



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:00 PM GMT

PDB ID : 4B7S
Title : PikC D50N mutant bound to the 10-DML analog with the 3-(N,N- dimethylamino)propanoate anchoring group
Authors : Podust, L.M.
Deposited on : 2012-08-21
Resolution : 1.84 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

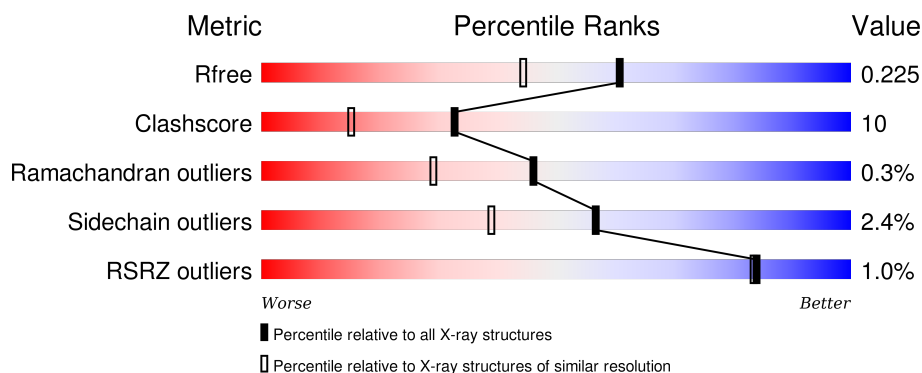
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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	436	<div> <div></div> <div>74% 16% • 9%</div> </div>
1	B	436	<div> <div></div> <div>79% 10% • 10%</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
3	SO4	A	1412	-	-	-	X
3	SO4	A	1414	-	-	-	X
3	SO4	B	1410	-	-	-	X
5	GOL	A	1417	-	-	X	X
5	GOL	A	1420	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7135 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 CYTOCHROME P450 HYDROXYLASE PIKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	3	0
			3084	1948	553	570	13			
1	B	393	Total	C	N	O	S	0	5	0
			3100	1959	554	574	13			

There are 42 discrepancies between the modelled and reference sequences:

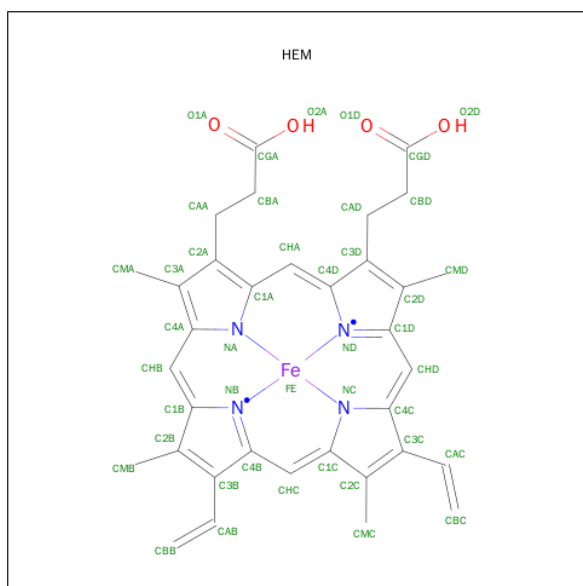
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O87605
A	-18	GLY	-	EXPRESSION TAG	UNP O87605
A	-17	SER	-	EXPRESSION TAG	UNP O87605
A	-16	SER	-	EXPRESSION TAG	UNP O87605
A	-15	HIS	-	EXPRESSION TAG	UNP O87605
A	-14	HIS	-	EXPRESSION TAG	UNP O87605
A	-13	HIS	-	EXPRESSION TAG	UNP O87605
A	-12	HIS	-	EXPRESSION TAG	UNP O87605
A	-11	HIS	-	EXPRESSION TAG	UNP O87605
A	-10	HIS	-	EXPRESSION TAG	UNP O87605
A	-9	SER	-	EXPRESSION TAG	UNP O87605
A	-8	SER	-	EXPRESSION TAG	UNP O87605
A	-7	GLY	-	EXPRESSION TAG	UNP O87605
A	-6	LEU	-	EXPRESSION TAG	UNP O87605
A	-5	VAL	-	EXPRESSION TAG	UNP O87605
A	-4	PRO	-	EXPRESSION TAG	UNP O87605
A	-3	ARG	-	EXPRESSION TAG	UNP O87605
A	-2	GLY	-	EXPRESSION TAG	UNP O87605
A	-1	SER	-	EXPRESSION TAG	UNP O87605
A	0	HIS	-	EXPRESSION TAG	UNP O87605
A	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
B	-19	MET	-	EXPRESSION TAG	UNP O87605
B	-18	GLY	-	EXPRESSION TAG	UNP O87605
B	-17	SER	-	EXPRESSION TAG	UNP O87605
B	-16	SER	-	EXPRESSION TAG	UNP O87605

