



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:44 AM UTC

PDB ID : 3SCF / pdb_00003scf
Title : Fe(II)-HppE with S-HPP and NO
Authors : Drennan, C.L.
Deposited on : 2011-06-07
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

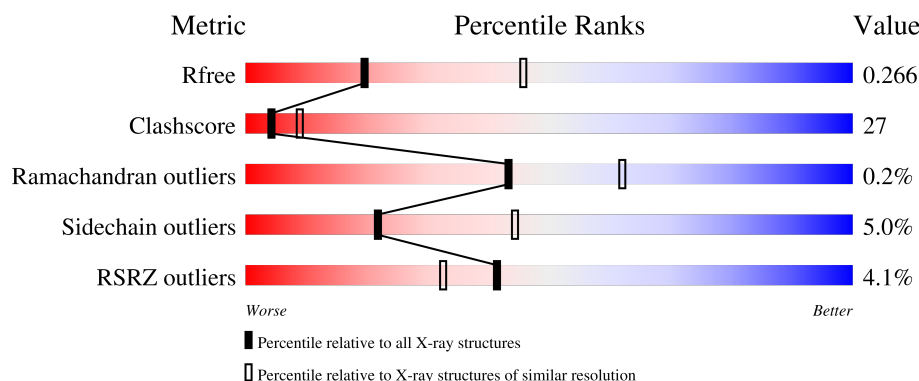
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	198	 6% 49% 42% 6% .
1	B	198	 4% 55% 36% 6% .
1	C	198	 2% 62% 32% . . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4427 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.

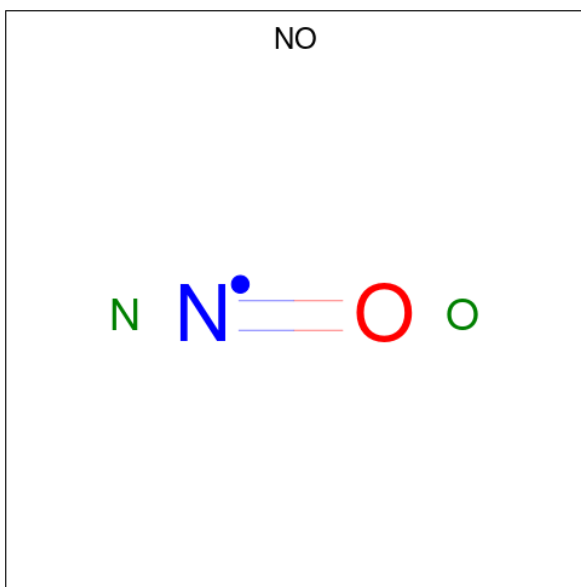
- Molecule 1 is a protein called Epoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1443	908	245	285	5			
1	B	193	Total	C	N	O	S	0	0	0
			1455	917	248	285	5			
1	C	193	Total	C	N	O	S	0	0	0
			1459	920	249	285	5			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

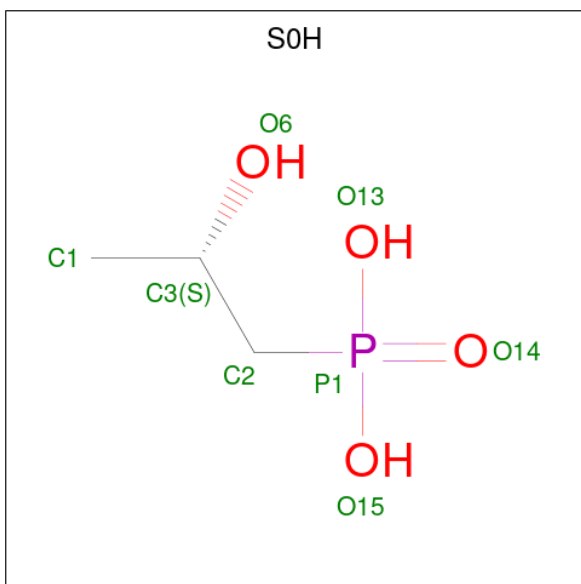
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is NITRIC OXIDE (CCD ID: NO) (formula: NO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			2	1	1		
3	B	1	Total	N	O	0	0
			2	1	1		

- Molecule 4 is (S)-2-HYDROXYPROPYLPHOSPHONIC ACID (CCD ID: S0H) (formula: $C_3H_9O_4P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			8	3	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			8	3	4	1		
4	C	1	Total	C	O	P	0	0
			8	3	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

