Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:34 AM EDT

PDB ID	:	1NEN
Title	:	Complex II (Succinate Dehydrogenase) From E. Coli with Dinitrophenol-17 inhibitor co-crystallized at the ubiquinone binding site
Authors	:	Yankovskaya, V.; Horsefield, R.; Tornroth, S.; Luna-Chavez, C.; Miyoshi, H.; Leger, C.; Byrne, B.; Cecchini, G.; Iwata, S.
Deposited on	:	2002-12-11
Resolution	:	2.90 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 (i) 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 (1)) were used in the production of this report:

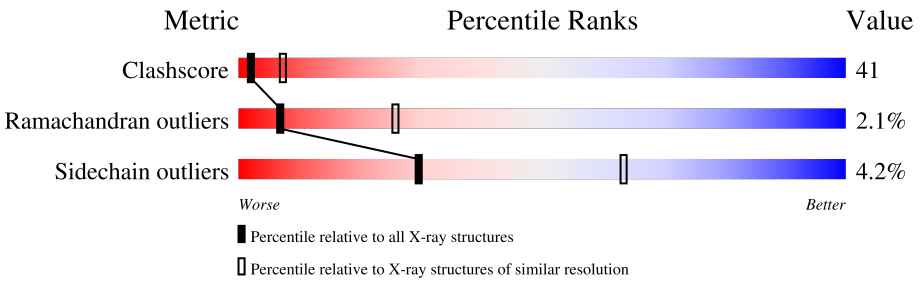
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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	588	36% 59% 5%
2	B	238	50% 48% .
3	C	129	59% 37% .
4	D	115	64% 33% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	F3S	B	304	-	-	X	-
12	DNT	C	306	X	-	-	-
13	CDN	C	308	X	-	-	-
5	OAA	A	589	-	-	X	-
8	FES	B	302	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 8695 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 Succinate dehydrogenase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	588	4522	2812	821	861	28	88	0	0

- Molecule 2 is a protein called Succinate dehydrogenase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	238	1869	1172	329	348	20	0	0	0

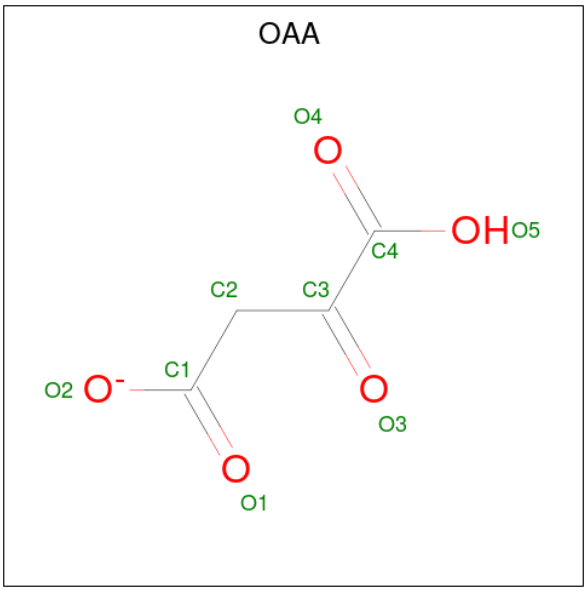
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b-556 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	129	1008	668	166	168	6	0	0	0

- Molecule 4 is a protein called Succinate dehydrogenase hydrophobic membrane anchor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	113	898	615	136	144	3	0	0	0

- Molecule 5 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).

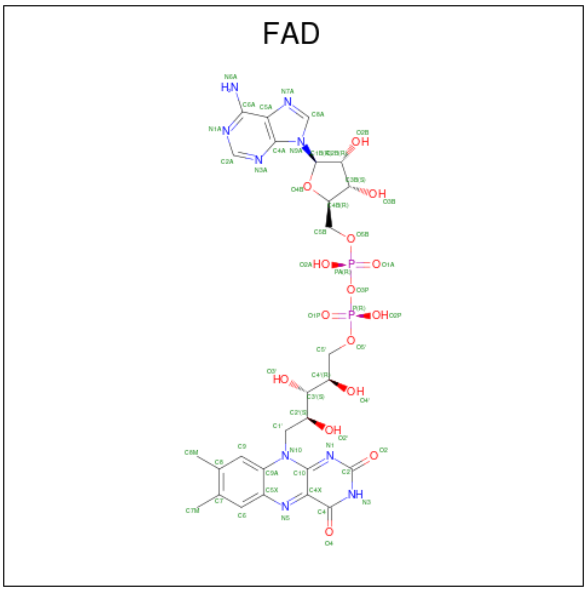


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 4 5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

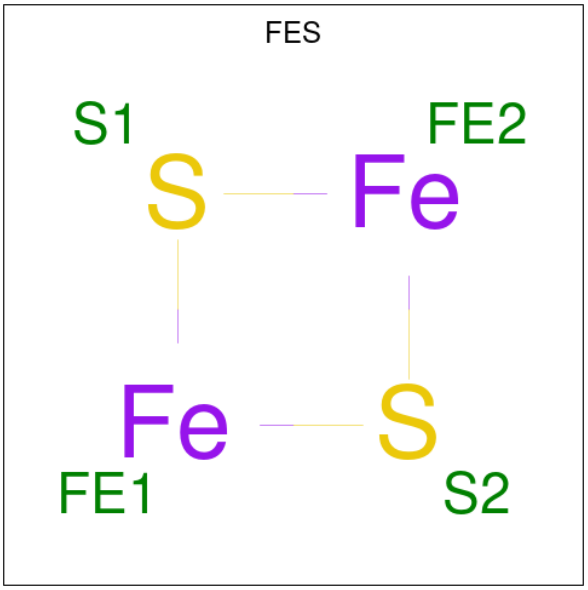
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



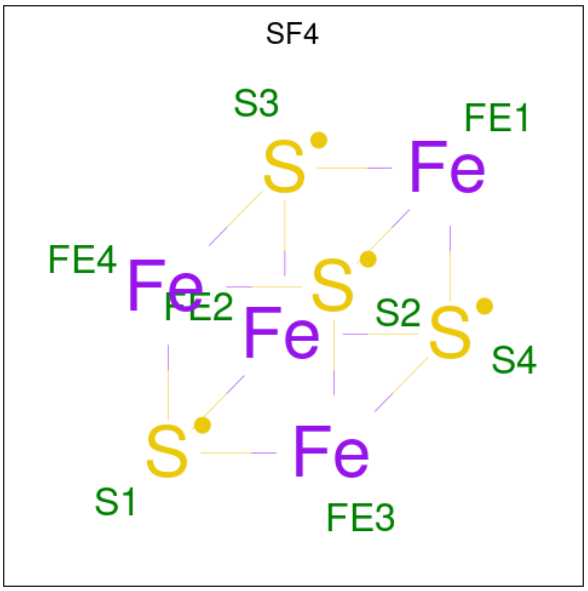
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	53	27	9	15	2	0	0

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



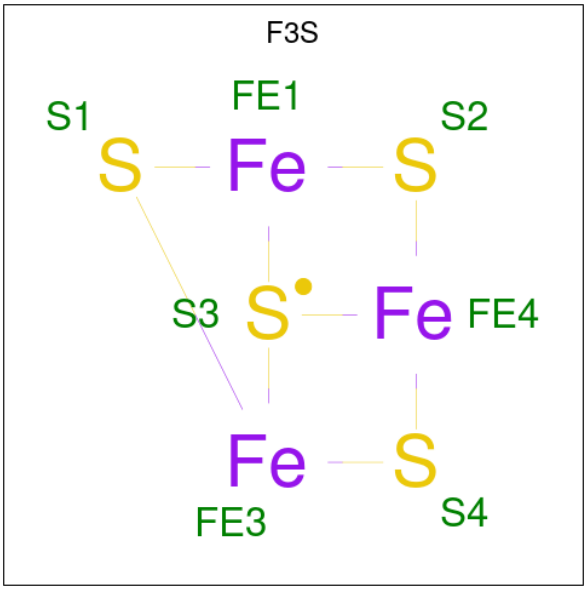
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	4	2	2	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



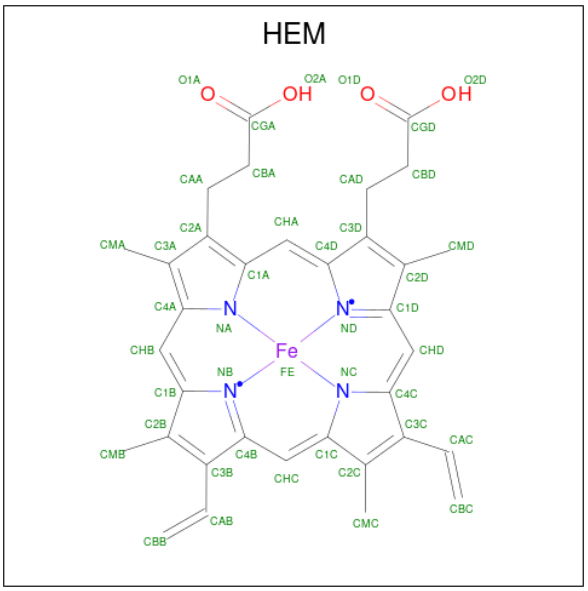
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	8	4	4	0	0

- Molecule 10 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



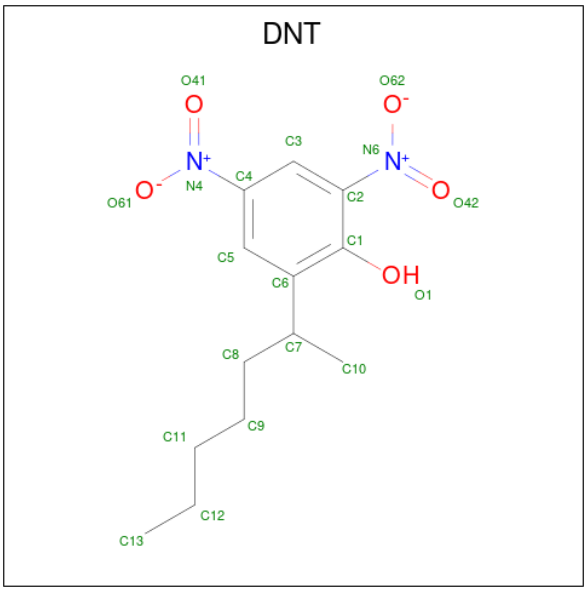
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
10	B	1	7	3	4	0	0

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



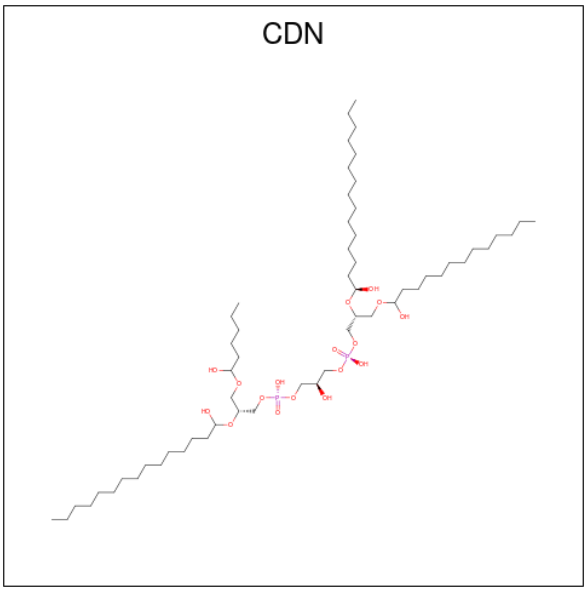
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
11	C	1	43	34	1	4	4	0	0

- Molecule 12 is 2-[1-METHYLHEXYL]-4,6-DINITROPHENOL (three-letter code: DNT) (formula: $C_{13}H_{18}N_2O_5$).



