



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:37 PM UTC

PDB ID : 1EGC / pdb_00001egc
Title : STRUCTURE OF T255E, E376G MUTANT OF HUMAN MEDIUM CHAIN
ACYL-COA DEHYDROGENASE COMPLEXED WITH OCTANOYL-COA
Authors : Lee, H.J.; Wang, M.; Paschke, R.; Nandy, A.; Ghisla, S.; Kim, J.P.
Deposited on : 1996-04-11
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

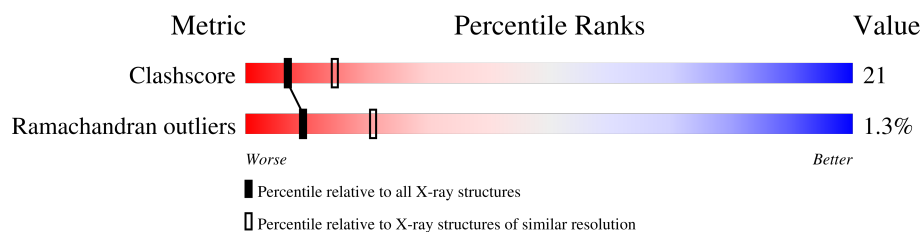
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	 55% 39% . .
1	B	396	 59% 36% . .
1	C	396	 62% 34% . .
1	D	396	 49% 43% 5% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12536 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.

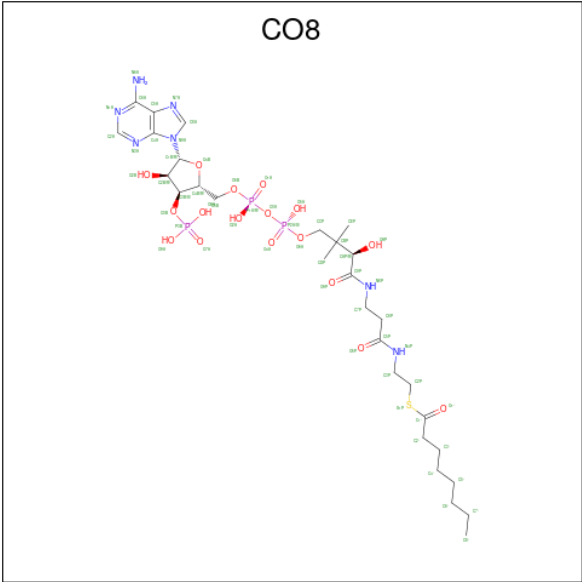
- Molecule 1 is a protein called MEDIUM CHAIN ACYL-COA DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2990	1892	515	565	18			
1	B	387	Total	C	N	O	S	0	0	0
			2990	1892	515	565	18			
1	C	387	Total	C	N	O	S	0	0	0
			2990	1892	515	565	18			
1	D	387	Total	C	N	O	S	5	0	0
			2990	1892	515	565	18			

There are 8 discrepancies between the modelled and reference sequences:

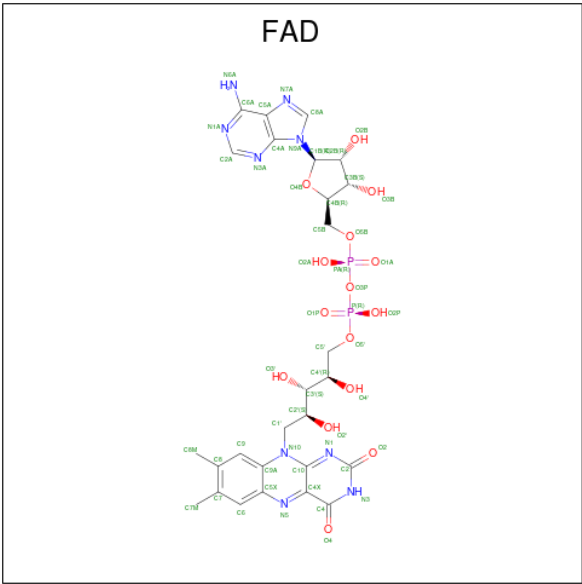
Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLU	THR	engineered mutation	UNP P11310
A	376	GLY	GLU	engineered mutation	UNP P11310
B	255	GLU	THR	engineered mutation	UNP P11310
B	376	GLY	GLU	engineered mutation	UNP P11310
C	255	GLU	THR	engineered mutation	UNP P11310
C	376	GLY	GLU	engineered mutation	UNP P11310
D	255	GLU	THR	engineered mutation	UNP P11310
D	376	GLY	GLU	engineered mutation	UNP P11310

- Molecule 2 is OCTANOYL-COENZYME A (CCD ID: CO8) (formula: C₂₉H₅₀N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is water.

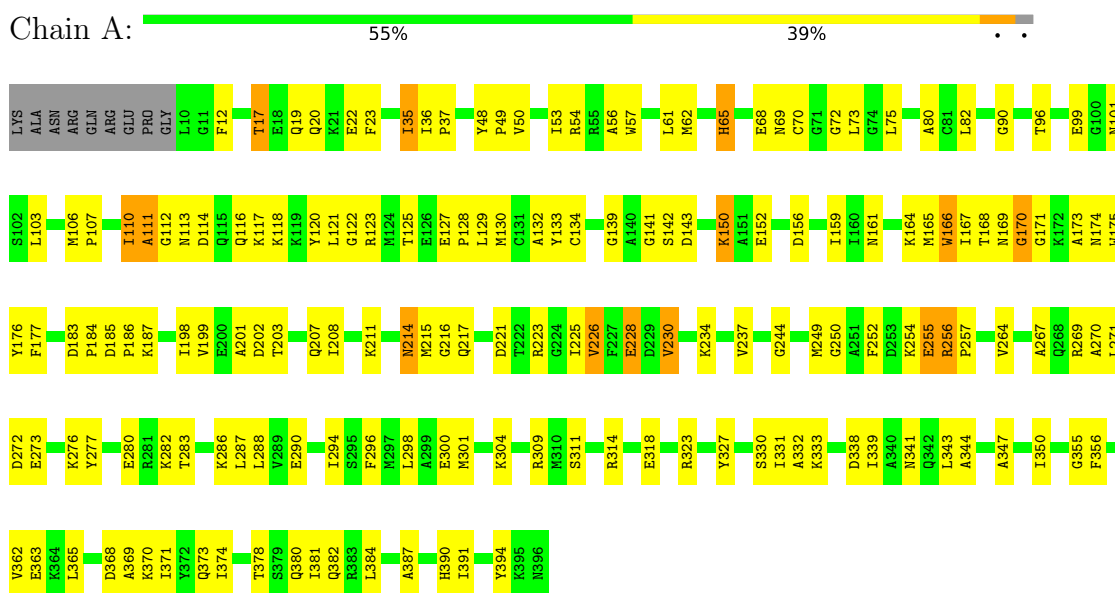
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		
4	B	33	Total	O	0	0
			33	33		
4	C	41	Total	O	0	0
			41	41		
4	D	35	Total	O	0	0
			35	35		

3 Residue-property plots

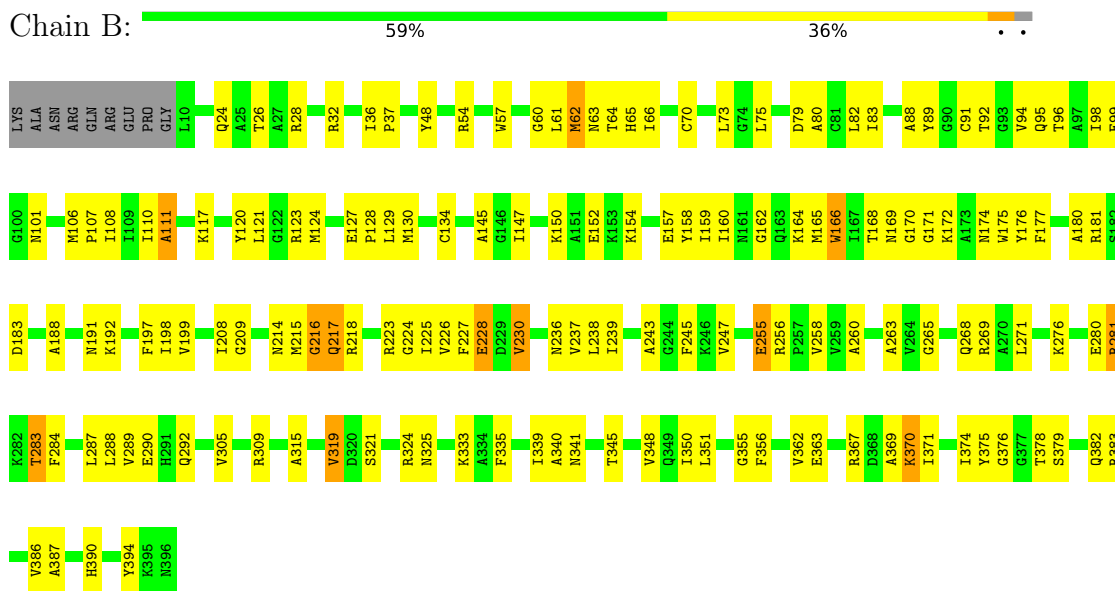
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

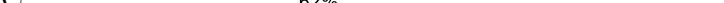
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

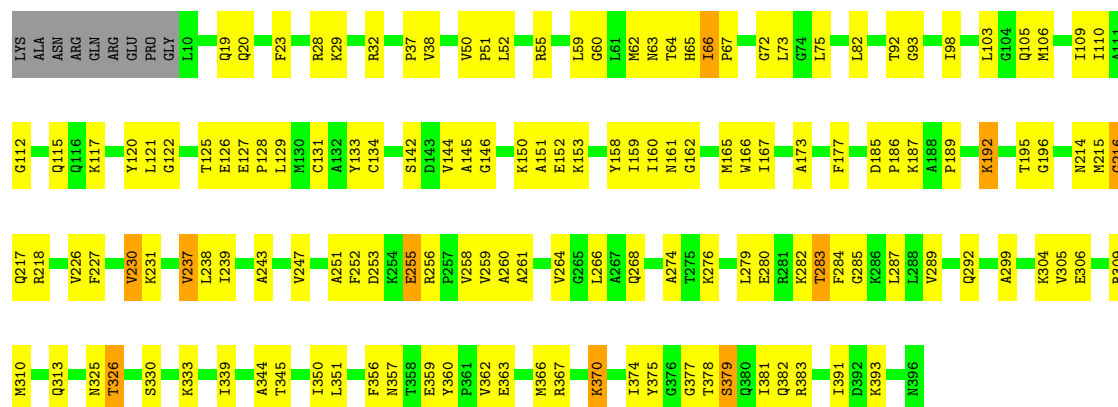


• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE



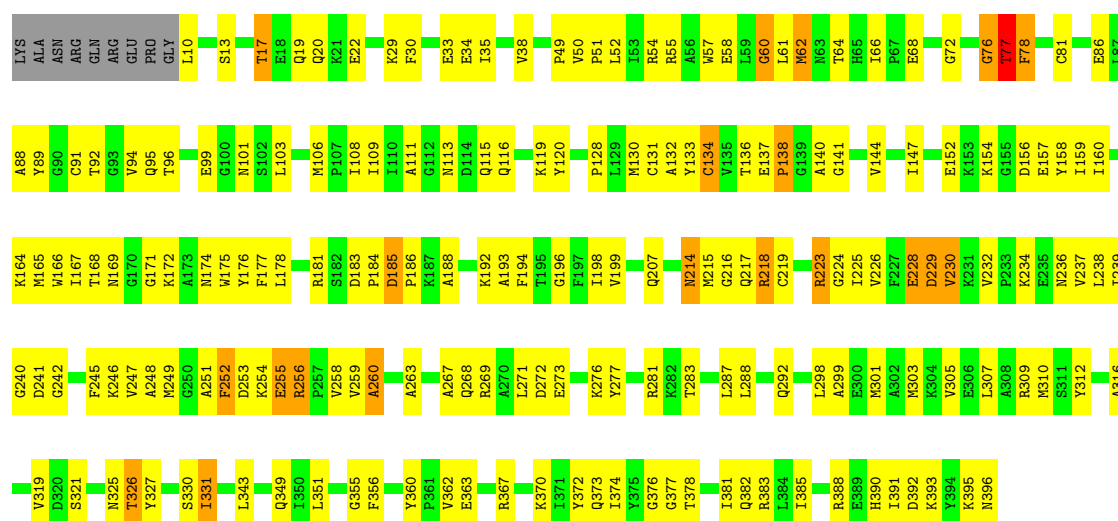
- Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain C:  62% 34% 4%



- Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain D: 49% 43% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.00 Å 170.00 Å 149.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.217 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12536	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, CO8

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	0.74	5/3045 (0.2%)	1.23	31/4102 (0.8%)
1	B	0.73	8/3045 (0.3%)	1.17	35/4102 (0.9%)
1	C	0.61	3/3045 (0.1%)	1.13	21/4102 (0.5%)
1	D	0.74	6/3045 (0.2%)	1.17	31/4102 (0.8%)
All	All	0.71	22/12180 (0.2%)	1.18	118/16408 (0.7%)

