Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:56 am BST

PDB ID	:	1NEK
Title	:	Complex II (Succinate Dehydrogenase) From E. Coli with ubiquinone bound
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	:	2.60 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:

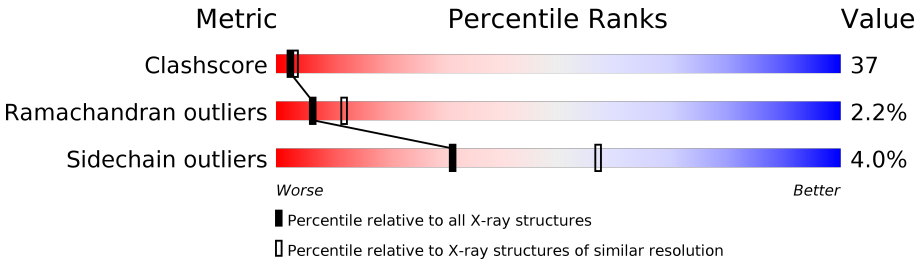
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	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 on 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	38% 57% 5%
2	B	238	54% 44% .
3	C	129	70% 29% .
4	D	115	63% 35% ..

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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CDN	C	308	X	-	-	-
8	FES	B	302	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 8698 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
1	A	588	Total	C	N	O	S	89	0	0
			4522	2812	821	861	28			

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

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

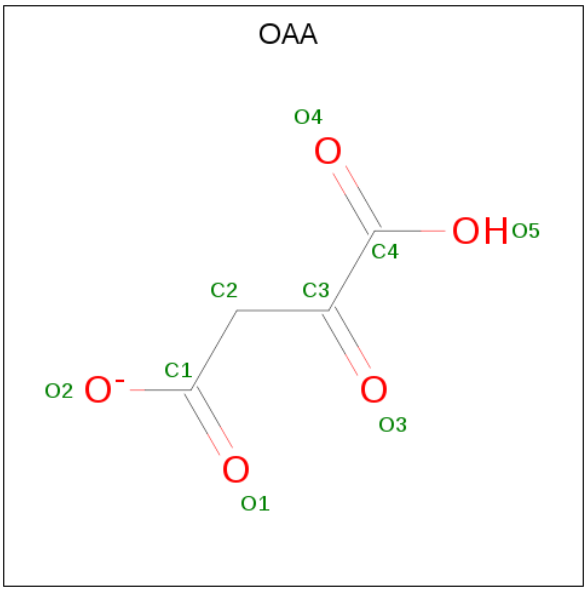
- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b-556 subunit.

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

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

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

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

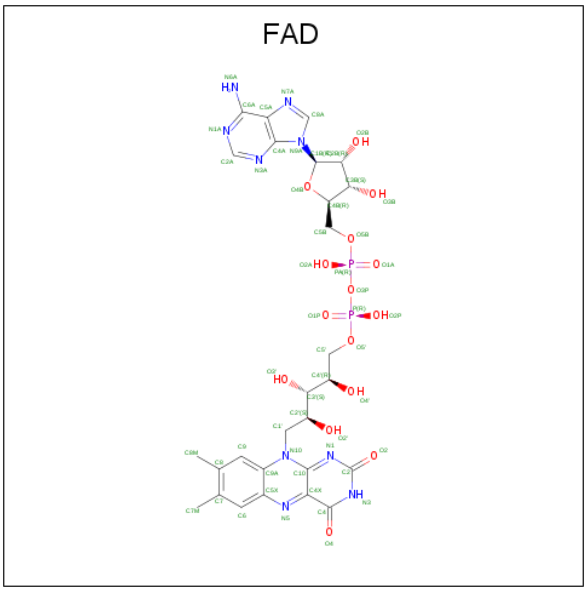


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 4 5	0	0

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

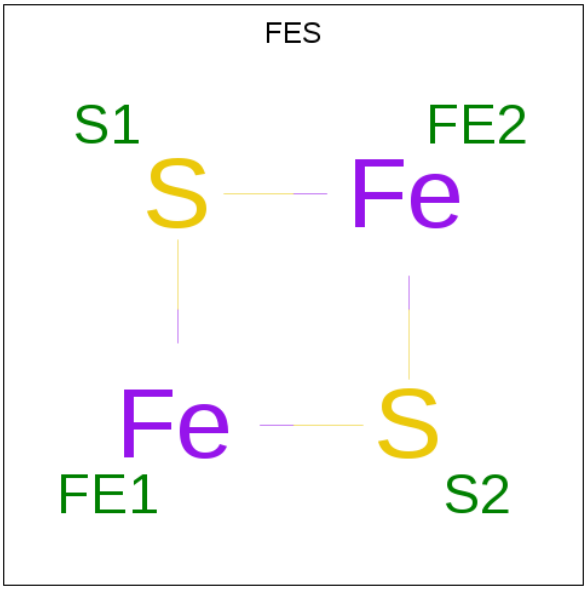
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0
6	A	1	Total Ca 1 1	0	0

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



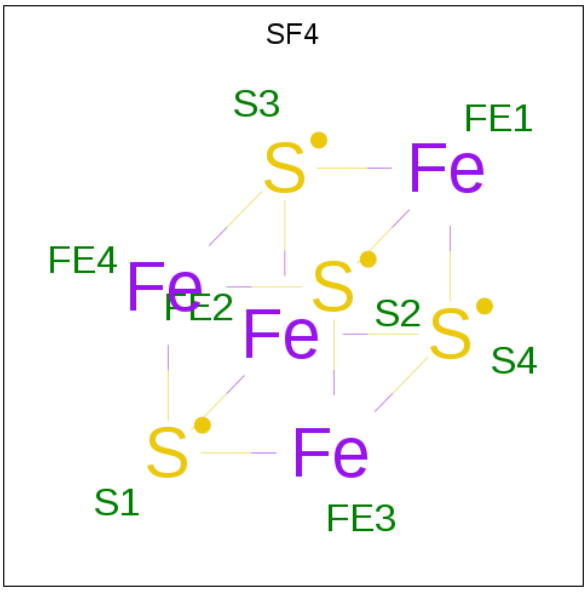
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



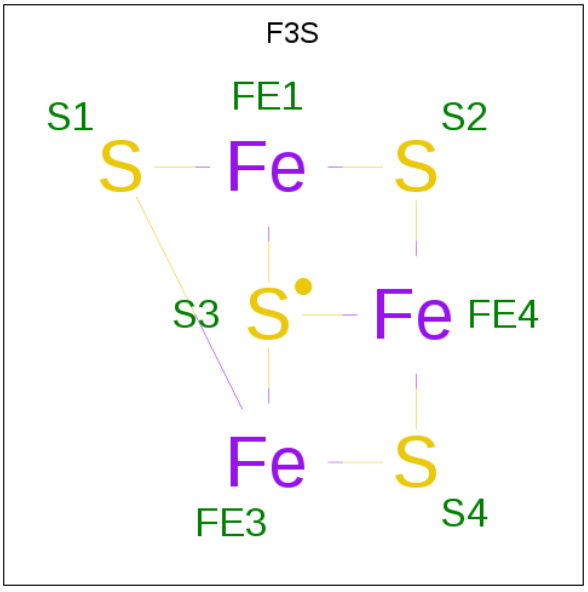
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			4	2	2		

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



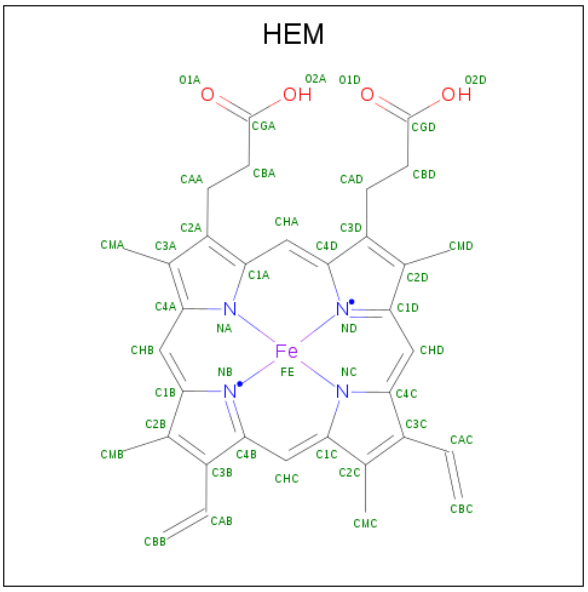
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 8 4 4	0	0

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



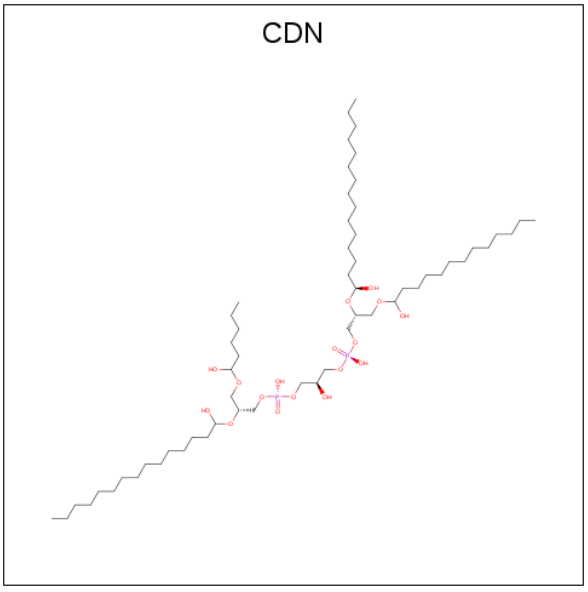
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Fe S 7 3 4	0	0

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



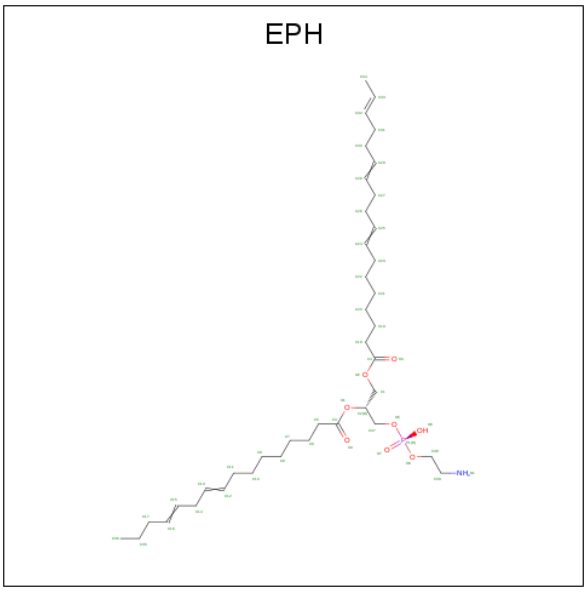
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 12 is CARDIOLIPIN (three-letter code: CDN) (formula: $C_{58}H_{120}O_{17}P_2$).



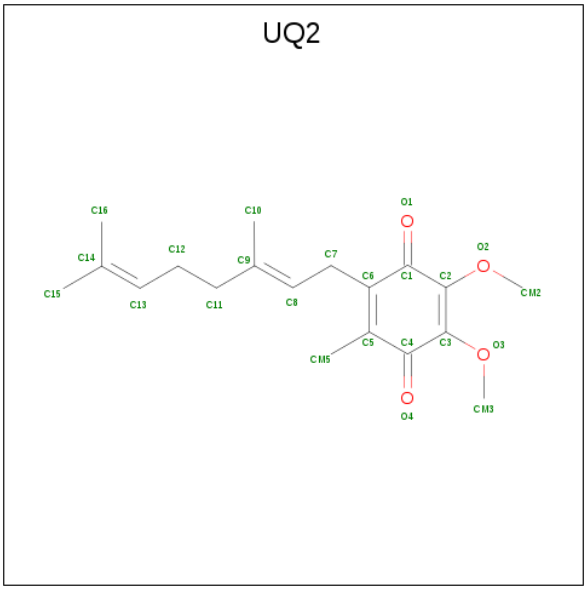
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	O	P	0	0
			77	58	17	2		

- Molecule 13 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
13	C	1	Total	C	N	O	P	0	0
			35	25	1	8	1		

- Molecule 14 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	C	O	0	0
			23	19	4		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	61	Total O 61 61	0	0
15	B	50	Total O 50 50	0	0
15	C	15	Total O 15 15	0	0
15	D	14	Total O 14 14	0	0

