



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 AM GMT

PDB ID : 2H89
Title : Avian Respiratory Complex II with Malonate Bound
Authors : Huang, L.S.; Shen, J.T.; Wang, A.C.; Berry, E.A.
Deposited on : 2006-06-06
Resolution : 2.40 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

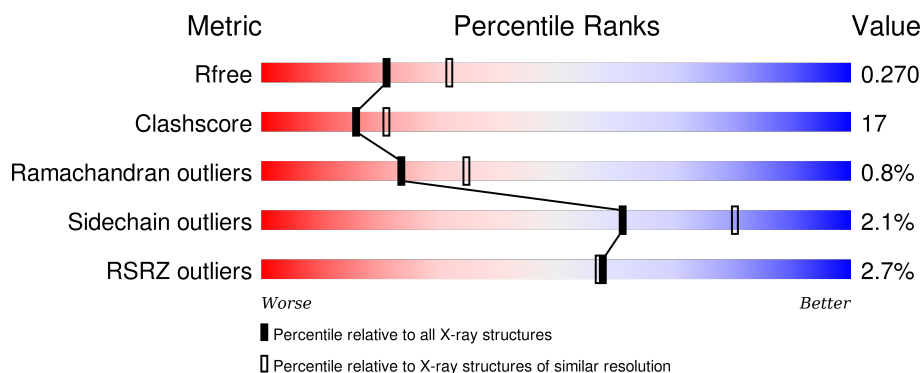
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 $\leq 5\%$. 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	621	<div> <div>2%</div> <div>64%</div> <div>34%</div> <div>..</div> </div>
2	B	252	<div> <div>6%</div> <div>67%</div> <div>26%</div> <div>..</div> </div>
3	C	140	<div> <div>%</div> <div>61%</div> <div>38%</div> <div>..</div> </div>
4	D	103	<div> <div>81%</div> <div>17%</div> <div>..</div> </div>

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
12	BHG	C	141	X	-	-	X
14	PEE	C	143	-	-	-	X
14	PEE	D	105	-	-	-	X
7	MLI	A	1002	-	-	X	-
8	UNL	A	1017	-	-	-	X
8	UNL	B	1005	-	-	-	X
8	UNL	B	1014	-	-	-	X
8	UNL	C	144	-	-	-	X
8	UNL	C	149	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 9302 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	613	Total	C	N	O	S	0	0	1
			4727	2957	843	898	29			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	ARG	CYS	CONFLICT	UNP Q9YHT1
A	556	LEU	PHE	CONFLICT	UNP Q9YHT1
A	560	GLU	ASP	CONFLICT	UNP Q9YHT1

- Molecule 2 is a protein called Succinate dehydrogenase Ip subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	1
			1925	1218	326	359	22			

- Molecule 3 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total	C	N	O	S	0	0	0
			1077	706	178	189	4			

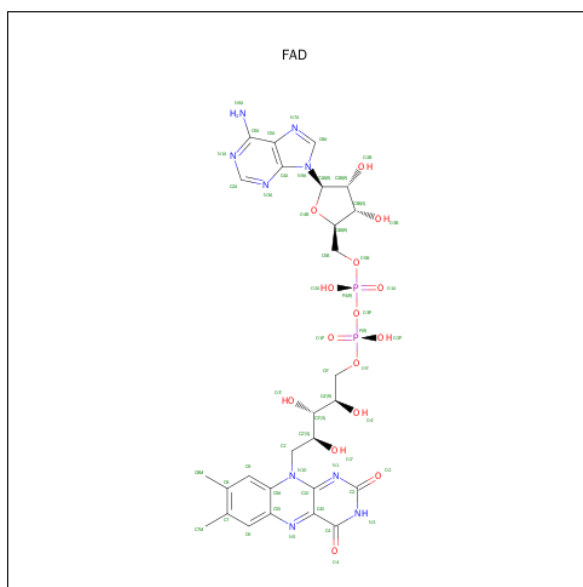
- Molecule 4 is a protein called SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			771	508	122	138	3			

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	A	1	Total K 1 1	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 7 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).

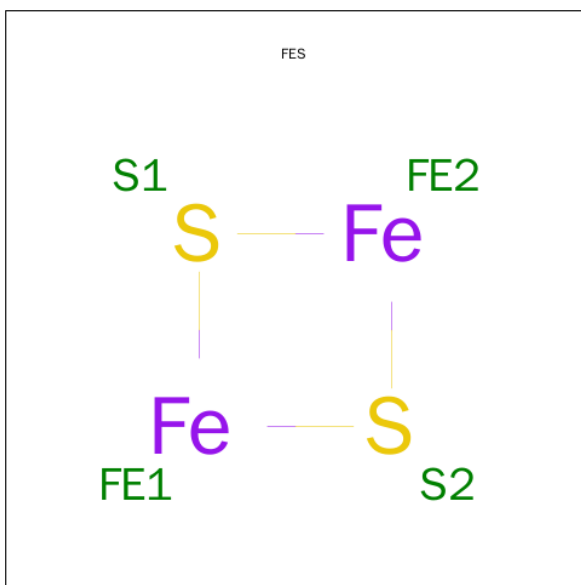


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 8 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

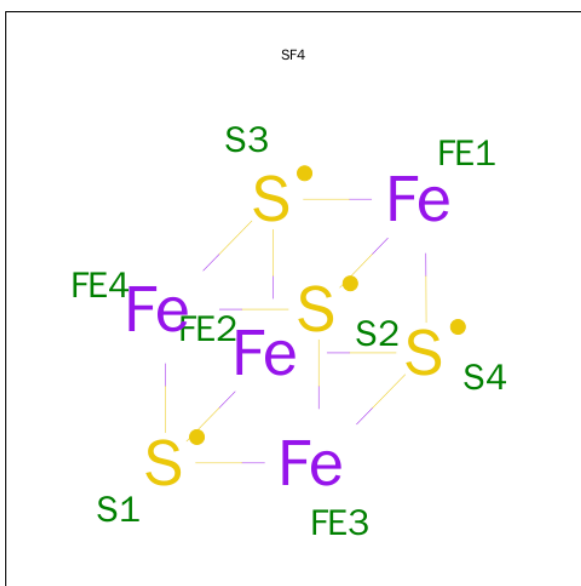
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	10	Total	C	O	0	0
			15	3	12		
8	A	15	Total	O		0	0
			15	15			
8	D	6	Total	O		0	0
			6	6			
8	C	9	Total	O		0	0
			11	11			

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



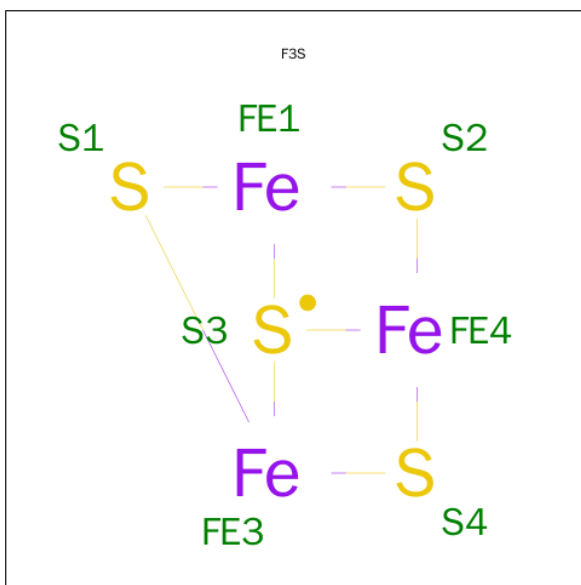
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



