



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 10:04 PM EDT

PDB ID : 4REU
Title : Revelation of Endogenously bound Fe²⁺ ions in the Crystal Structure of Ferritin from Escherichia coli
Authors : Thiruselvam, V.; Ponnuswamy, M.N.; Kumarevel, T.S.
Deposited on : 2014-09-24
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

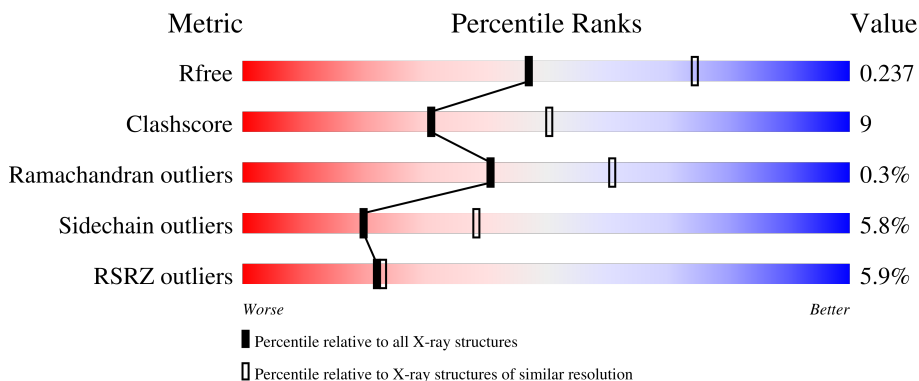
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

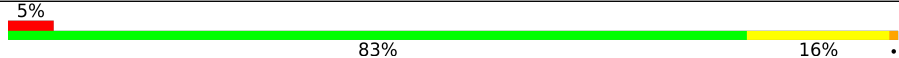


The reported resolution of this entry is 2.50 Å.

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	164	 4% 80% 20%
1	B	164	 5% 83% 16% .
1	C	164	 10% 79% 20% .
1	D	164	 5% 82% 17% .
1	E	164	 5% 81% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	164	

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	203	-	-	X	-
3	SO4	B	203	-	-	X	-
3	SO4	B	204	-	-	X	-
3	SO4	C	203	-	-	X	-
3	SO4	E	203	-	-	X	-
3	SO4	E	207	-	-	X	-
3	SO4	F	203	-	-	X	-
5	CL	B	207	-	-	X	-
5	CL	C	207	-	-	X	-
5	CL	E	209	-	-	X	-
5	CL	F	205	-	-	X	-
5	CL	F	206	-	-	X	-
5	CL	F	207	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8494 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 Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	164	1358	864	219	268	7	0	0	0
1	B	164	1358	864	219	268	7	0	0	0
1	C	164	1358	864	219	268	7	0	0	0
1	D	164	1358	864	219	268	7	0	0	0
1	E	164	1358	864	219	268	7	0	0	0
1	F	164	1358	864	219	268	7	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		
2	E	2	Total	Fe	0	0
			2	2		
2	F	2	Total	Fe	0	0
			2	2		

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



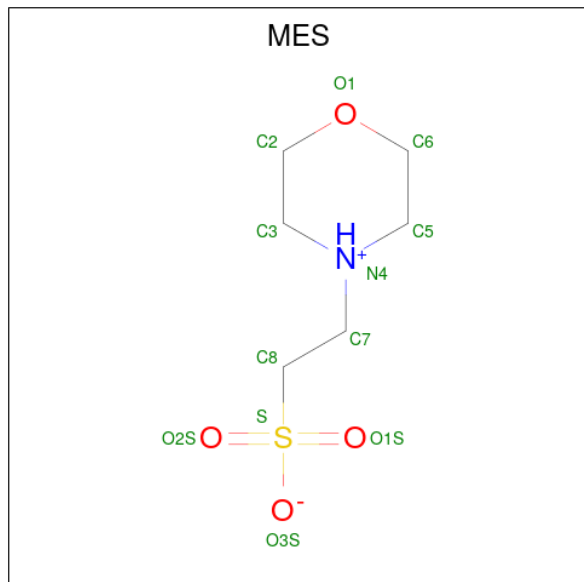
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total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

Continued on next page...

Continued from previous page...

