



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:23 pm GMT

PDB ID : 3NN4
Title : Structure of chlorite dismutase from Candidatus Nitrospira defluvii R173K mutant
Authors : Kostan, J.; Sjoebloom, B.; Maixner, F.; Mlynek, G.; Furtmueller, P.G.; Obinger, C.; Wagner, M.; Daims, H.; Djinovic-Carugo, K.
Deposited on : 2010-06-23
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

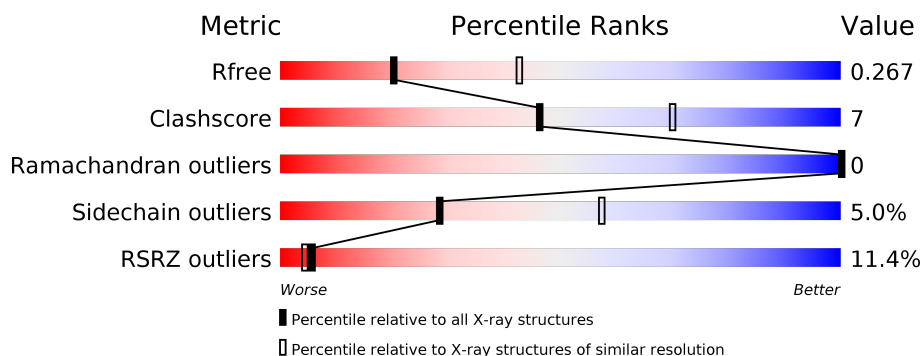
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	241	<div> <div>12%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
1	B	241	<div> <div>12%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	C	241	<div> <div>14%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	D	241	<div> <div>10%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	E	241	<div> <div>8%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10100 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 Chlorite dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1917	1223	333	355	6			
1	B	238	Total	C	N	O	S	0	0	0
			1917	1223	333	355	6			
1	C	238	Total	C	N	O	S	0	0	0
			1917	1223	333	355	6			
1	D	238	Total	C	N	O	S	0	0	0
			1917	1223	333	355	6			
1	E	238	Total	C	N	O	S	0	0	0
			1917	1223	333	355	6			

There are 20 discrepancies between the modelled and reference sequences:

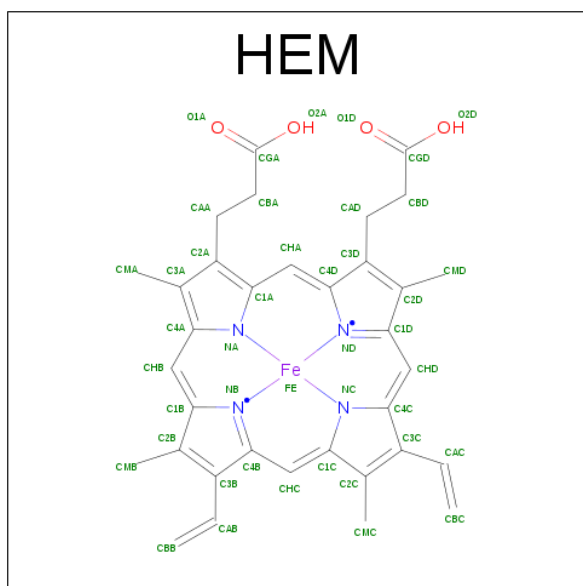
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP B3U4H7
A	-1	ALA	-	CLONING ARTIFACT	UNP B3U4H7
A	0	MET	-	CLONING ARTIFACT	UNP B3U4H7
A	173	LYS	ARG	ENGINEERED MUTATION	UNP B3U4H7
B	-2	GLY	-	CLONING ARTIFACT	UNP B3U4H7
B	-1	ALA	-	CLONING ARTIFACT	UNP B3U4H7
B	0	MET	-	CLONING ARTIFACT	UNP B3U4H7
B	173	LYS	ARG	ENGINEERED MUTATION	UNP B3U4H7
C	-2	GLY	-	CLONING ARTIFACT	UNP B3U4H7
C	-1	ALA	-	CLONING ARTIFACT	UNP B3U4H7
C	0	MET	-	CLONING ARTIFACT	UNP B3U4H7
C	173	LYS	ARG	ENGINEERED MUTATION	UNP B3U4H7
D	-2	GLY	-	CLONING ARTIFACT	UNP B3U4H7
D	-1	ALA	-	CLONING ARTIFACT	UNP B3U4H7
D	0	MET	-	CLONING ARTIFACT	UNP B3U4H7
D	173	LYS	ARG	ENGINEERED MUTATION	UNP B3U4H7
E	-2	GLY	-	CLONING ARTIFACT	UNP B3U4H7
E	-1	ALA	-	CLONING ARTIFACT	UNP B3U4H7
E	0	MET	-	CLONING ARTIFACT	UNP B3U4H7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	173	LYS	ARG	ENGINEERED MUTATION	UNP B3U4H7

- 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
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		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