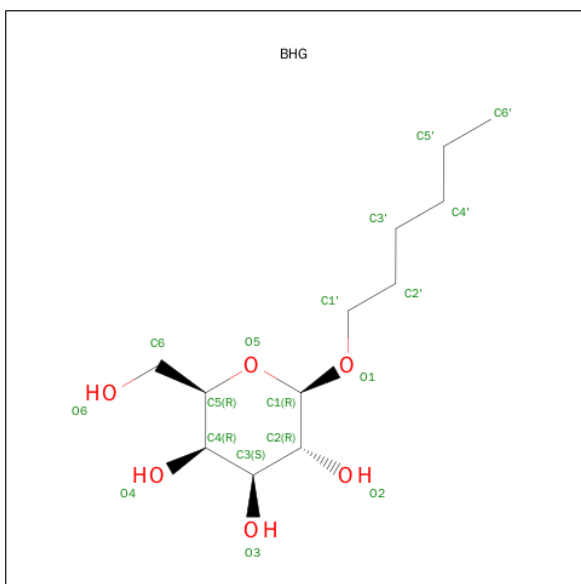
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 11 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



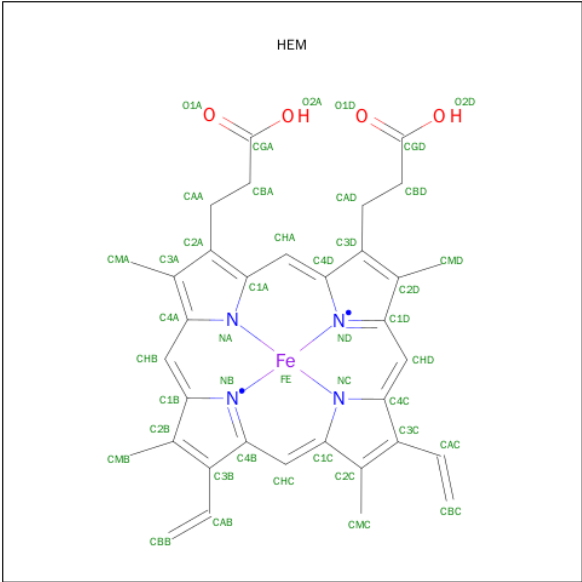
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 12 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula: $C_{12}H_{24}O_6$).



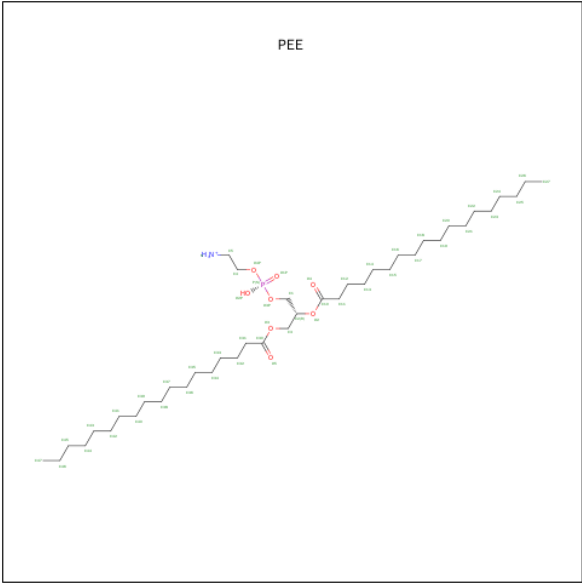
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			18	12	6		

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	
			41	32	1	4	4	

- Molecule 14 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	1	Total	C		
			11	11	0	0
14	D	1	Total	C		
			24	24	0	0

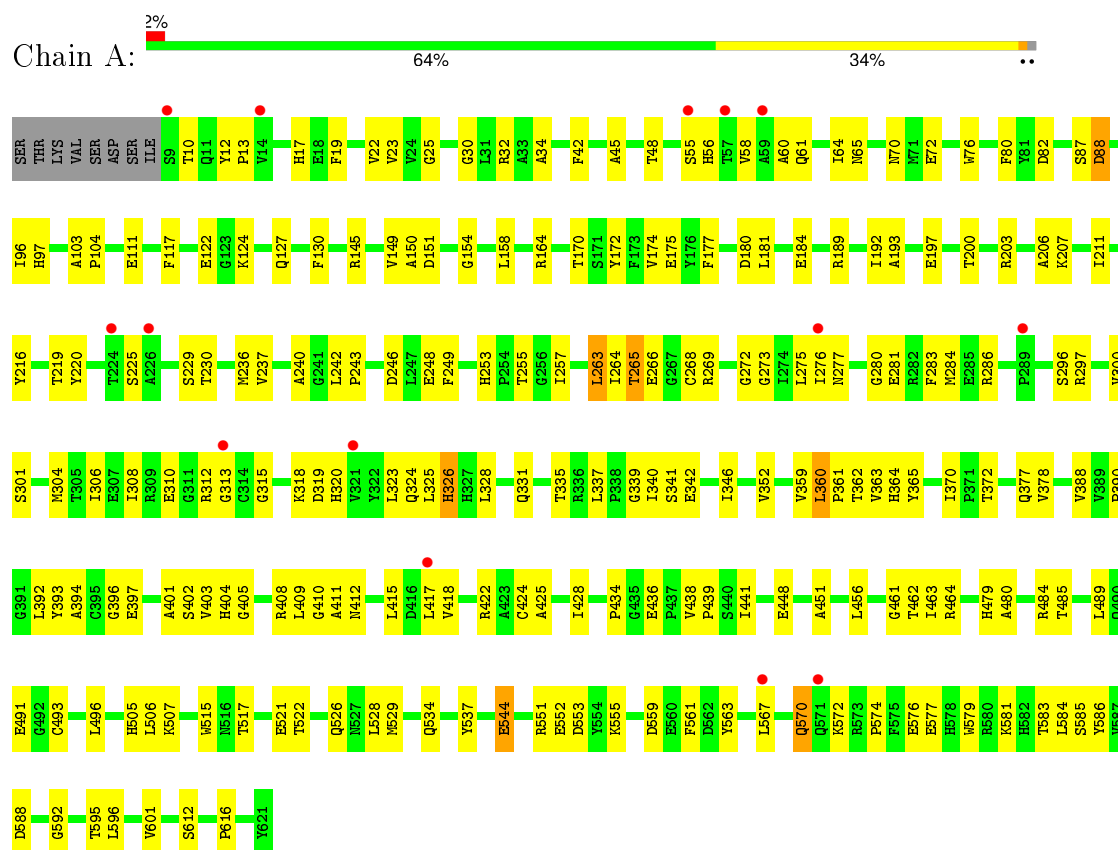
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	292	Total 292	O 292	0	0
15	B	166	Total 166	O 166	0	0
15	C	61	Total 61	O 61	0	0
15	D	61	Total 61	O 61	0	0