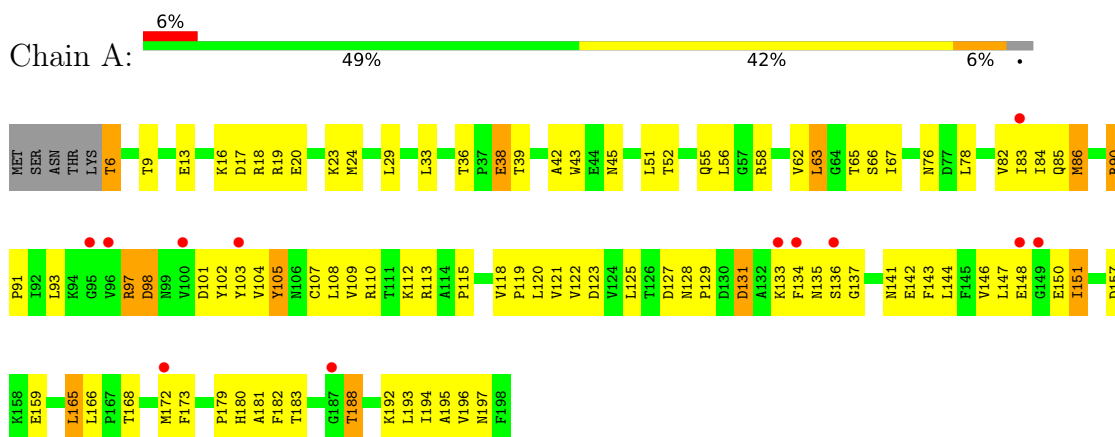
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	9	Total	O	0	0
			9	9		
6	C	14	Total	O	0	0
			14	14		

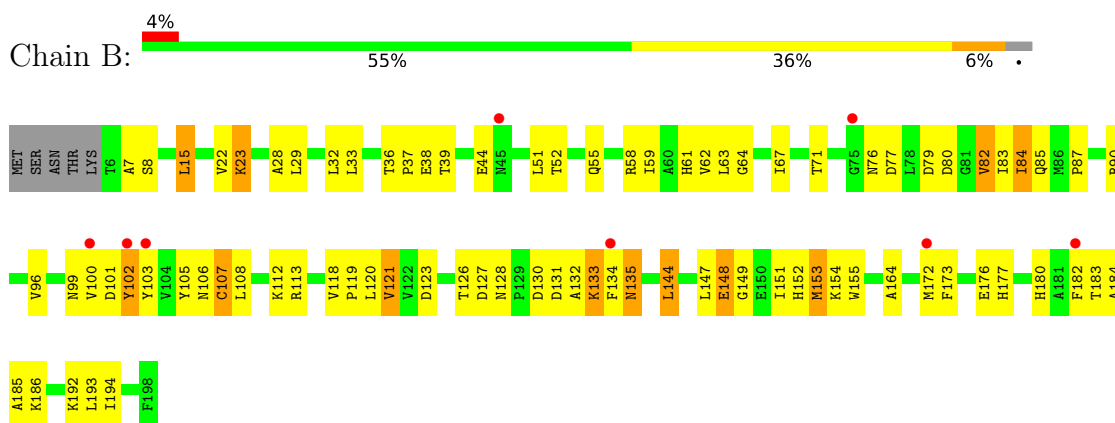
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

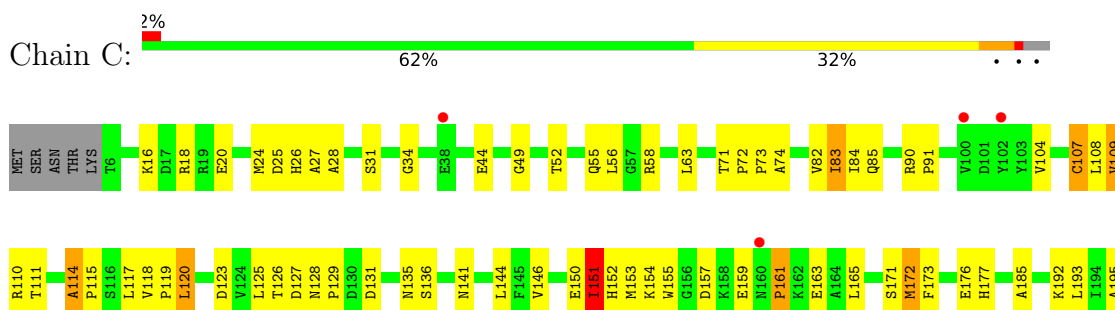
• Molecule 1: Epoxidase



• Molecule 1: Epoxidase



• Molecule 1: Epoxidase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.66Å 111.66Å 152.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.85) 98.2 (50.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.269 0.252 , 0.266	Depositor DCC
R_{free} test set	1166 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4427	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8227e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: FE2, S0H, GOL, NO

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	0.50	1/1473 (0.1%)	1.08	12/2009 (0.6%)
1	B	0.51	0/1485	1.18	16/2021 (0.8%)
1	C	0.57	0/1489	1.10	13/2025 (0.6%)
All	All	0.53	1/4447 (0.0%)	1.12	41/6055 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	PRO	N-CD	-5.42	1.40	1.47

