Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 09:50 PM EDT

PDB ID	:	4MLG
Title	:	Structure of RS223-Beta-xylosidase
Authors	:	Jordan, D.; Braker, J.; Wagschal, K.; Lee, C.; Dubrovska, I.; Anderson, S.; Wawrzak, Z.
Deposited on	:	2013-09-06
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
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:

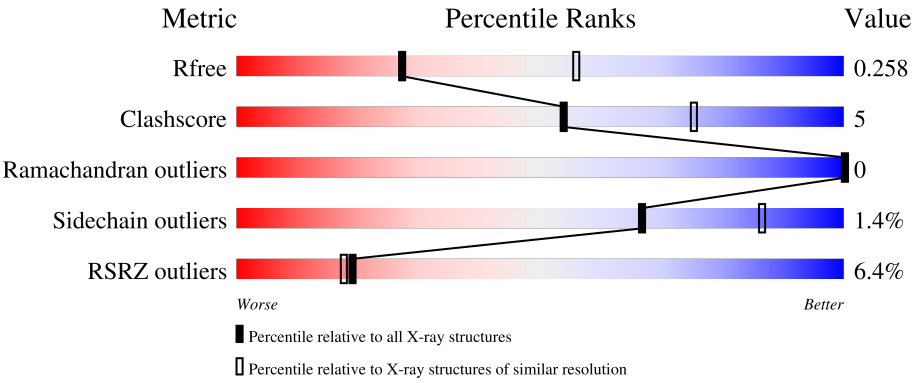
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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 <=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	324	3% 87% 13%
1	B	324	4% 86% 13%
1	C	324	8% 87% 12%
1	D	324	2% 84% 16%
1	E	324	6% 85% 15%

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Mol	Chain	Length	Quality of chain
1	F	324	9% 83% 17%
1	G	324	5% 85% 15%
1	H	324	8% 83% 17%
1	I	324	9% 86% 13%
1	J	324	4% 87% 13%
1	K	324	6% 83% 16%
1	L	324	14% 85% 14%

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	402	-	-	-	X
3	SO4	F	402	-	-	-	X
3	SO4	G	402	-	-	-	X
3	SO4	G	403	-	-	-	X
3	SO4	I	403	-	-	-	X
3	SO4	J	403	-	-	-	X
3	SO4	K	402	-	-	-	X
3	SO4	K	403	-	-	-	X
3	SO4	L	403	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32402 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 Beta-xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2640	1699	438	488	15			
1	B	323	Total	C	N	O	S	0	0	0
			2640	1699	438	488	15			
1	C	323	Total	C	N	O	S	0	0	0
			2636	1696	437	488	15			
1	D	322	Total	C	N	O	S	0	0	0
			2635	1696	437	487	15			
1	E	323	Total	C	N	O	S	0	0	0
			2640	1699	438	488	15			
1	F	323	Total	C	N	O	S	0	0	0
			2636	1696	437	488	15			
1	G	324	Total	C	N	O	S	0	0	0
			2641	1699	438	489	15			
1	H	324	Total	C	N	O	S	0	0	0
			2645	1701	438	491	15			
1	I	321	Total	C	N	O	S	0	0	0
			2615	1684	434	483	14			
1	J	323	Total	C	N	O	S	0	0	0
			2636	1696	437	488	15			
1	K	324	Total	C	N	O	S	0	0	0
			2645	1701	438	491	15			
1	L	322	Total	C	N	O	S	0	0	0
			2631	1694	436	486	15			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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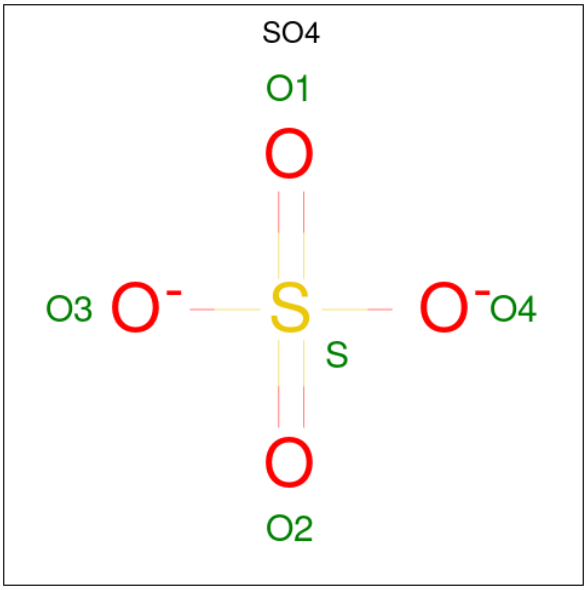
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	K	1	Total Ca 1 1	0	0
2	L	1	Total Ca 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
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	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0

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

- Molecule 4 is water.