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	4
1	C	0	1
1	D	0	1
All	All	0	6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	ASN	C-N	-13.66	1.15	1.33
1	D	260	ALA	C-N	13.15	1.51	1.33
1	A	230	VAL	C-N	11.95	1.50	1.33
1	A	226	VAL	C-N	-11.02	1.20	1.33
1	D	256	ARG	N-CA	9.81	1.56	1.46
1	D	214	ASN	C-N	-8.10	1.22	1.34
1	A	214	ASN	C-N	-7.56	1.22	1.33
1	C	226	VAL	C-N	-7.34	1.22	1.33
1	A	170	GLY	C-N	7.16	1.45	1.33
1	D	255	GLU	CA-C	6.61	1.61	1.52
1	B	281	ARG	C-N	-5.95	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	GLY	C-N	-5.90	1.26	1.33
1	C	60	GLY	C-N	-5.85	1.25	1.33
1	B	255	GLU	CA-CB	-5.76	1.43	1.53
1	B	226	VAL	C-N	-5.68	1.23	1.33
1	C	285	GLY	C-N	5.59	1.41	1.33
1	B	166	TRP	NE1-CE2	-5.41	1.31	1.37
1	D	158	TYR	C-N	-5.31	1.25	1.33
1	A	166	TRP	NE1-CE2	-5.27	1.31	1.37
1	D	229	ASP	N-CA	5.05	1.51	1.46
1	B	230	VAL	C-N	5.04	1.40	1.33
1	B	60	GLY	C-N	-5.01	1.25	1.33

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ILE	CA-C-O	-23.89	94.45	120.25
1	A	110	ILE	CB-CA-C	12.95	133.26	112.16
1	C	218	ARG	O-C-N	-12.84	105.64	122.33
1	A	170	GLY	O-C-N	-11.51	111.14	122.19
1	D	77	THR	N-CA-CB	-11.30	91.40	110.49
1	B	64	THR	O-C-N	-10.01	109.31	122.33
1	C	360	TYR	CA-C-N	8.67	129.20	119.32
1	C	360	TYR	C-N-CA	8.67	129.20	119.32
1	C	226	VAL	CA-C-N	8.45	135.88	123.13
1	C	226	VAL	C-N-CA	8.45	135.88	123.13
1	A	216	GLY	O-C-N	-8.43	111.75	122.70
1	D	60	GLY	CA-C-O	8.33	135.07	120.57
1	B	228	GLU	O-C-N	-8.17	111.73	122.59
1	D	360	TYR	CA-C-N	8.12	127.42	118.97
1	D	360	TYR	C-N-CA	8.12	127.42	118.97
1	D	77	THR	CB-CA-C	-7.95	94.61	110.42
1	A	65	HIS	O-C-N	-7.81	111.68	122.46
1	B	255	GLU	N-CA-CB	-7.77	97.73	110.40
1	B	62	MET	O-C-N	-7.71	112.33	122.59
1	A	203	THR	N-CA-C	-7.68	100.07	109.83
1	B	216	GLY	O-C-N	-7.54	112.89	122.70
1	A	111	ALA	CB-CA-C	7.53	125.39	110.42
1	B	177	PHE	N-CA-C	-7.49	97.48	109.76
1	A	228	GLU	O-C-N	-7.24	112.97	122.59
1	B	224	GLY	N-CA-C	-7.11	101.72	113.02
1	B	370	LYS	N-CA-C	7.10	119.93	111.33
1	A	177	PHE	N-CA-C	-6.96	99.26	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	177	PHE	N-CA-C	-6.92	97.93	109.07
1	C	362	VAL	N-CA-C	6.78	117.47	110.36
1	C	379	SER	N-CA-C	-6.72	103.95	111.28
1	B	255	GLU	O-C-N	-6.68	113.23	122.46
1	A	226	VAL	O-C-N	-6.58	116.09	123.20
1	D	78	PHE	N-CA-C	-6.57	96.80	110.80
1	D	167	ILE	N-CA-C	6.49	117.46	107.99
1	B	218	ARG	O-C-N	-6.46	113.99	122.59
1	B	217	GLN	O-C-N	6.42	130.77	121.78
1	B	283	THR	O-C-N	-6.40	115.52	121.79
1	A	226	VAL	CA-C-N	6.37	132.80	123.12
1	A	226	VAL	C-N-CA	6.37	132.80	123.12
1	A	369	ALA	N-CA-C	6.35	118.21	111.28
1	C	226	VAL	O-C-N	-6.30	115.52	122.83
1	B	111	ALA	N-CA-C	6.26	121.69	113.30
1	D	260	ALA	O-C-N	6.26	128.54	122.03
1	D	230	VAL	O-C-N	6.24	130.37	122.57
1	C	255	GLU	CB-CG-CD	6.21	123.16	112.60
1	A	283	THR	O-C-N	-6.18	114.37	122.59
1	C	351	LEU	N-CA-C	-6.11	105.47	113.17
1	D	134	CYS	N-CA-C	6.11	119.46	107.98
1	D	331	ILE	N-CA-C	-6.10	104.56	110.42
1	C	237	VAL	N-CA-C	-6.09	101.14	109.55
1	B	228	GLU	CA-C-N	-6.05	114.84	123.20
1	B	228	GLU	C-N-CA	-6.05	114.84	123.20
1	B	183	ASP	CA-C-N	6.05	125.75	119.82
1	B	183	ASP	C-N-CA	6.05	125.75	119.82
1	D	140	ALA	N-CA-C	6.05	119.09	108.75
1	A	50	VAL	CB-CA-C	-5.99	108.00	114.35
1	B	162	GLY	O-C-N	5.98	129.56	123.88
1	C	283	THR	O-C-N	-5.96	114.91	121.76
1	B	110	ILE	CB-CA-C	-5.90	104.34	112.24
1	B	281	ARG	CA-C-N	5.86	130.76	122.09
1	B	281	ARG	C-N-CA	5.86	130.76	122.09
1	B	321	SER	N-CA-C	-5.86	105.98	113.01
1	A	202	ASP	N-CA-C	5.78	119.10	112.97
1	A	120	TYR	N-CA-C	5.77	120.45	113.41
1	B	260	ALA	N-CA-C	-5.75	105.10	111.36
1	D	177	PHE	N-CA-C	-5.73	100.33	109.96
1	D	228	GLU	O-C-N	-5.67	115.05	122.59
1	B	369	ALA	N-CA-C	5.65	117.89	111.11
1	A	255	GLU	CB-CG-CD	5.62	122.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	GLY	N-CA-C	5.57	119.45	110.87
1	C	370	LYS	N-CA-C	5.57	117.79	111.11
1	D	223	ARG	N-CA-C	5.53	116.54	108.14
1	A	217	GLN	O-C-N	5.52	129.43	121.97
1	B	188	ALA	N-CA-C	5.48	116.31	109.57
1	A	121	LEU	N-CA-C	-5.46	106.75	113.41
1	B	319	VAL	CB-CA-C	-5.45	104.89	112.02
1	C	120	TYR	N-CA-C	5.44	118.13	111.82
1	B	281	ARG	O-C-N	-5.42	116.36	123.02
1	D	287	LEU	N-CA-C	-5.41	102.99	110.35
1	A	198	ILE	N-CA-C	-5.41	100.54	108.11
1	D	237	VAL	N-CA-C	-5.40	102.55	109.30
1	B	70	CYS	N-CA-C	-5.36	105.38	112.94
1	B	174	ASN	N-CA-C	-5.35	105.89	112.90
1	C	126	GLU	N-CA-C	5.33	118.00	111.82
1	A	17	THR	N-CA-C	-5.32	102.65	110.52
1	A	237	VAL	N-CA-C	-5.31	101.88	108.89
1	C	66	ILE	CA-C-N	5.30	125.31	119.90
1	C	66	ILE	C-N-CA	5.30	125.31	119.90
1	D	35	ILE	N-CA-C	5.30	115.56	110.74
1	C	292	GLN	N-CA-C	5.28	117.72	111.33
1	A	48	TYR	CA-C-N	5.28	126.44	119.84
1	A	48	TYR	C-N-CA	5.28	126.44	119.84
1	A	150	LYS	N-CA-C	5.26	117.33	108.96
1	C	255	GLU	CB-CA-C	-5.25	99.73	109.29
1	A	216	GLY	CA-C-N	-5.23	115.38	123.17
1	A	216	GLY	C-N-CA	-5.23	115.38	123.17
1	C	285	GLY	N-CA-C	-5.22	108.79	115.42
1	B	218	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	D	218	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	D	78	PHE	N-CA-CB	5.19	119.27	110.49
1	D	185	ASP	CA-C-N	5.19	126.33	119.84
1	D	185	ASP	C-N-CA	5.19	126.33	119.84
1	D	374	ILE	N-CA-C	5.19	116.36	111.48
1	D	77	THR	N-CA-C	5.17	121.80	110.80
1	B	238	LEU	N-CA-C	5.13	121.73	110.80
1	B	199	VAL	N-CA-C	5.12	115.34	108.17
1	D	174	ASN	N-CA-C	-5.09	105.43	111.69
1	D	321	SER	N-CA-C	-5.08	106.92	113.02
1	B	226	VAL	N-CA-C	5.06	115.60	108.36
1	B	48	TYR	CA-C-N	5.05	126.16	119.84
1	B	48	TYR	C-N-CA	5.05	126.16	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	256	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	A	256	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	362	VAL	N-CA-C	5.01	116.33	110.62
1	A	35	ILE	N-CA-C	5.01	115.30	110.74
1	D	17	THR	N-CA-C	-5.01	103.79	110.55
1	D	260	ALA	CA-C-N	-5.01	113.52	120.38
1	D	260	ALA	C-N-CA	-5.01	113.52	120.38

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ILE	Mainchain,Peptide
1	A	170	GLY	Mainchain
1	A	230	VAL	Mainchain
1	C	230	VAL	Mainchain
1	D	64	THR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2990	0	2978	136	0
1	B	2990	0	2978	112	0
1	C	2990	0	2978	122	0
1	D	2990	0	2978	171	0
2	A	57	0	46	11	0
2	B	57	0	46	8	0
2	C	57	0	46	9	0
2	D	57	0	46	14	0
3	A	53	0	30	4	0
3	B	53	0	31	4	0
3	C	53	0	31	2	0
3	D	53	0	31	4	0
4	A	27	0	0	1	0
4	B	33	0	0	0	0
4	C	41	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	35	0	0	3	0
All	All	12536	0	12219	518	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 21.