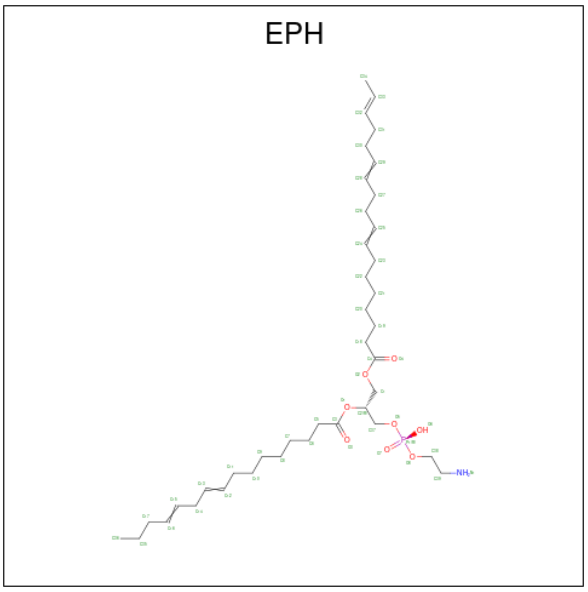
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	C	1	20	13	2	5	0	0

- Molecule 13 is CARDIOLIPIN (three-letter code: CDN) (formula: $C_{58}H_{120}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
13	C	1	77	58	17	2	0	0

- Molecule 14 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
14	C	1	35	25	1	8	1	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	61	61	61	0	0
			Total	O		
15	B	51	51	51	0	0
			Total	O		
15	C	13	13	13	0	0
			Total	O		
15	D	15	15	15	0	0

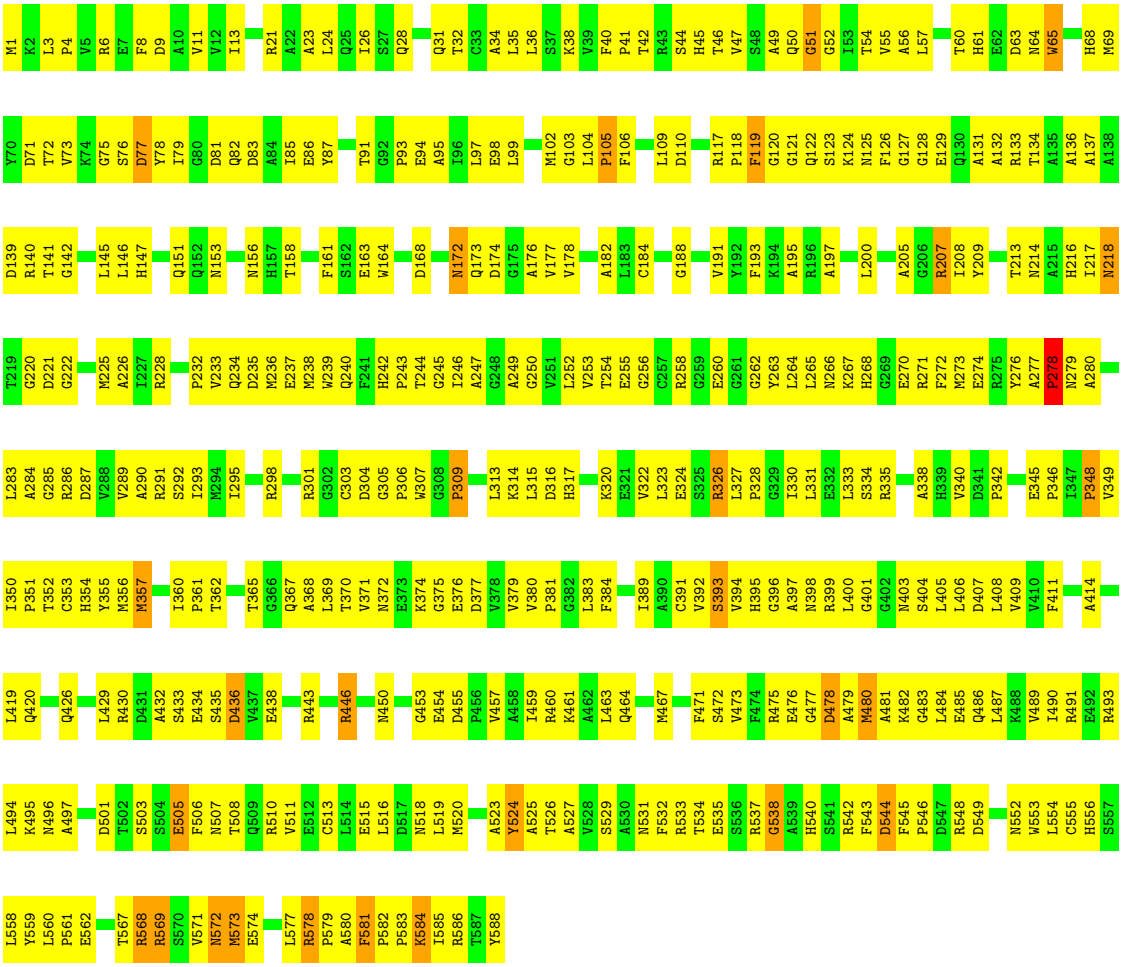
3 Residue-property plots (i)

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: Succinate dehydrogenase flavoprotein subunit

Chain A: 36% 59% 5%

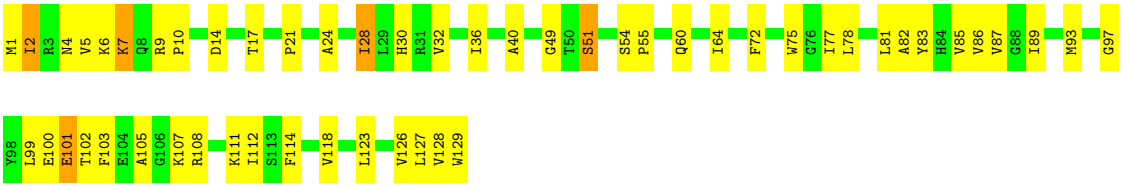


• Molecule 2: Succinate dehydrogenase iron-sulfur protein

Chain B: 50% 48% •

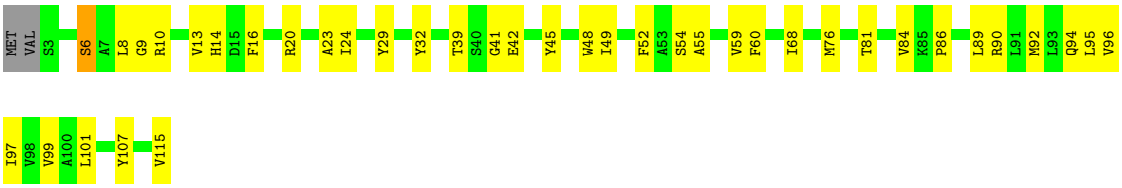
• Molecule 3: Succinate dehydrogenase cytochrome b-556 subunit

Chain C:



• Molecule 4: Succinate dehydrogenase hydrophobic membrane anchor protein

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	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	138.80Å 138.80Å 521.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8695	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OAA, CDN, F3S, FES, CA, FAD, HEM, EPH, SF4, DNT

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	0.45	0/4611	0.71	1/6237 (0.0%)
2	B	0.44	0/1908	0.69	0/2578
3	C	0.48	0/1030	0.67	0/1394
4	D	0.53	0/923	0.65	0/1262
All	All	0.46	0/8472	0.69	1/11471 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	GLY	N-CA-C	-5.42	99.54	113.10

There are no chirality outliers.

There are no planarity outliers.

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	4522	0	4426	469	0
2	B	1869	0	1850	149	0
3	C	1008	0	1066	58	0
4	D	898	0	936	37	0
5	A	9	0	2	6	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	53	0	29	8	0
8	B	4	0	0	3	0
9	B	8	0	0	1	0
10	B	7	0	0	4	0
11	C	43	0	30	10	0
12	C	20	0	16	3	0
13	C	77	0	112	13	0
14	C	35	0	40	2	0
15	A	61	0	0	9	0
15	B	51	0	0	0	0
15	C	13	0	0	1	0
15	D	15	0	0	1	0
All	All	8695	0	8507	690	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 41.

