE:HG23	1.48	0.95
1:C:587:LYS:H	1:D:220:HIS:HE1	1.13	0.95
1:D:105:MET:HE2	1:D:609:PRO:HD3	1.50	0.94
2:P:354:ARG:HH21	2:P:356:VAL:CG1	1.80	0.94
2:P:384:LEU:HA	2:P:468:PHE:O	1.66	0.94
2:N:722:ALA:HA	2:N:725:MET:HE3	1.50	0.93
2:O:363:ASP:HB2	2:O:462:ARG:HD2	1.52	0.92
1:D:279:VAL:HG11	1:D:315:ILE:CD1	2.00	0.91
1:B:577:VAL:HG21	1:B:645:ILE:HG23	1.53	0.90
1:B:110:ALA:O	1:B:114[A]:CYS:SG	2.30	0.89
2:O:334:ARG:HG3	9:O:1028:HOH:O	1.74	0.88
2:O:508:LEU:HB3	3:O:900:SF4:S1	2.14	0.88
2:P:490:ASP:C	2:P:492:MET:H	1.80	0.87
1:C:620:LEU:HD23	5:C:1004:XE:XE	2.52	0.87
7:O:950:CU1:CU	5:O:1009:XE:XE	2.02	0.87
1:A:114:CYS:HB2	9:A:1134:HOH:O	1.73	0.86
2:P:187:ASP:HA	2:P:211:ASN:HD22	1.39	0.86
2:P:588:MET:HE1	2:P:604:ILE:HD13	1.57	0.86
2:M:621:MET:HE1	2:M:625:GLY:HA2	1.55	0.86
2:O:407:ILE:HG23	2:O:408:HIS:H	1.40	0.86
1:D:335:ALA:H	1:D:471:ASN:HD22	1.19	0.85
2:N:163:ALA:H	2:N:192:GLN:HE22	1.25	0.85
1:C:114:CYS:HB2	9:C:1089:HOH:O	1.75	0.85
6:B:863:GOL:H32	2:N:27:HIS:CE1	2.12	0.85
1:A:105:MET:HE1	1:B:72:MET:HG3	1.59	0.85
1:C:126:GLU:OE1	1:C:390:THR:OG1	1.93	0.84
2:O:187:ASP:HA	2:O:211:ASN:HD22	1.40	0.84
2:O:373:ILE:HG22	2:O:440:ARG:CG	2.08	0.84
1:A:105:MET:HE1	1:B:72:MET:CG	2.08	0.83
1:B:400:ALA:HA	1:B:403:MET:CE	2.08	0.83
2:P:549:GLN:HG3	2:P:550:PRO:HD2	1.57	0.83
2:M:696:ILE:HA	2:M:699:ILE:HD12	1.61	0.82
1:D:102:VAL:HG13	5:D:1003[B]:XE:XE	2.57	0.82
2:M:621:MET:HE1	2:M:625:GLY:CA	2.10	0.82
2:P:95:ASN:C	2:P:95:ASN:HD22	1.86	0.82
1:D:105:MET:CE	1:D:609:PRO:CD	2.56	0.81
2:P:522:PRO:HD3	2:P:533:TRP:CD1	2.15	0.81
1:B:114[A]:CYS:SG	9:B:1161:HOH:O	2.38	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:CYS:SG	1:C:209:HIS:CD2	2.73	0.81
2:P:602:MET:HE1	2:P:645:MET:CE	2.10	0.80
2:O:371:PRO:HD2	2:O:469:THR:HB	1.63	0.79
2:O:468:PHE:HB2	2:O:474:VAL:HG23	1.63	0.79
1:C:620:LEU:HD21	5:C:1003[A]:XE:XE	2.61	0.79
1:D:470:CYS:HB3	4:D:800:XCC:S2	2.23	0.79
1:C:102:VAL:CG1	5:C:1003[B]:XE:XE	3.09	0.79
2:O:373:ILE:CG2	2:O:440:ARG:HG3	2.12	0.78
2:O:411:ILE:HD13	2:O:428:LEU:HD21	1.64	0.78
2:P:343:GLY:HA3	2:P:349:ALA:HB3	1.66	0.78
1:D:559:LEU:HG	1:D:563:MET:HE3	1.64	0.78
2:O:612:MET:SD	2:O:624:SER:HB3	2.24	0.78
1:C:411:ARG:HG3	1:C:416:ARG:HD3	1.64	0.78
2:M:451:LYS:NZ	2:M:454:GLU:OE1	2.14	0.77
2:O:396:GLN:HB2	2:O:399:PHE:CE2	2.18	0.77
1:C:114:CYS:SG	1:C:209:HIS:NE2	2.58	0.77
2:P:588:MET:CE	2:P:604:ILE:HD13	2.15	0.77
1:D:614:ASP:N	6:D:863:GOL:H11	2.00	0.77
2:M:163:ALA:H	2:M:192:GLN:HE22	1.33	0.76
1:C:563:MET:CE	1:C:576:PHE:HD2	1.97	0.76
2:N:187:ASP:HA	2:N:211:ASN:HD22	1.50	0.76
2:O:6:LYS:HA	2:O:9:GLU:HG3	1.67	0.76
1:A:335:ALA:H	1:A:471:ASN:HD22	1.31	0.76
1:B:580:ALA:HB2	5:B:1001:XE:XE	2.62	0.76
2:P:602:MET:HE3	2:P:645:MET:HB3	1.68	0.76
1:A:294:ALA:O	1:A:298:MET:HG3	1.86	0.75
2:P:156:GLU:HG2	5:P:1008:XE:XE	2.64	0.75
1:A:622:GLN:HB3	6:A:862:GOL:H11	1.67	0.75
2:M:640:GLN:HB2	9:M:1157:HOH:O	1.85	0.75
2:P:525:VAL:HG11	2:P:650:THR:CG2	2.15	0.75
1:C:470:CYS:HB3	4:C:800:XCC:S2	2.27	0.75
2:P:572:TYR:CE2	2:P:577:ARG:HG2	2.22	0.75
2:O:407:ILE:CG2	2:O:408:HIS:H	1.98	0.74
2:O:14:GLU:HA	9:O:1027:HOH:O	1.86	0.74
2:O:333:ILE:HG21	2:O:429:ARG:HB3	1.69	0.74
2:P:555:GLY:HA3	2:P:565:LYS:HB3	1.69	0.74
2:O:406:ARG:O	2:O:410:PHE:CD2	2.41	0.74
1:A:577:VAL:HG21	1:A:645:ILE:CG2	2.18	0.74
1:D:280:LEU:HD13	1:D:288:SER:HB2	1.69	0.74
1:C:105:MET:HE1	1:C:609:PRO:HD3	1.68	0.73
1:D:302:ALA:O	1:D:307:ALA:HB3	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:VAL:CG1	1:D:315:ILE:HD12	2.16	0.73
1:D:460:GLU:OE1	1:D:530:ARG:NH2	2.22	0.73
2:P:381:LYS:O	2:P:382:LEU:HD13	1.87	0.73
1:D:525:LYS:CE	9:D:1094:HOH:O	2.25	0.73
2:N:588:MET:HE3	2:N:728:ILE:HG12	1.70	0.73
2:P:568:ASN:HD21	2:P:581:GLN:HG3	1.52	0.73
1:B:400:ALA:HA	1:B:403:MET:HE3	1.69	0.73
1:A:68:CYS:HB2	1:A:97:ILE:HG23	1.71	0.73
1:A:33:VAL:HG21	1:A:477:GLN:HE22	1.54	0.72
2:M:344:GLY:O	2:M:345:ASN:HB2	1.88	0.72
2:O:469:THR:O	2:O:470:ASP:HB2	1.88	0.72
1:C:51:ARG:HD3	9:C:1137:HOH:O	1.89	0.72
2:M:3:ASP:CG	9:M:1198:HOH:O	2.32	0.72
2:O:418:TRP:O	2:O:428:LEU:HA	1.90	0.72
2:P:163:ALA:H	2:P:192:GLN:HE22	1.38	0.72
2:M:189:ALA:HA	2:M:192:GLN:HE21	1.53	0.72
1:D:32:ALA:HB1	1:D:268:MET:HG3	1.72	0.72
2:N:229:PHE:CD1	5:N:1009:XE:XE	3.21	0.71
2:O:407:ILE:HG23	2:O:408:HIS:N	2.05	0.71
2:P:95:ASN:ND2	2:P:98:ASN:H	1.87	0.71
1:D:114:CYS:SG	1:D:209:HIS:CD2	2.83	0.71
2:P:354:ARG:HH21	2:P:356:VAL:HG13	1.54	0.71
1:D:614:ASP:H	6:D:863:GOL:H11	1.55	0.71
1:C:102:VAL:HG13	5:C:1003[B]:XE:XE	2.69	0.71
2:O:361:ILE:HD13	2:O:391:TYR:HB2	1.73	0.71
2:P:383:PRO:HB2	2:P:474:VAL:HG21	1.73	0.71
2:P:560:ILE:O	2:P:660:ALA:HB2	1.90	0.71
1:B:77:ARG:HD3	9:B:1199:HOH:O	1.90	0.71
1:C:620:LEU:CD2	5:C:1004:XE:XE	3.17	0.70
2:M:408:HIS:HD2	2:M:419:HIS:ND1	1.90	0.70
2:O:181:PHE:HE2	2:O:306:MET:HE3	1.56	0.70
2:P:568:ASN:ND2	2:P:581:GLN:HA	2.07	0.70
2:N:150:ASP:OD1	2:N:152:THR:HG23	1.92	0.70
2:O:341:GLU:OE2	2:O:343:GLY:N	2.22	0.70
2:O:346:ARG:HB2	2:O:346:ARG:HH11	1.56	0.70
2:O:429:ARG:N	9:O:1018:HOH:O	2.25	0.70
1:D:364:ALA:HB1	1:D:369:THR:HB	1.74	0.70
2:O:62:LEU:HD12	2:O:65:ILE:HD12	1.72	0.70
2:O:580:GLU:O	2:O:581:GLN:HB2	1.90	0.70
1:C:577:VAL:HG21	1:C:645:ILE:HG23	1.73	0.69
2:M:150:ASP:OD1	2:M:152:THR:HG23	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ARG:HD2	1:C:418:VAL:HG23	1.74	0.69
2:N:588:MET:CE	2:N:728:ILE:HG12	2.21	0.69
2:P:150:ASP:OD1	2:P:152:THR:HG23	1.92	0.69
1:C:283:HIS:CD2	1:C:317:CYS:HB2	2.26	0.69
1:D:102:VAL:CG1	5:D:1003[B]:XE:XE	3.19	0.69
1:D:65:GLY:HA2	9:D:1089:HOH:O	1.92	0.69
2:N:588:MET:HE1	2:N:604:ILE:CG2	2.22	0.69
2:N:261:VAL:HG12	5:N:1006:XE:XE	2.70	0.69
1:A:24:ASN:O	1:A:27:ARG:HG2	1.93	0.69
1:B:470:CYS:HB3	4:B:800:XCC:S2	2.32	0.69
2:O:252:VAL:HB	2:O:276:VAL:HG22	1.74	0.69
2:O:509:CYS:SG	2:O:595:CYS:SG	2.91	0.69
1:C:482:LEU:HD13	1:C:486:LYS:HD2	1.75	0.69
1:B:577:VAL:HG21	1:B:645:ILE:CG2	2.23	0.68
2:P:490:ASP:C	2:P:492:MET:N	2.50	0.68
1:B:416:ARG:HG3	1:B:416:ARG:HH11	1.56	0.68
1:C:78:ILE:HD11	1:C:97:ILE:HD12	1.75	0.68
2:M:415:GLU:OE1	9:M:1206:HOH:O	2.11	0.68
2:O:491:ARG:HB2	2:O:491:ARG:HH11	1.58	0.68
2:O:675:LYS:HA	2:O:696:ILE:HD11	1.75	0.68
2:P:342:MET:HG3	2:P:384:LEU:HD22	1.75	0.68
1:A:2:PRO:N	6:A:862:GOL:HO1	1.92	0.67
2:M:445:GLY:HA2	2:M:465:VAL:HG11	1.76	0.67
1:C:12:ARG:O	6:C:861:GOL:H12	1.94	0.67
1:C:550:CYS:SG	4:C:800:XCC:NI	1.79	0.67
2:O:649:ARG:O	2:O:652:ILE:HD12	1.94	0.67
2:O:96:PHE:O	2:O:100:ARG:HG3	1.95	0.67
2:P:474:VAL:CG1	2:P:475:LYS:N	2.58	0.67
1:B:510:LEU:N	1:B:510:LEU:HD12	2.08	0.67
2:M:373:ILE:CG2	2:M:440:ARG:HD3	2.25	0.66
1:B:63:TYR:OH	9:B:1210:HOH:O	2.13	0.66
2:P:338:MET:SD	2:P:341:GLU:HB2	2.35	0.66
1:A:280:LEU:HD13	1:A:288:SER:HB2	1.77	0.66
1:B:468:CYS:SG	5:B:1001:XE:XE	3.32	0.66
2:N:354:ARG:HD2	2:N:389:ASP:OD1	1.95	0.66
2:O:63:PRO:HB2	2:O:220:ASN:HB2	1.78	0.66
2:O:488:ARG:C	2:O:490:ASP:H	2.02	0.66
2:P:143:ARG:O	2:P:146[A]:ILE:HD13	1.95	0.66
2:P:602:MET:CE	2:P:645:MET:HE2	2.19	0.66
1:A:105:MET:CE	1:B:72:MET:HG3	2.25	0.66
1:C:159:VAL:HG13	9:C:1052:HOH:O	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:516:HIS:CD2	2:O:593:THR:OG1	2.49	0.66
1:C:217:ASN:ND2	1:D:112:ALA:HA	2.10	0.66
1:C:563:MET:HE2	1:C:576:PHE:HD2	1.61	0.66
1:D:470:CYS:O	1:D:582:GLU:HB2	1.94	0.66
2:O:649:ARG:HA	2:O:652:ILE:CD1	2.26	0.66
2:N:315:LYS:HD3	9:N:1162:HOH:O	1.95	0.65
2:O:524:ARG:NH1	2:O:645:MET:HE3	2.11	0.65
2:P:474:VAL:CG1	2:P:475:LYS:H	2.10	0.65
2:P:316:ILE:HG23	2:P:316:ILE:O	1.96	0.65
1:B:400:ALA:HB2	5:B:1010:XE:XE	2.75	0.65
1:C:442:THR:HG21	1:C:537:ILE:HD11	1.79	0.65
2:M:428:LEU:N	2:M:428:LEU:HD12	2.11	0.65
2:P:387:LEU:O	2:P:465:VAL:HA	1.96	0.65
1:C:587:LYS:H	1:D:220:HIS:CE1	2.05	0.65
2:O:556:GLU:HG2	2:O:557:ILE:N	2.12	0.65
1:B:372:ILE:HD13	1:B:403:MET:HE3	1.77	0.65
2:M:617:ASP:HB2	9:M:1199:HOH:O	1.97	0.65
2:M:15:GLY:O	2:M:16:LYS:HD3	1.97	0.65
2:N:722:ALA:HA	2:N:725:MET:CE	2.26	0.65
2:O:374:ASP:HB2	2:O:440:ARG:HE	1.62	0.65
2:O:316:ILE:HG23	2:O:316:ILE:O	1.96	0.65
2:P:189:ALA:HA	2:P:192:GLN:HE21	1.62	0.65
1:C:2:PRO:N	1:C:625:SER:HG	1.95	0.64
1:D:105:MET:HE2	1:D:609:PRO:CG	2.28	0.64
1:A:102:VAL:CG1	5:A:1003[B]:XE:XE	3.24	0.64
1:A:220:HIS:HE1	1:B:587:LYS:H	1.43	0.64
2:N:146:ILE:O	2:N:146:ILE:HG13	1.96	0.64
2:O:568:ASN:ND2	2:O:581:GLN:HG2	2.12	0.64
2:O:346:ARG:HB2	2:O:346:ARG:NH1	2.12	0.64
2:O:181:PHE:CE2	2:O:306:MET:HE3	2.33	0.64
2:P:489:ASP:HA	2:P:492:MET:HB2	1.79	0.64
1:B:287:LEU:CD1	1:B:388:TYR:CE1	2.81	0.64
1:C:640:VAL:HG12	1:C:644:LYS:HE3	1.80	0.64
2:O:351:GLU:HA	2:O:386:ILE:HB	1.79	0.64
1:B:316:CYS:H	1:B:503:GLN:HE22	1.45	0.64
2:O:556:GLU:HG2	2:O:557:ILE:H	1.63	0.64
2:O:580:GLU:O	2:O:581:GLN:CB	2.46	0.64
2:O:334:ARG:HH11	2:O:335:LYS:HG3	1.63	0.63
2:P:588:MET:HE1	2:P:604:ILE:CD1	2.27	0.63
2:O:2:THR:HA	2:O:5:ASP:HB2	1.81	0.63
1:C:30:ASP:OD2	1:C:507:LYS:NZ	2.30	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:CYS:HA	1:D:503:GLN:HG3	1.79	0.63
2:P:666:ARG:HD2	2:P:728:ILE:HD13	1.80	0.63
1:A:357:MET:HG2	1:B:90:CYS:O	1.98	0.63
1:C:335:ALA:H	1:C:471:ASN:HD22	1.45	0.63
1:D:416:ARG:HB2	1:D:418:VAL:HG23	1.80	0.63
2:M:95:ASN:ND2	2:M:98:ASN:H	1.95	0.63
2:O:157:ALA:HB3	2:O:183:LEU:CD2	2.29	0.63
2:P:95:ASN:HD21	2:P:98:ASN:H	1.46	0.63
2:P:522:PRO:HD3	2:P:533:TRP:CG	2.34	0.63
2:O:584:LEU:HD23	2:O:592:MET:HE1	1.80	0.63
1:A:15:GLU:OE2	6:A:861:GOL:H12	1.99	0.63
2:P:474:VAL:HG13	2:P:475:LYS:N	2.14	0.62
1:C:316:CYS:H	1:C:503:GLN:HE22	1.47	0.62
1:D:18:ARG:CD	1:D:636:MET:HE3	2.30	0.62
1:C:615:LEU:O	1:C:615:LEU:HD23	1.99	0.62
1:D:658:VAL:O	1:D:662:VAL:HG23	1.99	0.62
2:M:498:GLU:OE2	2:M:656:LYS:NZ	2.27	0.62
2:O:556:GLU:HA	2:O:564:TRP:CD1	2.35	0.62
2:N:396:GLN:NE2	9:N:1215:HOH:O	2.30	0.62
2:O:384:LEU:HD12	2:O:385:GLY:H	1.65	0.62
6:B:863:GOL:H32	2:N:27:HIS:HE1	1.62	0.62
2:O:556:GLU:HA	2:O:564:TRP:HD1	1.63	0.62
1:B:281:HIS:HB3	1:B:351:VAL:HG12	1.82	0.62
2:O:149:VAL:HG11	2:O:509:CYS:HA	1.81	0.62
2:O:333:ILE:HG21	2:O:429:ARG:CB	2.30	0.62
2:P:605:LEU:HD21	2:P:623:PRO:HB2	1.80	0.62
1:B:335:ALA:H	1:B:471:ASN:HD22	1.46	0.62
2:O:346:ARG:HG3	2:O:381:LYS:NZ	2.15	0.62
1:C:11:CYS:HB2	1:C:621:THR:HB	1.83	0.61
1:D:182:GLU:HG2	1:D:204:VAL:HG11	1.82	0.61
1:C:12:ARG:HD3	9:C:1107:HOH:O	1.99	0.61