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	ASN	N-CA-C	-8.15	100.08	110.19
1	B	23	LYS	N-CA-C	7.32	121.16	111.28
1	B	118	VAL	CA-C-N	7.22	128.29	120.13
1	B	118	VAL	C-N-CA	7.22	128.29	120.13
1	B	7	ALA	N-CA-C	-7.10	103.72	112.38
1	A	131	ASP	N-CA-C	-6.82	104.84	113.02
1	C	135	ASN	N-CA-C	-6.81	99.89	110.17
1	C	71	THR	CA-C-N	6.59	124.41	119.66
1	C	71	THR	C-N-CA	6.59	124.41	119.66
1	C	72	PRO	N-CA-C	6.53	117.56	110.58
1	C	107	CYS	N-CA-C	6.37	118.95	109.59
1	A	86	MET	CA-C-N	6.36	127.80	119.84
1	A	86	MET	C-N-CA	6.36	127.80	119.84
1	B	184	ALA	N-CA-C	-6.28	100.33	110.32
1	B	39	THR	CB-CA-C	-6.16	100.96	110.81
1	A	137	GLY	N-CA-C	-6.15	103.93	112.18
1	B	121	VAL	N-CA-C	-6.13	98.91	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	LEU	N-CA-C	-6.10	104.55	111.07
1	A	188	THR	CB-CA-C	-5.86	98.05	110.31
1	A	56	LEU	N-CA-C	-5.83	104.93	111.28
1	A	90	ARG	CA-C-N	5.69	126.95	119.84
1	A	90	ARG	C-N-CA	5.69	126.95	119.84
1	B	102	TYR	N-CA-C	5.66	122.85	110.80
1	A	23	LYS	N-CA-C	5.66	118.09	111.02
1	A	121	VAL	N-CA-C	-5.58	99.19	107.51
1	B	90	ARG	N-CA-C	5.52	116.84	109.83
1	B	105	TYR	N-CA-C	5.51	117.62	108.20
1	B	87	PRO	N-CA-C	5.46	121.89	113.75
1	C	151	ILE	N-CA-C	5.45	116.43	108.53
1	A	122	VAL	N-CA-C	5.45	115.70	107.80
1	C	109	VAL	N-CA-C	5.38	116.64	109.37
1	C	49	GLY	N-CA-C	5.36	120.40	113.27
1	A	105	TYR	N-CA-C	5.34	117.45	107.99
1	C	90	ARG	CA-C-N	-5.31	114.26	119.99
1	C	90	ARG	C-N-CA	-5.31	114.26	119.99
1	C	114	ALA	CA-C-N	5.26	125.57	119.47
1	C	114	ALA	C-N-CA	5.26	125.57	119.47
1	B	39	THR	N-CA-C	5.20	117.35	111.11
1	B	130	ASP	CB-CA-C	-5.19	100.39	110.46
1	B	107	CYS	N-CA-C	5.09	117.08	109.59
1	C	34	GLY	N-CA-C	-5.08	106.74	115.08

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	1443	0	1387	99	0
1	B	1455	0	1420	95	0
1	C	1459	0	1431	53	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	8	0	2	0	0
4	B	8	0	2	0	0
4	C	8	0	2	0	0
5	A	6	0	8	3	0
5	C	6	0	8	0	0
6	A	4	0	0	0	0
6	B	9	0	0	0	0
6	C	14	0	0	0	0
All	All	4427	0	4260	235	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 27.