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

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



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	Cl	0	0
			6	6		
5	B	4	Total	Cl	0	0
			4	4		
5	C	2	Total	Cl	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	8	Total Cl 8 8	0	0
5	E	2	Total Cl 2 2	0	0
5	F	5	Total Cl 5 5	0	0

- Molecule 6 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Hg 1 1	0	0
6	D	1	Total Hg 1 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Mg 1 1	0	0

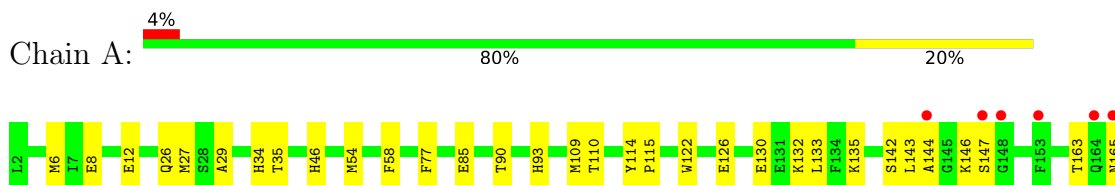
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	33	Total O 33 33	0	0
8	B	32	Total O 32 32	0	0
8	C	27	Total O 27 27	0	0
8	D	36	Total O 36 36	0	0
8	E	32	Total O 32 32	0	0
8	F	37	Total O 37 37	0	0

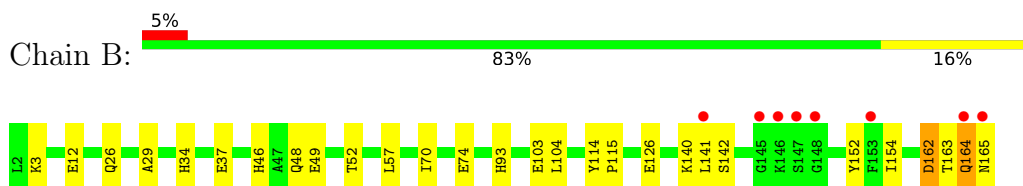
3 Residue-property plots [i](#)

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.

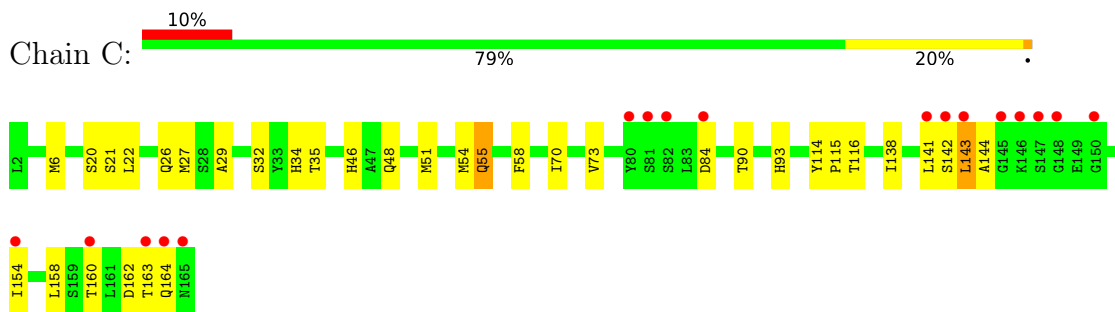
- Molecule 1: Ferritin



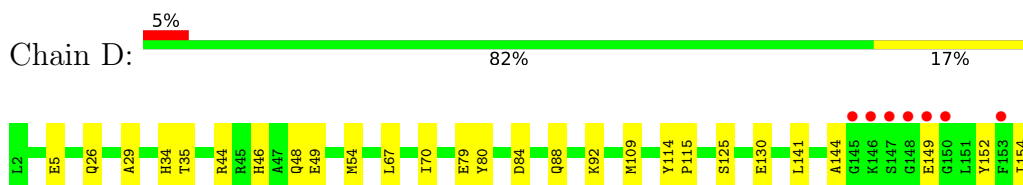
- Molecule 1: Ferritin



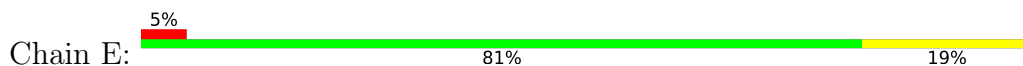
- Molecule 1: Ferritin

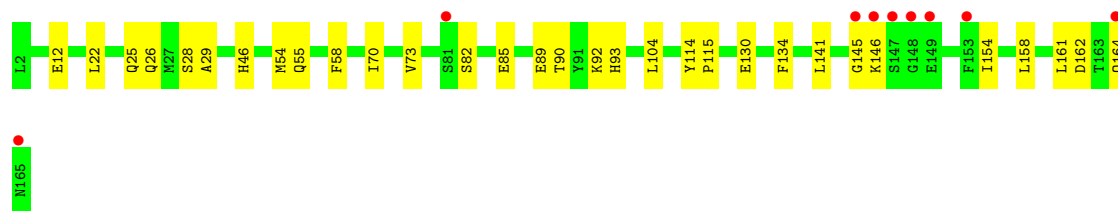


- Molecule 1: Ferritin

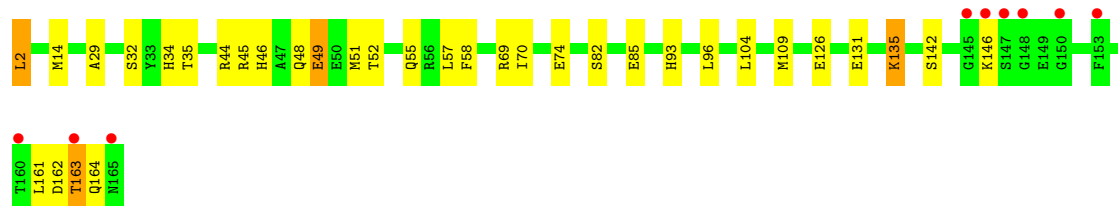
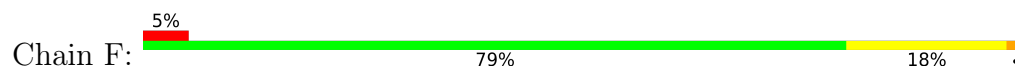