All (518) 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:C:274:ALA:HB1	1:C:350:ILE:HD11	1.29	1.13
1:C:216:GLY:HA3	1:D:356:PHE:HZ	1.12	1.11
1:C:216:GLY:HA3	1:D:356:PHE:CZ	1.89	1.07
1:D:256:ARG:CG	1:D:256:ARG:HH11	1.71	1.03
1:C:150:LYS:HD2	1:C:161:ASN:HB2	1.38	1.01
1:D:99:GLU:OE2	1:D:258:VAL:HG11	1.60	1.00
1:A:169:ASN:HD22	1:A:221:ASP:HB3	1.27	0.99
1:B:152:GLU:HG2	1:B:159:ILE:HB	1.46	0.95
1:B:62:MET:HG3	1:B:98:ILE:HG23	1.47	0.93
1:B:228:GLU:HA	1:B:228:GLU:OE1	1.67	0.93
1:A:142:SER:HB3	1:A:381:ILE:HD12	1.52	0.92
1:C:150:LYS:CD	1:C:161:ASN:HB2	2.02	0.90
1:A:36:ILE:HG22	1:A:90:GLY:HA2	1.55	0.88
1:A:169:ASN:ND2	1:A:221:ASP:HB3	1.89	0.87
1:D:381:ILE:HD13	2:D:400:CO8:H72	1.56	0.86
1:D:256:ARG:HH11	1:D:256:ARG:HG2	1.40	0.85
1:C:103:LEU:HD22	1:C:133:TYR:CD2	2.12	0.84
1:D:144:VAL:O	1:D:147:ILE:HG12	1.78	0.82
1:A:207:GLN:OE1	1:A:228:GLU:HG3	1.80	0.81
1:D:253:ASP:OD2	1:D:326:THR:OG1	1.99	0.79
1:D:256:ARG:HH11	1:D:256:ARG:HG3	1.45	0.79
1:A:159:ILE:HD11	1:A:161:ASN:OD1	1.83	0.79
1:B:130:MET:HG3	1:B:169:ASN:HD22	1.49	0.78
1:A:164:LYS:HB3	1:A:167:ILE:HD11	1.65	0.77
1:C:62:MET:HG3	1:C:98:ILE:HG23	1.66	0.77
1:D:62:MET:HE3	1:D:101:ASN:ND2	2.01	0.76
1:C:252:PHE:CE1	2:C:400:CO8:H21	2.20	0.76
1:A:65:HIS:HE1	1:A:80:ALA:HB2	1.51	0.76
1:B:130:MET:HG3	1:B:169:ASN:ND2	2.00	0.76
1:B:65:HIS:HE1	1:B:80:ALA:HB2	1.52	0.75
1:D:171:GLY:HA3	1:D:223:ARG:HD3	1.70	0.74
1:B:111:ALA:HB1	1:B:239:ILE:HD11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:THR:O	1:C:382:GLN:HG2	1.87	0.73
1:D:181:ARG:NH2	1:D:188:ALA:HB3	2.04	0.73
1:C:345:THR:HG23	1:C:366:MET:SD	2.29	0.73
1:A:73:LEU:HB3	1:A:75:LEU:HD23	1.70	0.73
1:D:272:ASP:O	1:D:276:LYS:HG3	1.89	0.72
1:A:73:LEU:HB3	1:A:75:LEU:CD2	2.20	0.72
1:A:374:ILE:HA	1:A:378:THR:HG22	1.71	0.71
1:B:36:ILE:HG13	1:B:37:PRO:HD3	1.71	0.71
1:C:279:LEU:HD23	1:C:289:VAL:HG21	1.72	0.71
1:D:254:LYS:HD2	1:D:319:VAL:HG21	1.71	0.71
1:C:231:LYS:H	1:C:231:LYS:HD2	1.54	0.71
1:D:136:THR:HG21	3:D:399:FAD:H1'1	1.72	0.70
1:A:62:MET:HE3	1:A:101:ASN:ND2	2.05	0.70
1:B:152:GLU:CG	1:B:159:ILE:HB	2.21	0.70
1:A:215:MET:HB2	1:B:363:GLU:HG3	1.73	0.70
1:D:160:ILE:HG21	1:D:178:LEU:HD21	1.72	0.70
1:B:283:THR:HG22	1:B:284:PHE:CD1	2.27	0.70
1:C:252:PHE:HE1	2:C:400:CO8:H21	1.55	0.70
1:A:57:TRP:HD1	1:A:62:MET:HE2	1.57	0.69
1:D:154:LYS:HB3	1:D:157:GLU:HG3	1.74	0.69
1:D:232:VAL:HG12	1:D:236:ASN:HD22	1.57	0.69
1:A:103:LEU:HD11	2:A:400:CO8:H2'1	1.74	0.69
1:A:150:LYS:HE2	1:A:184:PRO:HG3	1.75	0.68
1:C:131:CYS:HA	1:C:173:ALA:HB1	1.75	0.68
1:D:132:ALA:HB3	1:D:176:TYR:HD2	1.57	0.68
1:C:93:GLY:HA2	1:C:217:GLN:HB3	1.76	0.68
1:C:215:MET:HB3	1:D:363:GLU:HG3	1.75	0.68
1:D:101:ASN:HA	1:D:131:CYS:SG	2.33	0.68
1:C:216:GLY:CA	1:D:356:PHE:CZ	2.75	0.67
1:C:38:VAL:HG21	1:C:52:LEU:HD21	1.76	0.67
1:D:256:ARG:HG2	1:D:256:ARG:NH1	2.05	0.67
1:A:114:ASP:O	1:A:118:LYS:HG2	1.94	0.67
1:C:103:LEU:CD2	1:C:133:TYR:CD2	2.77	0.66
1:D:99:GLU:CD	1:D:258:VAL:HG11	2.19	0.66
3:A:399:FAD:N7A	1:B:283:THR:HG21	2.10	0.66
1:A:12:PHE:HA	1:D:13:SER:O	1.96	0.66
1:B:28:ARG:O	1:B:32:ARG:HG2	1.95	0.66
1:B:348:VAL:HG12	1:B:362:VAL:HB	1.79	0.65
1:D:252:PHE:CZ	2:D:400:CO8:H22	2.31	0.65
1:A:314:ARG:HD2	1:D:310:MET:SD	2.37	0.65
1:C:366:MET:HB3	1:D:215:MET:HE1	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ASP:HA	1:D:395:LYS:HB3	1.77	0.64
1:B:283:THR:HG22	1:B:284:PHE:HD1	1.62	0.64
1:C:150:LYS:HD2	1:C:161:ASN:CB	2.23	0.64
1:D:252:PHE:CE1	2:D:400:CO8:S1P	2.91	0.64
1:D:113:ASN:OD1	1:D:115:GLN:HB3	1.98	0.63
1:B:319:VAL:HG22	1:B:325:ASN:CG	2.24	0.62
1:B:99:GLU:HG3	2:B:400:CO8:H8'3	1.81	0.62
1:D:259:VAL:HG13	1:D:372:TYR:HE1	1.64	0.62
1:A:106:MET:HE1	1:A:254:LYS:HD3	1.80	0.62
1:D:246:LYS:O	1:D:247:VAL:C	2.38	0.62
1:B:106:MET:HE3	1:B:106:MET:HA	1.81	0.62
1:C:73:LEU:HB3	1:C:75:LEU:HD13	1.82	0.62
1:C:142:SER:HB3	1:C:381:ILE:HG21	1.80	0.62
1:C:370:LYS:HZ1	1:D:349:GLN:HG2	1.63	0.62
1:B:73:LEU:HB3	1:B:75:LEU:HD13	1.82	0.62
1:D:62:MET:HE3	1:D:101:ASN:HD22	1.64	0.62
1:A:20:GLN:HB2	1:A:82:LEU:HD13	1.82	0.61
1:D:49:PRO:HD3	1:D:219:CYS:SG	2.40	0.61
1:D:192:LYS:HA	1:D:242:GLY:O	2.00	0.61
1:A:370:LYS:HD2	1:B:348:VAL:HG23	1.82	0.61
1:D:108:ILE:CD1	1:D:198:ILE:HD12	2.29	0.61
1:D:188:ALA:HB1	1:D:193:ALA:HB2	1.83	0.61
1:A:165:MET:HG3	1:A:166:TRP:CD1	2.35	0.61
1:A:132:ALA:HB3	1:A:176:TYR:HD1	1.66	0.61
1:D:108:ILE:HD12	1:D:198:ILE:HD12	1.83	0.61
1:B:164:LYS:HB2	1:B:225:ILE:HG22	1.82	0.61
1:C:310:MET:HA	1:C:313:GLN:HE21	1.65	0.61
1:C:357:ASN:OD1	1:C:359:GLU:HB2	2.01	0.61
1:D:330:SER:HB3	1:D:385:ILE:HD11	1.81	0.61
2:A:400:CO8:O4A	2:A:400:CO8:H10	1.99	0.61
1:B:171:GLY:O	1:B:172:LYS:HD3	2.01	0.61
1:A:62:MET:HE3	1:A:101:ASN:HD22	1.65	0.60
1:A:294:ILE:HD11	3:B:399:FAD:H1B	1.83	0.60
1:D:156:ASP:C	1:D:234:LYS:HB2	2.25	0.60
1:B:209:GLY:O	1:B:223:ARG:HD3	2.00	0.60
1:A:333:LYS:HD3	1:A:333:LYS:C	2.26	0.60
1:C:115:GLN:H	1:C:115:GLN:NE2	1.99	0.60
1:C:153:LYS:HG3	1:C:158:TYR:CE1	2.36	0.60
1:D:147:ILE:HB	1:D:194:PHE:CE1	2.36	0.60
1:D:298:LEU:HA	1:D:301:MET:HE3	1.82	0.60
1:A:323:ARG:H	1:A:323:ARG:HD2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:PHE:HE1	2:D:400:CO8:S1P	2.24	0.60
1:A:287:LEU:HD23	1:A:287:LEU:H	1.67	0.60
1:B:154:LYS:O	1:B:157:GLU:HG3	2.02	0.60
1:D:137:GLU:HB2	1:D:138:PRO:HD2	1.83	0.60
1:D:254:LYS:CD	1:D:319:VAL:HG21	2.31	0.60
1:A:174:ASN:HD22	1:A:175:TRP:HD1	1.47	0.59
1:D:130:MET:HB3	1:D:169:ASN:OD1	2.02	0.59
2:D:400:CO8:H3'2	3:D:399:FAD:C4X	2.32	0.59
1:B:117:LYS:O	1:B:121:LEU:HB2	2.02	0.59
2:C:400:CO8:H8A	2:C:400:CO8:H51A	1.83	0.59
1:A:387:ALA:HB2	1:D:299:ALA:HB2	1.84	0.59
1:C:227:PHE:HD1	1:C:230:VAL:HG21	1.66	0.59
2:C:400:CO8:H31	3:C:399:FAD:O2'	2.02	0.59
1:C:268:GLN:NE2	1:C:305:VAL:HG11	2.18	0.59
1:A:252:PHE:CE1	2:A:400:CO8:H31	2.37	0.58
1:A:368:ASP:O	1:A:371:ILE:HG22	2.02	0.58
1:B:26:THR:HG22	1:B:61:LEU:HD11	1.84	0.58
1:B:180:ALA:HB3	1:B:197:PHE:HE1	1.67	0.58
1:D:268:GLN:HE21	1:D:309:ARG:HH12	1.49	0.58
1:D:138:PRO:HD3	1:D:165:MET:HB2	1.85	0.58
1:D:159:ILE:HG23	1:D:159:ILE:O	2.03	0.58
1:A:54:ARG:HD3	1:A:128:PRO:HG2	1.85	0.58
1:A:298:LEU:HD23	1:D:391:ILE:HD11	1.85	0.58
1:C:282:LYS:HA	1:C:287:LEU:HA	1.84	0.58
1:A:113:ASN:H	1:A:116:GLN:HE21	1.51	0.58
1:C:260:ALA:O	1:C:264:VAL:HG23	2.04	0.58
1:D:267:ALA:HB1	1:D:343:LEU:HD22	1.85	0.58
1:A:106:MET:CE	1:A:254:LYS:HD3	2.34	0.58
1:A:211:LYS:HA	1:A:223:ARG:HG2	1.86	0.58
1:A:355:GLY:O	1:A:363:GLU:HB2	2.04	0.58
1:B:176:TYR:OH	1:B:208:ILE:HD11	2.04	0.58
1:A:142:SER:HB3	1:A:381:ILE:CD1	2.30	0.57
1:C:253:ASP:HB3	1:C:325:ASN:HD21	1.68	0.57
1:D:134:CYS:HB3	1:D:164:LYS:HG3	1.86	0.57
1:A:370:LYS:HD2	1:B:348:VAL:CG2	2.35	0.57
1:D:81:CYS:HB3	1:D:312:TYR:CE1	2.39	0.57
1:C:64:THR:O	1:C:75:LEU:HB2	2.05	0.57
1:D:96:THR:HG23	2:D:400:CO8:H7'1	1.86	0.57
1:C:239:ILE:HB	1:C:243:ALA:CB	2.35	0.57
1:A:19:GLN:HG2	1:A:23:PHE:CE2	2.41	0.56
1:A:294:ILE:HG23	1:A:350:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:GLN:CG	1:D:309:ARG:HH22	2.16	0.56
1:D:303:MET:O	1:D:307:LEU:HD13	2.05	0.56
1:B:245:PHE:CE2	2:B:400:CO8:H52A	2.41	0.56
1:C:50:VAL:HB	1:C:51:PRO:HD3	1.86	0.56
1:C:214:ASN:HD22	1:D:356:PHE:HD2	1.51	0.56
1:D:214:ASN:O	1:D:218:ARG:HD2	2.06	0.56
1:A:99:GLU:HB3	2:A:400:CO8:H7'1	1.86	0.56
1:A:134:CYS:HA	1:A:167:ILE:HD12	1.88	0.56
1:C:127:GLU:HB3	1:C:129:LEU:HD13	1.88	0.56
1:A:134:CYS:HB3	1:A:164:LYS:HG3	1.88	0.56
1:A:381:ILE:HG12	1:A:384:LEU:HD12	1.87	0.56
1:D:68:GLU:HA	1:D:72:GLY:O	2.06	0.56
1:A:103:LEU:HD22	1:A:133:TYR:CG	2.40	0.56
1:D:165:MET:SD	1:D:165:MET:C	2.89	0.56
1:D:207:GLN:HB2	1:D:226:VAL:HG13	1.88	0.56
1:A:54:ARG:CD	1:A:128:PRO:HG2	2.36	0.55
1:C:151:ALA:HB2	1:C:160:ILE:HG12	1.88	0.55
1:C:231:LYS:NZ	1:C:231:LYS:HB3	2.21	0.55
1:B:292:GLN:HB2	1:D:292:GLN:HB3	1.88	0.55
1:A:255:GLU:O	1:A:256:ARG:C	2.46	0.55
1:C:150:LYS:HZ2	1:C:161:ASN:HB2	1.71	0.55
1:C:306:GLU:O	1:C:310:MET:HE2	2.05	0.55
1:C:109:ILE:HD13	1:C:121:LEU:HD21	1.87	0.55
1:B:66:ILE:HG23	1:B:121:LEU:HB3	1.89	0.55
1:C:127:GLU:HB3	1:C:129:LEU:CD1	2.36	0.55
1:D:171:GLY:C	1:D:172:LYS:HD2	2.31	0.55
1:D:383:ARG:HG3	1:D:383:ARG:HH11	1.71	0.55
1:A:68:GLU:HA	1:A:72:GLY:O	2.07	0.55
1:D:76:GLY:O	1:D:78:PHE:N	2.40	0.55
1:C:325:ASN:H	1:C:325:ASN:HD22	1.55	0.55
1:D:232:VAL:HG12	1:D:236:ASN:ND2	2.20	0.55
1:C:117:LYS:O	1:C:121:LEU:HB2	2.07	0.55
1:A:19:GLN:O	1:A:22:GLU:HB3	2.07	0.55
1:A:107:PRO:O	1:A:111:ALA:HB3	2.08	0.54
1:B:130:MET:CG	1:B:169:ASN:ND2	2.68	0.54
1:A:123:ARG:HD3	1:A:174:ASN:ND2	2.22	0.54
1:A:380:GLN:CD	1:A:380:GLN:H	2.13	0.54
1:D:216:GLY:O	1:D:218:ARG:N	2.37	0.54
1:D:88:ALA:HB2	1:D:95:GLN:HG3	1.90	0.54
1:D:115:GLN:O	1:D:119:LYS:HB2	2.08	0.54
1:C:375:TYR:HB2	2:C:400:CO8:O1'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:VAL:CG2	2:D:400:CO8:H62	2.37	0.54
1:D:159:ILE:HD11	1:D:229:ASP:OD1	2.08	0.54
1:B:243:ALA:O	1:B:247:VAL:HG23	2.07	0.54
1:B:387:ALA:HB2	1:C:299:ALA:HB2	1.90	0.54
1:D:252:PHE:O	1:D:255:GLU:N	2.41	0.54
1:D:377:GLY:HA2	1:D:381:ILE:HD11	1.89	0.54
1:A:288:LEU:HB3	1:A:294:ILE:HG21	1.90	0.54
1:B:281:ARG:HG2	1:B:288:LEU:HD22	1.90	0.54
1:A:69:ASN:ND2	1:A:70:CYS:SG	2.81	0.53
1:B:374:ILE:HA	1:B:378:THR:HG22	1.90	0.53
1:D:111:ALA:HB1	1:D:239:ILE:HG13	1.90	0.53
1:D:152:GLU:HB2	1:D:159:ILE:CG2	2.39	0.53
1:D:17:THR:H	1:D:20:GLN:HE21	1.56	0.53
1:A:36:ILE:HG22	1:A:90:GLY:CA	2.34	0.53
1:B:24:GLN:HB2	1:B:82:LEU:HD21	1.90	0.53
1:C:215:MET:CE	1:D:367:ARG:HG3	2.39	0.53
1:C:374:ILE:HA	1:C:378:THR:HG22	1.89	0.53
1:A:173:ALA:O	1:A:201:ALA:HB2	2.08	0.53
1:D:370:LYS:HZ3	1:D:373:GLN:NE2	2.07	0.53
1:D:92:THR:HB	1:D:217:GLN:OE1	2.09	0.53
1:A:139:GLY:HA2	1:B:281:ARG:HH22	1.74	0.52
1:D:260:ALA:O	1:D:263:ALA:HB3	2.10	0.52
1:C:215:MET:HE2	1:C:367:ARG:HG2	1.91	0.52
1:B:89:TYR:O	1:B:269:ARG:HG3	2.10	0.52
1:C:151:ALA:CB	1:C:160:ILE:HG12	2.40	0.52
1:D:327:TYR:O	1:D:331:ILE:HG13	2.09	0.52
1:B:91:CYS:SG	1:B:94:VAL:HG23	2.50	0.52
1:B:345:THR:O	1:B:348:VAL:HG22	2.10	0.52
1:D:370:LYS:NZ	1:D:373:GLN:NE2	2.57	0.52
1:A:112:GLY:O	1:A:117:LYS:HE3	2.09	0.52
1:B:276:LYS:O	1:B:280:GLU:HG3	2.09	0.52
1:C:65:HIS:HD2	4:C:2090:HOH:O	1.92	0.52
1:C:127:GLU:HG2	1:C:128:PRO:HD2	1.92	0.52
2:C:400:CO8:H4'1	2:C:400:CO8:H8'2	1.91	0.52
1:D:172:LYS:HD2	1:D:172:LYS:N	2.24	0.52
1:D:19:GLN:O	1:D:22:GLU:HB3	2.10	0.52
1:D:168:THR:OG1	3:D:399:FAD:H6	2.10	0.52
1:B:379:SER:O	1:B:383:ARG:HG2	2.09	0.52
1:C:189:PRO:HG2	1:C:192:LYS:HG2	1.91	0.52
1:C:112:GLY:O	1:C:117:LYS:HE3	2.10	0.51
1:C:122:GLY:O	1:C:125:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:HIS:CE1	1:B:80:ALA:HB2	2.40	0.51
2:B:400:CO8:O5P	2:B:400:CO8:H21	2.11	0.51
1:C:251:ALA:O	1:C:255:GLU:HB2	2.10	0.51
1:B:127:GLU:HB3	1:B:129:LEU:HG	1.93	0.51
1:D:38:VAL:CG2	1:D:52:LEU:HD11	2.41	0.51
1:A:250:GLY:O	1:A:254:LYS:HG3	2.11	0.51
1:D:57:TRP:CD2	1:D:128:PRO:HG3	2.45	0.51
1:B:111:ALA:HB1	1:B:239:ILE:CD1	2.38	0.51
1:C:67:PRO:HD3	1:C:109:ILE:CD1	2.41	0.51
1:C:152:GLU:HG2	1:C:159:ILE:HG23	1.93	0.50
1:C:252:PHE:O	1:C:256:ARG:HG3	2.12	0.50
1:C:333:LYS:HE2	1:C:377:GLY:O	2.10	0.50
1:A:68:GLU:HB2	4:A:2007:HOH:O	2.10	0.50
1:C:28:ARG:O	1:C:32:ARG:HB2	2.12	0.50
1:D:256:ARG:CG	1:D:256:ARG:NH1	2.43	0.50
1:A:183:ASP:OD1	1:A:185:ASP:HB3	2.11	0.50
1:B:383:ARG:HG3	1:B:383:ARG:HH11	1.76	0.50
1:C:370:LYS:NZ	1:D:349:GLN:HG2	2.25	0.50
1:A:150:LYS:CE	1:A:184:PRO:HG3	2.40	0.50
1:A:311:SER:HB2	1:A:332:ALA:HA	1.93	0.50
3:C:399:FAD:H8A	1:D:283:THR:HG21	1.94	0.50
1:B:375:TYR:HB2	2:B:400:CO8:O1'	2.12	0.50
1:A:169:ASN:HA	1:A:221:ASP:O	2.12	0.50
1:A:271:LEU:HD13	1:A:301:MET:HB3	1.94	0.50