2:M:587:LEU:HD23	2:M:588:MET:HE2	1.82	0.61
2:N:373:ILE:HD12	2:N:441:PHE:CZ	2.35	0.61
2:O:221:TYR:CA	2:O:224:ARG:HH21	2.13	0.61
2:O:431:SER:O	2:O:434:ALA:N	2.24	0.61
1:A:7:LEU:HD11	2:M:164:LYS:HB2	1.83	0.61
2:P:187:ASP:HA	2:P:211:ASN:ND2	2.15	0.61
2:N:156:GLU:HG3	2:N:182:MET:HB3	1.82	0.61
2:O:221:TYR:HA	2:O:224:ARG:HH21	1.66	0.61
2:P:174:LYS:HE2	2:P:323:ASN:OD1	2.00	0.61
1:B:102:VAL:HG13	5:B:1003[B]:XE:XE	2.79	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ASP:OD2	1:D:275:GLN:NE2	2.33	0.61
2:O:468:PHE:CB	2:O:474:VAL:HG23	2.31	0.61
2:P:164:LYS:NZ	9:P:1089:HOH:O	2.34	0.61
2:N:728:ILE:O	2:N:729:MET:HB2	1.98	0.61
2:P:611:ILE:O	2:P:611:ILE:HG13	2.01	0.61
2:M:657:PHE:O	2:M:658:ILE:C	2.44	0.60
2:N:300:LYS:HD2	9:N:1202:HOH:O	2.01	0.60
2:O:698:LYS:HA	2:O:718:LYS:CG	2.27	0.60
1:A:559:LEU:HG	1:A:563:MET:CE	2.31	0.60
2:P:681:GLU:HG3	2:P:684:ARG:HH21	1.64	0.60
1:B:220:HIS:HD2	1:B:221:MET:O	1.85	0.60
1:C:273:PRO:HD3	1:C:420:ILE:HD12	1.83	0.60
2:M:585:TYR:CZ	2:M:656:LYS:HE3	2.36	0.60
2:P:354:ARG:NH2	2:P:356:VAL:CG1	2.59	0.60
1:B:287:LEU:HD13	1:B:388:TYR:CE1	2.37	0.60
2:O:334:ARG:HH11	2:O:335:LYS:CG	2.14	0.60
2:O:549:GLN:HB3	2:O:550:PRO:HD2	1.83	0.60
2:O:560:ILE:O	2:O:660:ALA:HB2	2.01	0.60
2:P:342:MET:CG	2:P:384:LEU:HD22	2.31	0.60
1:B:114[A]:CYS:CB	9:B:1161:HOH:O	2.50	0.60
2:O:623:PRO:HB3	2:O:707:THR:C	2.25	0.60
2:P:672:LYS:HE3	2:P:676:ASP:OD2	2.01	0.60
1:C:7:LEU:HD11	2:O:164:LYS:HB2	1.84	0.60
2:M:587:LEU:HD23	2:M:588:MET:CE	2.32	0.60
2:O:346:ARG:HG3	2:O:381:LYS:HZ3	1.67	0.60
1:A:18:ARG:NE	1:A:636:MET:HE3	2.17	0.60
1:A:602:THR:CG2	5:A:1001:XE:XE	3.28	0.60
1:B:114[A]:CYS:HB3	9:B:1161:HOH:O	2.01	0.60
1:B:325:ARG:HD2	9:B:1067:HOH:O	2.02	0.60
2:N:124:ASP:OD2	2:N:125:GLU:HB2	2.02	0.60
2:N:163:ALA:N	2:N:192:GLN:HE22	1.96	0.60
1:A:112:ALA:HA	1:B:217:ASN:HD22	1.67	0.59
2:O:175:GLU:HG2	2:O:179:MET:HE2	1.83	0.59
2:P:523:GLU:O	2:P:654:SER:OG	2.17	0.59
1:A:102:VAL:HG13	5:A:1003[B]:XE:XE	2.80	0.59
1:B:400:ALA:HA	1:B:403:MET:HE2	1.81	0.59
1:D:114:CYS:SG	1:D:209:HIS:NE2	2.74	0.59
1:D:281:HIS:HB3	1:D:351:VAL:HG12	1.84	0.59
2:M:424:ASN:HD22	2:M:424:ASN:H	1.48	0.59
2:P:391:TYR:HD2	2:P:462:ARG:NH1	2.00	0.59
1:A:615:LEU:C	1:A:615:LEU:HD23	2.27	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ALA:O	1:C:298:MET:HG2	2.00	0.59
2:O:221:TYR:HA	2:O:224:ARG:NH2	2.18	0.59
2:O:429:ARG:HG3	9:O:1018:HOH:O	2.02	0.59
2:P:389:ASP:O	2:P:463:VAL:HA	2.01	0.59
2:P:525:VAL:HG11	2:P:650:THR:HG23	1.83	0.59
2:N:602:MET:HE2	2:N:647:ILE:HD13	1.82	0.59
2:O:407:ILE:CG2	2:O:408:HIS:N	2.65	0.59
1:B:466:LEU:HD22	1:B:595:TRP:CZ2	2.37	0.59
1:C:114:CYS:CB	9:C:1089:HOH:O	2.43	0.59
2:O:60:TYR:HE2	2:O:228:MET:HE3	1.68	0.59
1:C:384:TYR:HD1	1:C:384:TYR:H	1.51	0.59
1:D:36:MET:HE1	1:D:343:THR:HA	1.84	0.59
2:N:718:LYS:HD2	9:N:1200:HOH:O	2.03	0.59
2:M:602:MET:CE	2:M:647:ILE:HG21	2.33	0.59
2:O:170:ALA:O	2:O:174:LYS:HB2	2.02	0.59
2:P:720:HIS:O	2:P:723:LEU:HB2	2.03	0.59
1:B:641:ALA:O	1:B:645:ILE:HG13	2.02	0.58
2:O:250:ALA:H	2:O:309:ARG:HE	1.50	0.58
2:O:698:LYS:CA	2:O:718:LYS:HG2	2.29	0.58
2:P:484:LYS:HA	2:P:487:GLU:HG3	1.84	0.58
2:P:565:LYS:HD2	2:P:569:ASP:OD1	2.03	0.58
1:D:472:ASN:O	1:D:474:LYS:N	2.36	0.58
2:O:516:HIS:HD2	2:O:593:THR:OG1	1.85	0.58
1:D:235:ILE:HG23	1:D:597:SER:OG	2.03	0.58
2:P:344:GLY:O	2:P:346:ARG:NH2	2.36	0.58
2:P:537:LYS:HD3	2:P:541:GLU:OE2	2.03	0.58
1:B:102:VAL:CG1	5:B:1003[B]:XE:XE	3.29	0.58
1:C:280:LEU:HD13	1:C:288:SER:HB2	1.86	0.58
2:M:338:MET:SD	2:M:341:GLU:HB2	2.44	0.58
2:M:342:MET:HG3	2:M:384:LEU:HD22	1.86	0.58
2:M:354:ARG:HD2	2:M:389:ASP:OD1	2.04	0.58
2:M:372:ASP:OD1	2:M:373:ILE:N	2.32	0.58
2:N:261:VAL:CG1	5:N:1006:XE:XE	3.30	0.58
2:O:508:LEU:HD23	3:O:900:SF4:S1	2.43	0.58
2:P:144:PHE:O	2:P:148:MET:HG3	2.02	0.58
1:C:563:MET:HE1	1:C:576:PHE:HD2	1.66	0.58
1:A:278:PHE:HB3	1:A:312:LEU:HD23	1.84	0.58
1:A:283:HIS:CD2	1:A:317:CYS:HB2	2.38	0.58
2:M:315:LYS:HB2	9:M:1182:HOH:O	2.02	0.58
2:O:506:CYS:SG	2:O:508:LEU:HB2	2.42	0.58
2:O:525:VAL:HG13	2:O:531:VAL:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:602:MET:CE	2:P:645:MET:HB3	2.34	0.58
2:M:357:SER:OG	2:M:360:GLU:HG2	2.04	0.58
2:O:433:ASP:O	2:O:437:LYS:HG3	2.04	0.58
2:P:295:VAL:O	2:P:295:VAL:HG12	2.03	0.58
2:P:391:TYR:HA	2:P:395:MET:HG2	1.83	0.58
2:O:405:ARG:HH22	2:O:532:SER:HB3	1.67	0.58
1:C:573:LYS:HE2	1:C:671:CYS:O	2.04	0.57
6:D:863:GOL:H12	2:P:27:HIS:CE1	2.39	0.57
2:O:156:GLU:HG3	2:O:182:MET:HB3	1.85	0.57
1:D:525:LYS:NZ	9:D:1094:HOH:O	2.33	0.57
2:M:164:LYS:HD2	2:M:298:TYR:CE1	2.39	0.57
1:A:414:SER:O	1:A:415:ASN:C	2.47	0.57
2:P:369:ILE:HG22	2:P:370:GLY:H	1.69	0.57
1:A:114:CYS:SG	1:A:209:HIS:NE2	2.77	0.57
1:C:601:PRO:HD3	1:C:652:ARG:CZ	2.34	0.57
2:O:3:ASP:O	2:O:6:LYS:HG2	2.04	0.57
2:O:461:ASP:O	2:O:462:ARG:HG2	2.04	0.57
2:P:391:TYR:HD2	2:P:462:ARG:HH12	1.51	0.57
2:M:716:GLU:HG3	2:M:723:LEU:CD1	2.35	0.57
2:N:350:PHE:CD1	2:N:350:PHE:C	2.83	0.57
2:N:457:PRO:O	2:N:458:ALA:HB3	2.03	0.57
1:B:19:VAL:HG22	1:B:474:LYS:HG2	1.87	0.57
2:O:396:GLN:H	2:O:399:PHE:HD2	1.51	0.57
2:P:479:GLU:O	2:P:481:ALA:N	2.37	0.57
1:D:530:ARG:HG3	1:D:530:ARG:HH11	1.69	0.57
2:N:45:ARG:HD2	9:N:1216:HOH:O	2.03	0.57
2:O:316:ILE:HG22	2:O:454:GLU:OE1	2.04	0.57
1:D:98:VAL:HG21	1:D:613:SER:HB3	1.87	0.57
1:D:577:VAL:HG21	1:D:645:ILE:HG23	1.86	0.56
2:P:459:ILE:HG22	2:P:460:VAL:HG23	1.87	0.56
1:A:602:THR:HG23	5:A:1001:XE:XE	2.83	0.56
2:O:389:ASP:HB2	2:O:464:GLN:HB3	1.87	0.56
2:P:352:LEU:CD1	2:P:353:VAL:O	2.54	0.56
2:P:488:ARG:C	2:P:490:ASP:H	2.13	0.56
1:A:114:CYS:SG	1:A:209:HIS:CD2	2.98	0.56
1:B:274:ASP:OD1	1:B:412:LYS:NZ	2.38	0.56
1:C:126:GLU:HG3	1:C:131:LYS:HB2	1.87	0.56
2:M:261:VAL:HG12	5:M:1006:XE:XE	2.83	0.56
2:N:21:LEU:HB2	2:N:286:LYS:HA	1.87	0.56
2:P:352:LEU:HD11	2:P:353:VAL:O	2.05	0.56
2:P:369:ILE:CG2	2:P:370:GLY:N	2.68	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:626:MET:HB3	2:P:630:THR:HB	1.88	0.56
1:A:313:VAL:HB	1:A:331:VAL:HG22	1.88	0.56
1:B:15:GLU:HA	6:B:861:GOL:H12	1.88	0.56
1:D:149:ARG:NH2	1:D:250:ASP:OD2	2.38	0.56
1:D:357:MET:O	1:D:360:ILE:HG12	2.05	0.56
2:M:420:THR:HG22	2:M:427:TRP:HB3	1.88	0.56
2:P:478:MET:HE3	2:P:482:ARG:HH21	1.71	0.56
2:O:352:LEU:HD23	2:O:353:VAL:O	2.06	0.56
2:O:408:HIS:HA	2:O:419:HIS:ND1	2.21	0.56
2:O:510:GLN:O	2:O:514:PRO:HA	2.04	0.56
2:O:594:SER:HB3	2:O:598:PHE:HD2	1.70	0.56
2:P:318:LEU:HD22	2:P:320:LEU:HG	1.86	0.56
1:A:213:SER:OG	1:B:209:HIS:HD2	1.89	0.56
1:C:217:ASN:HD22	1:D:112:ALA:HA	1.70	0.56
1:D:303:LYS:HA	1:D:307:ALA:O	2.06	0.56
2:O:359:SER:O	2:O:360:GLU:HB2	2.06	0.56
2:O:376:ILE:HG12	2:O:382:LEU:HD21	1.86	0.56
2:O:449:VAL:O	2:O:449:VAL:HG12	2.05	0.56
2:O:180:GLY:HA2	2:O:326:PRO:HG2	1.88	0.56
2:P:347:THR:OG1	2:P:383:PRO:HA	2.06	0.56
1:B:190:ILE:HG13	1:B:195:LYS:HG3	1.86	0.56
1:B:235:ILE:HD11	5:B:1004:XE:XE	2.84	0.56
1:B:334:PHE:O	1:B:337:GLN:HG2	2.06	0.56
2:O:66:ARG:HG3	2:O:234:PRO:HB3	1.86	0.56
2:P:474:VAL:HG12	2:P:475:LYS:H	1.71	0.56
1:D:220:HIS:HD2	1:D:221:MET:O	1.89	0.56
2:M:357:SER:OG	2:M:360:GLU:CG	2.54	0.56
2:O:478:MET:HG3	2:O:482:ARG:HH21	1.71	0.56
2:M:17:GLU:HG2	9:M:1179:HOH:O	2.05	0.56
2:O:524:ARG:HH12	2:O:645:MET:HE3	1.71	0.56
2:O:564:TRP:HB2	2:O:567:VAL:HB	1.88	0.56
2:P:390:ILE:CG1	2:P:460:VAL:HG13	2.36	0.55
1:A:2:PRO:N	1:A:625:SER:HG	2.04	0.55
1:B:298:MET:CE	1:B:301:GLU:OE2	2.54	0.55
2:N:373:ILE:HG12	2:N:435:VAL:HG22	1.88	0.55
2:N:486:LYS:HG2	9:N:1156:HOH:O	2.05	0.55
2:O:515:ASN:OD1	2:O:576:ASN:HB2	2.06	0.55
2:O:522:PRO:HD3	2:O:533:TRP:CD1	2.41	0.55
2:P:24:GLU:CD	9:P:1085:HOH:O	2.50	0.55
2:P:343:GLY:HA2	2:P:347:THR:O	2.06	0.55
2:P:605:LEU:HD22	2:P:612:MET:HG2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:HIS:HD2	1:D:213:SER:OG	1.89	0.55
2:M:108:TYR:O	2:M:112:ILE:HG13	2.06	0.55
2:N:341:GLU:HG3	2:N:429:ARG:HG2	1.89	0.55
2:P:369:ILE:CG2	2:P:370:GLY:H	2.20	0.55
1:A:620:LEU:CD2	5:A:1004:XE:XE	3.33	0.55
1:D:504:ALA:O	1:D:505:ALA:C	2.50	0.55
2:N:150:ASP:OD1	2:N:152:THR:CG2	2.55	0.55
2:O:254:TYR:CZ	2:O:258:HIS:CD2	2.94	0.55
2:P:390:ILE:HG13	2:P:460:VAL:HG13	1.89	0.55
2:P:479:GLU:C	2:P:481:ALA:N	2.64	0.55
2:P:484:LYS:HA	2:P:487:GLU:CG	2.36	0.55
1:B:118:ASN:C	1:B:118:ASN:HD22	2.15	0.55
1:B:480:SER:HA	1:B:638:PRO:HB3	1.88	0.55
2:N:505:SER:HB3	2:N:551:ILE:HD11	1.87	0.55
2:O:472:ALA:O	2:O:476:GLU:HB2	2.07	0.55
1:B:283:HIS:NE2	1:B:587:LYS:NZ	2.55	0.55
2:O:418:TRP:HZ3	2:O:429:ARG:NE	2.05	0.55
1:C:281:HIS:HB3	1:C:351:VAL:HG12	1.89	0.55
2:M:95:ASN:HD22	2:M:95:ASN:C	2.15	0.55
2:P:254:TYR:O	2:P:278:THR:HA	2.07	0.55
2:P:373:ILE:HG13	2:P:441:PHE:CZ	2.42	0.55
1:A:142:LYS:HD3	1:A:253:ASP:HB3	1.89	0.55
1:A:368:HIS:HB2	9:A:1141:HOH:O	2.06	0.55
2:M:602:MET:HE3	2:M:647:ILE:HG21	1.89	0.55
2:N:95:ASN:ND2	2:N:98:ASN:H	2.05	0.55
2:O:670:MET:O	2:O:701:ASP:HB3	2.07	0.55
1:A:112:ALA:HA	1:B:217:ASN:ND2	2.22	0.54
1:D:470:CYS:N	9:D:1085:HOH:O	2.39	0.54
1:B:394:ILE:O	1:B:398:LYS:HG3	2.07	0.54
1:C:122:HIS:HD2	9:C:1127:HOH:O	1.88	0.54
2:M:615:THR:HG21	2:M:674:LEU:HG	1.89	0.54
2:P:21:LEU:HB2	2:P:286:LYS:HA	1.89	0.54
2:O:51:HIS:HB3	2:O:76:LEU:HD12	1.89	0.54
2:O:525:VAL:HG22	2:O:532:SER:HA	1.90	0.54
2:P:338:MET:CE	2:P:341:GLU:HB2	2.37	0.54
1:D:620:LEU:HD21	5:D:1003[A]:XE:XE	2.85	0.54
2:N:568:ASN:HD21	2:N:581:GLN:HE21	1.55	0.54
2:N:605:LEU:HD11	2:N:612:MET:HB3	1.89	0.54
2:M:426:ASN:C	2:M:426:ASN:HD22	2.16	0.54
1:C:587:LYS:N	1:D:220:HIS:HE1	1.94	0.54
1:D:208:ILE:HG21	9:D:1050:HOH:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ASN:N	1:D:330:LEU:O	2.41	0.54
2:O:593:THR:HB	2:O:638:GLY:HA2	1.89	0.54
1:A:72:MET:HG3	1:B:105:MET:CE	2.37	0.54
2:O:113:ILE:O	2:O:116:LEU:HB2	2.07	0.54
1:D:281:HIS:O	1:D:351:VAL:HA	2.07	0.54
2:M:424:ASN:HD22	2:M:424:ASN:N	2.04	0.54
2:O:283:PRO:HD2	2:O:286:LYS:HB2	1.90	0.54
2:O:402:VAL:C	2:O:404:GLU:N	2.65	0.54
2:P:275:PRO:HD2	2:P:309:ARG:HD3	1.89	0.54
2:P:319:ASP:O	2:P:320:LEU:HB2	2.07	0.54
2:P:479:GLU:C	2:P:481:ALA:H	2.16	0.54
2:P:717:GLU:O	2:P:717:GLU:HG2	2.07	0.54
1:C:215:LEU:HD13	1:C:233:SER:HB3	1.89	0.54
1:D:432:SER:HA	1:D:555:ARG:HD3	1.90	0.54
2:M:169:LEU:HD13	2:M:193:LEU:HG	1.90	0.54
2:N:583:CYS:HB3	2:N:586:THR:HG22	1.89	0.54
2:M:163:ALA:HB2	2:M:169:LEU:HG	1.90	0.54
2:N:221:TYR:CD1	2:N:221:TYR:C	2.86	0.54
