Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:51 PM GMT

PDB ID	:	4MWA
Title	:	1.85 Angstrom Crystal Structure of GCPE Protein from Bacillus anthracis
Authors	:	Minasov, G.; Wawrzak, Z.; Brunzelle, J.S.; Xu, X.; Cui, H.; Maltseva, N.; Bishop, B.; Kwon, K.; Savchenko, A.; Joachimiak, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2013-09-24
Resolution	:	1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

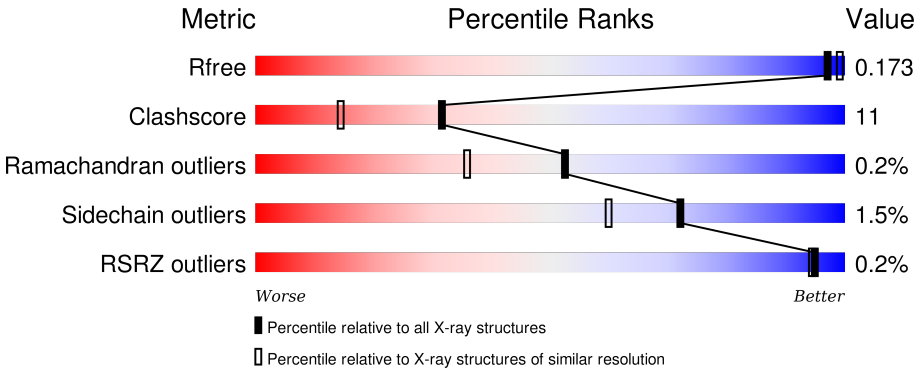
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	276	69% 25% • 5%
1	G	276	77% 15% • 7%
2	B	276	81% 12% • 6%
3	C	276	68% 24% • 7%
4	D	276	% 68% 23% 9%

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Mol	Chain	Length	Quality of chain
4	F	276	73% 21% • 5%
4	H	276	71% 22% 8%
5	E	276	79% 14% • 6%

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
6	SO4	E	401	-	-	X	-
6	SO4	G	402	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17202 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 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	Se	0	10	0
			2083	1305	376	395	1	6			
1	G	258	Total	C	N	O	S	Se	0	0	0
			1965	1235	354	371	1	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81LV7
A	-1	ASN	-	EXPRESSION TAG	UNP Q81LV7
A	0	ALA	-	EXPRESSION TAG	UNP Q81LV7
A	1	MSE	-	EXPRESSION TAG	UNP Q81LV7
A	2	ASN	-	EXPRESSION TAG	UNP Q81LV7
A	3	GLU	-	EXPRESSION TAG	UNP Q81LV7
G	-2	SER	-	EXPRESSION TAG	UNP Q81LV7
G	-1	ASN	-	EXPRESSION TAG	UNP Q81LV7
G	0	ALA	-	EXPRESSION TAG	UNP Q81LV7
G	1	MSE	-	EXPRESSION TAG	UNP Q81LV7
G	2	ASN	-	EXPRESSION TAG	UNP Q81LV7
G	3	GLU	-	EXPRESSION TAG	UNP Q81LV7

- Molecule 2 is a protein called 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	Se	0	2	0
			1990	1250	360	375	1	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	EXPRESSION TAG	UNP Q81LV7
B	-1	ASN	-	EXPRESSION TAG	UNP Q81LV7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	EXPRESSION TAG	UNP Q81LV7
B	1	MSE	-	EXPRESSION TAG	UNP Q81LV7
B	2	ASN	-	EXPRESSION TAG	UNP Q81LV7
B	3	GLU	-	EXPRESSION TAG	UNP Q81LV7

- Molecule 3 is a protein called 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	257	Total	C	N	O	S	Se	0	1	0
			1968	1236	354	373	1	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	EXPRESSION TAG	UNP Q81LV7
C	-1	ASN	-	EXPRESSION TAG	UNP Q81LV7
C	0	ALA	-	EXPRESSION TAG	UNP Q81LV7
C	1	MSE	-	EXPRESSION TAG	UNP Q81LV7
C	2	ASN	-	EXPRESSION TAG	UNP Q81LV7
C	3	GLU	-	EXPRESSION TAG	UNP Q81LV7

- Molecule 4 is a protein called 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	251	Total	C	N	O	S	Se	0	4	0
			1938	1222	344	367	1	4			
4	F	262	Total	C	N	O	S	Se	0	5	0
			2033	1274	371	383	1	4			
4	H	255	Total	C	N	O	S	Se	0	1	0
			1951	1226	352	368	1	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	EXPRESSION TAG	UNP Q81LV7
D	-1	ASN	-	EXPRESSION TAG	UNP Q81LV7
D	0	ALA	-	EXPRESSION TAG	UNP Q81LV7
D	1	MSE	-	EXPRESSION TAG	UNP Q81LV7
D	2	ASN	-	EXPRESSION TAG	UNP Q81LV7
D	3	GLU	-	EXPRESSION TAG	UNP Q81LV7
F	-2	SER	-	EXPRESSION TAG	UNP Q81LV7
F	-1	ASN	-	EXPRESSION TAG	UNP Q81LV7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	EXPRESSION TAG	UNP Q81LV7
F	1	MSE	-	EXPRESSION TAG	UNP Q81LV7
F	2	ASN	-	EXPRESSION TAG	UNP Q81LV7
F	3	GLU	-	EXPRESSION TAG	UNP Q81LV7
H	-2	SER	-	EXPRESSION TAG	UNP Q81LV7
H	-1	ASN	-	EXPRESSION TAG	UNP Q81LV7
H	0	ALA	-	EXPRESSION TAG	UNP Q81LV7
H	1	MSE	-	EXPRESSION TAG	UNP Q81LV7
H	2	ASN	-	EXPRESSION TAG	UNP Q81LV7
H	3	GLU	-	EXPRESSION TAG	UNP Q81LV7

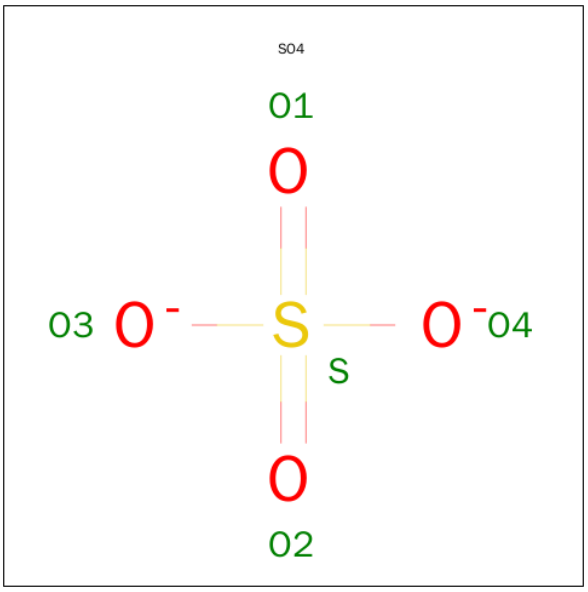
- Molecule 5 is a protein called 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	260	Total	C	N	O	S	Se	0	2	0
			2003	1256	363	379	1	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	SER	-	EXPRESSION TAG	UNP Q81LV7
E	-1	ASN	-	EXPRESSION TAG	UNP Q81LV7
E	0	ALA	-	EXPRESSION TAG	UNP Q81LV7
E	1	MSE	-	EXPRESSION TAG	UNP Q81LV7
E	2	ASN	-	EXPRESSION TAG	UNP Q81LV7
E	3	GLU	-	EXPRESSION TAG	UNP Q81LV7

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Cl 3 3	0	1
7	A	1	Total Cl 1 1	0	0
7	C	3	Total Cl 3 3	0	0
7	F	2	Total Cl 3 3	0	1

- Molecule 8 is water.

