



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:17 PM GMT

PDB ID : 2IVF
Title : ETHYLBENZENE DEHYDROGENASE FROM AROMATOLEUM AROMATICUM
Authors : Kloer, D.P.; Hagel, C.; Heider, J.; Schulz, G.E.
Deposited on : 2006-06-13
Resolution : 1.88 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

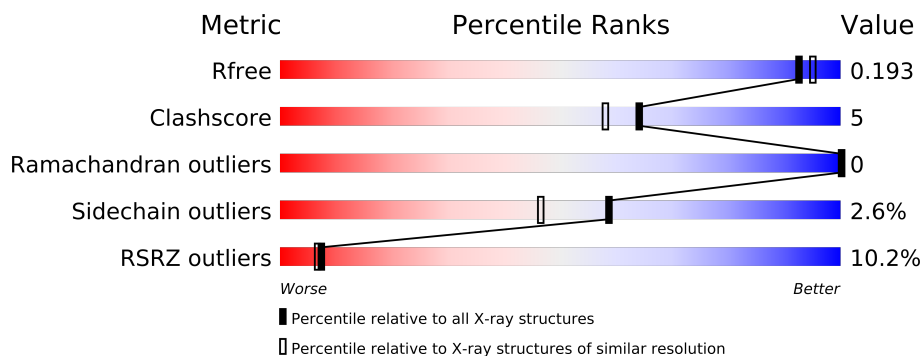
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.88 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}	66092	5260 (1.90-1.86)
Clashscore	79885	6268 (1.90-1.86)
Ramachandran outliers	78287	6195 (1.90-1.86)
Sidechain outliers	78261	6196 (1.90-1.86)
RSRZ outliers	66119	5262 (1.90-1.86)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	976	
2	B	352	
3	C	214	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	PO4	B	1354	-	X
6	GOL	A	1981	-	X
6	GOL	B	1353	-	X
6	GOL	B	1355	-	X

2 Entry composition i

There are 14 unique types of molecules in this entry. The entry contains 12639 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ETHYLBENZENE DEHYDROGENASE ALPHA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	912	Total	C	N	O	S	0	0	0
			7285	4651	1254	1331	49			

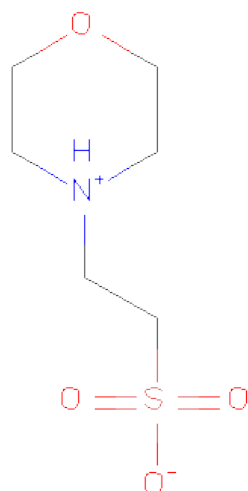
- Molecule 2 is a protein called ETHYLBENZENE DEHYDROGENASE BETA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2669	1686	479	484	20			

- Molecule 3 is a protein called ETHYLBENZENE DEHYDROGENASE GAMMA-SUBUNIT.

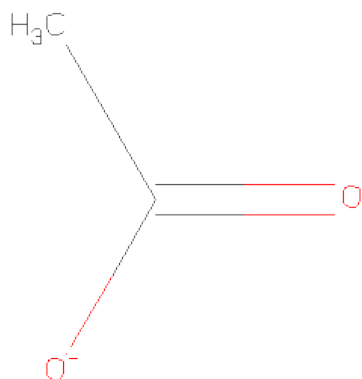
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1617	1026	288	293	10			

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



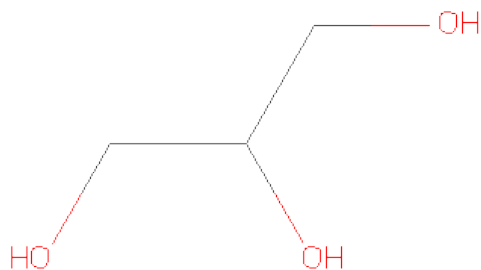
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



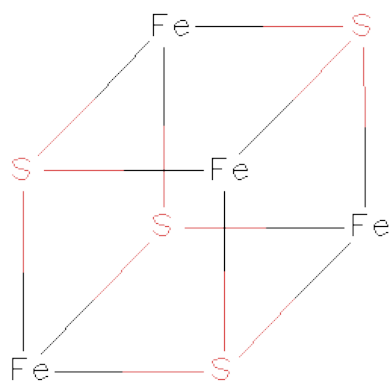
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

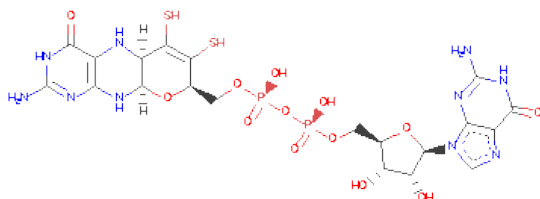


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Fe S 8 4 4	0	0
7	B	1	Total Fe S 8 4 4	0	0
7	B	1	Total Fe S 8 4 4	0	0
7	B	1	Total Fe S 8 4 4	0	0

- Molecule 8 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

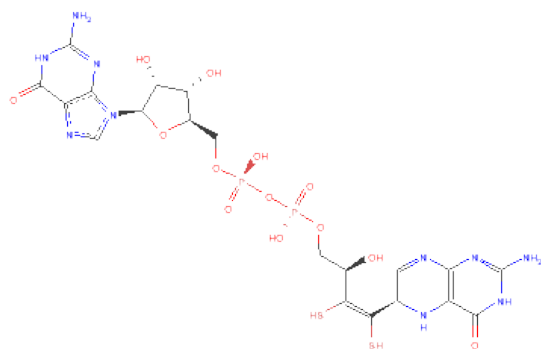
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mo	0	0
			1	1		

- Molecule 9 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONEGUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