All (690) 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)
11:C:305:HEM:HBB1	13:C:308:CDN:C24	1.73	1.17
1:A:559:TYR:HB2	1:A:569:ARG:NH2	1.69	1.07
1:A:584:LYS:HG2	1:A:585:ILE:H	1.17	1.04
3:C:6:LYS:HG2	3:C:7:LYS:H	1.21	1.02
2:B:223:THR:HG22	10:B:304:F3S:S1	2.00	1.01
1:A:534:THR:HB	1:A:553:TRP:HE1	1.28	0.97
1:A:9:ASP:H	1:A:32:THR:HG23	1.29	0.96
1:A:205:ALA:HB2	1:A:220:GLY:N	1.81	0.94
1:A:242:HIS:O	1:A:351:PRO:HA	1.67	0.94
3:C:6:LYS:HE3	3:C:7:LYS:HG3	1.51	0.93
1:A:516:LEU:HA	1:A:519:LEU:HD12	1.51	0.91
1:A:236:MET:HE3	1:A:236:MET:HA	1.50	0.90
2:B:94:LEU:HB3	2:B:157:THR:HG21	1.51	0.90
1:A:128:GLY:HA3	1:A:400:LEU:HD11	1.53	0.89
2:B:92:ARG:HH11	3:C:17:THR:HG21	1.37	0.89
1:A:79:ILE:HD13	1:A:397:ALA:HB2	1.56	0.88
11:C:305:HEM:HBB1	13:C:308:CDN:H241	1.52	0.88
1:A:324:GLU:O	1:A:328:PRO:HG3	1.74	0.87
1:A:272:PHE:CZ	1:A:293:ILE:HG22	2.09	0.86
11:C:305:HEM:CBB	13:C:308:CDN:C24	2.54	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD22	1:A:271:ARG:HG2	1.58	0.85
3:C:78:LEU:HD21	13:C:308:CDN:H162	1.57	0.85
1:A:172:ASN:HD21	1:A:430:ARG:HG3	1.40	0.85
1:A:534:THR:HB	1:A:553:TRP:NE1	1.91	0.85
3:C:28:ILE:HD11	12:C:306:DNT:H121	1.57	0.85
1:A:161:PHE:HB3	1:A:164:TRP:CD1	2.12	0.84
3:C:2:ILE:HG12	3:C:5:VAL:HB	1.59	0.83
1:A:42:THR:O	1:A:47:VAL:HG11	1.77	0.83
1:A:555:CYS:HB2	1:A:571:VAL:HG13	1.60	0.83
1:A:584:LYS:HG2	1:A:585:ILE:N	1.94	0.83
11:C:305:HEM:CBB	13:C:308:CDN:H241	2.09	0.83
1:A:559:TYR:HB2	1:A:569:ARG:HH21	1.38	0.82
1:A:126:PHE:HE2	1:A:401:GLY:HA3	1.45	0.82
2:B:172:PRO:HG3	10:B:304:F3S:S3	2.19	0.82
3:C:60:GLN:O	3:C:64:ILE:HG13	1.78	0.82
2:B:95:PRO:HD2	2:B:157:THR:HG22	1.60	0.82
3:C:51:SER:HB3	4:D:48:TRP:HE1	1.45	0.81
4:D:92:MET:O	4:D:96:VAL:HG23	1.80	0.81
1:A:126:PHE:O	1:A:283:LEU:HD11	1.81	0.81
1:A:139:ASP:OD2	1:A:330:ILE:HG12	1.82	0.80
2:B:25:LEU:HB2	2:B:42:LEU:HD21	1.61	0.80
4:D:9:GLY:HA2	4:D:14:HIS:CD2	2.16	0.80
1:A:277:ALA:HB1	1:A:588:TYR:O	1.81	0.80
1:A:584:LYS:CG	1:A:585:ILE:H	1.94	0.79
4:D:9:GLY:HA2	4:D:14:HIS:HD2	1.44	0.79
3:C:6:LYS:HG2	3:C:7:LYS:N	1.97	0.79
1:A:578:ARG:HB3	1:A:579:PRO:HD3	1.62	0.79
2:B:140:ARG:O	2:B:140:ARG:HD3	1.82	0.78
1:A:505:GLU:O	2:B:101:ARG:HD2	1.83	0.78
1:A:127:GLY:HA3	1:A:255:GLU:OE2	1.83	0.78
2:B:210:MET:HE2	3:C:103:PHE:HA	1.64	0.77
4:D:6:SER:HB3	4:D:94:GLN:NE2	1.99	0.77
1:A:265:LEU:CD2	1:A:271:ARG:HG2	2.14	0.77
1:A:9:ASP:OD2	1:A:32:THR:HG22	1.84	0.77
1:A:244:THR:HG23	1:A:258:ARG:HH21	1.49	0.77
11:C:305:HEM:HBB1	13:C:308:CDN:H242	1.62	0.77
1:A:534:THR:HG22	1:A:534:THR:O	1.84	0.76
1:A:520:MET:HE2	1:A:520:MET:HA	1.67	0.76
1:A:75:GLY:O	1:A:398:ASN:HB3	1.84	0.75
1:A:534:THR:HG23	1:A:545:PHE:CE2	2.22	0.75
1:A:446:ARG:NH2	1:A:497:ALA:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:MET:HA	2:B:34:MET:CE	2.16	0.75
2:B:37:ASP:O	2:B:41:GLN:HG2	1.85	0.75
1:A:280:ALA:HB3	1:A:588:TYR:O	1.86	0.75
1:A:69:MET:O	1:A:73:VAL:HG23	1.86	0.74
1:A:293:ILE:HD11	1:A:351:PRO:HG3	1.68	0.74
2:B:95:PRO:HD2	2:B:157:THR:CG2	2.17	0.74
1:A:205:ALA:HB2	1:A:220:GLY:CA	2.16	0.74
1:A:323:LEU:HB3	1:A:331:LEU:HD21	1.68	0.74
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.70	0.74
1:A:537:ARG:HH12	1:A:554:LEU:CD1	2.01	0.74
1:A:556:HIS:HB2	1:A:572:ASN:HB3	1.68	0.74
1:A:254:THR:HA	5:A:589:OAA:O5	1.88	0.74
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.71	0.73
1:A:119:PHE:HB2	2:B:135:GLN:H	1.54	0.73
4:D:115:VAL:OXT	4:D:115:VAL:HG12	1.87	0.73
1:A:365:THR:OG1	1:A:367:GLN:HG3	1.88	0.73
1:A:129:GLU:O	1:A:283:LEU:HD21	1.90	0.72
1:A:237:GLU:HB3	1:A:529:SER:HB2	1.70	0.72
3:C:2:ILE:CG1	3:C:5:VAL:HB	2.19	0.72
1:A:578:ARG:CB	1:A:579:PRO:HD3	2.19	0.72
2:B:129:PRO:HG2	2:B:133:HIS:CD2	2.24	0.72
1:A:177:VAL:HG21	1:A:383:LEU:HB2	1.69	0.72
1:A:255:GLU:N	5:A:589:OAA:O4	2.22	0.72
1:A:54:THR:HG22	1:A:134:THR:OG1	1.89	0.72
1:A:238:MET:HE3	1:A:397:ALA:HB1	1.70	0.72
1:A:331:LEU:O	1:A:335:ARG:HG3	1.89	0.72
1:A:434:GLU:O	1:A:438:GLU:HB2	1.90	0.72
3:C:6:LYS:CG	3:C:7:LYS:H	2.00	0.72
1:A:574:GLU:HG3	1:A:574:GLU:O	1.90	0.72
1:A:287:ASP:H	1:A:398:ASN:ND2	1.87	0.71
1:A:453:GLY:HA3	1:A:496:ASN:O	1.89	0.71
1:A:313:LEU:HD12	1:A:349:VAL:HG11	1.71	0.71
4:D:6:SER:HB3	4:D:94:GLN:HE22	1.52	0.71
1:A:560:LEU:HB3	1:A:568:ARG:HB2	1.71	0.71
2:B:2:ARG:HE	2:B:24:THR:HG21	1.55	0.71
2:B:34:MET:HA	2:B:34:MET:HE2	1.72	0.71
1:A:369:LEU:CD2	1:A:379:VAL:HG22	2.20	0.71
1:A:291:ARG:NH2	1:A:538:GLY:O	2.24	0.71
1:A:140:ARG:HH11	2:B:148:GLU:HG2	1.54	0.70
1:A:357:MET:HE2	1:A:357:MET:N	2.06	0.70
2:B:180:ARG:HG2	2:B:180:ARG:HH11	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASP:OD2	1:A:586:ARG:NH1	2.19	0.70
2:B:77:THR:HG22	2:B:82:LEU:HD11	1.70	0.70
1:A:119:PHE:CG	2:B:134:LEU:HA	2.26	0.70
2:B:92:ARG:NH1	3:C:17:THR:HG21	2.06	0.70
1:A:38:LYS:CE	1:A:217:ILE:HG23	2.21	0.69
1:A:104:LEU:HD23	1:A:106:PHE:CZ	2.27	0.69
1:A:126:PHE:CE2	1:A:401:GLY:HA3	2.27	0.69
1:A:534:THR:HG23	1:A:545:PHE:CD2	2.28	0.69
1:A:119:PHE:CD1	2:B:134:LEU:HD12	2.27	0.69
1:A:242:HIS:CE1	1:A:286:ARG:HH21	2.10	0.69
1:A:240:GLN:H	1:A:357:MET:HE1	1.58	0.69
2:B:210:MET:HE1	3:C:102:THR:O	1.93	0.69
1:A:36:LEU:HD22	1:A:161:PHE:HB2	1.73	0.69
2:B:77:THR:CG2	2:B:82:LEU:HD11	2.22	0.69
1:A:395:HIS:ND1	1:A:399:ARG:HG3	2.08	0.69
1:A:244:THR:HG23	1:A:258:ARG:NH2	2.07	0.68
1:A:244:THR:CG2	1:A:258:ARG:HH21	2.06	0.68
2:B:76:ILE:O	2:B:78:PRO:HD3	1.92	0.68
1:A:252:LEU:HG	1:A:253:VAL:N	2.07	0.68
1:A:392:VAL:HG13	1:A:394:VAL:HG13	1.75	0.68
1:A:272:PHE:CZ	1:A:293:ILE:CG2	2.76	0.68
1:A:285:GLY:O	1:A:289:VAL:HG23	1.94	0.68
1:A:234:GLN:HB2	1:A:361:PRO:HG3	1.74	0.68
1:A:567:THR:HG23	15:A:606:HOH:O	1.92	0.68
1:A:208:ILE:HG13	1:A:209:TYR:CD1	2.29	0.68
1:A:9:ASP:H	1:A:32:THR:CG2	2.06	0.67
3:C:82:ALA:O	3:C:86:VAL:HG23	1.95	0.67
1:A:81:ASP:HB3	1:A:83:ASP:OD1	1.93	0.67
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.29	0.67
1:A:544:ASP:HB2	1:A:545:PHE:CD1	2.30	0.67
1:A:255:GLU:HB2	1:A:286:ARG:HH22	1.59	0.67
1:A:511:VAL:O	1:A:515:GLU:HG3	1.95	0.67
1:A:208:ILE:HG13	1:A:209:TYR:CE1	2.30	0.66
1:A:253:VAL:HG13	1:A:330:ILE:HD12	1.75	0.66
1:A:293:ILE:HD11	1:A:351:PRO:CG	2.25	0.66
1:A:276:TYR:C	1:A:278:PRO:HD3	2.16	0.66
2:B:34:MET:HE1	2:B:78:PRO:HG3	1.77	0.66
4:D:84:VAL:HG13	4:D:89:LEU:HD23	1.78	0.66
2:B:35:LEU:HD12	2:B:35:LEU:O	1.96	0.66
3:C:1:MET:HG3	3:C:6:LYS:HA	1.77	0.65
1:A:238:MET:CE	1:A:397:ALA:HB1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLN:N	1:A:357:MET:HE1	2.12	0.65
3:C:72:PHE:O	3:C:75:TRP:HB3	1.97	0.65
1:A:573:MET:HA	15:A:640:HOH:O	1.97	0.65
1:A:578:ARG:HB3	1:A:579:PRO:CD	2.27	0.64
1:A:120:GLY:HA2	2:B:132:GLU:OE2	1.97	0.64
1:A:60:THR:HG21	1:A:123:SER:O	1.97	0.64
1:A:8:PHE:CE2	1:A:34:ALA:HB2	2.33	0.64
1:A:255:GLU:CD	1:A:286:ARG:HH22	1.99	0.64
1:A:287:ASP:H	1:A:398:ASN:HD21	1.45	0.64
1:A:544:ASP:HB2	1:A:545:PHE:CE1	2.33	0.64
1:A:233:VAL:HG11	1:A:236:MET:SD	2.37	0.64
4:D:86:PRO:HD3	15:D:117:HOH:O	1.98	0.63
1:A:559:TYR:CB	1:A:569:ARG:NH2	2.56	0.63
1:A:369:LEU:HD21	1:A:379:VAL:HG22	1.80	0.63
2:B:205:ARG:HH22	4:D:81:THR:HB	1.62	0.63
2:B:236:ARG:C	2:B:237:ASN:HD22	2.03	0.63
1:A:172:ASN:ND2	1:A:430:ARG:HG3	2.14	0.62
1:A:270:GLU:HG2	1:A:271:ARG:N	2.14	0.62
1:A:555:CYS:CB	1:A:571:VAL:HG13	2.28	0.62
1:A:104:LEU:HD12	1:A:105:PRO:HD2	1.82	0.62
1:A:242:HIS:HE1	1:A:286:ARG:HH21	1.44	0.62
3:C:30:HIS:CD2	3:C:87:VAL:HB	2.34	0.62
1:A:126:PHE:O	1:A:129:GLU:HG2	1.99	0.62
1:A:583:PRO:O	1:A:584:LYS:HB2	1.98	0.62
2:B:209:ILE:HG23	3:C:24:ALA:HA	1.80	0.62
1:A:139:ASP:OD1	1:A:139:ASP:O	2.18	0.62
1:A:263:TYR:HB2	1:A:314:LYS:HB3	1.82	0.62
1:A:567:THR:O	1:A:568:ARG:HG3	2.00	0.61
1:A:232:PRO:HB2	1:A:558:LEU:HD11	1.82	0.61
4:D:20:ARG:O	4:D:24:ILE:HG13	2.00	0.61
1:A:572:ASN:ND2	1:A:573:MET:H	1.99	0.61
1:A:572:ASN:C	1:A:573:MET:HG3	2.21	0.61
3:C:30:HIS:HD2	3:C:87:VAL:HB	1.63	0.61
1:A:571:VAL:HG12	1:A:572:ASN:N	2.16	0.61
1:A:537:ARG:HH21	1:A:548:ARG:CG	2.13	0.61
1:A:484:LEU:HD11	1:A:531:ASN:HB2	1.80	0.61
1:A:44:SER:O	1:A:47:VAL:HG22	2.01	0.61
1:A:242:HIS:CD2	1:A:252:LEU:HD11	2.35	0.61
4:D:95:LEU:O	4:D:99:VAL:HG23	1.99	0.61
1:A:320:LYS:HA	1:A:323:LEU:HD12	1.82	0.60
1:A:537:ARG:HA	1:A:586:ARG:HH12	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:HE2	1:A:401:GLY:CA	2.14	0.60
1:A:60:THR:CG2	1:A:123:SER:HB2	2.32	0.60
1:A:109:LEU:C	1:A:117:ARG:O	2.40	0.60
1:A:369:LEU:HD23	1:A:379:VAL:HA	1.83	0.60
1:A:537:ARG:HH12	1:A:554:LEU:HD12	1.65	0.59
1:A:537:ARG:HH12	1:A:554:LEU:HD13	1.67	0.59
1:A:579:PRO:O	1:A:580:ALA:HB3	2.02	0.59
2:B:58:GLY:HA2	8:B:302:FES:S2	2.42	0.59
2:B:67:MET:HE1	2:B:74:ALA:HA	1.84	0.59
1:A:486:GLN:O	1:A:489:VAL:HB	2.02	0.59
1:A:562:GLU:HB2	1:A:568:ARG:NH1	2.17	0.59
1:A:213:THR:HA	1:A:250:GLY:O	2.02	0.59
1:A:221:ASP:HA	1:A:518:ASN:ND2	2.17	0.59
2:B:56:ARG:O	2:B:56:ARG:HG2	2.02	0.59
2:B:180:ARG:HG2	2:B:180:ARG:NH1	2.16	0.59
1:A:408:LEU:HD11	7:A:601:FAD:H4'	1.82	0.59
1:A:571:VAL:CG1	1:A:572:ASN:N	2.66	0.59
1:A:38:LYS:HE2	1:A:217:ILE:HG23	1.82	0.59
1:A:221:ASP:O	1:A:225:MET:HG3	2.02	0.59
1:A:578:ARG:CG	1:A:579:PRO:HD3	2.32	0.59
1:A:350:ILE:HG13	1:A:350:ILE:O	2.02	0.59
1:A:245:GLY:HA3	1:A:352:THR:HG22	1.83	0.59
1:A:340:VAL:O	1:A:342:PRO:HD3	2.02	0.59
1:A:457:VAL:O	1:A:461:LYS:HG3	2.03	0.59
2:B:25:LEU:HB2	2:B:42:LEU:CD2	2.29	0.59
1:A:3:LEU:HD12	1:A:4:PRO:HD2	1.84	0.59
1:A:9:ASP:CG	1:A:32:THR:HG22	2.23	0.58
1:A:72:THR:HA	1:A:400:LEU:HD22	1.84	0.58
2:B:95:PRO:O	2:B:157:THR:HG23	2.02	0.58
13:C:308:CDN:H243	4:D:68:ILE:HD11	1.85	0.58
1:A:577:LEU:N	1:A:577:LEU:HD23	2.18	0.58
1:A:205:ALA:CB	1:A:220:GLY:N	2.62	0.58
1:A:293:ILE:CD1	1:A:351:PRO:HD3	2.33	0.58
1:A:463:LEU:HD13	1:A:520:MET:CE	2.33	0.58
2:B:25:LEU:HD21	2:B:41:GLN:HG3	1.86	0.58
2:B:70:LYS:HE3	2:B:215:VAL:HG12	1.86	0.58
2:B:146:LEU:CD1	2:B:183:ILE:HD11	2.33	0.58
3:C:85:VAL:O	3:C:89:ILE:HG13	2.03	0.58
2:B:82:LEU:HD12	2:B:82:LEU:N	2.19	0.58
1:A:63:ASP:OD1	1:A:64:ASN:N	2.37	0.58
1:A:399:ARG:NH2	5:A:589:OAA:O1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:THR:HG22	2:B:82:LEU:CD1	2.34	0.57
1:A:140:ARG:NH1	2:B:148:GLU:HG2	2.18	0.57
1:A:9:ASP:N	1:A:32:THR:HG23	2.11	0.57
