Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 09:23 AM EDT

PDB ID	:	1EGC
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 following versions of software and data (see references ⓘ) were used in the production of this report:

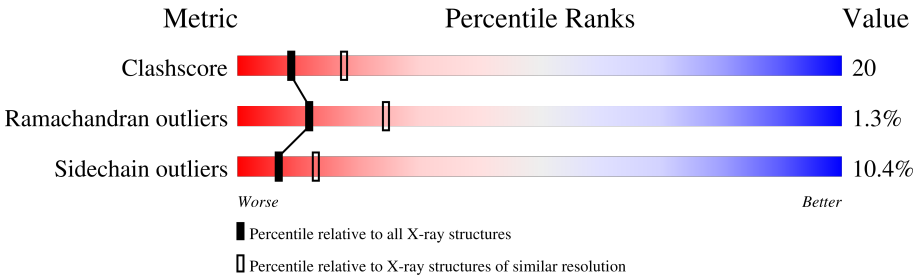
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	55% 36% 7% •
1	B	396	60% 33% 5% •
1	C	396	63% 30% • • •
1	D	396	51% 39% 7% • •

2 Entry composition (i)

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.

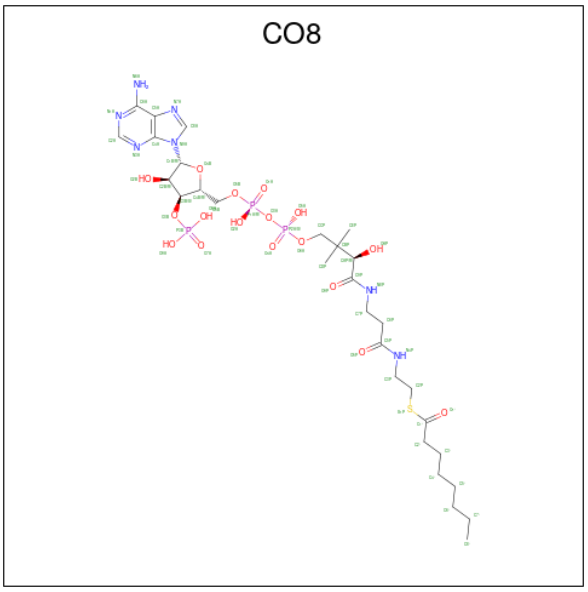
- Molecule 1 is a protein called MEDIUM CHAIN ACYL-COA DEHYDROGENASE.

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:

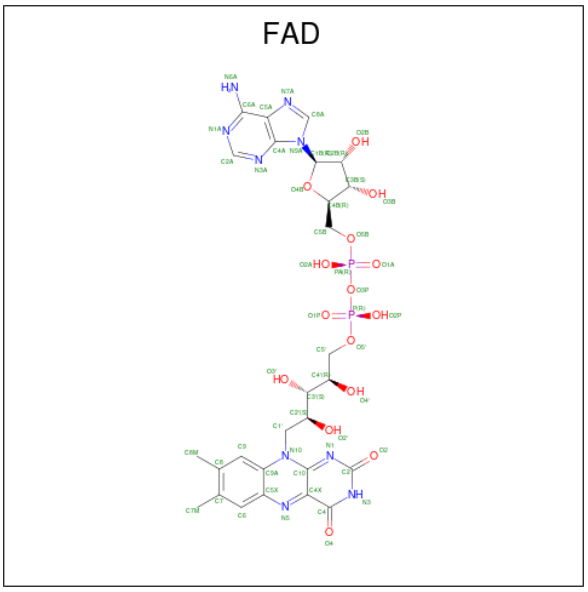
Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLU	THR	engineered mutation	UNP P11310
A	376	GLY	GLU	engineered mutation	UNP P11310
B	255	GLU	THR	engineered mutation	UNP P11310
B	376	GLY	GLU	engineered mutation	UNP P11310
C	255	GLU	THR	engineered mutation	UNP P11310
C	376	GLY	GLU	engineered mutation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

- Molecule 2 is OCTANOYL-COENZYME A (three-letter code: CO8) (formula: $C_{29}H_{50}N_7O_{17}P_3S$).



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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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		

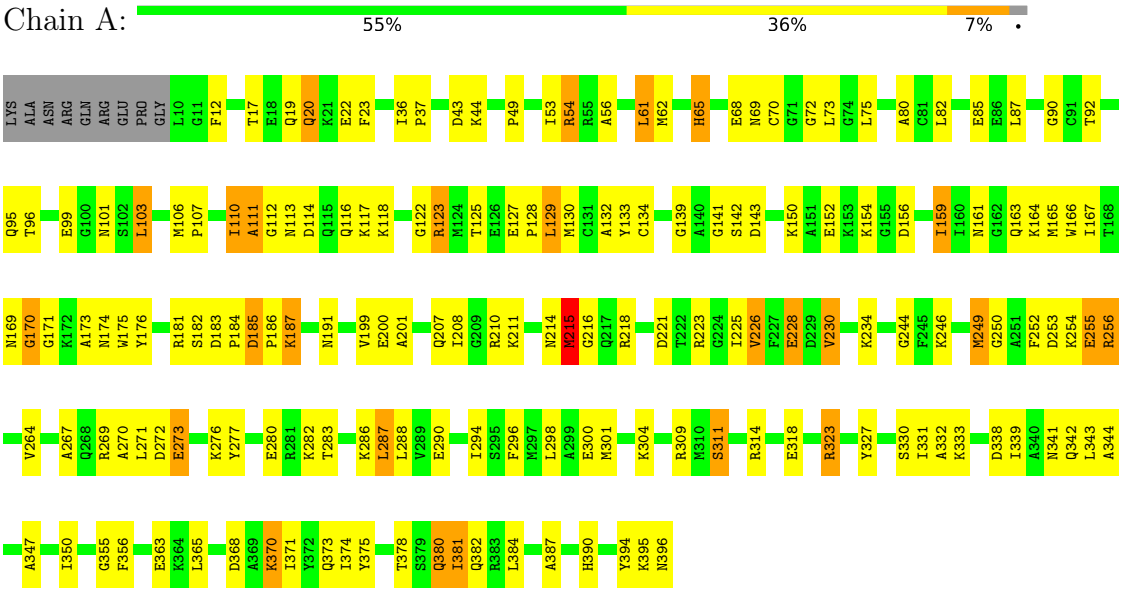
3 Residue-property plots (i)

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.

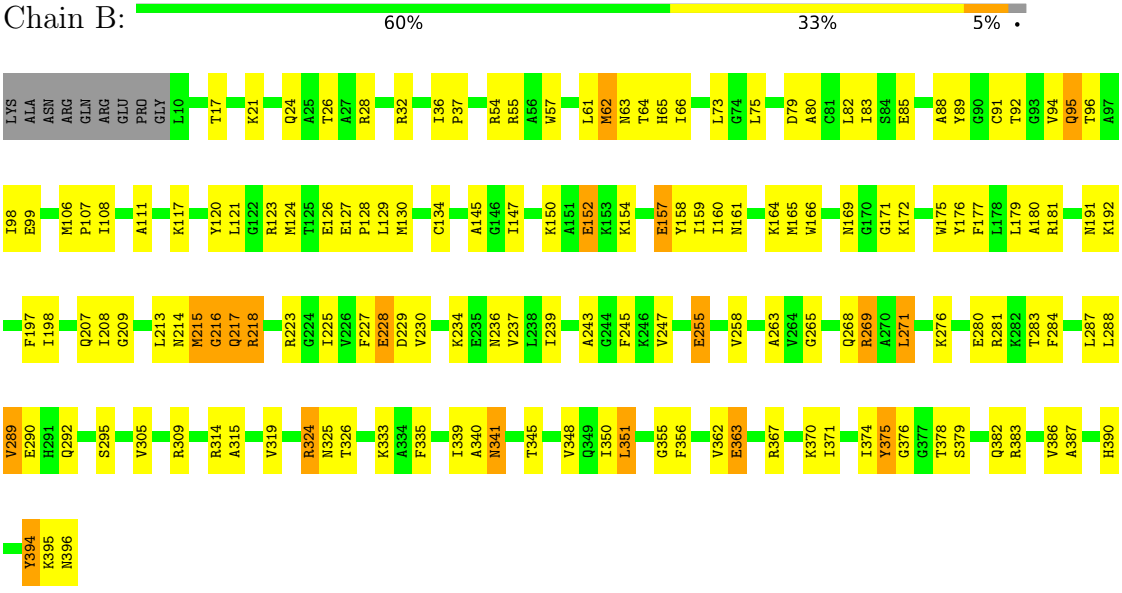
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain A:



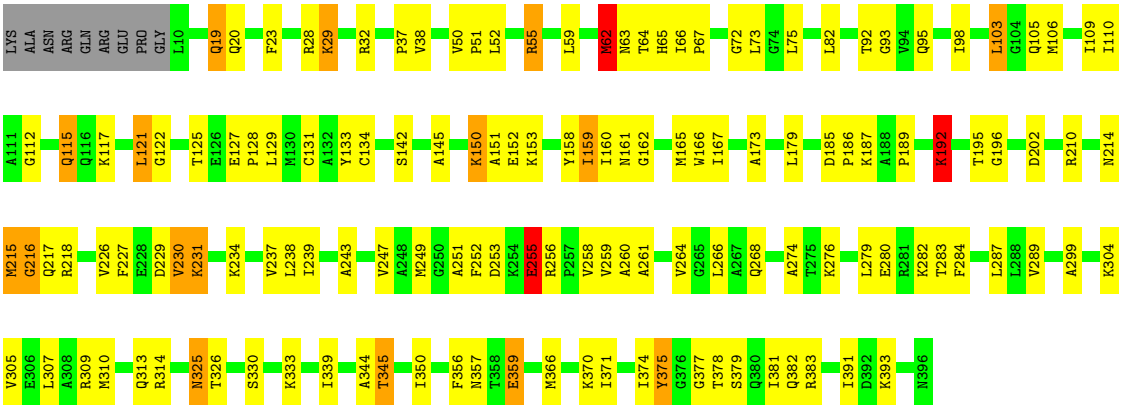
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain B:



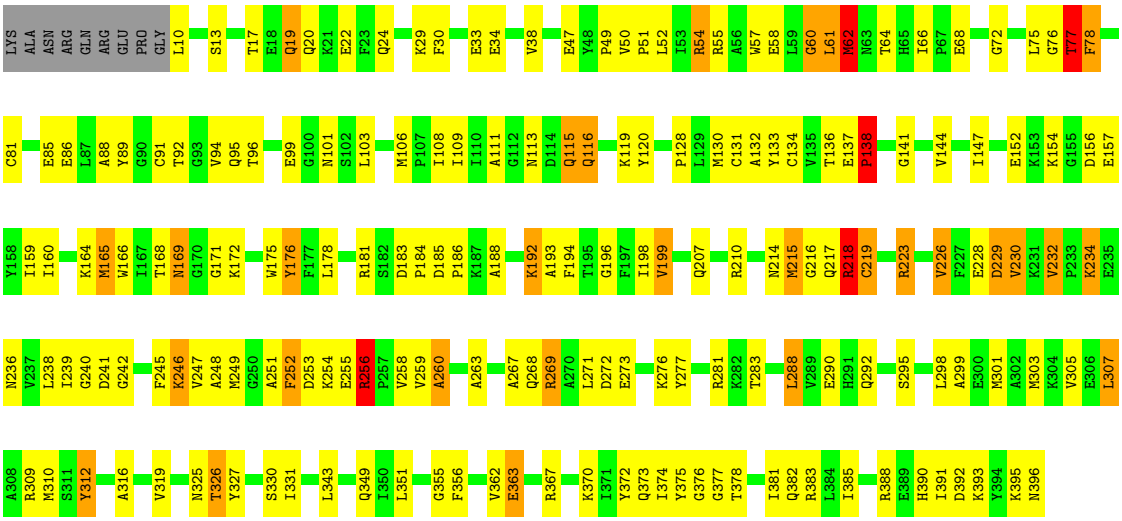
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain C:



• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain D:



4 Data and refinement statistics (i)

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	170.00Å 170.00Å 149.87Å 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: CO8, FAD

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	0.58	3/3045 (0.1%)	0.86	12/4102 (0.3%)
1	B	0.57	1/3045 (0.0%)	0.83	13/4102 (0.3%)
1	C	0.49	0/3045	0.77	7/4102 (0.2%)
1	D	0.56	2/3045 (0.1%)	0.82	10/4102 (0.2%)
All	All	0.55	6/12180 (0.0%)	0.82	42/16408 (0.3%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	ASN	C-N	-8.13	1.15	1.34
1	D	260	ALA	C-N	7.39	1.51	1.34
1	A	230	VAL	C-N	7.13	1.50	1.34
1	A	170	GLY	C-N	7.04	1.45	1.33
1	A	226	VAL	C-N	-5.85	1.20	1.34
1	D	256	ARG	N-CA	5.12	1.56	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	ILE	CA-C-O	-12.21	94.45	120.10
1	A	110	ILE	CB-CA-C	10.83	133.26	111.60
1	C	218	ARG	O-C-N	-10.66	105.64	122.70
1	A	111	ALA	CB-CA-C	10.20	125.39	110.10
1	D	77	THR	N-CA-CB	-9.95	91.40	110.30
1	B	64	THR	O-C-N	-8.37	109.31	122.70
1	D	60	GLY	CA-C-O	8.04	135.07	120.60
1	D	60	GLY	CA-C-N	-8.02	99.55	117.20
1	C	218	ARG	CA-C-N	7.80	134.36	117.20
1	B	218	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	D	218	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	B	255	GLU	N-CA-CB	-7.15	97.73	110.60
1	A	170	GLY	O-C-N	-7.09	111.14	123.20
1	A	65	HIS	O-C-N	-6.89	111.68	122.70
1	D	256	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	B	228	GLU	O-C-N	-6.86	111.73	122.70
1	A	216	GLY	O-C-N	-6.85	111.75	122.70
1	A	256	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	C	218	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	B	62	MET	O-C-N	-6.48	112.33	122.70
1	A	218	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	C	215	MET	CG-SD-CE	6.31	110.30	100.20
1	D	77	THR	CB-CA-C	-6.29	94.61	111.60
1	B	215	MET	CG-SD-CE	6.19	110.10	100.20
1	A	215	MET	CG-SD-CE	6.18	110.09	100.20
1	D	215	MET	CG-SD-CE	6.17	110.08	100.20
1	B	216	GLY	O-C-N	-6.13	112.89	122.70
1	A	228	GLU	O-C-N	-6.08	112.97	122.70
1	B	64	THR	CA-C-N	5.97	130.33	117.20
1	B	255	GLU	O-C-N	-5.92	113.23	122.70
1	C	226	VAL	C-N-CA	5.67	135.88	121.70
1	A	62	MET	CG-SD-CE	5.66	109.25	100.20
1	B	62	MET	CG-SD-CE	5.62	109.19	100.20
1	D	62	MET	CG-SD-CE	5.56	109.10	100.20
1	D	230	VAL	CA-C-N	-5.55	104.98	117.20
1	C	62	MET	CG-SD-CE	5.54	109.07	100.20
1	B	218	ARG	O-C-N	-5.44	113.99	122.70
1	C	255	GLU	CB-CA-C	-5.33	99.73	110.40
1	D	78	PHE	N-CA-C	-5.26	96.80	111.00
1	A	283	THR	O-C-N	-5.21	114.37	122.70
1	B	217	GLN	O-C-N	5.04	130.77	122.70
1	B	177	PHE	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ILE	Peptide,Mainchain
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 (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	2990	0	2977	128	0
1	B	2990	0	2975	110	0
1	C	2990	0	2977	116	0
1	D	2990	0	2978	167	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	5	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
4	D	35	0	0	3	0
All	All	12536	0	12214	499	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 20.