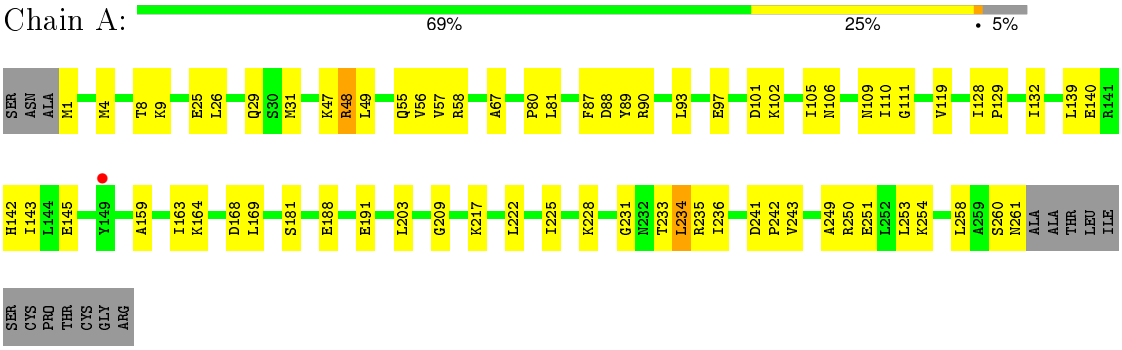
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	146	Total O 147 147	0	2
8	B	139	Total O 142 142	0	3
8	C	147	Total O 149 149	0	2
8	D	116	Total O 119 119	0	3
8	E	166	Total O 172 172	0	6
8	F	148	Total O 154 154	0	6
8	G	158	Total O 162 162	0	4
8	H	148	Total O 151 151	0	3

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.

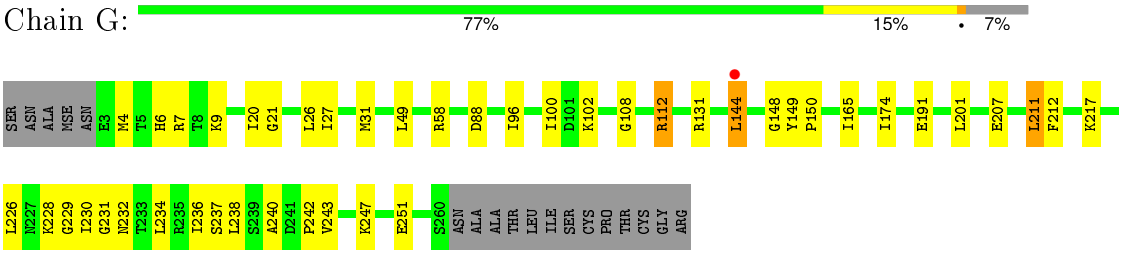
- Molecule 1: 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase

Chain A:



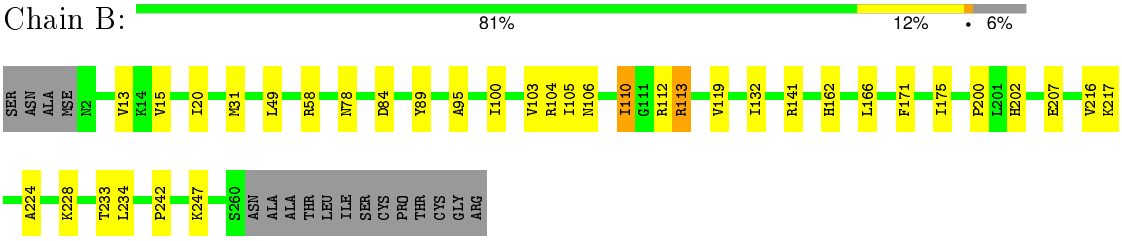
- Molecule 1: 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase

Chain G:



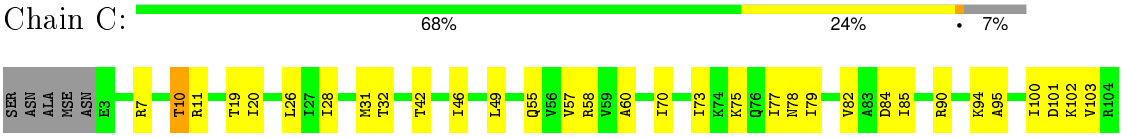
- Molecule 2: 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase

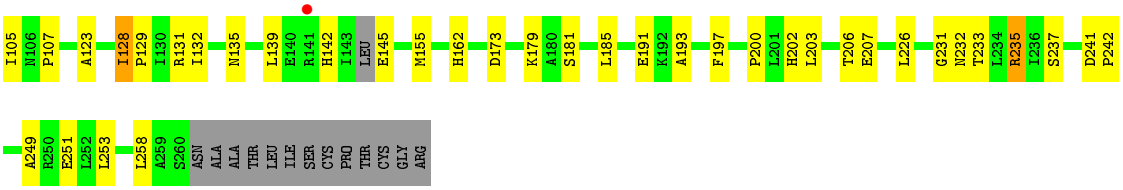
Chain B:



- Molecule 3: 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase

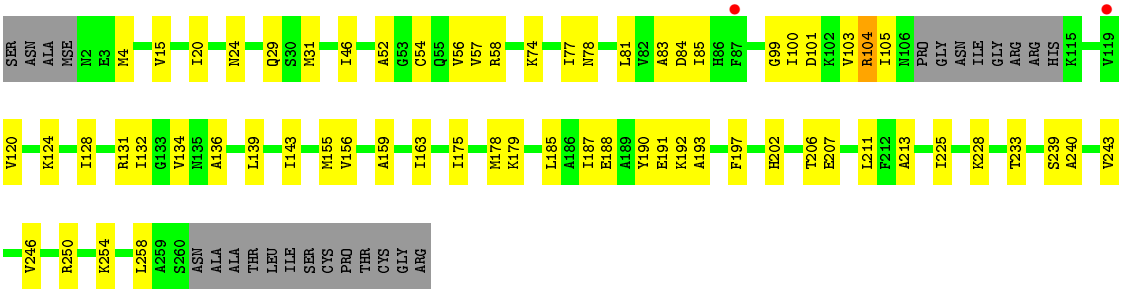
Chain C:





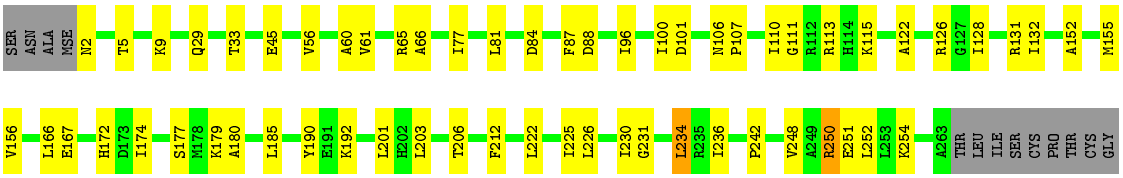
• Molecule 4: 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase

Chain D:



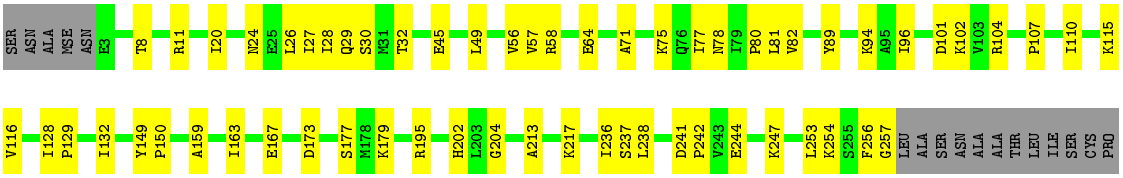
• Molecule 4: 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase

Chain F:



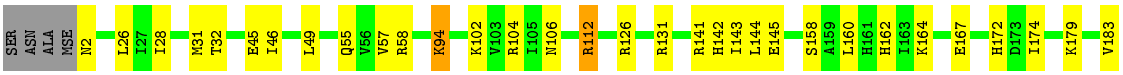
• Molecule 4: 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase

Chain H:



• Molecule 5: 4-hydroxy-3-methylbut-2-en-1-yl diphosphate synthase

Chain E:




P200
L203
L222
L234
R235
I236
A249
R250
E251
L258
N261
ALA
ALA
THR
LEU
ILE
SER
CYS
PRO
THR
CYS
GLY
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	162.68Å 162.68Å 76.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.77 – 1.85 29.77 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.77-1.85) 99.4 (29.77-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.66 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0046	Depositor
R, R_{free}	0.125 , 0.169 0.133 , 0.173	Depositor DCC
R_{free} test set	9677 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 19.4	EDS
Estimated twinning fraction	0.241 for H, K, L 0.260 for -K, -H, -L 0.268 for -H, -K, L 0.232 for K, H, -L 0.468 for -h,-k,l 0.479 for h,-h-k,-l 0.468 for -k,-h,-l	Xtriage
Reported twinning fraction	0.241 for H, K, L 0.260 for -K, -H, -L 0.268 for -H, -K, L 0.232 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 192077 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17202	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 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CL, KCX, 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	0.52	2/2093 (0.1%)	0.74	0/2817
1	G	0.53	0/1974	0.78	0/2660
2	B	0.45	0/2000	0.72	0/2696
3	C	0.46	0/1963	0.71	0/2643
4	D	0.45	0/1957	0.72	0/2636
4	F	0.50	0/2055	0.76	0/2770
4	H	0.52	0/1973	0.74	0/2659
5	E	0.52	0/2000	0.75	0/2694
All	All	0.50	2/16015 (0.0%)	0.74	0/21575

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48[A]	ARG	CD-NE	-5.32	1.37	1.46
1	A	48[B]	ARG	CD-NE	-5.32	1.37	1.46

There are no bond angle outliers.

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	2083	0	2132	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1965	0	2026	32	0
2	B	1990	0	2047	26	0
3	C	1968	0	2022	58	0
4	D	1938	0	2007	49	0
4	F	2033	0	2095	47	0
4	H	1951	0	2011	53	0
5	E	2003	0	2054	33	0
6	A	5	0	0	1	0
6	B	5	0	0	1	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
6	E	10	0	0	2	0
6	F	10	0	0	1	0
6	G	10	0	0	2	0
6	H	5	0	0	1	0
7	A	1	0	0	1	0
7	B	3	0	0	0	0
7	C	3	0	0	0	0
7	F	3	0	0	1	0
8	A	147	0	0	4	0
8	B	142	0	0	4	0
8	C	149	0	0	4	0
8	D	119	0	0	2	0
8	E	172	0	0	7	0
8	F	154	0	0	3	0
8	G	162	0	0	3	0
8	H	151	0	0	5	0
All	All	17202	0	16394	348	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 11.