1:A:287:ASP:HB2	1:A:538:GLY:O	2.04	0.57
2:B:114:TYR:O	2:B:117:ILE:HG13	2.05	0.57
1:A:47:VAL:HG13	1:A:146:LEU:CD2	2.34	0.57
1:A:54:THR:OG1	1:A:403:ASN:ND2	2.38	0.57
1:A:119:PHE:CB	2:B:135:GLN:H	2.17	0.57
1:A:362:THR:HG22	1:A:368:ALA:HA	1.85	0.57
1:A:228:ARG:HG3	15:A:602:HOH:O	2.05	0.57
1:A:245:GLY:HA3	1:A:352:THR:CG2	2.35	0.57
1:A:555:CYS:HB3	1:A:573:MET:HG2	1.86	0.57
2:B:65:LEU:HD12	2:B:74:ALA:HB2	1.85	0.57
1:A:78:TYR:CD2	1:A:583:PRO:HA	2.40	0.56
1:A:450:ASN:HB3	15:A:633:HOH:O	2.05	0.56
1:A:532:PHE:CD2	1:A:569:ARG:HB3	2.40	0.56
1:A:389:ILE:HG12	1:A:389:ILE:O	2.05	0.56
3:C:83:TYR:CE2	3:C:87:VAL:HG21	2.38	0.56
1:A:480:MET:HE2	1:A:542:ARG:NH1	2.20	0.56
2:B:165:ASN:HB3	2:B:168:LYS:HB2	1.88	0.56
2:B:34:MET:HE1	2:B:78:PRO:CG	2.35	0.56
1:A:65:TRP:O	1:A:68:HIS:HB3	2.06	0.55
1:A:559:TYR:O	1:A:561:PRO:HD3	2.05	0.55
1:A:255:GLU:HB2	1:A:286:ARG:NH2	2.19	0.55
1:A:304:ASP:OD1	1:A:305:GLY:N	2.39	0.55
1:A:574:GLU:O	1:A:574:GLU:CG	2.54	0.55
3:C:40:ALA:HB1	3:C:77:ILE:HG23	1.89	0.55
3:C:108:ARG:O	3:C:112:ILE:HG13	2.07	0.55
11:C:305:HEM:HAC	4:D:23:ALA:HB1	1.89	0.55
1:A:207:ARG:NH1	1:A:216:HIS:ND1	2.55	0.55
1:A:61:HIS:NE2	1:A:131:ALA:HB3	2.22	0.55
1:A:153:ASN:HD22	1:A:158:THR:CB	2.20	0.55
1:A:334:SER:O	1:A:338:ALA:N	2.39	0.55
1:A:559:TYR:CB	1:A:569:ARG:HH21	2.17	0.55
1:A:242:HIS:HB2	1:A:354:HIS:HB2	1.88	0.55
2:B:43:LYS:HA	2:B:46:ASP:O	2.07	0.55
4:D:10:ARG:H	4:D:14:HIS:CD2	2.24	0.54
1:A:54:THR:O	1:A:406:LEU:HD22	2.07	0.54
1:A:106:PHE:HA	1:A:137:ALA:HB2	1.89	0.54
1:A:532:PHE:CE2	1:A:569:ARG:HB3	2.42	0.54
1:A:578:ARG:CB	1:A:579:PRO:CD	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:NE	2:B:24:THR:HG21	2.23	0.54
1:A:238:MET:HE2	1:A:397:ALA:CB	2.37	0.54
2:B:34:MET:HA	2:B:34:MET:HE3	1.89	0.54
1:A:272:PHE:HZ	1:A:293:ILE:HG22	1.68	0.54
1:A:314:LYS:NZ	1:A:317:HIS:HB3	2.23	0.54
1:A:533:ARG:HB3	1:A:540:HIS:CE1	2.42	0.54
1:A:490:ILE:O	1:A:493:ARG:HB3	2.08	0.54
2:B:210:MET:HG2	2:B:223:THR:HG21	1.89	0.54
3:C:28:ILE:HG12	3:C:28:ILE:O	2.08	0.54
1:A:483:GLY:O	1:A:487:LEU:HD13	2.08	0.54
1:A:123:SER:HA	1:A:134:THR:O	2.07	0.54
1:A:255:GLU:OE1	1:A:286:ARG:NH2	2.41	0.54
1:A:357:MET:CE	1:A:357:MET:H	2.20	0.54
3:C:89:ILE:HG22	3:C:93:MET:CE	2.38	0.54
1:A:239:TRP:CZ3	1:A:356:MET:HB2	2.42	0.54
1:A:485:GLU:O	1:A:489:VAL:HG23	2.08	0.54
1:A:234:GLN:CB	1:A:361:PRO:HG3	2.37	0.53
1:A:584:LYS:HG2	1:A:585:ILE:HG12	1.90	0.53
2:B:43:LYS:HE2	2:B:47:PRO:O	2.08	0.53
1:A:79:ILE:HG23	1:A:396:GLY:HA3	1.91	0.53
1:A:295:ILE:HA	1:A:298:ARG:HG3	1.90	0.53
1:A:482:LYS:O	1:A:486:GLN:HG3	2.07	0.53
1:A:501:ASP:OD2	1:A:507:ASN:ND2	2.41	0.53
2:B:58:GLY:CA	8:B:302:FES:S2	2.97	0.53
1:A:47:VAL:HG13	1:A:146:LEU:HD22	1.89	0.53
2:B:94:LEU:HB3	2:B:157:THR:CG2	2.33	0.53
2:B:211:ASN:HD21	3:C:24:ALA:HB2	1.73	0.53
1:A:256:GLY:O	1:A:260:GLU:HG2	2.08	0.53
1:A:306:PRO:O	2:B:31:ARG:NH2	2.41	0.53
2:B:165:ASN:N	2:B:166:PRO:HD3	2.24	0.53
1:A:405:LEU:HG	7:A:601:FAD:C2	2.39	0.53
1:A:463:LEU:O	1:A:467:MET:HG2	2.09	0.53
1:A:182:ALA:HB3	1:A:193:PHE:CE1	2.43	0.52
3:C:83:TYR:O	3:C:87:VAL:HG23	2.09	0.52
4:D:10:ARG:H	4:D:14:HIS:HD2	1.57	0.52
1:A:372:ASN:HB3	1:A:376:GLU:H	1.74	0.52
4:D:29:TYR:O	4:D:32:TYR:HB3	2.09	0.52
1:A:23:ALA:HB2	1:A:35:LEU:HD13	1.92	0.52
1:A:94:GLU:HG3	1:A:95:ALA:N	2.23	0.52
1:A:173:GLN:HB3	1:A:430:ARG:HE	1.74	0.52
2:B:146:LEU:HD12	2:B:183:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HE21	1:A:420:GLN:HG2	1.75	0.52
1:A:454:GLU:OE1	1:A:493:ARG:HG3	2.10	0.52
2:B:29:GLU:HA	2:B:29:GLU:OE1	2.10	0.52
4:D:39:THR:O	4:D:39:THR:HG22	2.09	0.52
1:A:119:PHE:CD2	2:B:134:LEU:HA	2.45	0.52
1:A:476:GLU:HG3	1:A:478:ASP:OD1	2.09	0.52
2:B:180:ARG:HD3	2:B:181:PHE:CE2	2.44	0.52
1:A:21:ARG:O	1:A:21:ARG:NH1	2.43	0.52
1:A:172:ASN:HB3	1:A:176:ALA:H	1.74	0.52
1:A:476:GLU:HG3	1:A:478:ASP:CG	2.29	0.52
2:B:25:LEU:HD13	2:B:42:LEU:HD23	1.91	0.52
3:C:14:ASP:O	3:C:17:THR:HB	2.10	0.52
1:A:327:LEU:N	1:A:328:PRO:HD3	2.25	0.52
2:B:34:MET:HE1	2:B:78:PRO:CD	2.40	0.52
1:A:578:ARG:HG2	1:A:579:PRO:HD3	1.90	0.51
2:B:9:ARG:HH12	2:B:49:LEU:CA	2.23	0.51
1:A:11:VAL:HG23	1:A:195:ALA:HB2	1.93	0.51
2:B:223:THR:CG2	10:B:304:F3S:S1	2.87	0.51
1:A:370:THR:HG23	1:A:380:VAL:CG2	2.40	0.51
4:D:84:VAL:O	4:D:90:ARG:HD3	2.11	0.51
1:A:91:THR:O	1:A:91:THR:HG22	2.10	0.51
1:A:404:SER:O	1:A:408:LEU:HG	2.10	0.51
2:B:201:PHE:O	2:B:202:SER:C	2.49	0.51
1:A:82:GLN:NE2	1:A:581:PHE:HB3	2.25	0.51
1:A:238:MET:HE2	1:A:397:ALA:HB2	1.92	0.51
1:A:247:ALA:HB2	1:A:350:ILE:HG23	1.93	0.51
1:A:467:MET:SD	1:A:523:ALA:HB1	2.50	0.51
1:A:197:ALA:HB1	1:A:384:PHE:CE1	2.45	0.51
1:A:182:ALA:HB3	1:A:193:PHE:HE1	1.76	0.51
1:A:124:LYS:HE3	1:A:136:ALA:CB	2.41	0.51
1:A:49:ALA:HA	7:A:601:FAD:C5X	2.41	0.51
1:A:97:LEU:HD22	2:B:132:GLU:HB3	1.92	0.51
1:A:284:ALA:HB3	1:A:289:VAL:HG22	1.93	0.51
2:B:118:LYS:N	2:B:119:PRO:HD3	2.26	0.51
1:A:267:LYS:HE3	1:A:268:HIS:CE1	2.46	0.50
1:A:463:LEU:HD13	1:A:520:MET:HE2	1.92	0.50
3:C:81:LEU:O	3:C:85:VAL:HG23	2.11	0.50
1:A:520:MET:HA	1:A:520:MET:CE	2.40	0.50
1:A:372:ASN:O	1:A:375:GLY:N	2.45	0.50
1:A:476:GLU:HG3	1:A:478:ASP:OD2	2.12	0.50
1:A:98:GLU:O	1:A:102:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASN:N	1:A:376:GLU:O	2.45	0.50
1:A:221:ASP:HA	1:A:518:ASN:CG	2.32	0.50
1:A:207:ARG:HH12	1:A:216:HIS:CE1	2.28	0.50
1:A:556:HIS:N	1:A:572:ASN:O	2.37	0.50
1:A:205:ALA:HB2	1:A:220:GLY:HA3	1.91	0.50
1:A:537:ARG:O	1:A:540:HIS:N	2.45	0.50
2:B:82:LEU:O	2:B:89:ILE:HG12	2.11	0.50
1:A:272:PHE:HZ	1:A:293:ILE:CG2	2.20	0.50
1:A:46:THR:HB	1:A:146:LEU:HD13	1.93	0.50
1:A:222:GLY:HA3	1:A:389:ILE:HD12	1.94	0.50
1:A:236:MET:HG3	1:A:236:MET:O	2.12	0.50
2:B:34:MET:CE	2:B:34:MET:CA	2.87	0.49
2:B:35:LEU:HD21	2:B:91:ILE:CD1	2.42	0.49
4:D:16:PHE:O	4:D:20:ARG:HD3	2.12	0.49
4:D:45:TYR:O	4:D:49:ILE:HG22	2.12	0.49
1:A:63:ASP:CG	1:A:133:ARG:HH12	2.14	0.49
1:A:572:ASN:C	1:A:573:MET:CG	2.80	0.49
1:A:35:LEU:C	1:A:36:LEU:HD23	2.32	0.49
1:A:125:ASN:CG	1:A:132:ALA:HB2	2.32	0.49
1:A:274:GLU:O	1:A:278:PRO:HA	2.12	0.49
1:A:205:ALA:HA	1:A:218:ASN:O	2.12	0.49
1:A:207:ARG:NH1	1:A:216:HIS:CE1	2.80	0.49
1:A:56:ALA:O	1:A:93:PRO:HG3	2.12	0.49
1:A:222:GLY:HA2	1:A:225:MET:HE2	1.95	0.49
2:B:95:PRO:CD	2:B:157:THR:CG2	2.88	0.49
1:A:255:GLU:CB	1:A:286:ARG:HH22	2.22	0.49
1:A:379:VAL:HG12	1:A:380:VAL:N	2.27	0.49
1:A:404:SER:HB3	7:A:601:FAD:N1	2.28	0.49
2:B:35:LEU:HD11	2:B:91:ILE:CD1	2.42	0.49
2:B:52:ARG:NH2	2:B:105:VAL:O	2.46	0.49
11:C:305:HEM:CBB	13:C:308:CDN:H242	2.32	0.49
1:A:45:HIS:CE1	1:A:214:ASN:HA	2.47	0.49
2:B:9:ARG:HH11	2:B:49:LEU:HD13	1.77	0.49
2:B:35:LEU:HD11	2:B:91:ILE:HD11	1.93	0.49
1:A:126:PHE:CE2	1:A:255:GLU:OE1	2.66	0.49
1:A:232:PRO:HD2	1:A:370:THR:HG22	1.94	0.49
2:B:111:TYR:O	2:B:114:TYR:HB3	2.12	0.49
1:A:222:GLY:HA3	1:A:389:ILE:CD1	2.42	0.49
2:B:35:LEU:HD23	2:B:67:MET:CE	2.43	0.49
3:C:2:ILE:HD11	3:C:5:VAL:HG21	1.95	0.49
1:A:531:ASN:O	1:A:542:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:PHE:N	1:A:546:PRO:HD3	2.28	0.49
1:A:562:GLU:CD	1:A:568:ARG:NH2	2.67	0.48
2:B:3:LEU:HB3	2:B:5:PHE:CE1	2.48	0.48
1:A:392:VAL:CG1	1:A:394:VAL:HG13	2.42	0.48
1:A:443:ARG:NH1	15:A:602:HOH:O	2.40	0.48
1:A:472:SER:OG	1:A:473:VAL:N	2.45	0.48
1:A:537:ARG:NH1	1:A:554:LEU:HD12	2.26	0.48
1:A:555:CYS:HB2	1:A:571:VAL:CG1	2.40	0.48
2:B:3:LEU:HB3	2:B:5:PHE:HE1	1.78	0.48
3:C:6:LYS:HE3	3:C:7:LYS:CG	2.34	0.48
1:A:6:ARG:HB3	1:A:8:PHE:HE1	1.78	0.48
2:B:135:GLN:NE2	2:B:185:SER:HB2	2.28	0.48
3:C:28:ILE:O	3:C:32:VAL:HG23	2.13	0.48
1:A:79:ILE:HG21	1:A:397:ALA:CB	2.44	0.48
1:A:81:ASP:N	1:A:81:ASP:OD1	2.46	0.48
1:A:242:HIS:CE1	1:A:286:ARG:NH2	2.81	0.48
1:A:298:ARG:NH1	1:A:543:PHE:CZ	2.81	0.48
2:B:208:SER:HA	10:B:304:F3S:S1	2.53	0.48
1:A:454:GLU:OE2	1:A:493:ARG:NE	2.43	0.48
1:A:40:PHE:HD2	1:A:42:THR:HG1	1.62	0.48
1:A:81:ASP:O	1:A:85:ILE:HG13	2.14	0.48
3:C:101:GLU:HG2	15:C:312:HOH:O	2.14	0.48
1:A:81:ASP:CG	1:A:393:SER:HB2	2.34	0.48
1:A:237:GLU:OE1	1:A:529:SER:HB3	2.12	0.48
1:A:272:PHE:CE1	1:A:273:MET:HE1	2.48	0.48
1:A:63:ASP:OD2	1:A:133:ARG:NH1	2.47	0.48
1:A:238:MET:CE	1:A:397:ALA:CB	2.89	0.48
1:A:534:THR:HB	1:A:553:TRP:CD1	2.49	0.48
1:A:584:LYS:CG	1:A:585:ILE:N	2.64	0.48
1:A:124:LYS:HE3	1:A:136:ALA:HB3	1.95	0.48
1:A:264:LEU:C	1:A:265:LEU:HD23	2.34	0.48
2:B:6:SER:HB3	2:B:90:VAL:HA	1.96	0.48
2:B:201:PHE:CZ	4:D:81:THR:HG21	2.48	0.48
1:A:86:GLU:OE1	1:A:578:ARG:HB3	2.13	0.47
1:A:205:ALA:HB2	1:A:220:GLY:H	1.75	0.47
1:A:369:LEU:CD2	1:A:379:VAL:HA	2.44	0.47
1:A:532:PHE:HD2	1:A:569:ARG:HD3	1.78	0.47
1:A:567:THR:C	1:A:568:ARG:HD2	2.34	0.47
3:C:118:VAL:HG21	14:C:309:EPH:H221	1.96	0.47
1:A:232:PRO:CB	1:A:558:LEU:HD11	2.43	0.47
1:A:314:LYS:HG2	1:A:316:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:ALA:C	2:B:82:LEU:HD12	2.35	0.47
1:A:374:LYS:HB2	1:A:376:GLU:HG3	1.96	0.47
1:A:24:LEU:O	1:A:28:GLN:HG2	2.15	0.47
1:A:207:ARG:NH2	1:A:214:ASN:O	2.47	0.47
1:A:478:ASP:O	1:A:481:ALA:HB3	2.15	0.47
2:B:137:PRO:O	2:B:141:GLU:HG3	2.14	0.47
2:B:164:TRP:C	2:B:166:PRO:HD3	2.34	0.47
2:B:1:MET:HG3	2:B:29:GLU:OE2	2.14	0.47
2:B:234:LEU:HD23	4:D:13:VAL:HG13	1.96	0.47
1:A:38:LYS:HG3	7:A:601:FAD:C4A	2.43	0.47
1:A:263:TYR:CZ	1:A:271:ARG:CZ	2.97	0.47
1:A:307:TRP:HD1	1:A:348:PRO:HG2	1.80	0.47
1:A:322:VAL:HG13	1:A:326:ARG:HG3	1.97	0.47
1:A:463:LEU:HD13	1:A:520:MET:HE1	1.95	0.47
1:A:537:ARG:NH1	1:A:554:LEU:CD1	2.76	0.47
2:B:152:CYS:O	2:B:153:ALA:HB3	2.15	0.47
1:A:105:PRO:O	1:A:137:ALA:HB1	2.15	0.47
1:A:298:ARG:NH1	1:A:543:PHE:HZ	2.13	0.47
2:B:92:ARG:CD	3:C:17:THR:HG21	2.45	0.47
1:A:214:ASN:HD22	1:A:214:ASN:N	2.12	0.47
2:B:135:GLN:HE22	2:B:185:SER:HB2	1.79	0.47
2:B:157:THR:HG22	2:B:157:THR:O	2.14	0.47
1:A:26:ILE:HD13	1:A:419:LEU:HD22	1.97	0.47
1:A:68:HIS:O	1:A:72:THR:HG23	2.14	0.47
2:B:34:MET:HE1	2:B:78:PRO:N	2.29	0.47
2:B:94:LEU:CB	2:B:157:THR:HG21	2.33	0.47
3:C:100:GLU:HB2	3:C:105:ALA:CB	2.45	0.47
1:A:178:VAL:HG23	1:A:178:VAL:O	2.16	0.46
1:A:432:ALA:HB1	1:A:436:ASP:HB2	1.97	0.46
1:A:3:LEU:HD12	1:A:4:PRO:CD	2.45	0.46
2:B:32:ASP:OD2	2:B:80:SER:OG	2.33	0.46
1:A:234:GLN:HG3	1:A:361:PRO:CG	2.45	0.46
1:A:483:GLY:HA2	1:A:486:GLN:NE2	2.30	0.46