All (499) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:298:LEU:HA	1:D:301:MET:HE3	1.70	0.74
1:B:111:ALA:HB1	1:B:239:ILE:HD11	1.70	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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: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:B:73:LEU:HB3	1:B:75:LEU:HD13	1.82	0.62
1:D:99:GLU:CD	1:D:258:VAL:HG11	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:294:ILE:HD11	3:B:399:FAD:H1B	1.83	0.60
1:B:209:GLY:O	1:B:223:ARG:HD3	2.00	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:A:323:ARG:H	1:A:323:ARG:HD2	1.67	0.60
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:D:246:LYS:O	1:D:247:VAL:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:319:VAL:HG22	1:B:325:ASN:CG	2.24	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
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:C:215:MET:HE3	1:D:367:ARG:HG3	1.87	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:D:156:ASP:C	1:D:234:LYS:HB2	2.25	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: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:A:333:LYS:HD3	1:A:333:LYS:C	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLN:HB2	1:D:292:GLN:HB3	1.88	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:370:LYS:HZ3	1:D:373:GLN:NE2	2.05	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: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
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: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:B:89:TYR:O	1:B:269:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:370:LYS:NZ	1:D:349:GLN:HG2	2.25	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
1:A:380:GLN:CD	1:A:380:GLN:H	2.13	0.51
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:165:MET:SD	1:D:165:MET:C	2.89	0.51
1:D:57:TRP:CD2	1:D:128:PRO:HG3	2.45	0.51
1:A:255:GLU:O	1:A:256:ARG:C	2.46	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:C:370:LYS:HZ1	1:D:349:GLN:HG2	1.76	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:171:GLY:C	1:D:172:LYS:HD2	2.31	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:101:ASN:HA	1:D:131:CYS:HG	1.75	0.49
1:D:381:ILE:HG13	1:D:382:GLN:HE21	1.76	0.49
2:A:400:CO8:HO1	1:B:284:PHE:HZ	1.58	0.49
1:D:130:MET:HB2	1:D:172:LYS:O	2.13	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:THR:HG21	1:D:316:ALA:HA	1.99	0.45
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: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
1:C:186:PRO:HG2	1:C:187:LYS:HD2	1.99	0.44
1:C:307:LEU:HA	1:C:310:MET:HE2	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: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:B:99:GLU:C	2:B:400:CO8:H7'1	2.38	0.43
1:D:30:PHE:CD1	1:D:34:GLU:HB2	2.53	0.43
1:D:249:MET:HE1	1:D:252:PHE:HE2	1.83	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:239:ILE:HG22	1:D:240:GLY:N	2.34	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:57:TRP:HD1	1:D:62:MET:HE1	1.83	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
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:D:325:ASN:O	1:D:326:THR:C	2.58	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:A:371:ILE:HD13	3:A:399:FAD:HM83	2.01	0.42
1:C:64:THR:HB	1:C:75:LEU:HD22	2.01	0.42
1:C:366:MET:HB3	1:D:215:MET:CE	2.50	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: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:B:62:MET:HE3	1:B:130:MET:SD	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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:247:VAL:O	1:D:248:ALA:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:ILE:HG22	1:D:395:LYS:HE3	2.03	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:C:150:LYS:HZ3	1:C:161:ASN:N	2.19	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/396 (97%)	344 (89%)	39 (10%)	2 (0%)	29	52
1	B	385/396 (97%)	351 (91%)	33 (9%)	1 (0%)	41	64
1	C	385/396 (97%)	351 (91%)	29 (8%)	5 (1%)	12	24
1	D	385/396 (97%)	334 (87%)	39 (10%)	12 (3%)	4	6
All	All	1540/1584 (97%)	1380 (90%)	140 (9%)	20 (1%)	12	24

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

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Mol	Chain	Res	Type
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)

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	303/310 (98%)	265 (88%)	38 (12%)	4 8
1	B	303/310 (98%)	274 (90%)	29 (10%)	8 16
1	C	303/310 (98%)	278 (92%)	25 (8%)	11 22
1	D	303/310 (98%)	269 (89%)	34 (11%)	6 10
All	All	1212/1240 (98%)	1086 (90%)	126 (10%)	7 13

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	43	ASP
1	A	44	LYS
1	A	54	ARG
1	A	61	LEU
1	A	85	GLU
1	A	87	LEU
1	A	92	THR
1	A	95	GLN
1	A	103	LEU

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Mol	Chain	Res	Type
1	A	123	ARG
1	A	129	LEU
1	A	154	LYS
1	A	159	ILE
1	A	163	GLN
1	A	181	ARG
1	A	182	SER
1	A	185	ASP
1	A	187	LYS
1	A	191	ASN
1	A	200	GLU
1	A	210	ARG
1	A	215	MET
1	A	246	LYS
1	A	249	MET
1	A	253	ASP
1	A	255	GLU
1	A	273	GLU
1	A	287	LEU
1	A	311	SER
1	A	323	ARG
1	A	342	GLN
1	A	370	LYS
1	A	375	TYR
1	A	380	GLN
1	A	381	ILE
1	A	395	LYS
1	A	396	ASN
1	B	17	THR
1	B	21	LYS
1	B	55	ARG
1	B	85	GLU
1	B	95	GLN
1	B	126	GLU
1	B	152	GLU
1	B	157	GLU
1	B	161	ASN
1	B	179	LEU
1	B	207	GLN
1	B	213	LEU
1	B	218	ARG
1	B	229	ASP

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Mol	Chain	Res	Type
1	B	234	LYS
1	B	269	ARG
1	B	271	LEU
1	B	289	VAL
1	B	295	SER
1	B	314	ARG
1	B	324	ARG
1	B	326	THR
1	B	341	ASN
1	B	351	LEU
1	B	363	GLU
1	B	375	TYR
1	B	394	TYR
1	B	395	LYS
1	B	396	ASN
1	C	19	GLN
1	C	29	LYS
1	C	55	ARG
1	C	62	MET
1	C	95	GLN
1	C	103	LEU
1	C	115	GLN
1	C	121	LEU
1	C	150	LYS
1	C	159	ILE
1	C	179	LEU
1	C	192	LYS
1	C	202	ASP
1	C	210	ARG
1	C	229	ASP
1	C	231	LYS
1	C	234	LYS
1	C	249	MET
1	C	255	GLU
1	C	314	ARG
1	C	325	ASN
1	C	345	THR
1	C	359	GLU
1	C	371	ILE
1	C	375	TYR
1	D	19	GLN
1	D	24	GLN

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Mol	Chain	Res	Type
1	D	47	GLU
1	D	54	ARG
1	D	61	LEU
1	D	75	LEU
1	D	85	GLU
1	D	115	GLN
1	D	116	GLN
1	D	138	PRO
1	D	165	MET
1	D	169	ASN
1	D	176	TYR
1	D	192	LYS
1	D	199	VAL
1	D	210	ARG
1	D	218	ARG
1	D	219	CYS
1	D	223	ARG
1	D	226	VAL
1	D	229	ASP
1	D	232	VAL
1	D	234	LYS
1	D	246	LYS
1	D	256	ARG
1	D	269	ARG
1	D	288	LEU
1	D	290	GLU
1	D	295	SER
1	D	307	LEU
1	D	312	TYR
1	D	363	GLU
1	D	374	ILE
1	D	375	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	69	ASN
1	A	105	GLN
1	A	116	GLN
1	A	169	ASN
1	A	174	ASN

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Mol	Chain	Res	Type
1	A	341	ASN
1	A	349	GLN
1	A	396	ASN
1	B	65	HIS
1	B	161	ASN
1	B	169	ASN
1	B	174	ASN
1	B	191	ASN
1	B	217	GLN
1	B	236	ASN
1	B	349	GLN
1	B	354	ASN
1	B	380	GLN
1	C	19	GLN
1	C	63	ASN
1	C	65	HIS
1	C	105	GLN
1	C	115	GLN
1	C	214	ASN
1	C	268	GLN
1	C	313	GLN
1	C	325	ASN
1	C	373	GLN
1	D	20	GLN
1	D	65	HIS
1	D	105	GLN
1	D	163	GLN
1	D	236	ASN
1	D	268	GLN
1	D	291	HIS
1	D	342	GLN
1	D	349	GLN
1	D	354	ASN
1	D	373	GLN
1	D	382	GLN