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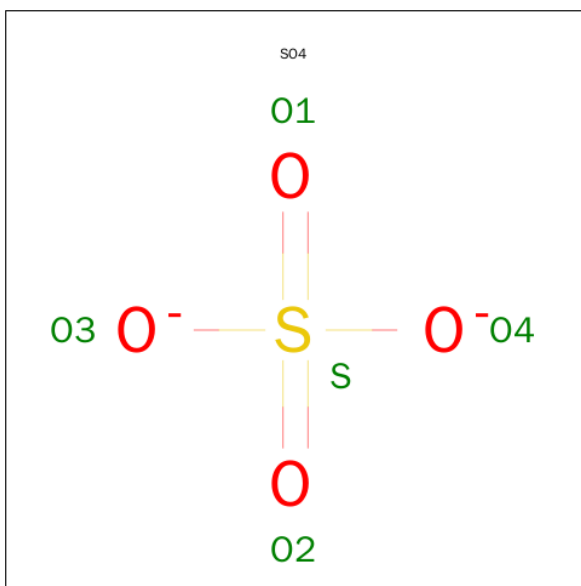
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP O87605
B	-14	HIS	-	EXPRESSION TAG	UNP O87605
B	-13	HIS	-	EXPRESSION TAG	UNP O87605
B	-12	HIS	-	EXPRESSION TAG	UNP O87605
B	-11	HIS	-	EXPRESSION TAG	UNP O87605
B	-10	HIS	-	EXPRESSION TAG	UNP O87605
B	-9	SER	-	EXPRESSION TAG	UNP O87605
B	-8	SER	-	EXPRESSION TAG	UNP O87605
B	-7	GLY	-	EXPRESSION TAG	UNP O87605
B	-6	LEU	-	EXPRESSION TAG	UNP O87605
B	-5	VAL	-	EXPRESSION TAG	UNP O87605
B	-4	PRO	-	EXPRESSION TAG	UNP O87605
B	-3	ARG	-	EXPRESSION TAG	UNP O87605
B	-2	GLY	-	EXPRESSION TAG	UNP O87605
B	-1	SER	-	EXPRESSION TAG	UNP O87605
B	0	HIS	-	EXPRESSION TAG	UNP O87605
B	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



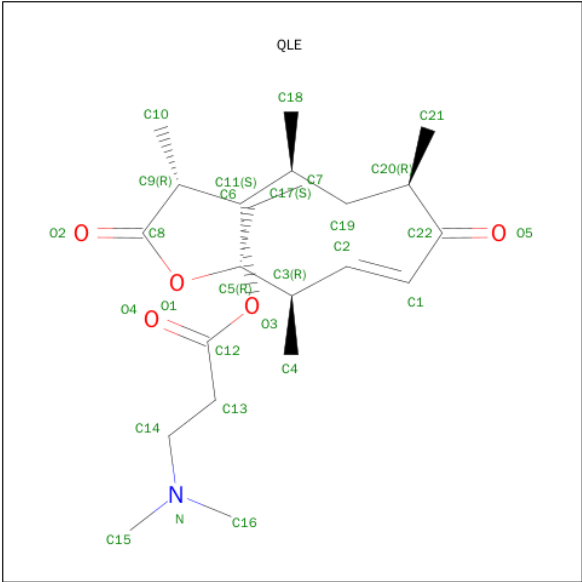
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



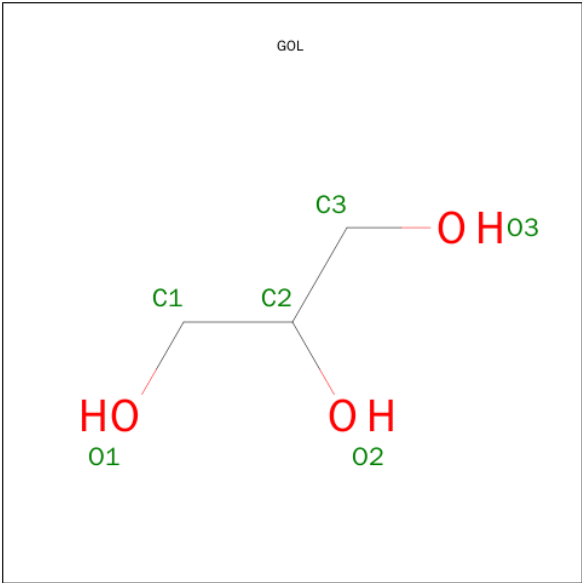
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is [(3R,4S,5S,7R,9E,11R,12R)-12-ETHYL-3,5,7,11-TETRAMETHYL-2,8-BIS(OXIDANYLIDENE)-1-OXACYCLODODEC-9-EN-4-YL] 3-(DIMETHYLAMINO)PROPANOATE (three-letter code: QLE) (formula: C₂₂H₃₇NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	22	1	5		
4	B	1	Total	C	N	O	0	0
			28	22	1	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