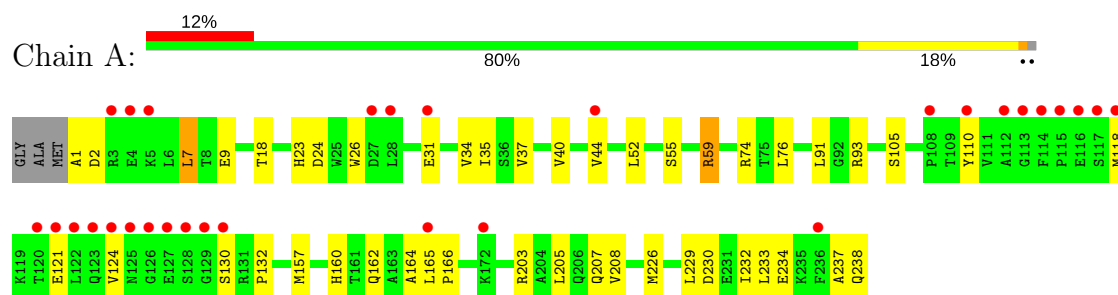
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	38	Total O 38 38	0	0
4	C	46	Total O 46 46	0	0
4	D	46	Total O 46 46	0	0
4	E	35	Total O 35 35	0	0

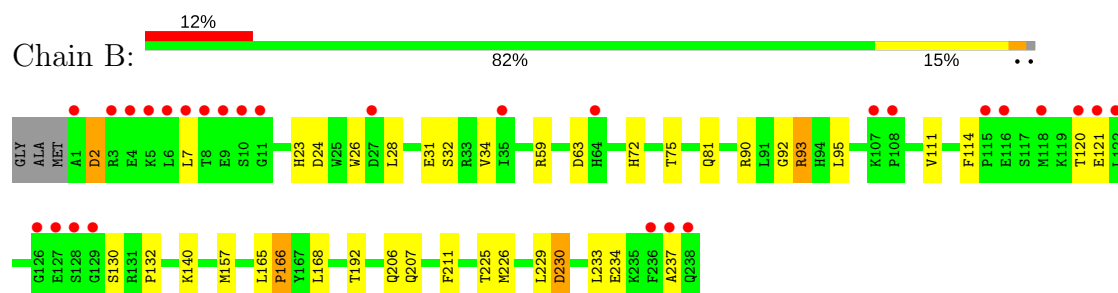
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

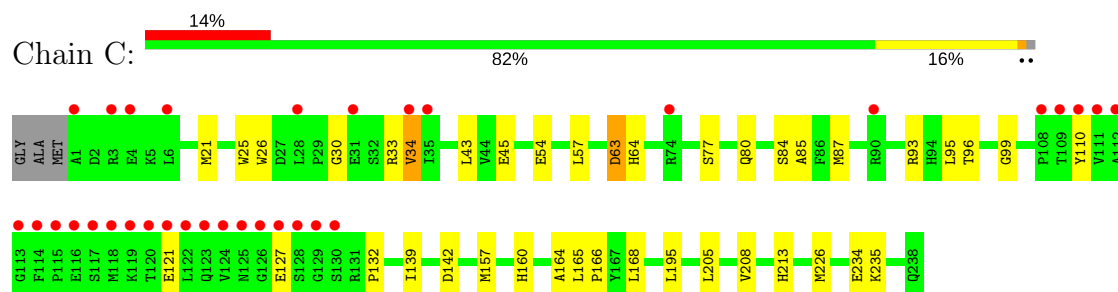
● Molecule 1: Chlorite dismutase



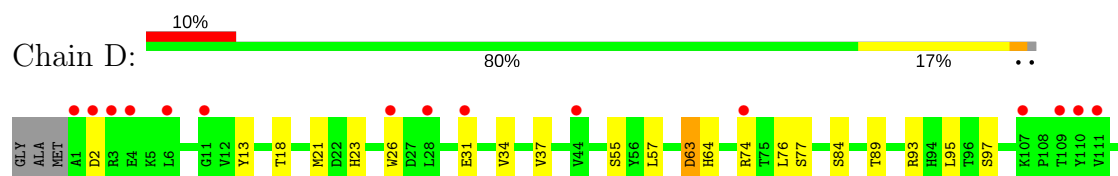
● Molecule 1: Chlorite dismutase

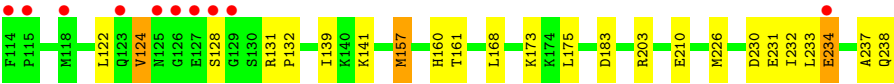


● Molecule 1: Chlorite dismutase

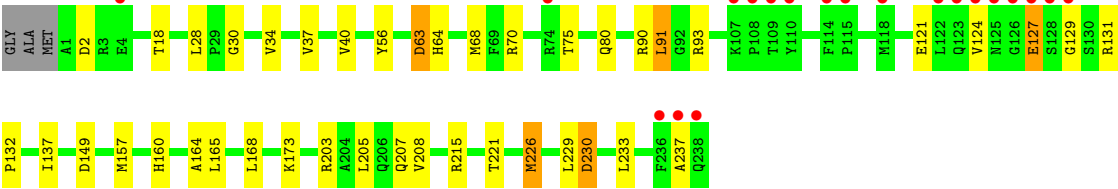
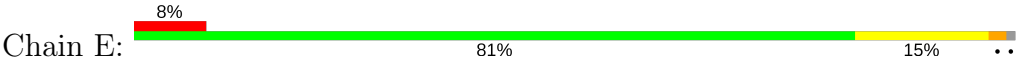