2:O:497:ASP:OD1	2:O:523:GLU:HG3	2.08	0.54
2:P:248:ILE:HD12	5:P:1008:XE:XE	2.86	0.54
2:P:650:THR:HG22	9:P:1070:HOH:O	2.08	0.54
1:A:587:LYS:H	1:B:220:HIS:HE1	1.56	0.53
2:N:339:TYR:CD2	2:N:435:VAL:HG21	2.43	0.53
2:O:4:PHE:N	2:O:238:GLU:OE2	2.41	0.53
2:P:61:TYR:HD2	2:P:66:ARG:HD2	1.72	0.53
1:A:32:ALA:O	1:A:36:MET:HG2	2.08	0.53
1:B:416:ARG:HG3	1:B:416:ARG:NH1	2.22	0.53
1:C:102:VAL:HG11	5:C:1003[B]:XE:XE	2.84	0.53
2:P:426:ASN:O	2:P:427:TRP:HB2	2.08	0.53
1:A:620:LEU:HD21	5:A:1003[A]:XE:XE	2.85	0.53
1:C:112:ALA:HA	1:D:217:ASN:ND2	2.24	0.53
1:C:281:HIS:ND1	1:C:282:GLY:N	2.57	0.53
2:N:613:ILE:O	2:N:671:PRO:HD3	2.07	0.53
2:O:60:TYR:CE2	2:O:228:MET:HE3	2.44	0.53
2:O:488:ARG:C	2:O:490:ASP:N	2.67	0.53
2:O:523:GLU:OE2	2:O:656:LYS:HE2	2.09	0.53
1:B:510:LEU:N	1:B:510:LEU:CD1	2.72	0.53
1:D:98:VAL:HG13	1:D:610:VAL:HA	1.89	0.53
2:P:623:PRO:HA	2:P:707:THR:HA	1.90	0.53
2:P:670:MET:HE3	2:P:675:LYS:HG2	1.91	0.53
2:M:87:ARG:HD2	9:M:1010:HOH:O	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HD11	5:A:1010:XE:XE	2.86	0.53
1:C:640:VAL:CG1	1:C:644:LYS:HE3	2.39	0.53
1:D:299:GLU:HA	1:D:299:GLU:OE1	2.09	0.53
1:D:2:PRO:HA	9:D:1040:HOH:O	2.09	0.53
2:M:621:MET:HE1	2:M:625:GLY:C	2.33	0.53
2:N:144:PHE:O	2:N:148:MET:HG3	2.08	0.53
2:O:345:ASN:C	2:O:348:PRO:HD3	2.34	0.53
2:P:341:GLU:OE2	2:P:427:TRP:CD1	2.61	0.53
1:C:118:ASN:OD1	1:C:209:HIS:HE1	1.92	0.53
2:O:491:ARG:HB2	2:O:491:ARG:NH1	2.22	0.53
2:O:686:SER:HB3	2:O:692:GLY:O	2.09	0.53
2:P:341:GLU:OE2	2:P:427:TRP:HD1	1.91	0.53
2:P:485:TYR:N	2:P:485:TYR:CD1	2.77	0.53
1:C:342:CYS:HA	1:C:367:TYR:CZ	2.44	0.53
1:C:411:ARG:O	1:C:416:ARG:HG2	2.08	0.53
1:A:426:ARG:NH2	1:A:539:ILE:HB	2.25	0.52
1:C:615:LEU:HD23	1:C:615:LEU:C	2.34	0.52
2:M:424:ASN:H	2:M:424:ASN:ND2	2.07	0.52
2:N:527:LEU:HD13	2:N:598:PHE:HB3	1.91	0.52
2:P:322:ILE:HG21	2:P:434:ALA:HB1	1.91	0.52
2:N:602:MET:HE3	2:N:647:ILE:HG21	1.91	0.52
2:O:233:THR:O	2:O:240:GLN:NE2	2.42	0.52
2:O:626:MET:HB3	2:O:630:THR:HB	1.91	0.52
2:N:417:LEU:O	9:N:1164:HOH:O	2.19	0.52
2:O:402:VAL:C	2:O:404:GLU:H	2.16	0.52
2:O:434:ALA:O	2:O:437:LYS:HB2	2.09	0.52
1:C:633:ILE:HA	9:C:1074:HOH:O	2.09	0.52
2:N:156:GLU:HG2	5:N:1008:XE:XE	2.87	0.52
2:O:221:TYR:N	2:O:224:ARG:HH21	2.07	0.52
2:O:460:VAL:HG13	2:O:463:VAL:HG13	1.90	0.52
2:P:395:MET:HE3	2:P:396:GLN:O	2.09	0.52
1:B:33:VAL:HG21	1:B:477:GLN:HE22	1.74	0.52
2:O:399:PHE:CE1	2:O:541:GLU:HG3	2.44	0.52
1:D:28:THR:HG21	1:D:33:VAL:HG12	1.91	0.52
2:P:585:TYR:CE1	2:P:656:LYS:HD3	2.45	0.52
1:A:96:THR:O	1:A:100:ARG:HG3	2.10	0.52
1:C:3:ARG:HG3	1:C:3:ARG:HH11	1.75	0.52
1:D:118:ASN:C	1:D:118:ASN:HD22	2.17	0.52
2:P:525:VAL:HB	9:P:1069:HOH:O	2.09	0.52
1:A:506:GLY:CA	1:A:511:LEU:HD12	2.39	0.52
2:O:136:ILE:HG21	2:O:221:TYR:CE2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:549:GLN:HB3	2:O:550:PRO:CD	2.40	0.52
2:O:554:GLU:HG3	2:O:566:SER:HB3	1.90	0.52
2:O:657:PHE:HE2	2:O:667:ILE:HD11	1.75	0.52
1:B:577:VAL:HG12	1:B:601:PRO:HG2	1.92	0.52
1:C:68:CYS:HB2	1:C:97:ILE:HG23	1.92	0.52
1:C:396:SER:HB3	5:C:1010:XE:XE	2.88	0.52
1:C:500:CYS:HA	1:C:503:GLN:HG3	1.91	0.52
2:N:95:ASN:C	2:N:95:ASN:HD22	2.17	0.52
2:O:672:LYS:C	2:O:674:LEU:H	2.16	0.52
2:P:364:GLY:N	2:P:463:VAL:O	2.42	0.52
1:A:177:LEU:HB2	1:A:180:GLU:CD	2.35	0.52
1:C:563:MET:HE2	1:C:576:PHE:CD2	2.44	0.52
2:O:356:VAL:HG11	2:O:360:GLU:OE2	2.10	0.52
2:P:142:ARG:HG2	2:P:142:ARG:HH11	1.75	0.52
2:P:333:ILE:HD12	2:P:418:TRP:HB2	1.92	0.52
2:P:681:GLU:CG	2:P:684:ARG:HH21	2.23	0.52
1:B:572:PRO:HG3	1:B:629:GLY:HA3	1.92	0.51
1:C:220:HIS:O	1:C:223:MET:HB2	2.11	0.51
1:D:283:HIS:CD2	1:D:317:CYS:HB2	2.45	0.51
2:O:183:LEU:HB2	2:O:206:ALA:HA	1.93	0.51
2:O:351:GLU:HG3	2:O:423:ARG:HA	1.92	0.51
2:O:508:LEU:CB	3:O:900:SF4:S1	2.95	0.51
2:O:590:ASN:N	2:O:591:PRO:HD3	2.26	0.51
2:P:412:ASN:ND2	2:P:419:HIS:HB3	2.25	0.51
1:C:9:HIS:CD2	1:C:644:LYS:HG2	2.45	0.51
1:D:332:THR:OG1	1:D:336:SER:OG	2.26	0.51
2:M:246:ARG:HE	2:M:247:ARG:NH1	2.08	0.51
2:N:408:HIS:HD2	2:N:419:HIS:ND1	2.08	0.51
2:O:382:LEU:HD23	2:O:469:THR:HG21	1.91	0.51
2:P:568:ASN:HD21	2:P:581:GLN:CG	2.22	0.51
1:C:114:CYS:HB2	1:C:208:ILE:HG21	1.92	0.51
2:M:95:ASN:HD21	2:M:98:ASN:H	1.57	0.51
1:D:191:ASN:ND2	9:D:1034:HOH:O	2.42	0.51
2:O:344:GLY:O	2:O:346:ARG:NH1	2.44	0.51
2:P:229:PHE:CD1	5:P:1009:XE:XE	3.41	0.51
1:B:256:PHE:CD1	1:B:289:GLU:HG3	2.46	0.51
1:D:292:VAL:HG11	1:D:326:GLN:HG3	1.93	0.51
1:C:611:GLU:HB2	9:C:1122:HOH:O	2.10	0.51
1:D:105:MET:HE2	1:D:609:PRO:HG3	1.92	0.51
2:O:152:THR:O	2:O:154:PRO:HD3	2.11	0.51
2:O:224:ARG:O	2:O:228:MET:HB2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:524:ARG:HB2	2:O:651:TYR:CE1	2.46	0.51
1:A:620:LEU:HD23	5:A:1004:XE:XE	2.88	0.51
2:O:254:TYR:CE2	2:O:258:HIS:CD2	2.98	0.51
2:O:430:VAL:HG11	2:O:439:PHE:CE2	2.45	0.51
2:P:343:GLY:O	2:P:346:ARG:NH1	2.43	0.51
1:D:68:CYS:HB2	1:D:97:ILE:HG23	1.93	0.51
2:N:335:LYS:HD3	2:N:429:ARG:HH12	1.76	0.51
2:O:277:ILE:N	2:O:277:ILE:HD12	2.25	0.51
2:P:288:ILE:O	2:P:289:PRO:C	2.54	0.51
2:O:612:MET:SD	2:O:622:THR:HB	2.51	0.51
2:P:385:GLY:O	2:P:467:ILE:HA	2.11	0.51
2:P:602:MET:HE2	2:P:647:ILE:HG21	1.93	0.51
1:A:592:GLY:HA2	5:A:1001:XE:XE	2.89	0.51
1:B:394:ILE:HG23	1:B:395:GLU:H	1.76	0.51
2:O:26:TYR:CE1	2:O:30:ILE:HD11	2.46	0.51
2:O:122:LYS:HB2	2:O:125:GLU:HG3	1.93	0.51
2:P:340:VAL:HG13	2:P:341:GLU:N	2.26	0.51
1:A:220:HIS:HD2	1:A:221:MET:O	1.94	0.50
1:B:298:MET:HE1	1:B:301:GLU:OE2	2.10	0.50
2:M:62:LEU:HD13	2:M:115:ALA:HB2	1.93	0.50
2:O:527:LEU:HA	2:O:648:GLY:N	2.26	0.50
2:P:403:LEU:N	2:P:403:LEU:HD23	2.26	0.50
2:P:564:TRP:HB2	2:P:567:VAL:HB	1.93	0.50
2:P:626:MET:SD	2:P:634:MET:HE3	2.52	0.50
1:A:72:MET:HG3	1:B:105:MET:HE1	1.93	0.50
1:D:266:ALA:HA	1:D:330:LEU:O	2.12	0.50
2:M:373:ILE:HG22	2:M:440:ARG:HD3	1.93	0.50
2:O:259:ASP:OD2	2:O:262:LYS:HD2	2.11	0.50
2:N:693:GLU:CD	2:N:693:GLU:H	2.19	0.50
2:O:391:TYR:HD2	2:O:462:ARG:HB2	1.77	0.50
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.26	0.50
1:A:305:ALA:HB1	1:A:409:LYS:HD2	1.93	0.50
1:B:620:LEU:CD2	5:B:1004:XE:XE	3.38	0.50
1:D:241:ASP:OD1	1:D:241:ASP:C	2.54	0.50
2:M:586:THR:HG1	2:M:661:ASP:CG	2.17	0.50
2:M:704:ILE:C	2:M:704:ILE:HD12	2.36	0.50
2:O:269:ALA:HB1	2:O:274:PHE:HB2	1.93	0.50
2:P:338:MET:HE3	2:P:341:GLU:HB2	1.91	0.50
2:P:358:GLU:HA	2:P:361:ILE:HG22	1.92	0.50
1:D:307:ALA:HB2	1:D:408:PHE:CE2	2.46	0.50
1:B:372:ILE:CD1	1:B:403:MET:HE3	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:MET:SD	1:D:127:MET:C	2.95	0.50
1:D:275:GLN:HG2	1:D:309:GLY:O	2.11	0.50
1:D:615:LEU:H	6:D:863:GOL:C1	2.25	0.50
2:M:373:ILE:HG21	2:M:439:PHE:O	2.11	0.50
2:N:679:HIS:HD2	2:N:680:ASP:OD1	1.94	0.50
1:B:620:LEU:HD22	5:B:1004:XE:XE	2.90	0.50
1:D:146:VAL:O	1:D:150:VAL:HG22	2.11	0.50
1:D:267:ASN:O	1:D:270:VAL:HG22	2.11	0.50
1:D:416:ARG:HB2	1:D:418:VAL:CG2	2.42	0.50
2:O:166:SER:HB3	2:O:192:GLN:HB3	1.93	0.50
2:O:362:THR:HB	2:O:365:LYS:HB2	1.94	0.50
2:O:392:GLY:HA2	2:O:461:ASP:HB2	1.93	0.50
2:O:725:MET:O	2:O:726:ASP:HB3	2.11	0.50
1:B:32:ALA:O	1:B:36:MET:HG2	2.11	0.50
1:D:41:LYS:O	1:D:41:LYS:HG2	2.12	0.50
1:B:341:ILE:HA	1:B:346:ILE:HG12	1.93	0.50
1:C:202:ASN:HA	9:C:1120:HOH:O	2.11	0.50
1:D:105:MET:HE1	1:D:609:PRO:HD3	1.88	0.50
2:N:272:THR:HG22	2:N:272:THR:O	2.11	0.50
1:B:549:SER:HB2	9:B:1019:HOH:O	2.12	0.49
2:O:95:ASN:C	2:O:95:ASN:HD22	2.20	0.49
2:O:497:ASP:HB2	2:O:656:LYS:NZ	2.28	0.49
2:O:597:CYS:SG	3:O:900:SF4:S3	3.10	0.49
2:P:353:VAL:HG13	2:P:388:VAL:HB	1.93	0.49
1:C:584:MET:O	1:D:71:CYS:HB2	2.11	0.49
2:N:602:MET:CE	2:N:647:ILE:HG21	2.42	0.49
2:O:144:PHE:O	2:O:148:MET:CG	2.49	0.49
2:O:163:ALA:HB2	2:O:255:LEU:HD13	1.92	0.49
2:O:373:ILE:C	2:O:375:GLN:H	2.20	0.49
2:O:504:TYR:OH	2:O:537:LYS:HG2	2.11	0.49
2:O:508:LEU:C	2:O:510:GLN:H	2.19	0.49
2:O:529:GLY:HA3	2:O:599:GLU:OE2	2.12	0.49
2:O:669:TRP:HD1	2:O:711:ILE:HG21	1.78	0.49
2:P:275:PRO:CD	2:P:309:ARG:HD3	2.42	0.49
2:P:391:TYR:CD2	2:P:462:ARG:NH1	2.78	0.49
2:P:403:LEU:HD22	2:P:456:PHE:CZ	2.48	0.49
2:P:525:VAL:HG11	2:P:650:THR:HG22	1.95	0.49
1:C:579:SER:HA	1:C:603:HIS:O	2.12	0.49
2:O:136:ILE:HG21	2:O:221:TYR:HE2	1.77	0.49
2:O:508:LEU:N	3:O:900:SF4:S2	2.84	0.49
1:C:220:HIS:HE1	1:D:587:LYS:H	1.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:CYS:O	1:D:321:GLU:HG2	2.11	0.49
2:M:184:PHE:C	2:M:185:ILE:HG13	2.36	0.49
2:M:373:ILE:CG2	2:M:440:ARG:HA	2.43	0.49
2:N:621:MET:HE1	9:N:1020:HOH:O	2.12	0.49
2:P:674:LEU:O	2:P:678:LEU:HD12	2.12	0.49
1:A:281:HIS:HB3	1:A:351:VAL:HG12	1.94	0.49
1:B:386:ILE:HD11	1:B:403:MET:HE1	1.95	0.49
1:C:18:ARG:NE	1:C:636:MET:HE3	2.28	0.49
1:D:282:GLY:HA3	1:D:352:ASP:OD1	2.13	0.49
1:D:333:SER:HA	1:D:503:GLN:NE2	2.28	0.49
2:N:365:LYS:HB3	2:N:464:GLN:HG3	1.95	0.49
2:O:184:PHE:HB3	2:O:209:LEU:HD11	1.95	0.49
2:O:457:PRO:O	2:O:458:ALA:CB	2.60	0.49
2:P:472:ALA:O	2:P:476:GLU:HB2	2.13	0.49
1:D:285:PRO:C	1:D:287:LEU:N	2.69	0.49
2:O:150:ASP:OD2	2:O:152:THR:HG23	2.13	0.49
2:O:579:LEU:HD22	2:O:593:THR:CG2	2.42	0.49
2:P:373:ILE:HD13	2:P:435:VAL:HG22	1.94	0.49
1:A:443:GLN:HB2	1:A:451:VAL:HG21	1.94	0.49
2:O:649:ARG:HA	2:O:652:ILE:HD12	1.94	0.49
2:P:261:VAL:HG12	5:P:1006:XE:XE	2.91	0.49
1:A:571:THR:OG1	1:A:572:PRO:HD3	2.13	0.49
2:N:558:ASP:C	2:N:558:ASP:OD1	2.56	0.49
1:C:52:PHE:CZ	1:C:474:LYS:HA	2.48	0.48
2:O:138:ASP:HB2	2:O:139:PRO:HD3	1.95	0.48
2:O:250:ALA:N	2:O:309:ARG:HE	2.10	0.48
2:O:416:GLY:O	2:O:430:VAL:HA	2.13	0.48
1:C:563:MET:CE	1:C:576:PHE:CD2	2.88	0.48
1:D:164:GLN:O	1:D:168[A]:GLU:HG3	2.12	0.48
2:O:316:ILE:CG2	2:O:454:GLU:OE1	2.61	0.48
2:O:649:ARG:C	2:O:651:TYR:H	2.20	0.48
2:P:354:ARG:HG2	2:P:484:LYS:NZ	2.28	0.48
2:P:605:LEU:HD11	2:P:624:SER:HA	1.95	0.48
2:O:19:VAL:O	2:O:22:PHE:HB2	2.13	0.48
2:O:66:ARG:HG3	2:O:66:ARG:O	2.12	0.48
2:O:602:MET:HE3	2:O:645:MET:HB3	1.94	0.48
2:P:170:ALA:O	2:P:174:LYS:HB2	2.13	0.48
2:P:667:ILE:O	2:P:699:ILE:HG12	2.13	0.48
2:P:681:GLU:HG3	2:P:684:ARG:NH2	2.28	0.48
1:B:587:LYS:HE3	4:B:800:XCC:S4	2.53	0.48
1:C:596:VAL:HG21	1:C:632:PHE:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:261:VAL:HG12	5:O:1006:XE:XE	2.91	0.48
2:P:343:GLY:HA3	2:P:349:ALA:CB	2.39	0.48
1:C:540:GLY:HA2	9:C:1136:HOH:O	2.13	0.48
2:N:182:MET:HB2	2:N:182:MET:HE3	1.67	0.48