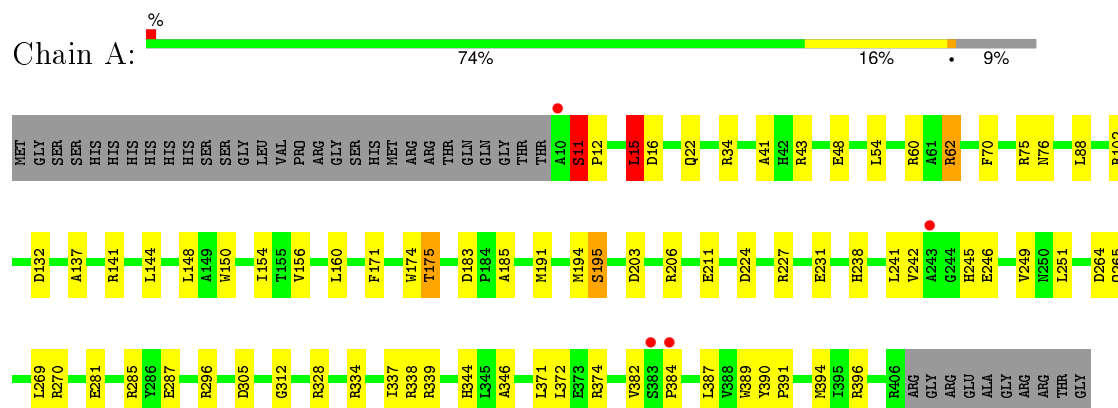
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	403	Total	O	0	0
			403	403		
6	B	324	Total	O	0	0
			324	324		

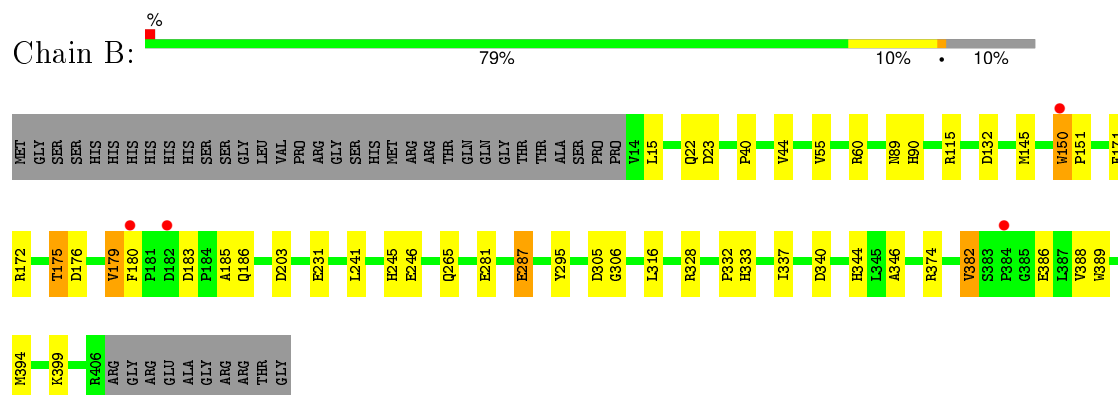
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.25Å 92.02Å 69.53Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	61.24 – 1.84 61.24 – 1.84	Depositor EDS
% Data completeness (in resolution range)	94.4 (61.24-1.84) 94.4 (61.24-1.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.166 , 0.224 0.167 , 0.225	Depositor DCC
R_{free} test set	3187 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.3	EDS
Estimated twinning fraction	0.076 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63120 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7135	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: GOL, QLE, SO4, HEM

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	1.02	2/3157 (0.1%)	0.95	8/4312 (0.2%)
1	B	0.97	0/3175	0.88	3/4336 (0.1%)
All	All	1.00	2/6332 (0.0%)	0.92	11/8648 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	GLU	CG-CD	6.83	1.62	1.51
1	A	249	VAL	CB-CG2	5.08	1.63	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	15	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	270	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	B	328	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	203	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	340	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	285	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	16	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	16	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	264	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	206	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3084	0	3037	68	0
1	B	3100	0	3049	55	0
2	A	43	0	30	1	0
2	B	43	0	30	4	0
3	A	30	0	0	2	0
3	B	10	0	0	0	0
4	A	28	0	37	5	0
4	B	28	0	37	4	0
5	A	36	0	48	21	0
5	B	6	0	8	0	0
6	A	403	0	0	10	0
6	B	324	0	0	6	0
All	All	7135	0	6276	132	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 10.