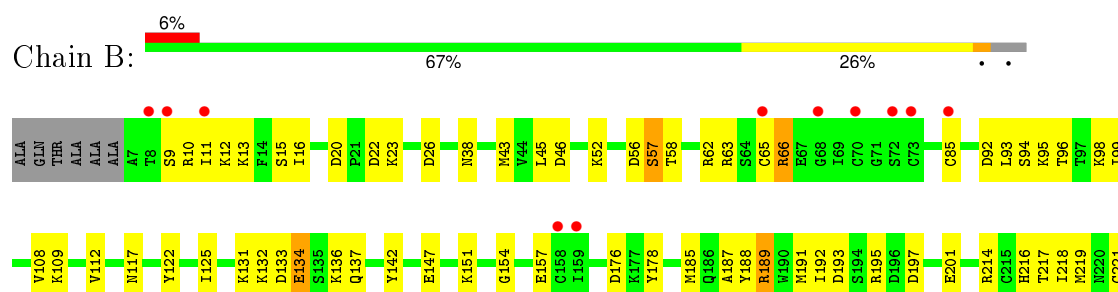
3 Residue-property plots

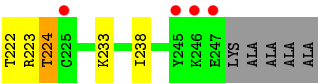
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 FLAVOPROTEIN SUBUNIT



• Molecule 2: Succinate dehydrogenase Ip subunit

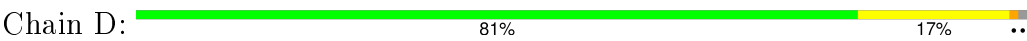




● Molecule 3: SUCCINATE DEHYDROGENASE CYTOCHROME B, LARGE SUBUNIT



● Molecule 4: SUCCINATE DEHYDROGENASE CYTOCHROME B, SMALL SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.52Å 84.12Å 292.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.74 – 2.40 50.74 – 2.29	Depositor EDS
% Data completeness (in resolution range)	86.3 (50.74-2.40) 79.7 (50.74-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.279 0.221 , 0.270	Depositor DCC
R_{free} test set	2909 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 63071 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9302	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: SF4, MLI, BHG, F3S, FES, PEE, HEM, UNL, K, 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	0.41	0/4827	0.66	0/6535
2	B	0.44	0/1966	0.68	0/2651
3	C	0.44	0/1106	0.61	0/1503
4	D	0.42	0/794	0.56	0/1089
All	All	0.42	0/8693	0.65	0/11778

There are no bond length outliers.

There are no bond angle outliers.

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	4727	0	4609	181	0
2	B	1925	0	1918	58	0
3	C	1077	0	1112	45	0
4	D	771	0	763	18	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	53	0	29	2	0
7	A	7	0	2	4	0
8	A	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	15	0	0	1	0
8	C	11	0	0	0	0
8	D	6	0	0	0	0
9	B	4	0	0	0	0
10	B	8	0	0	0	0
11	B	7	0	0	0	0
12	C	18	0	24	1	0
13	C	41	0	24	0	0
14	C	11	0	18	0	0
14	D	24	0	40	1	0
15	A	292	0	0	22	0
15	B	166	0	0	4	0
15	C	61	0	0	3	0
15	D	61	0	0	2	0
All	All	9302	0	8539	291	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 17.