1:D:60:GLY:O	1:D:62:MET:N	2.45	0.50
1:D:246:LYS:HE2	2:D:400:CO8:H1B	1.93	0.49
1:D:396:ASN:HB3	4:D:2088:HOH:O	2.11	0.49
1:A:17:THR:HB	1:A:20:GLN:HG2	1.93	0.49
1:D:381:ILE:HG13	1:D:382:GLN:HE21	1.76	0.49
1:D:130:MET:HB2	1:D:172:LYS:O	2.13	0.49
1:A:174:ASN:HD22	1:A:175:TRP:CD1	2.28	0.49
1:A:270:ALA:HB2	1:A:365:LEU:HD23	1.94	0.49
1:A:17:THR:HA	1:D:10:LEU:HD12	1.94	0.49
1:D:50:VAL:HB	1:D:51:PRO:HD3	1.95	0.49
1:B:225:ILE:HG23	1:B:227:PHE:CE1	2.48	0.49
1:B:255:GLU:OE2	1:B:258:VAL:HG21	2.13	0.49
1:C:55:ARG:O	1:C:59:LEU:HG	2.12	0.49
1:C:106:MET:O	1:C:110:ILE:HG12	2.13	0.49
1:A:36:ILE:N	1:A:37:PRO:HD2	2.28	0.49
1:B:263:ALA:HB1	1:B:340:ALA:HB2	1.95	0.48
1:C:134:CYS:HA	1:C:167:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ALA:HA	1:A:61:LEU:HD11	1.96	0.48
1:B:57:TRP:CH2	1:B:128:PRO:HD3	2.48	0.48
1:B:99:GLU:C	2:B:400:CO8:H7'1	2.38	0.48
1:D:57:TRP:HD1	1:D:62:MET:HE2	1.79	0.48
1:D:388:ARG:HH12	2:D:400:CO8:H143	1.78	0.48
1:B:79:ASP:O	1:B:83:ILE:HG13	2.13	0.48
1:B:147:ILE:O	1:B:181:ARG:NH1	2.47	0.48
1:A:171:GLY:H	1:A:223:ARG:HD2	1.77	0.48
1:B:268:GLN:CG	1:B:309:ARG:HH12	2.25	0.48
3:A:399:FAD:H4B	1:B:350:ILE:O	2.13	0.48
1:C:370:LYS:HB3	1:D:356:PHE:CE1	2.49	0.48
1:D:355:GLY:HA2	1:D:362:VAL:HG21	1.95	0.48
1:B:341:ASN:OD1	1:B:370:LYS:HA	2.13	0.48
1:A:114:ASP:OD2	1:A:118:LYS:HE2	2.13	0.48
1:A:269:ARG:HG3	1:A:365:LEU:HD21	1.94	0.48
1:B:374:ILE:O	3:B:399:FAD:H4'	2.13	0.48
1:D:198:ILE:HG23	1:D:198:ILE:O	2.14	0.48
1:A:96:THR:HG23	2:A:400:CO8:H6'2	1.95	0.48
1:A:286:LYS:HD3	1:A:290:GLU:HB2	1.96	0.48
1:A:327:TYR:O	1:A:331:ILE:HG13	2.13	0.48
1:B:394:TYR:CD1	1:B:394:TYR:N	2.82	0.48
1:D:188:ALA:CB	1:D:193:ALA:HB2	2.43	0.48
1:A:264:VAL:HG11	1:A:309:ARG:HG3	1.95	0.47
1:C:370:LYS:HB3	1:D:356:PHE:HE1	1.77	0.47
1:D:281:ARG:HB3	1:D:288:LEU:HD22	1.96	0.47
1:D:57:TRP:CD1	1:D:128:PRO:HA	2.49	0.47
1:A:380:GLN:HG2	3:A:399:FAD:O2B	2.13	0.47
1:C:284:PHE:CD1	1:C:284:PHE:N	2.82	0.47
1:A:341:ASN:HD21	1:A:370:LYS:HA	1.79	0.47
2:B:400:CO8:H22	3:B:399:FAD:O2'	2.14	0.47
1:C:67:PRO:HD3	1:C:109:ILE:HD12	1.97	0.47
1:D:245:PHE:HE2	2:D:400:CO8:H8A	1.80	0.47
1:B:355:GLY:HA2	1:B:362:VAL:HG21	1.95	0.47
1:D:391:ILE:CG2	1:D:395:LYS:HE3	2.45	0.47
1:A:333:LYS:HD3	1:A:333:LYS:O	2.15	0.47
1:B:92:THR:HB	1:B:217:GLN:HE21	1.79	0.47
1:C:66:ILE:O	1:C:72:GLY:HA3	2.14	0.47
1:D:325:ASN:O	1:D:326:THR:C	2.58	0.47
1:A:73:LEU:CB	1:A:75:LEU:HD23	2.43	0.47
1:A:152:GLU:HB2	1:A:159:ILE:HG23	1.97	0.47
1:A:249:MET:HE1	2:A:400:CO8:O9P	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ILE:HB	1:D:72:GLY:HA3	1.96	0.47
1:A:384:LEU:HD21	1:D:292:GLN:HE21	1.80	0.47
1:B:165:MET:HG3	1:B:166:TRP:CD1	2.49	0.47
1:B:333:LYS:HE3	1:B:376:GLY:O	2.15	0.47
1:B:351:LEU:HG	1:B:362:VAL:HG11	1.96	0.47
1:C:379:SER:O	1:C:383:ARG:HG2	2.14	0.47
1:A:294:ILE:O	1:A:298:LEU:HD13	2.15	0.47
1:C:344:ALA:HB1	1:C:366:MET:HA	1.96	0.47
1:B:217:GLN:NE2	1:B:371:ILE:HD11	2.30	0.47
1:D:183:ASP:OD1	1:D:185:ASP:HB3	2.15	0.47
1:D:160:ILE:HG21	1:D:178:LEU:CD2	2.42	0.46
1:D:178:LEU:O	1:D:196:GLY:HA2	2.15	0.46
1:A:185:ASP:OD1	1:A:187:LYS:HB2	2.15	0.46
1:C:165:MET:HG3	1:C:166:TRP:CD1	2.50	0.46
1:B:198:ILE:HG23	1:B:198:ILE:O	2.16	0.46
1:D:86:GLU:O	1:D:89:TYR:HB3	2.15	0.46
1:B:120:TYR:O	1:B:124:MET:HG2	2.15	0.46
1:D:184:PRO:O	1:D:186:PRO:HD3	2.16	0.46
1:C:268:GLN:HE21	1:C:309:ARG:HH22	1.63	0.46
2:C:400:CO8:O8A	2:C:400:CO8:H4B	2.15	0.46
1:D:144:VAL:HG23	2:D:400:CO8:H62	1.98	0.46
1:D:249:MET:O	1:D:252:PHE:HB2	2.16	0.46
1:D:160:ILE:HD13	1:D:232:VAL:HG23	1.97	0.46
1:A:176:TYR:HB2	1:A:199:VAL:HG12	1.96	0.46
1:B:382:GLN:O	1:B:386:VAL:HG23	2.16	0.46
1:C:367:ARG:HG3	1:D:215:MET:HE2	1.97	0.46
1:D:92:THR:HG21	1:D:372:TYR:HE2	1.80	0.46
1:D:152:GLU:HB2	1:D:159:ILE:HG22	1.97	0.46
1:D:171:GLY:CA	1:D:223:ARG:HD3	2.42	0.46
2:A:400:CO8:H3'2	3:A:399:FAD:C4X	2.46	0.46
1:B:191:ASN:HD22	1:B:192:LYS:HG3	1.80	0.46
1:B:315:ALA:O	1:B:319:VAL:HG23	2.16	0.46
2:C:400:CO8:H8A	2:C:400:CO8:C5B	2.46	0.46
1:D:216:GLY:O	1:D:218:ARG:HD3	2.16	0.46
1:B:54:ARG:HG2	1:B:54:ARG:HH11	1.81	0.45
1:A:390:HIS:CE1	1:A:394:TYR:HE2	2.33	0.45
1:C:63:ASN:HB3	1:C:66:ILE:HG13	1.98	0.45
1:C:162:GLY:O	1:C:227:PHE:HB2	2.16	0.45
1:A:249:MET:HG2	2:A:400:CO8:C5A	2.45	0.45
1:B:99:GLU:HG3	2:B:400:CO8:C8'	2.45	0.45
1:B:216:GLY:HA3	1:B:367:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:OD1	1:A:130:MET:HA	2.17	0.45
1:A:127:GLU:HG3	1:A:129:LEU:HD13	1.98	0.45
1:B:95:GLN:O	1:B:99:GLU:HB2	2.16	0.45
1:D:252:PHE:HZ	2:D:400:CO8:H22	1.77	0.45
1:A:122:GLY:O	1:A:125:THR:HG22	2.16	0.45
1:A:338:ASP:HA	1:A:373:GLN:HE21	1.82	0.45
1:A:381:ILE:HA	1:A:384:LEU:HD12	1.98	0.45
1:C:268:GLN:NE2	1:C:309:ARG:HH22	2.15	0.45
1:C:276:LYS:O	1:C:280:GLU:HG2	2.16	0.45
1:C:325:ASN:HD22	1:C:325:ASN:N	2.14	0.45
1:A:282:LYS:HA	1:A:287:LEU:HA	1.97	0.45
1:C:357:ASN:HB2	1:D:166:TRP:HH2	1.82	0.45
1:D:218:ARG:HA	4:D:2046:HOH:O	2.17	0.45
1:B:158:TYR:CE1	1:B:237:VAL:HG21	2.52	0.45
1:B:160:ILE:HB	1:B:230:VAL:HB	1.99	0.45
1:D:54:ARG:HG3	1:D:54:ARG:HH11	1.82	0.45
1:C:73:LEU:CB	1:C:75:LEU:HD13	2.45	0.45
1:D:29:LYS:O	1:D:33:GLU:HB2	2.16	0.45
1:D:268:GLN:HG3	1:D:309:ARG:HH22	1.79	0.45
1:A:255:GLU:C	1:A:257:PRO:HD2	2.42	0.45
1:A:267:ALA:HB1	1:A:343:LEU:HD22	1.99	0.45
1:C:186:PRO:HG2	1:C:187:LYS:CD	2.47	0.45
1:D:120:TYR:CD2	1:D:198:ILE:HD13	2.51	0.45
1:D:268:GLN:NE2	1:D:305:VAL:HG11	2.31	0.45
1:A:391:ILE:HD12	1:A:391:ILE:C	2.42	0.45
1:D:77:THR:HG21	1:D:316:ALA:HA	1.99	0.45
1:B:168:THR:C	1:B:170:GLY:H	2.25	0.44
1:A:171:GLY:HA2	1:A:208:ILE:HG21	1.99	0.44
1:A:287:LEU:H	1:A:287:LEU:CD2	2.30	0.44
1:B:335:PHE:O	1:B:339:ILE:HG23	2.17	0.44
1:C:266:LEU:HD23	1:C:266:LEU:O	2.17	0.44
1:B:289:VAL:HG21	1:C:391:ILE:HD12	1.99	0.44
1:C:150:LYS:HZ2	1:C:161:ASN:CB	2.29	0.44
1:D:120:TYR:CG	1:D:198:ILE:HD11	2.52	0.44
1:D:256:ARG:HG3	1:D:256:ARG:NH1	2.20	0.44
1:B:99:GLU:HB3	2:B:400:CO8:H7'1	1.99	0.44
1:A:143:ASP:HA	1:B:284:PHE:CZ	2.52	0.44
1:B:123:ARG:HD2	1:B:175:TRP:NE1	2.33	0.44
1:B:287:LEU:HB2	1:B:290:GLU:HG3	2.00	0.44
1:A:214:ASN:HB3	1:B:356:PHE:CD2	2.52	0.44
1:B:319:VAL:HG22	1:B:325:ASN:ND2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:PRO:HG2	1:C:187:LYS:HD2	1.99	0.44
1:A:252:PHE:HE1	2:A:400:CO8:S1P	2.40	0.44
1:A:318:GLU:O	1:A:323:ARG:HD2	2.18	0.44
1:A:370:LYS:HE3	1:A:370:LYS:O	2.18	0.44
1:A:35:ILE:C	1:A:37:PRO:HD2	2.42	0.44
1:A:186:PRO:HG2	1:A:187:LYS:CE	2.48	0.44
1:A:390:HIS:CE1	1:A:394:TYR:CE2	3.06	0.44
1:B:88:ALA:HB3	1:B:265:GLY:HA3	1.99	0.44
1:B:108:ILE:HG12	1:B:198:ILE:HD12	1.99	0.44
1:B:95:GLN:HG3	1:B:96:THR:N	2.33	0.44
1:A:277:TYR:HA	1:A:280:GLU:HG2	2.00	0.43
1:D:30:PHE:CD1	1:D:34:GLU:HB2	2.53	0.43
1:A:49:PRO:O	1:A:53:ILE:HG12	2.19	0.43
1:A:185:ASP:HA	1:A:186:PRO:HD2	1.83	0.43
2:A:400:CO8:OAP	1:B:284:PHE:HZ	2.01	0.43
1:C:19:GLN:HE21	1:C:23:PHE:HD2	1.66	0.43
1:B:160:ILE:N	1:B:230:VAL:O	2.47	0.43
1:D:247:VAL:O	1:D:248:ALA:C	2.59	0.43
1:B:255:GLU:O	1:B:256:ARG:C	2.60	0.43
1:A:122:GLY:HA2	1:A:125:THR:HG22	2.00	0.43
1:C:150:LYS:NZ	1:C:161:ASN:HB2	2.34	0.43
1:C:243:ALA:O	1:C:247:VAL:HG23	2.19	0.43
1:A:54:ARG:HH11	1:A:128:PRO:HB2	1.84	0.43
1:B:123:ARG:HD2	1:B:175:TRP:HE1	1.82	0.43
1:C:103:LEU:HD12	2:C:400:CO8:C5'	2.49	0.43
1:D:78:PHE:HB2	4:D:2030:HOH:O	2.17	0.43
1:A:296:PHE:O	1:A:300:GLU:HG3	2.19	0.43
1:B:271:LEU:HD12	1:B:305:VAL:HG11	2.00	0.43
1:A:344:ALA:O	1:A:347:ALA:HB3	2.18	0.43
1:B:106:MET:HB3	1:B:107:PRO:HD3	2.00	0.43
1:C:195:THR:CG2	1:C:237:VAL:HG23	2.49	0.43
1:A:20:GLN:HE21	1:A:20:GLN:HB3	1.69	0.43
1:D:378:THR:O	1:D:382:GLN:HG2	2.17	0.43
1:A:270:ALA:HB1	1:A:347:ALA:HB2	2.01	0.43
1:C:152:GLU:CG	1:C:159:ILE:HG23	2.48	0.43
1:C:189:PRO:HG2	1:C:192:LYS:CG	2.48	0.43
1:C:121:LEU:HD12	1:C:121:LEU:HA	1.89	0.42
1:D:390:HIS:CD2	1:D:391:ILE:HD12	2.54	0.42
1:B:355:GLY:HA2	1:B:362:VAL:CG2	2.49	0.42
1:D:259:VAL:CG1	1:D:372:TYR:CE1	3.02	0.42
1:A:225:ILE:HG22	1:A:226:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLU:OE1	1:A:255:GLU:HA	2.19	0.42
1:C:393:LYS:HG3	4:C:2047:HOH:O	2.18	0.42
1:B:63:ASN:HB3	1:B:66:ILE:CD1	2.50	0.42
1:B:166:TRP:O	3:B:399:FAD:C4X	2.66	0.42
1:C:20:GLN:HG2	1:C:82:LEU:HD21	2.01	0.42
1:C:92:THR:HG21	1:C:266:LEU:HD12	2.00	0.42
1:B:28:ARG:HG3	1:B:32:ARG:CZ	2.49	0.42
1:C:103:LEU:HD22	1:C:133:TYR:CG	2.54	0.42
1:C:127:GLU:O	1:C:129:LEU:N	2.51	0.42
1:C:64:THR:HB	1:C:75:LEU:HD22	2.01	0.42
1:D:256:ARG:NH1	1:D:376:GLY:O	2.53	0.42
1:D:377:GLY:CA	1:D:381:ILE:HD11	2.49	0.42
1:A:356:PHE:CZ	1:B:216:GLY:N	2.87	0.42
1:A:363:GLU:CG	1:B:215:MET:HB2	2.49	0.42
1:C:266:LEU:HD23	1:C:266:LEU:C	2.45	0.42
1:C:363:GLU:O	1:D:215:MET:HE3	2.20	0.42
1:A:272:ASP:O	1:A:276:LYS:HG3	2.19	0.42
1:C:187:LYS:HD2	1:C:187:LYS:N	2.34	0.42
1:C:231:LYS:HD2	1:C:231:LYS:N	2.29	0.42
1:D:239:ILE:HG22	1:D:240:GLY:N	2.34	0.42
1:C:29:LYS:HE2	1:C:29:LYS:HA	2.02	0.42
1:C:256:ARG:O	1:C:259:VAL:HG22	2.20	0.42
1:D:113:ASN:O	1:D:116:GLN:HG2	2.19	0.42
1:D:390:HIS:HA	1:D:393:LYS:HE3	2.01	0.42
1:C:196:GLY:O	1:C:238:LEU:HD23	2.20	0.42
1:D:106:MET:HG2	1:D:251:ALA:HA	2.01	0.42
1:C:66:ILE:HG23	1:C:121:LEU:HG	2.00	0.41
1:C:357:ASN:HB2	1:D:166:TRP:CH2	2.55	0.41
1:D:252:PHE:O	1:D:253:ASP:C	2.63	0.41
1:D:268:GLN:HG2	1:D:309:ARG:HH22	1.85	0.41
1:A:156:ASP:O	1:A:234:LYS:HG2	2.20	0.41
1:A:208:ILE:HA	1:A:225:ILE:HG23	2.02	0.41
2:A:400:CO8:O2A	2:A:400:CO8:H121	2.20	0.41
1:B:390:HIS:CE1	1:B:394:TYR:CE1	3.08	0.41
1:C:144:VAL:C	1:C:146:GLY:H	2.28	0.41
1:D:277:TYR:CE2	1:D:351:LEU:HA	2.55	0.41
1:A:304:LYS:HB3	1:A:339:ILE:HB	2.03	0.41
1:D:269:ARG:O	1:D:273:GLU:HG2	2.20	0.41
1:A:269:ARG:O	1:A:273:GLU:HB2	2.21	0.41
1:B:150:LYS:HD2	1:B:150:LYS:HA	1.79	0.41
1:D:183:ASP:HA	1:D:184:PRO:HD2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:MET:HE3	1:B:101:ASN:ND2	2.35	0.41
1:C:63:ASN:HB3	1:C:66:ILE:CD1	2.50	0.41
1:C:185:ASP:HA	1:C:186:PRO:HD2	1.85	0.41
1:D:91:CYS:SG	1:D:94:VAL:HG23	2.61	0.41
1:B:57:TRP:CD2	1:B:128:PRO:HB3	2.55	0.41
1:B:111:ALA:CB	1:B:239:ILE:HD11	2.45	0.41
1:C:304:LYS:HB3	1:C:339:ILE:HB	2.02	0.41
1:D:103:LEU:HD21	2:D:400:CO8:H2'1	2.03	0.41
1:C:258:VAL:O	1:C:261:ALA:HB3	2.21	0.41
1:D:224:GLY:C	1:D:225:ILE:HG13	2.46	0.41
1:A:169:ASN:HD22	1:A:169:ASN:HA	1.72	0.41
1:A:390:HIS:NE2	1:D:271:LEU:HD11	2.35	0.41
1:B:198:ILE:HG22	1:B:236:ASN:O	2.21	0.41
1:B:215:MET:O	1:B:367:ARG:HD2	2.21	0.41
1:C:63:ASN:ND2	1:C:105:GLN:OE1	2.53	0.41
1:C:356:PHE:HE1	1:D:370:LYS:HB3	1.85	0.41
1:D:103:LEU:HG	1:D:133:TYR:HB2	2.03	0.41
1:D:137:GLU:O	1:D:138:PRO:C	2.64	0.41
1:D:175:TRP:HB2	1:D:199:VAL:O	2.21	0.41
2:D:400:CO8:H32	3:D:399:FAD:O2'	2.21	0.41
1:A:254:LYS:NZ	1:A:254:LYS:HB3	2.36	0.41
1:A:363:GLU:HG3	1:B:215:MET:HB2	2.01	0.41
1:C:330:SER:HA	1:C:382:GLN:NE2	2.36	0.41
1:B:324:ARG:O	1:B:324:ARG:HG3	2.20	0.40
1:D:138:PRO:CD	1:D:165:MET:HB2	2.50	0.40
1:D:159:ILE:O	1:D:159:ILE:CG2	2.69	0.40
1:D:383:ARG:HG3	1:D:383:ARG:NH1	2.36	0.40
1:C:283:THR:HB	1:C:284:PHE:CD1	2.55	0.40
1:D:391:ILE:HG22	1:D:395:LYS:HE3	2.03	0.40
1:C:325:ASN:O	1:C:326:THR:C	2.64	0.40
1:A:167:ILE:O	1:A:168:THR:C	2.63	0.40
1:A:330:SER:O	1:A:382:GLN:HG3	2.22	0.40
1:B:134:CYS:SG	1:B:176:TYR:HB3	2.61	0.40
1:D:29:LYS:HE2	1:D:33:GLU:OE1	2.21	0.40
1:D:55:ARG:O	1:D:58:GLU:HG2	2.21	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	385/396 (97%)	344 (89%)	39 (10%)	2 (0%)	24	46
1	B	385/396 (97%)	351 (91%)	33 (9%)	1 (0%)	36	58
1	C	385/396 (97%)	351 (91%)	29 (8%)	5 (1%)	9	21
1	D	385/396 (97%)	334 (87%)	39 (10%)	12 (3%)	3	5
All	All	1540/1584 (97%)	1380 (90%)	140 (9%)	20 (1%)	9	21