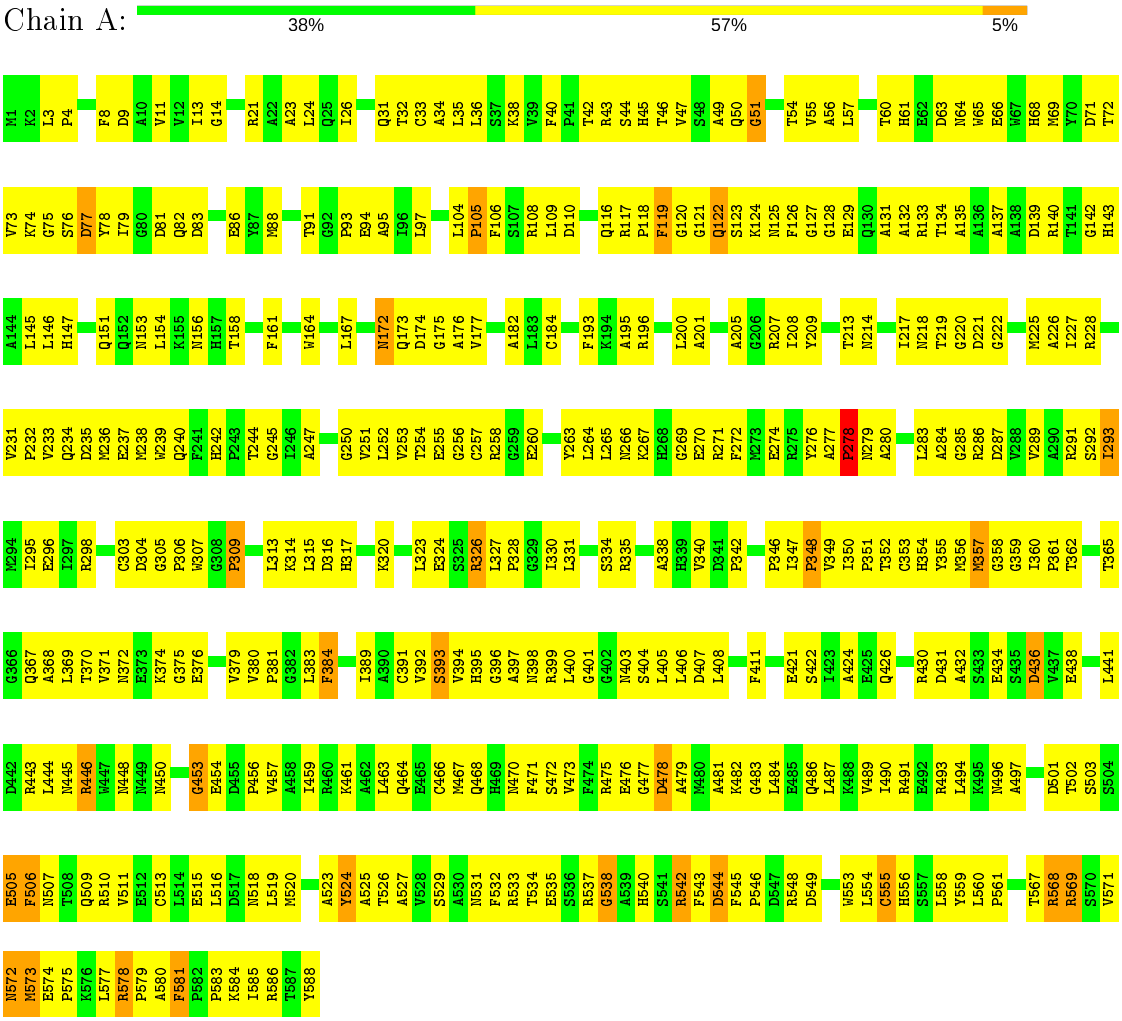
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

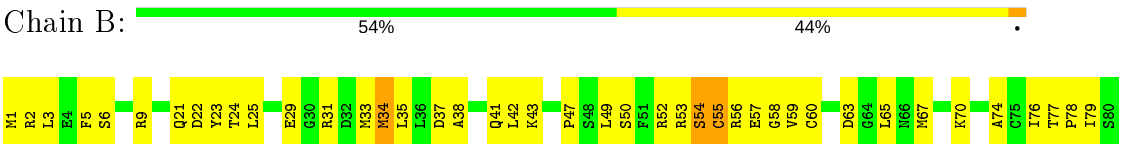
- Molecule 1: Succinate dehydrogenase flavoprotein subunit

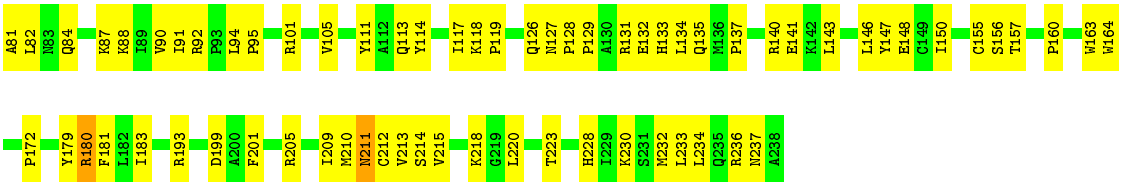
Chain A:



- Molecule 2: Succinate dehydrogenase iron-sulfur protein

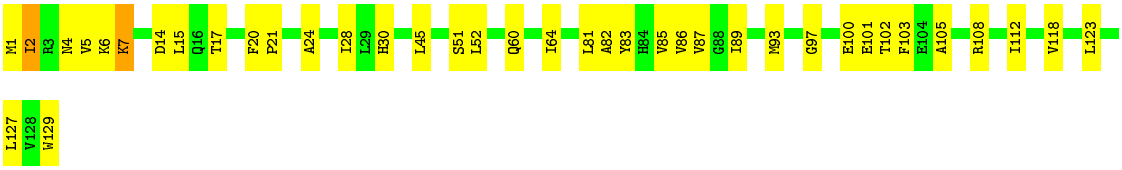
Chain B:





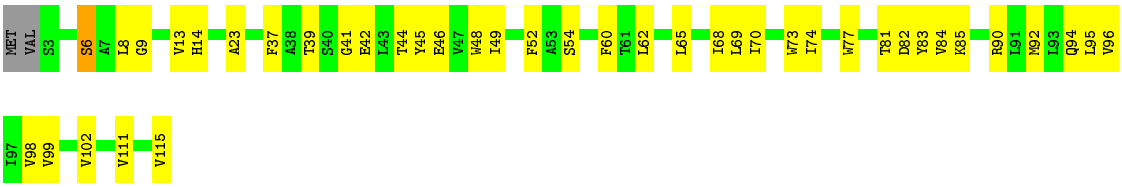
- Molecule 3: Succinate dehydrogenase cytochrome b-556 subunit

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 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8698	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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: SF4, OAA, CA, F3S, FES, EPH, HEM, UQ2, CDN, 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	0.36	0/4611	0.66	1/6237 (0.0%)
2	B	0.40	0/1908	0.64	0/2578
3	C	0.41	0/1030	0.63	0/1394
4	D	0.44	0/923	0.62	0/1262
All	All	0.38	0/8472	0.65	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	-5.09	100.37	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4522	0	4426	445	0
2	B	1869	0	1850	131	0
3	C	1008	0	1066	40	0
4	D	898	0	936	41	0
5	A	9	0	2	3	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	2	0
9	B	8	0	0	1	0
10	B	7	0	0	3	0
11	C	43	0	30	5	0
12	C	77	0	112	5	0
13	C	35	0	40	1	0
14	D	23	0	26	4	0
15	A	61	0	0	4	0
15	B	50	0	0	0	0
15	C	15	0	0	1	0
15	D	14	0	0	0	0
All	All	8698	0	8517	626	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 37.