● Molecule 1: Chlorite dismutase





● Molecule 1: Chlorite dismutase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.41Å 113.88Å 119.87Å 90.00° 118.02° 90.00°	Depositor
Resolution (Å)	43.72 – 2.70 43.72 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.72-2.70) 99.9 (43.72-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.258 0.221 , 0.267	Depositor DCC
R_{free} test set	2256 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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, 0.333 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: HEM, SO4

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	0.59	0/1963	0.66	1/2654 (0.0%)
1	B	0.64	0/1963	0.68	0/2654
1	C	0.65	0/1963	0.70	0/2654
1	D	0.63	0/1963	0.65	0/2654
1	E	0.62	0/1963	0.69	1/2654 (0.0%)
All	All	0.63	0/9815	0.68	2/13270 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	E	70	ARG	NE-CZ-NH1	5.10	122.85	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	1917	0	1893	34	1
1	B	1917	0	1893	26	0
1	C	1917	0	1893	34	0
1	D	1917	0	1893	25	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1917	0	1893	30	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	7	0
2	D	43	0	30	5	0
2	E	43	0	30	0	0
3	A	20	0	0	0	0
3	B	20	0	0	1	0
3	C	25	0	0	0	0
3	D	10	0	0	0	0
3	E	30	0	0	1	0
4	A	30	0	0	2	0
4	B	38	0	0	2	0
4	C	46	0	0	0	0
4	D	46	0	0	4	0
4	E	35	0	0	1	0
All	All	10100	0	9615	140	1

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 7.