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	61	LEU
1	D	77	THR
1	D	228	GLU
1	D	326	THR
1	A	141	GLY
1	B	145	ALA
1	D	62	MET
1	D	241	ASP
1	A	244	GLY
1	C	145	ALA
1	C	192	LYS
1	D	238	LEU
1	D	252	PHE
1	C	216	GLY
1	C	326	THR
1	D	109	ILE
1	D	141	GLY
1	C	37	PRO
1	D	138	PRO
1	D	230	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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
2	CO8	D	400	-	57,59,59	1.98	8 (14%)	79,85,85	1.37	11 (13%)
3	FAD	C	399	-	58,58,58	1.31	4 (6%)	85,89,89	1.32	11 (12%)
3	FAD	B	399	-	58,58,58	1.40	8 (13%)	85,89,89	1.34	9 (10%)
2	CO8	C	400	-	57,59,59	1.46	7 (12%)	79,85,85	2.52	21 (26%)
3	FAD	D	399	-	58,58,58	1.30	6 (10%)	85,89,89	1.22	7 (8%)
2	CO8	A	400	-	57,59,59	1.72	7 (12%)	79,85,85	1.57	9 (11%)
2	CO8	B	400	-	57,59,59	1.55	6 (10%)	79,85,85	1.98	13 (16%)
3	FAD	A	399	-	58,58,58	1.38	9 (15%)	85,89,89	1.68	17 (20%)