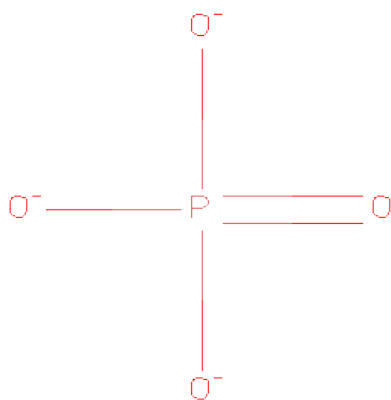
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 10 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PT ERIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YLESTER GUANYLATE ESTER (three-letter code: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



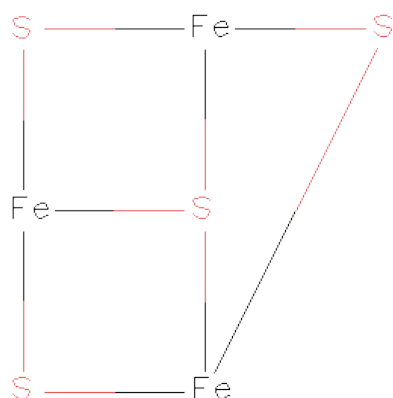
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
10	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



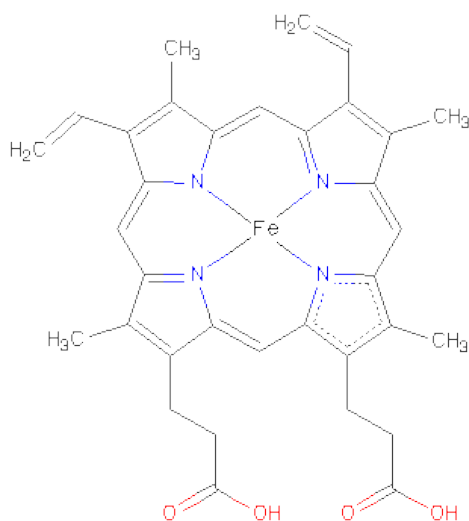
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	O P	0	0
			5	4 1		

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



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

- 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	
			43	34	1	4	4	

- Molecule 14 is water.

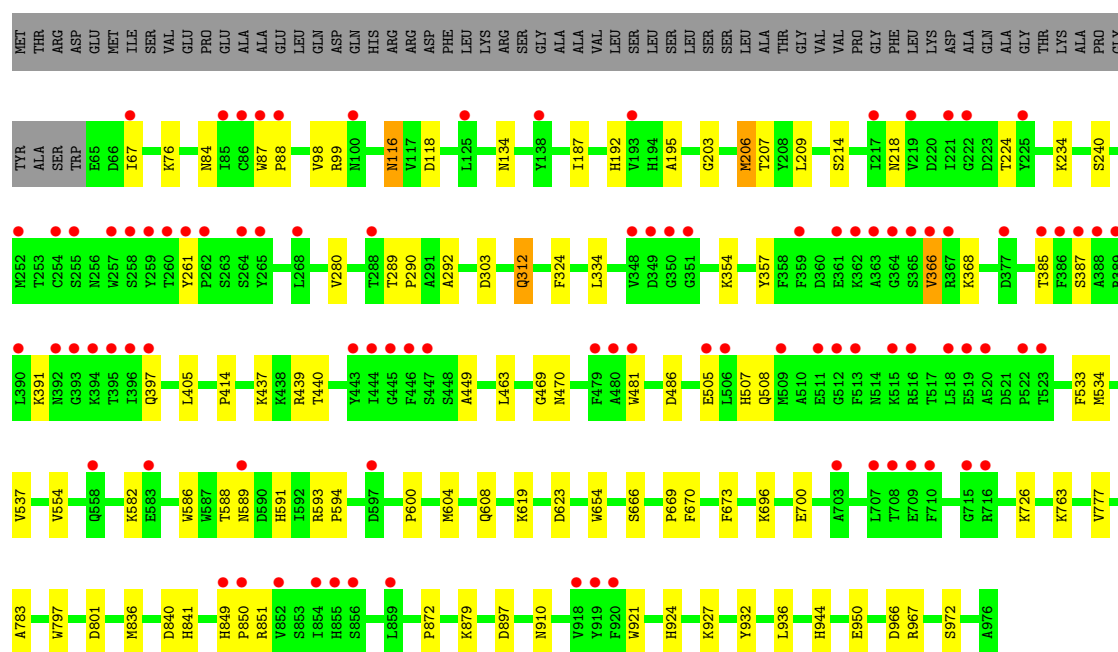
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	492	Total 492	O 492	0	0
14	B	237	Total 237	O 237	0	0
14	C	89	Total 89	O 89	0	0

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.

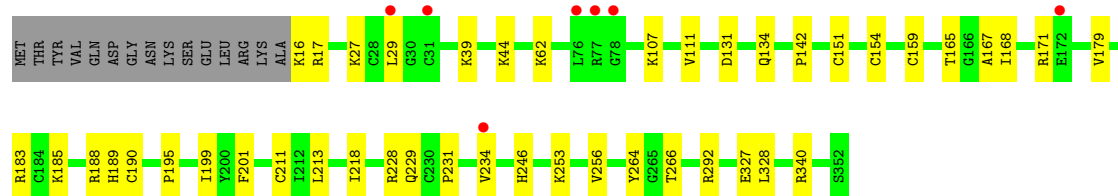
• Molecule 1: ETHYLBENZENE DEHYDROGENASE ALPHA-SUBUNIT

Chain A: 



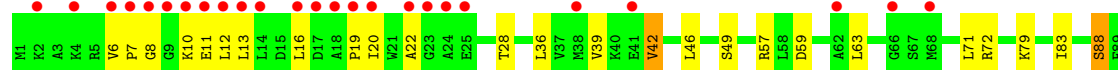
• Molecule 2: ETHYLBENZENE DEHYDROGENASE BETA-SUBUNIT