All (235) 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:78:LEU:HD23	1:A:83:ILE:HD11	1.31	1.11
1:A:93:LEU:HD22	1:B:23:LYS:O	1.51	1.09
1:A:123:ASP:OD1	1:A:192:LYS:HE2	1.58	1.02
1:B:133:LYS:HD3	1:B:134:PHE:H	1.31	0.96
1:B:76:ASN:ND2	1:B:113:ARG:HH11	1.63	0.96
1:B:133:LYS:HD3	1:B:134:PHE:N	1.80	0.96
1:A:90:ARG:NH2	5:A:199:GOL:H32	1.90	0.87
1:B:107:CYS:HA	1:B:120:LEU:HD23	1.59	0.84
1:B:133:LYS:CD	1:B:134:PHE:N	2.40	0.84
1:A:108:LEU:HB2	1:A:119:PRO:HB2	1.57	0.83
1:C:154:LYS:HG2	1:C:163:GLU:HG2	1.59	0.82
1:A:128:ASN:HB3	1:A:131:ASP:HB2	1.63	0.81
1:A:93:LEU:HD22	1:B:23:LYS:C	2.04	0.81
1:C:52:THR:OG1	1:C:55:GLN:HG3	1.81	0.80
1:C:128:ASN:ND2	1:C:131:ASP:HB2	1.96	0.80
1:B:151:ILE:HG13	1:B:193:LEU:HD23	1.62	0.79
1:B:36:THR:HG22	1:B:38:GLU:H	1.49	0.78
1:A:101:ASP:HB3	1:A:125:LEU:HD13	1.66	0.78
1:C:108:LEU:HG	1:C:120:LEU:HA	1.65	0.77
1:A:188:THR:O	1:A:188:THR:HG22	1.84	0.77
1:B:76:ASN:ND2	1:B:113:ARG:NH1	2.32	0.76
1:A:93:LEU:CD2	1:B:23:LYS:O	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:THR:HG23	1:B:183:THR:HG22	1.68	0.74
1:C:91:PRO:HG2	1:C:107:CYS:HB2	1.71	0.72
1:B:76:ASN:HD22	1:B:113:ARG:HH11	1.35	0.72
1:C:171:SER:C	1:C:172:MET:HE3	2.15	0.72
1:B:148:GLU:HG2	1:B:149:GLY:N	2.05	0.71
1:A:78:LEU:HA	1:A:83:ILE:CD1	2.20	0.71
1:C:128:ASN:HD22	1:C:131:ASP:HB2	1.54	0.71
1:B:76:ASN:HD22	1:B:113:ARG:HD3	1.53	0.70
1:B:32:LEU:HD12	1:B:32:LEU:H	1.57	0.69
1:C:157:ASP:OD2	1:C:159:GLU:HB2	1.91	0.69
1:A:16:LYS:O	1:A:20:GLU:HG3	1.92	0.69
1:B:108:LEU:HB2	1:B:119:PRO:HB2	1.74	0.69
1:A:112:LYS:NZ	1:B:61:HIS:CD2	2.60	0.69
1:A:93:LEU:CD2	1:B:23:LYS:C	2.66	0.68
1:B:76:ASN:HD22	1:B:113:ARG:NH1	1.90	0.68
1:B:153:MET:SD	1:B:172:MET:SD	2.91	0.68
1:A:6:THR:HB	1:A:9:THR:HB	1.76	0.68
1:C:104:VAL:HG23	1:C:125:LEU:HD11	1.74	0.68
1:A:78:LEU:HA	1:A:83:ILE:HD11	1.76	0.68
1:B:153:MET:HG3	1:B:154:LYS:N	2.09	0.68
1:C:144:LEU:HB2	1:C:172:MET:HG2	1.76	0.67
1:B:147:LEU:HG	1:B:194:ILE:HG12	1.75	0.67
1:C:152:HIS:ND1	1:C:165:LEU:HD21	2.09	0.67
1:A:123:ASP:OD1	1:A:192:LYS:CE	2.39	0.67
1:A:78:LEU:HD23	1:A:83:ILE:CD1	2.19	0.67
1:A:24:MET:HE1	1:A:29:LEU:HD13	1.77	0.67
1:A:110:ARG:CZ	1:B:22:VAL:HG13	2.25	0.66
1:A:146:VAL:HG22	1:A:151:ILE:HD13	1.79	0.65
1:C:104:VAL:HB	1:C:123:ASP:HB2	1.79	0.65
1:C:110:ARG:HD3	1:C:118:VAL:HG13	1.79	0.64
1:C:129:PRO:O	1:C:154:LYS:NZ	2.30	0.64
1:A:76:ASN:CG	1:A:113:ARG:HH11	2.05	0.64
1:B:153:MET:HE3	1:B:182:PHE:CZ	2.32	0.64
1:A:97:ARG:O	1:A:98:ASP:CG	2.40	0.64
1:A:104:VAL:HB	1:A:123:ASP:HB2	1.80	0.63
1:C:16:LYS:O	1:C:20:GLU:HG3	1.99	0.63
1:A:144:LEU:HD23	1:A:195:ALA:HA	1.80	0.62
1:C:83:ILE:HD13	1:C:84:ILE:N	2.14	0.62
1:A:188:THR:O	1:A:188:THR:CG2	2.47	0.62
1:A:134:PHE:HA	1:A:181:ALA:HB2	1.82	0.62
1:B:15:LEU:HD23	1:B:44:GLU:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LYS:CD	1:B:133:LYS:C	2.72	0.61
1:B:127:ASP:O	1:B:186:LYS:HA	2.01	0.61
1:B:38:GLU:OE1	1:B:38:GLU:HA	2.00	0.61
1:B:36:THR:HG22	1:B:38:GLU:N	2.17	0.60
1:B:76:ASN:ND2	1:B:113:ARG:HD3	2.16	0.60
1:B:84:ILE:CG2	1:B:85:GLN:N	2.65	0.60
1:A:165:LEU:HD12	1:A:165:LEU:C	2.27	0.60
1:B:33:LEU:HD23	1:B:62:VAL:HG21	1.83	0.60
1:C:128:ASN:HD22	1:C:131:ASP:CB	2.15	0.60
1:A:193:LEU:O	1:A:193:LEU:HD12	2.02	0.60
1:A:90:ARG:HB2	1:A:107:CYS:O	2.02	0.59
1:B:147:LEU:HD11	1:B:194:ILE:HD11	1.82	0.59
1:A:182:PHE:O	1:A:183:THR:HG23	2.02	0.59
1:B:126:THR:CG2	1:B:183:THR:HG22	2.31	0.59
1:B:76:ASN:HD21	1:B:113:ARG:HH11	1.48	0.58
1:B:22:VAL:HG12	1:B:22:VAL:O	2.03	0.58