All (140) 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:E:34:VAL:O	1:E:37:VAL:HG12	1.63	0.99
1:C:139:ILE:HD12	2:C:239:HEM:HMD2	1.51	0.91
1:A:40:VAL:HG21	1:A:91:LEU:HD13	1.53	0.90
1:B:157:MET:HE2	2:B:239:HEM:HBD2	1.57	0.86
1:C:54:GLU:OE2	1:C:226:MET:CE	2.26	0.83
1:E:40:VAL:HG21	1:E:91:LEU:HD12	1.62	0.79
1:E:164:ALA:HB2	1:E:205:LEU:HD21	1.65	0.78
1:C:139:ILE:HD12	2:C:239:HEM:CMD	2.17	0.74
1:B:34:VAL:HG22	1:B:237:ALA:HB1	1.71	0.72
1:A:34:VAL:HG22	1:A:237:ALA:HB1	1.73	0.71
1:D:63:ASP:OD1	1:D:64:HIS:ND1	2.22	0.71
1:A:91:LEU:HD11	1:A:233:LEU:HD22	1.74	0.70
1:D:124:VAL:HG12	4:D:268:HOH:O	1.92	0.69
1:D:139:ILE:HD12	2:D:239:HEM:HMD1	1.74	0.69
1:C:54:GLU:OE2	1:C:226:MET:HE1	1.92	0.68
1:B:165:LEU:HD23	1:B:168:LEU:HD12	1.76	0.67
1:C:30:GLY:O	1:C:34:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:GLU:OE2	1:C:226:MET:HE3	1.94	0.66
1:B:34:VAL:CG2	1:B:237:ALA:HB1	2.26	0.65
1:E:28:LEU:HD21	1:E:90:ARG:NH2	2.14	0.63
1:A:7:LEU:CD2	1:A:52:LEU:HD23	2.31	0.61
1:D:37:VAL:HG22	1:D:233:LEU:HB3	1.83	0.61
1:E:37:VAL:HG23	1:E:233:LEU:HB3	1.84	0.60
1:A:160:HIS:HD1	1:A:205:LEU:HD22	1.67	0.59
1:A:7:LEU:HD12	4:A:263:HOH:O	2.02	0.59
1:C:139:ILE:CD1	2:C:239:HEM:HMD2	2.29	0.59
1:B:59:ARG:O	1:C:80:GLN:HG3	2.04	0.58
1:E:230:ASP:OD1	1:E:230:ASP:N	2.37	0.58
1:A:205:LEU:O	1:A:208:VAL:HG22	2.04	0.58
1:A:31:GLU:O	1:A:35:ILE:HD12	2.04	0.57
1:C:165:LEU:N	1:C:166:PRO:HD2	2.21	0.56
1:B:28:LEU:HD22	1:B:32:SER:HB3	1.88	0.56
1:C:110:TYR:CD2	1:C:157:MET:HG3	2.41	0.56
1:C:160:HIS:HD1	1:C:205:LEU:HD22	1.71	0.55
1:E:18:THR:HG22	1:E:68:MET:HG3	1.88	0.55
1:C:121:GLU:OE1	1:C:165:LEU:HD13	2.07	0.55
1:A:160:HIS:ND1	1:A:205:LEU:HD22	2.23	0.54
1:D:168:LEU:HD13	4:D:268:HOH:O	2.08	0.54
1:D:183:ASP:OD1	1:E:221:THR:OG1	2.22	0.54
1:B:140:LYS:NZ	3:B:241:SO4:O3	2.40	0.53
1:B:165:LEU:N	1:B:166:PRO:HD2	2.23	0.53
1:E:137:ILE:HG12	1:E:221:THR:HG23	1.89	0.53
1:A:229:LEU:HG	1:A:233:LEU:HD11	1.90	0.53
1:B:26:TRP:CG	1:C:93:ARG:HD2	2.44	0.53
1:A:23:HIS:ND1	1:E:93:ARG:O	2.41	0.52
1:A:93:ARG:HD2	1:C:26:TRP:CD2	2.44	0.52
1:C:43:LEU:HD11	1:C:85:ALA:HB1	1.92	0.52
1:E:63:ASP:OD2	1:E:63:ASP:C	2.47	0.52
1:B:130:SER:HB2	4:B:279:HOH:O	2.10	0.52
1:B:111:VAL:HA	1:B:114:PHE:CD2	2.44	0.52
1:C:160:HIS:ND1	1:C:205:LEU:HD22	2.25	0.51
1:A:234:GLU:O	1:A:238:GLN:HG2	2.09	0.51
1:D:21:MET:HA	1:D:95:LEU:HD23	1.92	0.51
1:E:63:ASP:CG	1:E:64:HIS:HD1	2.13	0.51
1:D:55:SER:HB3	1:D:232:ILE:HD12	1.93	0.51
1:D:122:LEU:HD11	1:D:161:THR:HG21	1.92	0.50
1:E:30:GLY:O	1:E:34:VAL:HG23	2.10	0.50
1:B:206:GLN:HG2	1:B:211:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ASP:CG	1:C:64:HIS:HD1	2.14	0.50
1:B:93:ARG:O	1:D:23:HIS:HD2	1.95	0.49
1:A:26:TRP:CG	1:E:93:ARG:HD3	2.48	0.49
1:A:164:ALA:HB1	2:A:239:HEM:HAB	1.95	0.49
1:A:132:PRO:HD2	1:A:226:MET:HB3	1.95	0.49
2:A:239:HEM:CMC	2:A:239:HEM:HBC2	2.43	0.48
1:D:230:ASP:OD1	1:D:231:GLU:N	2.46	0.48
1:E:121:GLU:OE1	1:E:165:LEU:HD13	2.12	0.48
1:B:92:GLY:HA2	1:B:95:LEU:HD12	1.96	0.48
1:B:132:PRO:HD2	1:B:226:MET:HB3	1.96	0.48
1:D:34:VAL:HG22	1:D:237:ALA:HB1	1.95	0.48
2:C:239:HEM:HBD2	2:C:239:HEM:HHA	1.96	0.48