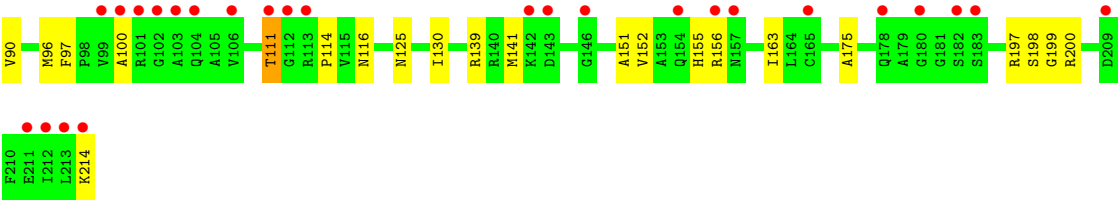
Chain B: 



• Molecule 3: ETHYLBENZENE DEHYDROGENASE GAMMA-SUBUNIT

Chain C: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.53Å 67.32Å 114.77Å 90.00° 111.30° 90.00°	Depositor
Resolution (Å)	46.42 – 1.88 43.36 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.1 (46.42-1.88) 98.1 (43.36-1.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.148 , 0.183 0.162 , 0.193	Depositor DCC
R_{free} test set	6423 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 52.5	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 127861 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12639	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: GOL, MGD, MO, PO4, F3S, MES, ACT, HEM, MD1, SF4