5.3.3 RNA

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 monosaccharides 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	B	400	-	51,59,59	1.29	6 (11%)	62,85,85	2.07	11 (17%)
3	FAD	C	399	-	51,58,58	1.76	10 (19%)	60,89,89	2.70	15 (25%)
3	FAD	A	399	-	51,58,58	1.52	10 (19%)	60,89,89	3.36	22 (36%)
3	FAD	B	399	-	51,58,58	1.31	4 (7%)	60,89,89	2.93	18 (30%)
2	CO8	D	400	-	51,59,59	1.36	5 (9%)	62,85,85	1.40	8 (12%)
2	CO8	C	400	-	51,59,59	1.30	6 (11%)	62,85,85	2.76	18 (29%)
2	CO8	A	400	-	51,59,59	1.60	7 (13%)	62,85,85	1.80	10 (16%)
3	FAD	D	399	-	51,58,58	1.35	7 (13%)	60,89,89	2.77	13 (21%)

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	B	400	-	-	16/54/74/74	0/3/3/3
3	FAD	C	399	-	-	2/30/50/50	0/6/6/6
3	FAD	A	399	-	-	3/30/50/50	0/6/6/6
3	FAD	B	399	-	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CO8	D	400	-	-	7/54/74/74	0/3/3/3
2	CO8	C	400	-	-	16/54/74/74	0/3/3/3
2	CO8	A	400	-	-	8/54/74/74	0/3/3/3
3	FAD	D	399	-	-	2/30/50/50	0/6/6/6

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	CO8	C5P-N4P	5.64	1.46	1.33
3	C	399	FAD	C4-N3	5.23	1.42	1.33
2	A	400	CO8	O1'-C1'	4.37	1.28	1.21
2	D	400	CO8	C2'-C1'	4.34	1.55	1.50
3	C	399	FAD	C1'-N10	-4.26	1.43	1.48
2	C	400	CO8	C5P-N4P	4.20	1.42	1.33
2	D	400	CO8	O4B-C1B	4.18	1.46	1.41
3	C	399	FAD	C4-C4X	4.16	1.48	1.41
2	A	400	CO8	C9P-N8P	4.11	1.42	1.33
3	C	399	FAD	C4X-N5	4.06	1.39	1.33
3	B	399	FAD	C4X-N5	3.85	1.38	1.33
2	B	400	CO8	O4B-C1B	3.81	1.46	1.41
2	C	400	CO8	C9P-N8P	3.79	1.41	1.33
3	A	399	FAD	C4-C4X	3.67	1.47	1.41
2	B	400	CO8	C5P-N4P	3.59	1.41	1.33
3	D	399	FAD	C9A-N10	3.42	1.43	1.38
3	A	399	FAD	O4B-C1B	3.38	1.45	1.41
3	A	399	FAD	C10-N1	3.36	1.37	1.33
2	A	400	CO8	P3B-O3B	3.28	1.65	1.59
3	B	399	FAD	C9A-N10	3.25	1.42	1.38
3	A	399	FAD	O2B-C2B	-3.22	1.35	1.43
3	A	399	FAD	C4X-N5	3.21	1.37	1.33
3	D	399	FAD	C4-N3	3.15	1.38	1.33
2	D	400	CO8	C9P-N8P	3.13	1.40	1.33
2	B	400	CO8	C9P-N8P	3.12	1.40	1.33
2	B	400	CO8	C1'-S1P	-3.05	1.68	1.76
2	C	400	CO8	O4B-C1B	3.01	1.45	1.41
3	D	399	FAD	C4X-N5	3.00	1.37	1.33
3	C	399	FAD	C5X-N5	2.98	1.40	1.35
3	A	399	FAD	C7M-C7	2.97	1.57	1.51
3	D	399	FAD	C8A-N7A	-2.97	1.29	1.34
3	C	399	FAD	C10-N1	2.95	1.37	1.33
2	B	400	CO8	P3B-O3B	2.85	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	399	FAD	C8A-N7A	-2.84	1.29	1.34
2	A	400	CO8	C8A-N7A	-2.83	1.29	1.34
3	A	399	FAD	C9A-N10	2.82	1.42	1.38
3	A	399	FAD	C8A-N7A	-2.79	1.29	1.34
3	C	399	FAD	C2A-N1A	-2.72	1.28	1.33
3	C	399	FAD	C8M-C8	2.64	1.56	1.51
2	C	400	CO8	O2B-C2B	2.64	1.49	1.43
3	D	399	FAD	C1'-N10	-2.61	1.45	1.48
2	A	400	CO8	O4B-C1B	2.60	1.44	1.41
2	D	400	CO8	P3B-O3B	2.54	1.64	1.59
2	A	400	CO8	C2'-C1'	2.53	1.53	1.50
3	B	399	FAD	O2B-C2B	-2.42	1.37	1.43
3	C	399	FAD	C2-N3	2.39	1.42	1.38
3	A	399	FAD	C4X-C10	2.37	1.41	1.38
2	B	400	CO8	C8A-N7A	-2.37	1.30	1.34
3	C	399	FAD	C4A-N3A	-2.33	1.32	1.35
3	A	399	FAD	C1'-N10	-2.31	1.45	1.48
3	D	399	FAD	C4-C4X	2.23	1.45	1.41
2	C	400	CO8	P3B-O3B	2.08	1.63	1.59
3	D	399	FAD	C5X-N5	2.05	1.38	1.35
2	D	400	CO8	C4A-N3A	2.03	1.38	1.35
2	C	400	CO8	C2B-C1B	2.02	1.56	1.53