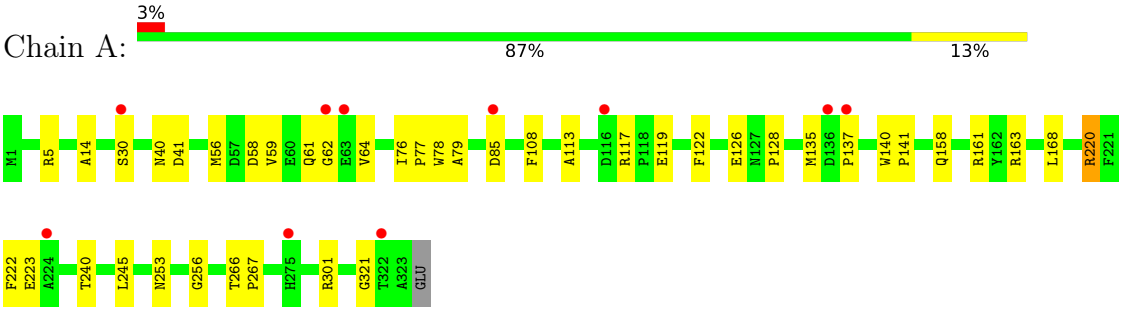
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	72	Total O 72 72	0	0
4	B	64	Total O 64 64	0	0
4	C	45	Total O 45 45	0	0
4	D	68	Total O 68 68	0	0
4	E	50	Total O 50 50	0	0
4	F	58	Total O 58 58	0	0
4	G	47	Total O 47 47	0	0
4	H	50	Total O 50 50	0	0
4	I	49	Total O 49 49	0	0
4	J	50	Total O 50 50	0	0
4	K	44	Total O 44 44	0	0
4	L	33	Total O 33 33	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.

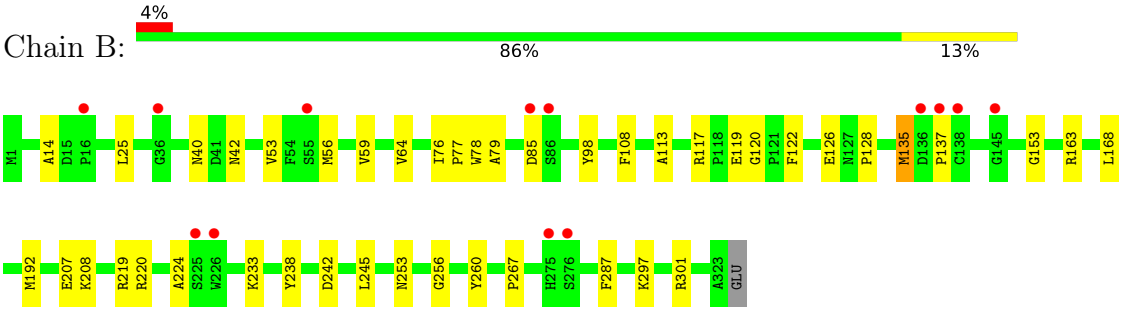
• Molecule 1: Beta-xylosidase

Chain A:



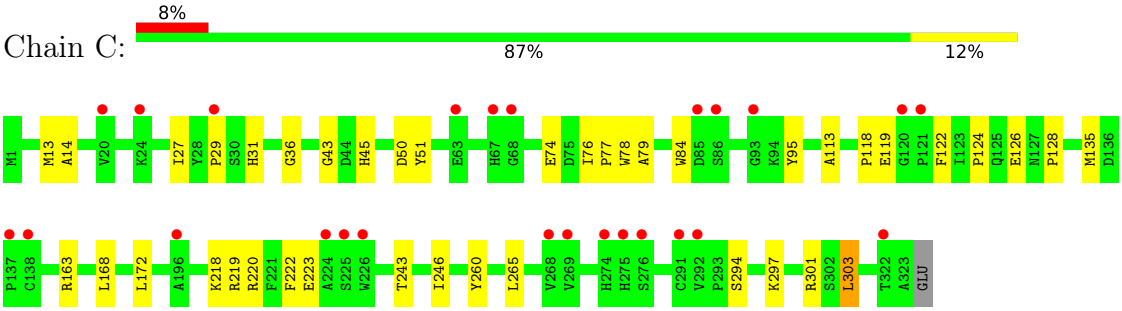
• Molecule 1: Beta-xylosidase

Chain B:



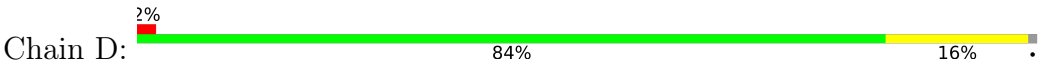
• Molecule 1: Beta-xylosidase

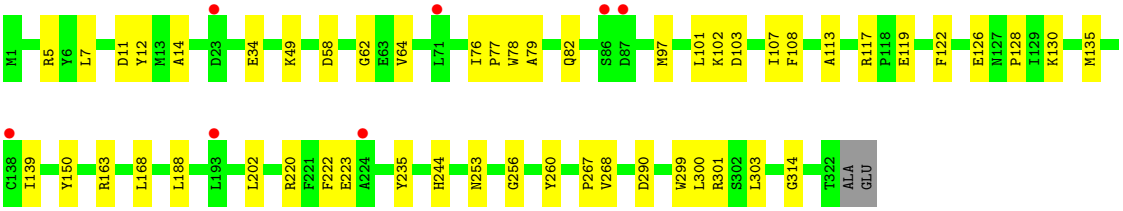
Chain C:



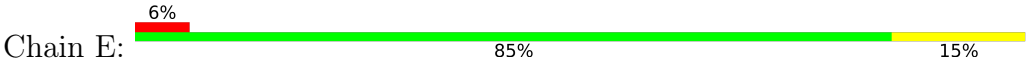
• Molecule 1: Beta-xylosidase

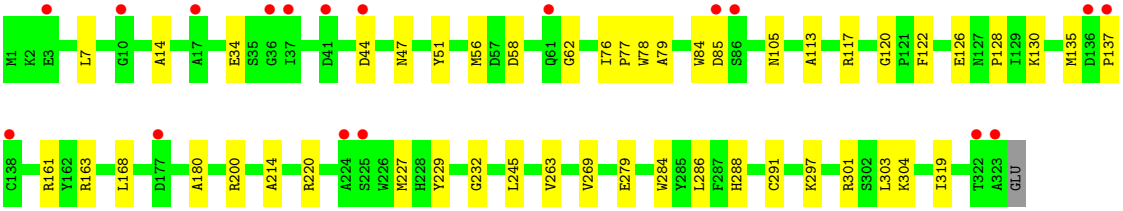
Chain D:



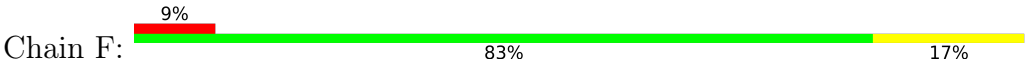


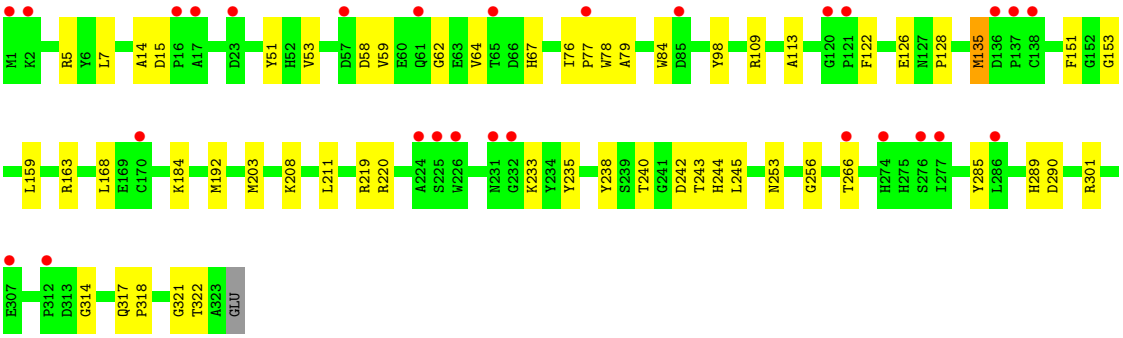
• Molecule 1: Beta-xylosidase



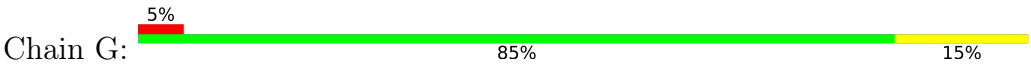


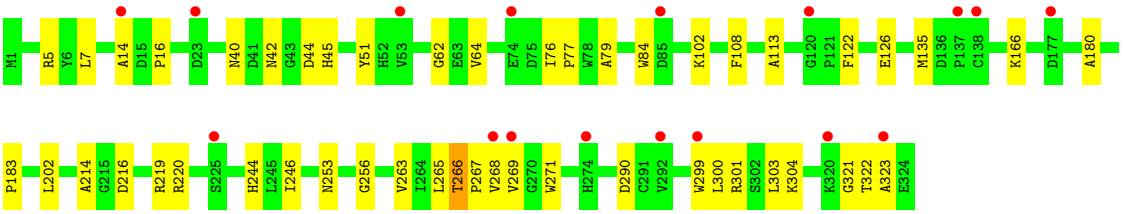
• Molecule 1: Beta-xylosidase



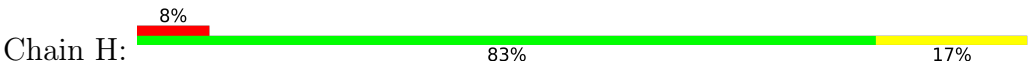


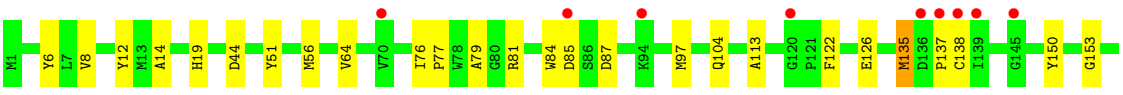
• Molecule 1: Beta-xylosidase

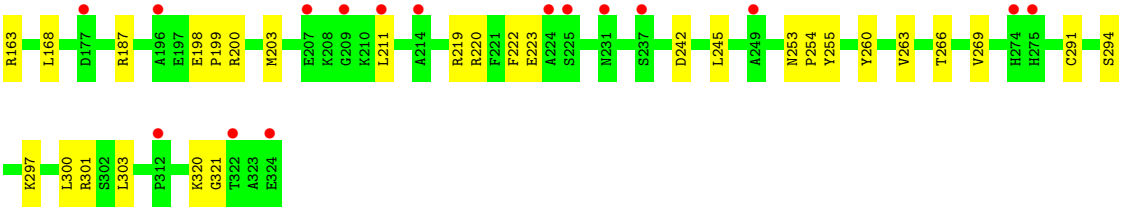




• Molecule 1: Beta-xylosidase

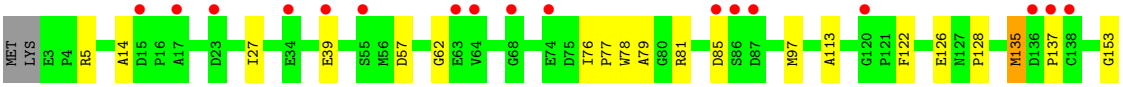


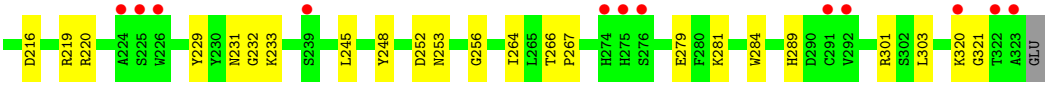




• Molecule 1: Beta-xylosidase

Chain I:



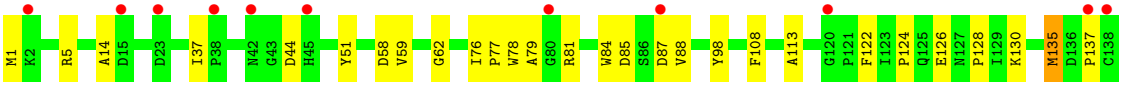


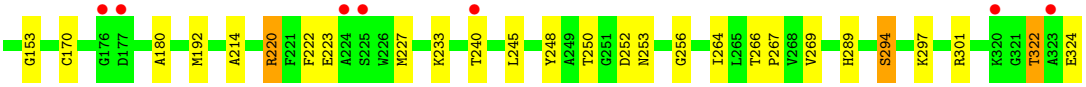
• Molecule 1: Beta-xylosidase

Chain J:

• Molecule 1: Beta-xylosidase

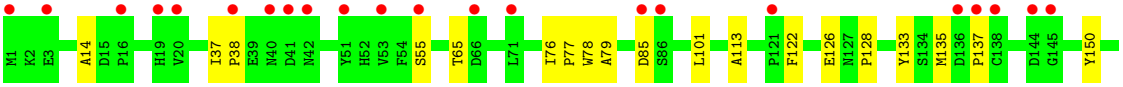
Chain K:

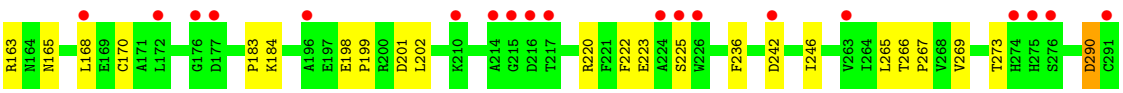


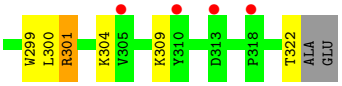


• Molecule 1: Beta-xylosidase

Chain L:






W299
L300
R301
K304
V305
K309
Y310
D313
P318
T322
ALA
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	124.53Å 148.70Å 125.65Å 90.00° 112.87° 90.00°	Depositor
Resolution (Å)	29.20 – 2.70 29.17 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.20-2.70) 91.8 (29.17-2.69)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.210 , 0.257 0.211 , 0.258	Depositor DCC
R_{free} test set	5761 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32402	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, 0.333 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: SO4, CA

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	0.22	0/2729	0.39	0/3706
1	B	0.22	0/2729	0.38	0/3706
1	C	0.21	0/2725	0.38	0/3702
1	D	0.22	0/2724	0.38	0/3699
1	E	0.22	0/2729	0.38	0/3706
1	F	0.23	0/2725	0.38	0/3702
1	G	0.21	0/2730	0.37	0/3709
1	H	0.22	0/2734	0.39	0/3714
1	I	0.21	0/2704	0.37	0/3675
1	J	0.22	0/2725	0.38	0/3702
1	K	0.22	0/2734	0.38	0/3714
1	L	0.21	0/2720	0.37	0/3694
All	All	0.22	0/32708	0.38	0/44429

There are no bond length outliers.

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	2640	0	2490	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2640	0	2490	21	0
1	C	2636	0	2479	25	0
1	D	2635	0	2485	26	0
1	E	2640	0	2490	28	0
1	F	2636	0	2479	41	0
1	G	2641	0	2481	34	0
1	H	2645	0	2485	30	0
1	I	2615	0	2455	26	0
1	J	2636	0	2479	27	0
1	K	2645	0	2485	30	0
1	L	2631	0	2479	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
3	G	10	0	0	0	0
3	H	10	0	0	0	0
3	I	10	0	0	0	0
3	J	10	0	0	0	0
3	K	10	0	0	0	0
3	L	10	0	0	0	0
4	A	72	0	0	0	0
4	B	64	0	0	0	0
4	C	45	0	0	0	0
4	D	68	0	0	0	0
4	E	50	0	0	2	0
4	F	58	0	0	0	0
4	G	47	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	50	0	0	2	0
4	I	49	0	0	1	0
4	J	50	0	0	1	0
4	K	44	0	0	1	0
4	L	33	0	0	0	0
All	All	32402	0	29777	328	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 5.