3:C:54:SER:HB2	3:C:55:PRO:CD	2.45	0.46
3:C:89:ILE:HG22	3:C:93:MET:HE2	1.96	0.46
1:A:82:GLN:HB2	1:A:577:LEU:HB3	1.98	0.46
11:C:305:HEM:CBB	4:D:68:ILE:HG12	2.45	0.46
2:B:71:ASN:OD1	2:B:94:LEU:HD23	2.16	0.46
2:B:123:ASN:O	2:B:125:GLY:N	2.49	0.46
1:A:76:SER:O	1:A:77:ASP:HB2	2.15	0.46
1:A:255:GLU:CD	1:A:286:ARG:NH2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LEU:CD2	2:B:103:LEU:HB3	2.46	0.46
2:B:213:VAL:HG23	2:B:223:THR:HG23	1.97	0.46
4:D:16:PHE:CE1	4:D:20:ARG:CZ	2.99	0.46
1:A:314:LYS:HA	1:A:346:PRO:HG3	1.97	0.46
2:B:179:TYR:O	2:B:183:ILE:HG12	2.15	0.46
2:B:190:THR:O	2:B:194:LEU:HG	2.16	0.46
3:C:128:VAL:HG12	3:C:128:VAL:O	2.15	0.46
1:A:533:ARG:HB3	1:A:540:HIS:HE1	1.78	0.46
1:A:571:VAL:CG1	1:A:572:ASN:H	2.29	0.46
2:B:100:ILE:HG12	3:C:9:ARG:CZ	2.46	0.46
13:C:308:CDN:HA21	4:D:41:GLY:O	2.16	0.46
1:A:426:GLN:NE2	1:A:429:LEU:HD11	2.30	0.46
1:A:559:TYR:HD1	1:A:569:ARG:HE	1.63	0.46
1:A:525:ALA:O	1:A:529:SER:OG	2.24	0.45
3:C:32:VAL:HG12	3:C:36:ILE:HD13	1.99	0.45
1:A:103:GLY:O	2:B:186:ARG:NH2	2.50	0.45
1:A:163:GLU:OE1	2:B:52:ARG:NH1	2.49	0.45
1:A:240:GLN:CB	1:A:357:MET:HE1	2.46	0.45
1:A:392:VAL:CG1	1:A:394:VAL:HG22	2.46	0.45
1:A:290:ALA:O	1:A:293:ILE:HG12	2.17	0.45
1:A:357:MET:N	1:A:357:MET:CE	2.75	0.45
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.66	0.45
1:A:459:ILE:HD13	1:A:494:LEU:HA	1.98	0.45
4:D:76:MET:HB3	4:D:97:ILE:HD13	1.98	0.45
1:A:8:PHE:CD2	1:A:34:ALA:HB2	2.52	0.45
1:A:234:GLN:CG	1:A:361:PRO:HG3	2.47	0.45
1:A:126:PHE:HZ	5:A:589:OAA:H21	1.81	0.45
1:A:255:GLU:CG	1:A:286:ARG:HH22	2.30	0.45
1:A:320:LYS:O	1:A:324:GLU:HG3	2.17	0.45
1:A:184:CYS:O	1:A:188:GLY:N	2.48	0.45
2:B:127:ASN:N	2:B:128:PRO:HD3	2.31	0.45
1:A:6:ARG:HD2	1:A:191:VAL:HG11	1.98	0.45
1:A:291:ARG:O	1:A:295:ILE:HG13	2.17	0.45
1:A:548:ARG:NH2	1:A:584:LYS:O	2.49	0.45
11:C:305:HEM:CAC	4:D:23:ALA:HB1	2.46	0.45
1:A:404:SER:O	1:A:407:ASP:HB3	2.16	0.45
2:B:5:PHE:HB2	2:B:23:TYR:HB2	1.98	0.45
2:B:9:ARG:NH1	2:B:49:LEU:HA	2.31	0.45
1:A:266:ASN:HD21	1:A:270:GLU:HB3	1.82	0.45
1:A:273:MET:HE3	1:A:292:SER:HB2	1.98	0.45
1:A:340:VAL:HG13	1:A:345:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:OG1	1:A:367:GLN:NE2	2.44	0.45
1:A:523:ALA:O	1:A:526:THR:HB	2.17	0.45
2:B:59:VAL:HG12	2:B:59:VAL:O	2.17	0.45
1:A:50:GLN:HA	1:A:139:ASP:O	2.17	0.45
1:A:534:THR:O	1:A:534:THR:CG2	2.56	0.45
2:B:84:GLN:OE1	2:B:87:LYS:HD2	2.16	0.45
2:B:201:PHE:CE2	4:D:81:THR:HG21	2.51	0.45
3:C:123:LEU:HB3	13:C:308:CDN:H521	1.99	0.45
1:A:61:HIS:NE2	1:A:131:ALA:CB	2.80	0.44
1:A:126:PHE:CZ	5:A:589:OAA:H21	2.53	0.44
1:A:494:LEU:HD23	1:A:520:MET:HG2	1.98	0.44
1:A:54:THR:HA	1:A:134:THR:HA	1.99	0.44
1:A:60:THR:HG23	1:A:123:SER:HB2	2.00	0.44
1:A:72:THR:HG22	1:A:400:LEU:HD23	1.98	0.44
1:A:463:LEU:HD22	1:A:520:MET:CE	2.47	0.44
1:A:555:CYS:CA	1:A:572:ASN:O	2.66	0.44
1:A:273:MET:CE	1:A:292:SER:CB	2.95	0.44
4:D:55:ALA:O	4:D:59:VAL:HG23	2.17	0.44
1:A:174:ASP:HB2	1:A:430:ARG:NH2	2.33	0.44
1:A:361:PRO:HA	1:A:391:CYS:O	2.17	0.44
1:A:476:GLU:O	1:A:479:ALA:HB3	2.17	0.44
1:A:586:ARG:HG2	15:A:645:HOH:O	2.17	0.44
2:B:75:CYS:SG	2:B:76:ILE:HG23	2.57	0.44
1:A:213:THR:HG23	1:A:353:CYS:O	2.17	0.44
1:A:411:PHE:HA	1:A:414:ALA:HB3	1.98	0.44
1:A:491:ARG:NH1	1:A:524:TYR:CE2	2.86	0.44
1:A:236:MET:HA	1:A:236:MET:CE	2.35	0.44
1:A:268:HIS:NE2	1:A:301:ARG:HD2	2.33	0.44
1:A:436:ASP:OD1	1:A:436:ASP:N	2.49	0.44
1:A:503:SER:O	1:A:510:ARG:NH2	2.51	0.44
1:A:76:SER:O	1:A:77:ASP:CB	2.65	0.44
1:A:234:GLN:HG3	1:A:361:PRO:HG3	1.98	0.44
1:A:71:ASP:HB3	1:A:128:GLY:O	2.18	0.43
1:A:242:HIS:HE1	5:A:589:OAA:H22	1.83	0.43
1:A:545:PHE:CD1	1:A:545:PHE:N	2.86	0.43
2:B:35:LEU:HD23	2:B:67:MET:HE1	2.00	0.43
2:B:155:CYS:SG	2:B:156:SER:N	2.91	0.43
1:A:97:LEU:CD1	2:B:131:ARG:HB3	2.48	0.43
1:A:529:SER:OG	1:A:569:ARG:NH2	2.52	0.43
1:A:537:ARG:HH21	1:A:548:ARG:CD	2.31	0.43
2:B:34:MET:HE3	2:B:78:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PHE:CE2	1:A:480:MET:HG3	2.54	0.43
3:C:9:ARG:HA	3:C:10:PRO:HD3	1.73	0.43
1:A:549:ASP:CG	1:A:552:ASN:HB2	2.39	0.43
2:B:9:ARG:HH12	2:B:49:LEU:HB2	1.84	0.43
2:B:34:MET:CE	2:B:78:PRO:HA	2.48	0.43
1:A:168:ASP:HB3	15:A:623:HOH:O	2.18	0.43
1:A:453:GLY:CA	1:A:496:ASN:O	2.64	0.43
1:A:477:GLY:HA2	1:A:542:ARG:NH2	2.34	0.43
2:B:82:LEU:N	2:B:82:LEU:CD1	2.82	0.43
1:A:252:LEU:HB3	7:A:601:FAD:HM73	2.01	0.43
1:A:479:ALA:O	1:A:480:MET:C	2.55	0.43
7:A:601:FAD:H9	7:A:601:FAD:H1'1	1.78	0.43
4:D:48:TRP:HA	4:D:48:TRP:CE3	2.53	0.43
1:A:99:LEU:HD11	1:A:409:VAL:HG21	2.01	0.43
1:A:320:LYS:HE3	1:A:324:GLU:OE2	2.19	0.43
1:A:535:GLU:OE1	1:A:549:ASP:N	2.52	0.43
2:B:220:LEU:HD12	9:B:303:SF4:S4	2.59	0.43
3:C:89:ILE:HG22	3:C:93:MET:HE3	2.01	0.43
1:A:49:ALA:HB3	1:A:142:GLY:CA	2.45	0.43
1:A:263:TYR:CZ	1:A:271:ARG:NH2	2.87	0.43
1:A:286:ARG:NE	15:A:614:HOH:O	2.52	0.43
2:B:209:ILE:HD13	12:C:306:DNT:O61	2.19	0.43
1:A:13:ILE:HB	1:A:200:LEU:HD23	2.01	0.42
1:A:242:HIS:HA	1:A:243:PRO:HD3	1.83	0.42
1:A:477:GLY:CA	1:A:542:ARG:NH2	2.82	0.42
1:A:483:GLY:HA2	1:A:486:GLN:HE21	1.84	0.42
2:B:236:ARG:C	2:B:237:ASN:ND2	2.70	0.42
1:A:41:PRO:O	1:A:146:LEU:HD21	2.17	0.42
1:A:104:LEU:HD12	1:A:105:PRO:CD	2.48	0.42
1:A:433:SER:C	1:A:435:SER:N	2.71	0.42
1:A:1:MET:CA	1:A:434:GLU:OE2	2.67	0.42
1:A:286:ARG:HB2	1:A:398:ASN:HD21	1.83	0.42
2:B:43:LYS:HG3	2:B:49:LEU:O	2.19	0.42
2:B:140:ARG:HD3	2:B:140:ARG:C	2.39	0.42
3:C:107:LYS:HB3	3:C:107:LYS:HE2	1.74	0.42
4:D:9:GLY:CA	4:D:14:HIS:HD2	2.25	0.42
1:A:177:VAL:CG2	1:A:383:LEU:HB2	2.45	0.42
1:A:560:LEU:HD23	1:A:568:ARG:HD3	2.01	0.42
2:B:205:ARG:NH2	4:D:81:THR:HB	2.32	0.42
1:A:208:ILE:HG13	1:A:209:TYR:HD1	1.83	0.42
1:A:554:LEU:HD12	1:A:554:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:THR:O	3:C:17:THR:HG22	2.18	0.42
1:A:357:MET:HE2	1:A:357:MET:H	1.75	0.42
1:A:471:PHE:CE2	1:A:527:ALA:HA	2.55	0.42
2:B:9:ARG:HH11	2:B:49:LEU:CD1	2.32	0.42
3:C:114:PHE:O	3:C:118:VAL:HG23	2.20	0.42
1:A:555:CYS:HA	1:A:572:ASN:O	2.20	0.42
1:A:118:PRO:O	1:A:120:GLY:N	2.50	0.42
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.78	0.42
1:A:480:MET:HG2	1:A:531:ASN:HA	2.02	0.42
2:B:54:SER:O	2:B:56:ARG:N	2.53	0.42
2:B:215:VAL:O	2:B:217:PRO:HD3	2.20	0.42
1:A:273:MET:HE3	1:A:292:SER:CB	2.50	0.41
1:A:313:LEU:CD2	1:A:315:LEU:HD21	2.50	0.41
1:A:508:THR:HB	2:B:43:LYS:NZ	2.35	0.41
2:B:9:ARG:NH1	2:B:49:LEU:HB2	2.35	0.41
2:B:59:VAL:N	8:B:302:FES:S2	2.93	0.41
1:A:572:ASN:ND2	1:A:573:MET:N	2.66	0.41
2:B:201:PHE:HA	2:B:205:ARG:HG2	2.02	0.41
1:A:24:LEU:HD11	1:A:156:ASN:ND2	2.36	0.41
1:A:314:LYS:HZ1	1:A:317:HIS:HB3	1.85	0.41
1:A:355:TYR:CD2	1:A:399:ARG:HD3	2.55	0.41
1:A:586:ARG:O	1:A:586:ARG:HG3	2.20	0.41
4:D:52:PHE:C	4:D:54:SER:N	2.72	0.41
1:A:277:ALA:O	1:A:279:ASN:N	2.53	0.41
1:A:303:CYS:O	1:A:309:PRO:HA	2.20	0.41
1:A:314:LYS:O	1:A:315:LEU:HD23	2.20	0.41
1:A:399:ARG:NH1	1:A:399:ARG:HG2	2.35	0.41
1:A:480:MET:HG2	1:A:531:ASN:CA	2.50	0.41
1:A:333:LEU:HG	15:A:613:HOH:O	2.19	0.41
1:A:463:LEU:HD11	1:A:523:ALA:CB	2.51	0.41
2:B:54:SER:HB3	2:B:60:CYS:SG	2.60	0.41
11:C:305:HEM:CAB	13:C:308:CDN:H241	2.50	0.41
1:A:76:SER:O	1:A:79:ILE:HG22	2.21	0.41
1:A:125:ASN:OD1	1:A:132:ALA:HB2	2.20	0.41
1:A:209:TYR:O	1:A:464:GLN:NE2	2.33	0.41
1:A:293:ILE:HD12	1:A:351:PRO:HD3	2.02	0.41
2:B:71:ASN:OD1	2:B:94:LEU:CD2	2.68	0.41
3:C:127:LEU:HB2	13:C:308:CDN:H512	2.02	0.41
1:A:42:THR:O	1:A:47:VAL:CG1	2.59	0.41
1:A:47:VAL:CG1	1:A:146:LEU:HD23	2.51	0.41
1:A:52:GLY:HA2	1:A:141:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ASP:OD1	1:A:552:ASN:HB2	2.20	0.41
1:A:579:PRO:O	1:A:580:ALA:CB	2.68	0.41
2:B:211:ASN:O	2:B:214:SER:HB3	2.20	0.41
1:A:8:PHE:CZ	1:A:34:ALA:HB2	2.55	0.41
1:A:50:GLN:O	1:A:51:GLY:C	2.58	0.41
1:A:164:TRP:CH2	1:A:184:CYS:HB2	2.56	0.41
1:A:246:ILE:HB	1:A:249:ALA:HB3	2.02	0.41
1:A:475:ARG:O	1:A:542:ARG:HA	2.21	0.41
4:D:52:PHE:C	4:D:54:SER:H	2.24	0.41
4:D:101:LEU:HD23	4:D:101:LEU:HA	1.92	0.41
1:A:258:ARG:HA	1:A:262:GLY:H	1.85	0.41
1:A:460:ARG:O	1:A:463:LEU:HB3	2.21	0.41
1:A:582:PRO:HA	1:A:583:PRO:HD3	1.89	0.41
2:B:218:LYS:HB2	2:B:220:LEU:HG	2.02	0.41
3:C:6:LYS:CG	3:C:7:LYS:N	2.68	0.41
1:A:455:ASP:OD1	1:A:457:VAL:HG23	2.21	0.41
1:A:513:CYS:O	1:A:516:LEU:HB3	2.21	0.41
2:B:36:LEU:O	2:B:40:ILE:HG13	2.20	0.41
2:B:95:PRO:CD	2:B:157:THR:HG22	2.40	0.41
2:B:126:GLN:O	2:B:127:ASN:HB2	2.21	0.41
3:C:54:SER:HB2	3:C:55:PRO:HD2	2.03	0.41
1:A:265:LEU:HD21	1:A:271:ARG:HG2	2.00	0.40
2:B:52:ARG:CZ	2:B:104:VAL:HG13	2.51	0.40
2:B:160:PRO:HA	2:B:163:TRP:CE3	2.56	0.40
1:A:49:ALA:HA	7:A:601:FAD:C6	2.50	0.40
1:A:145:LEU:C	1:A:145:LEU:HD23	2.42	0.40
1:A:226:ALA:HB2	1:A:360:ILE:HD11	2.04	0.40
1:A:544:ASP:OD1	1:A:544:ASP:N	2.54	0.40
2:B:143:LEU:N	2:B:143:LEU:CD1	2.85	0.40
3:C:24:ALA:HB1	12:C:306:DNT:O41	2.20	0.40
1:A:78:TYR:CD1	1:A:78:TYR:N	2.89	0.40
1:A:104:LEU:HA	1:A:105:PRO:HD3	1.85	0.40
1:A:147:HIS:O	1:A:151:GLN:HG3	2.21	0.40
1:A:256:GLY:O	1:A:260:GLU:N	2.50	0.40
1:A:577:LEU:HD11	1:A:580:ALA:C	2.42	0.40
2:B:9:ARG:HE	2:B:9:ARG:HB3	1.75	0.40
3:C:49:GLY:HA3	4:D:107:TYR:OH	2.21	0.40
1:A:47:VAL:HG13	1:A:146:LEU:HD23	2.02	0.40
1:A:87:TYR:CD1	1:A:87:TYR:C	2.95	0.40
1:A:124:LYS:N	1:A:134:THR:O	2.42	0.40
1:A:254:THR:HG21	1:A:327:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:O	1:A:393:SER:CB	2.69	0.40
1:A:577:LEU:HD21	1:A:580:ALA:HA	2.02	0.40
2:B:55:CYS:O	2:B:56:ARG:HB3	2.19	0.40
3:C:126:VAL:HG11	13:C:308:CDN:OB9	2.22	0.40
1:A:320:LYS:O	1:A:320:LYS:HG2	2.22	0.40
1:A:399:ARG:HD2	1:A:404:SER:HB2	2.03	0.40
1:A:491:ARG:O	1:A:495:LYS:HG3	2.21	0.40
1:A:559:TYR:OH	1:A:567:THR:CG2	2.69	0.40
2:B:1:MET:HB3	2:B:2:ARG:H	1.76	0.40
2:B:29:GLU:O	2:B:29:GLU:HG3	2.22	0.40
2:B:121:LEU:O	2:B:122:LEU:HD23	2.21	0.40
2:B:211:ASN:ND2	3:C:21:PRO:HD2	2.36	0.40
3:C:99:LEU:HD23	3:C:99:LEU:HA	1.93	0.40
3:C:111:LYS:HE2	14:C:309:EPH:H381	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	586/588 (100%)	503 (86%)	69 (12%)	14 (2%)	6 22
2	B	236/238 (99%)	209 (89%)	22 (9%)	5 (2%)	7 26
3	C	127/129 (98%)	115 (91%)	9 (7%)	3 (2%)	6 22
4	D	111/115 (96%)	109 (98%)	2 (2%)	0	100 100
All	All	1060/1070 (99%)	936 (88%)	102 (10%)	22 (2%)	7 26