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
2	CO8	D	400	-	-	7/58/74/74	0/3/3/3
3	FAD	C	399	-	-	2/34/50/50	0/6/6/6
3	FAD	B	399	-	-	0/34/50/50	0/6/6/6
2	CO8	C	400	-	-	15/58/74/74	0/3/3/3
3	FAD	D	399	-	-	2/34/50/50	0/6/6/6
2	CO8	A	400	-	-	8/58/74/74	0/3/3/3
2	CO8	B	400	-	-	17/58/74/74	0/3/3/3
3	FAD	A	399	-	-	4/34/50/50	0/6/6/6

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	CO8	P2A-O3A	8.38	1.68	1.59
2	D	400	CO8	P1A-O3A	8.12	1.68	1.59
2	B	400	CO8	P2A-O3A	6.04	1.66	1.59
2	A	400	CO8	P1A-O3A	5.73	1.65	1.59
2	A	400	CO8	C5P-N4P	5.41	1.46	1.33
2	B	400	CO8	P1A-O3A	5.31	1.65	1.59
2	C	400	CO8	P1A-O3A	4.91	1.64	1.59
2	A	400	CO8	O1'-C1'	4.56	1.28	1.21
2	D	400	CO8	C2'-C1'	4.42	1.55	1.50
2	A	400	CO8	P2A-O3A	4.30	1.64	1.59
3	D	399	FAD	C10-N10	4.23	1.46	1.37
3	A	399	FAD	C10-N10	4.22	1.46	1.37
3	C	399	FAD	C10-N10	4.20	1.46	1.37
2	C	400	CO8	C5P-N4P	4.03	1.42	1.33
3	B	399	FAD	P-O3P	3.99	1.63	1.59
3	C	399	FAD	C4X-N5	3.88	1.39	1.30
2	A	400	CO8	C9P-N8P	3.82	1.42	1.33
3	B	399	FAD	C4X-N5	3.74	1.38	1.30
2	C	400	CO8	C9P-N8P	3.52	1.41	1.33
2	B	400	CO8	C5P-N4P	3.44	1.41	1.33
2	A	400	CO8	P3B-O3B	3.41	1.65	1.59
3	D	399	FAD	C6-C7	-3.34	1.35	1.39
3	B	399	FAD	C9-C8	-3.32	1.35	1.39
3	A	399	FAD	C4X-N5	3.32	1.37	1.30
2	C	400	CO8	P2A-O3A	3.30	1.63	1.59
2	B	400	CO8	C1'-S1P	-3.21	1.68	1.76
3	A	399	FAD	C7M-C7	3.19	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	399	FAD	C4X-N5	3.18	1.37	1.30
3	D	399	FAD	C9-C8	-3.12	1.35	1.39
3	B	399	FAD	C10-N10	3.09	1.44	1.37
3	A	399	FAD	O2B-C2B	-3.06	1.35	1.43
2	B	400	CO8	P3B-O3B	2.95	1.64	1.59
2	D	400	CO8	C9P-N8P	2.91	1.40	1.33
2	C	400	CO8	C8A-N9A	2.90	1.42	1.37
2	B	400	CO8	C9P-N8P	2.90	1.40	1.33
3	C	399	FAD	C2A-N1A	-2.87	1.28	1.33
3	C	399	FAD	C8M-C8	2.84	1.56	1.51
3	B	399	FAD	PA-O3P	2.70	1.62	1.59
3	A	399	FAD	P-O3P	2.62	1.62	1.59
2	D	400	CO8	P3B-O3B	2.61	1.64	1.59
2	A	400	CO8	C2'-C1'	2.55	1.53	1.50
2	C	400	CO8	O2B-C2B	2.51	1.49	1.43
3	A	399	FAD	C6-C7	-2.32	1.36	1.39
3	B	399	FAD	O2B-C2B	-2.30	1.37	1.43
3	D	399	FAD	PA-O3P	-2.17	1.57	1.59
3	A	399	FAD	C5X-N5	-2.16	1.35	1.39
2	D	400	CO8	C4A-N3A	2.16	1.38	1.34
3	A	399	FAD	C10-N1	2.16	1.37	1.33
2	D	400	CO8	C1B-N9A	2.15	1.52	1.46
3	B	399	FAD	C5X-N5	-2.14	1.35	1.39
2	D	400	CO8	O4B-C1B	2.12	1.46	1.42
2	C	400	CO8	P3B-O3B	2.12	1.63	1.59
3	A	399	FAD	C4A-N3A	2.11	1.38	1.34
3	B	399	FAD	C2-N3	-2.09	1.34	1.39
3	D	399	FAD	P-O3P	-2.03	1.57	1.59

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	CO8	O1'-C1'-C2'	-14.34	107.43	123.98
2	C	400	CO8	C2'-C1'-S1P	8.01	122.95	113.40
2	B	400	CO8	O6A-CCP-CBP	7.90	123.25	110.55
2	B	400	CO8	O1'-C1'-S1P	-7.85	112.69	122.68
2	A	400	CO8	O6A-CCP-CBP	7.03	121.84	110.55
2	C	400	CO8	C6P-C7P-N8P	-6.13	98.95	112.00
3	A	399	FAD	C2B-C3B-C4B	-5.55	91.89	102.61
3	A	399	FAD	C9A-C5X-N5	5.20	127.97	122.45
3	B	399	FAD	O3'-C3'-C4'	-4.58	98.52	108.93
3	D	399	FAD	C9A-C5X-N5	4.53	127.27	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	CO8	C2'-C1'-S1P	4.49	118.75	113.40
2	B	400	CO8	C2B-C3B-C4B	-4.47	95.41	103.24
2	C	400	CO8	O1'-C1'-S1P	4.47	128.38	122.68
2	A	400	CO8	O1'-C1'-S1P	-4.45	117.02	122.68
3	B	399	FAD	C4'-C3'-C2'	4.36	120.83	113.57
3	B	399	FAD	C9A-C5X-N5	4.36	127.08	122.45
3	A	399	FAD	O5'-C5'-C4'	-4.28	97.93	109.36
2	B	400	CO8	C2B-C1B-N9A	-4.25	102.75	113.30
3	C	399	FAD	C9A-C5X-N5	4.24	126.95	122.45
2	A	400	CO8	C6P-C7P-N8P	4.21	120.95	112.00
2	B	400	CO8	O4B-C1B-N9A	4.15	116.06	108.09
3	C	399	FAD	O4B-C1B-N9A	-4.08	100.25	108.09
2	C	400	CO8	O6A-CCP-CBP	4.05	117.06	110.55
2	B	400	CO8	O1'-C1'-C2'	3.86	128.43	123.98
2	D	400	CO8	O6A-CCP-CBP	-3.83	104.38	110.55
3	A	399	FAD	O4-C4-N3	-3.78	113.01	120.11
3	D	399	FAD	O5B-C5B-C4B	3.62	121.31	108.99
2	C	400	CO8	C6P-C5P-N4P	-3.61	109.77	116.34
2	D	400	CO8	CDP-CBP-CAP	3.57	114.85	108.77
2	C	400	CO8	P3B-O3B-C3B	3.53	132.86	123.43
2	A	400	CO8	C2B-C3B-C4B	-3.47	97.16	103.24
2	D	400	CO8	C3P-N4P-C5P	-3.25	116.77	122.82
2	D	400	CO8	O4B-C1B-N9A	3.17	114.19	108.09
3	A	399	FAD	C5X-N5-C4X	-3.16	112.97	118.09
3	B	399	FAD	C5X-N5-C4X	-3.13	113.02	118.09
2	C	400	CO8	CEP-CBP-CCP	-3.09	103.12	108.22
3	C	399	FAD	C6-C5X-C9A	-3.09	114.81	119.05
2	D	400	CO8	O2A-P1A-O3A	3.02	115.45	107.27
2	B	400	CO8	CEP-CBP-CAP	2.96	113.81	108.77
3	A	399	FAD	O3P-PA-O1A	-2.94	101.85	110.70
3	A	399	FAD	C6-C5X-N5	-2.89	113.65	118.44
3	A	399	FAD	O5B-C5B-C4B	2.87	118.78	108.99
2	A	400	CO8	CDP-CBP-CCP	-2.85	103.52	108.22
3	A	399	FAD	O2-C2-N1	2.85	126.53	121.80
2	A	400	CO8	C2P-C3P-N4P	2.81	118.28	112.41
2	A	400	CO8	O1'-C1'-C2'	2.78	127.19	123.98
3	A	399	FAD	O2A-PA-O1A	2.73	125.16	112.44
2	C	400	CO8	CAP-C9P-N8P	2.73	121.66	116.48
2	C	400	CO8	C3B-C2B-C1B	-2.72	93.90	99.89
2	D	400	CO8	C6P-C5P-N4P	-2.70	111.41	116.34
2	B	400	CO8	C3'-C2'-C1'	2.67	118.16	112.27
3	C	399	FAD	C5X-N5-C4X	-2.66	113.78	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	399	FAD	C1'-N10-C9A	-2.65	115.48	120.63
2	C	400	CO8	O9A-P3B-O8A	2.61	117.60	107.80
2	C	400	CO8	O5P-C5P-N4P	2.61	128.14	123.03
3	C	399	FAD	O4B-C1B-C2B	-2.59	101.07	106.62
2	A	400	CO8	CEP-CBP-CAP	2.58	113.17	108.77
3	C	399	FAD	C2B-C1B-N9A	2.58	119.71	113.30
3	D	399	FAD	C5X-N5-C4X	-2.57	113.93	118.09
3	C	399	FAD	O2B-C2B-C3B	-2.55	103.64	111.82
2	C	400	CO8	O5B-C5B-C4B	2.52	117.57	108.99
3	C	399	FAD	O4-C4-N3	-2.50	115.40	120.11
3	A	399	FAD	C1'-N10-C9A	-2.48	115.81	120.63
3	A	399	FAD	PA-O5B-C5B	-2.48	107.13	121.35
2	C	400	CO8	O9P-C9P-N8P	-2.47	117.76	122.98
3	D	399	FAD	O4-C4-N3	-2.45	115.50	120.11
3	B	399	FAD	O4-C4-N3	-2.45	115.50	120.11
2	A	400	CO8	O4B-C1B-C2B	-2.43	101.43	106.62
2	C	400	CO8	O4B-C1B-N9A	-2.40	103.48	108.09
2	B	400	CO8	CDP-CBP-CAP	2.38	112.83	108.77
3	D	399	FAD	O2A-PA-O1A	2.37	123.48	112.44
2	C	400	CO8	C1B-N9A-C8A	2.36	132.32	127.09
3	A	399	FAD	O4B-C1B-C2B	-2.35	101.58	106.62
2	D	400	CO8	C2B-C1B-N9A	-2.33	107.52	113.30
2	B	400	CO8	O5B-C5B-C4B	2.31	116.85	108.99
2	C	400	CO8	C3P-N4P-C5P	2.30	127.10	122.82
2	C	400	CO8	O2A-P1A-O3A	2.29	113.47	107.27
2	D	400	CO8	O2B-C2B-C3B	-2.26	104.85	111.19
2	C	400	CO8	P1A-O5B-C5B	-2.26	108.41	121.35
3	B	399	FAD	C2B-C1B-N9A	-2.23	107.75	113.30
2	D	400	CO8	CDP-CBP-CCP	-2.23	104.54	108.22
3	A	399	FAD	O3'-C3'-C2'	2.22	113.97	108.93
3	A	399	FAD	O4'-C4'-C3'	2.19	114.37	109.25
3	B	399	FAD	C6-C5X-N5	-2.15	114.88	118.44
3	A	399	FAD	O2P-P-O3P	2.14	113.07	107.27
3	A	399	FAD	O4-C4-C4X	2.13	132.16	126.53
2	B	400	CO8	O2B-C2B-C3B	2.12	117.11	111.19
3	D	399	FAD	C5X-C9A-N10	-2.11	116.06	117.97
2	C	400	CO8	O3B-P3B-O7A	-2.09	101.89	109.33
3	B	399	FAD	C2B-C3B-C4B	-2.09	98.58	102.61
2	B	400	CO8	O3B-P3B-O7A	-2.08	101.92	109.33
2	C	400	CO8	O3B-C3B-C2B	2.05	119.04	111.68
2	D	400	CO8	O5A-P2A-O3A	2.04	112.79	107.27
3	B	399	FAD	O5B-C5B-C4B	2.03	115.90	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	CO8	O3B-C3B-C2B	-2.02	104.42	111.68
3	C	399	FAD	O2A-PA-O1A	2.02	121.83	112.44
3	D	399	FAD	O3P-P-O1P	-2.01	104.66	110.70
3	C	399	FAD	C4A-N9A-C8A	-2.00	103.63	105.74