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	0.76	0/7494	0.78	2/10140 (0.0%)
2	B	0.81	1/2744 (0.0%)	0.81	0/3715
3	C	0.58	0/1651	0.73	1/2225 (0.0%)
All	All	0.75	1/11889 (0.0%)	0.78	3/16080 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	292	ARG	CG-CD	-6.22	1.36	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	96	MET	CG-SD-CE	-7.68	87.92	100.20
1	A	99	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	851	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	11	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7285	0	7052	64	0
2	B	2669	0	2581	30	0
3	C	1617	0	1628	30	0
4	A	12	0	12	0	0
5	A	8	0	6	2	0
6	A	24	0	32	7	0
6	B	12	0	16	3	0
6	C	12	0	16	1	0
7	A	8	0	0	0	0
7	B	24	0	0	0	0
8	A	1	0	0	0	0
9	A	47	0	22	1	0
10	A	47	0	21	4	0
11	B	5	0	0	0	0
12	B	7	0	0	0	0
13	C	43	0	30	3	0
14	A	492	0	0	7	1
14	B	237	0	0	5	1
14	C	89	0	0	1	0
All	All	12639	0	11416	126	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (126) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:116:ASN:HD22	3:C:175:ALA:H	1.21	0.89
3:C:139:ARG:HG2	3:C:141:MET:HE2	1.61	0.82
1:A:944:HIS:HA	6:A:1981:GOL:H12	1.64	0.80
3:C:16:LEU:O	3:C:72:ARG:NH1	2.12	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:8:GLY:HA3	3:C:12:LEU:HD12	1.70	0.74
1:A:67:ILE:HB	14:A:2002:HOH:O	1.87	0.72
1:A:944:HIS:HA	6:A:1981:GOL:C1	2.23	0.68
1:A:206:MET:HE1	1:A:604:MET:SD	2.33	0.67
6:A:1981:GOL:H31	6:A:1982:GOL:O1	1.95	0.66
1:A:134:ASN:HD21	2:B:44:LYS:NZ	1.95	0.65
3:C:6:VAL:HG11	3:C:20:ILE:HG12	1.79	0.64
2:B:165:THR:HG22	13:C:1217:HEM:CGD	2.26	0.64
1:A:505:GLU:HA	1:A:508:GLN:HE21	1.63	0.64
10:A:1987:MD1:C7	10:A:1987:MD1:H11	2.29	0.62
1:A:209:LEU:HD22	1:A:726:LYS:HE3	1.82	0.61
6:B:1355:GOL:H12	14:B:2237:HOH:O	2.00	0.60
3:C:6:VAL:HG13	3:C:7:PRO:HD2	1.83	0.60
1:A:87:TRP:HA	1:A:88:PRO:C	2.22	0.59
1:A:554:VAL:HG12	1:A:554:VAL:O	2.04	0.58
3:C:39:VAL:O	3:C:42:VAL:HG13	2.04	0.57
1:A:841:HIS:HD2	1:A:972:SER:OG	1.87	0.57
1:A:588:THR:H	1:A:591:HIS:HD2	1.52	0.57
1:A:850:PRO:HB3	14:A:2463:HOH:O	2.05	0.57
2:B:340:ARG:CZ	14:B:2225:HOH:O	2.53	0.56
1:A:357:TYR:HB3	1:A:366:VAL:HG22	1.88	0.56
1:A:334:LEU:CD1	1:A:366:VAL:HG23	2.35	0.56
3:C:100:ALA:HB2	3:C:114:PRO:HD2	1.88	0.56
1:A:437:LYS:CE	14:A:2197:HOH:O	2.54	0.55
2:B:27:LYS:HB2	2:B:234:VAL:HG22	1.88	0.55
1:A:593:ARG:HA	1:A:594:PRO:C	2.26	0.55
3:C:116:ASN:ND2	3:C:175:ALA:H	1.99	0.55
3:C:36:LEU:O	3:C:39:VAL:HG22	2.07	0.55
1:A:849:HIS:HD1	9:A:1986:MGD:H15	1.56	0.54
1:A:783:ALA:HA	1:A:797:TRP:CE3	2.43	0.53
1:A:192:HIS:CE1	5:A:1978:ACT:H3	2.44	0.53
2:B:167:ALA:HA	2:B:183:ARG:HE	1.73	0.53
1:A:116:ASN:HD22	1:A:118:ASP:H	1.58	0.52
3:C:6:VAL:CG2	3:C:63:LEU:HD22	2.40	0.52
2:B:107:LYS:HD3	2:B:111:VAL:HG11	1.92	0.52
2:B:165:THR:HG22	13:C:1217:HEM:O1D	2.10	0.52
1:A:385:THR:HG21	1:A:397:GLN:OE1	2.10	0.52
1:A:192:HIS:HE1	5:A:1978:ACT:H3	1.74	0.51
2:B:189:HIS:CE1	3:C:46:LEU:HD13	2.45	0.51
1:A:195:ALA:HA	10:A:1987:MD1:C6	2.41	0.51
1:A:203:GLY:HA2	1:A:206:MET:HE2	1.93	0.51
1:A:841:HIS:HE1	1:A:897:ASP:OD1	1.95	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:207:THR:HG21	1:A:214:SER:OG	2.11	0.50
3:C:90:VAL:HG22	6:C:1215:GOL:H11	1.94	0.50
10:A:1987:MD1:H7	10:A:1987:MD1:H11	1.94	0.50
1:A:879:LYS:NZ	14:A:2440:HOH:O	2.44	0.49
1:A:927:LYS:NZ	14:A:2467:HOH:O	2.42	0.49
13:C:1217:HEM:HBB2	13:C:1217:HEM:HHC	1.94	0.49
3:C:79:LYS:HD3	3:C:155:HIS:HB3	1.94	0.49
1:A:936:LEU:HD13	1:A:966:ASP:HB2	1.94	0.49
1:A:696:LYS:NZ	1:A:700:GLU:OE2	2.27	0.49
1:A:586:TRP:O	6:A:1982:GOL:H2	2.13	0.49
1:A:289:THR:N	1:A:290:PRO:CD	2.76	0.48
3:C:198:SER:OG	3:C:199:GLY:N	2.44	0.47
1:A:673:PHE:CZ	1:A:763:LYS:HG2	2.49	0.47
3:C:49:SER:OG	3:C:200:ARG:NH1	2.45	0.47
2:B:218:ILE:C	2:B:218:ILE:HD12	2.35	0.47
1:A:134:ASN:HD21	2:B:44:LYS:HZ2	1.62	0.47
2:B:229:GLN:O	2:B:231:PRO:HD3	2.14	0.47
3:C:152:VAL:HG22	3:C:163:ILE:HB	1.97	0.47
2:B:195:PRO:HB2	2:B:264:TYR:CD2	2.51	0.46
2:B:62:LYS:HE2	14:B:2032:HOH:O	2.15	0.46
3:C:83:ILE:HA	3:C:88:SER:OG	2.15	0.46
1:A:218:ASN:ND2	1:A:481:TRP:HZ2	2.14	0.46
2:B:27:LYS:CB	2:B:234:VAL:HG22	2.46	0.45
1:A:534:MET:HG3	1:A:777:VAL:CG2	2.46	0.45
1:A:669:PRO:HG2	6:A:1979:GOL:H32	1.98	0.45
1:A:440:THR:H	1:A:470:ASN:ND2	2.15	0.45
1:A:836:MET:CE	1:A:840:ASP:HA	2.47	0.45
3:C:139:ARG:CG	3:C:141:MET:HE2	2.40	0.45
1:A:187:ILE:HD11	1:A:600:PRO:HB3	1.98	0.44
1:A:187:ILE:CD1	1:A:600:PRO:HB3	2.46	0.44
1:A:437:LYS:HE2	14:A:2197:HOH:O	2.17	0.44
1:A:589:ASN:OD1	1:A:589:ASN:O	2.34	0.44
6:A:1981:GOL:C3	6:A:1982:GOL:O1	2.63	0.44
1:A:533:PHE:CZ	1:A:537:VAL:HG11	2.53	0.44
1:A:354:LYS:NZ	1:A:950:GLU:OE1	2.50	0.44
1:A:439:ARG:HA	1:A:470:ASN:HD21	1.83	0.44
1:A:224:THR:O	1:A:449:ALA:HB2	2.18	0.44
1:A:872:PRO:HA	1:A:921:TRP:CE2	2.53	0.44
2:B:190:CYS:HB2	2:B:199:ILE:HD12	1.99	0.44
1:A:240:SER:HA	1:A:666:SER:O	2.18	0.44
1:A:224:THR:HG22	1:A:449:ALA:HB1	1.99	0.43
3:C:6:VAL:CG1	3:C:7:PRO:HD2	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:151:CYS:HB3	2:B:211:CYS:HB3	2.01	0.43
2:B:228:ARG:HE	6:B:1353:GOL:H31	1.83	0.43
1:A:218:ASN:ND2	1:A:481:TRP:CZ2	2.87	0.42
2:B:159:CYS:HB2	2:B:199:ILE:HD11	2.00	0.42
3:C:71:LEU:O	3:C:163:ILE:HA	2.19	0.42
3:C:28:THR:HG23	3:C:59:ASP:OD1	2.19	0.42
2:B:131:ASP:HA	2:B:134:GLN:OE1	2.20	0.42
1:A:368:LYS:NZ	14:A:2159:HOH:O	2.45	0.42
3:C:19:PRO:O	3:C:22:ALA:HB3	2.19	0.42
3:C:139:ARG:HG2	3:C:141:MET:CE	2.43	0.42
1:A:619:LYS:NZ	1:A:623:ASP:OD2	2.42	0.42
1:A:534:MET:HG3	1:A:777:VAL:HG22	2.02	0.42
2:B:154:CYS:HB3	2:B:266:THR:O	2.19	0.42
3:C:151:ALA:HA	3:C:163:ILE:O	2.20	0.42
3:C:28:THR:CG2	3:C:57:ARG:HG3	2.50	0.41
2:B:165:THR:HG21	2:B:185:LYS:HD2	2.02	0.41
2:B:340:ARG:NH2	14:B:2225:HOH:O	2.53	0.41
2:B:253:LYS:HZ3	2:B:327:GLU:CD	2.23	0.41
2:B:256:VAL:HG21	2:B:328:LEU:HD11	2.02	0.41
3:C:111:THR:HG23	14:C:2046:HOH:O	2.20	0.41
1:A:324:PHE:CD1	1:A:469:GLY:HA2	2.56	0.41
1:A:967:ARG:HH12	10:A:1987:MD1:H17	1.68	0.41
1:A:76:LYS:HE3	1:A:98:VAL:HG21	2.03	0.41
1:A:312:GLN:NE2	1:A:414:PRO:HD3	2.36	0.41
1:A:797:TRP:O	1:A:801:ASP:HB2	2.20	0.41
1:A:405:LEU:HD21	1:A:463:LEU:HD21	2.03	0.41
2:B:16:LYS:NZ	2:B:17:ARG:O	2.54	0.41
2:B:168:ILE:HG12	2:B:179:VAL:HG22	2.01	0.41
1:A:280:VAL:HG23	1:A:292:ALA:HB2	2.03	0.41
3:C:13:LEU:O	3:C:163:ILE:HD13	2.21	0.41
3:C:97:PHE:HB2	3:C:175:ALA:HB2	2.02	0.40
1:A:944:HIS:O	6:A:1981:GOL:H32	2.21	0.40
3:C:100:ALA:CB	3:C:114:PRO:HD2	2.51	0.40
2:B:188:ARG:HD3	2:B:201:PHE:CG	2.55	0.40
1:A:116:ASN:ND2	1:A:118:ASP:H	2.20	0.40
2:B:171:ARG:HD2	14:B:2118:HOH:O	2.21	0.40
2:B:228:ARG:HE	6:B:1353:GOL:C2	2.34	0.40
1:A:910:ASN:HA	2:B:142:PRO:HG3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:A:2120:HOH:O	14:B:2149:HOH:O[2.645]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	910/976 (93%)	887 (98%)	23 (2%)	0	100	100
2	B	335/352 (95%)	323 (96%)	12 (4%)	0	100	100
3	C	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	1457/1542 (94%)	1414 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	766/816 (94%)	748 (98%)	18 (2%)	63	52
2	B	285/298 (96%)	281 (99%)	4 (1%)	78	73
3	C	163/164 (99%)	154 (94%)	9 (6%)	30	15
All	All	1214/1278 (95%)	1183 (97%)	31 (3%)	59	46