All (626) 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:A:559:TYR:HB2	1:A:569:ARG:NH2	1.66	1.09
3:C:6:LYS:HG2	3:C:7:LYS:H	1.19	1.06
1:A:584:LYS:HG2	1:A:585:ILE:H	1.19	1.05
1:A:534:THR:HB	1:A:553:TRP:HE1	1.21	1.04
2:B:95:PRO:HD2	2:B:157:THR:HG22	1.38	1.04
2:B:92:ARG:HH11	3:C:17:THR:HG21	1.13	1.02
1:A:79:ILE:HD13	1:A:397:ALA:HB2	1.40	0.99
1:A:534:THR:HB	1:A:553:TRP:NE1	1.78	0.97
2:B:94:LEU:HB3	2:B:157:THR:HG21	1.44	0.97
1:A:172:ASN:HD21	1:A:430:ARG:HG3	1.33	0.93
2:B:223:THR:HG22	10:B:304:F3S:S1	2.09	0.93
4:D:6:SER:HB3	4:D:94:GLN:NE2	1.85	0.92
1:A:578:ARG:HB3	1:A:579:PRO:HD3	1.52	0.92
1:A:139:ASP:OD2	1:A:330:ILE:HG12	1.72	0.90
1:A:9:ASP:H	1:A:32:THR:HG23	1.38	0.89
2:B:140:ARG:HD3	2:B:140:ARG:O	1.73	0.89
1:A:242:HIS:O	1:A:351:PRO:HA	1.72	0.89
1:A:555:CYS:HB2	1:A:571:VAL:HG13	1.52	0.89
1:A:516:LEU:HA	1:A:519:LEU:HD12	1.56	0.88
2:B:77:THR:HG22	2:B:82:LEU:HD11	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:ARG:NH1	3:C:17:THR:HG21	1.89	0.88
4:D:9:GLY:HA2	4:D:14:HIS:HD2	1.37	0.88
2:B:25:LEU:HB2	2:B:42:LEU:HD21	1.56	0.87
1:A:126:PHE:HE2	1:A:401:GLY:HA3	1.38	0.86
1:A:126:PHE:O	1:A:283:LEU:HD11	1.76	0.86
1:A:9:ASP:OD2	1:A:32:THR:HG22	1.76	0.86
1:A:236:MET:HE3	1:A:236:MET:HA	1.56	0.85
4:D:6:SER:HB3	4:D:94:GLN:HE22	1.40	0.84
2:B:95:PRO:HD2	2:B:157:THR:CG2	2.08	0.84
1:A:233:VAL:HG11	1:A:236:MET:SD	2.18	0.83
3:C:51:SER:HB3	4:D:48:TRP:HE1	1.43	0.83
1:A:36:LEU:HD22	1:A:161:PHE:HB2	1.61	0.82
1:A:324:GLU:O	1:A:328:PRO:HG3	1.80	0.82
1:A:205:ALA:HB2	1:A:220:GLY:N	1.94	0.82
1:A:559:TYR:HB2	1:A:569:ARG:HH21	1.42	0.81
1:A:277:ALA:HB1	1:A:588:TYR:O	1.80	0.81
1:A:584:LYS:HG2	1:A:585:ILE:N	1.96	0.81
1:A:104:LEU:HD12	1:A:105:PRO:HD2	1.63	0.80
1:A:265:LEU:HD22	1:A:271:ARG:HG2	1.63	0.80
1:A:128:GLY:HA3	1:A:400:LEU:HD11	1.64	0.80
1:A:47:VAL:HG13	1:A:146:LEU:HD23	1.64	0.80
1:A:272:PHE:CZ	1:A:293:ILE:HG22	2.17	0.79
3:C:6:LYS:HE3	3:C:7:LYS:HG3	1.63	0.79
1:A:49:ALA:HB3	1:A:142:GLY:HA3	1.64	0.79
1:A:567:THR:O	1:A:568:ARG:HG3	1.82	0.78
1:A:254:THR:HA	5:A:589:OAA:O5	1.83	0.77
1:A:47:VAL:HG13	1:A:146:LEU:CD2	2.15	0.77
1:A:313:LEU:HD12	1:A:349:VAL:HG11	1.66	0.77
1:A:534:THR:CB	1:A:553:TRP:HE1	1.98	0.77
1:A:242:HIS:CD2	1:A:252:LEU:HD11	2.19	0.77
1:A:578:ARG:CB	1:A:579:PRO:HD3	2.14	0.76
1:A:126:PHE:CE2	1:A:401:GLY:HA3	2.21	0.76
1:A:42:THR:O	1:A:47:VAL:HG11	1.84	0.76
1:A:69:MET:O	1:A:73:VAL:HG23	1.86	0.76
1:A:245:GLY:HA3	1:A:352:THR:HG22	1.67	0.75
1:A:534:THR:HG22	1:A:534:THR:O	1.87	0.75
3:C:30:HIS:HD2	3:C:87:VAL:HB	1.52	0.75
1:A:272:PHE:CZ	1:A:293:ILE:CG2	2.70	0.74
2:B:77:THR:CG2	2:B:82:LEU:HD11	2.17	0.74
3:C:2:ILE:HG12	3:C:5:VAL:HB	1.70	0.74
1:A:127:GLY:HA3	1:A:255:GLU:OE2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:GLY:HA2	8:B:302:FES:S2	2.28	0.74
1:A:120:GLY:HA2	2:B:132:GLU:OE2	1.87	0.74
3:C:60:GLN:O	3:C:64:ILE:HG13	1.88	0.73
2:B:9:ARG:HH11	2:B:49:LEU:HD13	1.54	0.73
1:A:556:HIS:HB2	1:A:572:ASN:HB3	1.69	0.73
4:D:9:GLY:HA2	4:D:14:HIS:CD2	2.22	0.72
1:A:55:VAL:HG13	1:A:57:LEU:HG	1.71	0.72
3:C:30:HIS:CD2	3:C:87:VAL:HB	2.24	0.72
2:B:172:PRO:HG3	10:B:304:F3S:S3	2.29	0.72
1:A:453:GLY:HA3	1:A:496:ASN:O	1.89	0.71
1:A:395:HIS:ND1	1:A:399:ARG:HG3	2.04	0.71
2:B:34:MET:CE	2:B:34:MET:HA	2.20	0.71
1:A:77:ASP:OD2	1:A:586:ARG:NH1	2.20	0.71
1:A:172:ASN:ND2	1:A:430:ARG:HG3	2.06	0.71
1:A:392:VAL:HG13	1:A:394:VAL:HG13	1.73	0.71
1:A:463:LEU:O	1:A:467:MET:HG2	1.91	0.71
1:A:559:TYR:O	1:A:561:PRO:HD3	1.91	0.71
1:A:126:PHE:HE2	1:A:401:GLY:CA	2.04	0.70
2:B:146:LEU:CD1	2:B:183:ILE:HD11	2.21	0.70
1:A:147:HIS:O	1:A:151:GLN:HG3	1.92	0.69
1:A:482:LYS:O	1:A:486:GLN:HG3	1.92	0.69
1:A:240:GLN:N	1:A:357:MET:HE1	2.07	0.69
1:A:454:GLU:OE1	1:A:493:ARG:HG3	1.92	0.69
1:A:240:GLN:H	1:A:357:MET:HE1	1.57	0.69
1:A:293:ILE:HD11	1:A:351:PRO:HG3	1.75	0.69
3:C:6:LYS:CG	3:C:7:LYS:H	1.99	0.69
1:A:572:ASN:C	1:A:573:MET:HG3	2.12	0.69
1:A:446:ARG:NH2	1:A:497:ALA:O	2.24	0.68
1:A:221:ASP:HA	1:A:518:ASN:ND2	2.07	0.68
1:A:555:CYS:CB	1:A:571:VAL:HG13	2.23	0.68
1:A:245:GLY:HA3	1:A:352:THR:CG2	2.23	0.68
1:A:123:SER:HA	1:A:134:THR:O	1.91	0.68
1:A:139:ASP:O	1:A:139:ASP:OD1	2.10	0.68
1:A:255:GLU:HB2	1:A:286:ARG:HH22	1.57	0.68
1:A:291:ARG:NH2	1:A:538:GLY:O	2.27	0.68
2:B:164:TRP:HZ2	14:D:306:UQ2:H72	1.57	0.68
1:A:205:ALA:HB2	1:A:220:GLY:CA	2.22	0.68
2:B:94:LEU:HB3	2:B:157:THR:CG2	2.21	0.68
3:C:6:LYS:HG2	3:C:7:LYS:N	2.01	0.68
3:C:14:ASP:O	3:C:17:THR:HB	1.94	0.68
1:A:534:THR:HG23	1:A:545:PHE:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:C	1:A:117:ARG:O	2.32	0.67
1:A:47:VAL:CG1	1:A:146:LEU:HD23	2.23	0.67
1:A:537:ARG:HH21	1:A:548:ARG:CG	2.07	0.67
1:A:140:ARG:HH11	2:B:148:GLU:HG2	1.59	0.67
1:A:578:ARG:HB3	1:A:579:PRO:CD	2.25	0.67
1:A:280:ALA:HB3	1:A:588:TYR:O	1.94	0.67
1:A:285:GLY:O	1:A:289:VAL:HG23	1.95	0.67
1:A:323:LEU:HB3	1:A:331:LEU:HD21	1.76	0.67
1:A:454:GLU:OE2	1:A:493:ARG:NE	2.28	0.67
1:A:60:THR:CG2	1:A:123:SER:HB2	2.24	0.67
1:A:270:GLU:HG2	1:A:271:ARG:N	2.10	0.67
1:A:238:MET:HE3	1:A:397:ALA:HB1	1.77	0.66
1:A:520:MET:HE2	1:A:520:MET:HA	1.77	0.66
1:A:276:TYR:C	1:A:278:PRO:HD3	2.15	0.66
1:A:534:THR:HB	1:A:553:TRP:CD1	2.30	0.66
1:A:126:PHE:O	1:A:129:GLU:HG2	1.95	0.66
1:A:287:ASP:H	1:A:398:ASN:ND2	1.93	0.66
1:A:340:VAL:O	1:A:342:PRO:HD3	1.95	0.66
1:A:60:THR:HG21	1:A:123:SER:O	1.95	0.66
1:A:237:GLU:HB3	1:A:529:SER:HB2	1.77	0.66
1:A:571:VAL:HG12	1:A:572:ASN:N	2.11	0.66
2:B:65:LEU:HD12	2:B:74:ALA:HB2	1.77	0.65
1:A:537:ARG:HH21	1:A:548:ARG:HB2	1.61	0.65
1:A:237:GLU:OE1	1:A:529:SER:HB3	1.96	0.65
1:A:369:LEU:CD2	1:A:379:VAL:HG22	2.26	0.65
1:A:574:GLU:O	1:A:574:GLU:HG3	1.97	0.65
1:A:537:ARG:HA	1:A:586:ARG:HH12	1.60	0.65
2:B:37:ASP:O	2:B:41:GLN:HG2	1.97	0.65
1:A:255:GLU:CD	1:A:286:ARG:HH22	1.99	0.65
1:A:78:TYR:CD2	1:A:583:PRO:HA	2.32	0.65
2:B:1:MET:HG3	2:B:29:GLU:OE2	1.97	0.65
2:B:77:THR:HG22	2:B:82:LEU:CD1	2.24	0.65
3:C:2:ILE:CG1	3:C:5:VAL:HB	2.26	0.65
1:A:75:GLY:O	1:A:398:ASN:HB3	1.96	0.64
1:A:404:SER:O	1:A:407:ASP:HB3	1.97	0.64
1:A:251:VAL:HG13	2:B:57:GLU:OE1	1.96	0.64
1:A:537:ARG:HH12	1:A:554:LEU:HD13	1.62	0.64
1:A:129:GLU:O	1:A:283:LEU:HD21	1.98	0.64
4:D:92:MET:O	4:D:96:VAL:HG23	1.97	0.64
1:A:577:LEU:HD23	1:A:577:LEU:N	2.12	0.64
1:A:226:ALA:HB2	1:A:360:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:HIS:CE1	1:A:286:ARG:HH21	2.16	0.64
2:B:56:ARG:O	2:B:56:ARG:HG2	1.96	0.64
1:A:571:VAL:CG1	1:A:572:ASN:N	2.61	0.64
1:A:255:GLU:N	5:A:589:OAA:O4	2.25	0.64
2:B:129:PRO:HG2	2:B:133:HIS:CD2	2.34	0.63
1:A:63:ASP:OD1	1:A:64:ASN:N	2.31	0.63
4:D:98:VAL:O	4:D:102:VAL:HG23	1.99	0.63
1:A:529:SER:OG	1:A:569:ARG:NH2	2.31	0.63
1:A:239:TRP:CZ3	1:A:356:MET:HB2	2.33	0.63
1:A:252:LEU:HG	1:A:253:VAL:N	2.12	0.63
1:A:161:PHE:HB3	1:A:164:TRP:CD1	2.33	0.63
1:A:483:GLY:O	1:A:487:LEU:HD13	1.99	0.63
1:A:119:PHE:CD2	2:B:134:LEU:HD12	2.33	0.63
1:A:208:ILE:HG13	1:A:209:TYR:CD1	2.34	0.63
1:A:54:THR:OG1	1:A:403:ASN:ND2	2.32	0.63
2:B:1:MET:N	2:B:29:GLU:HB2	2.14	0.63
1:A:227:ILE:HG23	1:A:561:PRO:HB3	1.81	0.62
2:B:58:GLY:CA	8:B:302:FES:S2	2.87	0.62
1:A:23:ALA:HB2	1:A:35:LEU:HD13	1.80	0.62
1:A:119:PHE:HB2	2:B:135:GLN:H	1.64	0.62
11:C:305:HEM:HAC	4:D:23:ALA:HB1	1.81	0.62
1:A:544:ASP:HB2	1:A:545:PHE:CD1	2.35	0.62
2:B:25:LEU:HB2	2:B:42:LEU:CD2	2.27	0.62
1:A:255:GLU:HB2	1:A:286:ARG:NH2	2.14	0.62
4:D:39:THR:O	4:D:39:THR:HG22	1.98	0.62
1:A:584:LYS:CG	1:A:585:ILE:H	2.00	0.62
2:B:94:LEU:CB	2:B:157:THR:HG21	2.26	0.62
1:A:264:LEU:C	1:A:265:LEU:HD23	2.19	0.62
1:A:369:LEU:HD21	1:A:379:VAL:HG22	1.82	0.62
2:B:210:MET:HE2	3:C:103:PHE:HA	1.82	0.62
1:A:234:GLN:HB2	1:A:361:PRO:HG3	1.80	0.62
2:B:59:VAL:HG12	2:B:59:VAL:O	1.99	0.62
1:A:559:TYR:CB	1:A:569:ARG:NH2	2.55	0.61
1:A:76:SER:O	1:A:79:ILE:HG22	2.00	0.61
4:D:6:SER:HB2	4:D:77:TRP:CD1	2.35	0.61
1:A:265:LEU:CD2	1:A:271:ARG:HG2	2.30	0.61
1:A:272:PHE:HZ	1:A:293:ILE:CG2	2.11	0.61
1:A:38:LYS:CE	1:A:217:ILE:HG23	2.30	0.61
1:A:369:LEU:HD23	1:A:379:VAL:HA	1.82	0.61
1:A:572:ASN:ND2	1:A:573:MET:H	1.99	0.61
1:A:173:GLN:HB3	1:A:430:ARG:HE	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:THR:HG22	1:A:368:ALA:HA	1.81	0.61
1:A:79:ILE:HG23	1:A:396:GLY:HA3	1.83	0.61
1:A:79:ILE:HG21	1:A:397:ALA:CB	2.31	0.61
1:A:72:THR:HA	1:A:400:LEU:HD22	1.81	0.61
1:A:213:THR:HA	1:A:250:GLY:O	2.01	0.60
1:A:124:LYS:HE2	1:A:260:GLU:OE2	2.02	0.60
1:A:531:ASN:O	1:A:542:ARG:NH1	2.34	0.60
1:A:9:ASP:CG	1:A:32:THR:HG22	2.21	0.60
2:B:164:TRP:CZ2	14:D:306:UQ2:H72	2.36	0.60
2:B:34:MET:HA	2:B:34:MET:HE2	1.82	0.60
1:A:434:GLU:O	1:A:438:GLU:HB2	2.01	0.60
1:A:560:LEU:HB3	1:A:568:ARG:HB2	1.83	0.60
2:B:35:LEU:HD11	2:B:91:ILE:HD11	1.84	0.59
1:A:213:THR:HG23	1:A:353:CYS:O	2.02	0.59
1:A:511:VAL:O	1:A:515:GLU:HG3	2.03	0.59
1:A:293:ILE:HD11	1:A:351:PRO:CG	2.32	0.59
1:A:567:THR:HG23	15:A:606:HOH:O	2.01	0.59
4:D:94:GLN:O	4:D:98:VAL:HG23	2.02	0.59
1:A:537:ARG:HH12	1:A:554:LEU:CD1	2.15	0.59
1:A:295:ILE:HA	1:A:298:ARG:HG3	1.84	0.59
2:B:211:ASN:HD21	3:C:21:PRO:HD2	1.67	0.59
1:A:208:ILE:HG13	1:A:209:TYR:CE1	2.37	0.59
1:A:263:TYR:HB2	1:A:314:LYS:HB3	1.85	0.59
1:A:405:LEU:HG	7:A:601:FAD:C2	2.33	0.58
2:B:146:LEU:HD12	2:B:183:ILE:HD11	1.84	0.58
