Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:01 PM GMT

PDB ID	:	3SFD
Title	:	crystal structure of porcine mitochondrial respiratory complex II bound with oxaloacetate and pentachlorophenol
Authors	:	Zhou, Q.J.; Zhai, Y.J.; Liu, M.; Sun, F.
Deposited on	:	2011-06-13
Resolution	:	2.61 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

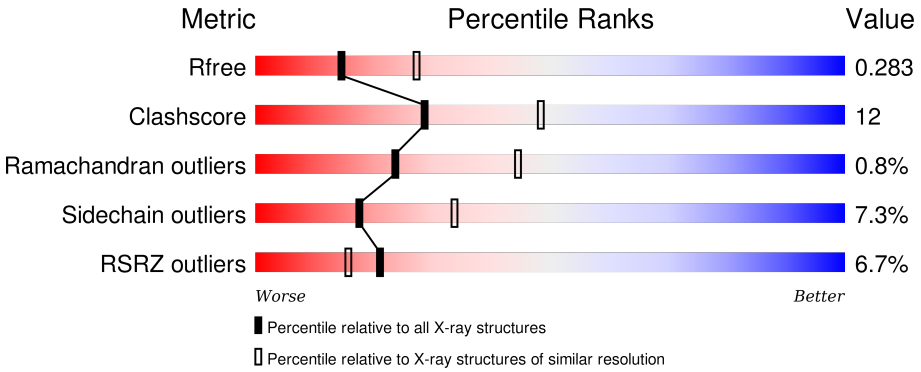
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.61 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))
R_{free}	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	622	6% 70% 26%
2	B	252	6% 71% 21% 5%
3	C	140	8% 80% 16%
4	D	103	7% 75% 21%

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
6	OAA	A	701	-	-	X	-
9	F3S	B	304	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8746 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 [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	613	4729	2954	848	895	32	0	0	0

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	239	1922	1214	326	360	22	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	252	VAL	ALA	SEE REMARK 999	UNP Q007T0

- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b560 subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	138	1064	695	179	183	7	0	0	0

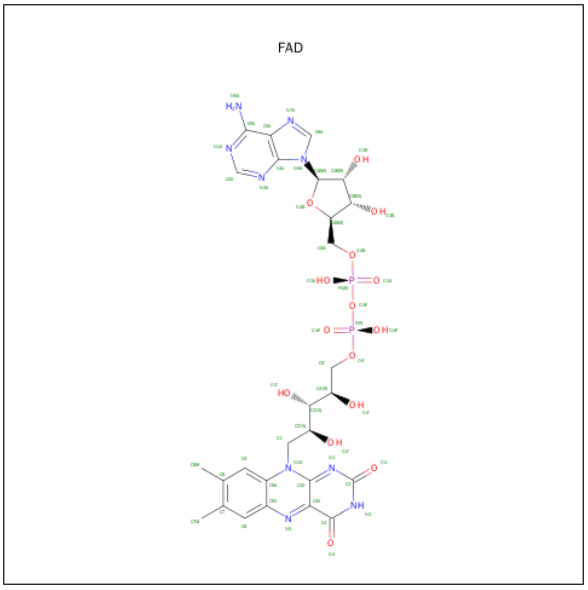
- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	102	765	499	128	133	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

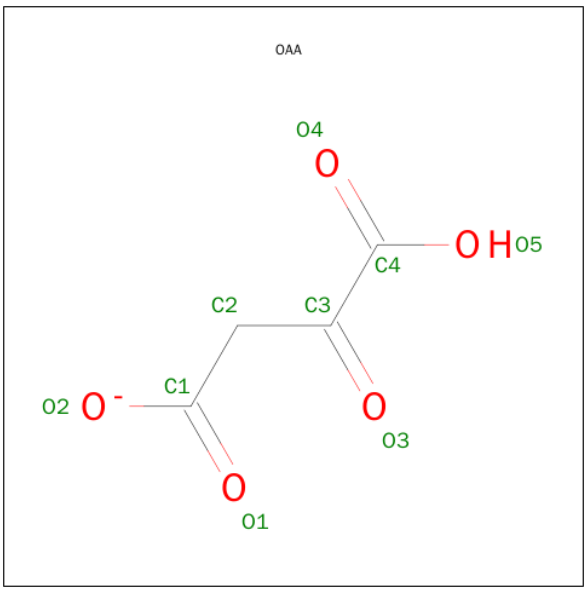
Chain	Residue	Modelled	Actual	Comment	Reference
D	100	ALA	VAL	SEE REMARK 999	UNP A5GZW8

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



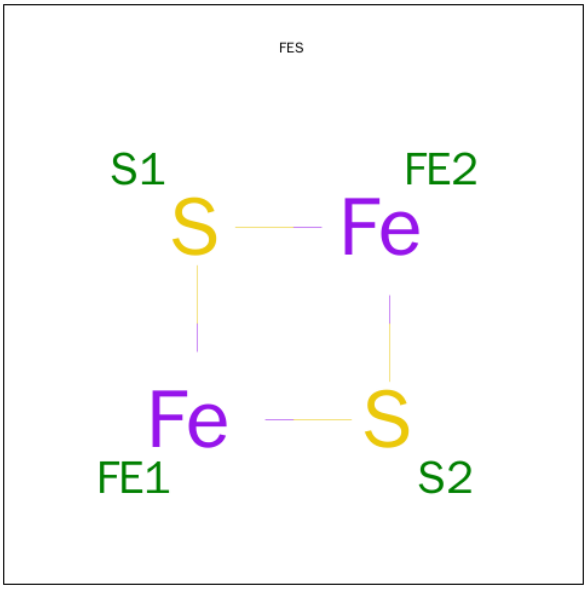
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	53	27	9	15	2	0	0