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	399	FAD	C4-N3-C2	15.60	128.31	115.14
2	C	400	CO8	O1'-C1'-C2'	-14.02	107.43	123.99
3	B	399	FAD	C4-N3-C2	13.97	126.94	115.14
3	D	399	FAD	C4-N3-C2	13.81	126.80	115.14
3	C	399	FAD	C4-N3-C2	12.80	125.95	115.14
3	A	399	FAD	C10-C4X-N5	8.76	127.32	121.26
3	B	399	FAD	C10-C4X-N5	8.50	127.14	121.26
2	C	400	CO8	C2'-C1'-S1P	8.15	122.95	113.46
3	A	399	FAD	C1'-N10-C10	7.91	125.50	118.41
2	B	400	CO8	O6A-CCP-CBP	7.90	123.25	110.55
2	B	400	CO8	O1'-C1'-S1P	-7.64	112.69	122.61
3	D	399	FAD	C10-C4X-N5	7.53	126.46	121.26
2	A	400	CO8	O6A-CCP-CBP	7.03	121.84	110.55
3	C	399	FAD	C4X-C4-N3	-6.50	114.53	123.43
2	C	400	CO8	C6P-C7P-N8P	-6.41	98.95	111.90
3	A	399	FAD	C4X-C4-N3	-6.33	114.77	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	399	FAD	C10-C4X-N5	6.13	125.50	121.26
3	C	399	FAD	C1'-N10-C10	6.10	123.88	118.41
3	B	399	FAD	C4X-C4-N3	-6.09	115.10	123.43
3	D	399	FAD	C4X-C4-N3	-5.99	115.23	123.43
3	D	399	FAD	C1'-N10-C10	5.76	123.56	118.41
3	A	399	FAD	C2B-C3B-C4B	-5.54	91.89	102.64
3	D	399	FAD	C4-C4X-C10	-5.41	116.37	119.95
3	B	399	FAD	C1'-N10-C10	5.38	123.23	118.41
3	B	399	FAD	C4-C4X-C10	-5.22	116.50	119.95
3	A	399	FAD	C6-C5X-N5	-4.90	113.65	119.05
2	B	400	CO8	C2'-C1'-S1P	4.55	118.75	113.46
2	A	400	CO8	C6P-C7P-N8P	4.49	120.95	111.90
2	C	400	CO8	O1'-C1'-S1P	4.44	128.38	122.61
2	B	400	CO8	C2B-C3B-C4B	-4.41	95.41	103.22
3	A	399	FAD	C4-C4X-C10	-4.32	117.09	119.95
2	A	400	CO8	O1'-C1'-S1P	-4.30	117.02	122.61
3	A	399	FAD	O5'-C5'-C4'	-4.28	97.93	109.36
3	B	399	FAD	O3'-C3'-C4'	-4.26	98.52	108.81
3	A	399	FAD	C4X-C10-N10	-4.07	116.12	120.30
2	C	400	CO8	O6A-CCP-CBP	4.05	117.06	110.55
3	C	399	FAD	C4-C4X-C10	-4.03	117.28	119.95
3	C	399	FAD	O4B-C1B-C2B	-4.01	101.07	106.93
2	C	400	CO8	C6P-C5P-N4P	-3.95	109.77	116.42
3	A	399	FAD	P-O3P-PA	-3.85	119.62	132.83
2	D	400	CO8	O6A-CCP-CBP	-3.83	104.38	110.55
3	A	399	FAD	C4X-N5-C5X	-3.80	112.97	116.77
3	B	399	FAD	C6-C5X-N5	-3.78	114.88	119.05
2	A	400	CO8	O4B-C1B-C2B	-3.76	101.43	106.93
2	B	400	CO8	O1'-C1'-C2'	3.76	128.43	123.99
3	B	399	FAD	C4X-N5-C5X	-3.75	113.02	116.77
3	A	399	FAD	O4B-C1B-C2B	-3.66	101.58	106.93
3	C	399	FAD	C4X-C10-N10	-3.60	116.60	120.30
3	C	399	FAD	P-O3P-PA	-3.59	120.50	132.83
3	B	399	FAD	C4'-C3'-C2'	3.59	120.83	113.36
3	A	399	FAD	C9A-C5X-N5	3.59	127.97	122.36
3	D	399	FAD	O5B-C5B-C4B	3.58	121.31	108.99
3	C	399	FAD	C1'-N10-C9A	-3.57	115.48	118.29
3	D	399	FAD	C4X-C10-N10	-3.50	116.71	120.30
2	D	400	CO8	CDP-CBP-CAP	3.48	114.85	108.82
3	B	399	FAD	C4X-C10-N10	-3.46	116.74	120.30
2	A	400	CO8	C2B-C3B-C4B	-3.42	97.16	103.22
2	D	400	CO8	C3P-N4P-C5P	-3.27	116.77	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	399	FAD	C6-C5X-C9A	-3.23	114.81	119.05
3	A	399	FAD	C1'-N10-C9A	-3.16	115.81	118.29
3	D	399	FAD	C9A-C5X-N5	3.14	127.27	122.36
2	C	400	CO8	CEP-CBP-CCP	-3.13	103.12	108.23
3	B	399	FAD	C9A-C5X-N5	3.02	127.08	122.36
3	C	399	FAD	C4X-N5-C5X	-3.00	113.78	116.77
2	D	400	CO8	C6P-C5P-N4P	-2.98	111.41	116.42
3	C	399	FAD	C9A-C5X-N5	2.94	126.95	122.36
3	A	399	FAD	C4A-C5A-N7A	2.93	112.45	109.40
3	D	399	FAD	C6-C5X-N5	-2.91	115.84	119.05
3	B	399	FAD	O4B-C1B-C2B	-2.90	102.69	106.93
2	A	400	CO8	CDP-CBP-CCP	-2.89	103.52	108.23
2	B	400	CO8	CEP-CBP-CAP	2.88	113.81	108.82
3	D	399	FAD	C4X-N5-C5X	-2.85	113.93	116.77
3	A	399	FAD	O5B-C5B-C4B	2.84	118.78	108.99
2	A	400	CO8	C4A-C5A-N7A	2.81	112.33	109.40
2	A	400	CO8	C2P-C3P-N4P	2.79	118.28	112.42
2	C	400	CO8	O5P-C5P-N4P	2.72	128.14	123.01
2	A	400	CO8	O1'-C1'-C2'	2.71	127.19	123.99
2	D	400	CO8	C5A-C6A-N6A	2.71	124.47	120.35
2	C	400	CO8	C3B-C2B-C1B	-2.70	93.90	99.89
3	B	399	FAD	C9A-N10-C10	-2.65	118.44	121.91
2	C	400	CO8	P2A-O3A-P1A	-2.64	123.76	132.83
3	A	399	FAD	C4-C4X-N5	-2.64	115.58	118.60
2	B	400	CO8	C3'-C2'-C1'	2.63	118.16	112.33
3	A	399	FAD	O2A-PA-O1A	2.61	125.16	112.24
2	C	400	CO8	O9A-P3B-O8A	2.61	117.60	107.64
2	C	400	CO8	CAP-C9P-N8P	2.55	121.66	116.58
3	A	399	FAD	C9A-N10-C10	-2.53	118.60	121.91
3	C	399	FAD	O2B-C2B-C3B	-2.53	103.64	111.82
3	D	399	FAD	P-O3P-PA	-2.51	124.20	132.83
2	A	400	CO8	CEP-CBP-CAP	2.51	113.17	108.82
2	C	400	CO8	O5B-C5B-C4B	2.49	117.57	108.99
3	A	399	FAD	PA-O5B-C5B	-2.48	107.13	121.68
2	C	400	CO8	O9P-C9P-N8P	-2.44	117.76	122.99
3	C	399	FAD	C5A-C6A-N6A	2.42	124.02	120.35
3	B	399	FAD	C4A-C5A-N7A	2.41	111.91	109.40
2	B	400	CO8	CDP-CBP-CAP	2.31	112.83	108.82
2	C	400	CO8	C3P-N4P-C5P	2.30	127.10	122.84
2	B	400	CO8	O5B-C5B-C4B	2.28	116.85	108.99
3	D	399	FAD	C5X-C9A-N10	-2.28	116.06	117.72
3	D	399	FAD	O2A-PA-O1A	2.27	123.48	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	400	CO8	P1A-O5B-C5B	-2.26	108.41	121.68
2	D	400	CO8	CDP-CBP-CCP	-2.26	104.54	108.23
2	D	400	CO8	O2B-C2B-C3B	-2.22	104.85	111.17
3	A	399	FAD	O4'-C4'-C3'	2.17	114.37	109.10
2	C	400	CO8	C1B-N9A-C4A	-2.14	122.88	126.64
3	A	399	FAD	O3'-C3'-C2'	2.13	113.97	108.81
3	C	399	FAD	C7-C6-C5X	2.13	124.23	121.22
2	B	400	CO8	O2B-C2B-C3B	2.10	117.11	111.17
3	B	399	FAD	C2B-C3B-C4B	-2.09	98.58	102.64
2	B	400	CO8	O4B-C1B-C2B	-2.07	103.90	106.93
2	C	400	CO8	O3B-C3B-C2B	2.03	119.04	111.68
3	B	399	FAD	C4-C4X-N5	-2.02	116.29	118.60
3	B	399	FAD	O5B-C5B-C4B	2.01	115.90	108.99
3	B	399	FAD	O2B-C2B-C1B	-2.01	103.44	110.85
2	D	400	CO8	O3B-C3B-C2B	-2.00	104.42	111.68

There are no chirality outliers.

All (54) 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	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	CCP-O6A-P2A-O3A
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	O1'-C1'-S1P-C2P
2	C	400	CO8	C2'-C1'-S1P-C2P
2	D	400	CO8	CCP-O6A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
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
2	A	400	CO8	CDP-CBP-CCP-O6A
2	A	400	CO8	CEP-CBP-CCP-O6A
2	A	400	CO8	O9P-C9P-CAP-OAP
3	C	399	FAD	PA-O3P-P-O1P
3	D	399	FAD	PA-O3P-P-O1P
2	D	400	CO8	S1P-C2P-C3P-N4P
2	B	400	CO8	N8P-C9P-CAP-CBP
2	C	400	CO8	C5'-C6'-C7'-C8'
2	B	400	CO8	O1'-C1'-S1P-C2P
2	C	400	CO8	C2B-C3B-O3B-P3B
2	D	400	CO8	O1'-C1'-S1P-C2P
2	D	400	CO8	C2'-C1'-S1P-C2P
2	D	400	CO8	CCP-O6A-P2A-O3A
2	B	400	CO8	CCP-O6A-P2A-O4A
2	B	400	CO8	CCP-O6A-P2A-O5A
3	A	399	FAD	C5B-O5B-PA-O1A
2	C	400	CO8	C3B-C4B-C5B-O5B
2	B	400	CO8	C4B-C5B-O5B-P1A
2	B	400	CO8	OAP-CAP-CBP-CDP
3	D	399	FAD	PA-O3P-P-O2P
2	B	400	CO8	CDP-CBP-CCP-O6A
2	D	400	CO8	C5'-C6'-C7'-C8'
2	C	400	CO8	C3P-C2P-S1P-C1'
2	B	400	CO8	C5B-O5B-P1A-O3A
2	C	400	CO8	C3B-O3B-P3B-O9A
3	C	399	FAD	PA-O3P-P-O2P
2	C	400	CO8	C5B-O5B-P1A-O1A
2	B	400	CO8	O9P-C9P-CAP-CBP

There are no ring outliers.