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	CO8	P1A-O3A-P2A-O6A
2	A	400	CO8	CCP-O6A-P2A-O4A
2	A	400	CO8	CBP-CCP-O6A-P2A
2	A	400	CO8	CDP-CBP-CCP-O6A
2	A	400	CO8	CEP-CBP-CCP-O6A
2	A	400	CO8	CAP-CBP-CCP-O6A
2	A	400	CO8	N8P-C9P-CAP-OAP
2	B	400	CO8	C5B-O5B-P1A-O1A
2	B	400	CO8	C5B-O5B-P1A-O2A
2	B	400	CO8	C5B-O5B-P1A-O3A
2	B	400	CO8	CCP-O6A-P2A-O5A
2	B	400	CO8	C5P-C6P-C7P-N8P
2	B	400	CO8	C2P-C3P-N4P-C5P
2	B	400	CO8	C3P-C2P-S1P-C1'
2	B	400	CO8	C2'-C1'-S1P-C2P
2	C	400	CO8	OAP-CAP-CBP-CCP
2	C	400	CO8	C9P-CAP-CBP-CCP
2	C	400	CO8	OAP-CAP-CBP-CDP
2	C	400	CO8	C9P-CAP-CBP-CDP
2	C	400	CO8	OAP-CAP-CBP-CEP
2	C	400	CO8	C9P-CAP-CBP-CEP
2	C	400	CO8	C2P-C3P-N4P-C5P
2	C	400	CO8	C3P-C2P-S1P-C1'
2	C	400	CO8	O1'-C1'-S1P-C2P
2	C	400	CO8	C2'-C1'-S1P-C2P
2	D	400	CO8	CCP-O6A-P2A-O3A
2	D	400	CO8	CCP-O6A-P2A-O4A
2	D	400	CO8	CCP-O6A-P2A-O5A
3	A	399	FAD	C5B-O5B-PA-O2A
3	A	399	FAD	C5B-O5B-PA-O3P
2	C	400	CO8	C4B-C3B-O3B-P3B
3	C	399	FAD	PA-O3P-P-O1P
3	D	399	FAD	PA-O3P-P-O1P

Continued on next page...

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Mol	Chain	Res	Type	Atoms
2	D	400	CO8	S1P-C2P-C3P-N4P
2	B	400	CO8	N8P-C9P-CAP-CBP
2	B	400	CO8	O1'-C1'-S1P-C2P
2	D	400	CO8	O1'-C1'-S1P-C2P
2	C	400	CO8	C5'-C6'-C7'-C8'
2	C	400	CO8	C2B-C3B-O3B-P3B
2	D	400	CO8	C2'-C1'-S1P-C2P
2	C	400	CO8	C3B-C4B-C5B-O5B
2	A	400	CO8	O9P-C9P-CAP-OAP
2	B	400	CO8	CDP-CBP-CCP-O6A
2	B	400	CO8	CCP-O6A-P2A-O3A
2	B	400	CO8	CCP-O6A-P2A-O4A
2	C	400	CO8	C5B-O5B-P1A-O1A
3	A	399	FAD	C5B-O5B-PA-O1A
2	B	400	CO8	OAP-CAP-CBP-CDP
3	D	399	FAD	PA-O3P-P-O2P
2	B	400	CO8	C4B-C5B-O5B-P1A
2	D	400	CO8	C5'-C6'-C7'-C8'
3	C	399	FAD	PA-O3P-P-O2P
2	B	400	CO8	O9P-C9P-CAP-CBP
2	B	400	CO8	CEP-CBP-CCP-O6A
3	A	399	FAD	PA-O3P-P-O1P

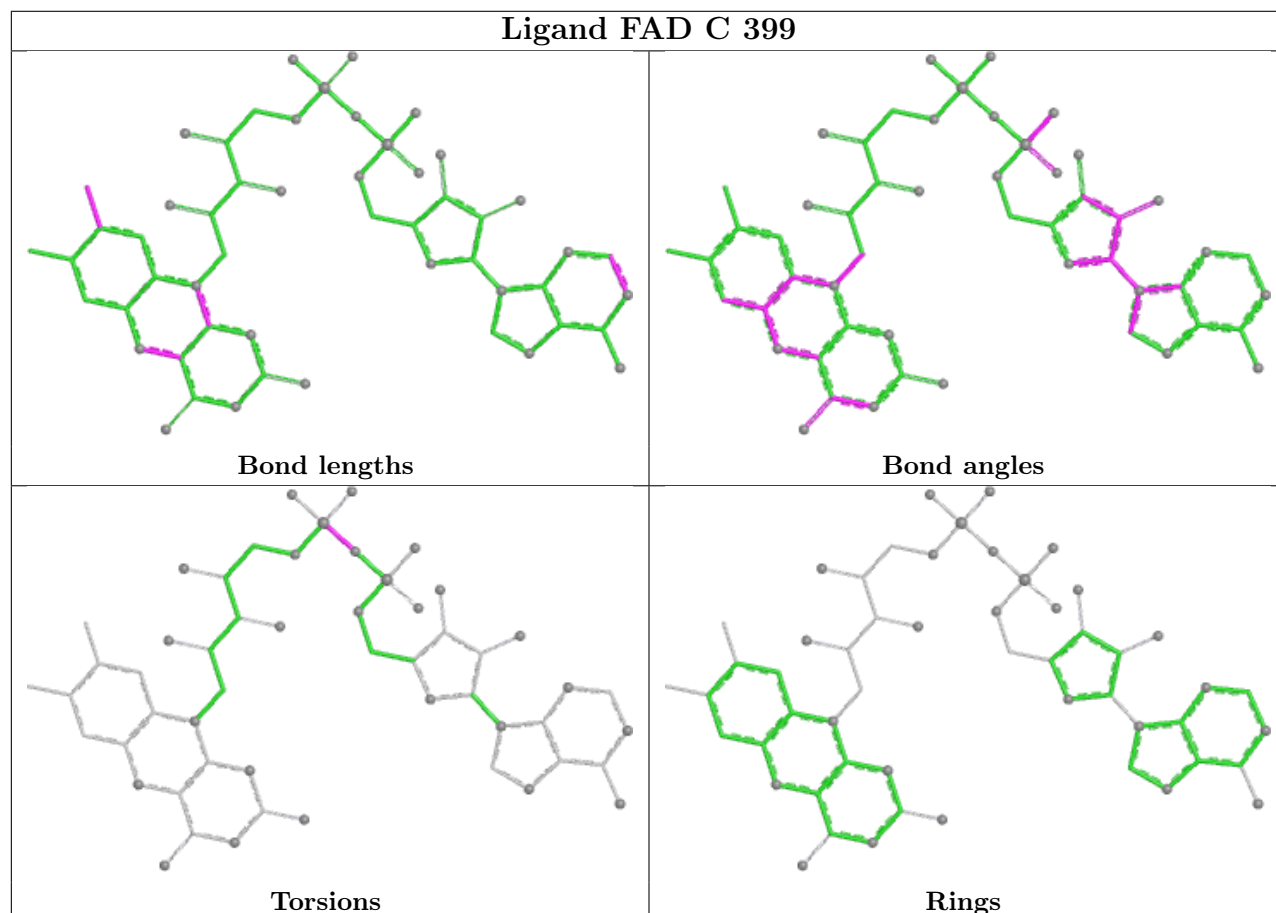
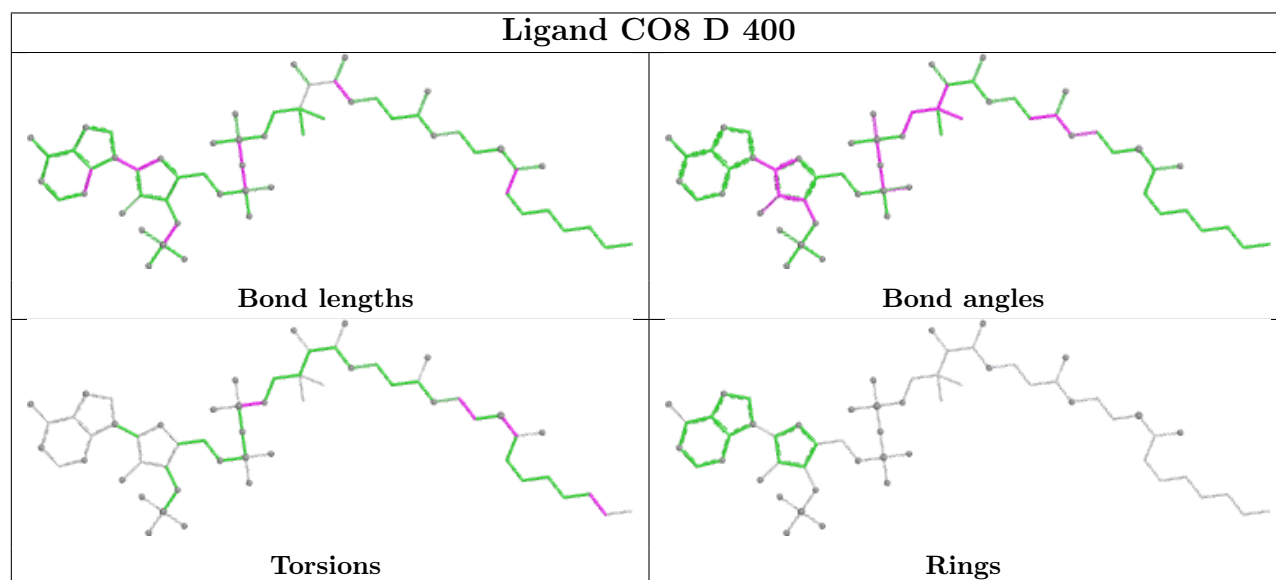
There are no ring outliers.