- Molecule 1: Ferritin





- Molecule 1: Ferritin



4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	128.00Å 128.00Å 170.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 45.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.50) 100.0 (45.25-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.172 , 0.235 0.174 , 0.237	Depositor DCC
R_{free} test set	2402 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.027 for -h,k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8494	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, CL, FE, MG, HG, 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	0.71	0/1389	0.74	1/1876 (0.1%)
1	B	0.72	0/1389	0.74	0/1876
1	C	0.68	0/1389	0.74	0/1876
1	D	0.71	0/1389	0.73	0/1876
1	E	0.70	1/1389 (0.1%)	0.74	0/1876
1	F	0.71	0/1389	0.77	0/1876
All	All	0.71	1/8334 (0.0%)	0.74	1/11256 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	12	GLU	CG-CD	5.89	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	MET	CG-SD-CE	-5.09	92.06	100.20

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	1358	0	1293	29	0
1	B	1358	0	1293	20	1
1	C	1358	0	1293	30	0
1	D	1358	0	1293	27	0
1	E	1358	0	1293	28	0
1	F	1358	0	1293	28	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	25	0	0	3	1
3	B	10	0	0	4	0
3	C	10	0	0	4	0
3	D	15	0	0	0	1
3	E	25	0	0	5	0
3	F	10	0	0	2	0
4	A	12	0	13	1	0
5	A	6	0	0	1	1
5	B	4	0	0	3	0
5	C	2	0	0	2	0
5	D	8	0	0	3	0
5	E	2	0	0	3	0
5	F	5	0	0	6	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	D	1	0	0	0	0
8	A	33	0	0	4	0
8	B	32	0	0	6	0
8	C	27	0	0	3	0
8	D	36	0	0	6	0
8	E	32	0	0	2	1
8	F	37	0	0	11	0
All	All	8494	0	7771	146	3

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 9.