All (132) 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:287:GLU:CB	5:A:1417:GOL:H31	1.63	1.27
1:B:180[B]:PHE:O	1:B:180[B]:PHE:CD1	2.05	1.09
5:A:1420:GOL:H12	6:A:2048:HOH:O	1.51	1.09
1:A:15:LEU:HD13	5:A:1420:GOL:O3	1.64	0.96
1:A:287:GLU:CB	5:A:1417:GOL:C3	2.44	0.95
1:A:396:ARG:NE	5:A:1417:GOL:H11	1.84	0.91
1:A:15:LEU:CD1	5:A:1420:GOL:O3	2.17	0.91
1:B:179:VAL:HG13	4:B:1408:QLE:H212	1.56	0.87
1:A:338:ARG:NH1	6:A:2363:HOH:O	2.06	0.86
1:A:242:VAL:HG11	4:A:1408:QLE:H181	1.55	0.86
1:B:333[A]:HIS:HE1	6:B:2298:HOH:O	1.58	0.86
1:A:34:ARG:HH21	5:A:1420:GOL:H31	1.40	0.84
1:B:22:GLN:HE22	1:B:389:TRP:H	1.26	0.84
1:A:396:ARG:HE	5:A:1417:GOL:H11	1.41	0.83
1:B:180[B]:PHE:O	1:B:180[B]:PHE:CG	2.34	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150[B]:TRP:CZ3	1:B:245:HIS:NE2	2.48	0.80
1:A:60:ARG:NH2	1:A:305:ASP:HB2	1.98	0.79
1:B:183[B]:ASP:OD2	1:B:185:ALA:HB3	1.85	0.76
1:A:171:PHE:O	1:A:175:THR:HB	1.87	0.75
1:B:145:MET:HG3	1:B:150[B]:TRP:CD1	2.22	0.75
1:A:102:ARG:HH21	5:A:1416:GOL:H32	1.51	0.75
1:A:34:ARG:NH2	5:A:1420:GOL:H31	2.03	0.74
1:B:145:MET:HG3	1:B:150[B]:TRP:HD1	1.52	0.74
1:A:22:GLN:HE22	1:A:389:TRP:H	1.36	0.73
1:B:60:ARG:NH2	1:B:305[B]:ASP:OD1	2.21	0.73
1:B:175:THR:HG21	1:B:245:HIS:CD2	2.24	0.72
1:B:145:MET:SD	1:B:150[B]:TRP:CD1	2.83	0.72
1:B:150[A]:TRP:CH2	1:B:172:ARG:HB2	2.25	0.72
1:A:11:SER:H	1:A:12:PRO:HD3	1.56	0.71
1:A:156:VAL:O	1:A:160:LEU:HD13	1.92	0.70
1:A:60:ARG:HH22	1:A:305:ASP:HB2	1.54	0.70
1:B:150[B]:TRP:HZ3	1:B:245:HIS:HE2	1.31	0.69
1:A:265:GLN:NE2	1:A:337:ILE:H	1.91	0.68
1:A:203[A]:ASP:OD1	6:A:2271:HOH:O	2.10	0.68
1:B:344:HIS:HD2	1:B:346:ALA:H	1.43	0.67
1:B:265:GLN:NE2	1:B:337:ILE:H	1.93	0.66
1:A:15:LEU:HD11	5:A:1420:GOL:O3	1.96	0.66
1:A:344:HIS:HD2	1:A:346:ALA:H	1.43	0.65
1:B:306:GLY:O	6:B:2286:HOH:O	2.14	0.65
1:B:150[B]:TRP:CE3	1:B:245:HIS:NE2	2.65	0.64
1:A:62:ARG:HH21	5:A:1419:GOL:C3	2.10	0.64
1:A:396:ARG:HE	5:A:1417:GOL:C1	2.10	0.64
1:A:396:ARG:CZ	5:A:1417:GOL:H11	2.28	0.64