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	116	ASN
1	A	206	MET
1	A	234	LYS

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Mol	Chain	Res	Type
1	A	261	TYR
1	A	303	ASP
1	A	312	GLN
1	A	366	VAL
1	A	387	SER
1	A	391	LYS
1	A	486	ASP
1	A	507	HIS
1	A	582	LYS
1	A	608	GLN
1	A	654	TRP
1	A	670	PHE
1	A	924	HIS
1	A	932	TYR
2	B	29	LEU
2	B	39	LYS
2	B	213	LEU
2	B	246	HIS
3	C	10	LYS
3	C	42	VAL
3	C	88	SER
3	C	111	THR
3	C	125	ASN
3	C	130	ILE
3	C	156	ARG
3	C	197	ARG
3	C	214	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	134	ASN
1	A	312	GLN
1	A	470	ASN
1	A	507	HIS
1	A	508	GLN
1	A	589	ASN
1	A	591	HIS
1	A	747	ASN
1	A	841	HIS
1	A	871	GLN

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Mol	Chain	Res	Type
2	B	55	ASN
2	B	269	ASN
3	C	116	ASN
3	C	161	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\# Z > 2$
4	MES	A	1977	-	12,12,12	1.63	1 (8%)	16,16,16	2.47	4 (25%)
5	ACT	A	1978	8	1,3,3	0.34	0	0,3,3	0.00	-
6	GOL	A	1979	-	5,5,5	0.49	0	5,5,5	0.75	0
6	GOL	A	1980	-	5,5,5	0.38	0	5,5,5	0.55	0
6	GOL	A	1981	-	5,5,5	0.36	0	5,5,5	1.64	1 (20%)
6	GOL	A	1982	-	5,5,5	0.26	0	5,5,5	0.66	0
5	ACT	A	1983	-	1,3,3	1.58	0	0,3,3	0.00	-
7	SF4	A	1984	1	12,12,12	6.96	11 (91%)	0,24,24	0.00	-
9	MGD	A	1986	8	52,52,52	1.53	8 (15%)	72,81,81	2.43	21 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MD1	A	1987	8	51,51,51	2.52	7 (13%)	64,78,78	2.00	15 (23%)
6	GOL	B	1353	-	5,5,5	0.74	0	5,5,5	2.12	3 (60%)
11	PO4	B	1354	-	4,4,4	0.18	0	6,6,6	0.32	0
6	GOL	B	1355	-	5,5,5	0.45	0	5,5,5	0.41	0
12	F3S	B	1356	2	3,9,9	21.98	3 (100%)	0,15,15	0.00	-
7	SF4	B	1357	2	12,12,12	6.44	12 (100%)	0,24,24	0.00	-
7	SF4	B	1358	2	12,12,12	7.21	11 (91%)	0,24,24	0.00	-
7	SF4	B	1359	2	12,12,12	6.16	9 (75%)	0,24,24	0.00	-
6	GOL	C	1215	-	5,5,5	0.28	0	5,5,5	0.68	0
6	GOL	C	1216	-	5,5,5	0.29	0	5,5,5	0.35	0
13	HEM	C	1217	3	49,50,50	1.97	11 (22%)	46,82,82	2.00	8 (17%)

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
4	MES	A	1977	-	-	0/6/14/14	0/1/1/1
5	ACT	A	1978	8	-	0/0/0/0	0/0/0/0
6	GOL	A	1979	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1980	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1981	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1982	-	-	0/4/4/4	0/0/0/0
5	ACT	A	1983	-	-	0/0/0/0	0/0/0/0
7	SF4	A	1984	1	-	0/0/48/48	0/0/5/5
9	MGD	A	1986	8	-	0/22/66/66	0/1/6/6
10	MD1	A	1987	8	1/1/10/12	0/22/59/59	0/1/5/5
6	GOL	B	1353	-	-	0/4/4/4	0/0/0/0
11	PO4	B	1354	-	-	0/0/0/0	0/0/0/0
6	GOL	B	1355	-	-	0/4/4/4	0/0/0/0
12	F3S	B	1356	2	-	0/0/24/24	0/0/3/3
7	SF4	B	1357	2	-	0/0/48/48	0/0/5/5
7	SF4	B	1358	2	-	0/0/48/48	0/0/5/5
7	SF4	B	1359	2	-	0/0/48/48	0/0/5/5
6	GOL	C	1215	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1216	-	-	0/4/4/4	0/0/0/0
13	HEM	C	1217	3	-	0/14/114/114	0/0/8/8