8 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	CO8	8	0
3	C	399	FAD	2	0
3	A	399	FAD	5	0
3	B	399	FAD	4	0
2	D	400	CO8	14	0

Continued on next page...

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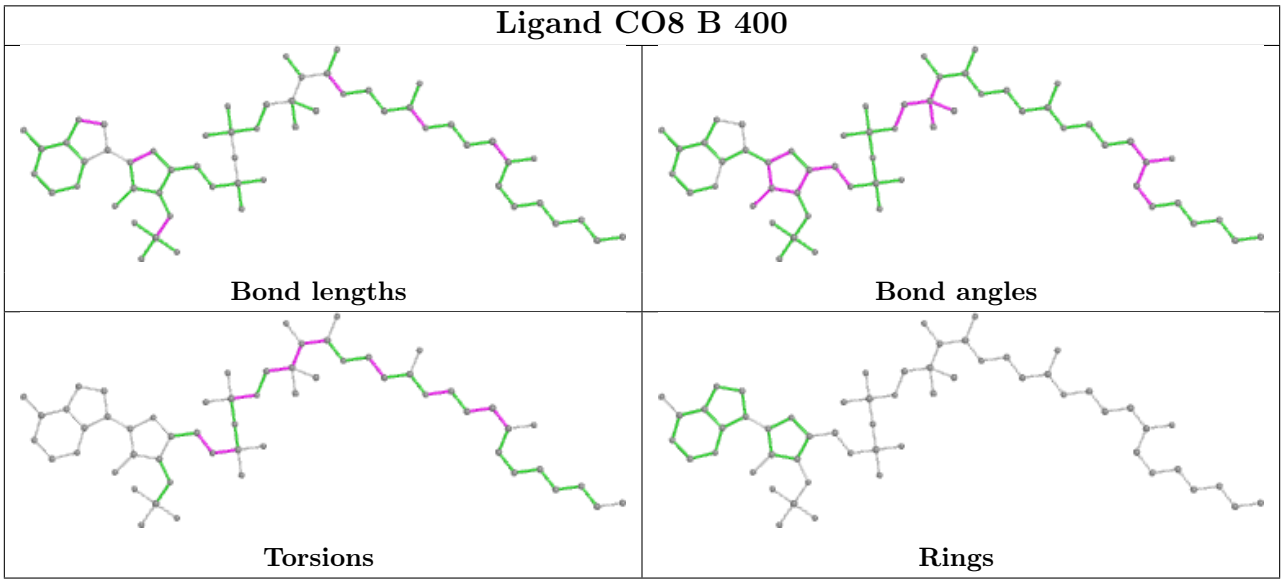
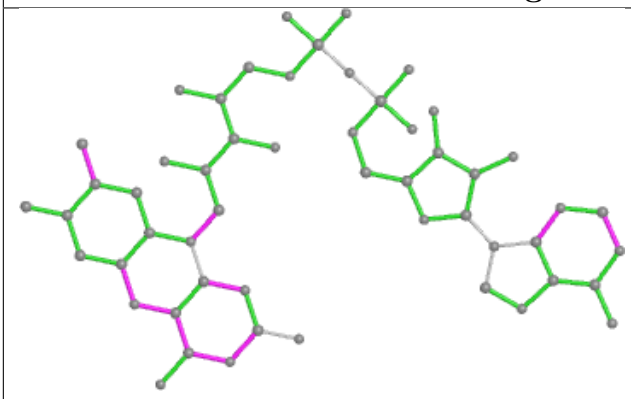
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400	CO8	9	0
2	A	400	CO8	11	0
3	D	399	FAD	4	0

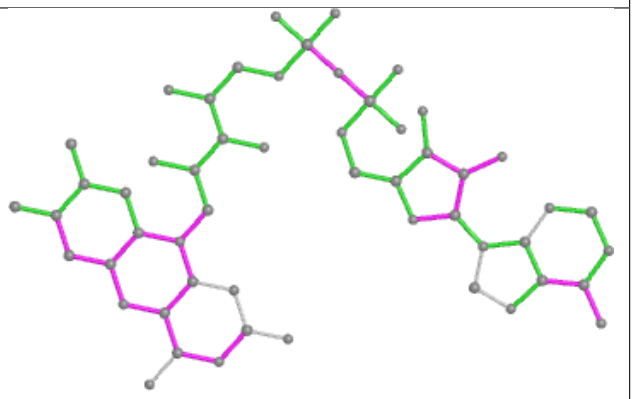
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