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	GLY

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Mol	Chain	Res	Type
1	A	77	ASP
1	A	110	ASP
1	A	119	PHE
1	A	278	PRO
3	C	7	LYS
1	A	505	GLU
1	A	538	GLY
2	B	54	SER
1	A	218	ASN
1	A	393	SER
1	A	578	ARG
1	A	584	LYS
2	B	124	ASN
3	C	97	GLY
1	A	309	PRO
2	B	55	CYS
2	B	119	PRO
2	B	30	GLY
3	C	2	ILE
1	A	105	PRO
1	A	348	PRO

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	473/473 (100%)	450 (95%)	23 (5%)	25 57
2	B	208/208 (100%)	203 (98%)	5 (2%)	49 79
3	C	109/109 (100%)	104 (95%)	5 (5%)	27 60
4	D	94/96 (98%)	90 (96%)	4 (4%)	29 62
All	All	884/886 (100%)	847 (96%)	37 (4%)	30 63

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	TRP
1	A	122	GLN
1	A	172	ASN
1	A	207	ARG
1	A	235	ASP
1	A	278	PRO
1	A	326	ARG
1	A	357	MET
1	A	371	VAL
1	A	377	ASP
1	A	381	PRO
1	A	436	ASP
1	A	446	ARG
1	A	478	ASP
1	A	480	MET
1	A	506	PHE
1	A	524	TYR
1	A	544	ASP
1	A	568	ARG
1	A	569	ARG
1	A	572	ASN
1	A	573	MET
1	A	581	PHE
2	B	34	MET
2	B	53	ARG
2	B	85	PRO
2	B	137	PRO
2	B	180	ARG
3	C	4	ASN
3	C	28	ILE
3	C	51	SER
3	C	101	GLU
3	C	129	TRP
4	D	6	SER
4	D	8	LEU
4	D	42	GLU
4	D	60	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	147	HIS

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Mol	Chain	Res	Type
1	A	153	ASN
1	A	172	ASN
1	A	210	GLN
1	A	218	ASN
1	A	242	HIS
1	A	367	GLN
1	A	398	ASN
1	A	403	ASN
1	A	420	GLN
1	A	445	ASN
1	A	470	ASN
1	A	486	GLN
1	A	540	HIS
1	A	572	ASN
2	B	123	ASN
2	B	133	HIS
2	B	135	GLN
2	B	211	ASN
2	B	237	ASN
3	C	4	ASN
3	C	30	HIS
4	D	14	HIS
4	D	78	GLN
4	D	94	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	F3S	B	304	2	0,9,9	-	-	-		
11	HEM	C	305	3,4	41,50,50	1.40	5 (12%)	45,82,82	2.03	13 (28%)
9	SF4	B	303	2	0,12,12	-	-	-		
5	OAA	A	589	-	8,8,8	4.54	4 (50%)	9,10,10	1.77	1 (11%)
8	FES	B	302	2	0,4,4	-	-	-		
13	CDN	C	308	-	76,76,76	2.14	8 (10%)	78,88,88	1.94	4 (5%)
12	DNT	C	306	-	18,20,20	5.22	12 (66%)	19,27,27	2.55	5 (26%)
7	FAD	A	601	1	53,58,58	2.36	14 (26%)	68,89,89	1.32	7 (10%)
14	EPH	C	309	-	34,34,48	1.18	3 (8%)	37,39,53	0.96	1 (2%)