2:O:449:VAL:O	2:O:449:VAL:CG1	2.62	0.48
2:O:657:PHE:CE2	2:O:667:ILE:HD11	2.48	0.48
2:P:585:TYR:CZ	2:P:656:LYS:HD3	2.49	0.48
2:M:716:GLU:HG3	2:M:723:LEU:HD12	1.95	0.48
2:O:7:ILE:HD12	2:O:245:ARG:HD2	1.96	0.48
2:O:270:ILE:O	2:O:271:PHE:C	2.55	0.48
2:P:339:TYR:CD1	2:P:339:TYR:C	2.91	0.48
2:P:350:PHE:CD1	2:P:351:GLU:N	2.82	0.48
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.79	0.48
1:B:415:ASN:CG	1:B:415:ASN:O	2.57	0.48
2:O:215:ILE:HG21	5:O:1006:XE:XE	2.92	0.48
2:P:95:ASN:C	2:P:95:ASN:ND2	2.56	0.48
1:A:272:ASP:C	1:A:272:ASP:OD1	2.56	0.48
1:A:506:GLY:HA2	1:A:511:LEU:HD12	1.96	0.48
1:C:112:ALA:HA	1:D:217:ASN:HD22	1.79	0.48
1:C:384:TYR:CD1	1:C:384:TYR:N	2.80	0.48
1:D:147:CYS:HB3	1:D:152:ILE:HB	1.95	0.48
1:D:275:GLN:HG2	1:D:309:GLY:C	2.39	0.48
2:O:229:PHE:CD1	5:O:1009:XE:XE	3.45	0.48
2:O:289:PRO:C	2:O:291:TRP:H	2.21	0.48
2:P:221:TYR:CD1	2:P:221:TYR:C	2.91	0.48
2:P:341:GLU:HG3	2:P:429:ARG:HB3	1.95	0.48
1:A:384:TYR:CD2	2:N:84:ASN:HB3	2.49	0.48
1:B:443:GLN:HB2	1:B:451:VAL:HG21	1.96	0.48
1:C:569:VAL:CG1	1:C:573:LYS:HD3	2.43	0.48
2:N:340:VAL:HG22	2:N:341:GLU:N	2.29	0.48
2:O:556:GLU:HG3	2:O:564:TRP:NE1	2.29	0.48
2:P:576:ASN:O	2:P:577:ARG:HB2	2.14	0.48
1:C:563:MET:HE3	1:C:574:VAL:HG11	1.96	0.48
2:O:408:HIS:HA	2:O:419:HIS:HD1	1.77	0.48
2:O:503:PHE:O	2:O:551:ILE:N	2.36	0.48
2:O:685:ARG:HA	2:O:688:GLU:HB2	1.95	0.48
2:P:117[A]:ARG:NH2	9:P:1051:HOH:O	2.47	0.48
2:P:701:ASP:O	2:P:702:GLU:C	2.57	0.48
1:B:394:ILE:HG23	1:B:395:GLU:N	2.29	0.47
1:C:3:ARG:HG3	1:C:3:ARG:NH1	2.29	0.47
1:C:384:TYR:HD1	1:C:384:TYR:N	2.11	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:568:ASN:ND2	2:N:581:GLN:HE21	2.11	0.47
2:O:485:TYR:HA	2:O:489:ASP:HB2	1.95	0.47
2:P:665:ALA:O	2:P:720:HIS:HE1	1.97	0.47
1:A:576:PHE:CD1	1:A:576:PHE:C	2.93	0.47
1:B:241:ASP:OD1	1:B:245:GLU:OE2	2.31	0.47
1:B:426:ARG:NH2	9:B:1216:HOH:O	2.46	0.47
1:D:46:ILE:HD12	6:D:860:GOL:H31	1.95	0.47
2:O:335:LYS:HD2	2:O:336:GLY:N	2.28	0.47
1:A:267:ASN:O	1:A:270:VAL:HG22	2.13	0.47
1:A:559:LEU:HG	1:A:563:MET:HE2	1.97	0.47
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.45	0.47
1:A:607:MET:HE3	1:A:611:GLU:CD	2.39	0.47
2:N:244:GLN:HG3	2:N:272:THR:CG2	2.45	0.47
1:A:658:VAL:O	1:A:662:VAL:HG23	2.15	0.47
1:C:420:ILE:O	1:C:421:PRO:C	2.56	0.47
2:N:187:ASP:HA	2:N:211:ASN:ND2	2.24	0.47
2:N:527:LEU:HD12	2:N:527:LEU:C	2.40	0.47
2:P:354:ARG:HD2	2:P:355:THR:H	1.79	0.47
2:P:491:ARG:O	2:P:495:LEU:HD12	2.15	0.47
2:P:527:LEU:HA	2:P:648:GLY:N	2.30	0.47
1:D:114:CYS:CA	9:D:1050:HOH:O	2.62	0.47
1:D:466:LEU:HD22	1:D:595:TRP:CZ2	2.49	0.47
2:O:295:VAL:CG1	2:O:301:ILE:HG12	2.45	0.47
2:O:376:ILE:HG21	2:O:382:LEU:HD11	1.97	0.47
2:O:418:TRP:CZ3	2:O:429:ARG:NE	2.82	0.47
1:B:317:CYS:O	1:B:321:GLU:HG2	2.15	0.47
1:B:654:TRP:HE1	2:N:195:GLU:CD	2.23	0.47
1:C:154:VAL:HG13	1:C:162:LEU:HD11	1.97	0.47
1:C:545:PHE:N	1:C:545:PHE:CD1	2.83	0.47
1:D:278:PHE:HB3	1:D:312:LEU:HD23	1.96	0.47
2:O:276:VAL:N	2:O:291:TRP:O	2.46	0.47
2:P:150:ASP:OD1	2:P:152:THR:CG2	2.62	0.47
2:P:400:GLU:C	2:P:402:VAL:H	2.21	0.47
2:P:412:ASN:OD1	2:P:418:TRP:HA	2.13	0.47
2:P:589:GLU:O	2:P:590:ASN:C	2.58	0.47
1:C:43:ASP:O	1:C:44:LYS:HB2	2.15	0.47
1:C:107:LEU:HD21	1:C:215:LEU:HB3	1.96	0.47
1:C:126:GLU:HG2	1:C:132:ALA:HB2	1.97	0.47
1:C:318:THR:O	1:C:322:VAL:HG22	2.15	0.47
1:D:52:PHE:CZ	1:D:474:LYS:HA	2.50	0.47
1:D:82:ASP:OD1	1:D:83:GLY:N	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:340:VAL:HG22	2:M:341:GLU:N	2.29	0.47
2:N:162:ARG:HB2	2:N:188:GLU:HB2	1.96	0.47
2:O:66:ARG:CZ	2:O:234:PRO:HG2	2.45	0.47
2:O:107:TRP:NE1	2:O:268:GLY:HA3	2.29	0.47
2:O:118:TYR:CD2	2:O:121:TYR:HB2	2.50	0.47
2:O:162:ARG:HG3	2:O:188:GLU:HB2	1.97	0.47
2:O:334:ARG:O	2:O:335:LYS:C	2.57	0.47
1:A:191:ASN:OD1	1:A:194:ARG:HG2	2.14	0.47
1:D:447:ASN:ND2	1:D:450:ARG:HB2	2.30	0.47
2:M:315:LYS:HG3	9:M:1153:HOH:O	2.14	0.47
2:O:563:ILE:HG12	2:O:583:CYS:SG	2.55	0.47
2:P:339:TYR:HB2	2:P:432:LYS:HA	1.96	0.47
1:C:292:VAL:HA	1:C:312:LEU:HD11	1.96	0.47
2:M:150:ASP:OD1	2:M:152:THR:CG2	2.62	0.47
2:M:341:GLU:HG3	2:M:429:ARG:HG2	1.97	0.47
2:M:675:LYS:NZ	2:M:699:ILE:O	2.40	0.47
2:P:354:ARG:HH21	2:P:356:VAL:HG11	1.73	0.47
1:A:287:LEU:HD13	1:A:388:TYR:CE1	2.50	0.47
1:D:182:GLU:OE2	1:D:199:ARG:HD3	2.15	0.47
1:D:373:THR:CG2	1:D:380:ILE:HD12	2.45	0.47
2:M:129:PRO:O	2:M:132:TRP:HB2	2.15	0.47
2:O:71:GLU:HG3	2:O:82:ILE:HD11	1.96	0.47
2:O:86:LYS:HA	2:O:86:LYS:HD3	1.62	0.47
2:P:490:ASP:O	2:P:492:MET:N	2.48	0.47
1:C:223:MET:SD	1:D:353:VAL:HB	2.54	0.46
2:M:206:ALA:O	2:M:208:PRO:HD3	2.15	0.46
2:O:124:ASP:OD1	2:O:124:ASP:N	2.40	0.46
1:C:279:VAL:HG22	1:C:313:VAL:HG23	1.96	0.46
1:D:30:ASP:HA	1:D:508:LEU:HD21	1.97	0.46
2:N:381:LYS:HE2	2:N:381:LYS:HB2	1.43	0.46
2:N:681:GLU:HB3	2:N:684:ARG:NH2	2.29	0.46
2:O:181:PHE:CE1	2:O:251:PHE:HE2	2.33	0.46
2:O:220:ASN:C	2:O:224:ARG:HH21	2.24	0.46
2:O:427:TRP:O	2:O:428:LEU:HB2	2.13	0.46
2:O:488:ARG:HB3	2:O:488:ARG:NH1	2.30	0.46
2:P:343:GLY:CA	2:P:349:ALA:HB3	2.40	0.46
1:B:607:MET:HG3	1:B:608:PRO:O	2.15	0.46
1:D:25:ARG:NH2	1:D:41:LYS:HB2	2.30	0.46
2:M:560:ILE:O	2:M:660:ALA:HB2	2.15	0.46
2:M:704:ILE:HD12	2:M:704:ILE:O	2.15	0.46
1:B:20:MET:HG3	9:B:1052:HOH:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:GLU:OE2	1:D:164:GLN:NE2	2.49	0.46
1:D:477:GLN:O	1:D:478:ASP:HB2	2.15	0.46
2:M:383:PRO:HG3	2:M:471:GLU:HG2	1.98	0.46
2:M:408:HIS:CD2	2:M:419:HIS:ND1	2.78	0.46
2:N:211:ASN:ND2	9:N:1016:HOH:O	2.39	0.46
2:N:657:PHE:O	2:N:663:GLY:HA2	2.15	0.46
2:O:169:LEU:HD13	2:O:193:LEU:HD21	1.97	0.46
2:P:488:ARG:HG2	2:P:491:ARG:NH2	2.30	0.46
1:D:107:LEU:HD21	1:D:215:LEU:HB3	1.98	0.46
1:D:555:ARG:HG2	9:D:1045:HOH:O	2.15	0.46
2:N:283:PRO:HG2	2:N:286:LYS:HG3	1.96	0.46
2:O:193:LEU:HD22	2:O:198:VAL:HG21	1.98	0.46
2:P:571:LEU:HD12	2:P:575:SER:HB3	1.97	0.46
1:B:87:ARG:HD3	1:B:91:GLY:O	2.16	0.46
1:D:145:GLU:OE1	1:D:145:GLU:HA	2.16	0.46
2:M:611:ILE:HD11	2:M:667:ILE:HG12	1.98	0.46
2:N:147:LYS:HB3	2:N:153:ILE:HD12	1.96	0.46
2:N:540:TYR:CE1	2:N:544:HIS:HA	2.51	0.46
2:O:333:ILE:HG13	2:O:418:TRP:HB2	1.98	0.46
2:O:603:ALA:HB3	2:O:612:MET:HG3	1.97	0.46
2:P:553:LYS:HG2	2:P:564:TRP:NE1	2.30	0.46
1:A:217:ASN:HD22	1:B:112:ALA:HA	1.81	0.46
1:B:7:LEU:HD11	2:N:164:LYS:HB2	1.97	0.46
1:B:661[A]:GLU:HG3	1:B:665[A]:ARG:HH21	1.80	0.46
2:N:681:GLU:HB3	2:N:684:ARG:HH21	1.80	0.46
2:O:354:ARG:HE	2:O:356:VAL:HG22	1.81	0.46
2:P:316:ILE:O	2:P:316:ILE:CG2	2.61	0.46
2:P:602:MET:HE2	2:P:647:ILE:CG2	2.45	0.46
1:D:416:ARG:C	1:D:418:VAL:H	2.24	0.46
2:O:79:LEU:O	2:O:80:PRO:C	2.57	0.46
2:P:457:PRO:O	2:P:458:ALA:HB3	2.16	0.46
1:A:31:PRO:HB2	1:A:423:ILE:HD13	1.98	0.46
1:C:316:CYS:N	1:C:503:GLN:HE22	2.13	0.46
1:C:381:PRO:HB2	9:C:1104:HOH:O	2.15	0.46
1:C:637:ASP:OD1	1:C:640:VAL:HG23	2.16	0.46
2:M:395:MET:C	2:M:396:GLN:HG3	2.41	0.46
2:N:64:VAL:HG13	2:N:111:GLU:OE2	2.16	0.46
2:O:158:ILE:HG22	2:O:252:VAL:HG13	1.97	0.46
2:O:247:ARG:O	2:O:512:PHE:CZ	2.69	0.46
2:P:95:ASN:O	2:P:96:PHE:C	2.59	0.46
2:P:609:ASN:OD1	2:P:728:ILE:HG22	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:674:LEU:O	2:P:674:LEU:HD22	2.15	0.46
1:B:466:LEU:HA	1:B:496:VAL:HG23	1.98	0.46
2:O:58:THR:HA	2:O:138:ASP:OD2	2.16	0.46
2:O:95:ASN:ND2	2:O:98:ASN:H	2.13	0.46
2:P:61:TYR:CD2	2:P:66:ARG:HD2	2.48	0.46
2:P:344:GLY:O	2:P:346:ARG:CZ	2.64	0.46
1:A:118:ASN:C	1:A:118:ASN:HD22	2.23	0.45
1:A:584:MET:HG3	1:B:73:ALA:HB2	1.96	0.45
1:D:9:HIS:C	1:D:9:HIS:CD2	2.93	0.45
2:M:21:LEU:HB2	2:M:286:LYS:HA	1.97	0.45
2:N:61:TYR:HD2	2:N:66:ARG:HD2	1.82	0.45
2:O:167:LYS:HD3	2:O:196:GLU:OE2	2.16	0.45
2:O:266:ALA:O	2:O:269:ALA:N	2.46	0.45
2:O:346:ARG:HB3	2:O:381:LYS:HD3	1.98	0.45
2:P:456:PHE:O	2:P:459:ILE:HB	2.15	0.45
1:A:287:LEU:HB3	9:A:1020:HOH:O	2.15	0.45
1:B:9:HIS:CE1	1:B:644:LYS:HB3	2.51	0.45
1:B:432:SER:HA	1:B:555:ARG:HD3	1.98	0.45
1:B:580:ALA:CB	5:B:1001:XE:XE	3.39	0.45
1:B:602:THR:HG23	5:B:1001:XE:XE	2.94	0.45
1:D:61:ILE:HG23	1:D:66:ILE:HD12	1.98	0.45
1:D:249:THR:O	1:D:250:ASP:C	2.58	0.45
2:N:189:ALA:HA	2:N:192:GLN:HE21	1.80	0.45
2:O:611:ILE:O	2:O:668:VAL:HG22	2.16	0.45
2:O:627:THR:O	2:O:628:PHE:C	2.58	0.45
2:P:79:LEU:O	2:P:80:PRO:C	2.59	0.45
2:P:538:ALA:O	2:P:542:ILE:HG23	2.16	0.45
1:C:105:MET:CE	1:C:609:PRO:HD3	2.42	0.45
1:C:256:PHE:CG	1:C:289:GLU:HG3	2.52	0.45
1:D:186:LEU:O	1:D:190:ILE:HG23	2.16	0.45
2:O:151:TRP:HA	2:O:151:TRP:CE3	2.51	0.45
2:O:216:VAL:O	2:O:219:ALA:HB3	2.16	0.45
2:O:505:SER:CB	2:O:570:TYR:HE2	2.28	0.45
2:O:609:ASN:O	2:O:666:ARG:NH1	2.50	0.45
2:P:344:GLY:O	2:P:346:ARG:NH1	2.50	0.45
1:A:338:GLU:OE2	1:A:359:SER:OG	2.30	0.45
1:A:569:VAL:HA	1:A:672:GLN:HE22	1.81	0.45
1:C:531:LEU:HD23	1:C:531:LEU:HA	1.53	0.45
1:C:569:VAL:HB	1:C:573:LYS:HD3	1.98	0.45
2:M:261:VAL:CG1	5:M:1006:XE:XE	3.42	0.45
2:M:657:PHE:O	2:M:663:GLY:HA2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:367:GLU:HB2	9:N:1171:HOH:O	2.17	0.45
2:O:144:PHE:HB3	2:O:153:ILE:HD11	1.97	0.45
2:O:639:THR:O	2:O:640:GLN:C	2.58	0.45
2:P:439:PHE:O	2:P:440:ARG:HD2	2.16	0.45
1:B:386:ILE:HD11	1:B:403:MET:CE	2.47	0.45
1:C:288:SER:O	1:C:292:VAL:HG23	2.15	0.45
1:C:587:LYS:NZ	4:C:800:XCC:S4	2.85	0.45
1:D:545:PHE:N	1:D:545:PHE:CD1	2.84	0.45
2:M:373:ILE:HG21	2:M:440:ARG:HA	1.99	0.45
1:B:370:ARG:HH11	1:B:370:ARG:HG2	1.81	0.45
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.47	0.45
2:O:183:LEU:HA	2:O:183:LEU:HD23	1.71	0.45
2:O:439:PHE:CG	2:O:440:ARG:N	2.84	0.45
2:O:524:ARG:NH2	2:O:645:MET:HE1	2.31	0.45
2:O:590:ASN:C	2:O:640:GLN:HE21	2.25	0.45
2:P:150:ASP:OD1	2:P:150:ASP:C	2.57	0.45
2:P:611:ILE:O	2:P:668:VAL:HG22	2.16	0.45
1:B:308:LYS:HA	1:B:308:LYS:HD3	1.57	0.45
1:C:552:ASP:C	1:C:554:SER:N	2.74	0.45
2:N:694:ASP:O	2:N:695:PHE:C	2.59	0.45
2:O:308:THR:O	2:O:309:ARG:C	2.58	0.45
2:O:346:ARG:HH22	2:O:427:TRP:HZ2	1.64	0.45
1:D:32:ALA:CB	1:D:268:MET:HG3	2.45	0.45
1:D:530:ARG:HH11	1:D:530:ARG:CG	2.30	0.45
1:D:572:PRO:O	1:D:652:ARG:CZ	2.65	0.45
1:D:600:VAL:HA	1:D:601:PRO:HD3	1.89	0.45
2:N:254:TYR:O	2:N:278:THR:HA	2.17	0.45
2:N:354:ARG:HB3	2:N:484:LYS:HE2	1.98	0.45
2:O:316:ILE:O	2:O:316:ILE:CG2	2.64	0.45
2:O:590:ASN:OD1	2:O:640:GLN:NE2	2.50	0.45
2:P:369:ILE:HG21	2:P:468:PHE:HD2	1.82	0.45
2:P:665:ALA:O	2:P:720:HIS:CE1	2.70	0.45
1:C:154:VAL:O	1:C:154:VAL:HG12	2.17	0.45