1:B:145:MET:CG	1:B:150[B]:TRP:CD1	2.81	0.63
1:B:175:THR:HG23	1:B:246:GLU:OE2	1.99	0.62
1:B:115:ARG:NH2	6:B:2148:HOH:O	2.31	0.62
1:B:179:VAL:CG1	4:B:1408:QLE:H212	2.30	0.61
1:A:241:LEU:O	1:A:245:HIS:HB2	2.00	0.61
1:B:132:ASP:OD1	1:B:374:ARG:NH2	2.24	0.61
1:B:179:VAL:HB	1:B:180[A]:PHE:CE1	2.35	0.61
1:A:11:SER:CB	6:A:2004:HOH:O	2.48	0.61
1:A:328:ARG:HH11	1:A:328:ARG:HG3	1.66	0.60
1:A:11:SER:H	1:A:12:PRO:CD	2.17	0.58
1:A:175:THR:HG23	1:A:246:GLU:OE2	2.04	0.57
1:B:150[A]:TRP:CZ3	1:B:172:ARG:HB2	2.40	0.56
1:A:11:SER:HB2	6:A:2004:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:MET:HE2	4:B:1408:QLE:H213	1.88	0.55
1:A:62:ARG:HE	5:A:1419:GOL:H32	1.69	0.55
4:A:1408:QLE:C7	4:A:1408:QLE:H42C	2.37	0.55
1:A:265:GLN:HE21	1:A:337:ILE:H	1.54	0.55
1:A:11:SER:N	1:A:12:PRO:CD	2.70	0.55
1:B:265:GLN:HE21	1:B:337:ILE:H	1.54	0.55
1:A:281:GLU:OE1	1:A:344:HIS:HE1	1.90	0.55
1:B:281:GLU:OE1	1:B:344:HIS:HE1	1.91	0.53
1:B:179:VAL:HB	1:B:180[A]:PHE:CD1	2.44	0.53
1:A:328:ARG:HG3	1:A:328:ARG:NH1	2.23	0.53
1:B:265:GLN:NE2	1:B:337:ILE:HG12	2.24	0.53
1:B:183[B]:ASP:OD1	1:B:186:GLN:HB2	2.09	0.53
1:B:246:GLU:HG2	6:B:2195:HOH:O	2.08	0.52
1:B:382:VAL:HG22	1:B:386:GLU:HB2	1.90	0.52
1:A:137:ALA:HB2	6:A:2221:HOH:O	2.10	0.51
1:A:269:LEU:HD23	1:A:372:LEU:HD21	1.92	0.51
1:B:332:PRO:HD2	1:B:333[B]:HIS:CE1	2.45	0.51
1:A:174:TRP:CB	1:A:194:MET:HE3	2.40	0.51
1:B:15:LEU:HB3	1:B:44:VAL:HG12	1.93	0.50
2:B:1407:HEM:HBC2	2:B:1407:HEM:HHD	1.93	0.50
1:B:333[A]:HIS:CE1	6:B:2298:HOH:O	2.45	0.50
1:B:145:MET:CG	1:B:150[B]:TRP:HD1	2.19	0.50
1:A:251:LEU:HD22	2:A:1407:HEM:HBB1	1.92	0.50
2:B:1407:HEM:CMB	2:B:1407:HEM:HBB2	2.42	0.50
1:B:388:VAL:HG22	1:B:399:LYS:HB3	1.93	0.50
1:A:102:ARG:NH2	5:A:1416:GOL:H32	2.23	0.50
1:B:171:PHE:O	1:B:175:THR:HB	2.12	0.50
1:B:171:PHE:CZ	1:B:241:LEU:HD13	2.46	0.49
3:A:1411:SO4:O1	6:A:2396:HOH:O	2.18	0.49
1:A:191:MET:O	1:A:195:SER:HB3	2.12	0.49
1:A:75:ARG:HD3	3:A:1413:SO4:O3	2.13	0.49