All (291) 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:297:ARG:HH22	7:A:1002:MLI:C3	1.65	1.08
1:A:365:TYR:CE1	1:A:397:GLU:HG3	2.11	0.86
3:C:4:THR:OG1	3:C:7:GLU:HG3	1.77	0.85
1:A:401:ALA:N	1:A:402:SER:HA	1.98	0.77
3:C:115:LYS:HB3	3:C:118:GLN:OE1	1.86	0.76
2:B:187:ALA:O	2:B:191:MET:HG3	1.88	0.73
3:C:70:TYR:O	3:C:74:VAL:HG23	1.87	0.73
3:C:74:VAL:HA	3:C:77:LEU:HD12	1.70	0.73
1:A:297:ARG:HH22	7:A:1002:MLI:C1	2.03	0.71
1:A:297:ARG:NH2	7:A:1002:MLI:C3	2.49	0.71
1:A:464:ARG:HB3	1:A:507:LYS:HE3	1.73	0.71
1:A:277:ASN:HD21	1:A:281:GLU:HB3	1.55	0.70
1:A:177:PHE:O	1:A:193:ALA:HB1	1.90	0.70
4:D:24:LEU:N	4:D:25:PRO:HD2	2.07	0.70
1:A:281:GLU:HG2	1:A:283:PHE:N	2.07	0.70
2:B:65:CYS:O	2:B:66:ARG:HG3	1.93	0.69
2:B:15:SER:HB3	2:B:98:LYS:HG2	1.76	0.68
2:B:216:HIS:HB2	15:C:1145:HOH:O	1.92	0.68
1:A:424:CYS:O	1:A:428:ILE:HG13	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HG21	1:A:370:ILE:HD13	1.77	0.67
2:B:23:LYS:HB3	2:B:26:ASP:HB2	1.75	0.67
3:C:34:LEU:HB3	3:C:35:PRO:HD3	1.75	0.67
1:A:207:LYS:NZ	1:A:436:GLU:HB3	2.10	0.66
3:C:8:GLU:HG2	3:C:11:ARG:NH2	2.10	0.66
3:C:5:ALA:O	3:C:9:MET:HG3	1.97	0.65
1:A:268:CYS:HB3	1:A:325:LEU:HD21	1.78	0.64
3:C:69:HIS:O	3:C:73:VAL:HG23	1.97	0.64
1:A:306:ILE:O	1:A:310:GLU:HB2	1.97	0.64
2:B:45:LEU:HD22	2:B:85:CYS:HB3	1.80	0.64
1:A:403:VAL:HG23	1:A:404:HIS:CE1	2.34	0.63
3:C:106:LEU:HD22	15:D:1267:HOH:O	1.97	0.63
2:B:134:GLU:CD	2:B:134:GLU:H	2.02	0.62
2:B:133:ASP:OD1	2:B:136:LYS:HE3	2.00	0.62
3:C:26:HIS:CD2	3:C:27:ILE:H	2.16	0.62
1:A:410:GLY:O	1:A:411:ALA:HB3	1.98	0.62
1:A:122:GLU:HG3	15:A:1062:HOH:O	1.98	0.62
2:B:10:ARG:HD3	2:B:38:ASN:HD21	1.66	0.61
1:A:103:ALA:HB3	1:A:104:PRO:HD3	1.81	0.61
1:A:237:VAL:HG12	1:A:242:LEU:HB2	1.84	0.60
1:A:61:GLN:HB3	1:A:151:ASP:O	2.01	0.60
1:A:127:GLN:NE2	1:A:145:ARG:HA	2.17	0.60
1:A:563:TYR:HE1	15:A:1258:HOH:O	1.85	0.59
1:A:324:GLN:HG3	1:A:326:HIS:CE1	2.37	0.59
1:A:197:GLU:HB2	15:A:1262:HOH:O	2.03	0.59
1:A:574:PRO:HD2	1:A:577:GLU:HB2	1.84	0.59
1:A:189:ARG:HH11	1:A:439:PRO:HB2	1.68	0.58
1:A:340:ILE:HD12	1:A:341:SER:N	2.18	0.58
1:A:32:ARG:HH22	1:A:422:ARG:NH1	2.02	0.58
1:A:296:SER:O	1:A:300:VAL:HG23	2.03	0.58
2:B:13:LYS:HB3	2:B:96:THR:HG23	1.86	0.58
1:A:230:THR:HG22	1:A:528:LEU:HD11	1.86	0.57
2:B:122:TYR:O	2:B:125:ILE:HG12	2.04	0.57
2:B:11:ILE:O	2:B:93:LEU:HD22	2.04	0.57
1:A:263:LEU:HG	1:A:264:ILE:N	2.19	0.57
1:A:64:ILE:HD11	1:A:415:LEU:HA	1.87	0.57
2:B:189:ARG:HD3	2:B:189:ARG:C	2.25	0.57
1:A:402:SER:HB2	15:A:1060:HOH:O	2.03	0.57
2:B:217:THR:HG22	2:B:217:THR:O	2.04	0.57
3:C:65:GLU:HB2	3:C:70:TYR:CE1	2.40	0.56
1:A:515:TRP:HD1	15:A:1271:HOH:O	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:GLY:O	4:D:65:ILE:HG13	2.04	0.56
1:A:25:GLY:HA2	6:A:1001:FAD:H1B	1.86	0.56
1:A:479:HIS:O	1:A:489:LEU:HD23	2.04	0.56
1:A:448:GLU:O	1:A:451:ALA:HB3	2.04	0.56
2:B:151:LYS:HB3	2:B:192:ILE:HD12	1.87	0.56
1:A:493:CYS:HB3	1:A:537:TYR:CZ	2.40	0.56
1:A:277:ASN:ND2	1:A:281:GLU:HB3	2.21	0.56
1:A:19:PHE:CD2	1:A:45:ALA:HB2	2.41	0.55
1:A:576:GLU:CD	1:A:576:GLU:H	2.10	0.55
1:A:563:TYR:CD1	1:A:616:PRO:HB2	2.41	0.55
1:A:10:THR:O	1:A:10:THR:HG23	2.07	0.55
1:A:377:GLN:HG2	1:A:393:TYR:CE1	2.41	0.55
1:A:207:LYS:HZ2	1:A:436:GLU:HB3	1.72	0.55
1:A:340:ILE:HD12	1:A:340:ILE:C	2.27	0.55
1:A:312:ARG:HG3	1:A:312:ARG:HH11	1.72	0.54
2:B:10:ARG:HD3	2:B:38:ASN:ND2	2.22	0.54
2:B:154:GLY:H	2:B:157:GLU:CD	2.10	0.54
1:A:174:VAL:HG12	1:A:175:GLU:HG3	1.89	0.54
2:B:147:GLU:CD	2:B:147:GLU:H	2.11	0.54
1:A:266:GLU:HG3	1:A:269:ARG:NH2	2.21	0.54
1:A:32:ARG:NH2	1:A:422:ARG:HD2	2.22	0.54
3:C:81:PRO:O	3:C:84:ILE:HB	2.07	0.54
1:A:22:VAL:HG23	1:A:206:ALA:CB	2.37	0.54
2:B:131:LYS:HE3	2:B:195:ARG:O	2.08	0.54
3:C:93:PHE:N	3:C:94:PRO:HD2	2.23	0.54
2:B:20:ASP:HB3	2:B:23:LYS:HB2	1.90	0.54
1:A:300:VAL:HG12	15:A:1279:HOH:O	2.07	0.54
1:A:184:GLU:HB3	1:A:189:ARG:HE	1.74	0.53
1:A:276:ILE:HA	1:A:281:GLU:O	2.09	0.53
4:D:63:THR:HB	4:D:64:PRO:HD3	1.89	0.53
1:A:372:THR:HG21	1:A:394:ALA:HB3	1.90	0.53
1:A:237:VAL:CG1	1:A:242:LEU:HB2	2.39	0.53
1:A:253:HIS:O	1:A:361:PRO:HA	2.07	0.53
1:A:266:GLU:HG3	1:A:269:ARG:CZ	2.38	0.53
1:A:70:ASN:ND2	1:A:124:LYS:HB3	2.24	0.53
1:A:60:ALA:HB3	1:A:154:GLY:HA3	1.91	0.53
1:A:243:PRO:HB3	1:A:586:TYR:CZ	2.44	0.53
4:D:9:HIS:O	4:D:13:GLU:HG3	2.08	0.53
2:B:136:LYS:HB2	15:B:1138:HOH:O	2.09	0.53
1:A:534:GLN:NE2	1:A:585:SER:OG	2.42	0.52