All (348) 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)
4:F:155:MSE:SE	4:F:185:LEU:HD21	2.10	1.02
4:H:236:ILE:HG22	4:H:238:LEU:CD1	1.95	0.97
4:H:29:GLN:HE22	4:H:58:ARG:NH1	1.68	0.91
3:C:241:ASP:HB3	8:C:554:HOH:O	1.73	0.87
4:H:28:ILE:HD11	4:H:253:LEU:HD12	1.61	0.82
5:E:28:ILE:HD13	5:E:234:LEU:HD21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:250:ARG:HH11	4:F:250:ARG:HG3	1.45	0.80
4:D:46[A]:ILE:HD12	4:D:57:VAL:HG11	1.61	0.80
4:H:128:ILE:HD11	8:H:507:HOH:O	1.82	0.78
4:F:5:THR:HG23	4:F:9:LYS:HG3	1.64	0.77
3:C:60:ALA:HA	3:C:84:ASP:HB3	1.66	0.77
4:H:236:ILE:HG22	4:H:238:LEU:HD11	1.65	0.77
4:H:177:SER:OG	4:H:202:HIS:HB3	1.84	0.77
3:C:70:ILE:HD12	3:C:100:ILE:HD11	1.65	0.76
4:D:187[B]:ILE:HA	4:D:225:ILE:HD11	1.68	0.75
1:A:140:GLU:HB2	1:A:143:ILE:HD13	1.69	0.75
3:C:10:THR:HG21	3:C:200:PRO:HA	1.67	0.74
2:B:141:ARG:NH1	8:B:586:HOH:O	2.21	0.74
3:C:19:THR:C	3:C:20:ILE:HD12	2.08	0.73
4:D:187[A]:ILE:HA	4:D:225:ILE:HD11	1.73	0.71
3:C:46:ILE:HD12	3:C:57:VAL:HG11	1.73	0.70
4:H:236:ILE:CG2	4:H:238:LEU:HD11	2.22	0.69
4:D:31:MSE:SE	4:D:58:ARG:HH12	2.24	0.69
5:E:28:ILE:HD12	5:E:249:ALA:HB1	1.74	0.69
2:B:15:VAL:HG21	2:B:20:ILE:HD12	1.74	0.69
4:D:202:HIS:HA	4:D:233:THR:HG23	1.74	0.69
3:C:75:LYS:HG3	8:C:619:HOH:O	1.93	0.68
1:A:203[A]:LEU:HD11	1:A:231:GLY:HA3	1.75	0.68
1:A:241:ASP:OD2	1:A:243:VAL:HG12	1.94	0.68
1:A:228[A]:LYS:HA	1:A:228[A]:LYS:HE2	1.75	0.67
4:F:5:THR:HG23	4:F:9:LYS:CG	2.24	0.66
4:F:236:ILE:HG21	4:F:248:VAL:HG11	1.77	0.66
2:B:49:LEU:HD21	2:B:242:PRO:HB2	1.77	0.66
4:D:240:ALA:HB1	8:D:528:HOH:O	1.95	0.66
1:G:4:MSE:SE	1:G:228:LYS:HG2	2.46	0.66
4:D:120:VAL:O	4:D:124:LYS:HG2	1.96	0.65
1:G:211:LEU:HG	1:G:240:ALA:HB2	1.78	0.65
3:C:123:ALA:HA	3:C:128:ILE:HG23	1.79	0.65
5:E:45:GLU:O	5:E:49:LEU:HD13	1.98	0.64
1:G:49:LEU:HD21	1:G:242:PRO:HB2	1.78	0.64
5:E:160:LEU:O	5:E:164:LYS:HG3	1.97	0.64
4:H:253:LEU:O	4:H:257:GLY:HA2	1.98	0.63
2:B:13:VAL:HG11	2:B:175:ILE:HD11	1.79	0.63
4:F:33:THR:HG22	4:F:45:GLU:OE2	1.98	0.62
5:E:179:LYS:HD2	6:E:401:SO4:O1	2.00	0.62
3:C:207:GLU:HG2	3:C:237:SER:HB3	1.82	0.62
4:F:185:LEU:O	4:F:185:LEU:HD23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:MSE:SE	4:D:58:ARG:NH1	2.82	0.62
3:C:20:ILE:N	3:C:20:ILE:HD12	2.15	0.61
5:E:28:ILE:CD1	5:E:234:LEU:HD21	2.30	0.61
5:E:94[A]:LYS:HZ3	5:E:94[A]:LYS:HB3	1.64	0.61
2:B:89:TYR:HB3	2:B:110:ILE:HG23	1.82	0.61
1:A:234:LEU:HD12	1:A:234:LEU:C	2.22	0.60
1:A:159:ALA:O	1:A:163:ILE:HG12	2.02	0.60
4:H:20:ILE:CD1	4:H:27:ILE:HG13	2.31	0.60
3:C:90:ARG:O	3:C:94:LYS:HG2	2.02	0.59
1:A:250:ARG:O	1:A:254:LYS:HG3	2.02	0.59
1:A:106:ASN:HB2	1:A:109:ASN:ND2	2.18	0.59
4:F:254:LYS:NZ	8:F:611:HOH:O	2.33	0.59
1:A:188[B]:GLU:OE1	1:A:188[B]:GLU:HA	2.02	0.59
1:G:88:ASP:CG	8:G:623:HOH:O	2.41	0.59
3:C:77:ILE:HG22	3:C:78:ASN:N	2.18	0.59
2:B:58:ARG:NH1	6:B:401:SO4:O2	2.35	0.59
5:E:32:THR:CG2	5:E:46:ILE:HD11	2.33	0.59
1:G:243:VAL:HG12	1:G:247:LYS:HE3	1.85	0.58
3:C:10:THR:HG21	3:C:200:PRO:CA	2.32	0.58
3:C:155:MSE:HE1	3:C:185:LEU:HD21	1.85	0.58
4:H:115:LYS:NZ	8:H:636[B]:HOH:O	2.32	0.58
5:E:112:ARG:NH1	8:E:630[A]:HOH:O	2.36	0.58
4:D:155:MSE:HE1	4:D:185:LEU:HD21	1.86	0.58
4:H:58:ARG:CZ	4:H:104:ARG:HD3	2.34	0.57
4:H:179:LYS:HZ3	4:H:204:GLY:HA3	1.68	0.57
3:C:103:VAL:HG23	3:C:128:ILE:HD11	1.84	0.57
4:H:56:VAL:HG22	4:H:80:PRO:HG2	1.86	0.57
4:H:107:PRO:O	4:H:110:ILE:HG22	2.04	0.57
4:D:178:MSE:HE3	4:D:193:ALA:HB2	1.86	0.57
4:H:29:GLN:HG2	4:H:30:SER:N	2.20	0.57
4:F:250:ARG:HH11	4:F:250:ARG:CG	2.16	0.57
1:G:4:MSE:SE	1:G:191:GLU:HG3	2.55	0.57
3:C:70:ILE:HG21	3:C:100:ILE:HG12	1.86	0.56
3:C:203:LEU:HD11	3:C:231:GLY:HA3	1.86	0.56
1:A:49:LEU:HD21	1:A:242:PRO:HB2	1.86	0.56
3:C:207:GLU:HG3	8:D:584:HOH:O	2.06	0.56
3:C:28:ILE:HD12	3:C:249:ALA:HB1	1.86	0.56
1:G:217:LYS:NZ	8:G:544:HOH:O	2.35	0.56
2:B:13:VAL:CG1	2:B:175:ILE:HD11	2.35	0.56
1:A:249:ALA:O	1:A:253:LEU:HD13	2.05	0.56
1:G:31:MSE:HE1	1:G:58:ARG:NH1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:241:ASP:OD1	4:H:242:PRO:HD2	2.06	0.55
3:C:102:KCX:OQ2	3:C:131:ARG:NE	2.37	0.55
2:B:95:ALA:HB1	2:B:100:ILE:HG13	1.89	0.55
1:G:102:KCX:OQ1	1:G:131:ARG:NE	2.35	0.55
1:A:89[B]:TYR:HB2	1:A:119:VAL:CG2	2.36	0.55
4:F:201:LEU:HD22	4:F:230:ILE:CG2	2.35	0.55
5:E:55:GLN:NE2	5:E:261:ASN:OD1	2.40	0.55
4:H:58:ARG:NH1	6:H:401:SO4:O1	2.40	0.55
3:C:207:GLU:CG	3:C:237:SER:HB3	2.36	0.55
2:B:103:VAL:HG12	2:B:105:ILE:HG23	1.88	0.55
4:H:236:ILE:CG2	4:H:238:LEU:CD1	2.77	0.55
5:E:28:ILE:HD13	5:E:234:LEU:CD2	2.33	0.54
5:E:179:LYS:HG3	8:E:625:HOH:O	2.06	0.54
3:C:155:MSE:CE	3:C:185:LEU:HD21	2.37	0.54
3:C:58:ARG:HG3	3:C:82:VAL:HB	1.89	0.54
4:F:226:LEU:HD12	4:F:252:LEU:HD21	1.89	0.54
4:H:110:ILE:CG2	4:H:116:VAL:HG22	2.36	0.54
4:D:207:GLU:OE1	4:D:239:SER:OG	2.24	0.54
4:F:65:ARG:HG3	8:F:622:HOH:O	2.07	0.54
1:A:132:ILE:HD12	1:A:163:ILE:HD13	1.89	0.54
4:F:77:ILE:CD1	4:F:81:LEU:HD21	2.38	0.54
4:H:58:ARG:NH2	4:H:82:VAL:HG11	2.23	0.53
3:C:32:THR:CG2	3:C:46:ILE:HD11	2.39	0.53
3:C:11:ARG:NH2	3:C:173:ASP:OD1	2.40	0.53
4:H:236:ILE:HG22	4:H:238:LEU:HD12	1.87	0.53
1:A:90[B]:ARG:NH2	7:A:402:CL:CL	2.78	0.53
4:D:178:MSE:HE2	4:D:197:PHE:HZ	1.73	0.52
4:F:115:LYS:NZ	7:F:404[B]:CL:CL	2.79	0.52
4:H:64:GLU:HG3	4:H:94:LYS:HE2	1.91	0.52
4:F:60:ALA:HA	4:F:84:ASP:HB3	1.91	0.52
4:D:4:MSE:HE1	4:D:228:LYS:HB3	1.90	0.52
1:G:4:MSE:SE	1:G:228:LYS:CG	3.07	0.52
1:G:7:ARG:NH1	1:G:226:LEU:O	2.41	0.52
3:C:135:ASN:ND2	8:C:510:HOH:O	2.28	0.52
4:H:96:ILE:HG23	4:H:128:ILE:CD1	2.39	0.52
4:H:179:LYS:NZ	8:H:506:HOH:O	2.42	0.52
4:H:11:ARG:NH2	4:H:173:ASP:OD1	2.42	0.52
1:A:26:LEU:HD11	1:A:258:LEU:HD13	1.91	0.52
3:C:49:LEU:HD21	3:C:242:PRO:HB2	1.90	0.52
1:G:27:ILE:HD11	8:G:539:HOH:O	2.09	0.52
4:F:155:MSE:SE	4:F:185:LEU:CD2	2.99	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:77:ILE:HD11	4:D:81:LEU:HG	1.91	0.52
1:A:25:GLU:N	1:A:25:GLU:OE1	2.43	0.52
4:F:251[B]:GLU:HG3	1:G:212:PHE:CE2	2.44	0.52
4:H:101:ASP:O	4:H:129:PRO:HD2	2.10	0.52
3:C:193:ALA:HB1	3:C:197:PHE:CZ	2.45	0.52
5:E:251:GLU:HG2	4:H:213:ALA:HA	1.91	0.51
4:H:29:GLN:HG2	4:H:30:SER:H	1.75	0.51
4:H:96:ILE:HG23	4:H:128:ILE:HD12	1.92	0.51
3:C:123:ALA:HA	3:C:128:ILE:CG2	2.40	0.51
3:C:77:ILE:HG22	3:C:78:ASN:H	1.75	0.51
4:F:152:ALA:O	4:F:156:VAL:HG23	2.11	0.51
1:A:89[A]:TYR:CE1	1:A:93:LEU:HD11	2.45	0.51
3:C:95:ALA:HB1	3:C:100:ILE:HG13	1.93	0.51
1:A:67:ALA:HB3	8:A:533:HOH:O	2.08	0.51
1:G:108:GLY:HA2	1:G:165:ILE:CD1	2.41	0.51
4:F:29:GLN:HG2	4:F:56:VAL:HB	1.93	0.51
4:H:57:VAL:HG13	4:H:81:LEU:HD23	1.93	0.50
3:C:20:ILE:N	3:C:20:ILE:CD1	2.74	0.50
4:D:74:LYS:NZ	4:D:101:ASP:OD2	2.43	0.50
1:G:144:LEU:O	1:G:148:GLY:N	2.41	0.50
4:D:211:LEU:HD23	4:D:211:LEU:C	2.31	0.50
2:B:106:ASN:ND2	2:B:162:HIS:CE1	2.80	0.50
4:H:49:LEU:HD21	4:H:242:PRO:HB2	1.93	0.50
3:C:235:ARG:HD3	3:C:235:ARG:C	2.31	0.50
1:A:139:LEU:O	2:B:78:ASN:ND2	2.37	0.50
3:C:73:ILE:O	3:C:77:ILE:HG12	2.11	0.50
3:C:181:SER:HA	3:C:206:THR:HB	1.94	0.50
4:H:244:GLU:HA	4:H:247:LYS:HD2	1.94	0.50
3:C:107:PRO:CD	3:C:132:ILE:HD12	2.41	0.50
1:A:209:GLY:HA2	2:B:247:LYS:HD2	1.94	0.50
4:D:100:ILE:HG21	4:D:103:VAL:HG22	1.94	0.50
1:A:48[B]:ARG:NH2	8:A:556:HOH:O	2.40	0.50
1:A:58:ARG:NH2	6:A:401:SO4:O4	2.45	0.50
1:A:203[A]:LEU:HD12	1:A:233:THR:O	2.12	0.49
4:F:234:LEU:HD12	4:F:234:LEU:C	2.33	0.49
4:F:166:LEU:HD13	4:F:174:ILE:HD11	1.94	0.49
4:H:159:ALA:O	4:H:163:ILE:HD13	2.12	0.49
4:F:203:LEU:HD22	4:F:225:ILE:HG21	1.93	0.49
3:C:85:ILE:O	3:C:105:ILE:HD12	2.12	0.49
4:H:256:PHE:N	4:H:257:GLY:HA2	2.28	0.49
3:C:78:ASN:OD1	8:C:620:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:ALA:CB	4:D:243:VAL:HG13	2.42	0.49
4:H:58:ARG:HD3	8:H:583:HOH:O	2.11	0.49
1:G:112:ARG:NE	6:G:402:SO4:S	2.84	0.49
4:F:87:PHE:CG	4:F:88:ASP:N	2.81	0.49
2:B:202:HIS:ND1	2:B:233:THR:HG23	2.27	0.49
1:G:230:ILE:HG22	1:G:231:GLY:N	2.28	0.49
8:E:536:HOH:O	4:H:217:LYS:HD2	2.11	0.49
1:A:181:SER:O	1:A:217:LYS:HE3	2.13	0.49
3:C:31:MSE:SE	3:C:58:ARG:NH2	2.96	0.48
2:B:216:VAL:HG11	3:C:251:GLU:HB3	1.95	0.48
1:G:96:ILE:HA	1:G:100:ILE:HG22	1.93	0.48
1:A:203[A]:LEU:HB3	1:A:222:LEU:HD22	1.94	0.48
1:G:6:HIS:H	1:G:9:LYS:CE	2.27	0.48
4:F:101:ASP:O	4:F:128[A]:ILE:HG23	2.13	0.48