1:A:165:LEU:N	1:A:166:PRO:HD2	2.29	0.47
1:C:164:ALA:HB1	2:C:239:HEM:CAB	2.44	0.47
1:D:26:TRP:C	4:D:270:HOH:O	2.53	0.47
1:D:13:TYR:CD1	1:D:76:LEU:HD13	2.49	0.47
1:E:229:LEU:HD11	1:E:233:LEU:HD11	1.97	0.47
1:A:7:LEU:CD2	1:A:52:LEU:CD2	2.93	0.47
1:C:132:PRO:HD2	1:C:226:MET:HB3	1.95	0.47
1:E:90:ARG:CZ	4:E:262:HOH:O	2.63	0.47
1:D:13:TYR:CG	1:D:76:LEU:HD13	2.50	0.47
1:A:59:ARG:O	1:E:80:GLN:HG3	2.15	0.47
2:D:239:HEM:HBD2	2:D:239:HEM:HHA	1.97	0.47
1:B:26:TRP:CD1	1:C:93:ARG:HD2	2.50	0.47
1:E:205:LEU:O	1:E:208:VAL:HG22	2.15	0.46
1:B:121:GLU:OE1	1:B:165:LEU:HD13	2.15	0.46
1:A:157:MET:HE3	1:A:160:HIS:CD2	2.51	0.46
1:C:205:LEU:O	1:C:208:VAL:HG22	2.16	0.46
1:D:175:LEU:HD21	2:D:239:HEM:HAD2	1.98	0.46
1:E:56:TYR:CE2	1:E:226:MET:HG3	2.50	0.46
1:E:131:ARG:N	1:E:132:PRO:HD3	2.30	0.46
1:B:230:ASP:O	1:B:234:GLU:HB2	2.17	0.45
1:E:127:GLU:OE2	1:E:129:GLY:N	2.49	0.45
1:A:9:GLU:O	1:A:105:SER:OG	2.34	0.45
1:A:34:VAL:CG2	1:A:237:ALA:HB1	2.43	0.45
1:D:132:PRO:HD2	1:D:226:MET:HB3	1.99	0.45
1:D:157:MET:HE3	1:D:160:HIS:CD2	2.52	0.45
1:D:89:THR:O	1:D:93:ARG:HG3	2.16	0.45
1:A:121:GLU:OE1	1:A:165:LEU:HD13	2.17	0.45
1:E:34:VAL:HG22	1:E:237:ALA:HB1	1.99	0.44
1:A:157:MET:CE	1:A:160:HIS:CD2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:HIS:O	1:B:26:TRP:HD1	2.01	0.44
1:A:1:ALA:HB3	4:A:268:HOH:O	2.18	0.44
1:A:44:VAL:HG21	1:A:229:LEU:CD2	2.48	0.44
1:A:37:VAL:HG22	1:A:233:LEU:HB3	1.99	0.43
1:D:234:GLU:O	1:D:238:GLN:HG2	2.18	0.43
1:A:55:SER:HB3	1:A:232:ILE:HD12	2.00	0.43
1:C:164:ALA:HB1	2:C:239:HEM:HAB	2.00	0.43
1:C:84:SER:HA	1:C:87:MET:HE3	1.99	0.43
1:D:57:LEU:HD22	4:D:245:HOH:O	2.18	0.43
1:B:90:ARG:HA	1:B:93:ARG:HG3	2.01	0.43
1:C:142:ASP:OD2	1:C:213:HIS:HA	2.19	0.43
1:D:57:LEU:HD13	1:D:232:ILE:HG23	2.00	0.43
1:A:118:MET:HE1	1:A:162:GLN:HB2	2.00	0.42
1:B:81:GLN:OE1	1:B:81:GLN:HA	2.19	0.42
1:E:168:LEU:HD21	1:E:173:LYS:HD3	2.02	0.42
1:E:215:ARG:NH1	3:E:241:SO4:O4	2.52	0.42
1:B:229:LEU:HD11	1:B:233:LEU:CD1	2.49	0.42
1:D:141:LYS:NZ	1:D:210:GLU:OE2	2.53	0.42
1:A:91:LEU:CD1	1:A:233:LEU:HD22	2.47	0.42
1:C:30:GLY:O	1:C:34:VAL:CG2	2.64	0.42
1:C:25:TRP:CZ2	1:C:33:ARG:HG2	2.55	0.42
1:C:164:ALA:HB1	2:C:239:HEM:C3B	2.55	0.42
1:B:7:LEU:HD23	1:B:72:HIS:CE1	2.55	0.41
1:B:120:THR:HG22	4:B:275:HOH:O	2.20	0.41
1:E:157:MET:O	1:E:160:HIS:HB3	2.20	0.41
1:D:139:ILE:HD12	2:D:239:HEM:CMD	2.47	0.41
1:A:110:TYR:CD2	1:A:157:MET:HG3	2.55	0.41
1:E:149:ASP:C	1:E:149:ASP:OD1	2.58	0.41
1:A:76:LEU:HD12	1:C:195:LEU:CD1	2.50	0.41
1:B:2:ASP:N	1:B:2:ASP:OD1	2.53	0.41
1:A:76:LEU:HD12	1:C:195:LEU:HD13	2.03	0.41
1:C:164:ALA:HB2	1:C:205:LEU:HD21	2.03	0.41
1:D:157:MET:HE2	2:D:239:HEM:O2D	2.21	0.41
1:C:21:MET:HA	1:C:95:LEU:HD23	2.02	0.41
1:E:127:GLU:HG3	1:E:127:GLU:O	2.20	0.41
1:E:37:VAL:HG23	1:E:233:LEU:CB	2.49	0.41
1:A:121:GLU:HB3	1:A:165:LEU:HD22	2.02	0.40
1:B:63:ASP:OD2	1:C:99:GLY:HA2	2.22	0.40
1:C:165:LEU:N	1:C:166:PRO:CD	2.84	0.40
1:C:57:LEU:HD22	1:C:235:LYS:HE2	2.04	0.40
1:E:34:VAL:O	1:E:37:VAL:CG1	2.51	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:SER:OG	1:D:31:GLU:OE2[4_454]	2.11	0.09