1:C:123:ASP:OD1	1:C:192:LYS:HE2	2.03	0.58
1:B:82:VAL:HG13	1:B:83:ILE:N	2.16	0.58
1:C:172:MET:HE3	1:C:172:MET:N	2.17	0.58
1:A:112:LYS:HZ3	1:B:61:HIS:CD2	2.21	0.57
1:B:36:THR:CG2	1:B:38:GLU:HB2	2.34	0.57
1:A:151:ILE:HG21	1:A:182:PHE:HD2	1.70	0.57
1:A:38:GLU:CD	1:A:38:GLU:H	2.11	0.57
1:A:52:THR:OG1	1:A:55:GLN:HG3	2.05	0.56
1:B:67:ILE:O	1:B:71:THR:HG23	2.06	0.56
1:A:97:ARG:C	1:A:98:ASP:CG	2.72	0.56
1:A:38:GLU:CD	1:A:38:GLU:N	2.62	0.56
1:B:133:LYS:HD2	1:B:134:PHE:N	2.18	0.56
1:B:36:THR:HG22	1:B:38:GLU:HB2	1.86	0.56
1:C:128:ASN:HD22	1:C:131:ASP:CG	2.14	0.55
1:B:58:ARG:O	1:B:62:VAL:HG23	2.05	0.55
1:A:83:ILE:C	1:A:84:ILE:HD12	2.31	0.55
1:B:152:HIS:HB2	1:B:185:ALA:HA	1.88	0.55
1:B:153:MET:HE3	1:B:182:PHE:CE1	2.41	0.55
1:A:128:ASN:ND2	1:A:131:ASP:OD2	2.40	0.55
1:A:90:ARG:NH2	5:A:199:GOL:O1	2.40	0.55
1:B:33:LEU:CD2	1:B:62:VAL:HG21	2.37	0.55
1:C:153:MET:HE2	1:C:155:TRP:CE3	2.41	0.55
1:B:176:GLU:O	1:B:177:HIS:HB2	2.06	0.54
1:A:112:LYS:HZ1	1:B:61:HIS:CD2	2.23	0.54
1:B:153:MET:HG3	1:B:154:LYS:H	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:MET:CG	1:B:154:LYS:N	2.69	0.54
1:C:117:LEU:HG	1:C:119:PRO:HD3	1.89	0.54
1:C:146:VAL:HG13	1:C:151:ILE:HD13	1.90	0.54
1:C:83:ILE:HG23	1:C:109:VAL:HG21	1.90	0.54
1:C:114:ALA:N	1:C:115:PRO:HD3	2.23	0.54
1:C:25:ASP:O	1:C:28:ALA:N	2.41	0.53
1:A:85:GLN:OE1	1:A:108:LEU:HA	2.08	0.53
1:A:151:ILE:CG2	1:A:182:PHE:HD2	2.22	0.53
1:B:107:CYS:HA	1:B:120:LEU:CD2	2.36	0.53
1:A:65:THR:HG23	1:A:66:SER:N	2.23	0.52
1:B:100:VAL:O	1:B:102:TYR:N	2.39	0.52
1:A:84:ILE:HG21	1:A:86:MET:HE2	1.91	0.52
1:C:24:MET:HB3	1:C:28:ALA:HB3	1.91	0.52
1:A:82:VAL:HG12	1:A:84:ILE:HD12	1.91	0.51
1:A:43:TRP:C	1:A:45:ASN:H	2.17	0.51
1:B:153:MET:SD	1:B:172:MET:HE1	2.51	0.51
1:B:123:ASP:OD1	1:B:192:LYS:HE3	2.11	0.51
1:B:99:ASN:N	1:B:99:ASN:HD22	2.08	0.51
1:A:146:VAL:CG1	1:A:168:THR:HA	2.41	0.50
1:C:126:THR:HG22	1:C:128:ASN:H	1.75	0.50
1:A:24:MET:HE3	1:A:29:LEU:HB2	1.91	0.50
1:B:147:LEU:H	1:B:193:LEU:HA	1.75	0.50
1:A:82:VAL:HG12	1:A:84:ILE:CD1	2.42	0.50
1:B:106:ASN:HB2	1:B:121:VAL:HB	1.92	0.50
1:A:147:LEU:HG	1:A:194:ILE:HG13	1.92	0.49
1:B:84:ILE:HG22	1:B:85:GLN:N	2.27	0.49
1:A:103:TYR:HD2	1:A:105:TYR:HH	1.60	0.49
1:A:109:VAL:HG13	1:A:109:VAL:O	2.13	0.49
1:A:157:ASP:OD2	1:A:159:GLU:HB2	2.12	0.49
1:A:193:LEU:HD12	1:A:193:LEU:C	2.37	0.49
1:B:82:VAL:CG1	1:B:83:ILE:N	2.76	0.49
1:A:119:PRO:O	1:A:120:LEU:HD23	2.13	0.49
1:A:142:GLU:OE2	1:A:144:LEU:HD21	2.12	0.49
1:B:99:ASN:N	1:B:99:ASN:ND2	2.59	0.49
1:B:193:LEU:HD12	1:B:193:LEU:C	2.38	0.49
1:C:27:ALA:O	1:C:31:SER:OG	2.24	0.49
1:A:90:ARG:HH22	5:A:199:GOL:C1	2.26	0.48
1:A:150:GLU:HG2	1:A:165:LEU:HD13	1.95	0.48
1:B:102:TYR:OH	1:B:132:ALA:HA	2.14	0.48
1:A:150:GLU:CG	1:A:165:LEU:HD13	2.43	0.48
1:B:182:PHE:O	1:B:183:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:VAL:HG13	1:A:151:ILE:CD1	2.44	0.48
1:A:102:TYR:HE2	1:A:133:LYS:H	1.62	0.47
1:A:151:ILE:HG21	1:A:182:PHE:CD2	2.48	0.47
1:B:51:LEU:HD23	1:B:55:GLN:OE1	2.15	0.47
1:C:25:ASP:O	1:C:26:HIS:C	2.58	0.47
1:C:120:LEU:CD1	1:C:195:ALA:HB3	2.45	0.47
1:C:120:LEU:HD11	1:C:195:ALA:HB3	1.97	0.47
1:C:141:ASN:HB3	1:C:173:PHE:CE1	2.50	0.47
1:C:144:LEU:HB2	1:C:172:MET:CG	2.44	0.47
1:A:150:GLU:CD	1:A:165:LEU:HD13	2.40	0.47
1:A:58:ARG:O	1:A:62:VAL:HG23	2.15	0.47
1:A:85:GLN:NE2	1:A:90:ARG:HA	2.30	0.46
1:C:128:ASN:ND2	1:C:131:ASP:CB	2.70	0.46
1:A:136:SER:O	1:A:179:PRO:HG3	2.16	0.46
1:B:15:LEU:HD23	1:B:44:GLU:CG	2.45	0.46
1:C:18:ARG:HG3	1:C:63:LEU:HD22	1.97	0.46