4:D:69:LEU:O	4:D:73:TRP:HB2	2.02	0.58
1:A:35:LEU:C	1:A:36:LEU:HD23	2.23	0.58
2:B:209:ILE:HG23	3:C:24:ALA:HA	1.85	0.58
2:B:95:PRO:CD	2:B:157:THR:CG2	2.82	0.58
2:B:9:ARG:HH11	2:B:49:LEU:CD1	2.15	0.58
1:A:436:ASP:N	1:A:436:ASP:OD1	2.36	0.58
1:A:544:ASP:HB2	1:A:545:PHE:CE1	2.39	0.58
1:A:357:MET:H	1:A:357:MET:CE	2.16	0.58
2:B:33:MET:O	2:B:79:ILE:HG12	2.03	0.58
4:D:95:LEU:O	4:D:99:VAL:HG23	2.03	0.57
1:A:331:LEU:O	1:A:335:ARG:HG3	2.04	0.57
3:C:100:GLU:HB2	3:C:105:ALA:CB	2.33	0.57
2:B:25:LEU:HD13	2:B:42:LEU:HD23	1.86	0.57
1:A:579:PRO:O	1:A:580:ALA:HB3	2.04	0.57
1:A:81:ASP:HB3	1:A:83:ASP:OD1	2.04	0.57
1:A:140:ARG:NH1	2:B:148:GLU:HG2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HE	2:B:24:THR:HG21	1.68	0.57
1:A:236:MET:CE	1:A:236:MET:HA	2.31	0.57
1:A:177:VAL:HG21	1:A:383:LEU:HB2	1.86	0.57
1:A:81:ASP:CG	1:A:393:SER:HB2	2.25	0.57
1:A:104:LEU:HD12	1:A:105:PRO:CD	2.34	0.57
1:A:463:LEU:HD13	1:A:520:MET:CE	2.35	0.57
3:C:108:ARG:O	3:C:112:ILE:HG13	2.05	0.57
1:A:463:LEU:HD13	1:A:520:MET:HE2	1.86	0.56
1:A:537:ARG:HH21	1:A:548:ARG:CB	2.18	0.56
1:A:534:THR:HG23	1:A:545:PHE:CD2	2.40	0.56
1:A:314:LYS:NZ	1:A:317:HIS:HB3	2.19	0.56
1:A:236:MET:HE3	1:A:358:GLY:HA3	1.86	0.56
1:A:60:THR:HG23	1:A:123:SER:HB2	1.86	0.56
1:A:459:ILE:HD13	1:A:494:LEU:HA	1.88	0.56
3:C:83:TYR:CZ	3:C:87:VAL:HG21	2.40	0.56
1:A:240:GLN:CB	1:A:357:MET:HE1	2.36	0.56
1:A:532:PHE:CD2	1:A:569:ARG:HB3	2.41	0.56
1:A:365:THR:OG1	1:A:367:GLN:HG3	2.06	0.56
1:A:139:ASP:OD2	1:A:330:ILE:CG1	2.52	0.56
1:A:255:GLU:CB	1:A:286:ARG:HH22	2.19	0.56
1:A:355:TYR:CD2	1:A:399:ARG:HD3	2.41	0.55
2:B:114:TYR:O	2:B:117:ILE:HG13	2.06	0.55
2:B:205:ARG:HH22	4:D:81:THR:HB	1.70	0.55
2:B:95:PRO:CD	2:B:157:THR:HG22	2.24	0.55
1:A:145:LEU:C	1:A:145:LEU:HD23	2.27	0.55
1:A:327:LEU:N	1:A:328:PRO:HD3	2.22	0.55
1:A:238:MET:CE	1:A:397:ALA:HB1	2.37	0.55
1:A:361:PRO:HA	1:A:391:CYS:O	2.06	0.55
1:A:532:PHE:CE2	1:A:569:ARG:HB3	2.42	0.55
2:B:179:TYR:O	2:B:183:ILE:HG12	2.07	0.55
1:A:44:SER:O	1:A:47:VAL:HG22	2.06	0.55
1:A:486:GLN:O	1:A:489:VAL:HB	2.07	0.55
3:C:123:LEU:HB3	12:C:308:CDN:H521	1.89	0.55
1:A:38:LYS:HG3	7:A:601:FAD:C4A	2.37	0.54
1:A:45:HIS:CE1	1:A:214:ASN:HA	2.41	0.54
3:C:82:ALA:O	3:C:86:VAL:HG23	2.07	0.54
1:A:293:ILE:CD1	1:A:351:PRO:HD3	2.37	0.54
2:B:9:ARG:HH12	2:B:49:LEU:CA	2.20	0.54
1:A:255:GLU:HG3	1:A:258:ARG:NH1	2.22	0.54
3:C:83:TYR:CE2	3:C:87:VAL:HG21	2.43	0.54
1:A:14:GLY:HA3	1:A:201:ALA:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:TYR:CZ	1:A:271:ARG:CZ	2.90	0.54
1:A:242:HIS:HE1	1:A:286:ARG:HH21	1.54	0.54
1:A:287:ASP:HB2	1:A:538:GLY:O	2.08	0.54
1:A:164:TRP:CH2	1:A:184:CYS:HB2	2.42	0.54
1:A:266:ASN:HD21	1:A:270:GLU:HB3	1.72	0.54
1:A:399:ARG:HG2	1:A:399:ARG:HH11	1.73	0.54
1:A:54:THR:O	1:A:406:LEU:HD22	2.07	0.54
1:A:255:GLU:CG	1:A:286:ARG:HH22	2.21	0.54
1:A:222:GLY:HA3	1:A:389:ILE:CD1	2.38	0.54
3:C:51:SER:HB3	4:D:48:TRP:NE1	2.20	0.54
1:A:252:LEU:HB3	7:A:601:FAD:HM73	1.90	0.53
1:A:535:GLU:OE1	1:A:549:ASP:N	2.41	0.53
1:A:556:HIS:N	1:A:572:ASN:O	2.35	0.53
1:A:263:TYR:HB3	1:A:265:LEU:HD21	1.90	0.53
1:A:571:VAL:CG1	1:A:572:ASN:H	2.21	0.53
1:A:586:ARG:HG3	1:A:586:ARG:O	2.09	0.53
4:D:45:TYR:O	4:D:49:ILE:HG22	2.08	0.53
1:A:221:ASP:HA	1:A:518:ASN:CG	2.29	0.53
2:B:180:ARG:HD3	2:B:181:PHE:CE1	2.44	0.53
3:C:1:MET:HG3	3:C:6:LYS:HA	1.90	0.53
1:A:466:CYS:SG	1:A:470:ASN:ND2	2.81	0.53
2:B:52:ARG:NH2	2:B:105:VAL:O	2.42	0.53
1:A:501:ASP:OD2	1:A:507:ASN:ND2	2.41	0.53
1:A:91:THR:O	1:A:91:THR:HG22	2.09	0.53
2:B:34:MET:HA	2:B:34:MET:HE3	1.90	0.53
2:B:111:TYR:O	2:B:114:TYR:HB3	2.08	0.53
2:B:55:CYS:HB3	2:B:60:CYS:HB3	1.91	0.53
1:A:244:THR:HG23	1:A:258:ARG:HH21	1.73	0.52
1:A:61:HIS:NE2	1:A:131:ALA:HB3	2.24	0.52
2:B:160:PRO:HA	2:B:163:TRP:CE3	2.43	0.52
1:A:350:ILE:HG13	1:A:350:ILE:O	2.08	0.52
1:A:444:LEU:HG	1:A:448:ASN:ND2	2.25	0.52
1:A:467:MET:SD	1:A:523:ALA:HB1	2.48	0.52
11:C:305:HEM:HBB1	12:C:308:CDN:C24	2.39	0.52
4:D:115:VAL:OXT	4:D:115:VAL:HG12	2.10	0.52
1:A:109:LEU:O	1:A:117:ARG:O	2.28	0.52
1:A:255:GLU:OE1	1:A:286:ARG:NH2	2.42	0.52
1:A:314:LYS:HZ1	1:A:317:HIS:HB3	1.75	0.52
1:A:578:ARG:CG	1:A:579:PRO:HD3	2.40	0.52
1:A:76:SER:O	1:A:77:ASP:CB	2.57	0.52
1:A:82:GLN:HB2	1:A:577:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ARG:HG2	1:A:399:ARG:NH1	2.24	0.52
1:A:272:PHE:CZ	1:A:293:ILE:HG23	2.44	0.52
2:B:67:MET:SD	2:B:77:THR:HG21	2.49	0.52
1:A:357:MET:H	1:A:357:MET:HE2	1.75	0.52
1:A:38:LYS:HE2	1:A:217:ILE:HG23	1.92	0.52
1:A:232:PRO:HB2	1:A:558:LEU:HD11	1.92	0.52
1:A:357:MET:HE2	1:A:357:MET:N	2.25	0.52
1:A:65:TRP:O	1:A:68:HIS:HB3	2.10	0.52
1:A:477:GLY:HA2	1:A:542:ARG:NH2	2.25	0.51
1:A:303:CYS:O	1:A:309:PRO:HA	2.11	0.51
1:A:389:ILE:O	1:A:389:ILE:HG12	2.11	0.51
1:A:534:THR:CB	1:A:553:TRP:NE1	2.62	0.51
1:A:76:SER:O	1:A:79:ILE:CG2	2.58	0.51
1:A:548:ARG:NH2	1:A:584:LYS:O	2.44	0.51
1:A:456:PRO:HG3	1:A:497:ALA:HB1	1.92	0.51
2:B:84:GLN:OE1	2:B:87:LYS:HD2	2.09	0.51
1:A:40:PHE:HD2	1:A:42:THR:HG1	1.59	0.51
1:A:71:ASP:HB3	1:A:128:GLY:O	2.11	0.51
4:D:6:SER:HB2	4:D:77:TRP:NE1	2.26	0.51
1:A:63:ASP:CG	1:A:133:ARG:HH12	2.13	0.51
1:A:81:ASP:N	1:A:81:ASP:OD1	2.44	0.51
1:A:97:LEU:HD22	2:B:132:GLU:HB3	1.93	0.51
4:D:52:PHE:C	4:D:54:SER:H	2.14	0.51
1:A:392:VAL:CG1	1:A:394:VAL:HG13	2.39	0.50
1:A:72:THR:HG22	1:A:400:LEU:HD23	1.92	0.50
1:A:63:ASP:OD2	1:A:133:ARG:NH1	2.44	0.50
2:B:76:ILE:O	2:B:78:PRO:HD3	2.11	0.50
2:B:234:LEU:HD23	4:D:13:VAL:HG13	1.94	0.50
1:A:176:ALA:HB1	1:A:381:PRO:HB2	1.94	0.50
1:A:242:HIS:HB2	1:A:354:HIS:HB2	1.91	0.50
1:A:484:LEU:HD11	1:A:531:ASN:HB2	1.93	0.50
1:A:555:CYS:HB3	1:A:573:MET:HG2	1.93	0.50
1:A:559:TYR:CE2	1:A:561:PRO:HG3	2.45	0.50
1:A:9:ASP:H	1:A:32:THR:CG2	2.18	0.50
2:B:25:LEU:HD21	2:B:41:GLN:HG3	1.93	0.50
2:B:54:SER:O	2:B:56:ARG:N	2.45	0.50
2:B:34:MET:HE1	2:B:78:PRO:HG3	1.93	0.50
1:A:370:THR:HG23	1:A:380:VAL:CG2	2.42	0.50
1:A:306:PRO:O	2:B:31:ARG:NH2	2.43	0.50
1:A:46:THR:HB	1:A:146:LEU:HD13	1.94	0.50
1:A:234:GLN:CB	1:A:361:PRO:HG3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:TYR:CE2	1:A:399:ARG:HD3	2.46	0.50
1:A:483:GLY:HA2	1:A:486:GLN:NE2	2.27	0.50
1:A:559:TYR:CB	1:A:569:ARG:HH21	2.18	0.50
1:A:209:TYR:HB3	1:A:468:GLN:OE1	2.12	0.50
2:B:201:PHE:CE2	4:D:81:THR:HG21	2.47	0.50
2:B:201:PHE:CZ	4:D:81:THR:HG21	2.46	0.50
1:A:372:ASN:HB3	1:A:376:GLU:H	1.76	0.50
1:A:79:ILE:CD1	1:A:397:ALA:HB2	2.28	0.50
1:A:483:GLY:HA2	1:A:486:GLN:HE21	1.77	0.50
1:A:108:ARG:HG3	2:B:135:GLN:O	2.11	0.50
1:A:513:CYS:O	1:A:516:LEU:N	2.44	0.49
2:B:70:LYS:HE3	2:B:215:VAL:HG12	1.94	0.49
2:B:35:LEU:HD21	2:B:91:ILE:CD1	2.42	0.49
1:A:560:LEU:HD23	1:A:568:ARG:HD3	1.94	0.49
1:A:8:PHE:CE2	1:A:34:ALA:HB2	2.48	0.49
12:C:308:CDN:HA21	4:D:41:GLY:O	2.12	0.49
1:A:221:ASP:O	1:A:225:MET:HG3	2.13	0.49
1:A:314:LYS:HA	1:A:346:PRO:HG3	1.94	0.49
1:A:545:PHE:N	1:A:546:PRO:HD3	2.27	0.49
1:A:119:PHE:CG	2:B:134:LEU:HA	2.47	0.49
1:A:293:ILE:HD12	1:A:351:PRO:HD3	1.95	0.49
1:A:574:GLU:O	1:A:574:GLU:CG	2.57	0.49
2:B:1:MET:H3	2:B:29:GLU:HB2	1.77	0.49
1:A:214:ASN:HD22	1:A:214:ASN:N	2.10	0.49
1:A:476:GLU:HG3	1:A:478:ASP:CG	2.33	0.49
1:A:584:LYS:HG2	1:A:585:ILE:HG12	1.95	0.49
1:A:244:THR:CG2	1:A:258:ARG:HH21	2.25	0.49
1:A:450:ASN:HB3	15:A:633:HOH:O	2.13	0.49
1:A:457:VAL:O	1:A:461:LYS:HG3	2.12	0.49
2:B:35:LEU:HD21	2:B:91:ILE:HD11	1.94	0.49
1:A:472:SER:OG	1:A:473:VAL:N	2.45	0.48
1:A:520:MET:CE	1:A:520:MET:HA	2.41	0.48
2:B:9:ARG:NH1	2:B:49:LEU:HA	2.28	0.48
2:B:218:LYS:HB2	2:B:220:LEU:HG	1.94	0.48
1:A:176:ALA:CB	1:A:381:PRO:HB2	2.44	0.48
1:A:443:ARG:NH1	15:A:602:HOH:O	2.42	0.48
1:A:49:ALA:HA	7:A:601:FAD:C5X	2.44	0.48
1:A:537:ARG:HH21	1:A:548:ARG:CD	2.26	0.48
1:A:583:PRO:O	1:A:584:LYS:HB2	2.13	0.48
1:A:314:LYS:HG2	1:A:316:ASP:OD1	2.13	0.48
1:A:525:ALA:O	1:A:529:SER:OG	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:LYS:HB2	2:B:193:ARG:HH12	1.79	0.48
2:B:210:MET:HE1	3:C:102:THR:O	2.13	0.48
1:A:205:ALA:CB	1:A:220:GLY:N	2.71	0.48
1:A:320:LYS:HA	1:A:323:LEU:HD12	1.95	0.48
1:A:384:PHE:CD1	1:A:384:PHE:N	2.82	0.48
1:A:408:LEU:HD11	7:A:601:FAD:H4'	1.96	0.48
2:B:220:LEU:HD12	9:B:303:SF4:S4	2.54	0.48
1:A:284:ALA:HB3	1:A:289:VAL:HG22	1.95	0.48
1:A:476:GLU:HG3	1:A:478:ASP:OD2	2.14	0.48
1:A:49:ALA:HB3	1:A:142:GLY:CA	2.40	0.48
4:D:83:TYR:OH	14:D:306:UQ2:O1	2.27	0.48
1:A:287:ASP:H	1:A:398:ASN:HD21	1.61	0.47
1:A:126:PHE:CE2	1:A:401:GLY:CA	2.90	0.47
2:B:82:LEU:N	2:B:82:LEU:HD12	2.28	0.47
2:B:211:ASN:HD21	3:C:24:ALA:HB2	1.79	0.47
1:A:209:TYR:O	1:A:464:GLN:NE2	2.38	0.47
1:A:537:ARG:O	1:A:540:HIS:N	2.47	0.47
1:A:21:ARG:O	1:A:21:ARG:NH1	2.47	0.47
1:A:533:ARG:HB3	1:A:540:HIS:CE1	2.50	0.47
2:B:9:ARG:HH12	2:B:49:LEU:HA	1.80	0.47
1:A:182:ALA:HB3	1:A:193:PHE:HE1	1.79	0.47
3:C:127:LEU:HB2	12:C:308:CDN:H512	1.97	0.47
3:C:2:ILE:HD11	3:C:5:VAL:HG21	1.96	0.47
11:C:305:HEM:CAC	4:D:23:ALA:HB1	2.44	0.47
1:A:490:ILE:O	1:A:493:ARG:HB3	2.15	0.47
2:B:211:ASN:ND2	3:C:21:PRO:HD2	2.30	0.47
1:A:124:LYS:N	1:A:134:THR:O	2.44	0.47
1:A:441:LEU:O	1:A:445:ASN:ND2	2.48	0.47
11:C:305:HEM:CBB	4:D:68:ILE:HG12	2.45	0.47
1:A:63:ASP:OD2	1:A:133:ARG:NH2	2.48	0.47
1:A:76:SER:O	1:A:77:ASP:HB2	2.14	0.47
2:B:1:MET:H1	2:B:29:GLU:HB2	1.79	0.47