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	236/241 (98%)	234 (99%)	2 (1%)	0	100	100
1	B	236/241 (98%)	234 (99%)	2 (1%)	0	100	100
1	C	236/241 (98%)	232 (98%)	4 (2%)	0	100	100
1	D	236/241 (98%)	233 (99%)	3 (1%)	0	100	100
1	E	236/241 (98%)	234 (99%)	2 (1%)	0	100	100
All	All	1180/1205 (98%)	1167 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	205/206 (100%)	196 (96%)	9 (4%)	33	63
1	B	205/206 (100%)	195 (95%)	10 (5%)	29	58
1	C	205/206 (100%)	197 (96%)	8 (4%)	37	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	205/206 (100%)	191 (93%)	14 (7%)	18	41
1	E	205/206 (100%)	195 (95%)	10 (5%)	29	58
All	All	1025/1030 (100%)	974 (95%)	51 (5%)	28	57

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	7	LEU
1	A	18	THR
1	A	24	ASP
1	A	74	ARG
1	A	124	VAL
1	A	203	ARG
1	A	207	GLN
1	A	230	ASP
1	B	2	ASP
1	B	24	ASP
1	B	31	GLU
1	B	75	THR
1	B	93	ARG
1	B	166	PRO
1	B	192	THR
1	B	207	GLN
1	B	225	THR
1	B	230	ASP
1	C	34	VAL
1	C	45	GLU
1	C	63	ASP
1	C	77	SER
1	C	96	THR
1	C	127	GLU
1	C	168	LEU
1	C	234	GLU
1	D	2	ASP
1	D	18	THR
1	D	63	ASP
1	D	74	ARG
1	D	77	SER
1	D	84	SER
1	D	97	SER

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Mol	Chain	Res	Type
1	D	124	VAL
1	D	128	SER
1	D	131	ARG
1	D	157	MET
1	D	173	LYS
1	D	203	ARG
1	D	234	GLU
1	E	2	ASP
1	E	63	ASP
1	E	75	THR
1	E	91	LEU
1	E	124	VAL
1	E	127	GLU
1	E	203	ARG
1	E	207	GLN
1	E	226	MET
1	E	230	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	158	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