All (146) 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)
5:B:207:CL:CL	5:B:208:CL:CL	2.29	1.24
1:C:163:THR:HG22	1:C:164:GLN:HG2	1.26	1.15
5:D:212:CL:CL	8:D:334:HOH:O	2.01	1.15
1:F:14:MET:HG2	8:F:337:HOH:O	1.44	1.15
1:F:109:MET:SD	8:F:336:HOH:O	2.03	1.14
1:F:14:MET:CE	8:F:337:HOH:O	1.97	1.10
1:F:93:HIS:ND1	3:F:203:SO4:O2	1.89	1.06
5:A:211:CL:CL	8:A:329:HOH:O	2.13	1.03
1:F:14:MET:CG	8:F:337:HOH:O	1.99	1.01
5:B:206:CL:CL	8:B:328:HOH:O	2.17	1.00
1:E:89:GLU:OE2	3:E:207:SO4:O4	1.88	0.90
1:C:55:GLN:HG3	8:C:327:HOH:O	1.73	0.89
1:B:162:ASP:CG	3:B:204:SO4:O4	2.14	0.85
1:F:162:ASP:OD2	5:F:205:CL:CL	2.35	0.81
1:A:144:ALA:HB2	1:D:152:TYR:HB2	1.63	0.80
1:A:142:SER:O	1:A:146:LYS:HE2	1.82	0.80
5:D:214:CL:CL	8:D:335:HOH:O	2.35	0.80
1:F:14:MET:HE2	8:F:337:HOH:O	1.68	0.79
1:E:89:GLU:CD	3:E:207:SO4:O4	2.21	0.79
5:F:207:CL:CL	8:F:333:HOH:O	2.38	0.78
1:E:93:HIS:ND1	3:E:203:SO4:O3	2.17	0.77
1:A:144:ALA:HB2	1:D:152:TYR:CB	2.14	0.76
1:C:162:ASP:OD2	5:C:207:CL:CL	2.42	0.75
1:B:34:HIS:CE1	8:B:331:HOH:O	2.38	0.74
1:C:163:THR:CG2	1:C:164:GLN:HG2	2.13	0.74
1:A:93:HIS:ND1	3:A:203:SO4:S	2.60	0.74
1:F:34:HIS:NE2	5:F:206:CL:CL	2.58	0.73
1:B:162:ASP:OD2	3:B:204:SO4:O4	2.05	0.73
1:C:93:HIS:CD2	3:C:203:SO4:O3	2.42	0.72
1:B:26:GLN:HE22	1:E:70:ILE:H	1.39	0.71
1:D:34:HIS:O	1:D:35:THR:HB	1.90	0.70
1:F:35:THR:HG22	1:F:35:THR:O	1.90	0.69
1:C:93:HIS:HD2	3:C:203:SO4:S	2.18	0.67
1:D:34:HIS:HE1	8:D:309:HOH:O	1.76	0.67
1:C:93:HIS:HD2	3:C:203:SO4:O3	1.79	0.66
1:D:46:HIS:HE1	1:D:130:GLU:OE2	1.81	0.63
1:B:46:HIS:HD2	8:B:323:HOH:O	1.82	0.63
1:B:70:ILE:H	1:E:26:GLN:HE22	1.46	0.62
1:A:142:SER:HA	1:A:146:LYS:HE2	1.82	0.61
1:E:162:ASP:OD2	5:E:209:CL:CL	2.56	0.61
1:A:144:ALA:HB2	1:D:152:TYR:CG	2.36	0.60
1:B:34:HIS:HE1	8:B:331:HOH:O	1.78	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:THR:HG21	8:D:333:HOH:O	2.01	0.59
1:A:27:MET:SD	1:A:90:THR:HG22	2.42	0.59
1:B:140:LYS:HG3	8:B:330:HOH:O	2.03	0.59
1:A:85:GLU:OE2	3:A:205:SO4:O2	2.21	0.58
1:A:93:HIS:ND1	3:A:203:SO4:O1	2.36	0.58
1:F:46:HIS:HD2	8:F:310:HOH:O	1.86	0.58
1:C:143:LEU:HD13	1:C:144:ALA:N	2.19	0.58
1:B:93:HIS:ND1	3:B:203:SO4:O1	2.35	0.58
1:F:93:HIS:CE1	3:F:203:SO4:O2	2.57	0.58
1:E:141:LEU:HD23	1:E:154:ILE:HD13	1.86	0.58
1:B:26:GLN:NE2	1:E:70:ILE:H	2.01	0.57
1:D:141:LEU:HD23	1:D:154:ILE:HD13	1.86	0.57
1:E:161:LEU:HD23	1:E:162:ASP:HB2	1.85	0.57
1:A:29:ALA:HB2	1:F:58:PHE:CZ	2.40	0.57
1:E:93:HIS:CE1	3:E:203:SO4:O3	2.58	0.57
1:C:70:ILE:H	1:D:26:GLN:NE2	2.03	0.56
1:D:34:HIS:CE1	8:D:309:HOH:O	2.56	0.55
1:A:77:PHE:CD1	1:F:69:ARG:HG3	2.41	0.55
1:C:26:GLN:NE2	1:D:70:ILE:H	2.04	0.55
1:C:70:ILE:H	1:D:26:GLN:HE22	1.56	0.54
1:E:22:LEU:HD12	1:E:73:VAL:HG11	1.89	0.54
1:A:26:GLN:HE22	1:F:70:ILE:H	1.55	0.54
1:C:27:MET:SD	1:C:90:THR:HG22	2.47	0.53
1:F:126:GLU:OE1	8:F:324:HOH:O	2.18	0.53
1:C:34:HIS:O	1:C:35:THR:OG1	2.24	0.53
1:C:93:HIS:CD2	3:C:203:SO4:S	3.01	0.52
1:F:34:HIS:CE1	5:F:206:CL:CL	3.00	0.52
1:B:12:GLU:OE1	8:B:327:HOH:O	2.19	0.52
1:B:141:LEU:HD23	1:B:154:ILE:HD13	1.92	0.52
1:F:51:MET:O	1:F:55:GLN:HG2	2.09	0.51
1:E:26:GLN:O	1:E:29:ALA:HB3	2.11	0.51