3:C:137:ILE:HA	3:C:140:GLU:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG23	1:A:206:ALA:HB2	1.92	0.52
2:B:52:LYS:HG2	2:B:57:SER:HA	1.90	0.52
3:C:77:LEU:O	3:C:78:SER:C	2.48	0.52
4:D:62:ASP:HA	15:D:1384:HOH:O	2.11	0.51
1:A:220:TYR:CG	1:A:363:VAL:HG21	2.45	0.51
2:B:15:SER:O	2:B:98:LYS:HA	2.11	0.51
1:A:461:GLY:H	1:A:507:LYS:HB3	1.76	0.51
1:A:263:LEU:HD13	1:A:364:HIS:CE1	2.46	0.51
4:D:61:GLY:O	4:D:64:PRO:HD2	2.11	0.51
1:A:378:VAL:HG21	1:A:392:LEU:HG	1.93	0.51
1:A:559:ASP:HB3	15:A:1258:HOH:O	2.10	0.50
1:A:19:PHE:O	1:A:206:ALA:HA	2.11	0.50
1:A:496:LEU:HD22	1:A:529:MET:CE	2.41	0.50
3:C:45:THR:O	3:C:49:LEU:HG	2.11	0.50
1:A:237:VAL:O	1:A:240:ALA:HB3	2.12	0.50
1:A:489:LEU:HD12	1:A:551:ARG:NH1	2.26	0.50
1:A:372:THR:CG2	1:A:394:ALA:HB3	2.42	0.50
1:A:342:GLU:OE2	1:A:346:ILE:HD11	2.12	0.50
1:A:269:ARG:HA	1:A:273:GLY:O	2.12	0.50
1:A:438:VAL:HG23	1:A:439:PRO:HD2	1.94	0.49
1:A:441:ILE:HG13	1:A:441:ILE:O	2.11	0.49
2:B:62:ARG:NH1	2:B:112:VAL:HG13	2.27	0.49
1:A:418:VAL:HB	15:A:1042:HOH:O	2.12	0.49
2:B:20:ASP:OD1	2:B:22:ASP:N	2.45	0.49
1:A:170:THR:HB	1:A:172:TYR:HE1	1.76	0.49
1:A:189:ARG:HH11	1:A:439:PRO:CB	2.25	0.49
2:B:12:LYS:NZ	2:B:95:LYS:O	2.34	0.49
1:A:308:ILE:HD13	1:A:319:ASP:O	2.12	0.49
1:A:275:LEU:HD12	1:A:284:MET:HG3	1.94	0.49
4:D:24:LEU:N	4:D:25:PRO:CD	2.75	0.49
2:B:189:ARG:NH1	2:B:193:ASP:OD2	2.38	0.49
1:A:117:PHE:HA	1:A:149:VAL:HG22	1.94	0.49
4:D:25:PRO:O	4:D:29:LEU:HG	2.12	0.49
4:D:63:THR:HG22	4:D:64:PRO:N	2.27	0.49
3:C:37:ALA:O	3:C:40:ILE:HG22	2.13	0.49
1:A:19:PHE:CE2	1:A:45:ALA:HB2	2.48	0.49
1:A:181:LEU:HD21	1:A:211:ILE:HD11	1.94	0.49
1:A:401:ALA:N	1:A:402:SER:CA	2.71	0.48
3:C:8:GLU:HG2	3:C:11:ARG:HH21	1.78	0.48
1:A:255:THR:HG22	1:A:359:VAL:HG21	1.94	0.48
1:A:87:SER:O	1:A:88:ASP:C	2.51	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:VAL:O	3:C:51:LEU:HG	2.13	0.48
2:B:176:ASP:HB3	3:C:13:TRP:CZ2	2.48	0.48
2:B:188:TYR:HD1	2:B:191:MET:CE	2.27	0.48
1:A:207:LYS:HZ3	1:A:436:GLU:HB3	1.77	0.48
1:A:82:ASP:HA	15:A:1125:HOH:O	2.12	0.48
1:A:266:GLU:HA	15:A:1092:HOH:O	2.13	0.48
1:A:55:SER:O	1:A:58:VAL:HG12	2.13	0.48
1:A:409:LEU:O	1:A:412:ASN:HB2	2.14	0.47
2:B:223:ARG:HG3	2:B:223:ARG:HH11	1.79	0.47
1:A:65:ASN:ND2	1:A:411:ALA:HB3	2.29	0.47
2:B:189:ARG:O	2:B:189:ARG:HD3	2.15	0.47
8:B:1013:UNL:O1	4:D:6:ALA:HB2	2.14	0.47
4:D:101:TRP:CD1	14:D:105:PEE:H28	2.49	0.47
1:A:584:LEU:O	1:A:596:LEU:HA	2.13	0.47
1:A:586:TYR:HB2	1:A:595:THR:HB	1.96	0.47
3:C:89:PHE:HE1	3:C:135:ALA:N	2.12	0.47
1:A:544:GLU:HG2	1:A:579:TRP:CG	2.49	0.47
2:B:56:ASP:C	2:B:58:THR:H	2.18	0.47
1:A:216:TYR:CD1	1:A:216:TYR:O	2.68	0.47
3:C:57:SER:HB2	4:D:82:GLY:HA3	1.96	0.47
1:A:266:GLU:HB2	7:A:1002:MLI:O6	2.15	0.47
1:A:13:PRO:HG2	1:A:200:THR:HG22	1.97	0.47
1:A:461:GLY:HA3	1:A:505:HIS:O	2.15	0.47
1:A:65:ASN:O	1:A:415:LEU:HD22	2.15	0.47
1:A:517:THR:O	1:A:521:GLU:HG3	2.15	0.47
1:A:242:LEU:HB3	15:A:1048:HOH:O	2.14	0.46
3:C:40:ILE:HG23	3:C:41:THR:N	2.30	0.46
3:C:41:THR:HG22	3:C:97:TYR:CE2	2.50	0.46
1:A:365:TYR:CE2	1:A:408:ARG:HD3	2.50	0.46
2:B:201:GLU:OE1	2:B:201:GLU:N	2.47	0.46
1:A:561:PHE:CZ	1:A:572:LYS:HB2	2.51	0.46
1:A:388:VAL:O	1:A:390:PRO:HD3	2.15	0.46
1:A:456:LEU:HD13	1:A:522:THR:HG22	1.98	0.46
1:A:61:GLN:HB2	1:A:265:THR:HB	1.98	0.46
2:B:108:VAL:HG23	2:B:112:VAL:O	2.15	0.46
3:C:13:TRP:O	3:C:17:THR:HG23	2.16	0.46
2:B:185:MET:HB3	15:B:1027:HOH:O	2.14	0.46
1:A:581:LYS:HA	1:A:601:VAL:HG23	1.96	0.46
3:C:67:PHE:N	3:C:68:PRO:CD	2.79	0.46
1:A:301:SER:HA	15:A:1279:HOH:O	2.15	0.46
2:B:43:MET:O	2:B:46:ASP:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ARG:HG3	1:A:312:ARG:NH1	2.31	0.45
1:A:265:THR:HG22	1:A:340:ILE:HG21	1.98	0.45
1:A:422:ARG:O	1:A:425:ALA:HB3	2.16	0.45
2:B:223:ARG:HA	3:C:116:LEU:HD22	1.98	0.45
1:A:479:HIS:HE1	1:A:491:GLU:OE1	2.00	0.45
1:A:17:HIS:HB3	1:A:19:PHE:HE1	1.80	0.45
1:A:403:VAL:HG23	1:A:404:HIS:ND1	2.31	0.45
1:A:58:VAL:HB	1:A:158:LEU:HD23	1.99	0.45
1:A:56:HIS:CE1	1:A:225:SER:HA	2.52	0.45
1:A:561:PHE:N	15:A:1258:HOH:O	2.37	0.45
1:A:76:TRP:HH2	1:A:97:HIS:NE2	2.14	0.45
1:A:276:ILE:CG2	1:A:280:GLY:HA2	2.47	0.45
2:B:62:ARG:HD2	15:B:1067:HOH:O	2.16	0.44
3:C:107:VAL:HA	3:C:110:MET:CE	2.46	0.44
1:A:177:PHE:O	1:A:193:ALA:CB	2.63	0.44
2:B:221:CYS:O	2:B:224:THR:HG22	2.16	0.44
1:A:111:GLU:OE2	2:B:142:TYR:HB2	2.16	0.44
2:B:219:MET:HE3	2:B:222:THR:HB	1.99	0.44