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1356	F3S	S3-FE1	-24.39	2.16	2.33
12	B	1356	F3S	S3-FE3	-23.52	2.17	2.33
12	B	1356	F3S	S3-FE4	-17.34	2.21	2.33
10	A	1987	MD1	C7-N8	15.79	1.44	1.27
7	A	1984	SF4	S3-FE2	-13.69	2.24	2.33
7	B	1359	SF4	S4-FE2	-12.33	2.25	2.33
7	B	1358	SF4	S2-FE3	-11.81	2.25	2.33
7	B	1358	SF4	S1-FE4	-11.07	2.25	2.33
7	B	1357	SF4	S3-FE2	-10.09	2.26	2.33
7	A	1984	SF4	S1-FE4	-9.65	2.26	2.33
7	A	1984	SF4	S2-FE1	-9.60	2.26	2.33
7	B	1357	SF4	S3-FE4	-9.31	2.27	2.33
7	B	1357	SF4	S2-FE1	-8.99	2.27	2.33
7	B	1358	SF4	S4-FE1	-8.63	2.27	2.33
7	B	1359	SF4	S4-FE1	-8.61	2.27	2.33
7	A	1984	SF4	S2-FE3	-8.19	2.27	2.33
7	B	1357	SF4	S3-FE1	-8.18	2.27	2.33
7	B	1359	SF4	S2-FE1	-7.83	2.28	2.33
7	B	1358	SF4	S4-FE2	-7.83	2.28	2.33
7	B	1357	SF4	S2-FE3	-7.70	2.28	2.33
7	B	1359	SF4	S2-FE4	-7.58	2.28	2.33
7	B	1359	SF4	S1-FE3	-7.44	2.28	2.33
7	B	1358	SF4	S1-FE2	-6.76	2.28	2.33
7	B	1358	SF4	S1-FE3	-6.47	2.28	2.33
7	B	1358	SF4	S3-FE4	-6.45	2.28	2.33
7	B	1357	SF4	S1-FE3	-6.30	2.29	2.33
7	A	1984	SF4	S3-FE4	-6.12	2.29	2.33
7	A	1984	SF4	S4-FE2	-5.61	2.29	2.33
13	C	1217	HEM	C3B-C2B	-5.46	1.34	1.43
13	C	1217	HEM	C3D-C2D	5.45	1.53	1.43
7	B	1358	SF4	S2-FE4	-5.41	2.29	2.33
7	B	1359	SF4	S1-FE4	-5.03	2.29	2.33
7	B	1358	SF4	S3-FE2	-4.95	2.29	2.33
7	B	1358	SF4	S3-FE1	-4.66	2.30	2.33
13	C	1217	HEM	C3C-CAC	4.53	1.54	1.40
13	C	1217	HEM	C3C-C2C	-4.49	1.35	1.43
9	A	1986	MGD	C4-N9	-4.33	1.31	1.37
7	B	1358	SF4	S2-FE1	-4.26	2.30	2.33
7	A	1984	SF4	S3-FE1	-4.26	2.30	2.33
13	C	1217	HEM	C3B-CAB	4.24	1.53	1.40
9	A	1986	MGD	O11-C11	-4.23	1.37	1.43
4	A	1977	MES	C8-S	-4.16	1.70	1.78
7	A	1984	SF4	S2-FE4	3.89	2.35	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1986	MGD	C2-N2	3.71	1.38	1.32
7	B	1357	SF4	S4-FE1	-3.70	2.30	2.33
7	A	1984	SF4	S4-FE3	-3.67	2.30	2.33
7	B	1357	SF4	S4-FE2	-3.67	2.30	2.33
7	A	1984	SF4	S1-FE3	-3.62	2.30	2.33
7	B	1359	SF4	S2-FE3	-3.58	2.30	2.33
7	A	1984	SF4	S1-FE2	3.42	2.35	2.33
7	B	1357	SF4	S4-FE3	-3.41	2.31	2.33
10	A	1987	MD1	C4-N9	-3.29	1.32	1.37
7	B	1359	SF4	S3-FE2	-3.18	2.31	2.33
7	B	1357	SF4	S1-FE2	-3.10	2.31	2.33
7	B	1357	SF4	S2-FE4	-2.95	2.31	2.33
13	C	1217	HEM	C4A-C3A	2.86	1.43	1.40
9	A	1986	MGD	C14-N15	2.75	1.49	1.45
13	C	1217	HEM	CMD-C2D	2.74	1.55	1.47
10	A	1987	MD1	C14-C13	-2.64	1.48	1.51
10	A	1987	MD1	C2-N2	2.59	1.36	1.32
13	C	1217	HEM	FE-ND	2.58	2.07	1.97
13	C	1217	HEM	CMC-C2C	2.54	1.55	1.47
9	A	1986	MGD	C2-N1	2.52	1.40	1.36
9	A	1986	MGD	C17-N18	2.49	1.41	1.37
9	A	1986	MGD	C21-N22	2.40	1.39	1.35
13	C	1217	HEM	CMB-C2B	2.37	1.54	1.47
10	A	1987	MD1	C13-C12	2.36	1.37	1.34
7	B	1357	SF4	S1-FE4	-2.23	2.31	2.33
7	B	1359	SF4	S4-FE3	2.14	2.34	2.33
9	A	1986	MGD	PA-O2A	-2.12	1.45	1.55
10	A	1987	MD1	C17-N17	2.05	1.40	1.36
10	A	1987	MD1	C20-N18	-2.04	1.32	1.35
13	C	1217	HEM	FE-NB	2.01	2.05	1.97