1:C:46:HIS:HD2	8:C:312:HOH:O	1.94	0.51
5:F:207:CL:CL	8:F:332:HOH:O	2.57	0.50
1:A:144:ALA:CB	1:D:152:TYR:CG	2.94	0.50
1:C:20:SER:OG	1:C:93:HIS:HE1	1.94	0.50
1:A:122:TRP:CH2	1:A:126:GLU:HG3	2.46	0.50
1:C:141:LEU:HD23	1:C:154:ILE:HG21	1.93	0.50
1:B:29:ALA:HB2	1:E:58:PHE:CZ	2.47	0.50
1:D:34:HIS:O	1:D:35:THR:CB	2.60	0.50
1:A:142:SER:CA	1:A:146:LYS:HE2	2.41	0.50
1:A:142:SER:C	1:A:146:LYS:HE2	2.33	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:MET:SD	8:F:337:HOH:O	2.38	0.49
1:C:21:SER:CB	1:C:51:MET:HE2	2.43	0.49
8:A:319:HOH:O	1:F:44:ARG:HD2	2.12	0.49
1:B:103:GLU:OE1	5:B:207:CL:CL	2.68	0.49
1:F:35:THR:O	1:F:35:THR:CG2	2.59	0.48
1:D:49:GLU:OE2	1:D:164:GLN:NE2	2.47	0.48
1:C:58:PHE:CZ	1:D:29:ALA:HB2	2.49	0.48
1:E:90:THR:HG21	1:E:134:PHE:CE1	2.48	0.48
1:A:27:MET:SD	1:A:90:THR:CG2	3.02	0.47
1:E:161:LEU:HD23	1:E:162:ASP:N	2.29	0.47
1:A:26:GLN:NE2	1:F:70:ILE:H	2.12	0.47
1:C:21:SER:OG	1:C:51:MET:HE2	2.14	0.47
1:C:26:GLN:HE22	1:D:70:ILE:H	1.63	0.47
1:A:12:GLU:HG2	4:A:208:MES:H22	1.96	0.47
1:C:29:ALA:HB1	1:D:67:LEU:HD12	1.96	0.47
1:B:70:ILE:H	1:E:26:GLN:NE2	2.10	0.47
1:E:90:THR:HG21	1:E:134:PHE:CD1	2.50	0.46
1:F:49:GLU:O	1:F:52:THR:HB	2.15	0.46
1:A:58:PHE:CZ	1:F:29:ALA:HB2	2.50	0.46
1:F:162:ASP:CG	5:F:205:CL:CL	2.91	0.46
1:E:162:ASP:OD1	5:E:209:CL:CL	2.71	0.45
1:A:34:HIS:CE1	8:A:331:HOH:O	2.69	0.45
1:A:132:LYS:NZ	8:A:303:HOH:O	2.49	0.45
1:B:93:HIS:CE1	3:B:203:SO4:O1	2.70	0.45
1:C:55:GLN:HE22	1:D:44:ARG:HD2	1.81	0.45
5:C:207:CL:CL	8:C:326:HOH:O	2.58	0.45
1:A:163:THR:HG22	1:A:163:THR:O	2.16	0.45
1:C:22:LEU:HD12	1:C:73:VAL:HG11	1.98	0.44
1:E:85:GLU:OE2	3:E:204:SO4:S	2.76	0.44
1:D:35:THR:O	1:D:35:THR:HG22	2.16	0.44
1:E:25:GLN:O	1:E:28:SER:HB3	2.18	0.44
1:E:145:GLY:N	8:E:314:HOH:O	2.51	0.44
1:A:147:SER:OG	1:D:149:GLU:OE1	2.29	0.44
1:E:90:THR:CG2	1:E:134:PHE:CD1	3.01	0.44
1:F:163:THR:N	1:F:164:GLN:HA	2.32	0.43
1:B:49:GLU:O	1:B:52:THR:HB	2.19	0.43
1:D:164:GLN:O	1:D:164:GLN:HG2	2.19	0.43
1:B:152:TYR:CG	1:D:144:ALA:HB2	2.53	0.43
1:C:143:LEU:HD22	1:C:143:LEU:C	2.39	0.43
1:D:80:TYR:HA	8:D:301:HOH:O	2.18	0.43
1:C:114:TYR:N	1:C:115:PRO:CD	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:LEU:HA	1:E:161:LEU:HB2	2.01	0.42
1:A:143:LEU:HB2	1:D:35:THR:HG21	2.01	0.42
1:D:79:GLU:OE1	5:D:213:CL:CL	2.74	0.42
1:B:114:TYR:N	1:B:115:PRO:CD	2.82	0.42
1:D:114:TYR:N	1:D:115:PRO:CD	2.82	0.42
1:A:114:TYR:N	1:A:115:PRO:CD	2.83	0.42
1:B:163:THR:O	1:B:165:ASN:N	2.53	0.42
1:A:142:SER:HA	1:A:146:LYS:CE	2.49	0.42
1:C:141:LEU:CD2	1:C:154:ILE:HG21	2.48	0.42
1:A:46:HIS:HE1	1:A:130:GLU:OE2	2.03	0.41
1:F:131:GLU:O	1:F:135:LYS:HB2	2.20	0.41
1:A:133:LEU:HD22	1:A:163:THR:HG23	2.02	0.41
1:C:160:THR:O	1:C:163:THR:HB	2.21	0.41
1:C:6:MET:HE2	1:C:116:THR:HG21	2.02	0.41
1:E:114:TYR:N	1:E:115:PRO:CD	2.84	0.41
1:E:146:LYS:N	8:E:314:HOH:O	2.53	0.41
1:F:46:HIS:CD2	8:F:310:HOH:O	2.67	0.41
1:E:162:ASP:CG	5:E:209:CL:CL	2.97	0.41
1:E:46:HIS:HE1	1:E:130:GLU:OE1	2.04	0.40
1:E:161:LEU:CD2	1:E:162:ASP:HB2	2.49	0.40
1:F:2:LEU:HD23	1:F:2:LEU:HA	1.92	0.40
1:C:138:ILE:O	1:C:141:LEU:HB2	2.21	0.40