26 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	239	1,4	28,50,50	2.23	7 (25%)	17,82,82	1.70	4 (23%)
3	SO4	A	240	-	4,4,4	0.14	0	6,6,6	0.36	0
3	SO4	A	241	-	4,4,4	0.23	0	6,6,6	0.49	0
3	SO4	A	242	-	4,4,4	0.18	0	6,6,6	0.22	0
3	SO4	A	243	-	4,4,4	0.15	0	6,6,6	0.21	0
2	HEM	B	239	1	28,50,50	2.19	6 (21%)	17,82,82	1.96	6 (35%)
3	SO4	B	240	-	4,4,4	0.17	0	6,6,6	0.19	0
3	SO4	B	241	-	4,4,4	0.18	0	6,6,6	0.40	0
3	SO4	B	242	-	4,4,4	0.19	0	6,6,6	0.24	0
3	SO4	B	243	-	4,4,4	0.16	0	6,6,6	0.14	0
2	HEM	C	239	1	28,50,50	2.22	10 (35%)	17,82,82	1.89	4 (23%)
3	SO4	C	240	-	4,4,4	0.18	0	6,6,6	0.45	0
3	SO4	C	241	-	4,4,4	0.16	0	6,6,6	0.26	0
3	SO4	C	242	-	4,4,4	0.16	0	6,6,6	0.22	0
3	SO4	C	243	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	C	244	-	4,4,4	0.19	0	6,6,6	0.23	0
2	HEM	D	239	1	28,50,50	2.23	6 (21%)	17,82,82	1.76	4 (23%)
3	SO4	D	240	-	4,4,4	0.19	0	6,6,6	0.45	0
3	SO4	D	241	-	4,4,4	0.24	0	6,6,6	0.35	0
2	HEM	E	239	1	28,50,50	2.13	6 (21%)	17,82,82	1.46	2 (11%)
3	SO4	E	240	-	4,4,4	0.18	0	6,6,6	0.50	0
3	SO4	E	241	-	4,4,4	0.19	0	6,6,6	0.33	0
3	SO4	E	242	-	4,4,4	0.16	0	6,6,6	0.45	0
3	SO4	E	243	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	E	244	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	E	245	-	4,4,4	0.16	0	6,6,6	0.22	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	239	1,4	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	240	-	-	0/0/0/0	0/0/0/0
3	SO4	A	241	-	-	0/0/0/0	0/0/0/0
3	SO4	A	242	-	-	0/0/0/0	0/0/0/0
3	SO4	A	243	-	-	0/0/0/0	0/0/0/0
2	HEM	B	239	1	-	0/6/54/54	0/0/8/8
3	SO4	B	240	-	-	0/0/0/0	0/0/0/0
3	SO4	B	241	-	-	0/0/0/0	0/0/0/0
3	SO4	B	242	-	-	0/0/0/0	0/0/0/0
3	SO4	B	243	-	-	0/0/0/0	0/0/0/0
2	HEM	C	239	1	-	0/6/54/54	0/0/8/8
3	SO4	C	240	-	-	0/0/0/0	0/0/0/0
3	SO4	C	241	-	-	0/0/0/0	0/0/0/0
3	SO4	C	242	-	-	0/0/0/0	0/0/0/0
3	SO4	C	243	-	-	0/0/0/0	0/0/0/0
3	SO4	C	244	-	-	0/0/0/0	0/0/0/0
2	HEM	D	239	1	-	0/6/54/54	0/0/8/8
3	SO4	D	240	-	-	0/0/0/0	0/0/0/0
3	SO4	D	241	-	-	0/0/0/0	0/0/0/0
2	HEM	E	239	1	-	0/6/54/54	0/0/8/8
3	SO4	E	240	-	-	0/0/0/0	0/0/0/0
3	SO4	E	241	-	-	0/0/0/0	0/0/0/0
3	SO4	E	242	-	-	0/0/0/0	0/0/0/0
3	SO4	E	243	-	-	0/0/0/0	0/0/0/0
3	SO4	E	244	-	-	0/0/0/0	0/0/0/0
3	SO4	E	245	-	-	0/0/0/0	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	239	HEM	C3B-C2B	-6.50	1.31	1.40
2	D	239	HEM	C3B-C2B	-6.22	1.32	1.40
2	C	239	HEM	C3B-C2B	-5.97	1.32	1.40
2	B	239	HEM	C3C-C2C	-5.80	1.32	1.40
2	B	239	HEM	C3B-C2B	-5.72	1.32	1.40
2	E	239	HEM	C3B-C2B	-5.13	1.33	1.40
2	E	239	HEM	C3C-C2C	-5.00	1.33	1.40
2	A	239	HEM	C3C-C2C	-4.86	1.33	1.40
2	D	239	HEM	C3C-C2C	-4.37	1.34	1.40
2	C	239	HEM	C3C-C2C	-3.78	1.35	1.40
2	A	239	HEM	CAA-C2A	2.02	1.55	1.52
2	A	239	HEM	C1B-NB	2.02	1.39	1.36
2	E	239	HEM	C4C-NC	2.11	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	239	HEM	CMA-C3A	2.14	1.56	1.51
2	C	239	HEM	C4D-ND	2.14	1.39	1.36
2	D	239	HEM	C1B-NB	2.22	1.39	1.36
2	C	239	HEM	CMB-C2B	2.26	1.56	1.51
2	C	239	HEM	CMD-C2D	2.43	1.56	1.51
2	C	239	HEM	C3B-CAB	2.44	1.52	1.47
2	C	239	HEM	C4C-NC	2.44	1.39	1.36
2	B	239	HEM	C3B-CAB	2.72	1.53	1.47
2	B	239	HEM	C1C-NC	2.79	1.40	1.36
2	D	239	HEM	C3B-CAB	2.86	1.53	1.47
2	B	239	HEM	C3C-CAC	2.87	1.53	1.47
2	A	239	HEM	C3B-CAB	3.07	1.54	1.47
2	A	239	HEM	C3C-CAC	3.28	1.54	1.47
2	D	239	HEM	C3C-CAC	3.37	1.54	1.47
2	E	239	HEM	C3C-CAC	3.52	1.54	1.47
2	C	239	HEM	C3C-CAC	3.56	1.54	1.47
2	E	239	HEM	C3B-CAB	3.63	1.55	1.47
2	B	239	HEM	C3D-C2D	4.53	1.51	1.37
2	A	239	HEM	C3D-C2D	4.61	1.51	1.37
2	E	239	HEM	C3D-C2D	4.76	1.51	1.37
2	C	239	HEM	C3D-C2D	4.92	1.52	1.37
2	D	239	HEM	C3D-C2D	4.92	1.52	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	239	HEM	CAD-CBD-CGD	-4.33	105.26	112.66
2	B	239	HEM	CAD-CBD-CGD	-4.03	105.77	112.66
2	D	239	HEM	CAD-CBD-CGD	-3.65	106.42	112.66
2	A	239	HEM	C1D-C2D-C3D	-3.59	104.50	107.00
2	D	239	HEM	C1D-C2D-C3D	-3.49	104.56	107.00
2	C	239	HEM	CAA-CBA-CGA	-3.21	107.17	112.66
2	E	239	HEM	CAA-CBA-CGA	-3.15	107.28	112.66
2	B	239	HEM	C1D-C2D-C3D	-3.06	104.87	107.00
2	A	239	HEM	CMA-C3A-C4A	-2.86	124.06	128.46
2	C	239	HEM	CAD-C3D-C2D	-2.80	121.02	129.00
2	D	239	HEM	CAA-CBA-CGA	-2.68	108.07	112.66
2	A	239	HEM	CAD-CBD-CGD	-2.35	108.64	112.66
2	B	239	HEM	CMA-C3A-C4A	-2.15	125.15	128.46
2	B	239	HEM	CAD-C3D-C2D	-2.06	123.12	129.00
2	E	239	HEM	C4C-C3C-C2C	2.08	108.35	106.90
2	B	239	HEM	C4A-C3A-C2A	2.29	108.59	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	239	HEM	C4C-C3C-C2C	2.30	108.50	106.90