1:C:241:ASP:OD1	1:C:245:GLU:OE2	2.34	0.45
1:D:219:ALA:O	1:D:220:HIS:C	2.58	0.45
1:D:241:ASP:OD1	1:D:245:GLU:OE2	2.34	0.45
1:D:614:ASP:H	6:D:863:GOL:H32	1.82	0.45
2:O:534:LEU:O	2:O:537:LYS:HB3	2.16	0.45
2:P:212:PHE:O	2:P:215:ILE:HG22	2.17	0.45
1:D:138:LYS:HG3	1:D:255:LEU:O	2.17	0.45
1:D:287:LEU:HD13	1:D:388:TYR:CE1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:551:ILE:HG21	2:M:567:VAL:HG22	1.98	0.45
2:N:79:LEU:HD22	2:N:112:ILE:HG12	1.99	0.45
2:P:488:ARG:HG2	2:P:491:ARG:HH22	1.82	0.45
2:M:95:ASN:ND2	2:M:95:ASN:C	2.74	0.44
2:O:483:GLU:HA	2:O:486:LYS:HB2	1.99	0.44
2:O:675:LYS:CA	2:O:696:ILE:HD11	2.46	0.44
2:P:342:MET:HE2	2:P:384:LEU:HD13	2.00	0.44
1:C:316:CYS:SG	4:C:800:XCC:S3	3.11	0.44
1:D:82:ASP:CG	1:D:83:GLY:N	2.75	0.44
1:D:105:MET:H	1:D:105:MET:HG2	1.56	0.44
2:M:621:MET:CE	9:M:1140:HOH:O	2.65	0.44
2:M:621:MET:CE	2:M:625:GLY:HA2	2.37	0.44
2:N:389:ASP:HB2	2:N:464:GLN:HB3	1.99	0.44
2:O:598:PHE:CE1	2:O:601:ILE:HD11	2.52	0.44
2:P:309:ARG:HB3	2:P:311:ILE:HG13	1.99	0.44
2:P:723:LEU:HD23	2:P:723:LEU:HA	1.50	0.44
1:B:380:ILE:HG22	1:B:381:PRO:O	2.18	0.44
2:N:622:THR:HB	2:N:623:PRO:HD2	1.99	0.44
2:P:326:PRO:O	2:P:327:ALA:C	2.58	0.44
2:P:352:LEU:HG	2:P:353:VAL:N	2.33	0.44
2:P:474:VAL:HG13	2:P:475:LYS:HG3	2.00	0.44
2:P:604:ILE:O	2:P:605:LEU:HD13	2.17	0.44
2:P:605:LEU:HD12	2:P:605:LEU:HA	1.75	0.44
1:A:89:ILE:HG12	1:B:52:PHE:HA	1.99	0.44
1:A:220:HIS:CE1	1:B:587:LYS:HG3	2.51	0.44
1:C:114:CYS:CA	9:C:1089:HOH:O	2.63	0.44
2:P:655:LYS:HA	2:P:685:ARG:HH12	1.82	0.44
1:A:218:GLN:HE22	1:A:233:SER:CB	2.30	0.44
1:B:18:ARG:HH21	6:B:861:GOL:H2	1.83	0.44
1:D:552:ASP:O	1:D:555:ARG:HB2	2.17	0.44
1:D:620:LEU:CD2	5:D:1004:XE:XE	3.43	0.44
2:N:327:ALA:HB2	9:N:1172:HOH:O	2.17	0.44
2:O:431:SER:C	2:O:433:ASP:N	2.76	0.44
1:A:549:SER:N	1:A:552:ASP:HB2	2.32	0.44
1:C:470:CYS:SG	1:C:588:ALA:HB2	2.58	0.44
1:D:431:TRP:O	1:D:547:MET:HG2	2.18	0.44
2:M:114:GLU:O	2:M:115:ALA:C	2.57	0.44
2:N:229:PHE:CE1	5:N:1009:XE:XE	3.49	0.44
2:O:169:LEU:CD1	2:O:193:LEU:HG	2.48	0.44
2:O:641:THR:O	2:O:642:PRO:C	2.61	0.44
2:P:138:ASP:N	2:P:139:PRO:CD	2.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:657:PHE:CE2	2:P:667:ILE:HD11	2.53	0.44
1:A:27:ARG:CZ	1:A:27:ARG:HB3	2.48	0.44
1:A:137:VAL:HG13	1:A:254:ILE:HG23	1.99	0.44
1:A:226:ASP:C	1:A:226:ASP:OD1	2.61	0.44
1:B:587:LYS:NZ	4:B:800:XCC:S4	2.91	0.44
2:N:626:MET:HB3	2:N:630:THR:HB	1.99	0.44
2:O:191:GLU:O	2:O:195:GLU:HB2	2.18	0.44
2:O:622:THR:OG1	2:O:626:MET:O	2.29	0.44
2:P:373:ILE:HD13	2:P:435:VAL:CG2	2.47	0.44
1:B:384:TYR:HD2	1:B:403:MET:SD	2.41	0.44
1:B:537:ILE:C	1:B:539:ILE:H	2.25	0.44
1:C:650:GLU:HA	1:C:653:THR:OG1	2.18	0.44
1:D:285:PRO:C	1:D:287:LEU:H	2.24	0.44
2:M:424:ASN:N	2:M:424:ASN:ND2	2.66	0.44
2:N:185:ILE:HD12	2:N:185:ILE:N	2.33	0.44
2:O:174:LYS:HA	9:O:1030:HOH:O	2.17	0.44
2:P:371:PRO:HD2	2:P:469:THR:HB	1.99	0.44
2:P:585:TYR:O	2:P:658:ILE:HA	2.17	0.44
1:D:636:MET:HE2	9:D:1043:HOH:O	2.18	0.44
2:N:621:MET:HE1	2:N:622:THR:O	2.18	0.44
2:O:491:ARG:HH11	2:O:491:ARG:CB	2.30	0.44
2:O:572:TYR:CE2	2:O:577:ARG:HB3	2.53	0.44
2:P:354:ARG:O	2:P:390:ILE:HG22	2.18	0.44
1:B:537:ILE:HD13	1:B:537:ILE:HA	1.94	0.43
1:C:287:LEU:HB3	9:C:1118:HOH:O	2.17	0.43
1:D:66:ILE:H	1:D:66:ILE:HG13	1.65	0.43
2:N:58:THR:HA	2:N:138:ASP:CG	2.43	0.43
2:O:6:LYS:O	2:O:9:GLU:HB2	2.18	0.43
2:O:180:GLY:HA2	2:O:326:PRO:CG	2.48	0.43
2:O:356:VAL:HG23	2:O:361:ILE:HD12	2.00	0.43
2:O:720:HIS:C	2:O:722:ALA:H	2.26	0.43
2:P:674:LEU:HD13	2:P:678:LEU:HD11	2.00	0.43
1:A:342:CYS:HA	1:A:367:TYR:CZ	2.53	0.43
1:B:283:HIS:CD2	1:B:317:CYS:HB2	2.53	0.43
1:D:607:MET:HG3	1:D:608:PRO:O	2.18	0.43
1:D:615:LEU:H	6:D:863:GOL:H11	1.83	0.43
2:N:558:ASP:OD1	2:N:560:ILE:N	2.51	0.43
2:O:193:LEU:O	2:O:198:VAL:HG13	2.18	0.43
2:P:3:ASP:O	2:P:6:LYS:HB3	2.18	0.43
1:A:9:HIS:CD2	1:A:9:HIS:C	2.96	0.43
1:B:114[A]:CYS:HB3	1:B:208:ILE:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:PRO:HA	1:D:429:ALA:O	2.18	0.43
2:M:604:ILE:HG23	2:M:611:ILE:HG22	2.01	0.43
2:N:384:LEU:HA	2:N:468:PHE:O	2.18	0.43
2:O:361:ILE:HD13	2:O:391:TYR:CB	2.46	0.43
2:P:613:ILE:HD13	2:P:652:ILE:HG12	1.99	0.43
1:A:220:HIS:CD2	1:A:221:MET:O	2.71	0.43
1:A:567:LEU:HD12	1:A:574:VAL:HG22	2.01	0.43
1:B:18:ARG:HD2	1:B:636:MET:HE3	2.00	0.43
1:B:287:LEU:HD12	1:B:388:TYR:CE1	2.54	0.43
1:D:322:VAL:O	1:D:326:GLN:HB2	2.18	0.43
2:N:478:MET:HG3	2:N:478:MET:O	2.18	0.43
2:O:142:ARG:NH1	2:O:228:MET:HG2	2.33	0.43
2:O:603:ALA:O	2:O:604:ILE:C	2.60	0.43
2:P:541:GLU:H	2:P:541:GLU:HG2	1.54	0.43
1:B:483:THR:HB	1:B:638:PRO:HB2	2.01	0.43
1:B:525:LYS:O	1:B:526:GLY:C	2.61	0.43
1:C:280:LEU:HD23	1:C:280:LEU:HA	1.74	0.43
1:D:217:ASN:O	1:D:223:MET:HG3	2.18	0.43
1:D:531:LEU:HD23	1:D:531:LEU:HA	1.75	0.43
2:N:315:LYS:CE	9:N:1162:HOH:O	2.67	0.43
2:O:491:ARG:O	2:O:495:LEU:HB2	2.19	0.43
2:P:558:ASP:OD1	2:P:558:ASP:C	2.62	0.43
1:A:238:ALA:O	1:A:241:ASP:HB3	2.19	0.43
1:C:223:MET:HG2	1:D:354:GLN:HA	2.01	0.43
1:C:559:LEU:O	1:C:563:MET:HG3	2.18	0.43
2:N:51:HIS:HB3	2:N:76:LEU:HD12	2.01	0.43
2:O:334:ARG:NH1	2:O:335:LYS:CG	2.82	0.43
2:P:369:ILE:HG21	2:P:468:PHE:CD2	2.54	0.43
2:P:479:GLU:O	2:P:480:VAL:C	2.61	0.43
1:A:394:ILE:HD12	1:A:394:ILE:HA	1.75	0.43
1:B:47:THR:HB	1:B:338:GLU:OE1	2.19	0.43
1:B:298:MET:HE2	1:B:301:GLU:OE2	2.18	0.43
1:C:626:ASP:HB3	2:O:212:PHE:CG	2.53	0.43
2:M:335:LYS:HG3	2:M:429:ARG:HH22	1.83	0.43
2:O:608:CYS:SG	2:O:712:LEU:HD12	2.58	0.43
1:A:283:HIS:CE1	4:A:800:XCC:S3	3.11	0.43
1:A:426:ARG:HH22	1:A:539:ILE:HB	1.82	0.43
1:B:484:VAL:O	1:B:488:LEU:HG	2.19	0.43
1:C:281:HIS:O	1:C:351:VAL:HA	2.18	0.43
1:C:436:LEU:HD23	1:C:436:LEU:HA	1.74	0.43
1:D:637:ASP:OD1	1:D:637:ASP:C	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:85:ARG:HD2	9:N:1043:HOH:O	2.18	0.43
2:N:423:ARG:HB3	2:N:485:TYR:CE2	2.53	0.43
2:N:674:LEU:HD22	2:N:678:LEU:HG	2.00	0.43
2:P:358:GLU:HA	2:P:361:ILE:CG2	2.49	0.43
2:P:412:ASN:HD21	2:P:419:HIS:HB3	1.82	0.43
2:P:626:MET:HE3	2:P:631:LEU:HD13	2.00	0.43
1:C:87:ARG:HD3	1:C:91:GLY:O	2.19	0.43
2:M:419:HIS:HE1	2:M:421:GLY:O	2.02	0.43
2:M:427:TRP:C	2:M:428:LEU:HD12	2.42	0.43
2:M:428:LEU:N	2:M:428:LEU:CD1	2.81	0.43
2:O:263:THR:O	2:O:266:ALA:HB3	2.19	0.43
2:O:569:ASP:O	2:O:573:THR:HG23	2.18	0.43
2:P:199:LYS:HG2	2:P:204:TYR:CZ	2.54	0.43
2:P:256:GLY:O	2:P:257:GLU:C	2.61	0.43
1:A:549:SER:O	1:A:552:ASP:HB2	2.19	0.43
1:B:280:LEU:HD13	1:B:288:SER:HB2	2.01	0.43
1:D:124:LEU:HD12	1:D:255:LEU:HD21	2.00	0.43
2:O:508:LEU:C	2:O:510:GLN:N	2.76	0.43
2:P:378:GLU:O	2:P:380:SER:N	2.52	0.43
2:P:426:ASN:O	2:P:427:TRP:CB	2.67	0.43
1:A:110:ALA:HA	1:A:241:ASP:OD2	2.19	0.42
1:A:470:CYS:HB3	4:A:800:XCC:S2	2.59	0.42
1:B:18:ARG:CD	1:B:636:MET:HE3	2.48	0.42
1:B:50:ASP:OD2	9:B:1055:HOH:O	2.21	0.42
1:B:317:CYS:HB3	9:B:1019:HOH:O	2.19	0.42
1:D:279:VAL:CG1	1:D:315:ILE:CD1	2.84	0.42
2:M:55:TYR:HB3	2:M:56:PRO:HD2	2.00	0.42
2:M:623:PRO:HA	2:M:707:THR:HA	2.01	0.42
2:N:160:LEU:HD21	2:N:262:LYS:HG2	2.01	0.42
2:N:316:ILE:HD13	2:N:317:LYS:O	2.19	0.42
2:O:527:LEU:HA	2:O:648:GLY:H	1.84	0.42
2:P:182:MET:HB2	2:P:205:ILE:HG22	2.00	0.42
1:A:186:LEU:HD22	1:A:205:PRO:HD2	2.00	0.42
1:A:574:VAL:O	1:A:576:PHE:N	2.51	0.42
1:D:285:PRO:O	1:D:286:LEU:C	2.61	0.42
2:M:604:ILE:HG22	2:M:610:GLY:O	2.19	0.42
2:O:409:ASP:O	2:O:410:PHE:C	2.62	0.42
2:O:509:CYS:CB	2:O:595:CYS:SG	3.07	0.42
2:P:492:MET:O	2:P:493:ARG:C	2.63	0.42
1:B:268:MET:HA	1:B:331:VAL:HG23	2.01	0.42
1:B:287:LEU:HA	1:B:388:TYR:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:HIS:CD2	1:D:213:SER:OG	2.69	0.42
2:N:382:LEU:HD12	2:N:382:LEU:HA	1.88	0.42
2:N:439:PHE:CD2	2:N:439:PHE:C	2.97	0.42
2:O:79:LEU:N	2:O:80:PRO:CD	2.82	0.42
2:O:160:LEU:HD13	2:O:215:ILE:HD13	2.02	0.42
2:O:356:VAL:HG11	2:O:360:GLU:CD	2.45	0.42
2:P:448:LEU:O	2:P:452:MET:HG2	2.20	0.42
1:A:453:ASN:ND2	1:A:566:ASP:HB3	2.34	0.42
1:B:467:ILE:O	1:B:497:ALA:HA	2.19	0.42
1:C:574:VAL:O	1:C:576:PHE:N	2.50	0.42
1:D:134:ASP:HB3	1:D:290:ILE:HD12	2.00	0.42
2:M:592:MET:HE3	2:M:592:MET:HB2	1.92	0.42
2:N:66:ARG:HD3	9:N:1029:HOH:O	2.19	0.42
2:O:174:LYS:HE2	2:O:323:ASN:ND2	2.34	0.42
2:O:430:VAL:HG12	2:O:434:ALA:HB3	2.01	0.42
2:O:468:PHE:HB2	2:O:474:VAL:CG2	2.41	0.42
2:P:315[A]:LYS:HD3	9:P:1080:HOH:O	2.19	0.42
2:P:323:ASN:HB2	2:P:415:GLU:OE1	2.19	0.42
2:P:359:SER:C	2:P:361:ILE:H	2.27	0.42
1:A:2:PRO:N	6:A:862:GOL:O1	2.52	0.42
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.72	0.42
1:B:579:SER:HA	1:B:603:HIS:O	2.20	0.42
1:B:602:THR:CG2	5:B:1001:XE:XE	3.46	0.42
1:C:190:ILE:HG13	1:C:195:LYS:HG3	2.01	0.42
1:D:592:GLY:HA2	5:D:1001:XE:XE	2.98	0.42
2:M:448:LEU:HD12	2:M:448:LEU:HA	1.90	0.42
2:M:503:PHE:CG	2:M:521:THR:HG22	2.54	0.42
2:N:466:THR:HG21	2:N:468:PHE:CZ	2.55	0.42
2:O:114:GLU:HG3	2:O:216:VAL:HG12	2.01	0.42
2:O:397:ALA:HA	2:O:400:GLU:HG3	2.01	0.42
2:P:722:ALA:HA	2:P:725:MET:SD	2.60	0.42
1:A:6:ASP:OD1	1:A:6:ASP:C	2.63	0.42
1:A:106:ILE:HD11	5:A:1003[A]:XE:XE	2.98	0.42
1:A:515:ASN:HA	1:A:518:THR:HG23	2.02	0.42
1:D:292:VAL:HG22	1:D:312:LEU:HD13	2.01	0.42
1:D:400:ALA:HB2	5:D:1010:XE:XE	2.98	0.42
2:N:107:TRP:CZ3	2:N:219:ALA:HB1	2.54	0.42
2:N:405:ARG:HD2	9:N:1219:HOH:O	2.18	0.42
2:O:470:ASP:O	2:O:474:VAL:HB	2.19	0.42
2:P:528:CYS:HB3	3:P:900:SF4:S3	2.59	0.42
2:P:668:VAL:HB	2:P:715:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLU:HB2	9:A:1023:HOH:O	2.20	0.42
1:B:637:ASP:HA	1:B:638:PRO:HD2	1.75	0.42
1:C:655:LYS:NZ	1:C:674:TYR:O	2.38	0.42
2:M:121:TYR:CD1	2:M:121:TYR:C	2.98	0.42
2:M:525:VAL:HG23	2:M:532:SER:HA	2.01	0.42
2:N:199:LYS:HD2	2:N:204:TYR:CE2	2.55	0.42
2:N:478:MET:O	2:N:482:ARG:HG3	2.20	0.42
2:O:182:MET:HG3	2:O:205:ILE:HG22	2.01	0.42
2:O:482:ARG:HH12	2:O:485:TYR:HE1	1.67	0.42
2:O:497:ASP:HB2	2:O:656:LYS:HZ1	1.84	0.42
2:O:669:TRP:CD1	2:O:711:ILE:HG21	2.53	0.42
2:P:184:PHE:HD1	2:P:209:LEU:HD21	1.84	0.42
2:P:392:GLY:H	2:P:395:MET:HB2	1.84	0.42
1:A:2:PRO:HB2	1:A:651:TYR:CE2	2.55	0.42
1:B:287:LEU:HD13	1:B:388:TYR:CD1	2.54	0.42
1:B:572:PRO:CG	1:B:629:GLY:HA3	2.50	0.42
1:C:283:HIS:CD2	1:C:317:CYS:CB	3.00	0.42
2:N:26:TYR:CE1	2:N:30:ILE:HD11	2.55	0.42
2:N:150:ASP:OD1	2:N:150:ASP:C	2.59	0.42
2:N:243:TYR:CZ	2:N:247:ARG:HD3	2.54	0.42
2:O:118:TYR:CE2	2:O:121:TYR:CD2	3.08	0.42