All (3) 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)
5:A:212:CL:CL	8:E:331:HOH:O[7_555]	2.06	0.14
1:F:74:GLU:OE2	3:D:203:SO4:O2[8_455]	2.11	0.09
1:B:74:GLU:OE2	3:A:206:SO4:O4[8_454]	2.12	0.08

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	162/164 (99%)	157 (97%)	4 (2%)	1 (1%)	25	43
1	B	162/164 (99%)	160 (99%)	1 (1%)	1 (1%)	25	43
1	C	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	D	162/164 (99%)	159 (98%)	2 (1%)	1 (1%)	25	43
1	E	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	F	162/164 (99%)	160 (99%)	2 (1%)	0	100	100
All	All	972/984 (99%)	946 (97%)	23 (2%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	164	GLN
1	A	35	THR
1	D	163	THR

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	149/149 (100%)	143 (96%)	6 (4%)	31	56
1	B	149/149 (100%)	140 (94%)	9 (6%)	19	37
1	C	149/149 (100%)	141 (95%)	8 (5%)	22	42
1	D	149/149 (100%)	141 (95%)	8 (5%)	22	42
1	E	149/149 (100%)	143 (96%)	6 (4%)	31	56
1	F	149/149 (100%)	134 (90%)	15 (10%)	7	14
All	All	894/894 (100%)	842 (94%)	52 (6%)	20	38

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	54	MET
1	A	109	MET
1	A	110	THR
1	A	135	LYS
1	A	165	ASN
1	B	3	LYS
1	B	37	GLU
1	B	48	GLN
1	B	57	LEU
1	B	104	LEU
1	B	126	GLU
1	B	142	SER
1	B	162	ASP
1	B	164	GLN
1	C	32	SER
1	C	48	GLN
1	C	54	MET
1	C	55	GLN
1	C	84	ASP
1	C	142	SER
1	C	143	LEU
1	C	158	LEU
1	D	5	GLU
1	D	48	GLN
1	D	54	MET
1	D	84	ASP
1	D	88	GLN
1	D	92	LYS
1	D	109	MET
1	D	125	SER
1	E	54	MET
1	E	55	GLN
1	E	82	SER
1	E	92	LYS
1	E	104	LEU
1	E	164	GLN
1	F	2	LEU
1	F	32	SER
1	F	45	ARG
1	F	48	GLN
1	F	49	GLU
1	F	57	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	82	SER
1	F	85	GLU
1	F	96	LEU
1	F	104	LEU
1	F	135	LYS
1	F	142	SER
1	F	146	LYS
1	F	161	LEU
1	F	163	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	46	HIS
1	A	95	GLN
1	A	111	ASN
1	A	165	ASN
1	B	26	GLN
1	B	164	GLN
1	C	25	GLN
1	C	26	GLN
1	C	46	HIS
1	C	88	GLN
1	C	93	HIS
1	D	26	GLN
1	D	34	HIS
1	D	46	HIS
1	D	99	GLN
1	D	164	GLN
1	E	26	GLN
1	E	34	HIS
1	E	46	HIS
1	E	55	GLN
1	E	121	GLN
1	E	165	ASN
1	F	46	HIS
1	F	112	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 62 ligands modelled in this entry, 42 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	E	205	-	4,4,4	0.38	0	6,6,6	0.70	0
3	SO4	B	203	-	4,4,4	0.49	0	6,6,6	0.76	0
3	SO4	A	206	-	4,4,4	0.47	0	6,6,6	0.53	0
3	SO4	E	204	-	4,4,4	0.15	0	6,6,6	1.45	2 (33%)
3	SO4	C	204	-	4,4,4	0.41	0	6,6,6	1.60	1 (16%)
3	SO4	F	203	-	4,4,4	0.32	0	6,6,6	0.38	0
3	SO4	D	205	-	4,4,4	0.35	0	6,6,6	0.82	0
3	SO4	A	203	-	4,4,4	0.49	0	6,6,6	1.15	1 (16%)
3	SO4	A	204	-	4,4,4	0.44	0	6,6,6	0.60	0
3	SO4	A	207	-	4,4,4	0.54	0	6,6,6	1.07	1 (16%)
3	SO4	F	204	-	4,4,4	0.56	0	6,6,6	0.52	0
3	SO4	D	203	-	4,4,4	0.29	0	6,6,6	0.61	0
3	SO4	C	203	-	4,4,4	0.40	0	6,6,6	0.92	0
3	SO4	D	204	-	4,4,4	0.40	0	6,6,6	1.20	1 (16%)
3	SO4	E	206	-	4,4,4	0.29	0	6,6,6	0.14	0
3	SO4	B	204	-	4,4,4	0.56	0	6,6,6	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	E	203	-	4,4,4	0.63	0	6,6,6	1.45	1 (16%)
3	SO4	A	205	-	4,4,4	0.28	0	6,6,6	0.60	0
3	SO4	E	207	-	4,4,4	0.58	0	6,6,6	1.13	0
4	MES	A	208	-	12,12,12	1.96	1 (8%)	14,16,16	1.95	5 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	A	208	-	-	4/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	208	MES	C8-S	-6.31	1.68	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	208	MES	O1S-S-C8	4.53	112.37	106.92
4	A	208	MES	O2S-S-C8	3.58	111.22	106.92
3	C	204	SO4	O4-S-O1	3.16	125.80	109.31
3	E	203	SO4	O4-S-O3	2.88	121.36	109.06
3	D	204	SO4	O4-S-O2	2.61	122.95	109.31
3	E	204	SO4	O4-S-O2	2.41	121.90	109.31
4	A	208	MES	O3S-S-C8	2.30	109.49	105.77
3	A	207	SO4	O3-S-O1	2.23	120.93	109.31
4	A	208	MES	O2S-S-O1S	-2.19	106.36	113.95
3	E	204	SO4	O3-S-O2	-2.08	98.43	109.31
4	A	208	MES	C6-O1-C2	2.04	116.69	109.89
3	A	203	SO4	O4-S-O2	2.03	119.92	109.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	208	MES	N4-C7-C8-S
4	A	208	MES	C7-C8-S-O1S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	208	MES	C7-C8-S-O3S
4	A	208	MES	C7-C8-S-O2S