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
10	F3S	B	304	2	-	-	0/3/3/3
11	HEM	C	305	3,4	-	5/12/54/54	-
9	SF4	B	303	2	-	-	0/6/5/5
5	OAA	A	589	-	-	2/8/8/8	-
8	FES	B	302	2	-	-	0/1/1/1
13	CDN	C	308	-	3/3/9/9	26/87/87/87	-
12	DNT	C	306	-	1/1/3/3	1/13/17/17	0/1/1/1
7	FAD	A	601	1	-	3/30/50/50	0/6/6/6
14	EPH	C	309	-	-	9/38/38/52	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	589	OAA	C3-C4	-11.78	1.37	1.53
12	C	306	DNT	C2-N6	-10.32	1.26	1.45
12	C	306	DNT	C5-C4	8.59	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	306	DNT	C3-C4	8.44	1.53	1.39
7	A	601	FAD	C4X-N5	8.41	1.47	1.30
13	C	308	CDN	OB8-CB7	8.08	1.54	1.40
12	C	306	DNT	C1-C6	7.95	1.51	1.39
13	C	308	CDN	OA8-CA7	7.56	1.53	1.40
12	C	306	DNT	C4-N4	-7.22	1.27	1.45
13	C	308	CDN	OA9-CA7	-6.18	1.21	1.39
13	C	308	CDN	OB7-CB5	-6.18	1.21	1.39
13	C	308	CDN	OA6-CA5	-5.97	1.24	1.41
13	C	308	CDN	OB9-CB7	-5.94	1.22	1.39
7	A	601	FAD	C4A-N3A	5.92	1.43	1.35
7	A	601	FAD	C2A-N3A	5.88	1.41	1.32
12	C	306	DNT	C2-C1	5.86	1.53	1.40
7	A	601	FAD	C9A-N10	5.16	1.50	1.41
12	C	306	DNT	C8-C7	-5.11	1.37	1.52
13	C	308	CDN	OA7-CA5	4.57	1.51	1.39
11	C	305	HEM	CBB-CAB	4.31	1.51	1.30
13	C	308	CDN	OB6-CB5	4.05	1.53	1.41
12	C	306	DNT	O42-N6	4.05	1.29	1.22
12	C	306	DNT	O1-C1	-3.94	1.27	1.37
14	C	309	EPH	C25-C24	3.79	1.54	1.28
12	C	306	DNT	O41-N4	3.63	1.29	1.22
7	A	601	FAD	C9A-C5X	3.60	1.47	1.41
11	C	305	HEM	C4D-ND	-3.57	1.34	1.40
7	A	601	FAD	C5'-C4'	-3.57	1.46	1.51
7	A	601	FAD	C6-C7	3.54	1.44	1.39
7	A	601	FAD	C5A-C4A	-3.40	1.31	1.40
14	C	309	EPH	C12-C13	3.20	1.53	1.29
7	A	601	FAD	C10-N1	3.14	1.39	1.33
5	A	589	OAA	O4-C4	2.99	1.30	1.22
7	A	601	FAD	C5X-N5	2.70	1.44	1.39
7	A	601	FAD	C2B-C3B	-2.66	1.46	1.53
5	A	589	OAA	O3-C3	2.64	1.28	1.23
7	A	601	FAD	O4-C4	2.61	1.28	1.23
12	C	306	DNT	C9-C8	-2.60	1.41	1.52
11	C	305	HEM	FE-ND	2.55	2.09	1.96
11	C	305	HEM	C3C-C2C	-2.49	1.36	1.40
14	C	309	EPH	P1-O7	2.38	1.59	1.50
7	A	601	FAD	C8A-N7A	-2.32	1.30	1.34
7	A	601	FAD	C9-C9A	2.31	1.43	1.39
12	C	306	DNT	C3-C2	2.31	1.43	1.39
11	C	305	HEM	C4B-NB	-2.26	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	589	OAA	O2-C1	-2.01	1.24	1.30

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	308	CDN	OB7-CB5-C51	8.61	125.07	109.12
13	C	308	CDN	OB9-CB7-C71	8.47	124.81	109.12
13	C	308	CDN	OA9-CA7-C31	8.40	124.69	109.12
12	C	306	DNT	C9-C8-C7	7.26	129.39	114.79
12	C	306	DNT	C10-C7-C8	5.30	130.52	112.94
11	C	305	HEM	C4D-ND-C1D	5.17	110.42	105.07
11	C	305	HEM	C1B-NB-C4B	5.06	110.30	105.07
13	C	308	CDN	OA7-CA5-C11	4.59	117.63	109.12
7	A	601	FAD	C1'-N10-C9A	-4.55	112.93	120.51
11	C	305	HEM	CHC-C4B-NB	4.51	129.33	124.43
5	A	589	OAA	O3-C3-C2	4.00	126.37	120.58
12	C	306	DNT	C5-C4-N4	3.62	121.94	118.75
11	C	305	HEM	CHD-C1D-ND	3.50	128.24	124.43
11	C	305	HEM	C2C-C3C-C4C	3.33	109.23	106.90
11	C	305	HEM	CHA-C4D-ND	3.18	128.31	124.38
11	C	305	HEM	CHB-C1B-NB	3.17	128.30	124.38
7	A	601	FAD	C1'-C2'-C3'	3.10	118.44	109.79
12	C	306	DNT	O41-N4-C4	3.03	123.08	118.80
11	C	305	HEM	CBB-CAB-C3B	-2.94	113.00	127.62
11	C	305	HEM	CMC-C2C-C3C	2.81	129.94	124.68
12	C	306	DNT	C3-C2-C1	-2.69	118.96	122.51
7	A	601	FAD	O2B-C2B-C3B	2.61	120.28	111.82
7	A	601	FAD	N3A-C2A-N1A	-2.61	124.59	128.68
7	A	601	FAD	O4B-C1B-C2B	-2.42	103.39	106.93
11	C	305	HEM	C2D-C1D-ND	-2.32	107.10	109.88
7	A	601	FAD	C6-C5X-C9A	-2.24	115.76	118.94
7	A	601	FAD	C5X-C9A-N10	-2.23	115.66	117.95
11	C	305	HEM	C3C-C4C-NC	-2.14	106.91	110.94
11	C	305	HEM	CBA-CAA-C2A	2.12	116.24	112.62
14	C	309	EPH	C6-C5-C3	-2.12	105.92	113.62
11	C	305	HEM	C2B-C1B-NB	-2.01	107.45	109.84

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	306	DNT	C7
13	C	308	CDN	CB5

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Mol	Chain	Res	Type	Atom
13	C	308	CDN	CB7
13	C	308	CDN	CA7

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	589	OAA	O2-C1-C2-C3
11	C	305	HEM	C2B-C3B-CAB-CBB
11	C	305	HEM	C4B-C3B-CAB-CBB
13	C	308	CDN	CB2-OB2-PB2-OB3
13	C	308	CDN	CB2-OB2-PB2-OB4
13	C	308	CDN	OB7-CB5-OB6-CB4
13	C	308	CDN	C52-C51-CB5-OB7
13	C	308	CDN	OA7-CA5-OA6-CA4
11	C	305	HEM	C2A-CAA-CBA-CGA
13	C	308	CDN	CB2-OB2-PB2-OB5
13	C	308	CDN	C58-C59-C60-C61
13	C	308	CDN	C15-C16-C17-C18
13	C	308	CDN	C60-C61-C62-C63
13	C	308	CDN	C55-C56-C57-C58
14	C	309	EPH	C9-C10-C11-C12
14	C	309	EPH	C11-C10-C9-C8
13	C	308	CDN	CB3-CB4-CB6-OB8
13	C	308	CDN	C32-C31-CA7-OA8
5	A	589	OAA	O1-C1-C2-C3
14	C	309	EPH	O8-C38-C39-N1
12	C	306	DNT	C6-C7-C8-C9
13	C	308	CDN	C19-C20-C21-C22
13	C	308	CDN	C54-C55-C56-C57
13	C	308	CDN	C61-C62-C63-C64
14	C	309	EPH	C18-C19-C20-C21
13	C	308	CDN	C1-CB2-OB2-PB2
13	C	308	CDN	C72-C71-CB7-OB8
14	C	309	EPH	C11-C12-C13-C14
14	C	309	EPH	C37-O5-P1-O8
13	C	308	CDN	C31-CA7-OA8-CA6
13	C	308	CDN	OB6-CB4-CB6-OB8
13	C	308	CDN	CB3-OB5-PB2-OB2
13	C	308	CDN	CA3-OA5-PA1-OA2
13	C	308	CDN	CA2-OA2-PA1-OA5
7	A	601	FAD	P-O3P-PA-O1A
13	C	308	CDN	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
11	C	305	HEM	CAA-CBA-CGA-O1A
7	A	601	FAD	O4B-C4B-C5B-O5B
13	C	308	CDN	C35-C36-C37-C38
7	A	601	FAD	P-O3P-PA-O2A
13	C	308	CDN	C52-C51-CB5-OB6
11	C	305	HEM	CAA-CBA-CGA-O2A
14	C	309	EPH	C21-C22-C23-C24
14	C	309	EPH	C10-C11-C12-C13
13	C	308	CDN	CB2-C1-CA2-OA2
14	C	309	EPH	C19-C18-C4-O2

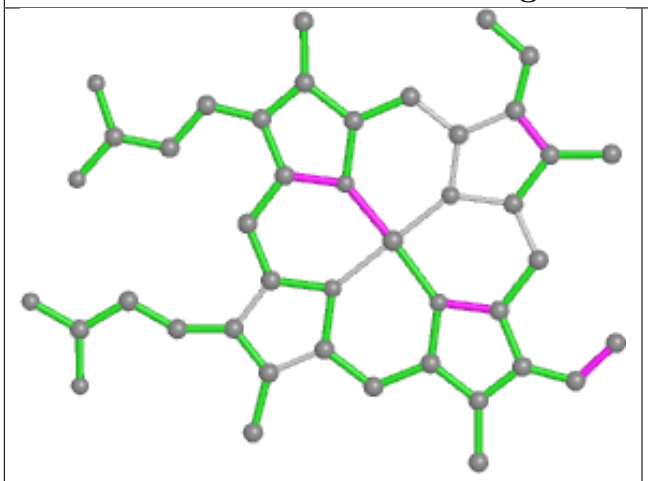
There are no ring outliers.

9 monomers are involved in 43 short contacts:

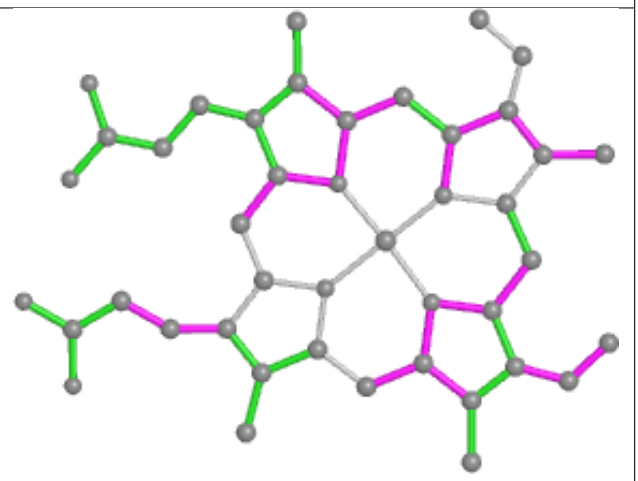
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	304	F3S	4	0
11	C	305	HEM	10	0
9	B	303	SF4	1	0
5	A	589	OAA	6	0
8	B	302	FES	3	0
13	C	308	CDN	13	0
12	C	306	DNT	3	0
7	A	601	FAD	8	0
14	C	309	EPH	2	0

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.