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1986	MGD	C6-C5-N7	13.49	135.96	134.14
13	C	1217	HEM	C3B-C4B-NB	-9.03	107.54	114.00
4	A	1977	MES	C5-N4-C3	6.63	122.89	109.75
10	A	1987	MD1	O4'-C1'-N9	6.39	114.39	108.44
9	A	1986	MGD	C4'-O4'-C1'	-6.18	103.03	109.75
10	A	1987	MD1	C6-C5-N7	5.27	134.85	134.14
10	A	1987	MD1	C4'-O4'-C1'	-4.98	104.34	109.75
10	A	1987	MD1	C14-C7-N8	-4.91	113.04	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	1217	HEM	C4D-ND-C1D	4.31	109.57	105.16
4	A	1977	MES	C7-N4-C5	3.80	121.61	111.66
9	A	1986	MGD	C2-N3-C4	3.70	120.29	115.09
9	A	1986	MGD	N1-C2-N3	-3.64	116.69	121.78
10	A	1987	MD1	C2-N3-C4	3.58	120.12	115.09
13	C	1217	HEM	CHD-C4C-NC	3.42	127.70	124.73
4	A	1977	MES	C2-C3-N4	3.40	114.33	109.96
9	A	1986	MGD	C17-C16-C21	3.29	117.60	114.56
10	A	1987	MD1	C15-C16-C20	3.24	122.09	114.53
9	A	1986	MGD	N18-C19-N20	-3.22	117.27	121.78
9	A	1986	MGD	C10-C11-C12	3.20	114.76	110.98
9	A	1986	MGD	C14-C23-N22	-3.18	105.66	110.01
9	A	1986	MGD	N19-C19-N20	3.18	124.60	120.31
10	A	1987	MD1	C7-C14-N15	3.16	119.42	109.53
13	C	1217	HEM	C1B-NB-C4B	3.09	108.33	105.16
10	A	1987	MD1	N2-C2-N1	3.07	121.24	117.86
9	A	1986	MGD	C23-O11-C11	-3.06	106.05	112.03
9	A	1986	MGD	C19-N20-C21	3.03	121.91	117.61
9	A	1986	MGD	C6-N1-C2	3.01	124.77	119.51
9	A	1986	MGD	C5'-C4'-C3'	-2.99	103.22	115.21
10	A	1987	MD1	C6-N1-C2	2.93	124.64	119.51
6	B	1353	GOL	O1-C1-C2	2.80	123.38	109.71
13	C	1217	HEM	C1A-CHA-C4D	-2.79	123.79	127.47
9	A	1986	MGD	C13-C14-N15	-2.75	106.51	111.70
9	A	1986	MGD	C17-C16-N15	2.73	123.07	119.10
6	A	1981	GOL	O1-C1-C2	2.68	122.80	109.71
13	C	1217	HEM	CBD-CAD-C3D	-2.68	108.53	114.37
10	A	1987	MD1	N1-C2-N3	-2.63	118.10	121.78
4	A	1977	MES	O2S-S-C8	2.56	114.26	106.36
10	A	1987	MD1	O11-C11-C10	-2.56	103.67	109.77
9	A	1986	MGD	N22-C21-N20	2.54	120.49	116.51
10	A	1987	MD1	C20-N8-C7	2.51	124.95	114.57
9	A	1986	MGD	C8-N9-C4	2.35	108.69	106.90
13	C	1217	HEM	CMA-C3A-C4A	-2.32	125.05	128.62
6	B	1353	GOL	O2-C2-C3	-2.32	97.65	108.22
9	A	1986	MGD	C1'-N9-C4	-2.31	122.64	126.64
9	A	1986	MGD	N2-C2-N1	2.27	120.36	117.86
6	B	1353	GOL	C3-C2-C1	2.26	121.23	111.26
9	A	1986	MGD	C4-C5-N7	-2.24	107.61	109.52
13	C	1217	HEM	CHD-C1D-ND	2.23	126.44	124.58
9	A	1986	MGD	O11-C23-N22	-2.15	106.42	109.22
10	A	1987	MD1	C4-C5-N7	-2.14	107.69	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1987	MD1	C1'-N9-C4	-2.03	123.12	126.64
10	A	1987	MD1	C5-C4-N3	-2.01	123.04	125.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	1987	MD1	C14

There are no torsion outliers.

There are no ring outliers.