- Molecule 6 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



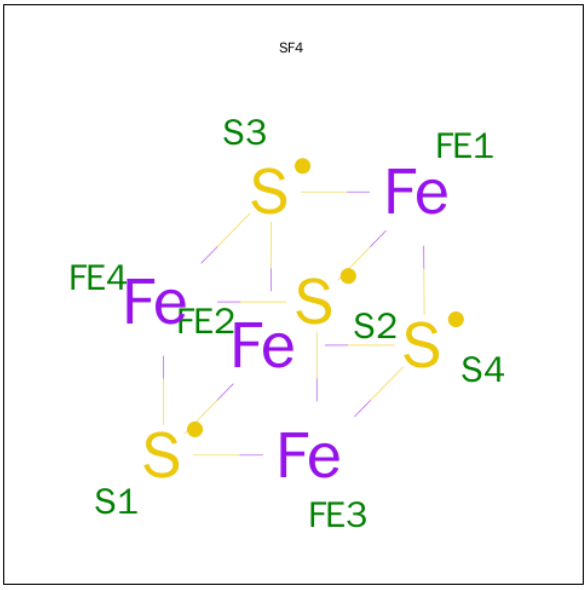
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 4 5	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



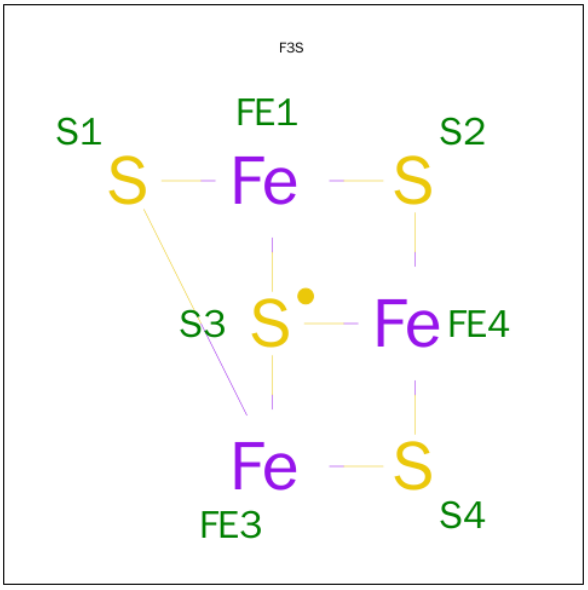
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Fe S 4 2 2	0	0

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



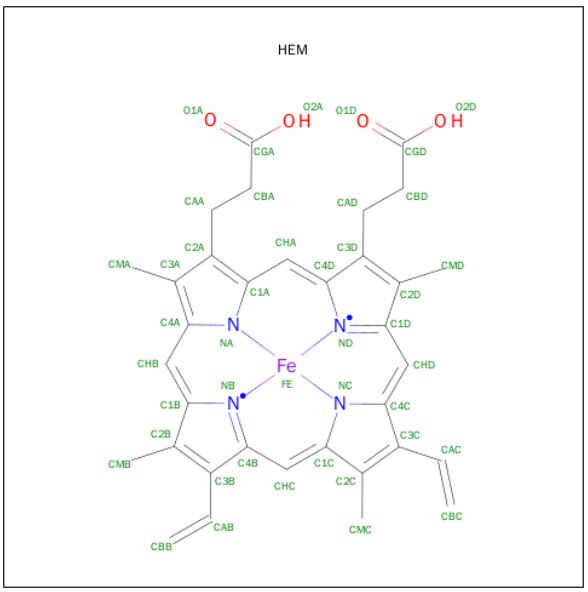
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe S 8 4 4	0	0

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



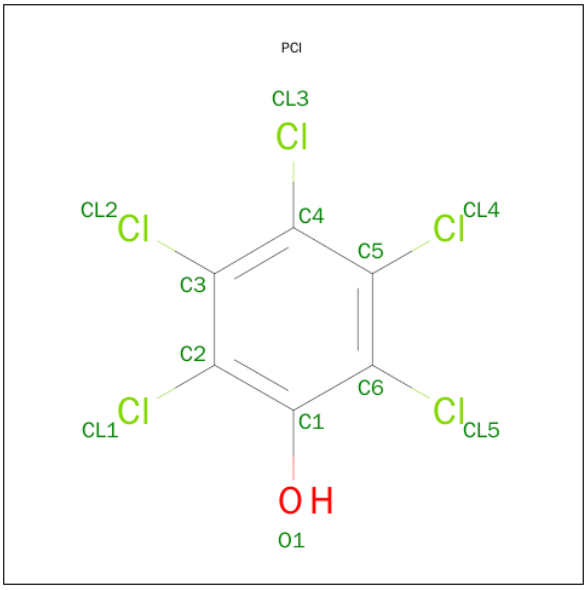
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 7 3 4	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 11 is PENTACHLOROPHENOL (three-letter code: PCI) (formula: C_6HCl_5O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	Cl	O	0	0
			12	6	5	1		

- Molecule 12 is water.