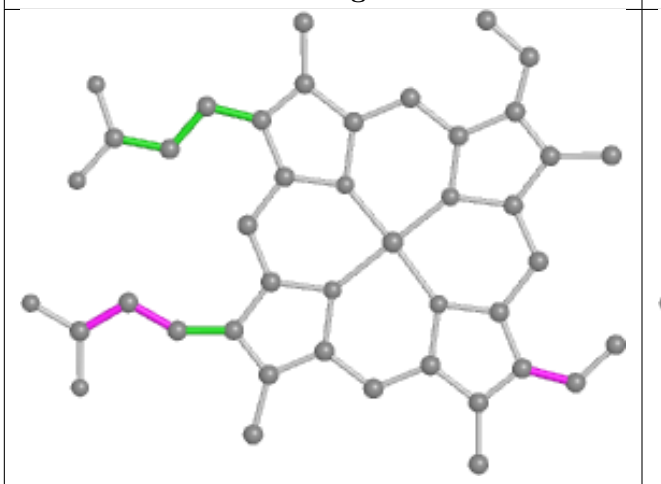
Ligand HEM C 305



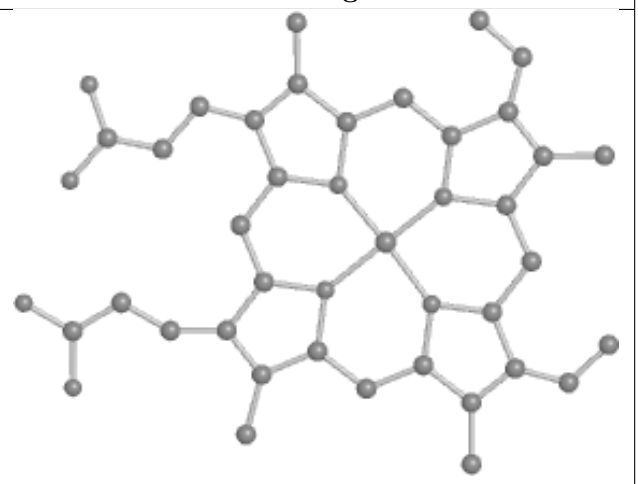
Bond lengths



Bond angles

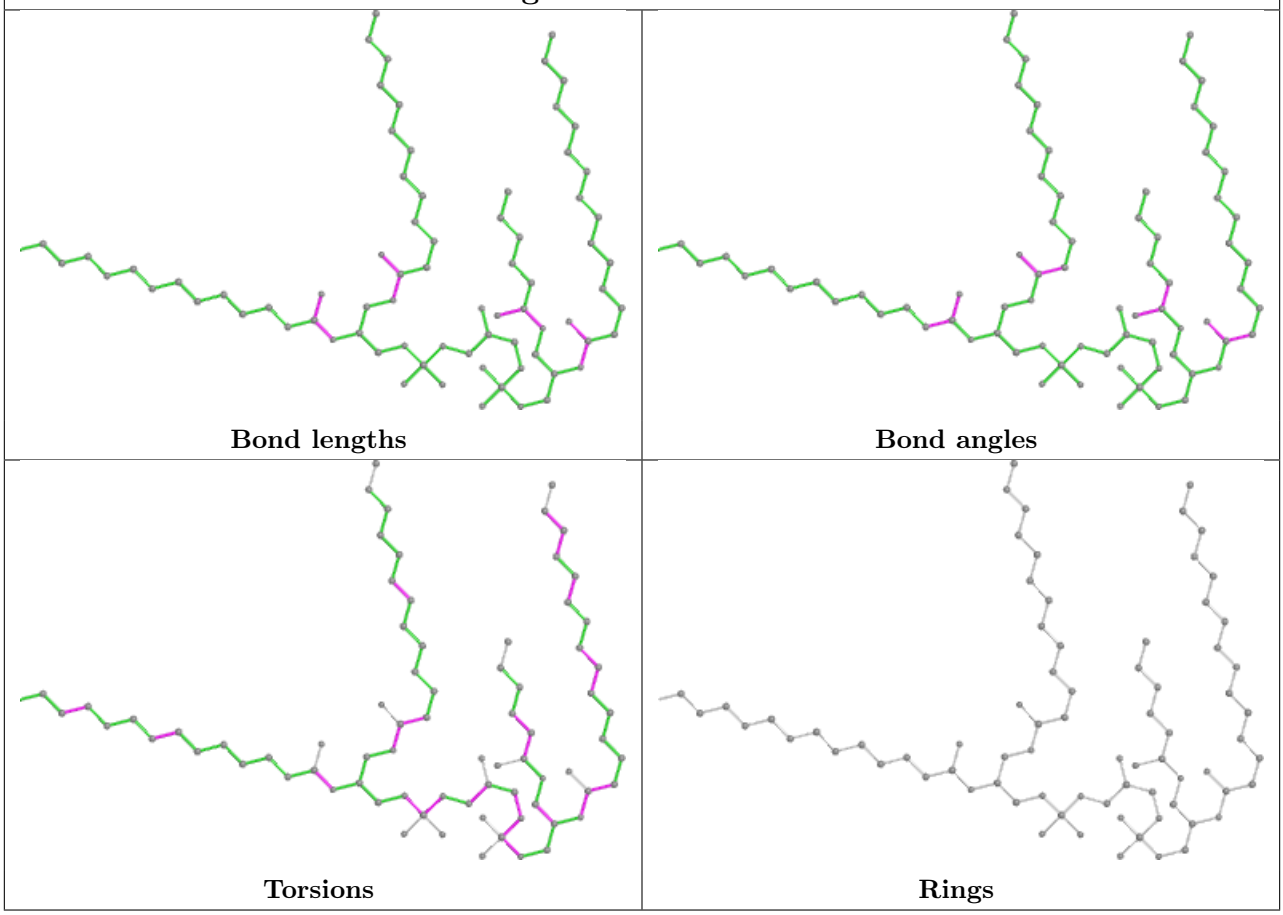


Torsions

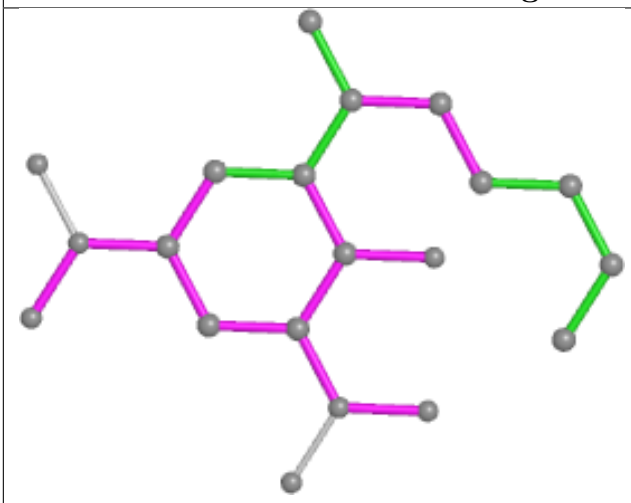


Rings

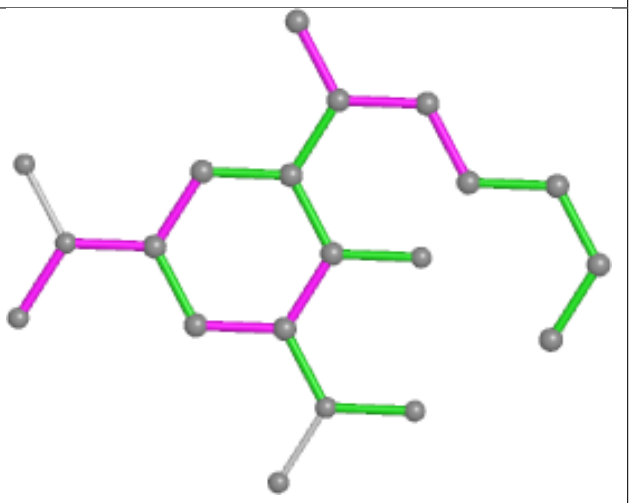
Ligand CDN C 308



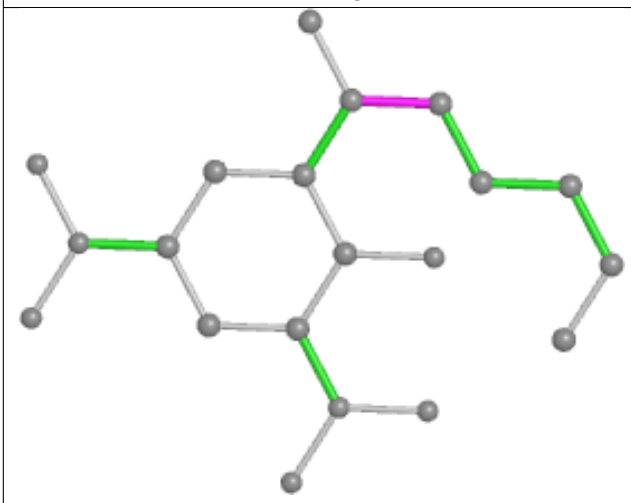
Ligand DNT C 306



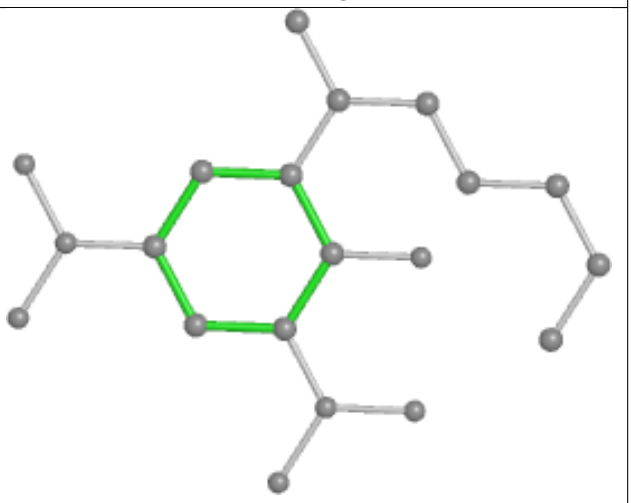
Bond lengths



Bond angles

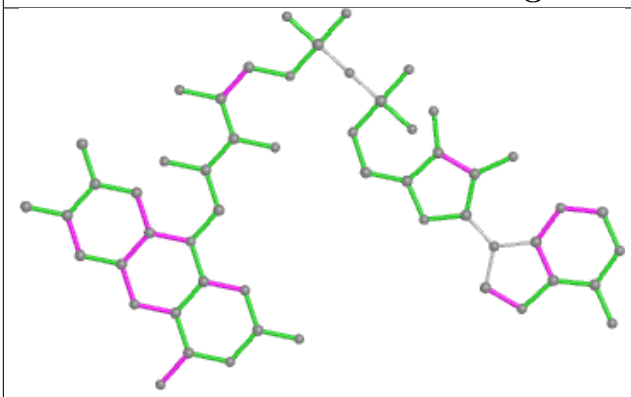


Torsions

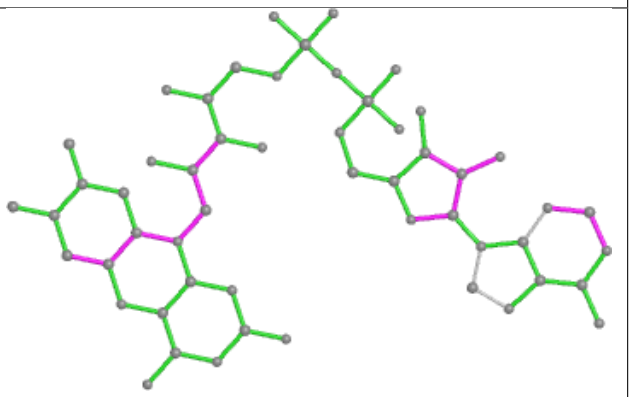


Rings

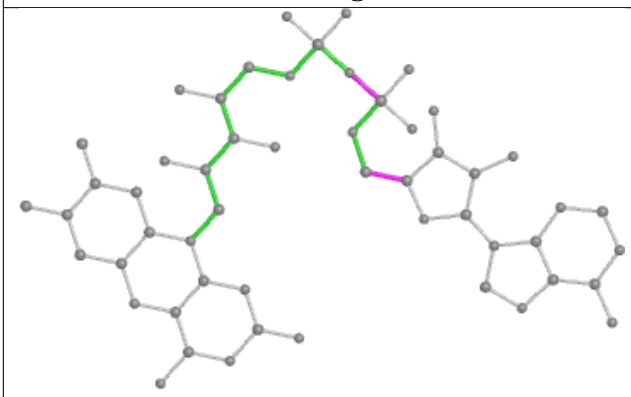
Ligand FAD A 601



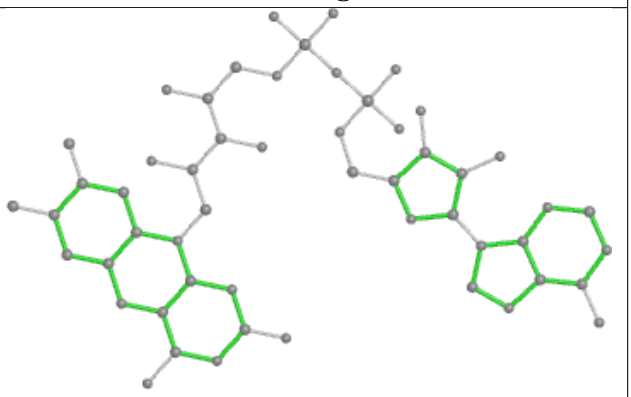
Bond lengths



Bond angles

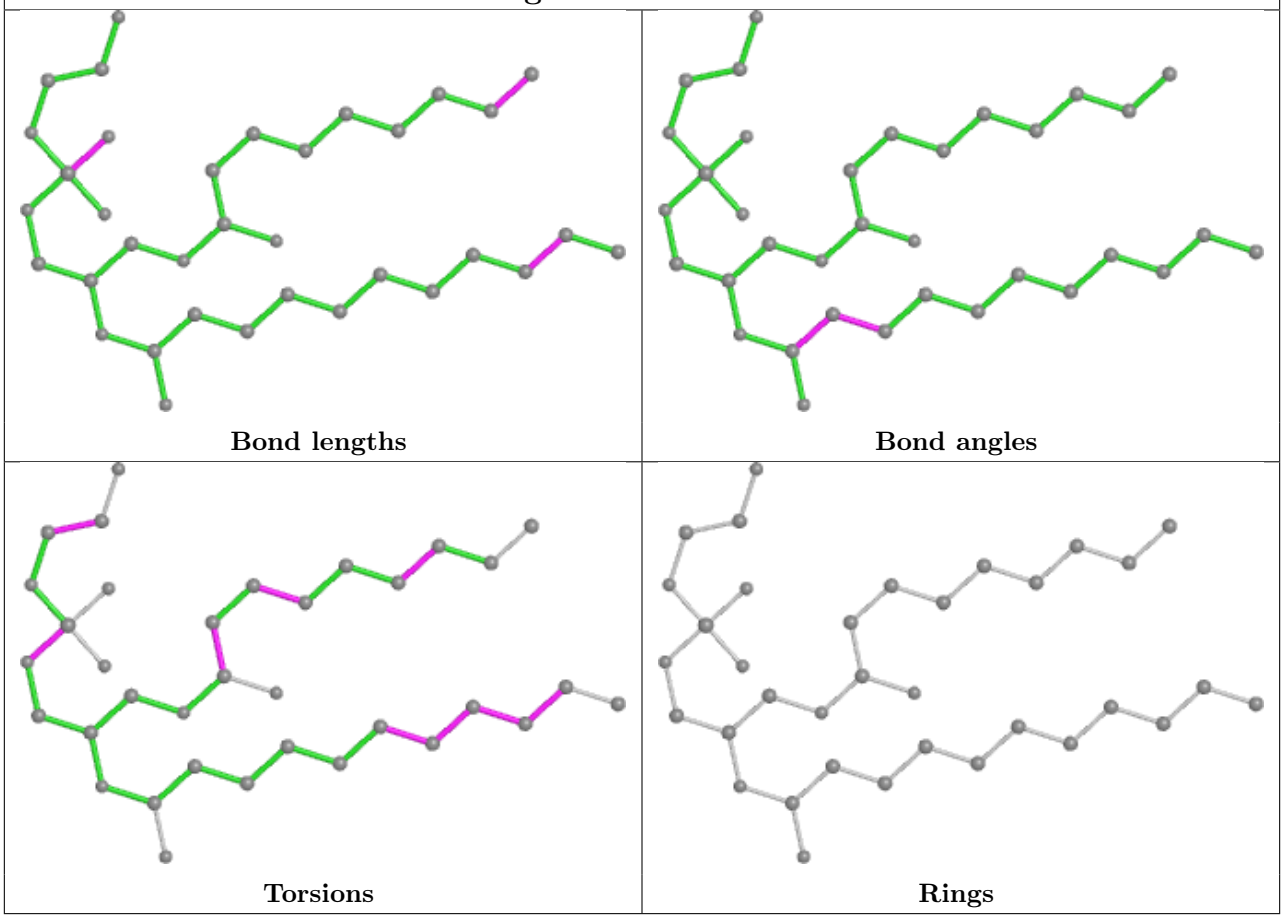


Torsions



Rings

Ligand EPH C 309



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.