There are no ring outliers.

12 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	SO4	2	0
3	A	206	SO4	0	1
3	E	204	SO4	1	0
3	F	203	SO4	2	0
3	A	203	SO4	2	0
3	D	203	SO4	0	1
3	C	203	SO4	4	0
3	B	204	SO4	2	0
3	E	203	SO4	2	0
3	A	205	SO4	1	0
3	E	207	SO4	2	0
4	A	208	MES	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	164/164 (100%)	-0.14	6 (3%) 41 45	27, 42, 98, 136	0
1	B	164/164 (100%)	-0.01	8 (4%) 29 31	26, 41, 96, 147	0
1	C	164/164 (100%)	0.22	17 (10%) 6 6	28, 43, 97, 153	0
1	D	164/164 (100%)	-0.16	9 (5%) 25 26	26, 41, 97, 148	0
1	E	164/164 (100%)	0.00	9 (5%) 25 26	29, 44, 99, 162	0
1	F	164/164 (100%)	-0.00	9 (5%) 25 26	24, 39, 96, 143	0
All	All	984/984 (100%)	-0.01	58 (5%) 22 23	24, 42, 101, 162	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	165	ASN	9.6
1	F	145	GLY	9.0
1	D	148	GLY	6.8
1	D	165	ASN	6.7
1	C	145	GLY	6.6
1	E	145	GLY	6.3
1	A	165	ASN	6.3
1	B	146	LYS	5.8
1	F	148	GLY	5.6
1	E	146	LYS	5.5
1	B	165	ASN	5.4
1	C	147	SER	5.1
1	C	146	LYS	5.1
1	E	153	PHE	4.8
1	D	164	GLN	4.7
1	C	81	SER	4.5
1	C	141	LEU	4.4
1	F	165	ASN	4.4
1	D	147	SER	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	147	SER	4.2
1	B	145	GLY	4.1
1	E	164	GLN	4.1
1	C	165	ASN	4.0
1	B	148	GLY	3.8
1	F	146	LYS	3.8
1	E	147	SER	3.7
1	C	80	TYR	3.4
1	B	153	PHE	3.2
1	D	149	GLU	3.1
1	D	150	GLY	3.1
1	A	148	GLY	3.0
1	E	148	GLY	3.0
1	C	84	ASP	2.9
1	A	153	PHE	2.9
1	C	143	LEU	2.9
1	A	164	GLN	2.8
1	C	164	GLN	2.8
1	B	147	SER	2.7
1	C	160	THR	2.7
1	C	163	THR	2.6
1	F	163	THR	2.6
1	D	145	GLY	2.6
1	A	144	ALA	2.5
1	F	153	PHE	2.5
1	C	150	GLY	2.5
1	D	146	LYS	2.4
1	A	147	SER	2.3
1	F	150	GLY	2.3
1	F	160	THR	2.3
1	B	164	GLN	2.2
1	C	82	SER	2.2
1	C	148	GLY	2.2
1	D	153	PHE	2.2
1	E	81	SER	2.2
1	C	142	SER	2.1
1	C	154	ILE	2.0
1	B	141	LEU	2.0
1	E	149	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 monosaccharides 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
4	MES	A	208	12/12	0.76	0.20	85,90,106,107	0
5	CL	D	215	1/1	0.89	0.14	66,66,66,66	0
5	CL	B	207	1/1	0.91	0.12	61,61,61,61	0
5	CL	A	214	1/1	0.92	0.10	56,56,56,56	0
5	CL	B	205	1/1	0.93	0.16	65,65,65,65	0
3	SO4	B	204	5/5	0.93	0.11	68,68,91,93	0
3	SO4	E	206	5/5	0.93	0.20	142,142,145,145	5
5	CL	F	206	1/1	0.93	0.10	71,71,71,71	0
5	CL	B	208	1/1	0.94	0.11	51,51,51,51	0