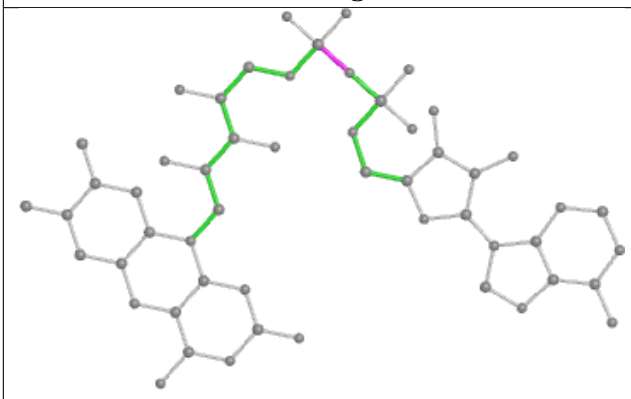
Ligand FAD C 399



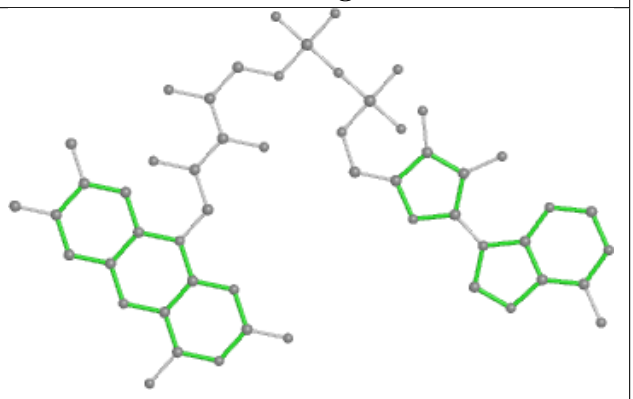
Bond lengths



Bond angles

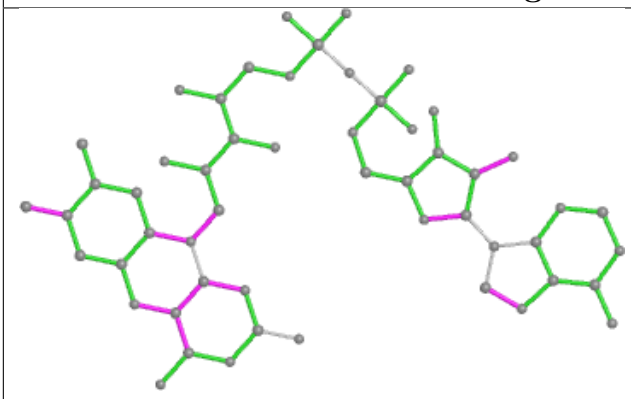


Torsions

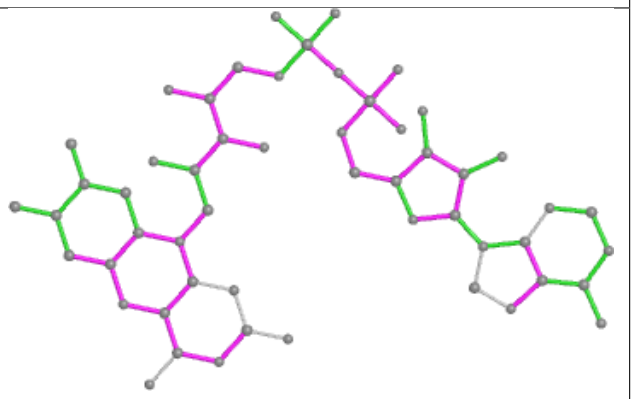


Rings

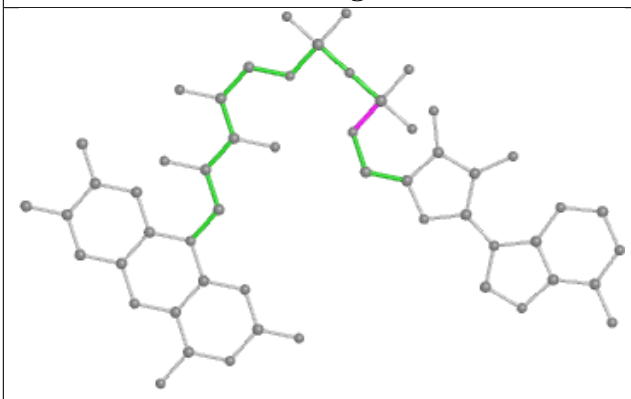
Ligand FAD A 399



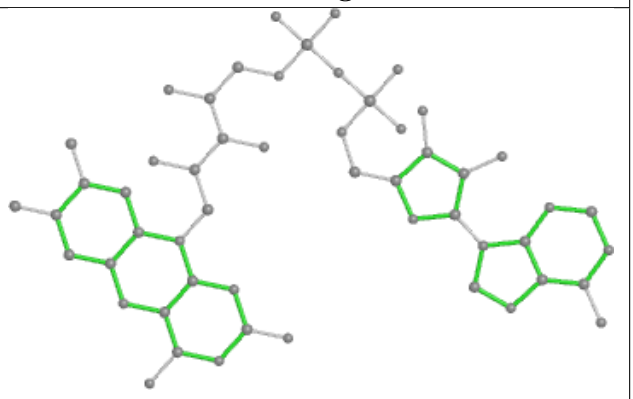
Bond lengths



Bond angles

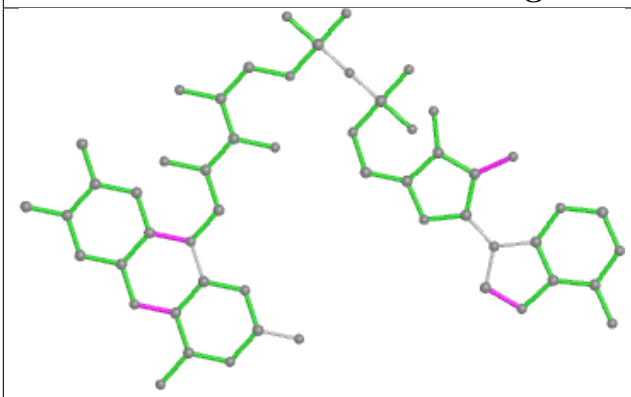


Torsions

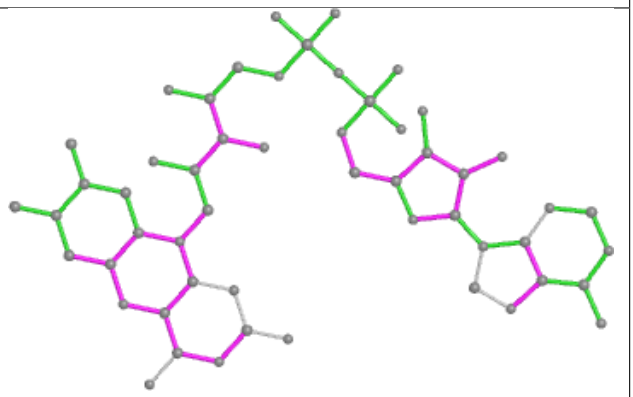


Rings

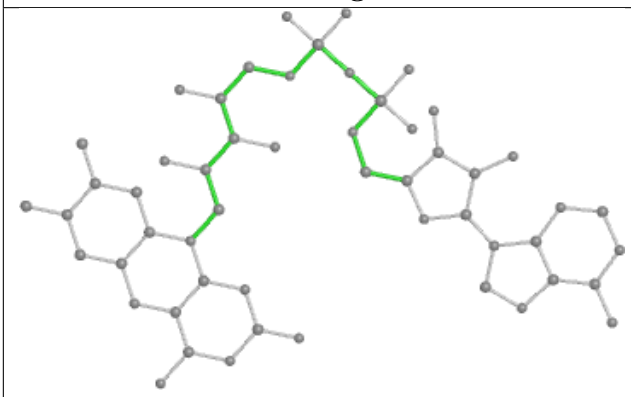
Ligand FAD B 399



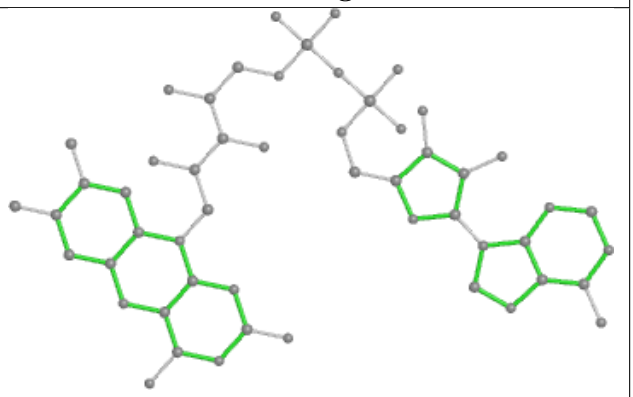
Bond lengths



Bond angles

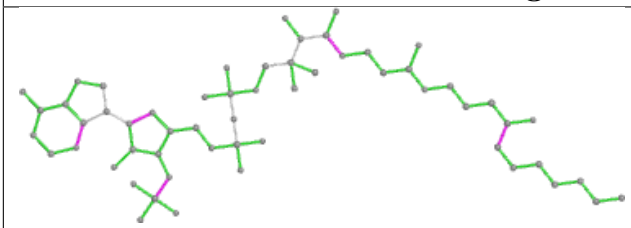


Torsions

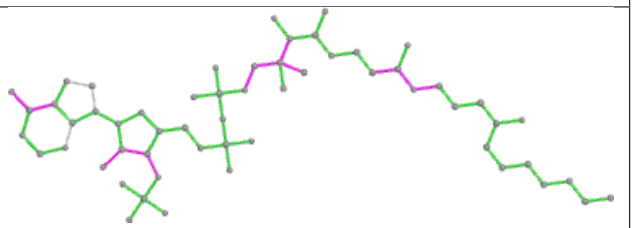


Rings

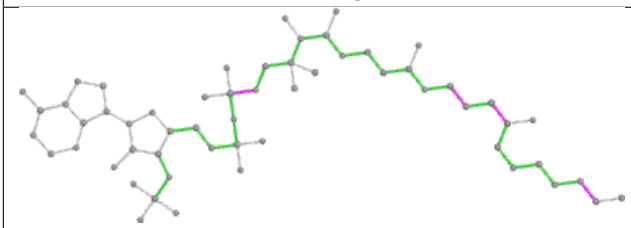
Ligand CO8 D 400



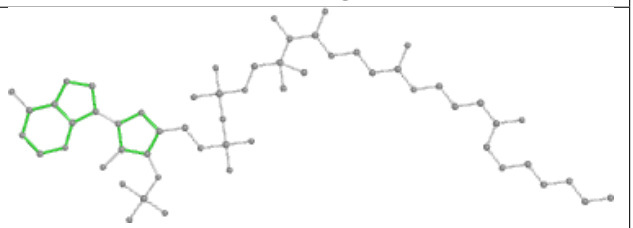