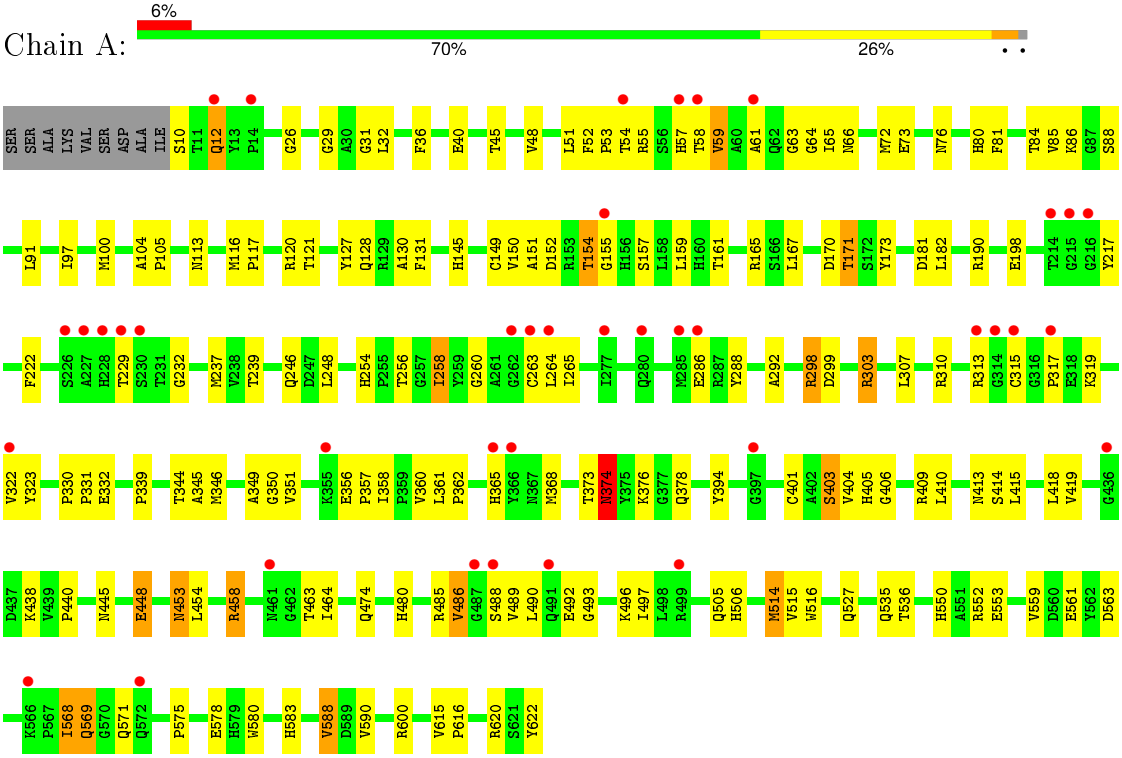
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	76	Total	O	0	0
			76	76		
12	B	30	Total	O	0	0
			30	30		
12	C	15	Total	O	0	0
			15	15		
12	D	9	Total	O	0	0
			9	9		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

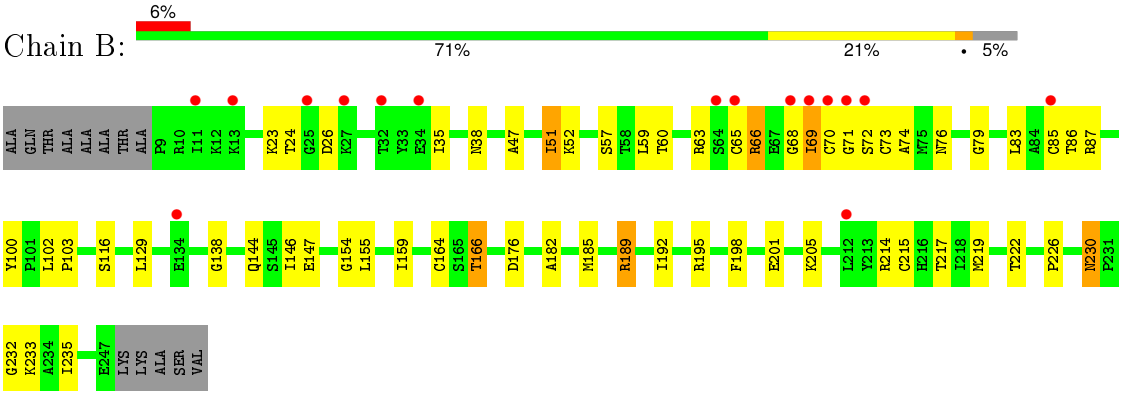
• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain A:



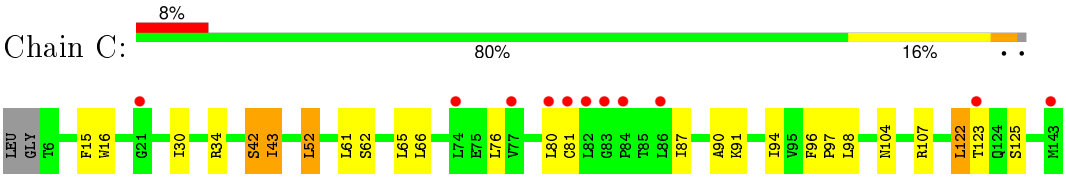
• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B:



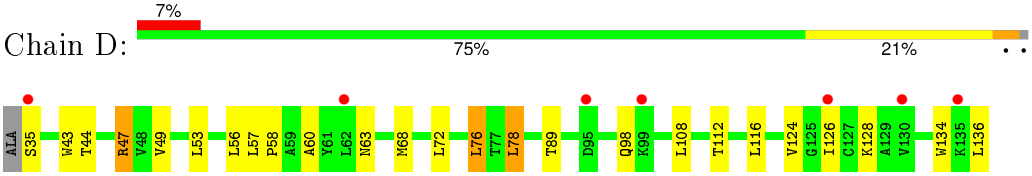
• Molecule 3: Succinate dehydrogenase cytochrome b560 subunit, mitochondrial

Chain C:



• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.31Å 83.36Å 293.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 48.85 – 2.61	Depositor EDS
% Data completeness (in resolution range)	75.3 (50.00-2.61) 75.5 (48.85-2.61)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.57 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.242 , 0.286 0.242 , 0.283	Depositor DCC
R_{free} test set	2055 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 40348 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8746	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCI, OAA, SF4, F3S, FES, HEM, 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	0.37	0/4828	0.57	1/6531 (0.0%)
2	B	0.40	0/1964	0.54	0/2648
3	C	0.37	0/1091	0.52	0/1483
4	D	0.38	0/784	0.54	0/1066
All	All	0.38	0/8667	0.55	1/11728 (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	454	LEU	CA-CB-CG	5.09	127.01	115.30

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	4729	0	4618	127	0
2	B	1922	0	1900	47	0
3	C	1064	0	1104	17	0
4	D	765	0	773	13	0
5	A	53	0	31	14	0
6	A	9	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	4	0	0	1	0
8	B	8	0	0	1	0
9	B	7	0	0	3	0
10	C	43	0	30	1	0
11	D	12	0	0	1	0
12	A	76	0	0	6	0
12	B	30	0	0	2	0
12	C	15	0	0	0	0
12	D	9	0	0	1	0
All	All	8746	0	8456	196	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 12.