1:B:536:ASN:HD22	1:C:23:LYS:HB3	1.85	0.42
1:C:154:VAL:O	1:C:154:VAL:CG1	2.67	0.42
1:C:187:MET:HE3	1:C:195:LYS:HG2	2.02	0.42
1:D:215:LEU:HD22	1:D:234:ALA:HA	2.02	0.42
1:D:324:MET:HE3	1:D:324:MET:HB3	1.95	0.42
1:D:496:VAL:HG11	1:D:547:MET:SD	2.60	0.42
2:M:64:VAL:HB	2:M:223:LEU:HD12	2.02	0.42
2:O:278:THR:O	2:O:294:SER:HA	2.20	0.42
2:P:316:ILE:HD13	2:P:454:GLU:CD	2.45	0.42
1:A:105:MET:HE3	1:A:105:MET:HB3	1.86	0.42
1:A:414:SER:O	1:A:416:ARG:HD2	2.19	0.42
1:A:577:VAL:HG13	1:A:649:LEU:CD2	2.50	0.42
1:B:637:ASP:OD1	1:B:637:ASP:C	2.63	0.42
1:D:287:LEU:HA	1:D:388:TYR:OH	2.19	0.42
2:M:152:THR:O	2:M:154:PRO:HD3	2.20	0.42
2:O:338:MET:SD	2:O:341:GLU:HB2	2.60	0.42
2:O:628:PHE:O	2:O:632:ALA:N	2.39	0.42
2:O:712:LEU:HA	2:O:715:LEU:HB2	2.00	0.42
2:P:289:PRO:O	2:P:290:ASP:HB2	2.20	0.42
2:P:395:MET:SD	2:P:459:ILE:HG23	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ILE:O	1:A:381:PRO:C	2.61	0.41
1:B:176:ARG:O	1:B:207:GLY:HA3	2.20	0.41
1:B:577:VAL:HG13	1:B:649:LEU:CD2	2.50	0.41
1:B:620:LEU:HD21	5:B:1003[A]:XE:XE	2.98	0.41
1:D:353:VAL:O	1:D:354:GLN:HB2	2.19	0.41
2:M:16:LYS:HA	2:M:16:LYS:HD2	1.37	0.41
2:N:43:ALA:O	2:N:47:TYR:HD2	2.03	0.41
2:O:121:TYR:CD1	2:O:121:TYR:C	2.98	0.41
2:O:504:TYR:HA	2:O:549:GLN:O	2.20	0.41
2:O:592:MET:HB2	2:O:592:MET:HE3	1.61	0.41
2:O:672:LYS:C	2:O:674:LEU:N	2.77	0.41
2:O:675:LYS:H	2:O:675:LYS:HG2	1.61	0.41
2:P:349:ALA:C	2:P:426:ASN:HD22	2.28	0.41
2:P:392:GLY:C	2:P:394:LYS:H	2.27	0.41
1:B:88:GLY:HA3	3:B:700:SF4:S3	2.60	0.41
1:C:603:HIS:HA	1:C:633:ILE:HB	2.01	0.41
2:M:357:SER:O	2:M:360:GLU:HB2	2.20	0.41
2:N:349:ALA:HA	2:N:384:LEU:O	2.20	0.41
2:N:549:GLN:NE2	2:N:570:TYR:OH	2.53	0.41
2:O:127:LEU:O	2:O:128:LEU:HD23	2.20	0.41
2:O:368:VAL:HG22	2:O:442:LYS:HB3	2.01	0.41
2:P:369:ILE:HG23	2:P:370:GLY:N	2.36	0.41
2:P:481:ALA:HB1	2:P:485:TYR:CZ	2.55	0.41
1:A:213:SER:CB	1:B:209:HIS:HD2	2.33	0.41
1:D:28:THR:HG21	1:D:33:VAL:CG1	2.51	0.41
2:O:500:VAL:HG22	2:O:501:ASP:H	1.85	0.41
2:P:351:GLU:O	2:P:485:TYR:OH	2.31	0.41
1:A:142:LYS:NZ	1:A:253:ASP:OD2	2.44	0.41
1:A:607:MET:HG3	1:A:608:PRO:O	2.21	0.41
1:B:18:ARG:NE	1:B:636:MET:HE3	2.34	0.41
1:C:144:LYS:HG2	1:C:154:VAL:HG11	2.02	0.41
2:M:669:TRP:HA	2:M:700:ALA:O	2.20	0.41
2:N:615:THR:HG21	2:N:674:LEU:HG	2.02	0.41
2:O:335:LYS:HG3	2:O:336:GLY:H	1.85	0.41
2:O:683:VAL:O	2:O:686:SER:HB2	2.21	0.41
1:A:23:LYS:HE3	9:A:1176:HOH:O	2.20	0.41
1:C:348:ALA:HA	1:C:370:ARG:O	2.21	0.41
2:M:278:THR:O	2:M:294:SER:HA	2.21	0.41
2:N:223:LEU:HD23	2:N:223:LEU:HA	1.88	0.41
2:N:243:TYR:CE2	2:N:247:ARG:HD3	2.56	0.41
2:P:268:GLY:O	2:P:272:THR:HG22	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASN:HB2	1:A:345:ALA:O	2.20	0.41
1:A:560:LEU:HD22	1:A:600:VAL:HG21	2.02	0.41
1:B:574:VAL:HA	1:B:575:PRO:HD3	1.89	0.41
1:D:557:VAL:O	1:D:558:ASP:C	2.64	0.41
2:N:87:ARG:HD2	9:N:1013:HOH:O	2.20	0.41
2:N:314:THR:O	2:N:315:LYS:C	2.63	0.41
2:N:403:LEU:O	2:N:452:MET:HE1	2.19	0.41
2:O:302:VAL:O	2:O:306:MET:HG3	2.20	0.41
2:P:358:GLU:HG3	2:P:462:ARG:NH1	2.36	0.41
1:A:125:VAL:HG23	1:A:167:GLY:HA3	2.02	0.41
1:A:235:ILE:HD11	5:A:1004:XE:XE	2.98	0.41
1:A:603:HIS:HA	1:A:633:ILE:O	2.20	0.41
1:B:447:ASN:O	1:B:450:ARG:HB3	2.21	0.41
1:C:332:THR:HG23	1:C:333:SER:N	2.36	0.41
1:D:573:LYS:HE2	1:D:671:CYS:O	2.21	0.41
2:M:463:VAL:HG12	2:M:464:GLN:N	2.36	0.41
2:M:606:PRO:O	2:M:608:CYS:N	2.54	0.41
2:O:142:ARG:CZ	2:O:228:MET:HG2	2.50	0.41
2:O:335:LYS:CD	2:O:336:GLY:N	2.83	0.41
2:O:482:ARG:NH1	2:O:482:ARG:HA	2.35	0.41
2:O:527:LEU:HD12	2:O:528:CYS:N	2.36	0.41
2:P:3:ASP:HB2	9:P:1058:HOH:O	2.20	0.41
2:P:393:ARG:HB3	2:P:393:ARG:CZ	2.49	0.41
2:P:556:GLU:OE1	2:P:559:PRO:HG3	2.21	0.41
2:P:602:MET:HE3	2:P:602:MET:HB2	1.92	0.41
1:B:14:SER:O	6:B:861:GOL:H12	2.21	0.41
1:B:256:PHE:CG	1:B:289:GLU:HG3	2.56	0.41
1:B:353:VAL:O	1:B:354:GLN:HB2	2.19	0.41
1:D:416:ARG:C	1:D:418:VAL:N	2.78	0.41
2:N:607:GLU:HB3	9:N:1067:HOH:O	2.21	0.41
2:N:678:LEU:O	2:N:679:HIS:C	2.63	0.41
2:O:340:VAL:HG12	2:O:380:SER:O	2.19	0.41
2:O:342:MET:HG3	2:O:384:LEU:HD23	2.02	0.41
2:O:396:GLN:HB2	2:O:399:PHE:CD2	2.55	0.41
2:O:408:HIS:O	2:O:412:ASN:HB2	2.21	0.41
2:P:163:ALA:CB	2:P:169:LEU:HB2	2.50	0.41
2:P:424:ASN:ND2	2:P:485:TYR:HD2	2.19	0.41
1:A:90:CYS:O	1:B:357:MET:HG2	2.21	0.41
1:B:466:LEU:HA	1:B:496:VAL:O	2.21	0.41
1:C:439:LEU:HD21	1:C:531:LEU:HD13	2.03	0.41
2:M:182:MET:HG3	2:M:205:ILE:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:309:ARG:HA	2:M:309:ARG:HD2	1.82	0.41
2:M:651:TYR:O	2:M:654:SER:HB3	2.21	0.41
2:N:16:LYS:HE2	2:N:16:LYS:HB3	1.63	0.41
2:N:61:TYR:CD2	2:N:66:ARG:HD2	2.56	0.41
2:N:245:ARG:HD2	9:N:1137:HOH:O	2.21	0.41
2:N:288:ILE:O	2:N:289:PRO:C	2.64	0.41
2:N:570:TYR:CD1	2:N:570:TYR:C	2.98	0.41
2:O:71:GLU:HG3	2:O:82:ILE:CD1	2.51	0.41
2:O:79:LEU:HD22	2:O:112:ILE:HG12	2.03	0.41
2:O:151:TRP:HA	2:O:151:TRP:HE3	1.86	0.41
2:O:521:THR:O	2:O:522:PRO:C	2.62	0.41
2:O:602:MET:HG2	2:O:611:ILE:HD12	2.03	0.41
2:P:64:VAL:HB	2:P:223:LEU:HD12	2.03	0.41
2:P:147:LYS:NZ	2:P:329:GLU:OE1	2.54	0.41
2:P:230:GLY:HA3	2:P:243:TYR:CE2	2.56	0.41
2:P:605:LEU:O	2:P:606:PRO:C	2.63	0.41
2:P:626:MET:CE	2:P:631:LEU:HD13	2.50	0.41
1:A:401:ILE:HG22	1:A:405:ILE:HD12	2.03	0.41
1:B:316:CYS:HB3	1:B:317:CYS:H	1.66	0.41
1:C:73:ALA:HB2	1:D:584:MET:HG3	2.03	0.41
1:C:256:PHE:CD1	1:C:289:GLU:HG3	2.55	0.41
1:C:260:GLN:O	1:C:261:PRO:C	2.64	0.41
2:N:146:ILE:HG22	9:N:1044:HOH:O	2.21	0.41
2:O:111:GLU:HB2	2:O:216:VAL:HG21	2.02	0.41
2:O:243:TYR:CE2	2:O:247:ARG:HD2	2.56	0.41
2:O:407:ILE:O	2:O:410:PHE:N	2.54	0.41
2:P:64:VAL:HG13	2:P:111:GLU:CD	2.46	0.41
1:A:655:LYS:NZ	1:A:674:TYR:O	2.51	0.40
1:C:316:CYS:HB3	1:C:317:CYS:H	1.78	0.40
2:M:282:LEU:HA	2:M:283:PRO:HD2	1.86	0.40
2:N:353:VAL:HG22	2:N:388:VAL:HB	2.02	0.40
2:N:424:ASN:HD22	2:N:425:ILE:N	2.19	0.40
2:O:444:TYR:O	2:O:448:LEU:HG	2.20	0.40
2:P:18:PRO:HB2	2:P:21:LEU:HB3	2.03	0.40
2:P:316:ILE:HD12	2:P:316:ILE:HA	1.94	0.40
1:A:68:CYS:HB2	1:A:97:ILE:CG2	2.46	0.40
1:B:127:MET:HA	1:B:132:ALA:HB3	2.03	0.40
1:B:299:GLU:O	1:B:303:LYS:HG3	2.21	0.40
1:C:261:PRO:HA	1:C:429:ALA:O	2.21	0.40
1:D:36:MET:CE	1:D:343:THR:HA	2.50	0.40
2:M:67:CYS:SG	2:M:223:LEU:HB3	2.61	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:655:LYS:HG2	2:M:685:ARG:NH1	2.36	0.40
2:N:206:ALA:O	2:N:208:PRO:HD3	2.21	0.40
2:N:607:GLU:CB	9:N:1067:HOH:O	2.69	0.40
2:O:51:HIS:HA	2:O:52:PRO:HD3	1.91	0.40
2:O:343:GLY:O	2:O:346:ARG:NH1	2.55	0.40
2:O:602:MET:O	2:O:644:PHE:HA	2.21	0.40
2:P:607:GLU:HB3	2:P:708:VAL:HG11	2.03	0.40
1:A:2:PRO:HD3	1:A:625:SER:CB	2.51	0.40
1:B:218:GLN:HE22	1:B:233:SER:CB	2.34	0.40
1:B:576:PHE:C	1:B:576:PHE:CD1	2.99	0.40
1:D:399:THR:O	1:D:403:MET:HG3	2.22	0.40
1:D:564:ALA:HB1	1:D:569:VAL:O	2.21	0.40
2:M:184:PHE:HB3	2:M:209:LEU:HD11	2.03	0.40
2:M:571:LEU:HD23	2:M:571:LEU:HA	1.91	0.40
2:O:245:ARG:O	2:O:245:ARG:HG3	2.16	0.40
2:O:317:LYS:HA	2:O:318:LEU:HD23	2.03	0.40
2:P:505:SER:CB	2:P:570:TYR:CE2	3.05	0.40
1:C:325:ARG:HH11	1:C:325:ARG:HD2	1.67	0.40
1:C:483:THR:HB	1:C:638:PRO:HB2	2.03	0.40
1:D:287:LEU:HA	1:D:388:TYR:CZ	2.56	0.40
2:M:342:MET:HB3	2:M:382:LEU:O	2.21	0.40
2:N:521:THR:O	2:N:522:PRO:C	2.65	0.40
2:N:621:MET:HB3	2:N:621:MET:HE3	1.30	0.40
2:O:649:ARG:HG2	2:O:674:LEU:HD11	2.03	0.40
2:P:201:GLY:HA2	9:P:1017:HOH:O	2.20	0.40
2:P:266:ALA:O	2:P:269:ALA:HB3	2.21	0.40
2:P:419:HIS:C	2:P:419:HIS:ND1	2.80	0.40
2:P:510:GLN:HA	2:P:513:ALA:O	2.22	0.40
1:C:122:HIS:CD2	9:C:1127:HOH:O	2.71	0.40
1:C:515:ASN:HD22	1:C:515:ASN:HA	1.71	0.40
1:C:596:VAL:HG21	1:C:632:PHE:CD2	2.56	0.40
1:D:271:LEU:O	1:D:420:ILE:HD13	2.22	0.40
2:M:343:GLY:C	2:M:345:ASN:H	2.29	0.40
2:N:4:PHE:O	2:N:7:ILE:HG12	2.20	0.40
2:O:142:ARG:O	2:O:143:ARG:C	2.65	0.40
2:O:169:LEU:HD12	2:O:193:LEU:HG	2.04	0.40
2:P:277:ILE:HD12	2:P:277:ILE:N	2.37	0.40
2:P:399:PHE:CD1	2:P:399:PHE:N	2.88	0.40
2:P:604:ILE:HG22	2:P:643:GLY:O	2.20	0.40
2:P:627:THR:O	2:P:631:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	671/674 (100%)	637 (95%)	31 (5%)	3 (0%)	30	49
1	B	671/674 (100%)	638 (95%)	31 (5%)	2 (0%)	36	55
1	C	671/674 (100%)	636 (95%)	33 (5%)	2 (0%)	36	55
1	D	671/674 (100%)	632 (94%)	36 (5%)	3 (0%)	30	49
2	M	726/729 (100%)	678 (93%)	41 (6%)	7 (1%)	12	24
2	N	726/729 (100%)	692 (95%)	27 (4%)	7 (1%)	12	24
2	O	725/729 (100%)	592 (82%)	104 (14%)	29 (4%)	2	3
2	P	726/729 (100%)	622 (86%)	78 (11%)	26 (4%)	2	3
All	All	5587/5612 (100%)	5127 (92%)	381 (7%)	79 (1%)	9	17

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	316	ILE
2	O	335	LYS
2	O	348	PRO
2	O	372	ASP
2	O	408	HIS
2	O	428	LEU
2	O	458	ALA
2	O	470	ASP
2	O	581	GLN
2	O	726	ASP
2	P	423	ARG
2	P	424	ASN
2	P	427	TRP
1	A	267	ASN
1	A	415	ASN
1	B	473	LEU
1	C	416	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	473	LEU
2	M	315	LYS
2	N	290	ASP
2	N	315	LYS
2	N	316	ILE
2	N	658	ILE
2	O	319	ASP
2	O	358	GLU
2	O	373	ILE
2	O	478	MET
2	O	650	THR
2	O	657	PHE
2	P	319	ASP
2	P	338	MET
2	P	359	SER
2	P	370	GLY
2	P	380	SER
2	P	474	VAL
2	P	480	VAL
2	P	491	ARG
2	M	228	MET
2	M	316	ILE
2	M	345	ASN
2	M	596	GLY
2	M	658	ILE
2	N	228	MET
2	O	123	PRO
2	O	154	PRO
2	O	187	ASP
2	O	290	ASP
2	O	527	LEU
2	O	556	GLU
2	P	187	ASP
2	P	346	ARG
2	P	360	GLU
2	P	449	VAL
2	P	489	ASP
1	C	354	GLN
2	M	187	ASP
2	N	187	ASP
2	N	596	GLY
2	O	338	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	374	ASP
2	O	493	ARG
2	O	509	CYS
2	P	320	LEU
2	P	337	ASP
2	P	378	GLU
2	P	596	GLY
1	A	316	CYS
1	B	354	GLN
1	D	267	ASN
1	D	354	GLN
2	O	345	ASN
2	O	406	ARG
2	P	10	GLY
2	P	393	ARG
2	P	379	GLY
2	P	522	PRO
2	P	336	GLY
2	O	727	PRO
2	P	638	GLY

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	542/543 (100%)	507 (94%)	35 (6%)	15	32
1	B	542/543 (100%)	517 (95%)	25 (5%)	24	48
1	C	542/543 (100%)	500 (92%)	42 (8%)	12	25
1	D	542/543 (100%)	504 (93%)	38 (7%)	14	29
2	M	610/611 (100%)	551 (90%)	59 (10%)	8	17
2	N	610/611 (100%)	561 (92%)	49 (8%)	11	24
2	O	608/611 (100%)	463 (76%)	145 (24%)	1	1
2	P	610/611 (100%)	513 (84%)	97 (16%)	2	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4606/4616 (100%)	4116 (89%)	490 (11%)	6 14

All (490) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	27	ARG
1	A	118	ASN
1	A	126	GLU
1	A	145	GLU
1	A	148[A]	ARG
1	A	153	GLU
1	A	168	GLU