Bond lengths



Bond angles

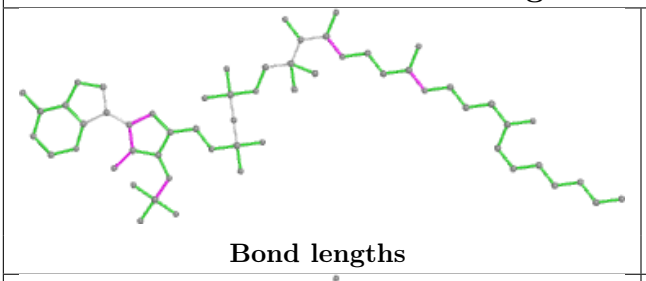


Torsions

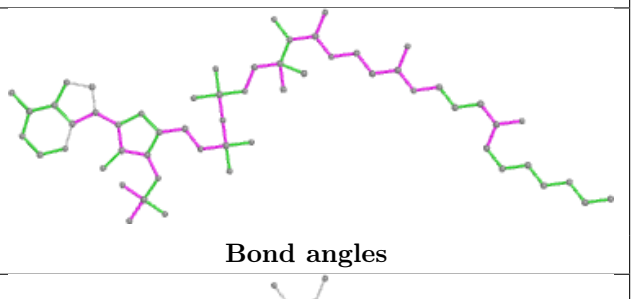


Rings

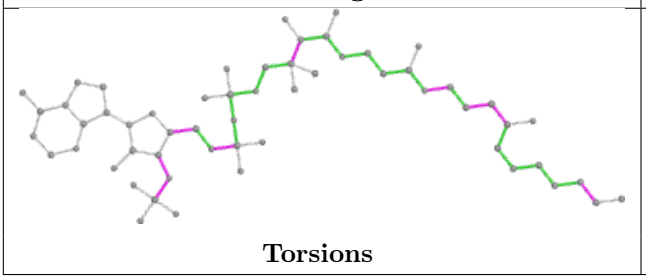
Ligand CO8 C 400



Bond lengths



Bond angles



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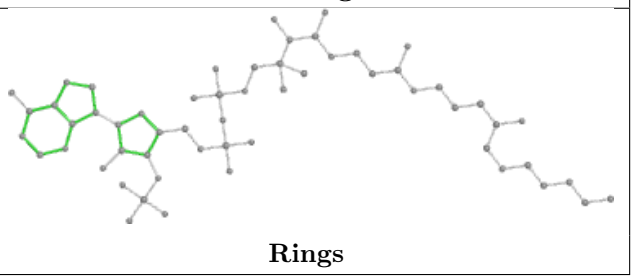
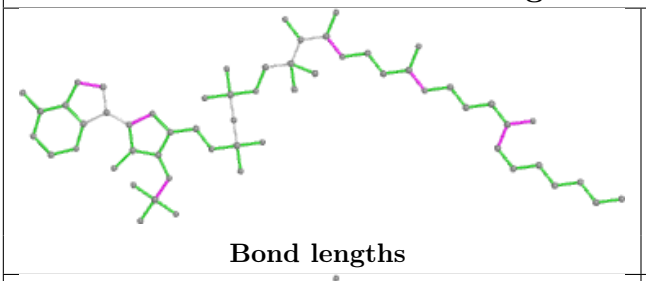
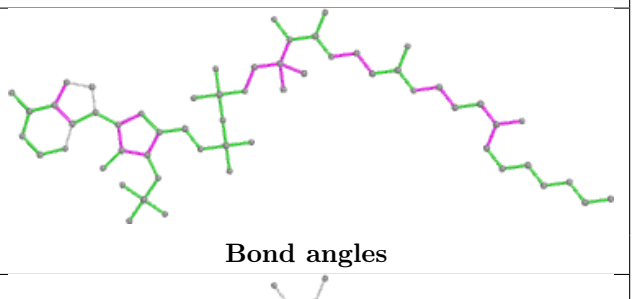


Rings

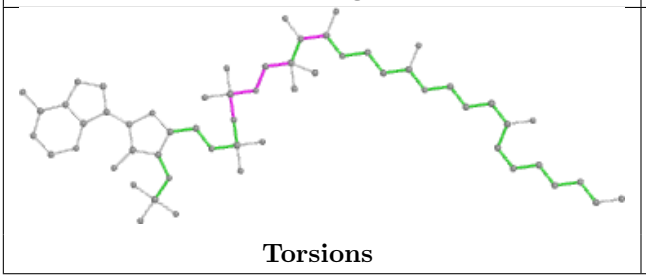
Ligand CO8 A 400



Bond lengths



Bond angles



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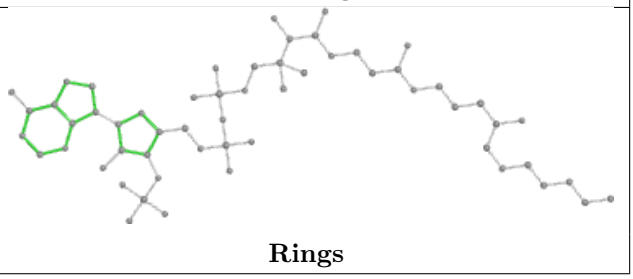
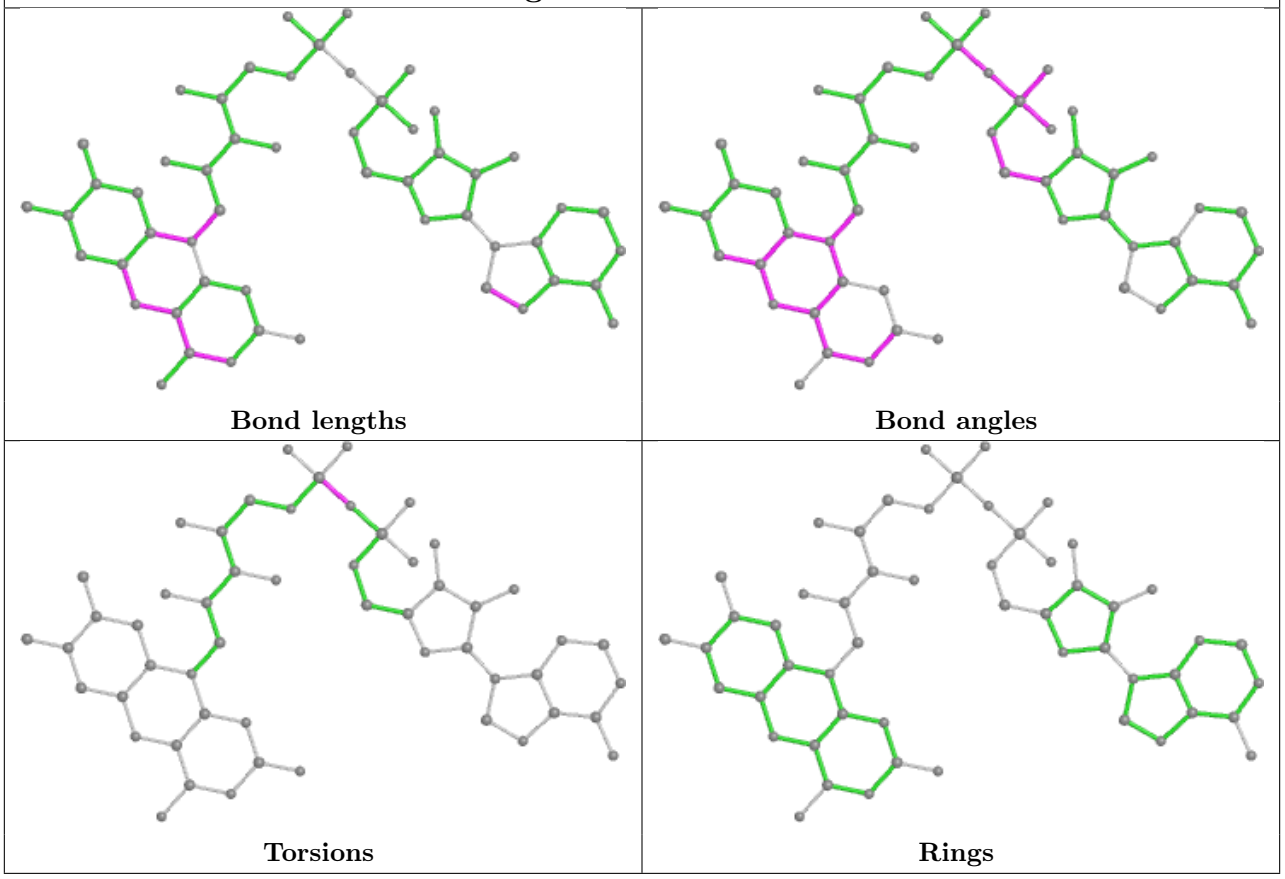


Rings

Ligand FAD D 399



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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.