1:C:150:GLU:HG2	1:C:185:ALA:HB2	1.97	0.46
1:A:43:TRP:C	1:A:45:ASN:N	2.73	0.46
1:B:63:LEU:O	1:B:64:GLY:C	2.58	0.46
1:A:146:VAL:HG12	1:A:168:THR:HA	1.98	0.46
1:B:22:VAL:O	1:B:22:VAL:CG1	2.63	0.46
1:B:128:ASN:OD1	1:B:131:ASP:CG	2.59	0.46
1:C:146:VAL:HA	1:C:193:LEU:HD23	1.98	0.46
1:A:165:LEU:HD12	1:A:165:LEU:O	2.16	0.46
1:C:84:ILE:HG22	1:C:85:GLN:N	2.31	0.46
1:A:82:VAL:O	1:A:83:ILE:HD13	2.17	0.45
1:C:171:SER:CA	1:C:172:MET:HE3	2.47	0.45
1:B:29:LEU:HD12	1:B:29:LEU:O	2.17	0.45
1:A:135:ASN:ND2	1:A:180:HIS:O	2.50	0.44
1:C:58:ARG:HH11	1:C:58:ARG:HG2	1.81	0.44
1:B:134:PHE:C	1:B:135:ASN:O	2.57	0.44
1:A:36:THR:OG1	1:A:38:GLU:HG2	2.17	0.44
1:A:110:ARG:NH1	1:B:22:VAL:HG13	2.32	0.44
1:A:147:LEU:H	1:A:193:LEU:HA	1.82	0.44
1:B:33:LEU:HD21	1:B:59:ILE:HA	2.00	0.44
1:B:172:MET:CG	1:B:173:PHE:N	2.80	0.44
1:C:84:ILE:CG2	1:C:85:GLN:N	2.80	0.44
1:B:32:LEU:HD22	1:B:62:VAL:HG13	1.99	0.44
1:B:32:LEU:HD12	1:B:32:LEU:N	2.29	0.44
1:B:147:LEU:HD23	1:B:147:LEU:HA	1.67	0.44
1:C:126:THR:HG22	1:C:127:ASP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASP:O	1:B:80:ASP:HB2	2.17	0.44
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.87	0.43
1:A:141:ASN:HB3	1:A:173:PHE:CE1	2.53	0.43
1:C:176:GLU:O	1:C:177:HIS:HB2	2.18	0.43
1:B:36:THR:O	1:B:37:PRO:C	2.60	0.43
1:A:19:ARG:HG2	1:A:24:MET:O	2.17	0.43
1:A:107:CYS:HA	1:A:120:LEU:HD23	1.99	0.43
1:A:18:ARG:HG3	1:A:63:LEU:HG	2.01	0.43
1:A:103:TYR:HD2	1:A:105:TYR:OH	2.02	0.43
1:A:166:LEU:CD1	1:A:172:MET:HE3	2.48	0.43
1:B:144:LEU:HA	1:B:194:ILE:O	2.18	0.43
1:B:153:MET:CE	1:B:182:PHE:CZ	3.02	0.43
1:B:173:PHE:CD1	1:B:173:PHE:C	2.97	0.43
1:A:127:ASP:O	1:A:129:PRO:HD3	2.18	0.42
1:A:147:LEU:N	1:A:192:LYS:O	2.52	0.42
1:C:128:ASN:ND2	1:C:131:ASP:CG	2.77	0.42
1:B:155:TRP:HZ3	1:B:164:ALA:HB2	1.84	0.42
1:C:120:LEU:O	1:C:120:LEU:HD12	2.20	0.42
1:A:39:THR:O	1:A:42:ALA:HB3	2.19	0.42
1:A:67:ILE:HD12	1:B:71:THR:HB	2.02	0.42
1:A:90:ARG:HA	1:A:91:PRO:HD3	1.85	0.42
1:B:172:MET:HG2	1:B:173:PHE:N	2.35	0.42
1:C:73:PRO:O	1:C:74:ALA:C	2.63	0.42
1:B:28:ALA:O	1:B:32:LEU:HD12	2.19	0.42
1:B:96:VAL:HG13	1:B:96:VAL:O	2.20	0.42
1:B:193:LEU:HD12	1:B:193:LEU:O	2.20	0.42
1:A:84:ILE:CG2	1:A:86:MET:HE2	2.50	0.42
1:B:77:ASP:OD2	1:B:112:LYS:HB2	2.19	0.42
1:B:32:LEU:H	1:B:32:LEU:CD1	2.30	0.41
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.94	0.41
1:A:33:LEU:CD2	1:A:62:VAL:HG21	2.50	0.41
1:A:51:LEU:O	1:B:52:THR:HA	2.20	0.41
1:A:118:VAL:HB	1:A:197:ASN:HB2	2.02	0.41
1:A:180:HIS:ND1	1:A:180:HIS:N	2.69	0.41
1:C:25:ASP:C	1:C:27:ALA:N	2.75	0.41
1:C:83:ILE:HG23	1:C:109:VAL:CG2	2.51	0.41
1:C:82:VAL:CG1	1:C:83:ILE:N	2.83	0.41
1:C:152:HIS:ND1	1:C:165:LEU:CD2	2.81	0.41
1:A:146:VAL:HG13	1:A:151:ILE:HD12	2.03	0.41
1:A:101:ASP:C	1:A:125:LEU:HD12	2.46	0.41
1:A:78:LEU:HA	1:A:83:ILE:HD13	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:TYR:HD1	1:B:103:TYR:CD1	2.39	0.40
1:A:143:PHE:HB3	1:A:196:VAL:HB	2.03	0.40
1:A:13:GLU:O	1:A:17:ASP:OD1	2.40	0.40
1:A:93:LEU:HD23	1:B:23:LYS:HB3	2.03	0.40
1:B:180:HIS:ND1	1:B:180:HIS:N	2.70	0.40
1:C:16:LYS:HA	1:C:44:GLU:OE2	2.21	0.40
1:A:84:ILE:HD12	1:A:84:ILE:N	2.35	0.40
1:B:107:CYS:SG	1:B:120:LEU:HD21	2.61	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	191/198 (96%)	174 (91%)	17 (9%)	0	100	100
1	B	191/198 (96%)	174 (91%)	17 (9%)	0	100	100
1	C	191/198 (96%)	182 (95%)	8 (4%)	1 (0%)	24	42
All	All	573/594 (96%)	530 (92%)	42 (7%)	1 (0%)	43	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	PRO