1	A	206	PHE
1	A	293	GLN
1	A	299	GLU
1	A	318	THR
1	A	331	VAL
1	A	336	SER
1	A	339	LEU
1	A	370	ARG
1	A	395	GLU
1	A	398	LYS
1	A	405	ILE
1	A	415	ASN
1	A	416	ARG
1	A	426	ARG
1	A	438	LYS
1	A	461	LEU
1	A	466	LEU
1	A	482	LEU
1	A	501	SER
1	A	518	THR
1	A	530	ARG
1	A	538	GLU
1	A	585	SER
1	A	647	ASP
1	A	656	LEU
1	A	664	GLU
1	A	665[A]	ARG
1	B	82[A]	ASP
1	B	114[A]	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	159	VAL
1	B	206	PHE
1	B	298	MET
1	B	318	THR
1	B	336	SER
1	B	394	ILE
1	B	395	GLU
1	B	406	GLU
1	B	413	GLU
1	B	415	ASN
1	B	416	ARG
1	B	418	VAL
1	B	427	VAL
1	B	447	ASN
1	B	466	LEU
1	B	470	CYS
1	B	482	LEU
1	B	518	THR
1	B	531	LEU
1	B	539	ILE
1	B	600	VAL
1	B	647	ASP
1	B	656	LEU
1	C	12	ARG
1	C	23	LYS
1	C	66	ILE
1	C	82	ASP
1	C	86	SER
1	C	114	CYS
1	C	118	ASN
1	C	159	VAL
1	C	196	GLU
1	C	206	PHE
1	C	218	GLN
1	C	233	SER
1	C	260	GLN
1	C	291	ILE
1	C	331	VAL
1	C	359	SER
1	C	360	ILE
1	C	370	ARG
1	C	384	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	409	LYS
1	C	411	ARG
1	C	412	LYS
1	C	413	GLU
1	C	416	ARG
1	C	427	VAL
1	C	438	LYS
1	C	466	LEU
1	C	470	CYS
1	C	482	LEU
1	C	501	SER
1	C	503	GLN
1	C	507	LYS
1	C	533	GLU
1	C	539[A]	ILE
1	C	579	SER
1	C	585	SER
1	C	600	VAL
1	C	647	ASP
1	C	653	THR
1	C	656	LEU
1	C	664	GLU
1	C	669	LYS
1	D	3	ARG
1	D	12	ARG
1	D	40	SER
1	D	61	ILE
1	D	66	ILE
1	D	77	ARG
1	D	82	ASP
1	D	105	MET
1	D	155	GLU
1	D	159	VAL
1	D	190	ILE
1	D	199	ARG
1	D	206	PHE
1	D	275	GLN
1	D	293	GLN
1	D	296	ARG
1	D	298	MET
1	D	299	GLU
1	D	326	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	331	VAL
1	D	395	GLU
1	D	396	SER
1	D	409	LYS
1	D	418	VAL
1	D	427	VAL
1	D	466	LEU
1	D	470	CYS
1	D	482	LEU
1	D	496	VAL
1	D	518	THR
1	D	529	LYS
1	D	533	GLU
1	D	539	ILE
1	D	600	VAL
1	D	613	SER
1	D	647	ASP
1	D	656	LEU
1	D	664	GLU
2	M	6	LYS
2	M	16	LYS
2	M	17	GLU
2	M	19	VAL
2	M	62	LEU
2	M	64	VAL
2	M	66	ARG
2	M	95	ASN
2	M	127	LEU
2	M	152	THR
2	M	164	LYS
2	M	169	LEU
2	M	174	LYS
2	M	198	VAL
2	M	214	GLN
2	M	215	ILE
2	M	221	TYR
2	M	245	ARG
2	M	249	ARG
2	M	262	LYS
2	M	284	GLU
2	M	315	LYS
2	M	317	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	334	ARG
2	M	335	LYS
2	M	342	MET
2	M	354	ARG
2	M	373	ILE
2	M	375	GLN
2	M	381	LYS
2	M	382	LEU
2	M	422	GLN
2	M	424	ASN
2	M	425	ILE
2	M	426	ASN
2	M	442	LYS
2	M	448	LEU
2	M	470	ASP
2	M	475	LYS
2	M	478	MET
2	M	479	GLU
2	M	486	LYS
2	M	539	SER
2	M	571	LEU
2	M	602	MET
2	M	604	ILE
2	M	621	MET
2	M	631	LEU
2	M	634	MET
2	M	672	LYS
2	M	674	LEU
2	M	686	SER
2	M	693	GLU
2	M	702	GLU
2	M	704	ILE
2	M	711	ILE
2	M	723	LEU
2	M	726	ASP
2	M	729	MET
2	N	6	LYS
2	N	14	GLU
2	N	64	VAL
2	N	66	ARG
2	N	95	ASN
2	N	122	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	147	LYS
2	N	152	THR
2	N	167	LYS
2	N	174	LYS
2	N	198	VAL
2	N	205	ILE
2	N	249	ARG
2	N	262	LYS
2	N	313	LEU
2	N	314	THR
2	N	316	ILE
2	N	334	ARG
2	N	335	LYS
2	N	354	ARG
2	N	362	THR
2	N	373	ILE
2	N	381	LYS
2	N	396	GLN
2	N	405	ARG
2	N	424	ASN
2	N	425	ILE
2	N	437	LYS
2	N	440	ARG
2	N	442	LYS
2	N	448	LEU
2	N	451	LYS
2	N	462	ARG
2	N	470	ASP
2	N	475	LYS
2	N	478	MET
2	N	495	LEU
2	N	571	LEU
2	N	588	MET
2	N	604	ILE
2	N	606	PRO
2	N	631	LEU
2	N	639	THR
2	N	674	LEU
2	N	675	LYS
2	N	686	SER
2	N	693	GLU
2	N	704	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	729	MET
2	O	2	THR
2	O	3	ASP
2	O	5	ASP
2	O	7	ILE
2	O	14	GLU
2	O	16	LYS
2	O	17	GLU
2	O	19	VAL
2	O	34	SER
2	O	39	LEU
2	O	62	LEU
2	O	64	VAL
2	O	66	ARG
2	O	86	LYS
2	O	95	ASN
2	O	97	GLU
2	O	122	LYS
2	O	125	GLU
2	O	127	LEU
2	O	164	LYS
2	O	174	LYS
2	O	198	VAL
2	O	205	ILE
2	O	224	ARG
2	O	228	MET
2	O	245	ARG
2	O	262	LYS
2	O	284	GLU
2	O	285	ASP
2	O	286	LYS
2	O	303	GLN
2	O	307	GLU
2	O	313	LEU
2	O	314	THR
2	O	318	LEU
2	O	320	LEU
2	O	323	ASN
2	O	332	SER
2	O	334	ARG
2	O	335	LYS
2	O	340	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	342	MET
2	O	346	ARG
2	O	347	THR
2	O	350	PHE
2	O	352	LEU
2	O	354	ARG
2	O	356	VAL
2	O	357	SER
2	O	358	GLU
2	O	359	SER
2	O	361	ILE
2	O	362	THR
2	O	366	ILE
2	O	367	GLU
2	O	368	VAL
2	O	373	ILE
2	O	375	GLN
2	O	376	ILE
2	O	378	GLU
2	O	384	LEU
2	O	386	ILE
2	O	388	VAL
2	O	393	ARG
2	O	394	LYS
2	O	399	PHE
2	O	402	VAL
2	O	403	LEU
2	O	405	ARG
2	O	406	ARG
2	O	409	ASP
2	O	420	THR
2	O	425	ILE
2	O	426	ASN
2	O	427	TRP
2	O	428	LEU
2	O	429	ARG
2	O	432	LYS
2	O	451	LYS
2	O	461	ASP
2	O	463	VAL
2	O	465	VAL
2	O	466	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	469	THR
2	O	473	LYS
2	O	474	VAL
2	O	476	GLU
2	O	478	MET
2	O	482	ARG
2	O	485	TYR
2	O	486	LYS
2	O	487	GLU
2	O	488	ARG
2	O	489	ASP
2	O	490	ASP
2	O	491	ARG
2	O	492	MET
2	O	493	ARG
2	O	495	LEU
2	O	496	THR
2	O	497	ASP
2	O	523	GLU
2	O	524	ARG
2	O	525	VAL
2	O	527	LEU
2	O	534	LEU
2	O	544	HIS
2	O	560	ILE
2	O	565	LYS
2	O	567	VAL
2	O	575	SER
2	O	577	ARG
2	O	579	LEU
2	O	582	VAL
2	O	586	THR
2	O	594	SER
2	O	598	PHE
2	O	604	ILE
2	O	609	ASN
2	O	612	MET
2	O	614	THR
2	O	615	THR
2	O	621	MET
2	O	631	LEU
2	O	634	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	635	ILE
2	O	639	THR
2	O	640	GLN
2	O	641	THR
2	O	658	ILE
2	O	664	ILE
2	O	670	MET
2	O	672	LYS
2	O	675	LYS
2	O	681	GLU
2	O	683	VAL
2	O	687	VAL
2	O	689	GLU
2	O	693	GLU
2	O	704	ILE
2	O	708	VAL
2	O	710	GLU
2	O	712	LEU
2	O	725	MET
2	O	728	ILE
2	P	6	LYS
2	P	9	GLU
2	P	39	LEU
2	P	64	VAL
2	P	66	ARG
2	P	95	ASN
2	P	125	GLU
2	P	130	PRO
2	P	146[A]	ILE
2	P	152	THR
2	P	171	LYS
2	P	174	LYS
2	P	182	MET
2	P	183	LEU
2	P	198	VAL
2	P	199	LYS
2	P	205	ILE
2	P	245	ARG
2	P	262	LYS
2	P	284	GLU
2	P	286	LYS
2	P	312	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	313	LEU
2	P	314	THR
2	P	316	ILE
2	P	318	LEU
2	P	331	GLU
2	P	334	ARG
2	P	335	LYS
2	P	340	VAL
2	P	342	MET
2	P	346	ARG
2	P	347	THR
2	P	351	GLU
2	P	353	VAL
2	P	354	ARG
2	P	355	THR
2	P	362	THR
2	P	365	LYS
2	P	366	ILE
2	P	369	ILE
2	P	373	ILE
2	P	382	LEU
2	P	388	VAL
2	P	390	ILE
2	P	393	ARG
2	P	398	ASP
2	P	403	LEU
2	P	422	GLN
2	P	424	ASN
2	P	428	LEU
2	P	431	SER
2	P	435	VAL
2	P	442	LYS
2	P	448	LEU
2	P	462	ARG
2	P	463	VAL
2	P	464	GLN
2	P	469	THR
2	P	473	LYS
2	P	474	VAL
2	P	485	TYR
2	P	486	LYS
2	P	487	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	490	ASP
2	P	495	LEU
2	P	501	ASP
2	P	527	LEU
2	P	537	LYS
2	P	541	GLU
2	P	542	ILE
2	P	551	ILE
2	P	556	GLU
2	P	563	ILE
2	P	565	LYS
2	P	567	VAL
2	P	569	ASP
2	P	571	LEU
2	P	579	LEU
2	P	605	LEU
2	P	631	LEU
2	P	639	THR
2	P	652	ILE
2	P	656	LYS
2	P	661	ASP
2	P	672	LYS
2	P	674	LEU
2	P	678	LEU
2	P	681	GLU
2	P	685	ARG
2	P	704	ILE
2	P	707	THR
2	P	717	GLU
2	P	718	LYS
2	P	726	ASP
2	P	728	ILE
2	P	729	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	118	ASN
1	A	209	HIS
1	A	217	ASN
1	A	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	220	HIS
1	A	260	GLN
1	A	275	GLN
1	A	471	ASN
1	A	477	GLN
1	A	479	ASN
1	A	515	ASN
1	A	565	ASN
1	A	622	GLN
1	A	672	GLN
1	B	58	GLN
1	B	119	HIS
1	B	122	HIS
1	B	209	HIS
1	B	217	ASN
1	B	218	GLN
1	B	220	HIS
1	B	293	GLN
1	B	415	ASN
1	B	447	ASN
1	B	454	GLN
1	B	471	ASN
1	B	477	GLN
1	B	479	ASN
1	B	503	GLN
1	B	515	ASN
1	B	565	ASN
1	B	622	GLN
1	B	672	GLN
1	C	56	GLN
1	C	58	GLN
1	C	209	HIS
1	C	217	ASN
1	C	218	GLN
1	C	443	GLN
1	C	454	GLN
1	C	471	ASN
1	C	477	GLN
1	C	479	ASN
1	C	503	GLN
1	C	515	ASN
1	C	639	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	672	GLN
1	D	56	GLN
1	D	58	GLN
1	D	118	ASN
1	D	164	GLN
1	D	209	HIS
1	D	217	ASN
1	D	218	GLN
1	D	220	HIS
1	D	446	GLN
1	D	471	ASN
1	D	477	GLN
1	D	503	GLN
1	D	515	ASN
1	D	639	GLN
2	M	95	ASN
2	M	192	GLN
2	M	197	ASN
2	M	211	ASN
2	M	287	GLN
2	M	408	HIS
2	M	424	ASN
2	M	426	ASN
2	M	510	GLN
2	M	581	GLN
2	M	590	ASN
2	N	95	ASN
2	N	192	GLN
2	N	211	ASN
2	N	408	HIS
2	N	424	ASN
2	N	510	GLN
2	N	515	ASN
2	N	549	GLN
2	N	576	ASN
2	N	581	GLN
2	N	590	ASN
2	N	679	HIS
2	O	51	HIS
2	O	95	ASN
2	O	211	ASN
2	O	244	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	258	HIS
2	O	323	ASN
2	O	396	GLN
2	O	515	ASN
2	O	516	HIS
2	O	568	ASN
2	O	578	ASN
2	O	590	ASN
2	O	618	HIS
2	O	640	GLN
2	O	679	HIS
2	P	27	HIS
2	P	95	ASN
2	P	192	GLN
2	P	211	ASN
2	P	303	GLN
2	P	396	GLN
2	P	424	ASN
2	P	426	ASN
2	P	510	GLN
2	P	515	ASN
2	P	544	HIS
2	P	548	ASN
2	P	549	GLN
2	P	568	ASN
2	P	576	ASN
2	P	618	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 75 ligands modelled in this entry, 50 are monoatomic - leaving 25 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	$\# Z > 2$
4	XCC	A	800	1	0,12,12	-	-	-		
3	SF4	M	900	2	0,12,12	-	-	-		
3	SF4	A	750	1	0,12,12	-	-	-		
3	SF4	A	700	1	0,12,12	-	-	-		
3	SF4	B	700	1	0,12,12	-	-	-		
6	GOL	C	861	-	5,5,5	0.62	0	5,5,5	0.81	0
4	XCC	D	800	1	0,12,12	-	-	-		
6	GOL	B	863	-	5,5,5	0.79	0	5,5,5	1.75	2 (40%)
4	XCC	C	800	1	0,12,12	-	-	-		
6	GOL	D	860	-	5,5,5	0.54	0	5,5,5	0.38	0
3	SF4	N	900	2	0,12,12	-	-	-		
3	SF4	C	750	1	0,12,12	-	-	-		
3	SF4	P	900	2	0,12,12	-	-	-		
6	GOL	C	860	-	5,5,5	0.53	0	5,5,5	0.70	0
6	GOL	A	860	-	5,5,5	1.01	0	5,5,5	1.78	2 (40%)
6	GOL	B	860	-	5,5,5	0.84	0	5,5,5	1.24	1 (20%)
6	GOL	A	863	-	5,5,5	0.63	0	5,5,5	2.11	2 (40%)
3	SF4	C	700	1	0,12,12	-	-	-		
6	GOL	A	861	-	5,5,5	0.74	0	5,5,5	1.36	1 (20%)
6	GOL	A	862	-	5,5,5	1.04	0	5,5,5	1.16	0
6	GOL	D	863	-	5,5,5	0.88	0	5,5,5	1.42	1 (20%)
3	SF4	D	700	1	0,12,12	-	-	-		
4	XCC	B	800	1	0,12,12	-	-	-		
3	SF4	O	900	2	0,12,12	-	-	-		
6	GOL	B	861	-	5,5,5	0.73	0	5,5,5	1.00	0

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
4	XCC	A	800	1	-	-	0/4/4/4
3	SF4	M	900	2	-	-	0/6/5/5
3	SF4	A	750	1	-	-	0/6/5/5
3	SF4	B	700	1	-	-	0/6/5/5
3	SF4	A	700	1	-	-	0/6/5/5
6	GOL	C	861	-	-	2/4/4/4	-
4	XCC	D	800	1	-	-	0/4/4/4
6	GOL	B	863	-	-	0/4/4/4	-
4	XCC	C	800	1	-	-	0/4/4/4
6	GOL	D	860	-	-	2/4/4/4	-
6	GOL	C	860	-	-	2/4/4/4	-
3	SF4	C	750	1	-	-	0/6/5/5
3	SF4	N	900	2	-	-	0/6/5/5
3	SF4	P	900	2	-	-	0/6/5/5
6	GOL	B	860	-	-	4/4/4/4	-
6	GOL	A	860	-	-	2/4/4/4	-
6	GOL	A	863	-	-	0/4/4/4	-
3	SF4	C	700	1	-	-	0/6/5/5
6	GOL	A	861	-	-	2/4/4/4	-
6	GOL	A	862	-	-	4/4/4/4	-
6	GOL	D	863	-	-	4/4/4/4	-
3	SF4	D	700	1	-	-	0/6/5/5
4	XCC	B	800	1	-	-	0/4/4/4
3	SF4	O	900	2	-	-	0/6/5/5
6	GOL	B	861	-	-	4/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	863	GOL	O3-C3-C2	-3.96	92.56	110.38
6	A	860	GOL	O1-C1-C2	2.98	123.80	110.38
6	B	863	GOL	O2-C2-C1	-2.85	97.36	109.18
6	D	863	GOL	O2-C2-C3	2.84	120.95	109.18