1:G:6:HIS:HB3	1:G:9:LYS:HE2	1.95	0.48
1:A:110:ILE:HB	1:A:111:GLY:HA2	1.94	0.48
2:B:84:ASP:HA	2:B:104:ARG:HB3	1.95	0.48
4:D:188:GLU:O	4:D:192:LYS:HB2	2.14	0.48
4:D:139:LEU:HB3	4:D:143:ILE:HD11	1.95	0.48
4:F:185:LEU:HD23	4:F:185:LEU:C	2.34	0.48
1:G:21:GLY:HA2	1:G:232:ASN:ND2	2.29	0.47
5:E:203:LEU:HB3	5:E:222:LEU:HD22	1.96	0.47
5:E:28:ILE:HD12	5:E:249:ALA:CB	2.44	0.47
2:B:89:TYR:HD1	8:B:547:HOH:O	1.96	0.47
1:A:234:LEU:HD11	1:A:249:ALA:HB1	1.96	0.47
4:D:85:ILE:HD12	4:D:85:ILE:N	2.29	0.47
1:A:169:LEU:HG	8:A:588:HOH:O	2.14	0.47
5:E:31:MSE:SE	5:E:58:ARG:NH2	2.98	0.47
1:A:203[B]:LEU:HB3	1:A:222:LEU:HD22	1.97	0.47
4:F:236:ILE:HG13	4:F:248:VAL:HG13	1.96	0.47
1:G:6:HIS:CB	1:G:9:LYS:HE2	2.45	0.47
4:D:132:ILE:HD12	4:D:163:ILE:HD13	1.96	0.47
2:B:113:ARG:HD2	2:B:113:ARG:H	1.80	0.47
5:E:46:ILE:HD12	5:E:57:VAL:HG21	1.96	0.47
3:C:31:MSE:SE	3:C:58:ARG:CZ	3.13	0.47
4:D:159:ALA:O	4:D:163:ILE:HG12	2.14	0.47
5:E:142[B]:HIS:HE1	8:E:600:HOH:O	1.95	0.47
3:C:101:ASP:O	3:C:129:PRO:HD2	2.15	0.47
1:A:97[B]:GLU:OE1	1:A:97[B]:GLU:HA	2.14	0.47
4:H:26:LEU:N	4:H:26:LEU:HD12	2.30	0.47
4:F:156:VAL:HG21	4:F:192:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:190:TYR:HD1	4:F:201:LEU:HD23	1.80	0.47
4:F:110:ILE:O	4:F:115:LYS:HE2	2.14	0.46
4:D:101:ASP:O	4:D:128:ILE:HG23	2.14	0.46
4:H:71:ALA:O	4:H:75:LYS:HG3	2.15	0.46
1:A:142:HIS:HA	1:A:145[A]:GLU:HG2	1.97	0.46
1:G:228:LYS:HG3	1:G:228:LYS:O	2.15	0.46
1:A:143:ILE:HD12	1:A:143:ILE:N	2.31	0.46
5:E:26:LEU:CD1	5:E:258:LEU:HD13	2.45	0.46
1:A:164:LYS:HE2	1:A:168:ASP:OD1	2.15	0.46
3:C:139:LEU:O	4:D:78:ASN:OD1	2.34	0.46
3:C:28:ILE:HD11	3:C:253:LEU:HD12	1.96	0.46
1:G:7:ARG:HG3	1:G:229:GLY:O	2.16	0.46
4:D:74:LYS:HA	4:D:77:ILE:HG12	1.98	0.46
4:D:104:ARG:HD3	4:D:104:ARG:O	2.16	0.46
2:B:132:ILE:HG21	2:B:162:HIS:HB2	1.97	0.46
4:D:58:ARG:HE	4:D:84:ASP:HB3	1.81	0.46
1:A:29:GLN:HG2	1:A:56:VAL:HB	1.98	0.45
2:B:217:KCX:CX	8:B:581:HOH:O	2.64	0.45
4:H:254:LYS:O	4:H:257:GLY:CA	2.64	0.45
1:G:149:TYR:HB2	1:G:150:PRO:CD	2.47	0.45
4:D:58:ARG:NE	4:D:84:ASP:HB3	2.31	0.45
1:G:20:ILE:CD1	1:G:27:ILE:HG13	2.46	0.45
4:D:202:HIS:HA	4:D:233:THR:CG2	2.46	0.45
4:D:85:ILE:HB	4:D:105:ILE:CG2	2.47	0.45
5:E:174:ILE:O	5:E:200:PRO:HD2	2.17	0.45
4:F:132:ILE:HD11	4:F:166:LEU:HD12	1.97	0.45
1:G:112:ARG:NE	6:G:402:SO4:O2	2.50	0.45
4:D:156:VAL:HG21	4:D:192:LYS:HB3	1.97	0.45
4:D:131:ARG:HA	4:D:175:ILE:O	2.17	0.45
4:H:237:SER:C	4:H:238:LEU:HD12	2.37	0.45
3:C:42:THR:O	3:C:46:ILE:HG12	2.17	0.45
1:A:132:ILE:CD1	1:A:163:ILE:HD13	2.47	0.45
1:A:128:ILE:HG23	1:A:129:PRO:HD2	1.98	0.45
1:A:203[A]:LEU:H	1:A:203[A]:LEU:HD12	1.82	0.45
5:E:102:KCX:OQ2	5:E:131:ARG:NE	2.47	0.45
4:F:113:ARG:HB3	6:F:402:SO4:O4	2.17	0.45
4:F:167:GLU:HG2	4:F:172:HIS:CE1	2.52	0.45
4:F:230:ILE:HG22	4:F:231:GLY:N	2.33	0.44
4:F:106:ASN:HA	4:F:107:PRO:HD3	1.88	0.44
4:F:222:LEU:CD1	4:F:236:ILE:HD12	2.47	0.44
3:C:28:ILE:HD12	3:C:249:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:74:LYS:NZ	4:D:99:GLY:O	2.38	0.44
4:H:89:TYR:HB3	4:H:110:ILE:HD11	2.00	0.44
3:C:202:HIS:HA	3:C:233:THR:HG23	1.99	0.44
4:H:254:LYS:O	4:H:257:GLY:HA3	2.17	0.44
4:D:190:TYR:HB2	4:D:225:ILE:HD12	2.00	0.44
4:F:111:GLY:HA3	4:F:115:LYS:HE2	2.00	0.44
5:E:144:LEU:C	8:E:647:HOH:O	2.56	0.44
5:E:106:ASN:HB3	5:E:162:HIS:CE1	2.53	0.44
2:B:224:ALA:O	2:B:228:LYS:HG2	2.17	0.44
4:D:179:LYS:HE3	4:D:206:THR:HG22	1.98	0.44
4:H:58:ARG:HH21	4:H:82:VAL:HG11	1.81	0.44
3:C:107:PRO:HD2	3:C:132:ILE:HD12	1.99	0.44
1:A:105:ILE:HD11	1:A:110:ILE:CD1	2.48	0.44
4:F:131[B]:ARG:HD3	4:F:177:SER:OG	2.17	0.43
3:C:142:HIS:O	3:C:145:GLU:N	2.51	0.43
1:A:203[B]:LEU:HD22	1:A:225:ILE:HG21	2.00	0.43
1:A:88[A]:ASP:OD1	1:A:88[A]:ASP:C	2.56	0.43
1:G:236:ILE:HG22	1:G:238:LEU:HG	2.00	0.43
3:C:7:ARG:HB2	3:C:232:ASN:ND2	2.34	0.43
1:A:251:GLU:OE2	4:D:213:ALA:HB1	2.18	0.43
4:F:250:ARG:CG	4:F:250:ARG:NH1	2.81	0.43
4:F:122:ALA:HA	4:F:126:ARG:HH21	1.83	0.43
1:G:26:LEU:HD22	1:G:226:LEU:HD21	2.01	0.43
2:B:175:ILE:HD12	2:B:200:PRO:HB2	2.00	0.43
4:D:134:VAL:HG21	4:D:159:ALA:HB2	2.01	0.43
1:A:8:THR:C	1:A:9:LYS:HD2	2.39	0.43
1:G:207:GLU:HB3	1:G:237:SER:OG	2.18	0.43
3:C:55:GLN:O	3:C:79:ILE:HB	2.18	0.43
5:E:126:ARG:HB3	5:E:126:ARG:CZ	2.48	0.43
2:B:207:GLU:HA	8:B:533:HOH:O	2.18	0.43
4:H:77:ILE:HD11	4:H:81:LEU:HG	1.99	0.42
3:C:26:LEU:HD12	3:C:258:LEU:HD13	2.01	0.42
4:H:195:ARG:NE	8:H:637:HOH:O	2.51	0.42
4:F:61:VAL:HG12	4:F:61:VAL:O	2.18	0.42
1:A:89[A]:TYR:HD2	1:A:90[A]:ARG:HG3	1.85	0.42
4:D:77:ILE:HD13	4:D:81:LEU:HD21	2.02	0.42
1:A:228[A]:LYS:CE	1:A:228[A]:LYS:HA	2.45	0.42
5:E:31:MSE:SE	5:E:58:ARG:CZ	3.17	0.42
2:B:105:ILE:HD13	2:B:119:VAL:HG11	2.00	0.42
4:F:234:LEU:CD1	4:F:234:LEU:C	2.88	0.42
5:E:143:ILE:CD1	5:E:158:SER:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:32:THR:HB	4:H:45:GLU:OE1	2.19	0.42
4:D:74:LYS:HE2	4:D:81:LEU:HD12	2.01	0.42
4:D:29:GLN:HG2	4:D:56:VAL:HB	2.02	0.42
4:F:212:PHE:CE2	1:G:251:GLU:HG3	2.55	0.42
4:D:84:ASP:HB3	4:D:104:ARG:HD2	2.01	0.42
1:A:260:SER:O	1:A:261:ASN:CB	2.67	0.42
4:H:107:PRO:HD2	4:H:132:ILE:HD12	2.02	0.42
4:H:163:ILE:HG22	4:H:167:GLU:OE2	2.20	0.42
1:A:4:MSE:SE	1:A:191:GLU:HB2	2.69	0.42
4:F:66:ALA:HB2	8:F:575[B]:HOH:O	2.20	0.42
4:F:180:ALA:CB	4:F:185:LEU:HD22	2.50	0.42
5:E:235:ARG:HG2	5:E:236:ILE:N	2.34	0.42
1:G:201:LEU:HD12	1:G:230:ILE:CG2	2.50	0.42
1:A:47:LYS:HD2	8:A:623:HOH:O	2.20	0.42
1:A:57:VAL:HG13	1:A:81:LEU:HD12	2.02	0.41
1:A:102:KCX:HA	1:A:128:ILE:CG2	2.50	0.41
1:A:55:GLN:O	1:A:80:PRO:HD2	2.20	0.41
3:C:107:PRO:HD3	3:C:132:ILE:CD1	2.50	0.41
3:C:107:PRO:HD2	3:C:162:HIS:HB3	2.02	0.41
4:D:15:VAL:HG12	4:D:20:ILE:HG12	2.02	0.41
4:H:28:ILE:N	4:H:28:ILE:HD12	2.35	0.41
5:E:236:ILE:HG12	5:E:249:ALA:HB2	2.01	0.41
5:E:179:LYS:HD2	6:E:401:SO4:S	2.61	0.41
4:D:54:CYS:HB2	4:D:246:VAL:HG21	2.03	0.41
4:F:96:ILE:HA	4:F:100:ILE:HG22	2.03	0.41
4:H:149:TYR:HB2	4:H:150:PRO:CD	2.51	0.41
3:C:179:LYS:HE2	3:C:206:THR:HA	2.01	0.41
4:H:8:THR:HG22	4:H:24:ASN:HB2	2.02	0.41
1:A:235:ARG:HG2	1:A:236:ILE:N	2.35	0.41
5:E:142[B]:HIS:CE1	8:E:600:HOH:O	2.71	0.41
5:E:141:ARG:O	5:E:145:GLU:HG2	2.20	0.41
4:H:82:VAL:HG22	4:H:102:LYS:HB3	2.03	0.41
1:A:234:LEU:CD1	1:A:234:LEU:C	2.88	0.41
1:A:234:LEU:HD12	1:A:234:LEU:O	2.19	0.41
3:C:26:LEU:HD11	3:C:226:LEU:HD22	2.02	0.41
3:C:46:ILE:CD1	3:C:57:VAL:HG21	2.51	0.41
3:C:102:KCX:HA	3:C:128:ILE:HG13	2.02	0.41
1:A:234:LEU:HD11	1:A:249:ALA:CB	2.50	0.41
1:A:89[B]:TYR:CE1	1:A:90[B]:ARG:HG3	2.55	0.41
2:B:103:VAL:CG1	2:B:105:ILE:HG23	2.51	0.41
4:D:24:ASN:O	4:D:258:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:187[B]:ILE:O	4:D:191:GLU:HG3	2.21	0.41
5:E:2:ASN:N	8:E:603:HOH:O	2.53	0.41
4:D:250:ARG:O	4:D:254:LYS:HB3	2.21	0.40
1:A:203[A]:LEU:HD11	1:A:231:GLY:CA	2.48	0.40
4:F:236:ILE:CG1	4:F:248:VAL:HG13	2.51	0.40
4:H:179:LYS:NZ	4:H:204:GLY:HA3	2.35	0.40
1:A:80:PRO:HA	1:A:101:ASP:OD2	2.21	0.40
4:D:136:ALA:HB2	4:D:155:MSE:CE	2.52	0.40
4:D:83:ALA:HB2	4:D:100:ILE:HG12	2.02	0.40
4:F:179:LYS:HE2	4:F:206:THR:HA	2.03	0.40
2:B:15:VAL:CG2	2:B:20:ILE:HD12	2.46	0.40
5:E:167:GLU:HG2	5:E:172:HIS:CE1	2.56	0.40
1:A:89[B]:TYR:HB2	1:A:119:VAL:HG21	2.04	0.40
2:B:166:LEU:HB3	2:B:171:PHE:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	268/276 (97%)	260 (97%)	7 (3%)	1 (0%)	39 22
1	G	255/276 (92%)	246 (96%)	9 (4%)	0	100 100
2	B	258/276 (94%)	245 (95%)	11 (4%)	2 (1%)	24 9
3	C	252/276 (91%)	242 (96%)	10 (4%)	0	100 100
4	D	251/276 (91%)	241 (96%)	10 (4%)	0	100 100
4	F	265/276 (96%)	260 (98%)	4 (2%)	1 (0%)	39 22
4	H	254/276 (92%)	247 (97%)	7 (3%)	0	100 100
5	E	258/276 (94%)	251 (97%)	7 (3%)	0	100 100
All	All	2061/2208 (93%)	1992 (97%)	65 (3%)	4 (0%)	52 36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	110	ILE
1	A	87	PHE
2	B	112	ARG
4	F	242	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	219/215 (102%)	215 (98%)	4 (2%)	66	52
1	G	206/215 (96%)	201 (98%)	5 (2%)	57	39
2	B	209/215 (97%)	206 (99%)	3 (1%)	74	63
3	C	205/214 (96%)	201 (98%)	4 (2%)	63	47
4	D	206/216 (95%)	205 (100%)	1 (0%)	92	90
4	F	214/216 (99%)	211 (99%)	3 (1%)	74	63
4	H	206/216 (95%)	205 (100%)	1 (0%)	92	90
5	E	209/214 (98%)	204 (98%)	5 (2%)	57	39
All	All	1674/1721 (97%)	1648 (98%)	26 (2%)	72	57