8 monomers are involved in 51 short contacts:

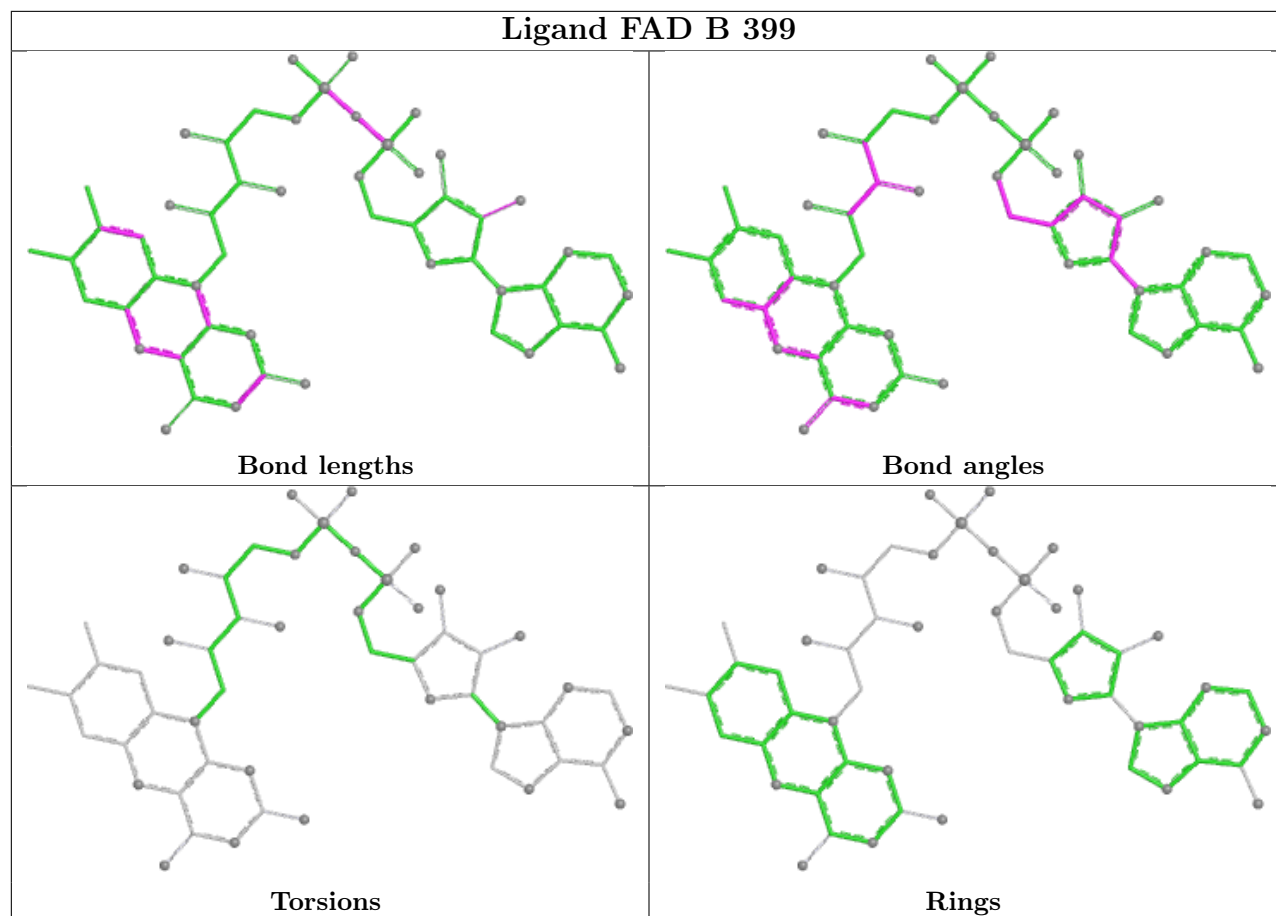
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	400	CO8	14	0
3	C	399	FAD	2	0
3	B	399	FAD	4	0
2	C	400	CO8	9	0
3	D	399	FAD	4	0
2	A	400	CO8	11	0
2	B	400	CO8	8	0
3	A	399	FAD	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

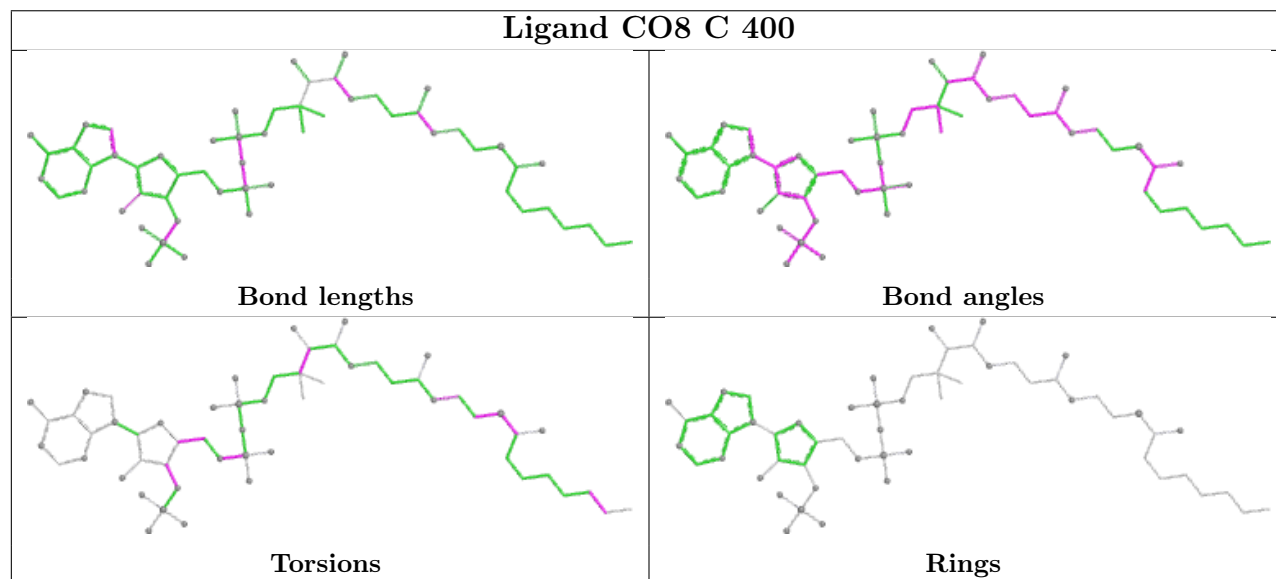
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



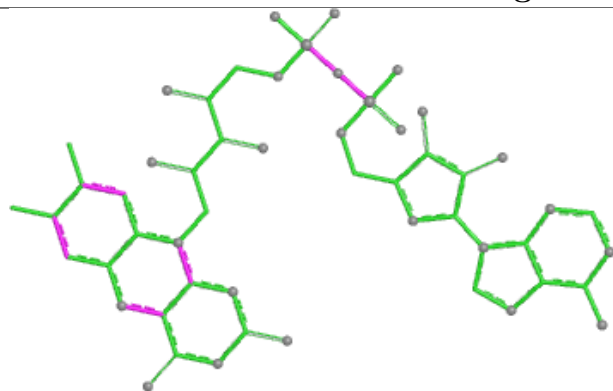
Ligand FAD B 399



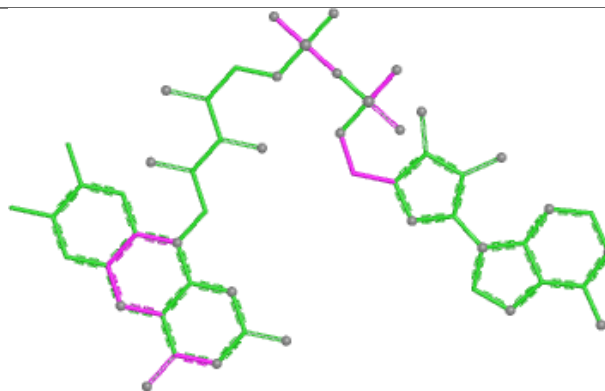
Ligand CO8 C 400



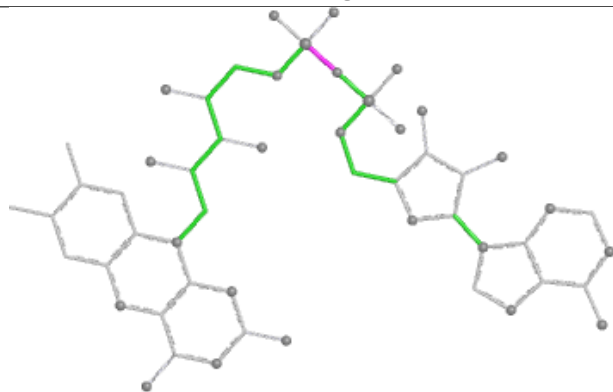
Ligand FAD D 399



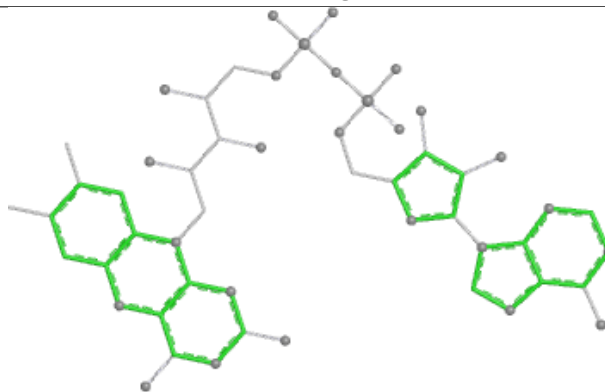
Bond lengths



Bond angles

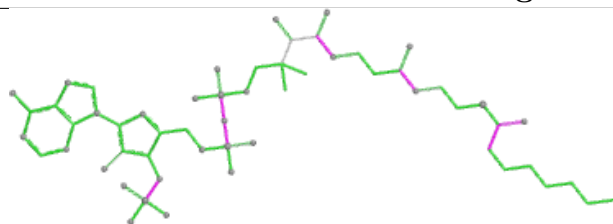


Torsions

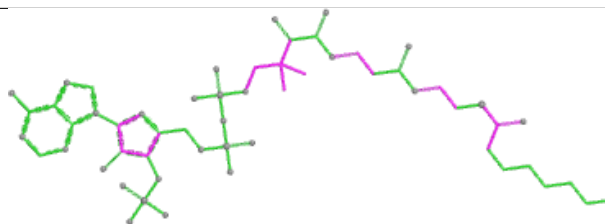


Rings

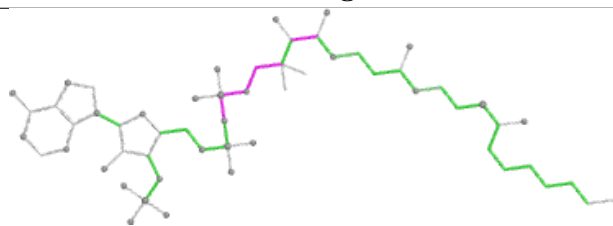
Ligand CO8 A 400



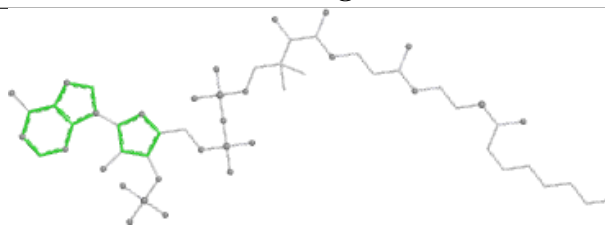
Bond lengths



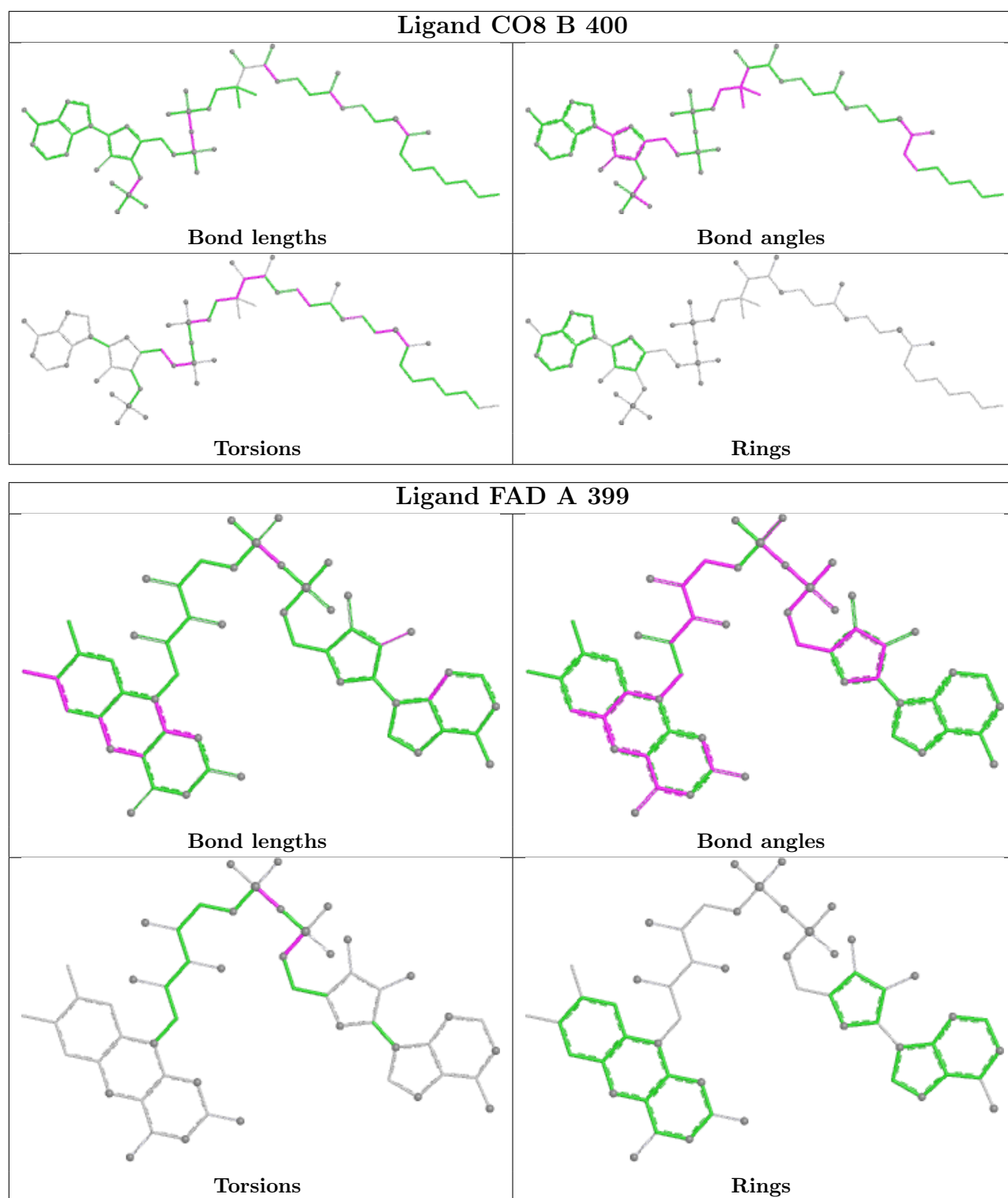
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	214:ASN	C	215:MET	N	1.15

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.