5	CL	F	209	1/1	0.94	0.17	68,68,68,68	0
5	CL	D	212	1/1	0.95	0.14	51,51,51,51	0
3	SO4	F	204	5/5	0.95	0.14	52,70,75,76	0
5	CL	C	207	1/1	0.95	0.16	69,69,69,69	0
5	CL	D	208	1/1	0.95	0.15	57,57,57,57	0
3	SO4	B	203	5/5	0.96	0.13	48,52,63,67	0
5	CL	E	209	1/1	0.96	0.07	54,54,54,54	0
5	CL	F	205	1/1	0.96	0.16	62,62,62,62	0
3	SO4	D	204	5/5	0.96	0.14	37,40,55,57	0
5	CL	D	214	1/1	0.96	0.12	69,69,69,69	0
3	SO4	A	205	5/5	0.97	0.10	36,40,46,51	0
5	CL	A	213	1/1	0.97	0.08	50,50,50,50	0
3	SO4	E	205	5/5	0.97	0.12	34,42,49,56	0
3	SO4	A	207	5/5	0.97	0.14	33,36,47,48	0
5	CL	F	207	1/1	0.97	0.29	52,52,52,52	0
3	SO4	C	204	5/5	0.97	0.19	32,39,43,46	0
5	CL	D	213	1/1	0.98	0.14	51,51,51,51	0
3	SO4	C	203	5/5	0.98	0.12	35,45,46,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CL	A	209	1/1	0.98	0.17	53,53,53,53	0
5	CL	E	208	1/1	0.98	0.14	52,52,52,52	0
5	CL	C	206	1/1	0.98	0.04	50,50,50,50	0
3	SO4	D	205	5/5	0.98	0.14	36,42,49,52	0
3	SO4	F	203	5/5	0.98	0.09	47,52,58,65	0
5	CL	D	211	1/1	0.98	0.11	49,49,49,49	0
3	SO4	E	204	5/5	0.98	0.12	35,37,42,45	0
5	CL	A	212	1/1	0.99	0.14	49,49,49,49	0
2	FE	A	201	1/1	0.99	0.13	25,25,25,25	0
3	SO4	A	206	5/5	0.99	0.10	37,42,45,45	0
3	SO4	E	207	5/5	0.99	0.15	26,28,36,37	0
5	CL	B	206	1/1	0.99	0.17	58,58,58,58	0
3	SO4	D	203	5/5	0.99	0.13	39,39,46,48	0
2	FE	F	202	1/1	0.99	0.14	32,32,32,32	0
3	SO4	A	203	5/5	0.99	0.15	20,30,32,34	0
3	SO4	A	204	5/5	0.99	0.11	29,31,39,39	0
5	CL	A	211	1/1	0.99	0.18	47,47,47,47	0
5	CL	F	208	1/1	0.99	0.19	51,51,51,51	0
5	CL	D	210	1/1	0.99	0.10	51,51,51,51	0
5	CL	A	210	1/1	1.00	0.07	42,42,42,42	0
2	FE	B	201	1/1	1.00	0.15	28,28,28,28	0
2	FE	B	202	1/1	1.00	0.13	34,34,34,34	0
3	SO4	E	203	5/5	1.00	0.15	18,25,29,30	0
2	FE	C	201	1/1	1.00	0.12	27,27,27,27	0
2	FE	C	202	1/1	1.00	0.10	32,32,32,32	0
2	FE	D	201	1/1	1.00	0.13	28,28,28,28	0
2	FE	D	202	1/1	1.00	0.12	33,33,33,33	0
2	FE	E	201	1/1	1.00	0.11	29,29,29,29	0
2	FE	E	202	1/1	1.00	0.11	33,33,33,33	0
2	FE	F	201	1/1	1.00	0.14	27,27,27,27	0
2	FE	A	202	1/1	1.00	0.09	30,30,30,30	0
5	CL	D	209	1/1	1.00	0.10	39,39,39,39	0
6	HG	C	205	1/1	1.00	0.10	56,56,56,56	0
6	HG	D	206	1/1	1.00	0.12	46,46,46,46	1
7	MG	D	207	1/1	1.00	0.23	33,33,33,33	1

6.5 Other polymers [i](#)

There are no such residues in this entry.