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	31[A]	MSE
1	A	31[B]	MSE
1	A	234	LEU
2	B	31	MSE
2	B	113	ARG
2	B	234	LEU
3	C	10	THR
3	C	128	ILE
3	C	191	GLU

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Mol	Chain	Res	Type
3	C	235	ARG
4	D	104	ARG
5	E	94[A]	LYS
5	E	94[B]	LYS
5	E	104	ARG
5	E	112	ARG
5	E	183	VAL
4	F	2	ASN
4	F	234	LEU
4	F	250	ARG
1	G	112	ARG
1	G	144	LEU
1	G	174	ILE
1	G	211	LEU
1	G	234	LEU
4	H	78	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	162	HIS
5	E	2	ASN
4	F	37	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	KCX	A	102	1	7,11,12	0.49	0	7,12,14	0.96	1 (14%)
2	KCX	B	217	2	7,11,12	0.44	0	7,12,14	0.95	0
3	KCX	C	102	3	7,11,12	0.55	0	7,12,14	0.83	1 (14%)
3	KCX	C	247	3	7,11,12	0.67	0	7,12,14	1.05	1 (14%)
5	KCX	E	102	5	7,11,12	0.88	0	7,12,14	0.96	1 (14%)
5	KCX	E	35	5	7,11,12	1.04	1 (14%)	7,12,14	1.21	0
1	KCX	G	102	1	7,11,12	0.60	0	7,12,14	1.30	2 (28%)