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	912/976 (93%)	0.48	94 (10%) 7 6	19, 24, 33, 50	0
2	B	337/352 (95%)	-0.01	7 (2%) 60 61	18, 24, 31, 46	0
3	C	214/214 (100%)	1.13	51 (23%) 1 1	17, 25, 34, 43	0
All	All	1463/1542 (94%)	0.46	152 (10%) 7 6	17, 24, 33, 50	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	11	GLU	6.2
3	C	101	ARG	5.5
3	C	12	LEU	5.3
3	C	7	PRO	5.1
3	C	19	PRO	4.8
1	A	389	ARG	4.5
1	A	363	ALA	4.5
1	A	854	ILE	4.4
1	A	221	ILE	4.4
3	C	17	ASP	4.3
2	B	77	ARG	4.1
1	A	362	LYS	4.1
3	C	22	ALA	4.1
1	A	392	ASN	4.0
2	B	76	LEU	4.0
3	C	8	GLY	4.0
3	C	6	VAL	3.9
3	C	182	SER	3.9
3	C	24	ALA	3.9
1	A	361	GLU	3.8
1	A	365	SER	3.8
3	C	10	LYS	3.8
1	A	385	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	520	ALA	3.7
1	A	261	TYR	3.7
3	C	178	GLN	3.6
1	A	518	LEU	3.6
3	C	20	ILE	3.6
1	A	395	THR	3.6
1	A	516	ARG	3.6
3	C	102	GLY	3.5
3	C	214	LYS	3.5
3	C	111	THR	3.5
3	C	25	GLU	3.4
3	C	23	GLY	3.4
1	A	259	TYR	3.4
1	A	522	PRO	3.3
1	A	481	TRP	3.3
1	A	708	THR	3.3
3	C	18	ALA	3.3
1	A	85	ILE	3.3
1	A	515	LYS	3.2
1	A	446	PHE	3.2
3	C	146	GLY	3.2
3	C	157	ASN	3.2
1	A	260	THR	3.1
1	A	265	TYR	3.1
3	C	68	MET	3.1
3	C	99	VAL	3.1
1	A	480	ALA	3.1
1	A	386	PHE	3.1
1	A	348	VAL	3.0
3	C	156	ARG	3.0
1	A	583	GLU	3.0
1	A	445	GLY	3.0
3	C	180	GLY	3.0
1	A	217	ILE	3.0
3	C	213	LEU	3.0
3	C	62	ALA	3.0
3	C	100	ALA	3.0
1	A	849	HIS	2.9
1	A	393	GLY	2.9
1	A	597	ASP	2.9
3	C	209	ASP	2.9
2	B	31	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	219	VAL	2.9
3	C	9	GLY	2.9
1	A	67	ILE	2.9
1	A	87	TRP	2.9
1	A	225	TYR	2.9
1	A	366	VAL	2.9
1	A	262	PRO	2.8
1	A	257	TRP	2.8
1	A	387	SER	2.8
1	A	359	PHE	2.8
2	B	29	LEU	2.8
1	A	350	GLY	2.8
3	C	142	LYS	2.8
1	A	920	PHE	2.8
3	C	113	ARG	2.7
1	A	519	GLU	2.7
1	A	506	LEU	2.7
3	C	112	GLY	2.7
1	A	86	CYS	2.7
3	C	16	LEU	2.7
1	A	377	ASP	2.7
1	A	258	SER	2.7
1	A	388	ALA	2.6
1	A	589	ASN	2.6
1	A	390	LEU	2.6
1	A	479	PHE	2.6
1	A	397	GLN	2.6
1	A	138	TYR	2.6
1	A	852	VAL	2.6
3	C	212	ILE	2.6
1	A	443	TYR	2.6
3	C	13	LEU	2.6
1	A	918	VAL	2.6
1	A	715	GLY	2.5
1	A	855	HIS	2.5
3	C	106	VAL	2.5
1	A	444	ILE	2.5
1	A	558	GLN	2.5
1	A	707	LEU	2.4
1	A	523	THR	2.4
1	A	856	SER	2.4
1	A	512	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	509	MET	2.4
1	A	268	LEU	2.4
1	A	710	PHE	2.4
3	C	103	ALA	2.4
1	A	511	GLU	2.3
1	A	703	ALA	2.3
1	A	859	LEU	2.3
1	A	100	ASN	2.3
1	A	351	GLY	2.3
1	A	193	VAL	2.3
1	A	716	ARG	2.3
2	B	172	GLU	2.3
3	C	14	LEU	2.3
1	A	88	PRO	2.3
1	A	850	PRO	2.3
1	A	264	SER	2.3
1	A	394	LYS	2.3
2	B	78	GLY	2.3
3	C	38	MET	2.3
3	C	143	ASP	2.3
3	C	211	GLU	2.3
3	C	66	GLY	2.3
1	A	396	ILE	2.3
1	A	364	GLY	2.2
1	A	349	ASP	2.2
1	A	255	SER	2.2
1	A	288	THR	2.2
3	C	154	GLN	2.2
1	A	367	ARG	2.2
3	C	4	LYS	2.2
1	A	254	CYS	2.2
1	A	222	GLY	2.2
3	C	104	GLN	2.1
3	C	2	LYS	2.1
1	A	447	SER	2.1
1	A	513	PHE	2.1
1	A	709	GLU	2.1
3	C	41	GLU	2.1
3	C	183	SER	2.1
1	A	919	TYR	2.1
1	A	252	MET	2.1
3	C	165	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	234	VAL	2.0
1	A	125	LEU	2.0
1	A	505	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
11	PO4	B	1354	5/5	0.23	8.21	44,47,47,48	0
6	GOL	A	1981	6/6	0.18	2.52	32,36,38,39	0
6	GOL	B	1353	6/6	0.14	2.07	24,31,33,37	0
6	GOL	B	1355	6/6	0.12	2.01	45,46,47,47	0
6	GOL	C	1216	6/6	0.10	1.08	33,34,35,36	0
5	ACT	A	1983	4/4	0.13	1.04	34,37,38,38	0
6	GOL	A	1980	6/6	0.21	1.02	33,36,36,37	0
6	GOL	A	1982	6/6	0.12	0.34	40,41,43,44	0
7	SF4	B	1359	8/8	0.12	0.03	23,24,24,26	0
13	HEM	C	1217	43/43	0.10	-0.24	21,24,27,28	0
6	GOL	C	1215	6/6	0.09	-0.42	23,27,30,30	0
7	SF4	B	1357	8/8	0.08	-0.70	21,22,23,24	0
6	GOL	A	1979	6/6	0.09	-1.00	16,20,23,24	0
7	SF4	B	1358	8/8	0.16	-1.04	24,24,25,25	0
7	SF4	A	1984	8/8	0.15	-1.06	23,25,26,26	0
10	MD1	A	1987	47/47	0.11	-1.35	14,16,18,18	0
12	F3S	B	1356	7/7	0.04	-1.52	20,21,22,22	0
4	MES	A	1977	12/12	0.08	-1.64	24,27,28,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	MGD	A	1986	47/47	0.11	-2.05	10,14,16,17	0
5	ACT	A	1978	4/4	0.15	-3.10	23,25,26,28	0
8	MO	A	1985	1/1	0.03	-6.43	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.