4:D:70:ILE:O	4:D:74:ILE:HG13	2.14	0.46
1:A:233:VAL:CG1	1:A:236:MET:SD	2.99	0.46
1:A:234:GLN:CG	1:A:361:PRO:HG3	2.46	0.46
1:A:172:ASN:O	1:A:175:GLY:N	2.42	0.46
1:A:372:ASN:O	1:A:375:GLY:N	2.49	0.46
1:A:40:PHE:O	1:A:43:ARG:HG2	2.15	0.46
1:A:572:ASN:C	1:A:573:MET:CG	2.81	0.46
1:A:356:MET:HG2	1:A:356:MET:O	2.15	0.46
2:B:95:PRO:O	2:B:157:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ARG:NH1	2:B:49:LEU:CD1	2.78	0.46
2:B:213:VAL:HG23	2:B:223:THR:HG23	1.98	0.46
1:A:238:MET:CE	1:A:397:ALA:CB	2.94	0.46
1:A:559:TYR:OH	1:A:567:THR:HG21	2.16	0.46
1:A:404:SER:HB3	7:A:601:FAD:N1	2.31	0.46
1:A:126:PHE:CE2	1:A:401:GLY:C	2.88	0.46
1:A:238:MET:HE2	1:A:397:ALA:CB	2.46	0.46
2:B:211:ASN:O	2:B:214:SER:HB3	2.16	0.46
3:C:52:LEU:HD13	4:D:115:VAL:HG21	1.96	0.46
12:C:308:CDN:H152	4:D:37:PHE:CE2	2.49	0.46
1:A:470:ASN:HD21	1:A:486:GLN:HE22	1.63	0.46
2:B:29:GLU:HG3	2:B:29:GLU:O	2.16	0.46
11:C:305:HEM:HBB1	4:D:68:ILE:HG12	1.98	0.46
4:D:84:VAL:O	4:D:90:ARG:HD3	2.16	0.46
2:B:113:GLN:OE1	2:B:113:GLN:HA	2.16	0.46
2:B:150:ILE:HD13	2:B:218:LYS:HD3	1.97	0.46
2:B:6:SER:HB3	2:B:90:VAL:HA	1.98	0.46
1:A:372:ASN:N	1:A:376:GLU:O	2.49	0.46
1:A:432:ALA:HB1	1:A:436:ASP:HB2	1.98	0.46
2:B:210:MET:HE1	3:C:102:THR:C	2.36	0.46
3:C:118:VAL:HG21	13:C:309:EPH:H221	1.98	0.46
1:A:559:TYR:HD1	1:A:569:ARG:HE	1.64	0.45
1:A:182:ALA:HB3	1:A:193:PHE:CE1	2.51	0.45
1:A:94:GLU:HG3	1:A:95:ALA:N	2.30	0.45
1:A:236:MET:HG3	1:A:236:MET:O	2.15	0.45
1:A:47:VAL:HG13	1:A:146:LEU:HD22	1.94	0.45
1:A:471:PHE:CE2	1:A:527:ALA:HA	2.51	0.45
2:B:228:HIS:O	2:B:232:MET:HG3	2.17	0.45
1:A:13:ILE:HB	1:A:200:LEU:HD23	1.99	0.45
1:A:56:ALA:O	1:A:93:PRO:HG3	2.16	0.45
4:D:48:TRP:CH2	4:D:52:PHE:HE1	2.34	0.45
1:A:126:PHE:HB2	1:A:134:THR:OG1	2.17	0.45
1:A:559:TYR:CD2	1:A:561:PRO:HG3	2.52	0.45
1:A:509:GLN:N	2:B:43:LYS:HZ1	2.15	0.45
1:A:244:THR:HG23	1:A:258:ARG:NH2	2.31	0.45
1:A:277:ALA:O	1:A:279:ASN:N	2.49	0.45
1:A:475:ARG:O	1:A:542:ARG:HA	2.17	0.45
1:A:505:GLU:O	2:B:101:ARG:HD2	2.16	0.45
1:A:122:GLN:O	1:A:135:ALA:HA	2.16	0.45
1:A:151:GLN:O	1:A:154:LEU:HB2	2.17	0.45
1:A:334:SER:O	1:A:338:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:GLN:O	2:B:127:ASN:HB2	2.16	0.45
2:B:34:MET:CA	2:B:34:MET:CE	2.91	0.45
1:A:106:PHE:HA	1:A:137:ALA:HB2	1.99	0.45
1:A:476:GLU:HG3	1:A:478:ASP:OD1	2.16	0.45
4:D:8:LEU:HG	4:D:73:TRP:CD2	2.52	0.45
2:B:21:GLN:NE2	2:B:23:TYR:OH	2.50	0.45
4:D:62:LEU:HD23	4:D:65:LEU:HD12	1.99	0.45
1:A:104:LEU:HA	1:A:105:PRO:HD3	1.76	0.44
1:A:119:PHE:CD2	2:B:134:LEU:CD1	3.00	0.44
1:A:222:GLY:HA3	1:A:389:ILE:HD11	1.98	0.44
1:A:255:GLU:CD	1:A:286:ARG:NH2	2.69	0.44
1:A:298:ARG:NH1	1:A:543:PHE:CZ	2.85	0.44
1:A:327:LEU:O	1:A:331:LEU:HG	2.17	0.44
1:A:125:ASN:CG	1:A:132:ALA:HB2	2.37	0.44
1:A:133:ARG:HH11	1:A:133:ARG:HB2	1.83	0.44
1:A:61:HIS:NE2	1:A:131:ALA:CB	2.80	0.44
1:A:304:ASP:OD1	1:A:305:GLY:N	2.51	0.44
1:A:88:MET:HB2	1:A:411:PHE:CZ	2.52	0.44
1:A:478:ASP:O	1:A:481:ALA:HB3	2.17	0.44
1:A:50:GLN:O	1:A:51:GLY:C	2.55	0.44
1:A:252:LEU:CB	7:A:601:FAD:HM73	2.46	0.44
2:B:236:ARG:O	2:B:236:ARG:HG2	2.17	0.44
1:A:578:ARG:CB	1:A:579:PRO:CD	2.85	0.44
1:A:68:HIS:O	1:A:72:THR:HG23	2.17	0.44
2:B:180:ARG:HG2	2:B:180:ARG:HH11	1.83	0.44
2:B:55:CYS:O	2:B:56:ARG:HB3	2.16	0.44
3:C:28:ILE:O	3:C:28:ILE:HG12	2.17	0.44
2:B:160:PRO:HA	2:B:163:TRP:CD2	2.52	0.44
2:B:79:ILE:O	2:B:79:ILE:HG22	2.16	0.44
3:C:81:LEU:O	3:C:85:VAL:HG23	2.18	0.44
4:D:52:PHE:C	4:D:54:SER:N	2.70	0.44
1:A:60:THR:HG21	1:A:123:SER:HB2	1.97	0.44
1:A:36:LEU:HD23	1:A:36:LEU:N	2.33	0.44
1:A:97:LEU:CD1	2:B:131:ARG:HB3	2.48	0.44
4:D:111:VAL:O	4:D:115:VAL:HG23	2.17	0.44
1:A:172:ASN:N	1:A:176:ALA:O	2.51	0.44
1:A:234:GLN:HG3	1:A:361:PRO:HG3	1.99	0.44
1:A:3:LEU:HA	1:A:4:PRO:HD3	1.88	0.44
1:A:82:GLN:NE2	1:A:581:PHE:HB3	2.32	0.44
2:B:127:ASN:N	2:B:128:PRO:HD3	2.32	0.44
1:A:13:ILE:HD12	1:A:200:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ARG:NH2	1:A:548:ARG:HB2	2.29	0.43
1:A:571:VAL:HG13	1:A:572:ASN:H	1.83	0.43
2:B:143:LEU:N	2:B:143:LEU:HD12	2.33	0.43
1:A:167:LEU:O	1:A:225:MET:HG2	2.18	0.43
1:A:222:GLY:HA3	1:A:389:ILE:HD12	2.00	0.43
1:A:257:CYS:HB3	1:A:315:LEU:HD21	2.00	0.43
1:A:567:THR:C	1:A:568:ARG:HG3	2.38	0.43
4:D:82:ASP:O	4:D:85:LYS:HE3	2.19	0.43
1:A:26:ILE:O	1:A:31:GLN:HB2	2.18	0.43
1:A:532:PHE:HD2	1:A:569:ARG:HD3	1.83	0.43
2:B:210:MET:CE	3:C:103:PHE:HA	2.48	0.43
1:A:392:VAL:CG1	1:A:394:VAL:HG22	2.49	0.43
1:A:502:THR:C	1:A:510:ARG:NH2	2.72	0.43
1:A:238:MET:HE2	1:A:397:ALA:HB2	2.00	0.43
2:B:236:ARG:O	2:B:237:ASN:ND2	2.51	0.43
2:B:223:THR:CG2	10:B:304:F3S:S1	2.95	0.43
3:C:45:LEU:HA	3:C:45:LEU:HD23	1.83	0.43
1:A:164:TRP:CZ3	1:A:184:CYS:HB2	2.54	0.43
1:A:370:THR:HG23	1:A:380:VAL:HG22	2.01	0.43
1:A:395:HIS:CG	1:A:399:ARG:HG3	2.52	0.43
1:A:453:GLY:CA	1:A:496:ASN:O	2.63	0.43
1:A:74:LYS:O	1:A:74:LYS:HG2	2.18	0.43
1:A:292:SER:O	1:A:296:GLU:HG2	2.18	0.43
1:A:79:ILE:HG21	1:A:397:ALA:HB3	1.98	0.43
2:B:179:TYR:CE2	2:B:183:ILE:HD13	2.54	0.43
2:B:54:SER:O	2:B:55:CYS:C	2.57	0.43
1:A:129:GLU:HG3	1:A:131:ALA:O	2.18	0.43
1:A:529:SER:OG	1:A:569:ARG:CZ	2.67	0.43
1:A:79:ILE:HG21	1:A:397:ALA:N	2.33	0.43
2:B:155:CYS:SG	2:B:156:SER:N	2.92	0.43
1:A:11:VAL:HG23	1:A:195:ALA:HB2	2.01	0.42
1:A:133:ARG:HH11	1:A:133:ARG:CB	2.32	0.42
1:A:491:ARG:NH1	1:A:524:TYR:CE2	2.87	0.42
1:A:234:GLN:HG3	1:A:361:PRO:CG	2.48	0.42
1:A:253:VAL:HG13	1:A:330:ILE:HD12	2.00	0.42
1:A:357:MET:H	1:A:357:MET:HE3	1.84	0.42
1:A:503:SER:O	1:A:510:ARG:NH2	2.52	0.42
1:A:572:ASN:HD22	1:A:573:MET:H	1.65	0.42
2:B:210:MET:HG2	2:B:223:THR:HG21	2.01	0.42
1:A:255:GLU:CD	1:A:286:ARG:HH12	2.22	0.42
2:B:137:PRO:O	2:B:141:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:CYS:SG	2:B:223:THR:HG23	2.59	0.42
1:A:228:ARG:HG3	15:A:602:HOH:O	2.18	0.42
1:A:326:ARG:C	1:A:328:PRO:HD3	2.39	0.42
2:B:21:GLN:HG2	2:B:23:TYR:CE1	2.55	0.42
1:A:24:LEU:HD11	1:A:156:ASN:ND2	2.35	0.42
2:B:29:GLU:OE1	2:B:29:GLU:HA	2.20	0.42
2:B:37:ASP:O	2:B:38:ALA:C	2.56	0.42
1:A:231:VAL:HA	1:A:232:PRO:HD3	1.81	0.42
1:A:219:THR:HG21	1:A:515:GLU:OE1	2.19	0.42
2:B:67:MET:HB3	2:B:82:LEU:HD21	2.02	0.42
1:A:72:THR:HG22	1:A:400:LEU:CD2	2.49	0.42
1:A:560:LEU:HD23	1:A:568:ARG:HB2	2.01	0.42
3:C:20:PHE:HA	3:C:21:PRO:HD3	1.86	0.42
1:A:338:ALA:O	1:A:340:VAL:HG23	2.19	0.42
2:B:50:SER:OG	2:B:101:ARG:HD3	2.20	0.42
1:A:392:VAL:O	1:A:393:SER:CB	2.67	0.41
1:A:572:ASN:ND2	1:A:573:MET:N	2.66	0.41
1:A:264:LEU:O	1:A:265:LEU:HD23	2.20	0.41
1:A:463:LEU:HD11	1:A:523:ALA:CB	2.51	0.41
1:A:502:THR:HA	1:A:510:ARG:HH21	1.85	0.41
7:A:601:FAD:H1'1	7:A:601:FAD:H9	1.80	0.41
2:B:34:MET:HE3	2:B:78:PRO:HA	2.01	0.41
1:A:421:GLU:O	1:A:424:ALA:HB3	2.20	0.41
1:A:476:GLU:O	1:A:479:ALA:HB3	2.20	0.41
1:A:42:THR:O	1:A:47:VAL:CG1	2.63	0.41
1:A:477:GLY:CA	1:A:542:ARG:NH2	2.83	0.41
4:D:85:LYS:HA	4:D:85:LYS:HD3	1.74	0.41
1:A:360:ILE:HA	1:A:361:PRO:HD3	1.85	0.41
3:C:89:ILE:HG22	3:C:93:MET:CE	2.50	0.41
4:D:44:THR:HG22	4:D:46:GLU:H	1.84	0.41
1:A:267:LYS:C	1:A:269:GLY:H	2.23	0.41
1:A:422:SER:O	1:A:426:GLN:HG2	2.20	0.41
1:A:277:ALA:CB	1:A:588:TYR:O	2.62	0.41
1:A:79:ILE:HG23	1:A:396:GLY:CA	2.49	0.41
2:B:22:ASP:OD1	2:B:88:LYS:NZ	2.51	0.41
2:B:3:LEU:HB3	2:B:5:PHE:CE1	2.56	0.41
1:A:133:ARG:NH1	1:A:133:ARG:CB	2.84	0.41
1:A:274:GLU:O	1:A:278:PRO:HA	2.20	0.41
1:A:463:LEU:HD22	1:A:520:MET:CE	2.50	0.41
1:A:545:PHE:N	1:A:545:PHE:CD1	2.89	0.41
1:A:574:GLU:N	1:A:575:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:THR:CA	5:A:589:OAA:O5	2.63	0.41
1:A:79:ILE:CG2	1:A:397:ALA:N	2.84	0.41
2:B:43:LYS:HE2	2:B:47:PRO:O	2.20	0.41
1:A:143:HIS:HE1	2:B:147:TYR:O	2.03	0.41
1:A:151:GLN:HB3	2:B:119:PRO:O	2.21	0.41
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.88	0.41
3:C:15:LEU:HD13	14:D:306:UQ2:H5M1	2.02	0.41
4:D:48:TRP:CE3	4:D:48:TRP:HA	2.55	0.41
4:D:65:LEU:HA	4:D:68:ILE:HD12	2.02	0.41
1:A:205:ALA:HA	1:A:218:ASN:O	2.21	0.41
1:A:334:SER:O	1:A:338:ALA:N	2.53	0.41
1:A:374:LYS:HB2	1:A:376:GLU:HG3	2.03	0.41
1:A:359:GLY:O	1:A:391:CYS:HB3	2.21	0.41
1:A:544:ASP:C	1:A:546:PRO:HD3	2.41	0.41
2:B:180:ARG:HG2	2:B:180:ARG:NH1	2.36	0.41
2:B:230:LYS:HA	2:B:233:LEU:HD12	2.01	0.41
2:B:81:ALA:C	2:B:82:LEU:HD12	2.41	0.41
1:A:307:TRP:HA	1:A:307:TRP:CE3	2.56	0.40
1:A:307:TRP:HA	1:A:307:TRP:HE3	1.86	0.40
1:A:86:GLU:OE1	1:A:578:ARG:HB3	2.21	0.40
1:A:78:TYR:O	1:A:554:LEU:HD11	2.21	0.40
1:A:153:ASN:HD22	1:A:158:THR:CB	2.34	0.40
1:A:256:GLY:O	1:A:260:GLU:HG2	2.21	0.40
1:A:247:ALA:HB2	1:A:350:ILE:HG23	2.03	0.40
1:A:236:MET:O	1:A:526:THR:HA	2.21	0.40
3:C:101:GLU:HG2	15:C:312:HOH:O	2.20	0.40
1:A:347:ILE:HA	1:A:348:PRO:HD3	1.97	0.40
1:A:174:ASP:HB2	1:A:430:ARG:NH2	2.36	0.40
1:A:272:PHE:HZ	1:A:293:ILE:HG22	1.74	0.40
1:A:470:ASN:HB2	1:A:471:PHE:CE1	2.57	0.40
1:A:579:PRO:O	1:A:580:ALA:CB	2.70	0.40
1:A:64:ASN:OD1	1:A:66:GLU:HB2	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	586/588 (100%)	504 (86%)	65 (11%)	17 (3%)	4 7
2	B	236/238 (99%)	205 (87%)	28 (12%)	3 (1%)	12 24
3	C	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	6 10
4	D	111/115 (96%)	107 (96%)	4 (4%)	0	100 100
All	All	1060/1070 (99%)	933 (88%)	104 (10%)	23 (2%)	6 12