All (196) 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:57:HIS:NE2	5:A:700:FAD:HM82	1.54	1.23
1:A:57:HIS:CE1	5:A:700:FAD:HM82	1.95	1.01
1:A:58:THR:HG23	5:A:700:FAD:O1A	1.65	0.94
1:A:298:ARG:HH22	6:A:701:OAA:C1	1.86	0.89
1:A:373:THR:HG22	1:A:374:ASN:O	1.72	0.88
1:A:64:GLY:HA2	1:A:154:THR:HG21	1.58	0.84
1:A:171:THR:HB	1:A:173:TYR:CE1	2.12	0.82
2:B:102:LEU:HD22	2:B:166:THR:HG21	1.61	0.82
1:A:303:ARG:HH11	1:A:303:ARG:HG2	1.44	0.81
1:A:152:ASP:HB2	1:A:339:PRO:HD2	1.64	0.80
2:B:164:CYS:SG	2:B:182:ALA:HB2	2.22	0.79
1:A:29:GLY:H	1:A:58:THR:HG21	1.52	0.73
1:A:181:ASP:HA	1:A:237:MET:HG2	1.72	0.72
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.72	0.71
3:C:42:SER:HB3	11:D:1:PCI:CL4	2.28	0.70
1:A:150:VAL:H	1:A:154:THR:HG23	1.54	0.70
1:A:299:ASP:O	1:A:303:ARG:HB2	1.92	0.69
1:A:58:THR:HG22	5:A:700:FAD:O4'	1.93	0.68
2:B:215:CYS:HA	9:B:304:F3S:S4	2.33	0.68
2:B:69:ILE:O	2:B:159:ILE:HD12	1.94	0.67
1:A:319:LYS:HA	12:A:696:HOH:O	1.95	0.66
3:C:61:LEU:O	3:C:65:LEU:HG	1.96	0.65
1:A:409:ARG:HH22	6:A:701:OAA:C1	2.09	0.65
1:A:222:PHE:HA	1:A:474:GLN:HE21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:CYS:SG	2:B:72:SER:OG	2.46	0.64
2:B:129:LEU:HD11	2:B:195:ARG:HB2	1.80	0.64
1:A:51:LEU:HD21	1:A:229:THR:HG21	1.80	0.64
1:A:113:ASN:HD22	2:B:138:GLY:H	1.45	0.64
2:B:52:LYS:HD2	2:B:57:SER:HA	1.80	0.63
1:A:171:THR:HB	1:A:173:TYR:HE1	1.62	0.63
1:A:130:ALA:HB2	1:A:145:HIS:HD2	1.62	0.63
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.82	0.62
2:B:219:MET:HE1	9:B:304:F3S:S1	2.40	0.62
1:A:57:HIS:NE2	5:A:700:FAD:HM81	2.08	0.62
4:D:60:ALA:HA	4:D:68:MET:HG2	1.82	0.61
2:B:219:MET:HG3	3:C:122:LEU:HD21	1.83	0.61
1:A:26:GLY:O	1:A:31:GLY:HA3	2.01	0.61
2:B:219:MET:HE1	2:B:232:GLY:HA3	1.83	0.60
5:A:700:FAD:H8A	12:A:650:HOH:O	2.01	0.60
3:C:52:LEU:HD21	3:C:98:LEU:HA	1.84	0.60
1:A:414:SER:O	1:A:418:LEU:HD13	2.02	0.60
1:A:72:MET:HE1	1:A:121:THR:HG21	1.84	0.59
1:A:415:LEU:HG	5:A:700:FAD:C2	2.32	0.59
1:A:182:LEU:HD22	1:A:237:MET:HB3	1.85	0.59
2:B:230:ASN:ND2	2:B:233:LYS:H	1.99	0.59
1:A:86:LYS:O	1:A:620:ARG:HD2	2.03	0.58
2:B:35:ILE:HD11	2:B:51:ILE:HG22	1.85	0.58
1:A:361:LEU:HD12	1:A:362:PRO:HD2	1.84	0.58
1:A:113:ASN:ND2	2:B:138:GLY:H	2.01	0.58
3:C:91:LYS:HG3	4:D:134:TRP:CH2	2.37	0.58
2:B:176:ASP:HB3	3:C:16:TRP:CZ2	2.39	0.58
1:A:303:ARG:O	1:A:307:LEU:HB2	2.05	0.57
1:A:150:VAL:H	1:A:154:THR:CG2	2.18	0.56
1:A:72:MET:CE	1:A:121:THR:HG21	2.36	0.56
2:B:154:GLY:O	2:B:185:MET:HE1	2.05	0.56
1:A:322:VAL:HG12	1:A:323:TYR:N	2.20	0.55
1:A:48:VAL:HG12	5:A:700:FAD:H2A	1.87	0.55
2:B:103:PRO:HD2	2:B:166:THR:HG23	1.88	0.55
1:A:486:VAL:HG13	1:A:553:GLU:HB2	1.89	0.55
1:A:264:LEU:CB	5:A:700:FAD:HM73	2.36	0.54
1:A:130:ALA:HB2	1:A:145:HIS:CD2	2.42	0.54
1:A:52:PHE:HB3	1:A:55:ARG:HG2	1.88	0.54
4:D:89:THR:HA	4:D:98:GLN:HE22	1.73	0.54
1:A:463:THR:HG22	1:A:506:HIS:HB3	1.90	0.54
1:A:463:THR:HG23	1:A:464:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:ARG:HD2	3:C:125:SER:HB2	1.91	0.53