1:A:164:ARG:HH22	2:B:137:GLN:HE22	1.65	0.44
1:A:552:GLU:O	1:A:555:LYS:HE3	2.17	0.44
1:A:42:PHE:CD1	1:A:434:PRO:HG3	2.53	0.44
1:A:276:ILE:HG23	1:A:280:GLY:HA2	1.98	0.44
1:A:192:ILE:HD12	1:A:203:ARG:HG2	1.99	0.44
1:A:365:TYR:HE1	1:A:397:GLU:HG3	1.76	0.44
1:A:339:GLY:HA3	15:A:1090:HOH:O	2.18	0.44
3:C:65:GLU:O	3:C:70:TYR:HE1	2.00	0.44
1:A:464:ARG:HB3	1:A:507:LYS:CE	2.46	0.44
2:B:191:MET:HB2	2:B:191:MET:HE3	1.83	0.43
3:C:107:VAL:HA	3:C:110:MET:HE3	1.99	0.43
1:A:315:GLY:HA3	1:A:320:HIS:CE1	2.53	0.43
2:B:188:TYR:HA	2:B:191:MET:HE2	2.00	0.43
1:A:283:PHE:O	1:A:286:ARG:HB3	2.18	0.43
1:A:567:LEU:O	1:A:570:GLN:HB2	2.17	0.43
1:A:396:GLY:HA2	1:A:417:LEU:CD2	2.48	0.43
1:A:313:GLY:O	1:A:318:LYS:HD2	2.18	0.43
1:A:170:THR:O	3:C:2:ALA:HB2	2.18	0.43
1:A:87:SER:HB2	1:A:405:GLY:HA3	2.00	0.43
3:C:63:LEU:HB3	3:C:70:TYR:OH	2.19	0.43
1:A:401:ALA:H	1:A:402:SER:HA	1.78	0.43
2:B:191:MET:CE	2:B:238:ILE:HG12	2.49	0.43
1:A:25:GLY:O	1:A:30:GLY:HA3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:ARG:NH1	4:D:58:TYR:OH	2.48	0.43
3:C:68:PRO:HA	4:D:99:MET:HE1	2.01	0.43
3:C:74:VAL:HG11	4:D:103:ILE:HD13	2.00	0.43
1:A:275:LEU:HD12	1:A:284:MET:CG	2.49	0.43
3:C:81:PRO:HA	3:C:84:ILE:HB	2.00	0.43
1:A:463:ILE:O	1:A:506:LEU:HA	2.19	0.43
1:A:246:ASP:HB3	1:A:249:PHE:HD1	1.84	0.43
1:A:284:MET:HB2	15:A:1074:HOH:O	2.19	0.43
1:A:246:ASP:HB3	1:A:249:PHE:CD1	2.54	0.43
2:B:233:LYS:HB2	3:C:114:PHE:HB3	2.00	0.42
1:A:237:VAL:HG21	1:A:370:ILE:CD1	2.47	0.42
1:A:403:VAL:CG2	1:A:404:HIS:CE1	3.02	0.42
1:A:275:LEU:HB2	15:A:1074:HOH:O	2.18	0.42
2:B:20:ASP:HB2	15:B:1080:HOH:O	2.18	0.42
3:C:137:ILE:O	3:C:140:GLU:HG2	2.18	0.42
2:B:178:TYR:CD1	2:B:214:ARG:HB2	2.55	0.42
2:B:117:ASN:HB2	3:C:12:PHE:CD2	2.55	0.42
1:A:362:THR:O	1:A:363:VAL:C	2.56	0.42
2:B:108:VAL:O	2:B:109:LYS:HB2	2.19	0.42
1:A:456:LEU:HD11	1:A:526:GLN:CD	2.40	0.42
1:A:313:GLY:O	1:A:318:LYS:CD	2.67	0.42
1:A:180:ASP:HA	1:A:236:MET:HG2	2.00	0.42
2:B:16:ILE:HG12	2:B:99:ILE:HB	2.02	0.42
1:A:255:THR:HG21	1:A:323:LEU:HD22	2.01	0.42
1:A:588:ASP:O	1:A:592:GLY:N	2.36	0.42
2:B:132:LYS:HE2	2:B:197:ASP:O	2.20	0.42
1:A:331:GLN:NE2	1:A:335:THR:OG1	2.53	0.42
1:A:310:GLU:OE1	1:A:312:ARG:NH2	2.42	0.42
1:A:10:THR:OG1	1:A:12:TYR:O	2.38	0.42
1:A:216:TYR:HD1	1:A:216:TYR:O	2.03	0.42
12:C:141:BHG:H6'1	15:C:1339:HOH:O	2.20	0.42
1:A:229:SER:HA	15:A:1257:HOH:O	2.18	0.42
1:A:263:LEU:HD22	6:A:1001:FAD:H6	2.02	0.41
1:A:304:MET:HE1	1:A:360:LEU:HA	2.02	0.41
4:D:63:THR:CB	4:D:64:PRO:HD3	2.50	0.41
1:A:304:MET:CE	1:A:361:PRO:HD3	2.50	0.41
1:A:484:ARG:HA	15:A:1070:HOH:O	2.19	0.41
1:A:268:CYS:HA	1:A:337:LEU:HD11	2.02	0.41
15:A:1269:HOH:O	3:C:15:LYS:HD2	2.21	0.41
15:A:1271:HOH:O	2:B:108:VAL:HG12	2.19	0.41
1:A:23:VAL:HG21	1:A:34:ALA:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:VAL:HG21	4:D:99:MET:CE	2.50	0.41
4:D:44:THR:HG21	4:D:80:PHE:HB2	2.03	0.41
3:C:115:LYS:HG3	15:C:1096:HOH:O	2.21	0.41
1:A:378:VAL:HG11	1:A:392:LEU:HD23	2.02	0.41
1:A:485:THR:HG22	15:A:1274:HOH:O	2.19	0.41
1:A:534:GLN:HG2	1:A:585:SER:HB2	2.02	0.41
1:A:76:TRP:CH2	1:A:97:HIS:CD2	3.08	0.41
3:C:27:ILE:HG23	3:C:28:SER:N	2.36	0.41
1:A:438:VAL:CG2	1:A:439:PRO:HD2	2.50	0.41
1:A:284:MET:HE1	1:A:300:VAL:HA	2.03	0.41
2:B:191:MET:HE2	2:B:238:ILE:HG12	2.04	0.40
1:A:61:GLN:CD	1:A:263:LEU:HD23	2.41	0.40
1:A:170:THR:HB	1:A:172:TYR:CE1	2.55	0.40
2:B:92:ASP:OD1	2:B:94:SER:OG	2.33	0.40
1:A:272:GLY:HA3	1:A:328:LEU:HD21	2.03	0.40
3:C:65:GLU:HG3	3:C:69:HIS:CE1	2.56	0.40
1:A:319:ASP:N	1:A:319:ASP:OD1	2.55	0.40
2:B:218:ILE:O	2:B:219:MET:HB2	2.20	0.40
1:A:553:ASP:N	1:A:553:ASP:OD1	2.48	0.40
15:A:1270:HOH:O	2:B:137:GLN:HG2	2.22	0.40
1:A:410:GLY:O	1:A:411:ALA:CB	2.63	0.40
2:B:131:LYS:HD2	2:B:142:TYR:CE2	2.57	0.40
1:A:248:GLU:OE2	1:A:583:THR:OG1	2.30	0.40
3:C:106:LEU:HA	3:C:106:LEU:HD23	1.89	0.40
1:A:149:VAL:O	1:A:150:ALA:C	2.60	0.40
1:A:80:PHE:CD1	1:A:96:ILE:HG22	2.57	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	610/621 (98%)	551 (90%)	53 (9%)	6 (1%)	19	28
2	B	238/252 (94%)	216 (91%)	20 (8%)	2 (1%)	24	35
3	C	137/140 (98%)	130 (95%)	6 (4%)	1 (1%)	26	38
4	D	100/103 (97%)	94 (94%)	6 (6%)	0	100	100
All	All	1085/1116 (97%)	991 (91%)	85 (8%)	9 (1%)	24	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	SER
1	A	326	HIS
2	B	9	SER
1	A	480	ALA
3	C	78	SER
1	A	88	ASP
1	A	265	THR
1	A	257	ILE
1	A	352	VAL