1:A:231:GLU:HG3	6:A:2310:HOH:O	2.11	0.49
1:A:328:ARG:HD3	6:A:2084:HOH:O	2.13	0.49
1:B:150[B]:TRP:CH2	1:B:176:ASP:OD1	2.66	0.49
4:A:1408:QLE:H42C	4:A:1408:QLE:H73C	1.94	0.49
1:B:145:MET:SD	1:B:150[B]:TRP:NE1	2.86	0.49
1:B:394:MET:HE3	4:B:1408:QLE:H43C	1.95	0.49
1:B:295:TYR:CE1	1:B:316:LEU:HD21	2.48	0.48
1:A:154:ILE:HB	1:A:245:HIS:HE1	1.79	0.48
1:A:382:VAL:HG11	1:A:387:LEU:HD21	1.95	0.48
1:B:60:ARG:NH2	1:B:305[B]:ASP:CG	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:THR:HG21	1:A:245:HIS:HD2	1.78	0.48
1:A:396:ARG:NE	5:A:1417:GOL:C1	2.67	0.48
1:A:175:THR:HG21	1:A:245:HIS:CD2	2.50	0.47
1:A:141:ARG:NH2	6:A:2226:HOH:O	2.39	0.47
1:A:238:HIS:CE1	1:A:242:VAL:HG21	2.48	0.47
1:B:150[A]:TRP:CD1	1:B:151:PRO:HD3	2.50	0.47
1:A:224:ASP:OD2	1:A:227:ARG:HG3	2.14	0.47
1:A:62:ARG:HH21	5:A:1419:GOL:H32	1.79	0.46
1:A:102:ARG:HE	5:A:1416:GOL:H32	1.82	0.45
1:B:90:HIS:CG	1:B:231:GLU:HG3	2.52	0.44
2:B:1407:HEM:HBC2	2:B:1407:HEM:CHD	2.49	0.43
1:A:148:LEU:HD23	1:A:371:LEU:HD11	2.00	0.43
1:A:396:ARG:NH2	5:A:1417:GOL:H11	2.34	0.43
1:B:60:ARG:HH21	1:B:305[B]:ASP:CG	2.23	0.43
1:A:144:LEU:HD11	1:A:371:LEU:HD11	2.01	0.42
1:B:183[B]:ASP:OD1	1:B:183[B]:ASP:N	2.53	0.42
1:A:41:ALA:HA	1:A:54:LEU:O	2.19	0.42
1:B:23:ASP:HB2	6:B:2004:HOH:O	2.19	0.42
1:A:34:ARG:HH21	5:A:1420:GOL:C3	2.20	0.42
1:B:374:ARG:HB3	1:B:374:ARG:HE	1.75	0.41
1:A:132:ASP:OD1	1:A:374:ARG:NH2	2.48	0.41
1:A:183:ASP:OD1	1:A:185:ALA:HB3	2.20	0.41
1:A:174:TRP:CB	1:A:194:MET:CE	2.97	0.41
1:A:174:TRP:HB2	1:A:194:MET:CE	2.50	0.41
1:B:60:ARG:HA	1:B:60:ARG:HD3	1.90	0.41
1:A:88:LEU:HD21	1:A:195:SER:HB2	2.03	0.41
1:B:145:MET:HE2	1:B:145:MET:HB2	1.93	0.41
1:B:287:GLU:HA	1:B:287:GLU:OE1	2.20	0.41
1:A:76:ASN:O	1:A:312:GLY:HA2	2.21	0.40
4:A:1408:QLE:C4	4:A:1408:QLE:C7	2.99	0.40
2:B:1407:HEM:HHD	2:B:1407:HEM:CBC	2.52	0.40
1:B:40:PRO:O	1:B:55:VAL:HA	2.21	0.40
1:A:394:MET:HE2	4:A:1408:QLE:H1	2.03	0.40
1:A:70:PHE:HB3	1:A:296:ARG:HB3	2.02	0.40
1:A:390:TYR:HA	1:A:391:PRO:HD3	1.79	0.40