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	GLY
1	A	110	ASP
1	A	119	PHE
1	A	278	PRO
3	C	7	LYS
1	A	77	ASP
1	A	431	ASP
1	A	538	GLY
1	A	393	SER
1	A	506	PHE
2	B	54	SER
2	B	55	CYS
3	C	2	ILE
1	A	505	GLU
2	B	199	ASP
1	A	116	GLN
1	A	578	ARG
1	A	118	PRO
1	A	453	GLY
3	C	97	GLY
1	A	105	PRO
1	A	309	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%)	448 (95%)	25 (5%)	22 45
2	B	208/208 (100%)	203 (98%)	5 (2%)	49 74
3	C	109/109 (100%)	107 (98%)	2 (2%)	59 80
4	D	94/96 (98%)	91 (97%)	3 (3%)	39 65
All	All	884/886 (100%)	849 (96%)	35 (4%)	31 57

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	CYS
1	A	122	GLN
1	A	172	ASN
1	A	196	ARG
1	A	207	ARG
1	A	235	ASP
1	A	278	PRO
1	A	293	ILE
1	A	326	ARG
1	A	357	MET
1	A	371	VAL
1	A	384	PHE
1	A	436	ASP
1	A	446	ARG
1	A	478	ASP
1	A	506	PHE
1	A	524	TYR
1	A	542	ARG
1	A	544	ASP
1	A	555	CYS
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	63	ASP