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/160 (94%)	142 (95%)	8 (5%)	20	42
1	B	153/160 (96%)	145 (95%)	8 (5%)	21	43
1	C	154/160 (96%)	147 (96%)	7 (4%)	24	48
All	All	457/480 (95%)	434 (95%)	23 (5%)	22	44

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	38	GLU
1	A	63	LEU
1	A	97	ARG
1	A	98	ASP
1	A	148	GLU
1	A	151	ILE
1	A	165	LEU
1	B	8	SER
1	B	82	VAL
1	B	84	ILE
1	B	101	ASP
1	B	133	LYS
1	B	144	LEU
1	B	148	GLU
1	B	153	MET
1	C	83	ILE
1	C	111	THR
1	C	120	LEU
1	C	136	SER
1	C	151	ILE
1	C	161	PRO
1	C	172	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	106	ASN
1	A	128	ASN
1	A	197	ASN

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Mol	Chain	Res	Type
1	B	61	HIS
1	B	76	ASN
1	B	99	ASN
1	B	106	ASN
1	C	128	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	S0H	C	207	2	7,7,7	4.30	4 (57%)	6,10,10	2.45	2 (33%)
4	S0H	B	206	2	7,7,7	4.59	4 (57%)	6,10,10	2.45	2 (33%)
3	NO	B	210	2	0,1,1	-	-	-	-	-
4	S0H	A	205	2	7,7,7	4.44	4 (57%)	6,10,10	2.36	1 (16%)
5	GOL	C	199	-	5,5,5	0.47	0	5,5,5	0.47	0
3	NO	A	209	2	0,1,1	-	-	-	-	-
5	GOL	A	199	-	5,5,5	0.37	0	5,5,5	0.31	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
4	S0H	C	207	2	-	0/5/5/5	-
4	S0H	B	206	2	-	1/5/5/5	-
4	S0H	A	205	2	-	0/5/5/5	-
5	GOL	C	199	-	-	4/4/4/4	-
5	GOL	A	199	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	206	S0H	C1-C3	-10.12	1.09	1.51
4	A	205	S0H	C1-C3	-9.92	1.10	1.51
4	C	207	S0H	C1-C3	-9.89	1.10	1.51
4	B	206	S0H	P1-O13	-4.39	1.45	1.55
4	A	205	S0H	P1-O13	-4.18	1.45	1.55
4	C	207	S0H	P1-O13	-3.86	1.46	1.55
4	B	206	S0H	P1-O14	3.65	1.57	1.50
4	B	206	S0H	P1-C2	3.46	1.82	1.79
4	A	205	S0H	P1-C2	3.31	1.82	1.79
4	A	205	S0H	P1-O14	3.29	1.56	1.50
4	C	207	S0H	P1-O14	2.92	1.56	1.50
4	C	207	S0H	P1-C2	2.66	1.81	1.79