6	A	861	GOL	O3-C3-C2	2.68	122.46	110.38
6	B	863	GOL	O1-C1-C2	-2.50	99.13	110.38
6	A	863	GOL	C3-C2-C1	2.25	120.06	111.80
6	A	860	GOL	O2-C2-C3	-2.07	100.61	109.18
6	B	860	GOL	O2-C2-C3	-2.02	100.82	109.18

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	861	GOL	C1-C2-C3-O3
6	A	861	GOL	O2-C2-C3-O3
6	A	862	GOL	O1-C1-C2-O2
6	A	862	GOL	O1-C1-C2-C3
6	A	862	GOL	C1-C2-C3-O3
6	B	860	GOL	O1-C1-C2-C3
6	B	860	GOL	C1-C2-C3-O3
6	B	861	GOL	O1-C1-C2-C3
6	B	861	GOL	C1-C2-C3-O3
6	C	861	GOL	C1-C2-C3-O3
6	D	860	GOL	C1-C2-C3-O3
6	D	863	GOL	O1-C1-C2-C3
6	D	863	GOL	C1-C2-C3-O3
6	D	863	GOL	O2-C2-C3-O3
6	C	860	GOL	O2-C2-C3-O3
6	D	860	GOL	O2-C2-C3-O3
6	A	860	GOL	C1-C2-C3-O3
6	C	860	GOL	C1-C2-C3-O3
6	A	860	GOL	O2-C2-C3-O3
6	A	862	GOL	O2-C2-C3-O3
6	B	860	GOL	O2-C2-C3-O3
6	B	861	GOL	O1-C1-C2-O2
6	B	861	GOL	O2-C2-C3-O3
6	C	861	GOL	O2-C2-C3-O3
6	B	860	GOL	O1-C1-C2-O2
6	D	863	GOL	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	XCC	2	0
3	B	700	SF4	1	0
6	C	861	GOL	1	0
4	D	800	XCC	1	0
6	B	863	GOL	2	0
4	C	800	XCC	4	0
6	D	860	GOL	1	0
3	P	900	SF4	1	0
6	A	861	GOL	1	0
6	A	862	GOL	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	863	GOL	6	0
4	B	800	XCC	3	0
3	O	900	SF4	5	0
6	B	861	GOL	3	0

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
1	A	673/674 (99%)	-0.73	0	100	100	9, 18, 36, 61	2 (0%)
1	B	673/674 (99%)	-0.77	1 (0%)	92	90	8, 18, 35, 67	7 (1%)
1	C	673/674 (99%)	-0.54	2 (0%)	90	87	10, 23, 40, 61	3 (0%)
1	D	673/674 (99%)	-0.45	2 (0%)	90	87	11, 25, 46, 70	2 (0%)
2	M	728/729 (99%)	-0.45	4 (0%)	87	85	9, 25, 49, 70	4 (0%)
2	N	728/729 (99%)	-0.54	3 (0%)	88	86	7, 23, 48, 64	3 (0%)
2	O	727/729 (99%)	1.17	178 (24%)	2	1	22, 58, 90, 130	1 (0%)
2	P	728/729 (99%)	0.40	90 (12%)	8	6	12, 40, 84, 112	3 (0%)
All	All	5603/5612 (99%)	-0.22	280 (4%)	34	30	7, 25, 71, 130	25 (0%)

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	728	ILE	6.0
2	O	480	VAL	5.4
2	O	356	VAL	5.3
2	P	480	VAL	4.9
2	P	356	VAL	4.7
2	O	350	PHE	4.7
2	O	723	LEU	4.6
2	O	399	PHE	4.6
2	O	465	VAL	4.3
2	P	387	LEU	4.3
1	B	539	ILE	4.3
2	P	485	TYR	4.3
2	P	335	LYS	4.2
2	O	485	TYR	4.2
2	O	384	LEU	4.2
2	P	346	ARG	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	539[A]	ILE	4.1
2	O	382	LEU	4.1
2	O	402	VAL	4.0
2	P	355	THR	3.9
2	P	399	PHE	3.8
2	O	353	VAL	3.8
2	P	474	VAL	3.8
2	P	352	LEU	3.8
2	O	469	THR	3.8
2	P	343	GLY	3.8
2	P	459	ILE	3.8
2	O	474	VAL	3.7
2	P	353	VAL	3.7
2	O	457	PRO	3.7
2	O	486	LYS	3.7
2	M	314	THR	3.7
2	O	488	ARG	3.7
2	M	729	MET	3.6
2	P	391	TYR	3.6
2	P	475	LYS	3.6
2	O	318	LEU	3.6
2	P	481	ALA	3.5
2	O	459	ILE	3.5
2	O	579	LEU	3.5
2	O	472	ALA	3.5
2	P	425	ILE	3.5
2	O	460	VAL	3.4
2	P	384	LEU	3.4
2	O	377	PRO	3.4
2	P	458	ALA	3.4
2	O	369	ILE	3.4
2	P	316	ILE	3.4
2	O	492	MET	3.4
2	P	486	LYS	3.4
2	O	463	VAL	3.4
2	P	463	VAL	3.4
1	D	539	ILE	3.4
2	O	519	ILE	3.3
2	P	484	LYS	3.3
2	O	520	VAL	3.3
2	P	457	PRO	3.3
2	O	340	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	692	GLY	3.3
2	O	725	MET	3.3
2	P	472	ALA	3.3
2	O	566	SER	3.2
2	O	504	TYR	3.2
2	P	345	ASN	3.2
2	O	724	THR	3.2
2	O	495	LEU	3.2
2	P	357	SER	3.2
2	O	314	THR	3.2
2	O	653	VAL	3.2
2	O	366	ILE	3.2
2	O	481	ALA	3.1
2	P	336	GLY	3.1
2	O	530	ALA	3.1
2	P	315[A]	LYS	3.1
2	P	350	PHE	3.1
2	O	533	TRP	3.1
2	O	403	LEU	3.1
2	P	488	ARG	3.1
2	O	401	GLY	3.1
2	O	376	ILE	3.1
2	O	355	THR	3.0
2	P	342	MET	3.0
2	O	545	ALA	3.0
2	P	344	GLY	3.0
2	P	390	ILE	3.0
2	P	467	ILE	3.0
2	O	482	ARG	3.0
2	P	461	ASP	3.0
2	O	316	ILE	3.0
2	O	368	VAL	3.0
2	P	460	VAL	3.0
2	P	427	TRP	3.0
2	O	339	TYR	3.0
2	O	491	ARG	3.0
2	P	482	ARG	3.0
2	O	529	GLY	3.0
2	O	447	ILE	2.9
2	O	542	ILE	2.9
2	P	354	ARG	2.9
2	O	428	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	359	SER	2.9
2	O	467	ILE	2.9
2	P	729	MET	2.9
2	O	687	VAL	2.9
2	O	420	THR	2.9
2	O	371	PRO	2.9
2	P	469	THR	2.9
2	P	724	THR	2.9
2	O	564	TRP	2.9
2	O	655	LYS	2.9
2	P	381	LYS	2.9
2	O	410	PHE	2.9
2	O	448	LEU	2.8
2	O	470	ASP	2.8
2	P	728	ILE	2.8
2	O	500	VAL	2.8
2	O	362	THR	2.8
2	O	450	ALA	2.8
2	O	342	MET	2.8
2	O	348	PRO	2.8
2	O	2	THR	2.8
2	O	567	VAL	2.7
2	P	314	THR	2.7
2	O	494	GLY	2.7
2	P	338	MET	2.7
2	O	390	ILE	2.7
2	N	318	LEU	2.7
2	P	395	MET	2.7
2	P	477	TYR	2.7
1	D	416	ARG	2.7
2	O	466	THR	2.7
2	O	373	ILE	2.7
2	O	468	PHE	2.7
2	O	380	SER	2.7
2	O	582	VAL	2.7
2	O	572	TYR	2.7
2	O	427	TRP	2.7
2	P	573	THR	2.7
2	O	596	GLY	2.6
2	O	484	LYS	2.6
2	O	550	PRO	2.6
2	P	424	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	691	LEU	2.6
2	P	495	LEU	2.6
2	O	538	ALA	2.6
2	O	344	GLY	2.6
2	O	379	GLY	2.6
2	P	394	LYS	2.6
2	P	473	LYS	2.6
2	O	383	PRO	2.6
2	P	557	ILE	2.6
2	O	378	GLU	2.6
2	O	388	VAL	2.6
2	O	668	VAL	2.6
2	P	347	THR	2.6
2	O	391	TYR	2.6
2	P	364	GLY	2.6
2	P	552	PRO	2.6
2	O	551	ILE	2.6
2	O	534	LEU	2.6
2	P	723	LEU	2.6
2	O	525	VAL	2.6
2	O	475	LYS	2.6
2	P	348	PRO	2.6
2	O	696	ILE	2.6
2	O	431	SER	2.6
2	O	570	TYR	2.6
2	P	471	GLU	2.5
2	P	639	THR	2.5
2	O	338	MET	2.5
2	O	361	ILE	2.5
2	P	340	VAL	2.5
1	C	416	ARG	2.5
2	O	605	LEU	2.5
2	O	683	VAL	2.5
2	O	349	ALA	2.5
2	O	665	ALA	2.5
2	O	650	THR	2.5
2	O	664	ILE	2.5
2	P	369	ILE	2.5
2	O	387	LEU	2.5
2	P	491	ARG	2.5
2	O	395	MET	2.5
2	O	407	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	490	ASP	2.4
2	O	478	MET	2.4
2	O	727	PRO	2.4
2	O	473	LYS	2.4
2	N	316	ILE	2.4
2	M	313	LEU	2.4
2	O	313	LEU	2.4
2	O	444	TYR	2.4
2	O	393	ARG	2.4
2	O	151	TRP	2.4
2	P	581	GLN	2.4
2	O	315	LYS	2.4
2	O	586	THR	2.4
2	O	385	GLY	2.4
2	O	456	PHE	2.4
2	O	540	TYR	2.4
2	P	478	MET	2.4
2	O	708	VAL	2.4
2	O	317	LYS	2.4
2	P	341	GLU	2.4
2	O	357	SER	2.3
2	O	548	ASN	2.3
2	O	343	GLY	2.3
2	O	610	GLY	2.3
2	O	333	ILE	2.3
2	O	560	ILE	2.3
2	P	398	ASP	2.3
2	O	381	LYS	2.3
2	O	430	VAL	2.3
2	P	400	GLU	2.3
2	O	392	GLY	2.3
2	O	322	ILE	2.3
2	O	358	GLU	2.3
2	O	663	GLY	2.3
2	O	386	ILE	2.3
2	O	435	VAL	2.3
2	P	388	VAL	2.3
2	O	522	PRO	2.3
2	P	383	PRO	2.3
2	O	477	TYR	2.3
2	O	573	THR	2.2
2	O	719	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	425	ILE	2.2
2	O	715	LEU	2.2
2	O	595	CYS	2.2
2	O	347	THR	2.2
2	O	320	LEU	2.2
2	O	584	LEU	2.2
2	O	645	MET	2.2
2	O	489	ASP	2.2
2	O	406	ARG	2.2
2	O	453	LYS	2.2
2	P	719	GLY	2.2
2	P	359	SER	2.2
2	O	389	ASP	2.2
2	O	524	ARG	2.2
2	O	713	PRO	2.2
2	O	464	GLN	2.2
2	O	557	ILE	2.2
2	O	563	ILE	2.2
2	O	331	GLU	2.2
2	O	547	PRO	2.2
2	M	335	LYS	2.2
2	P	402	VAL	2.1
2	P	492	MET	2.1
2	O	483	GLU	2.1
2	O	398	ASP	2.1
2	P	317	LYS	2.1
2	O	345	ASN	2.1
2	O	336	GLY	2.1
2	P	366	ILE	2.1
2	P	462	ARG	2.1
2	O	505	SER	2.1
2	O	592	MET	2.1
2	P	493	ARG	2.1
2	P	542	ILE	2.1
2	P	570	TYR	2.1
2	O	553	LYS	2.1
2	P	623	PRO	2.1
2	O	439	PHE	2.1
2	O	458	ALA	2.1
2	P	349	ALA	2.1
2	N	335	LYS	2.1
2	O	612	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	544	HIS	2.1
2	O	695	PHE	2.0
2	O	397	ALA	2.0
2	P	397	ALA	2.0
2	P	650	THR	2.0
2	O	497	ASP	2.0
2	P	371	PRO	2.0
2	O	452	MET	2.0
2	O	324	PHE	2.0
2	P	379	GLY	2.0
2	P	496	THR	2.0
2	P	533	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	C	861	6/6	0.79	0.14	53,59,59,60	0
6	GOL	D	860	6/6	0.84	0.13	47,51,52,52	0
6	GOL	B	861	6/6	0.85	0.16	45,51,52,54	0
6	GOL	C	860	6/6	0.85	0.14	39,48,50,51	0
6	GOL	D	863	6/6	0.89	0.14	28,36,42,42	0
6	GOL	B	863	6/6	0.91	0.12	30,34,37,37	0
4	XCC	D	800	9/9	0.92	0.09	52,61,69,69	0
6	GOL	A	861	6/6	0.92	0.12	34,47,51,53	0
6	GOL	B	860	6/6	0.93	0.09	27,27,30,30	0
6	GOL	A	863	6/6	0.94	0.10	22,26,32,35	0
4	XCC	C	800	9/9	0.94	0.08	40,54,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SF4	O	900	8/8	0.95	0.06	59,60,62,62	0
4	XCC	A	800	9/9	0.95	0.07	37,48,56,57	0
5	XE	C	1001	1/1	0.95	0.14	13,13,13,13	1
4	XCC	B	800	9/9	0.95	0.07	37,52,54,57	0
5	XE	O	1007	1/1	0.96	0.04	33,33,33,33	1
5	XE	P	1008	1/1	0.96	0.07	19,19,19,19	1
5	XE	B	1001	1/1	0.96	0.08	32,32,32,32	1
6	GOL	A	862	6/6	0.96	0.12	27,30,35,35	0
5	XE	D	1010	1/1	0.96	0.05	25,25,25,25	1
5	XE	M	1006	1/1	0.96	0.06	29,29,29,29	1
7	CU1	O	950	1/1	0.96	0.06	88,88,88,88	0
5	XE	O	1006	1/1	0.97	0.12	30,30,30,30	1
5	XE	D	1001	1/1	0.97	0.22	34,34,34,34	1
5	XE	N	1006	1/1	0.97	0.04	27,27,27,27	1
6	GOL	A	860	6/6	0.97	0.06	17,20,23,27	0
5	XE	N	1008	1/1	0.97	0.09	25,25,25,25	1
7	CU1	P	950	1/1	0.97	0.04	52,52,52,52	0
8	NI	O	951	1/1	0.97	0.09	75,75,75,75	0
5	XE	P	1006	1/1	0.98	0.07	29,29,29,29	1
7	CU1	M	950	1/1	0.98	0.03	30,30,30,30	0
5	XE	C	1005	1/1	0.98	0.02	31,31,31,31	1
5	XE	A	1001	1/1	0.98	0.12	23,23,23,23	1
5	XE	O	1009	1/1	0.98	0.05	42,42,42,42	1
3	SF4	B	700	8/8	0.99	0.03	7,9,11,15	0
5	XE	M	1008	1/1	0.99	0.02	30,30,30,30	1
3	SF4	C	700	8/8	0.99	0.03	21,23,24,24	0
3	SF4	C	750	8/8	0.99	0.03	22,26,28,28	0
3	SF4	D	700	8/8	0.99	0.03	18,19,20,22	0
5	XE	A	1002	1/1	0.99	0.01	27,27,27,27	0
5	XE	A	1003[A]	1/1	0.99	0.03	30,30,30,30	1
5	XE	A	1003[B]	1/1	0.99	0.03	14,14,14,14	1
5	XE	P	1007	1/1	0.99	0.02	29,29,29,29	0
5	XE	A	1010	1/1	0.99	0.09	31,31,31,31	1
5	XE	P	1009	1/1	0.99	0.04	31,31,31,31	1
3	SF4	M	900	8/8	0.99	0.02	13,14,17,20	0
5	XE	B	1002	1/1	0.99	0.02	25,25,25,25	0
5	XE	B	1010	1/1	0.99	0.08	24,24,24,24	1
3	SF4	N	900	8/8	0.99	0.03	12,14,16,17	0
5	XE	C	1002	1/1	0.99	0.04	33,33,33,33	0
5	XE	C	1003[A]	1/1	0.99	0.02	29,29,29,29	1
5	XE	C	1003[B]	1/1	0.99	0.02	33,33,33,33	1
3	SF4	A	700	8/8	0.99	0.03	10,12,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	XE	C	1010	1/1	0.99	0.04	35,35,35,35	1
3	SF4	P	900	8/8	0.99	0.04	31,34,36,37	0
5	XE	D	1002	1/1	0.99	0.03	29,29,29,29	1
5	XE	D	1003[A]	1/1	0.99	0.04	28,28,28,28	1
7	CU1	N	950	1/1	0.99	0.02	28,28,28,28	0
5	XE	D	1003[B]	1/1	0.99	0.04	30,30,30,30	1
5	XE	D	1004	1/1	0.99	0.02	28,28,28,28	1
3	SF4	A	750	8/8	0.99	0.02	12,15,16,17	0
8	NI	P	951	1/1	0.99	0.02	44,44,44,44	0
5	XE	D	1005	1/1	1.00	0.02	27,27,27,27	0
5	XE	B	1005	1/1	1.00	0.02	21,21,21,21	0
5	XE	A	1005	1/1	1.00	0.02	24,24,24,24	0
5	XE	M	1007	1/1	1.00	0.02	27,27,27,27	0
5	XE	A	1004	1/1	1.00	0.03	30,30,30,30	1
5	XE	B	1003[A]	1/1	1.00	0.02	26,26,26,26	1
5	XE	N	1007	1/1	1.00	0.01	21,21,21,21	0
5	XE	B	1003[B]	1/1	1.00	0.02	25,25,25,25	1
5	XE	N	1009	1/1	1.00	0.01	34,34,34,34	1
8	NI	M	951	1/1	1.00	0.03	18,18,18,18	0
8	NI	N	951	1/1	1.00	0.02	17,17,17,17	0
5	XE	B	1004	1/1	1.00	0.02	29,29,29,29	1
5	XE	C	1004	1/1	1.00	0.01	30,30,30,30	1

6.5 Other polymers ⓘ

There are no such residues in this entry.