5.3.2 Protein sidechains ⓘ

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	497/506 (98%)	487 (98%)	10 (2%)	63	81
2	B	215/219 (98%)	210 (98%)	5 (2%)	58	78
3	C	118/119 (99%)	116 (98%)	2 (2%)	68	85
4	D	78/79 (99%)	76 (97%)	2 (3%)	54	74
All	All	908/923 (98%)	889 (98%)	19 (2%)	61	80

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	72	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	130	PHE
1	A	219	THR
1	A	263	LEU
1	A	360	LEU
1	A	462	THR
1	A	544	GLU
1	A	570	GLN
1	A	612	SER
2	B	63	ARG
2	B	66	ARG
2	B	134	GLU
2	B	189	ARG
2	B	224	THR
3	C	50	SER
3	C	91	LEU
4	D	14	ARG
4	D	101	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	155	HIS
1	A	159	HIS
1	A	251	GLN
1	A	326	HIS
1	A	331	GLN
1	A	479	HIS
1	A	534	GLN
2	B	38	ASN
2	B	121	GLN
2	B	137	GLN
3	C	26	HIS
4	D	9	HIS
4	D	69	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 40 are unknown and 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
6	FAD	A	1001	1	48,58,58	2.70	18 (37%)	54,89,89	2.55	11 (20%)
7	MLI	A	1002	-	0,6,6	0.00	-	0,7,7	0.00	-
9	FES	B	1002	2	0,4,4	0.00	-	0,4,4	0.00	-
10	SF4	B	1003	2	0,12,12	0.00	-	0,24,24	0.00	-
11	F3S	B	1004	2	0,9,9	0.00	-	0,15,15	0.00	-
12	BHG	C	141	-	18,18,18	1.85	5 (27%)	23,23,23	0.85	0
13	HEM	C	142	3,4	29,48,50	2.28	7 (24%)	24,80,82	2.26	10 (41%)
14	PEE	C	143	-	10,10,50	1.15	1 (10%)	9,9,55	1.38	2 (22%)
14	PEE	D	105	-	22,22,50	0.89	1 (4%)	20,20,55	0.97	2 (10%)

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
6	FAD	A	1001	1	-	0/30/50/50	0/6/6/6
7	MLI	A	1002	-	-	0/0/4/4	0/0/0/0
9	FES	B	1002	2	-	0/0/4/4	0/1/1/1
10	SF4	B	1003	2	-	0/0/48/48	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	F3S	B	1004	2	-	0/0/24/24	0/0/3/3
12	BHG	C	141	-	1/1/5/5	0/9/29/29	0/1/1/1
13	HEM	C	142	3,4	-	0/6/50/54	0/0/8/8
14	PEE	C	143	-	-	0/8/8/54	0/0/0/0
14	PEE	D	105	-	-	0/18/18/54	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	142	HEM	CAC-C3C	-6.03	1.39	1.53
13	C	142	HEM	C2D-C3D	-5.68	1.37	1.54
13	C	142	HEM	CAB-C3B	-5.62	1.40	1.53
6	A	1001	FAD	PA-O2A	-5.59	1.31	1.54
6	A	1001	FAD	PA-O1A	-4.21	1.35	1.51
13	C	142	HEM	C3C-C4C	-3.49	1.46	1.52
13	C	142	HEM	C3D-C4D	-3.25	1.47	1.51
14	C	143	PEE	C19-C18	-2.80	1.35	1.51
14	D	105	PEE	C19-C18	-2.64	1.36	1.51
13	C	142	HEM	C2C-C1C	-2.53	1.47	1.52
12	C	141	BHG	O1-C1'	2.00	1.48	1.42
12	C	141	BHG	C4-C5	2.14	1.57	1.53
6	A	1001	FAD	C8-C7	2.14	1.46	1.41
13	C	142	HEM	C4C-NC	2.34	1.38	1.36
12	C	141	BHG	C3-C2	2.45	1.58	1.52
6	A	1001	FAD	C2A-N1A	2.49	1.38	1.33
6	A	1001	FAD	C5X-N5	2.53	1.39	1.35
6	A	1001	FAD	C9-C8	2.72	1.45	1.37
6	A	1001	FAD	O4B-C1B	2.80	1.44	1.41
6	A	1001	FAD	C10-N1	2.84	1.40	1.35
12	C	141	BHG	O5-C1	2.90	1.49	1.41
6	A	1001	FAD	C4A-N3A	3.12	1.40	1.35
6	A	1001	FAD	C6-C7	3.28	1.46	1.37
6	A	1001	FAD	C6-C5X	3.40	1.46	1.41
6	A	1001	FAD	C4-C4X	3.40	1.48	1.41
6	A	1001	FAD	C2A-N3A	3.56	1.38	1.32
6	A	1001	FAD	C1'-N10	4.45	1.53	1.48
6	A	1001	FAD	C9A-N10	4.56	1.45	1.38
12	C	141	BHG	O1-C1	4.62	1.48	1.40
6	A	1001	FAD	C4X-N5	4.81	1.40	1.33
6	A	1001	FAD	C4-N3	5.70	1.43	1.33
6	A	1001	FAD	C10-N10	8.18	1.48	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	FAD	N3A-C2A-N1A	-11.69	119.94	128.89
6	A	1001	FAD	C4X-C10-N10	-5.64	117.19	120.52
6	A	1001	FAD	C4-C4X-C10	-4.39	117.13	119.94
13	C	142	HEM	CAA-C2A-C1A	-3.34	123.38	127.01
6	A	1001	FAD	C4X-C4-N3	-2.82	119.73	123.59
6	A	1001	FAD	O3P-P-O5'	-2.06	97.47	102.94
13	C	142	HEM	CMD-C2D-C3D	2.09	123.59	114.35
6	A	1001	FAD	C1'-C2'-C3'	2.21	116.15	109.82
6	A	1001	FAD	O2P-P-O3P	2.32	115.63	105.09
13	C	142	HEM	C4B-CHC-C1C	2.34	129.73	125.82
13	C	142	HEM	C2D-C3D-C4D	2.48	105.70	101.50
14	C	143	PEE	C19-C18-C17	2.55	127.70	114.53
14	D	105	PEE	C19-C18-C17	2.65	128.24	114.53
14	C	143	PEE	C20-C19-C18	2.71	128.50	114.53
14	D	105	PEE	C20-C19-C18	2.82	129.09	114.53
13	C	142	HEM	CMC-C2C-C3C	2.92	123.19	116.20
13	C	142	HEM	CAB-C3B-C2B	3.44	124.45	116.20
13	C	142	HEM	CAC-C3C-C2C	3.53	124.66	116.20
6	A	1001	FAD	P-O3P-PA	3.66	143.02	132.73
13	C	142	HEM	CMB-C2B-C3B	3.92	125.58	116.20
6	A	1001	FAD	C4-C4X-N5	4.07	123.66	118.72
13	C	142	HEM	CAD-C3D-C4D	4.26	127.51	112.47
13	C	142	HEM	CAD-C3D-C2D	4.69	126.71	113.22
6	A	1001	FAD	C4-N3-C2	5.04	119.61	115.25
6	A	1001	FAD	C4X-N5-C5X	6.77	124.55	116.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	C	141	BHG	C4