2	D	239	HEM	C4C-C3C-C2C	2.56	108.69	106.90
2	C	239	HEM	CMC-C2C-C3C	2.57	129.66	124.89
2	B	239	HEM	C4C-C3C-C2C	3.14	109.09	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	239	HEM	2	0
2	B	239	HEM	1	0
3	B	241	SO4	1	0
2	C	239	HEM	7	0
2	D	239	HEM	5	0
3	E	241	SO4	1	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	238/241 (98%)	0.75	30 (12%) 4 3	56, 78, 108, 137	0
1	B	238/241 (98%)	0.73	28 (11%) 5 4	54, 72, 97, 125	0
1	C	238/241 (98%)	0.79	33 (13%) 3 2	57, 72, 101, 117	0
1	D	238/241 (98%)	0.63	25 (10%) 7 5	57, 78, 106, 136	1 (0%)
1	E	238/241 (98%)	0.58	20 (8%) 12 9	57, 75, 103, 122	0
All	All	1190/1205 (98%)	0.69	136 (11%) 6 4	54, 75, 105, 137	1 (0%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	MET	7.7
1	C	127	GLU	6.5
1	C	124	VAL	6.2
1	A	129	GLY	6.2
1	B	107	LYS	6.1
1	C	110	TYR	6.0
1	C	112	ALA	5.7
1	C	120	THR	5.7
1	E	115	PRO	5.5
1	C	122	LEU	5.4
1	A	126	GLY	5.3
1	E	109	THR	5.2
1	E	110	TYR	5.2
1	B	126	GLY	5.2
1	C	114	PHE	5.2
1	A	27	ASP	5.1
1	E	236	PHE	5.1
1	A	128	SER	5.0
1	E	118	MET	5.0
1	D	110	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	128	SER	4.9
1	D	126	GLY	4.7
1	E	237	ALA	4.7
1	A	125	ASN	4.6
1	E	125	ASN	4.6
1	C	123	GLN	4.5
1	C	129	GLY	4.5
1	D	125	ASN	4.4
1	E	124	VAL	4.4
1	B	4	GLU	4.3
1	B	3	ARG	4.3
1	A	117	SER	4.2
1	B	129	GLY	4.2
1	A	113	GLY	4.1
1	B	237	ALA	4.1
1	D	28	LEU	4.1
1	E	129	GLY	4.1
1	A	115	PRO	4.0
1	A	122	LEU	4.0
1	E	128	SER	4.0
1	D	118	MET	4.0
1	B	127	GLU	3.9
1	B	108	PRO	3.9
1	B	120	THR	3.8
1	D	1	ALA	3.8
1	A	124	VAL	3.8
1	E	122	LEU	3.8
1	B	10	SER	3.8
1	A	114	PHE	3.7
1	D	6	LEU	3.7
1	A	123	GLN	3.6
1	A	4	GLU	3.6
1	B	118	MET	3.6
1	B	1	ALA	3.6
1	E	127	GLU	3.6
1	E	126	GLY	3.6
1	A	118	MET	3.6
1	B	6	LEU	3.6
1	A	28	LEU	3.5
1	D	127	GLU	3.5
1	C	121	GLU	3.5
1	C	128	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	238	GLN	3.4
1	B	27	ASP	3.4
1	C	116	GLU	3.4
1	C	117	SER	3.3
1	B	5	LYS	3.3
1	C	108	PRO	3.3
1	D	26	TRP	3.3
1	E	107	LYS	3.2
1	E	114	PHE	3.2
1	A	127	GLU	3.2
1	C	111	VAL	3.2
1	A	120	THR	3.1
1	A	130	SER	3.1
1	C	125	ASN	3.1
1	D	111	VAL	3.1
1	C	28	LEU	3.1
1	D	129	GLY	2.9
1	D	107	LYS	2.9
1	E	108	PRO	2.9
1	C	1	ALA	2.8
1	C	34	VAL	2.8
1	B	8	THR	2.8
1	B	236	PHE	2.8
1	B	128	SER	2.8
1	B	122	LEU	2.7
1	D	114	PHE	2.7
1	C	109	THR	2.6
1	C	113	GLY	2.6
1	A	116	GLU	2.6
1	A	3	ARG	2.6
1	A	121	GLU	2.6
1	C	74	ARG	2.6
1	B	238	GLN	2.6
1	C	6	LEU	2.6
1	D	44	VAL	2.5
1	D	234	GLU	2.5
1	C	90	ARG	2.5
1	B	7	LEU	2.5
1	C	4	GLU	2.5
1	E	4	GLU	2.4
1	C	119	LYS	2.4
1	A	165	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	44	VAL	2.4
1	A	31	GLU	2.4
1	E	123	GLN	2.4
1	C	126	GLY	2.4
1	B	9	GLU	2.4
1	C	31	GLU	2.3
1	A	5	LYS	2.3
1	B	115	PRO	2.3
1	D	115	PRO	2.2
1	C	3	ARG	2.2
1	B	35	ILE	2.2
1	D	123	GLN	2.2
1	D	11	GLY	2.2
1	D	4	GLU	2.2
1	D	74	ARG	2.2
1	A	112	ALA	2.2
1	A	172	LYS	2.2
1	C	115	PRO	2.2
1	B	64	HIS	2.1
1	D	2	ASP	2.1
1	A	110	TYR	2.1
1	B	116	GLU	2.1
1	C	35	ILE	2.1
1	C	130	SER	2.1
1	E	74	ARG	2.1
1	D	3	ARG	2.1
1	D	109	THR	2.1
1	B	11	GLY	2.1
1	D	31	GLU	2.0
1	A	236	PHE	2.0
1	A	108	PRO	2.0
1	B	121	GLU	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	E	243	5/5	0.88	0.28	0.42	134,134,135,135	0
3	SO4	E	244	5/5	0.90	0.25	-0.03	124,124,124,124	0
3	SO4	C	243	5/5	0.78	0.29	-0.19	141,142,142,142	0
2	HEM	D	239	43/43	0.97	0.21	-0.25	59,62,71,75	0
2	HEM	B	239	43/43	0.97	0.20	-0.26	50,55,65,68	0
2	HEM	E	239	43/43	0.96	0.21	-0.33	52,57,67,70	0
2	HEM	C	239	43/43	0.97	0.19	-0.50	55,61,67,70	0
2	HEM	A	239	43/43	0.97	0.20	-0.64	59,63,73,79	0
3	SO4	B	242	5/5	0.92	0.15	-1.04	101,102,102,103	0
3	SO4	B	243	5/5	0.81	0.14	-1.09	147,147,147,148	0
3	SO4	C	244	5/5	0.83	0.16	-1.10	119,119,120,120	0
3	SO4	C	242	5/5	0.92	0.16	-1.13	105,106,107,107	0
3	SO4	D	241	5/5	0.89	0.13	-1.68	102,102,102,103	0
3	SO4	A	242	5/5	0.92	0.14	-1.88	120,120,120,121	0
3	SO4	E	245	5/5	0.89	0.10	-1.97	133,133,134,134	0
3	SO4	A	243	5/5	0.91	0.12	-2.39	118,119,119,119	0
3	SO4	C	240	5/5	0.95	0.13	-	78,79,80,82	0
3	SO4	E	240	5/5	0.94	0.10	-	81,81,83,85	0
3	SO4	E	242	5/5	0.93	0.25	-	110,110,111,111	0
3	SO4	C	241	5/5	0.81	0.28	-	120,120,121,122	0
3	SO4	A	240	5/5	0.89	0.17	-	97,98,99,99	0
3	SO4	E	241	5/5	0.82	0.30	-	110,111,112,112	0
3	SO4	B	240	5/5	0.96	0.10	-	83,84,84,84	0
3	SO4	D	240	5/5	0.96	0.12	-	81,83,83,84	0
3	SO4	A	241	5/5	0.91	0.21	-	98,98,98,99	0
3	SO4	B	241	5/5	0.82	0.29	-	113,114,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.