3:C:87:ILE:O	3:C:91:LYS:HB2	2.08	0.53
1:A:254:HIS:HB2	1:A:365:HIS:HB2	1.90	0.53
1:A:298:ARG:NH2	6:A:701:OAA:C1	2.66	0.52
2:B:83:LEU:HB2	2:B:86:THR:HG22	1.92	0.52
4:D:47:ARG:NH1	12:D:6:HOH:O	2.41	0.52
1:A:563:ASP:HB3	1:A:571:GLN:HE22	1.75	0.51
1:A:405:HIS:ND1	1:A:409:ARG:HG3	2.26	0.50
1:A:45:THR:HB	1:A:171:THR:HG23	1.93	0.50
1:A:323:TYR:HD2	1:A:357:PRO:HB2	1.76	0.50
2:B:230:ASN:CG	2:B:233:LYS:HB3	2.32	0.50
2:B:51:ILE:HD11	2:B:59:LEU:HD22	1.93	0.50
1:A:258:ILE:HG22	1:A:263:CYS:H	1.76	0.50
1:A:303:ARG:HG2	1:A:303:ARG:NH1	2.22	0.50
1:A:453:ASN:HD21	1:A:527:GLN:HE22	1.59	0.50
1:A:346:MET:O	1:A:350:GLY:N	2.35	0.50
1:A:568:ILE:O	1:A:569:GLN:HB2	2.12	0.50
1:A:288:TYR:HE2	1:A:307:LEU:HD23	1.75	0.49
2:B:230:ASN:ND2	2:B:233:LYS:HB3	2.27	0.49
2:B:76:ASN:HB3	2:B:100:TYR:HB2	1.94	0.49
1:A:254:HIS:HB2	1:A:365:HIS:CB	2.42	0.49
2:B:198:PHE:HD2	2:B:201:GLU:HG3	1.78	0.49
1:A:117:PRO:HA	12:A:629:HOH:O	2.12	0.49
1:A:248:LEU:HD12	1:A:535:GLN:HB2	1.93	0.49
1:A:445:ASN:O	1:A:448:GLU:HB2	2.13	0.49
1:A:374:ASN:OD1	1:A:378:GLN:NE2	2.40	0.48
1:A:265:ILE:HD13	1:A:360:VAL:HG12	1.95	0.48
1:A:66:ASN:HB3	1:A:80:HIS:CE1	2.48	0.48
2:B:219:MET:CE	9:B:304:F3S:S1	3.00	0.48
1:A:88:SER:HB2	1:A:406:GLY:HA3	1.95	0.48
2:B:23:LYS:HB3	2:B:26:ASP:HB2	1.95	0.48
2:B:79:GLY:HA3	3:C:34:ARG:HB2	1.94	0.48
1:A:378:GLN:HG2	1:A:394:TYR:CE2	2.49	0.48
1:A:264:LEU:HB3	5:A:700:FAD:HM73	1.96	0.48
2:B:222:THR:OG1	2:B:230:ASN:ND2	2.47	0.48
2:B:219:MET:CE	2:B:232:GLY:HA3	2.44	0.47
1:A:248:LEU:O	1:A:536:THR:HG23	2.14	0.47
2:B:47:ALA:O	2:B:51:ILE:HG23	2.14	0.47
1:A:52:PHE:O	1:A:53:PRO:C	2.53	0.47
2:B:155:LEU:HD13	2:B:189:ARG:HA	1.96	0.47
1:A:410:LEU:O	1:A:413:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:HD22	5:A:700:FAD:C6	2.44	0.47
3:C:90:ALA:O	3:C:94:ILE:HG12	2.15	0.47
1:A:492:GLU:O	1:A:496:LYS:HB2	2.14	0.47
12:B:262:HOH:O	4:D:35:SER:HB3	2.15	0.46
1:A:29:GLY:HA3	1:A:418:LEU:HD23	1.97	0.46
2:B:232:GLY:HA2	2:B:235:ILE:HD12	1.96	0.46
1:A:303:ARG:HH11	1:A:303:ARG:CG	2.22	0.46
1:A:493:GLY:O	1:A:497:ILE:HG12	2.15	0.46
4:D:57:LEU:HB2	4:D:58:PRO:HD3	1.97	0.46
1:A:292:ALA:HB3	1:A:622:TYR:HB3	1.97	0.46
1:A:246:GLN:HE22	1:A:600:ARG:HE	1.64	0.46
1:A:480:HIS:HD2	1:A:489:VAL:O	1.99	0.46
1:A:217:TYR:HB3	1:A:232:GLY:HA3	1.97	0.46
2:B:226:PRO:HD2	8:B:303:SF4:S1	2.56	0.46
3:C:104:ASN:ND2	3:C:107:ARG:HE	2.14	0.45
1:A:485:ARG:NE	12:A:673:HOH:O	2.48	0.45
1:A:120:ARG:HG3	2:B:144:GLN:O	2.15	0.45
1:A:310:ARG:HA	12:A:684:HOH:O	2.15	0.45
2:B:116:SER:HB2	3:C:15:PHE:HD1	1.80	0.45
1:A:52:PHE:CE2	1:A:54:THR:HB	2.50	0.45
2:B:65:CYS:O	2:B:66:ARG:HG3	2.16	0.45
2:B:70:CYS:SG	2:B:72:SER:CB	3.04	0.45
2:B:38:ASN:HB2	12:B:264:HOH:O	2.16	0.45
1:A:322:VAL:HG12	1:A:323:TYR:H	1.81	0.45
1:A:97:ILE:HA	1:A:404:VAL:HG23	1.98	0.45
1:A:458:ARG:NH2	1:A:514:MET:HG2	2.32	0.45
4:D:72:LEU:HB3	4:D:126:ILE:HD11	1.98	0.45
1:A:84:THR:HA	1:A:410:LEU:HD22	1.99	0.45
1:A:458:ARG:HH22	1:A:514:MET:HG2	1.81	0.45
1:A:190:ARG:CD	1:A:440:PRO:HB2	2.47	0.44