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Mol	Chain	Res	Type
2	B	180	ARG
2	B	211	ASN
3	C	4	ASN
3	C	129	TRP
4	D	6	SER
4	D	42	GLU
4	D	60	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	147	HIS
1	A	153	ASN
1	A	172	ASN
1	A	210	GLN
1	A	218	ASN
1	A	234	GLN
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	448	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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
8	FES	B	302	2	0,4,4	0.00	-	-		
13	EPH	C	309	-	34,34,48	1.11	3 (8%)	37,39,53	0.96	1 (2%)
10	F3S	B	304	2	0,9,9	0.00	-	-		
14	UQ2	D	306	-	23,23,23	2.88	9 (39%)	28,31,31	1.39	3 (10%)
12	CDN	C	308	-	76,76,76	2.21	10 (13%)	78,88,88	2.06	10 (12%)
7	FAD	A	601	1	51,58,58	2.89	16 (31%)	60,89,89	2.44	13 (21%)
5	OAA	A	589	-	2,8,8	4.62	2 (100%)	2,10,10	5.03	2 (100%)
11	HEM	C	305	3,4	27,50,50	1.36	4 (14%)	17,82,82	1.62	5 (29%)
9	SF4	B	303	2	0,12,12	0.00	-	-		

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
14	UQ2	D	306	-	-	4/15/39/39	0/1/1/1
13	EPH	C	309	-	-	6/38/38/52	-
10	F3S	B	304	2	-	-	0/3/3/3
8	FES	B	302	2	-	-	0/1/1/1
12	CDN	C	308	-	3/3/9/9	26/87/87/87	-
9	SF4	B	303	2	-	-	0/6/5/5
5	OAA	A	589	-	-	0/2/8/8	-
11	HEM	C	305	3,4	-	1/6/54/54	-
7	FAD	A	601	1	-	3/30/50/50	0/6/6/6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	306	UQ2	C7-C8	-10.96	1.34	1.50
7	A	601	FAD	C4X-N5	9.59	1.47	1.33
7	A	601	FAD	C9A-N10	7.95	1.49	1.38
12	C	308	CDN	OA8-CA7	7.57	1.53	1.40
12	C	308	CDN	OA6-CA5	-7.12	1.21	1.41
12	C	308	CDN	OB8-CB7	7.09	1.52	1.40
12	C	308	CDN	OB7-CB5	-6.21	1.21	1.39
7	A	601	FAD	C2A-N3A	6.16	1.42	1.32
12	C	308	CDN	OA7-CA5	6.11	1.56	1.39
12	C	308	CDN	OA9-CA7	-6.10	1.22	1.39
12	C	308	CDN	OB9-CB7	-5.98	1.22	1.39
5	A	589	OAA	C2-C3	5.81	1.57	1.51
7	A	601	FAD	C1'-N10	-5.61	1.42	1.48
7	A	601	FAD	C4A-N3A	5.46	1.43	1.35
7	A	601	FAD	C5X-N5	5.17	1.43	1.35
7	A	601	FAD	C4-N3	4.81	1.41	1.33
7	A	601	FAD	C10-N1	4.61	1.39	1.33
7	A	601	FAD	C4X-C10	4.08	1.42	1.38
7	A	601	FAD	C5'-C4'	-4.08	1.46	1.51
12	C	308	CDN	OB6-CB5	3.99	1.53	1.41
13	C	309	EPH	C25-C24	3.67	1.53	1.28
11	C	305	HEM	CBB-CAB	3.63	1.53	1.29
14	D	306	UQ2	O4-C4	3.60	1.31	1.23
7	A	601	FAD	C5A-C4A	-3.41	1.31	1.40
5	A	589	OAA	O3-C3	3.00	1.27	1.22
11	C	305	HEM	C3C-C2C	-2.99	1.36	1.40
14	D	306	UQ2	C13-C14	2.98	1.40	1.32
13	C	309	EPH	C12-C13	2.95	1.51	1.29
14	D	306	UQ2	O3-CM3	-2.71	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	306	UQ2	C8-C9	2.66	1.39	1.33
14	D	306	UQ2	C16-C14	2.65	1.57	1.50
7	A	601	FAD	C2B-C3B	-2.59	1.46	1.53
7	A	601	FAD	C6-C7	2.56	1.44	1.37
7	A	601	FAD	C8A-N7A	-2.53	1.30	1.34
12	C	308	CDN	OB6-CB4	-2.48	1.41	1.44
11	C	305	HEM	C3B-C2B	-2.45	1.37	1.40
14	D	306	UQ2	CM5-C5	2.45	1.56	1.50
12	C	308	CDN	OA6-CA4	-2.31	1.41	1.44
13	C	309	EPH	P1-O7	2.29	1.59	1.50
14	D	306	UQ2	C6-C5	2.29	1.39	1.35
7	A	601	FAD	C2'-C3'	-2.24	1.49	1.53
14	D	306	UQ2	O3-C3	2.07	1.41	1.36
7	A	601	FAD	C9A-C5X	2.04	1.46	1.42
11	C	305	HEM	C4A-CHB	-2.03	1.35	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	601	FAD	C4-N3-C2	12.49	125.68	115.14
12	C	308	CDN	OB9-CB7-C71	8.69	125.22	109.12
12	C	308	CDN	OB7-CB5-C51	8.49	124.84	109.12
12	C	308	CDN	OA9-CA7-C31	8.46	124.80	109.12
7	A	601	FAD	C1'-N10-C9A	-6.45	113.22	118.29
7	A	601	FAD	C4X-C4-N3	-6.22	114.92	123.43
5	A	589	OAA	C1-C2-C3	-5.71	105.33	115.51
7	A	601	FAD	C1'-N10-C10	5.51	123.35	118.41
14	D	306	UQ2	CM3-O3-C3	4.40	132.05	116.47
5	A	589	OAA	O3-C3-C2	4.23	127.44	120.75
12	C	308	CDN	C19-C18-C17	-3.82	95.02	114.42
12	C	308	CDN	OA7-CA5-C11	3.71	116.00	109.12
12	C	308	CDN	C15-C14-C13	-3.61	96.10	114.42
11	C	305	HEM	C4C-C3C-C2C	3.09	109.06	106.90
7	A	601	FAD	C5X-C9A-N10	-3.05	115.50	117.72
14	D	306	UQ2	C12-C13-C14	3.01	138.03	127.75
7	A	601	FAD	C1'-C2'-C3'	2.76	117.51	109.79
11	C	305	HEM	CMC-C2C-C3C	2.61	129.56	124.68
7	A	601	FAD	N3A-C2A-N1A	-2.51	124.76	128.68
12	C	308	CDN	C21-C20-C19	-2.48	101.83	114.42
7	A	601	FAD	O2B-C2B-C3B	2.40	119.58	111.82
12	C	308	CDN	C22-C21-C20	-2.39	102.31	114.42
7	A	601	FAD	C6-C5X-C9A	-2.36	115.96	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	601	FAD	O4B-C1B-C2B	-2.18	103.74	106.93
13	C	309	EPH	C6-C5-C3	-2.16	105.77	113.62
11	C	305	HEM	CBD-CAD-C3D	2.14	116.42	112.48
12	C	308	CDN	C16-C15-C14	-2.10	103.74	114.42
11	C	305	HEM	C3C-C4C-NC	-2.09	106.99	110.94
12	C	308	CDN	CA6-OA8-CA7	-2.06	109.82	113.80
7	A	601	FAD	C3B-C2B-C1B	2.06	104.08	100.98
7	A	601	FAD	C6-C5X-N5	2.05	121.31	119.05
7	A	601	FAD	C10-C4X-N5	2.04	122.67	121.26
11	C	305	HEM	CMA-C3A-C4A	-2.02	125.36	128.46
14	D	306	UQ2	C6-C5-C4	2.01	120.78	119.18

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	308	CDN	CB5
12	C	308	CDN	CB7
12	C	308	CDN	CA7

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	C	309	EPH	C37-O5-P1-O8
12	C	308	CDN	CB2-OB2-PB2-OB3
12	C	308	CDN	CB2-OB2-PB2-OB4
12	C	308	CDN	OB7-CB5-OB6-CB4
12	C	308	CDN	C52-C51-CB5-OB7
12	C	308	CDN	OA7-CA5-OA6-CA4
11	C	305	HEM	C2A-CAA-CBA-CGA
12	C	308	CDN	CB2-OB2-PB2-OB5
12	C	308	CDN	C58-C59-C60-C61
12	C	308	CDN	C60-C61-C62-C63
12	C	308	CDN	C55-C56-C57-C58
13	C	309	EPH	C21-C22-C23-C24
13	C	309	EPH	C9-C10-C11-C12
13	C	309	EPH	C11-C10-C9-C8
13	C	309	EPH	C18-C19-C20-C21
12	C	308	CDN	CB3-CB4-CB6-OB8
12	C	308	CDN	C54-C55-C56-C57
12	C	308	CDN	C14-C15-C16-C17
12	C	308	CDN	C61-C62-C63-C64
12	C	308	CDN	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
14	D	306	UQ2	C12-C11-C9-C10
12	C	308	CDN	C1-CB2-OB2-PB2
12	C	308	CDN	C31-CA7-OA8-CA6
12	C	308	CDN	OB6-CB4-CB6-OB8
14	D	306	UQ2	C12-C11-C9-C8
12	C	308	CDN	CB3-OB5-PB2-OB2
12	C	308	CDN	CA3-OA5-PA1-OA2
12	C	308	CDN	CA2-OA2-PA1-OA5
12	C	308	CDN	C32-C31-CA7-OA8
12	C	308	CDN	CB7-C71-C72-C73
7	A	601	FAD	O4B-C4B-C5B-O5B
14	D	306	UQ2	C4-C3-O3-CM3
12	C	308	CDN	CB2-C1-CA2-OA2
7	A	601	FAD	P-O3P-PA-O1A
12	C	308	CDN	C35-C36-C37-C38
12	C	308	CDN	C56-C57-C58-C59
13	C	309	EPH	C10-C11-C12-C13
7	A	601	FAD	P-O3P-PA-O2A
12	C	308	CDN	C52-C51-CB5-OB6
14	D	306	UQ2	C6-C7-C8-C9

There are no ring outliers.

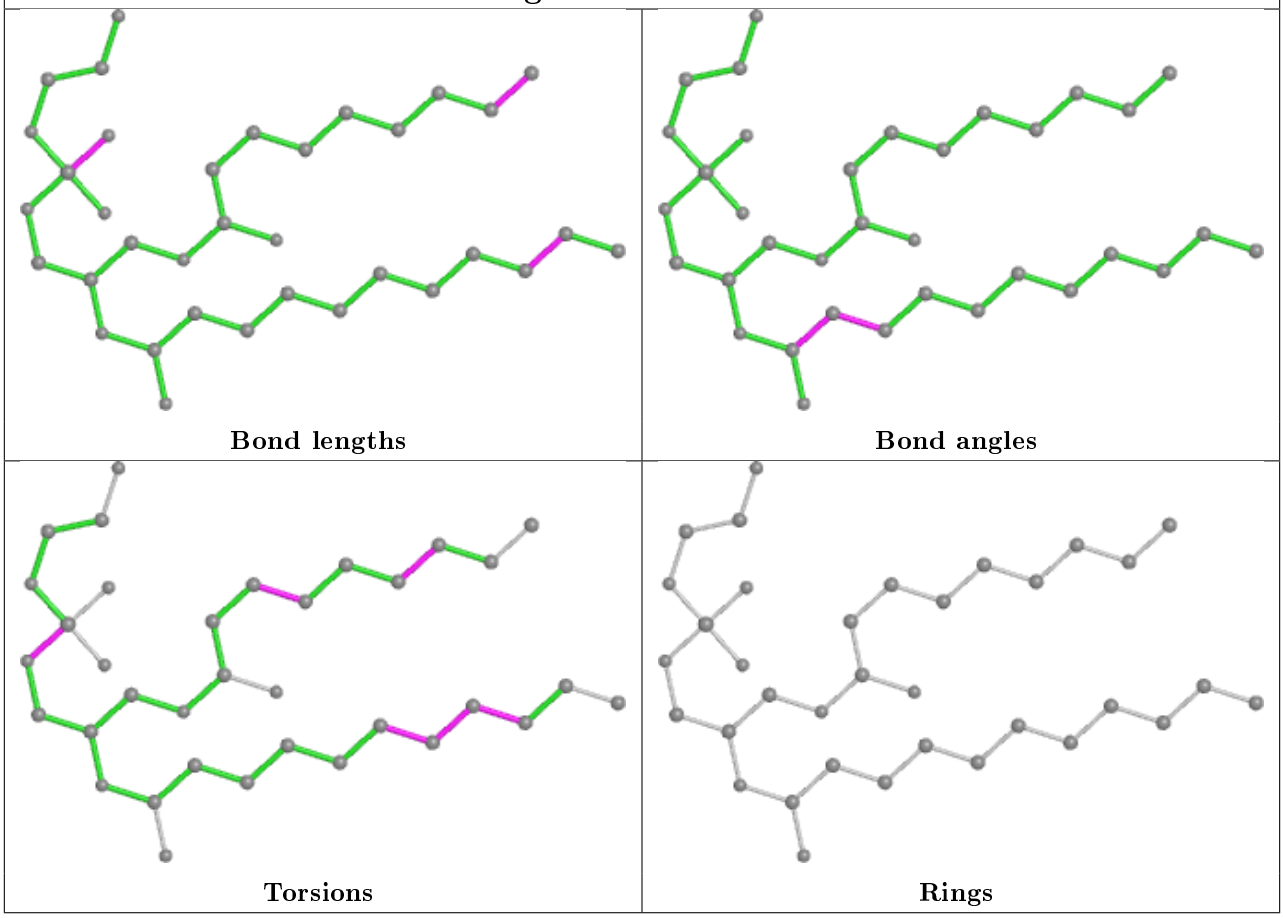
9 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	302	FES	2	0
13	C	309	EPH	1	0
10	B	304	F3S	3	0
14	D	306	UQ2	4	0
12	C	308	CDN	5	0
7	A	601	FAD	8	0
5	A	589	OAA	3	0
11	C	305	HEM	5	0
9	B	303	SF4	1	0