There are no symmetry-related clashes.

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	398/436 (91%)	388 (98%)	8 (2%)	2 (0%)	34	17
1	B	396/436 (91%)	388 (98%)	8 (2%)	0	100	100
All	All	794/872 (91%)	776 (98%)	16 (2%)	2 (0%)	46	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	PRO
1	A	11	SER

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	319/355 (90%)	310 (97%)	9 (3%)	51	32
1	B	323/355 (91%)	316 (98%)	7 (2%)	60	43
All	All	642/710 (90%)	626 (98%)	16 (2%)	57	37

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	15	LEU
1	A	43	ARG
1	A	48	GLU

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Mol	Chain	Res	Type
1	A	150	TRP
1	A	175	THR
1	A	195	SER
1	A	334	ARG
1	A	339	ARG
1	B	89	ASN
1	B	150[A]	TRP
1	B	150[B]	TRP
1	B	175	THR
1	B	179	VAL
1	B	287	GLU
1	B	382	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	188	GLN
1	A	245	HIS
1	A	265	GLN
1	A	344	HIS
1	B	22	GLN
1	B	89	ASN
1	B	188	GLN
1	B	265	GLN
1	B	344	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	HEM	A	1407	1	30,50,50	2.32	10 (33%)	24,82,82	2.75	10 (41%)
4	QLE	A	1408	-	26,28,28	1.35	3 (11%)	27,38,38	2.09	5 (18%)
3	SO4	A	1409	-	4,4,4	0.24	0	6,6,6	0.43	0
3	SO4	A	1410	-	4,4,4	0.19	0	6,6,6	0.87	0
3	SO4	A	1411	-	4,4,4	0.64	0	6,6,6	1.23	1 (16%)
3	SO4	A	1412	-	4,4,4	0.12	0	6,6,6	0.17	0
3	SO4	A	1413	-	4,4,4	0.12	0	6,6,6	0.09	0
3	SO4	A	1414	-	4,4,4	0.28	0	6,6,6	0.51	0
5	GOL	A	1415	-	5,5,5	0.46	0	5,5,5	0.79	0
5	GOL	A	1416	-	5,5,5	0.50	0	5,5,5	0.57	0
5	GOL	A	1417	-	5,5,5	0.58	0	5,5,5	1.05	0
5	GOL	A	1418	-	5,5,5	0.58	0	5,5,5	0.46	0
5	GOL	A	1419	-	5,5,5	0.43	0	5,5,5	0.71	0
5	GOL	A	1420	-	5,5,5	0.47	0	5,5,5	0.94	0
2	HEM	B	1407	1	30,50,50	2.37	10 (33%)	24,82,82	2.99	12 (50%)
4	QLE	B	1408	-	26,28,28	1.35	2 (7%)	27,38,38	1.85	6 (22%)
3	SO4	B	1409	-	4,4,4	0.24	0	6,6,6	0.35	0
3	SO4	B	1410	-	4,4,4	0.14	0	6,6,6	0.46	0
5	GOL	B	1411	-	5,5,5	0.62	0	5,5,5	0.82	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
2	HEM	A	1407	1	-	0/10/54/54	0/0/8/8
4	QLE	A	1408	-	-	0/44/44/44	0/0/1/1
3	SO4	A	1409	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1410	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1411	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1412	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1413	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1414	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1415	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1416	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1417	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1418	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1419	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1420	-	-	0/4/4/4	0/0/0/0
2	HEM	B	1407	1	-	0/10/54/54	0/0/8/8
4	QLE	B	1408	-	-	0/44/44/44	0/0/1/1
3	SO4	B	1409	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1410	-	-	0/0/0/0	0/0/0/0
5	GOL	B	1411	-	-	0/4/4/4	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1407	HEM	C3B-C4B	-6.93	1.45	1.51
2	A	1407	HEM	C3D-C4D	-6.41	1.43	1.51
2	A	1407	HEM	C3B-C4B	-5.35	1.47	1.51
2	B	1407	HEM	C3D-C4D	-5.22	1.44	1.51
2	A	1407	HEM	C2C-C1C	-4.01	1.45	1.52
2	B	1407	HEM	C2C-C1C	-3.27	1.46	1.52
2	B	1407	HEM	C2D-C1D	-2.81	1.42	1.51
2	A	1407	HEM	C2D-C1D	-2.35	1.44	1.51
2	B	1407	HEM	C2B-C1B	-2.12	1.44	1.51
4	A	1408	QLE	O5-C22	2.05	1.25	1.22
2	B	1407	HEM	C4C-NC	2.10	1.38	1.36
2	B	1407	HEM	C3B-CAB	2.34	1.55	1.51
2	A	1407	HEM	C1C-NC	2.55	1.39	1.36
2	B	1407	HEM	CAA-C2A	2.69	1.56	1.52
2	A	1407	HEM	CMA-C3A	2.82	1.57	1.51
2	A	1407	HEM	FE-NC	2.86	2.07	1.95