1:A:322:VAL:CG1	1:A:323:TYR:N	2.79	0.44
1:A:36:PHE:O	1:A:40:GLU:HB2	2.17	0.44
1:A:322:VAL:CG1	1:A:323:TYR:H	2.31	0.44
1:A:563:ASP:H	1:A:571:GLN:NE2	2.16	0.44
2:B:230:ASN:C	2:B:230:ASN:HD22	2.20	0.44
1:A:415:LEU:O	1:A:419:VAL:HG23	2.18	0.44
1:A:59:VAL:HB	1:A:159:LEU:HD23	1.98	0.44
3:C:52:LEU:HB3	10:C:1305:HEM:HAC	2.00	0.43
1:A:52:PHE:CD1	1:A:53:PRO:HD2	2.53	0.43
3:C:43:ILE:H	3:C:43:ILE:HG13	1.42	0.43
2:B:102:LEU:HA	2:B:103:PRO:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:CD2	1:A:54:THR:HB	2.53	0.43
1:A:615:VAL:HA	1:A:616:PRO:HD3	1.88	0.43
2:B:66:ARG:HA	2:B:85:CYS:HB2	2.00	0.43
4:D:49:VAL:HG11	4:D:78:LEU:HD13	2.00	0.43
1:A:516:TRP:HB3	2:B:60:THR:HG21	2.01	0.43
1:A:26:GLY:HA2	5:A:700:FAD:H1B	2.00	0.43
4:D:124:VAL:HG13	4:D:128:LYS:CG	2.49	0.43
1:A:514:MET:HA	1:A:514:MET:CE	2.49	0.43
4:D:53:LEU:HD11	4:D:76:LEU:CD1	2.49	0.43
1:A:76:ASN:HA	12:A:657:HOH:O	2.19	0.42
1:A:550:HIS:CE1	1:A:552:ARG:HG2	2.54	0.42
1:A:559:VAL:HB	1:A:580:TRP:HB2	1.99	0.42
1:A:264:LEU:HD13	1:A:365:HIS:CE1	2.54	0.42
4:D:43:TRP:O	4:D:47:ARG:HG2	2.19	0.42
1:A:72:MET:H	1:A:128:GLN:HE21	1.67	0.42
2:B:68:GLY:HA2	7:B:302:FES:S1	2.59	0.42
2:B:198:PHE:CD2	2:B:201:GLU:HG3	2.54	0.42
1:A:91:LEU:O	1:A:583:HIS:CE1	2.72	0.42
1:A:239:THR:CG2	1:A:588:VAL:HG13	2.49	0.42
2:B:65:CYS:SG	2:B:68:GLY:N	2.92	0.42
1:A:254:HIS:HB2	1:A:365:HIS:CG	2.55	0.42
1:A:63:GLY:N	6:A:701:OAA:O5	2.52	0.42
3:C:52:LEU:CD1	3:C:97:PRO:HB2	2.50	0.42
1:A:149:CYS:HA	1:A:154:THR:CG2	2.50	0.42
1:A:72:MET:HE3	1:A:127:TYR:HA	2.01	0.42
1:A:485:ARG:HB3	1:A:490:LEU:HD11	2.02	0.42
2:B:102:LEU:HD22	2:B:166:THR:CG2	2.41	0.42
1:A:100:MET:SD	1:A:404:VAL:HG21	2.60	0.42
1:A:264:LEU:HD22	5:A:700:FAD:H6	2.01	0.41
2:B:66:ARG:HD2	2:B:66:ARG:O	2.20	0.41
1:A:198:GLU:O	1:A:515:VAL:HG13	2.21	0.41
4:D:124:VAL:HG13	4:D:128:LYS:HG2	2.02	0.41
1:A:81:PHE:O	1:A:85:VAL:HG12	2.20	0.41
1:A:116:MET:HA	1:A:161:THR:HG21	2.02	0.41
1:A:374:ASN:HB3	1:A:376:LYS:H	1.84	0.41
1:A:346:MET:HA	1:A:351:VAL:H	1.85	0.41
1:A:409:ARG:NH2	6:A:701:OAA:O1	2.54	0.41
3:C:96:PHE:HB3	3:C:97:PRO:CD	2.51	0.41
1:A:351:VAL:HG13	1:A:356:GLU:HG3	2.02	0.41
3:C:62:SER:HB2	3:C:66:LEU:HD12	2.02	0.40
4:D:112:THR:O	4:D:116:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:HIS:NE2	5:A:700:FAD:C8	2.82	0.40
1:A:330:PRO:HA	1:A:331:PRO:HD3	1.96	0.40
1:A:10:SER:C	1:A:12:GLN:H	2.24	0.40
1:A:345:ALA:O	1:A:349:ALA:HB3	2.20	0.40
1:A:575:PRO:HG2	1:A:578:GLU:HB2	2.02	0.40
1:A:254:HIS:CD2	1:A:256:THR:H	2.39	0.40
2:B:71:GLY:HA3	2:B:159:ILE:CG2	2.52	0.40
1:A:401:CYS:C	1:A:403:SER:H	2.23	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	611/622 (98%)	559 (92%)	46 (8%)	6 (1%)	19	37
2	B	237/252 (94%)	217 (92%)	17 (7%)	3 (1%)	15	29
3	C	136/140 (97%)	130 (96%)	6 (4%)	0	100	100
4	D	100/103 (97%)	97 (97%)	3 (3%)	0	100	100
All	All	1084/1117 (97%)	1003 (92%)	72 (7%)	9 (1%)	24	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ASN
1	A	151	ALA
1	A	569	GLN
2	B	24	THR
2	B	74	ALA
1	A	317	PRO
2	B	73	CYS