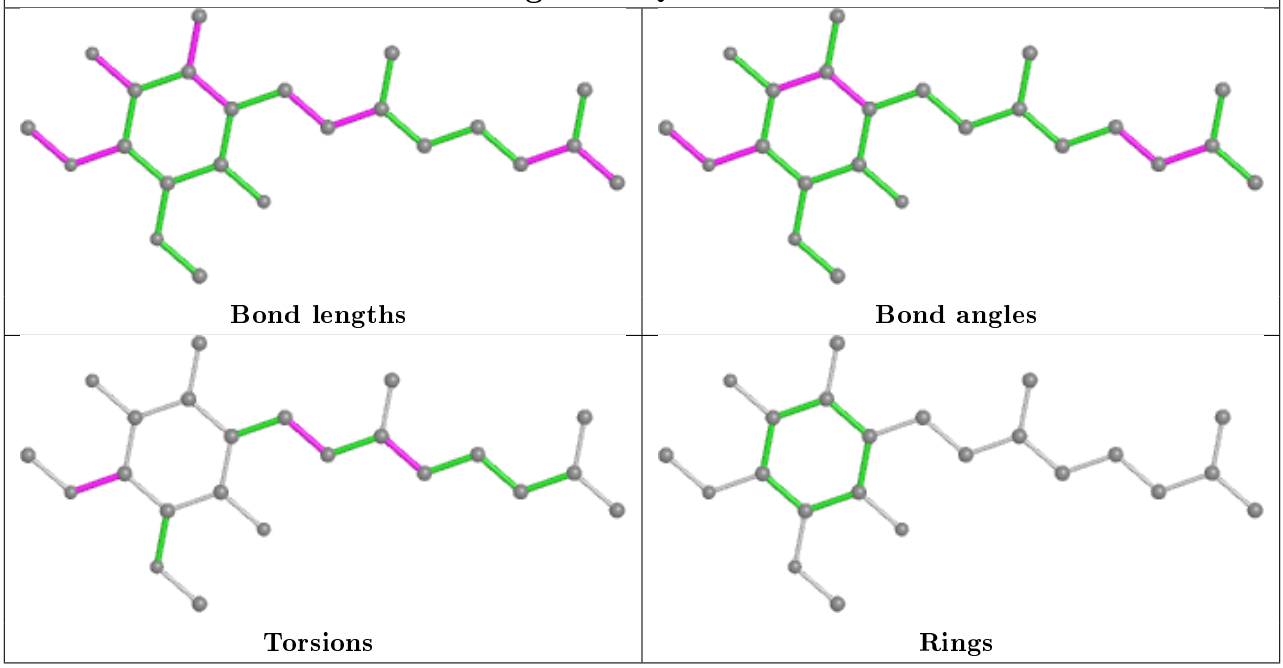
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

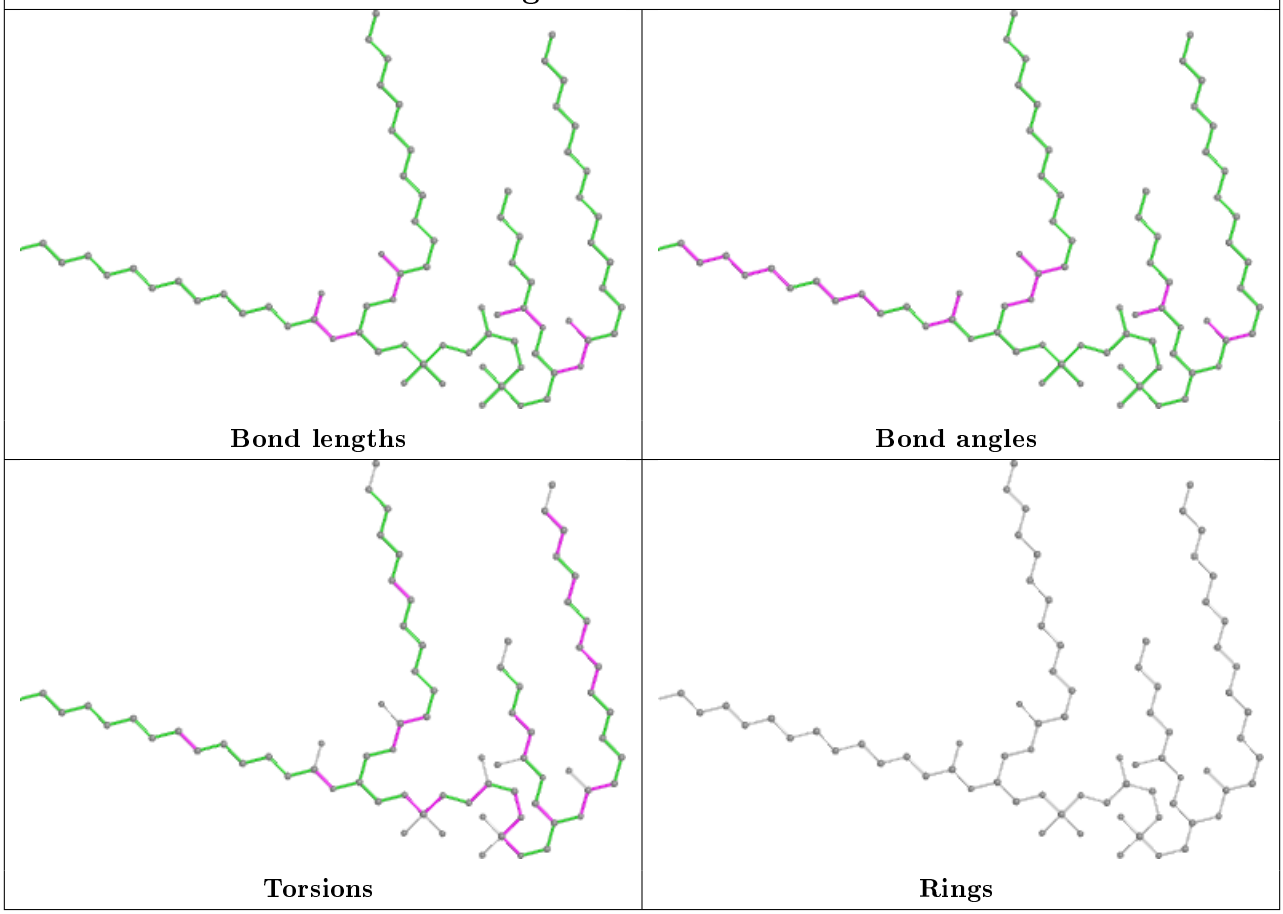
Ligand EPH C 309



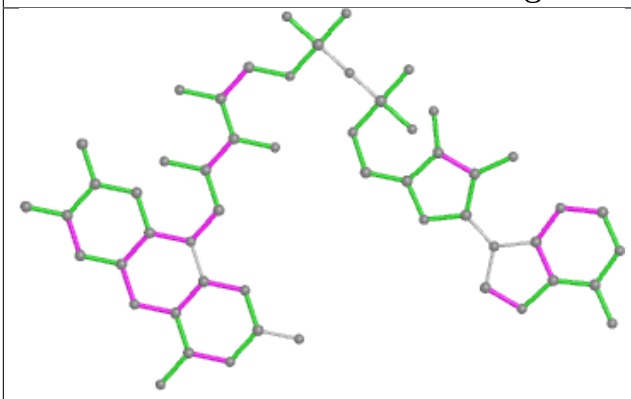
Ligand UQ2 D 306



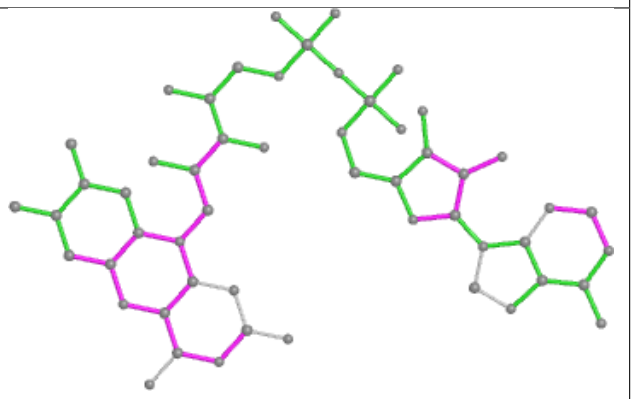
Ligand CDN C 308



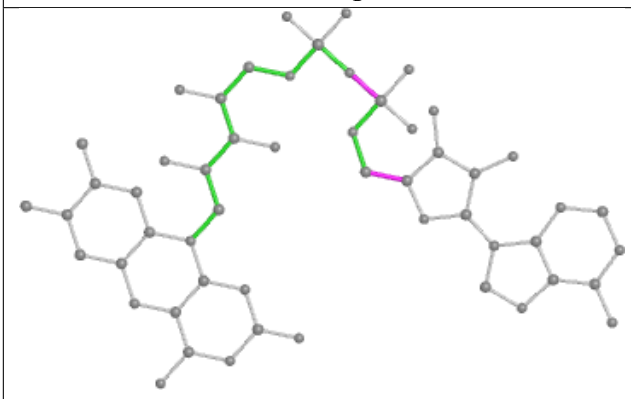
Ligand FAD A 601



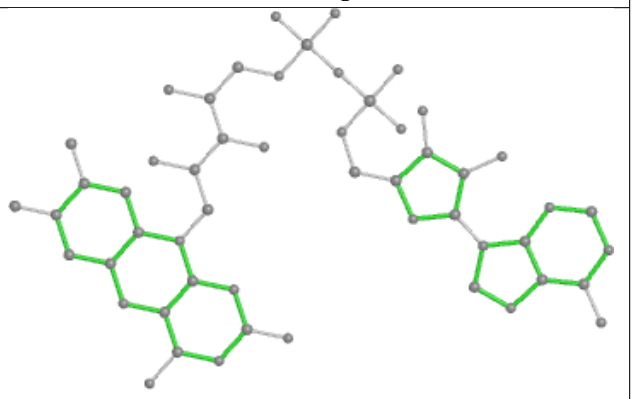
Bond lengths



Bond angles

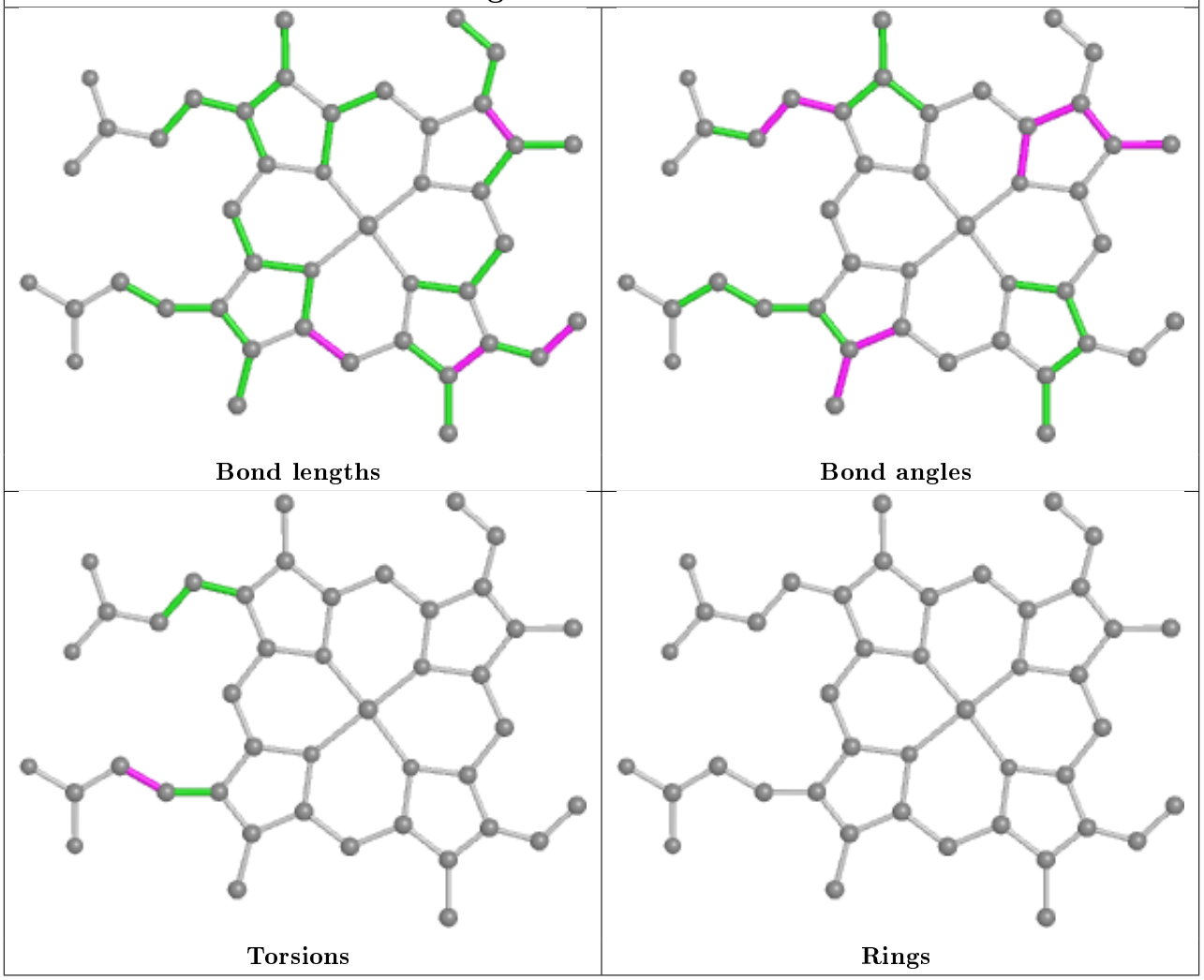


Torsions



Rings

Ligand HEM C 305



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.