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1001	FAD	2	0
7	A	1002	MLI	4	0
12	C	141	BHG	1	0
14	D	105	PEE	1	0

5.7 Other polymers

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, 95th 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	613/621 (98%)	-0.23	14 (2%) 64 63	34, 58, 92, 123	0
2	B	241/252 (95%)	-0.15	15 (6%) 24 25	34, 50, 86, 115	0
3	C	139/140 (99%)	-0.49	1 (0%) 89 88	35, 55, 82, 93	0
4	D	102/103 (99%)	-0.66	0 100 100	39, 53, 78, 96	0
All	All	1095/1116 (98%)	-0.28	30 (2%) 58 57	34, 56, 89, 123	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	8	THR	4.4
1	A	289	PRO	3.9
2	B	9	SER	3.8
2	B	247	GLU	3.7
2	B	11	ILE	3.1
2	B	245	TYR	3.1
1	A	9	SER	3.0
2	B	65	CYS	3.0
2	B	68	GLY	2.8
2	B	246	LYS	2.8
1	A	59	ALA	2.8
2	B	225	CYS	2.7
1	A	417	LEU	2.6
1	A	567	LEU	2.5
3	C	79	LEU	2.5
1	A	276	ILE	2.5
1	A	57	THR	2.5
2	B	85	CYS	2.4
1	A	14	VAL	2.4
2	B	159	ILE	2.4
1	A	226	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	321	VAL	2.3
1	A	55	SER	2.2
2	B	73	CYS	2.2
1	A	313	GLY	2.2
2	B	72	SER	2.1
1	A	571	GLN	2.1
2	B	70	CYS	2.1
2	B	158	CYS	2.0
1	A	224	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, 95th 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
8	UNL	B	1014	1/-	0.92	0.38	15.41	65,65,65,65	0
8	UNL	B	1005	6/-	0.37	0.87	9.07	154,157,158,158	0
8	UNL	A	1017	1/-	0.92	0.30	8.23	56,56,56,56	0
8	UNL	C	144	2/-	0.80	0.25	5.15	74,74,74,75	0
14	PEE	C	143	11/51	0.74	0.34	4.52	57,60,65,66	0
8	UNL	C	149	1/-	0.97	0.22	3.35	54,54,54,54	0
14	PEE	D	105	24/51	0.74	0.29	2.89	59,70,82,83	0
12	BHG	C	141	18/18	0.88	0.17	2.02	49,52,59,60	0
7	MLI	A	1002	7/7	0.96	0.21	1.69	59,60,62,62	0
8	UNL	C	148	2/-	0.76	0.19	1.69	68,68,68,71	0
6	FAD	A	1001	53/53	0.98	0.24	0.76	35,46,54,58	0
13	HEM	C	142	41/43	0.97	0.12	0.18	41,52,59,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	F3S	B	1004	7/7	0.99	0.14	-0.13	31,36,37,43	0
8	UNL	A	1016	1/-	0.97	0.09	-0.63	43,43,43,43	0
10	SF4	B	1003	8/8	0.99	0.17	-0.76	39,46,50,51	0
5	K	A	622	1/1	0.99	0.14	-1.03	50,50,50,50	0
9	FES	B	1002	4/4	0.99	0.18	-1.20	38,44,48,52	0
5	K	B	253	1/1	0.94	0.06	-1.85	91,91,91,91	0
8	UNL	B	1008	1/-	0.60	0.25	-	74,74,74,74	0
8	UNL	A	1010	1/-	0.69	0.32	-	63,63,63,63	0
8	UNL	D	109	1/-	0.98	0.19	-	53,53,53,53	0
8	UNL	C	147	1/-	0.99	0.20	-	49,49,49,49	0
8	UNL	D	110	1/-	0.87	0.23	-	79,79,79,79	0
8	UNL	A	1015	1/-	0.62	0.57	-	84,84,84,84	0
8	UNL	A	1008	1/-	0.78	0.65	-	63,63,63,63	0
8	UNL	D	132	1/-	0.86	0.30	-	47,47,47,47	0
8	UNL	C	146	1/-	0.74	0.38	-	147,147,147,147	0
8	UNL	A	1013	1/-	0.93	0.04	-	61,61,61,61	0
8	UNL	B	1012	1/-	0.81	0.12	-	57,57,57,57	0
8	UNL	A	1009	1/-	0.53	0.20	-	70,70,70,70	0
8	UNL	A	1004	1/-	0.74	0.09	-	56,56,56,56	0
8	UNL	A	1005	1/-	0.67	0.13	-	73,73,73,73	0
8	UNL	B	1007	1/-	0.87	0.22	-	58,58,58,58	0
8	UNL	D	142	1/-	0.96	0.11	-	54,54,54,54	0
8	UNL	B	1010	1/-	0.88	0.18	-	55,55,55,55	0
8	UNL	B	1009	1/-	0.79	0.28	-	70,70,70,70	0
8	UNL	B	1006	1/-	0.97	0.07	-	41,41,41,41	0
8	UNL	C	152	1/-	0.92	0.28	-	53,53,53,53	0
8	UNL	B	1011	1/-	0.68	0.24	-	71,71,71,71	0
8	UNL	D	122	1/-	0.95	0.14	-	54,54,54,54	0
8	UNL	C	145	1/-	0.97	0.24	-	43,43,43,43	0
8	UNL	A	1014	1/-	0.31	0.55	-	91,91,91,91	0
8	UNL	A	1003	1/-	0.92	0.32	-	58,58,58,58	0
8	UNL	A	1007	1/-	0.94	0.12	-	60,60,60,60	0
8	UNL	B	1013	1/-	0.89	0.20	-	63,63,63,63	0
8	UNL	C	150	1/-	0.77	0.26	-	48,48,48,48	0
8	UNL	D	125	1/-	0.93	0.14	-	50,50,50,50	0
8	UNL	A	1006	1/-	0.90	0.18	-	69,69,69,69	0
8	UNL	A	1012	1/-	0.81	0.20	-	49,49,49,49	0
8	UNL	A	1011	1/-	0.95	0.10	-	68,68,68,68	0
8	UNL	C	151	1/-	0.68	0.25	-	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.