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
1	KCX	A	102	1	-	0/6/10/12	0/0/0/0
2	KCX	B	217	2	-	0/6/10/12	0/0/0/0
3	KCX	C	102	3	-	0/6/10/12	0/0/0/0
3	KCX	C	247	3	-	0/6/10/12	0/0/0/0
5	KCX	E	102	5	-	0/6/10/12	0/0/0/0
5	KCX	E	35	5	-	0/6/10/12	0/0/0/0
1	KCX	G	102	1	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	35	KCX	CB-CA	-2.29	1.51	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	247	KCX	O-C-CA	-2.34	119.39	125.49
5	E	102	KCX	O-C-CA	-2.18	119.82	125.49
1	A	102	KCX	O-C-CA	-2.13	119.94	125.49
3	C	102	KCX	O-C-CA	-2.12	119.96	125.49
1	G	102	KCX	O-C-CA	-2.07	120.11	125.49
1	G	102	KCX	CE-NZ-CX	2.62	126.46	123.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	102	KCX	1	0
2	B	217	KCX	1	0
3	C	102	KCX	2	0
5	E	102	KCX	1	0
1	G	102	KCX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
6	SO4	A	401	-	4,4,4	0.28	0	6,6,6	0.21	0
6	SO4	B	401	-	4,4,4	0.39	0	6,6,6	0.27	0
6	SO4	C	401	-	4,4,4	0.32	0	6,6,6	0.20	0
6	SO4	C	402	-	4,4,4	0.52	0	6,6,6	0.12	0
6	SO4	D	401	-	4,4,4	0.30	0	6,6,6	0.16	0
6	SO4	D	402	-	4,4,4	0.29	0	6,6,6	0.08	0
6	SO4	E	401	-	4,4,4	0.38	0	6,6,6	0.44	0
6	SO4	E	402	-	4,4,4	0.30	0	6,6,6	0.22	0
6	SO4	F	401	-	4,4,4	0.28	0	6,6,6	0.29	0
6	SO4	F	402	-	4,4,4	0.39	0	6,6,6	0.15	0
6	SO4	G	401	-	4,4,4	0.39	0	6,6,6	0.43	0
6	SO4	G	402	-	4,4,4	0.45	0	6,6,6	0.07	0
6	SO4	H	401	-	4,4,4	0.42	0	6,6,6	0.19	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
6	SO4	A	401	-	-	0/0/0/0	0/0/0/0
6	SO4	B	401	-	-	0/0/0/0	0/0/0/0
6	SO4	C	401	-	-	0/0/0/0	0/0/0/0
6	SO4	C	402	-	-	0/0/0/0	0/0/0/0
6	SO4	D	401	-	-	0/0/0/0	0/0/0/0
6	SO4	D	402	-	-	0/0/0/0	0/0/0/0
6	SO4	E	401	-	-	0/0/0/0	0/0/0/0
6	SO4	E	402	-	-	0/0/0/0	0/0/0/0
6	SO4	F	401	-	-	0/0/0/0	0/0/0/0
6	SO4	F	402	-	-	0/0/0/0	0/0/0/0
6	SO4	G	401	-	-	0/0/0/0	0/0/0/0
6	SO4	G	402	-	-	0/0/0/0	0/0/0/0
6	SO4	H	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	SO4	1	0
6	B	401	SO4	1	0
6	E	401	SO4	2	0
6	F	402	SO4	1	0
6	G	402	SO4	2	0
6	H	401	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, 95^{th} 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	255/276 (92%)	-0.39	1 (0%) 93 92	12, 21, 33, 42	0
1	G	253/276 (91%)	-0.49	1 (0%) 93 92	11, 17, 26, 32	0
2	B	254/276 (92%)	-0.33	0 100 100	15, 24, 40, 49	0
3	C	251/276 (90%)	-0.36	1 (0%) 93 92	14, 22, 32, 54	0
4	D	247/276 (89%)	-0.24	2 (0%) 87 87	13, 24, 41, 51	0
4	F	258/276 (93%)	-0.41	0 100 100	12, 19, 29, 43	0
4	H	251/276 (90%)	-0.44	0 100 100	13, 19, 29, 37	0
5	E	254/276 (92%)	-0.49	0 100 100	10, 17, 24, 30	0
All	All	2023/2208 (91%)	-0.40	5 (0%) 95 94	10, 20, 33, 54	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	87	PHE	3.2
1	A	149	TYR	2.7
4	D	119	VAL	2.4
3	C	141	ARG	2.3
1	G	144	LEU	2.2