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Mol	Chain	Res	Type
1	A	286	GLU
1	A	260	GLY

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	499/506 (99%)	464 (93%)	35 (7%)	19	36
2	B	214/221 (97%)	200 (94%)	14 (6%)	21	41
3	C	117/118 (99%)	108 (92%)	9 (8%)	16	30
4	D	76/76 (100%)	68 (90%)	8 (10%)	8	15
All	All	906/921 (98%)	840 (93%)	66 (7%)	17	34

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	32	LEU
1	A	59	VAL
1	A	65	ILE
1	A	73	GLU
1	A	131	PHE
1	A	154	THR
1	A	157	SER
1	A	165	ARG
1	A	167	LEU
1	A	170	ASP
1	A	171	THR
1	A	258	ILE
1	A	298	ARG
1	A	303	ARG
1	A	313	ARG
1	A	315	CYS
1	A	332	GLU
1	A	344	THR

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Mol	Chain	Res	Type
1	A	358	ILE
1	A	368	MET
1	A	374	ASN
1	A	403	SER
1	A	438	LYS
1	A	448	GLU
1	A	453	ASN
1	A	458	ARG
1	A	486	VAL
1	A	488	SER
1	A	505	GLN
1	A	514	MET
1	A	561	GLU
1	A	568	ILE
1	A	588	VAL
1	A	590	VAL
2	B	51	ILE
2	B	63	ARG
2	B	66	ARG
2	B	69	ILE
2	B	87	ARG
2	B	146	ILE
2	B	147	GLU
2	B	166	THR
2	B	189	ARG
2	B	192	ILE
2	B	205	LYS
2	B	214	ARG
2	B	217	THR
2	B	230	ASN
3	C	30	ILE
3	C	42	SER
3	C	43	ILE
3	C	52	LEU
3	C	76	LEU
3	C	80	LEU
3	C	81	CYS
3	C	122	LEU
3	C	123	THR
4	D	44	THR
4	D	47	ARG
4	D	56	LEU

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Mol	Chain	Res	Type
4	D	63	ASN
4	D	76	LEU
4	D	78	LEU
4	D	108	LEU
4	D	136	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	44	ASN
1	A	80	HIS
1	A	113	ASN
1	A	128	GLN
1	A	143	GLN
1	A	156	HIS
1	A	160	HIS
1	A	246	GLN
1	A	254	HIS
1	A	321	HIS
1	A	384	ASN
1	A	408	ASN
1	A	453	ASN
1	A	474	GLN
1	A	480	HIS
1	A	527	GLN
1	A	550	HIS
1	A	571	GLN
1	A	579	HIS
2	B	39	ASN
2	B	92	ASN
2	B	121	GLN
2	B	174	ASN
2	B	220	ASN
2	B	230	ASN
3	C	17	ASN
3	C	23	ASN
3	C	29	HIS
3	C	104	ASN
4	D	98	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

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FAD	A	700	1	48,58,58	1.10	5 (10%)	54,89,89	2.08	11 (20%)
6	OAA	A	701	-	2,8,8	19.70	2 (100%)	2,10,10	20.46	1 (50%)
7	FES	B	302	2	0,4,4	0.00	-	0,4,4	0.00	-
8	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-
9	F3S	B	304	2	0,9,9	0.00	-	0,15,15	0.00	-
10	HEM	C	1305	3,4	30,50,50	4.04	15 (50%)	24,82,82	2.51	9 (37%)
11	PCI	D	1	-	12,12,12	2.07	5 (41%)	18,18,18	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	A	700	1	-	0/30/50/50	0/6/6/6
6	OAA	A	701	-	-	0/2/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	B	302	2	-	0/0/4/4	0/1/1/1
8	SF4	B	303	2	-	0/0/48/48	0/6/5/5
9	F3S	B	304	2	-	0/0/24/24	0/0/3/3
10	HEM	C	1305	3,4	-	0/10/54/54	0/0/8/8
11	PCI	D	1	-	-	0/0/0/0	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	OAA	C2-C3	-27.15	1.26	1.51
10	C	1305	HEM	C3B-C4B	-14.39	1.39	1.51
10	C	1305	HEM	C3D-C4D	-9.62	1.39	1.51
10	C	1305	HEM	C2D-C3D	-5.03	1.39	1.54
10	C	1305	HEM	C2B-C1B	-3.73	1.39	1.51
10	C	1305	HEM	C2D-C1D	-3.73	1.39	1.51
5	A	700	FAD	C9A-N10	2.06	1.41	1.38
5	A	700	FAD	O4B-C1B	2.13	1.43	1.41
10	C	1305	HEM	FE-NB	2.30	2.09	1.97
10	C	1305	HEM	FE-ND	2.35	2.09	1.97
11	D	1	PCI	C2-CL1	2.73	1.78	1.72
10	C	1305	HEM	C4A-CHB	2.85	1.47	1.39
11	D	1	PCI	C5-CL4	2.88	1.78	1.72
11	D	1	PCI	C3-CL2	2.90	1.79	1.72
10	C	1305	HEM	C1A-CHA	2.95	1.48	1.39
5	A	700	FAD	C8-C7	3.17	1.49	1.41
5	A	700	FAD	C9A-C5X	3.26	1.49	1.42
11	D	1	PCI	C6-CL5	3.27	1.79	1.72
10	C	1305	HEM	CHD-C1D	3.30	1.48	1.38
10	C	1305	HEM	CHC-C4B	3.41	1.48	1.38
5	A	700	FAD	C10-N10	3.43	1.43	1.39
10	C	1305	HEM	C2A-C3A	3.60	1.48	1.37
11	D	1	PCI	C4-CL3	3.64	1.80	1.72
10	C	1305	HEM	FE-NC	3.66	2.10	1.95
10	C	1305	HEM	CHD-C4C	4.99	1.48	1.36
10	C	1305	HEM	CHC-C1C	5.25	1.48	1.36
6	A	701	OAA	O3-C3	6.22	1.33	1.22