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	207	S0H	O15-P1-O14	-5.26	98.79	112.39
4	B	206	S0H	O15-P1-O14	-5.09	99.21	112.39
4	A	205	S0H	O15-P1-O14	-4.97	99.53	112.39
4	B	206	S0H	O14-P1-C2	-2.21	107.42	111.56
4	C	207	S0H	O15-P1-O13	2.04	113.77	107.96

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	199	GOL	O1-C1-C2-C3
5	C	199	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	199	GOL	O2-C2-C3-O3
5	C	199	GOL	O1-C1-C2-C3
5	A	199	GOL	O1-C1-C2-O2
5	C	199	GOL	O1-C1-C2-O2
4	B	206	S0H	P1-C2-C3-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	199	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	193/198 (97%)	0.50	12 (6%) 26 19	56, 81, 113, 122	0
1	B	193/198 (97%)	0.33	8 (4%) 41 32	51, 75, 96, 115	0
1	C	193/198 (97%)	-0.04	4 (2%) 63 55	47, 63, 90, 99	0
All	All	579/594 (97%)	0.26	24 (4%) 41 32	47, 72, 103, 122	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	VAL	4.7
1	A	172	MET	3.6
1	C	160	ASN	3.5
1	C	38	GLU	3.4
1	A	103	TYR	3.2
1	B	172	MET	3.0
1	B	134	PHE	2.7
1	A	187	GLY	2.7
1	B	102	TYR	2.6
1	C	100	VAL	2.4
1	B	103	TYR	2.4
1	B	100	VAL	2.4
1	C	102	TYR	2.4
1	B	75	GLY	2.3
1	B	182	PHE	2.3
1	B	45	ASN	2.3
1	A	134	PHE	2.2
1	A	148	GLU	2.2
1	A	83	ILE	2.2
1	A	96	VAL	2.2
1	A	136	SER	2.2
1	A	133	LYS	2.1
1	A	95	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLY	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
5	GOL	A	199	6/6	0.72	0.23	87,89,90,91	0
4	S0H	B	206	8/8	0.94	0.10	76,79,81,82	0
3	NO	B	210	2/2	0.95	0.09	75,75,75,76	0
5	GOL	C	199	6/6	0.95	0.10	74,76,77,77	0
4	S0H	A	205	8/8	0.97	0.07	86,88,89,89	0
4	S0H	C	207	8/8	0.97	0.07	64,65,67,68	0
2	FE2	A	201	1/1	0.99	0.03	82,82,82,82	0
2	FE2	B	202	1/1	0.99	0.02	74,74,74,74	0
3	NO	A	209	2/2	0.99	0.04	79,79,79,80	0
2	FE2	C	203	1/1	1.00	0.02	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.