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

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, 95^{th} 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
1	KCX	A	102	12/13	0.95	0.08	-	15,16,18,18	0
5	KCX	E	35	12/13	0.95	0.08	-	15,17,27,28	0
5	KCX	E	102	12/13	0.96	0.07	-	10,11,13,14	0
1	KCX	G	102	12/13	0.94	0.13	-	16,20,28,32	0
3	KCX	C	247	12/13	0.95	0.09	-	16,23,32,35	0
3	KCX	C	102	12/13	0.95	0.08	-	17,18,19,20	0
2	KCX	B	217	12/13	0.93	0.09	-	18,24,36,37	0

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, 95^{th} 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
6	SO4	G	402	5/5	0.94	0.14	1.73	34,43,45,46	0
6	SO4	E	402	5/5	0.96	0.11	0.46	38,42,43,45	0
6	SO4	D	401	5/5	0.97	0.08	0.10	32,34,37,38	0
6	SO4	F	401	5/5	0.97	0.10	-0.02	33,36,41,42	0
6	SO4	H	401	5/5	0.98	0.07	-0.74	25,30,31,36	0
6	SO4	B	401	5/5	0.97	0.07	-0.96	29,31,35,35	0
6	SO4	G	401	5/5	0.99	0.07	-0.97	16,19,20,21	0
6	SO4	C	402	5/5	0.97	0.06	-1.19	29,31,35,38	0
6	SO4	A	401	5/5	0.99	0.07	-1.26	18,21,23,23	0
6	SO4	E	401	5/5	0.99	0.06	-3.26	18,19,21,21	0
6	SO4	C	401	5/5	0.99	0.06	-5.70	25,26,27,27	0
7	CL	F	404[A]	1/1	0.97	0.14	-	31,31,31,31	1
7	CL	F	404[B]	1/1	0.97	0.14	-	23,23,23,23	1
6	SO4	F	402	5/5	0.97	0.07	-	37,37,39,39	0
7	CL	B	402[B]	1/1	0.95	0.09	-	21,21,21,21	1
7	CL	B	402[A]	1/1	0.95	0.09	-	32,32,32,32	1
7	CL	B	403	1/1	0.99	0.15	-	42,42,42,42	1
6	SO4	D	402	5/5	0.98	0.07	-	39,39,39,40	5
7	CL	A	402	1/1	0.95	0.14	-	53,53,53,53	0
7	CL	F	403	1/1	0.99	0.10	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	CL	C	405	1/1	0.89	0.08	-	50,50,50,50	0
7	CL	C	404	1/1	0.96	0.09	-	44,44,44,44	0
7	CL	C	403	1/1	0.98	0.12	-	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.