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	700	FAD	N3A-C2A-N1A	-9.20	121.85	128.89
10	C	1305	HEM	C3C-CAC-CBC	-3.22	119.52	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	1305	HEM	C3B-CAB-CBB	-2.64	120.41	124.46
5	A	700	FAD	C1B-N9A-C4A	-2.59	123.03	126.94
5	A	700	FAD	C4X-C4-N3	-2.59	120.05	123.59
10	C	1305	HEM	CAA-CBA-CGA	-2.40	108.36	112.75
5	A	700	FAD	C4A-C5A-N7A	-2.32	107.34	109.48
5	A	700	FAD	P-O3P-PA	-2.23	126.48	132.73
5	A	700	FAD	C2B-C1B-N9A	-2.22	110.90	114.29
5	A	700	FAD	C4-C4X-C10	-2.01	118.65	119.94
5	A	700	FAD	C1'-C2'-C3'	2.24	116.23	109.82
10	C	1305	HEM	C2C-C1C-NC	2.79	114.92	110.21
10	C	1305	HEM	CMD-C2D-C3D	3.06	127.88	114.35
5	A	700	FAD	O4B-C1B-N9A	3.65	115.74	108.10
10	C	1305	HEM	CAD-C3D-C4D	4.16	127.13	112.47
5	A	700	FAD	C4X-N5-C5X	4.60	122.06	116.76
10	C	1305	HEM	CMC-C2C-C3C	4.92	128.82	116.53
10	C	1305	HEM	CMB-C2B-C3B	5.01	129.03	116.53
10	C	1305	HEM	CAD-C3D-C2D	5.45	128.88	113.22
5	A	700	FAD	C4-N3-C2	7.03	121.32	115.25
6	A	701	OAA	C1-C2-C3	28.92	168.16	115.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	FAD	14	0
6	A	701	OAA	5	0
7	B	302	FES	1	0
8	B	303	SF4	1	0
9	B	304	F3S	3	0
10	C	1305	HEM	1	0
11	D	1	PCI	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	613/622 (98%)	0.37	39 (6%)	23 17	33, 56, 98, 108	0
2	B	239/252 (94%)	0.32	16 (6%)	21 16	37, 52, 72, 76	0
3	C	138/140 (98%)	0.26	11 (7%)	15 10	50, 64, 89, 92	0
4	D	102/103 (99%)	0.36	7 (6%)	20 14	48, 65, 74, 77	0
All	All	1092/1117 (97%)	0.34	73 (6%)	21 16	33, 58, 92, 108	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	80	LEU	6.3
4	D	35	SER	6.2
3	C	82	LEU	6.0
1	A	280	GLN	4.9
2	B	11	ILE	4.6
3	C	84	PRO	4.0
1	A	226	SER	4.0
2	B	65	CYS	3.8
1	A	317	PRO	3.6
2	B	69	ILE	3.6
3	C	81	CYS	3.6
2	B	70	CYS	3.5
3	C	77	VAL	3.4
2	B	25	GLY	3.3
1	A	263	CYS	3.2
2	B	13	LYS	2.9
1	A	487	GLY	2.9
3	C	143	MET	2.9
3	C	74	LEU	2.9
1	A	227	ALA	2.8
4	D	130	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	229	THR	2.8
1	A	14	PRO	2.8
4	D	126	ILE	2.7
1	A	436	GLY	2.7
1	A	57	HIS	2.7
4	D	95	ASP	2.6
1	A	366	TYR	2.6
1	A	61	ALA	2.6
1	A	12	GLN	2.6
4	D	99	LYS	2.6
1	A	488	SER	2.6
2	B	68	GLY	2.6
2	B	34	GLU	2.5
1	A	277	ILE	2.5
1	A	230	SER	2.5
1	A	566	LYS	2.5
2	B	134	GLU	2.5
2	B	64	SER	2.5
1	A	54	THR	2.5
1	A	313	ARG	2.4
1	A	215	GLY	2.4
1	A	355	LYS	2.4
2	B	212	LEU	2.4
4	D	62	LEU	2.4
1	A	365	HIS	2.4
1	A	286	GLU	2.4
1	A	491	GLN	2.4
1	A	314	GLY	2.3
1	A	397	GLY	2.3
1	A	155	GLY	2.3
2	B	71	GLY	2.3
1	A	285	MET	2.3
2	B	72	SER	2.3
1	A	572	GLN	2.3
1	A	216	GLY	2.3
1	A	322	VAL	2.3
3	C	86	LEU	2.2
1	A	214	THR	2.2
1	A	228	HIS	2.2
1	A	461	ASN	2.2
1	A	499	ARG	2.2
1	A	58	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	123	THR	2.1
3	C	21	GLY	2.1
4	D	135	LYS	2.1
2	B	27	LYS	2.1
1	A	315	CYS	2.1
2	B	85	CYS	2.1
3	C	83	GLY	2.1
1	A	264	LEU	2.0
1	A	262	GLY	2.0
2	B	32	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	HEM	C	1305	43/43	0.94	0.21	0.93	69,73,74,75	0
6	OAA	A	701	9/9	0.94	0.28	0.71	77,77,78,78	0
5	FAD	A	700	53/53	0.96	0.25	-0.12	34,38,41,42	0
9	F3S	B	304	7/7	0.98	0.14	-0.82	35,40,41,43	0
8	SF4	B	303	8/8	0.98	0.16	-0.92	34,35,36,36	0
7	FES	B	302	4/4	0.98	0.20	-1.76	38,39,41,42	0
11	PCI	D	1	12/12	0.95	0.13	-1.89	34,35,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.