2	A	1407	HEM	C3C-CAC	2.86	1.56	1.51
2	A	1407	HEM	FE-ND	2.94	2.13	1.97
2	A	1407	HEM	C3B-CAB	2.96	1.56	1.51
4	A	1408	QLE	O3-C12	3.25	1.44	1.34
4	B	1408	QLE	O3-C12	3.60	1.45	1.34
2	B	1407	HEM	C1C-NC	3.62	1.40	1.36
2	B	1407	HEM	FE-NC	4.49	2.13	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1408	QLE	O1-C8	4.87	1.45	1.34
4	B	1408	QLE	O1-C8	4.94	1.46	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1408	QLE	C2-C1-C22	-6.80	114.25	123.22
4	A	1408	QLE	C13-C14-N	-6.06	104.95	113.42
2	B	1407	HEM	C3B-CAB-CBB	-6.05	115.18	124.46
4	B	1408	QLE	C13-C14-N	-5.45	105.81	113.42
2	B	1407	HEM	C3C-CAC-CBC	-5.20	116.48	124.46
2	A	1407	HEM	CAA-C2A-C1A	-4.72	121.89	127.01
2	A	1407	HEM	CBD-CAD-C3D	-4.16	101.45	113.55
2	B	1407	HEM	CBA-CAA-C2A	-3.73	105.84	112.53
2	A	1407	HEM	C3B-CAB-CBB	-3.10	119.70	124.46
2	B	1407	HEM	CAA-C2A-C1A	-2.93	123.82	127.01
4	A	1408	QLE	C18-C17-C19	-2.66	106.62	110.76
4	B	1408	QLE	C2-C1-C22	-2.57	119.83	123.22
2	B	1407	HEM	CBD-CAD-C3D	-2.53	106.20	113.55
4	B	1408	QLE	C21-C20-C19	-2.36	106.69	111.42
2	B	1407	HEM	CMA-C3A-C4A	-2.23	124.68	128.36
4	A	1408	QLE	C7-C6-C5	-2.14	106.53	113.14
4	A	1408	QLE	O1-C5-C6	2.10	110.17	106.59
2	A	1407	HEM	CHD-C1D-ND	2.26	129.96	124.52
3	A	1411	SO4	O2-S-O1	2.30	116.79	109.50
4	B	1408	QLE	C4-C3-C2	2.34	115.80	110.07
2	B	1407	HEM	CMD-C2D-C3D	2.46	125.25	114.35
4	B	1408	QLE	O1-C8-C9	2.75	117.13	111.47
2	B	1407	HEM	C2D-C3D-C4D	2.98	106.54	101.50
2	A	1407	HEM	CMD-C2D-C3D	3.48	129.74	114.35
2	A	1407	HEM	CAD-C3D-C2D	3.88	124.36	113.22
2	A	1407	HEM	C2D-C3D-C4D	4.11	108.47	101.50
2	B	1407	HEM	CMC-C2C-C3C	4.14	126.88	116.53
2	A	1407	HEM	CAD-C3D-C4D	4.16	127.15	112.47
2	B	1407	HEM	CAD-C3D-C2D	4.25	125.43	113.22
4	B	1408	QLE	O1-C5-C6	4.28	113.87	106.59
2	B	1407	HEM	CAD-C3D-C4D	4.40	127.99	112.47
2	A	1407	HEM	CMB-C2B-C3B	4.94	128.86	116.53
2	A	1407	HEM	CMC-C2C-C3C	5.51	130.28	116.53
2	B	1407	HEM	CMB-C2B-C3B	5.87	131.18	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1407	HEM	1	0
4	A	1408	QLE	5	0
3	A	1411	SO4	1	0
3	A	1413	SO4	1	0
5	A	1416	GOL	3	0
5	A	1417	GOL	8	0
5	A	1419	GOL	3	0
5	A	1420	GOL	7	0
2	B	1407	HEM	4	0
4	B	1408	QLE	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	397/436 (91%)	-0.47	4 (1%) 84 83	11, 18, 34, 49	0
1	B	393/436 (90%)	-0.41	4 (1%) 84 83	12, 21, 36, 49	0
All	All	790/872 (90%)	-0.44	8 (1%) 84 83	11, 20, 35, 49	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ALA	5.4
1	B	180[A]	PHE	3.6
1	A	384	PRO	3.3
1	A	243	ALA	2.3
1	B	384	PRO	2.1
1	B	182	ASP	2.0
1	A	383	SER	2.0
1	B	150[A]	TRP	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
3	SO4	A	1414	5/5	0.75	0.27	48.71	80,81,83,83	0
3	SO4	A	1412	5/5	0.87	0.16	17.08	82,82,82,82	0
5	GOL	A	1417	6/6	0.91	0.17	11.05	34,38,39,41	0
3	SO4	B	1410	5/5	0.91	0.23	7.63	70,70,70,71	0
5	GOL	A	1420	6/6	0.91	0.20	4.31	32,34,39,43	0
4	QLE	B	1408	28/28	0.95	0.09	0.57	15,24,27,29	0
2	HEM	B	1407	43/43	0.98	0.08	0.33	9,13,16,20	0
4	QLE	A	1408	28/28	0.94	0.10	0.21	17,24,31,32	0
2	HEM	A	1407	43/43	0.98	0.09	0.21	7,12,16,24	0
5	GOL	B	1411	6/6	0.97	0.10	-	19,27,31,39	0
5	GOL	A	1419	6/6	0.90	0.16	-	32,42,45,45	0
3	SO4	A	1411	5/5	0.75	0.19	-	51,54,56,59	0
5	GOL	A	1418	6/6	0.73	0.20	-	55,56,57,58	0
3	SO4	A	1410	5/5	0.91	0.16	-	63,63,65,66	0
3	SO4	A	1413	5/5	0.87	0.21	-	89,89,90,90	0
5	GOL	A	1416	6/6	0.92	0.12	-	32,40,42,43	0
5	GOL	A	1415	6/6	0.97	0.10	-	17,26,31,37	0
3	SO4	B	1409	5/5	0.89	0.27	-	63,64,65,66	0
3	SO4	A	1409	5/5	0.93	0.17	-	62,64,65,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.