All (328) 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:G:265:LEU:HD12	1:G:266:THR:H	1.21	1.05
1:F:240:THR:CG2	1:F:243:THR:HB	2.13	0.79
1:G:265:LEU:HD12	1:G:266:THR:N	1.98	0.78
1:F:240:THR:HG22	1:F:243:THR:HB	1.69	0.74
1:L:266:THR:HG23	1:L:267:PRO:HD2	1.70	0.72
1:H:104:GLN:HG3	4:H:507:HOH:O	1.90	0.71
1:J:118:PRO:HG2	1:J:119:GLU:OE1	1.89	0.71
1:F:243:THR:HG22	1:F:245:LEU:HG	1.75	0.67
1:A:220:ARG:NH2	1:A:240:THR:O	2.28	0.67
1:G:290:ASP:HB2	1:G:304:LYS:HD2	1.75	0.66
1:G:76:ILE:HB	1:G:79:ALA:HB2	1.76	0.66
1:E:77:PRO:HG2	1:E:126:GLU:HA	1.78	0.66
1:C:76:ILE:HB	1:C:79:ALA:HB2	1.78	0.66
1:K:76:ILE:HB	1:K:79:ALA:HB2	1.78	0.66
1:J:76:ILE:HB	1:J:79:ALA:HB2	1.78	0.65
1:H:203:MET:HB2	1:H:211:LEU:HD21	1.79	0.64
1:E:269:VAL:HG23	1:E:291:CYS:H	1.62	0.64
1:I:77:PRO:HG2	1:I:126:GLU:HA	1.80	0.64
1:E:44:ASP:O	1:E:47:ASN:ND2	2.32	0.62
1:H:76:ILE:HB	1:H:79:ALA:HB2	1.80	0.62
1:F:76:ILE:HB	1:F:79:ALA:HB2	1.81	0.62
1:B:253:ASN:HD21	1:B:256:GLY:HA3	1.65	0.62
1:E:117:ARG:HG3	1:E:120:GLY:H	1.66	0.61
1:I:57:ASP:O	1:I:281:LYS:NZ	2.33	0.61
1:G:246:ILE:HB	1:G:265:LEU:HB3	1.82	0.61
1:L:266:THR:CG2	1:L:267:PRO:HD2	2.30	0.61
1:E:14:ALA:HB2	1:E:301:ARG:HB2	1.83	0.61
1:H:320:LYS:NZ	4:H:535:HOH:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:76:ILE:HB	1:L:79:ALA:HB2	1.83	0.61
1:L:77:PRO:HG2	1:L:126:GLU:HA	1.81	0.61
1:K:14:ALA:HB2	1:K:301:ARG:HB2	1.83	0.60
1:K:294:SER:HB3	1:K:297:LYS:HB2	1.84	0.60
1:I:113:ALA:HB1	1:I:122:PHE:HB3	1.82	0.60
1:K:269:VAL:HG23	1:K:322:THR:HB	1.85	0.59
1:B:14:ALA:HB2	1:B:301:ARG:HB2	1.85	0.59
1:F:240:THR:HG22	1:F:240:THR:O	2.03	0.59
1:A:76:ILE:HB	1:A:79:ALA:HB2	1.84	0.59
1:J:52:HIS:NE2	4:J:510:HOH:O	2.32	0.59
1:F:113:ALA:HB1	1:F:122:PHE:HB3	1.85	0.59
1:C:95:TYR:CZ	1:C:118:PRO:HG3	2.38	0.58
1:A:14:ALA:HB2	1:A:301:ARG:HB2	1.85	0.58
1:C:51:TYR:OH	1:C:84:TRP:O	2.20	0.58
1:J:117:ARG:HB3	1:J:119:GLU:OE2	2.03	0.58
1:E:7:LEU:HD13	1:E:56:MET:CE	2.34	0.58
1:C:77:PRO:HG2	1:C:126:GLU:HA	1.86	0.58
1:F:14:ALA:HB2	1:F:301:ARG:HB2	1.86	0.58
1:J:77:PRO:HG2	1:J:126:GLU:HA	1.86	0.58
1:H:297:LYS:HD2	1:H:300:LEU:HD12	1.86	0.58
1:D:7:LEU:HB3	1:D:64:VAL:HG21	1.86	0.57
1:B:77:PRO:HG2	1:B:126:GLU:HA	1.86	0.57
1:C:113:ALA:HB1	1:C:122:PHE:HB3	1.87	0.57
1:F:243:THR:HG21	1:F:245:LEU:HD12	1.86	0.56
1:D:103:ASP:OD1	1:D:107:ILE:N	2.33	0.56
1:G:113:ALA:HB1	1:G:122:PHE:HB3	1.87	0.56
1:L:113:ALA:HB1	1:L:122:PHE:HB3	1.87	0.56
1:E:7:LEU:HD12	1:E:303:LEU:CD1	2.35	0.56
1:L:37:ILE:HD12	1:L:38:PRO:HD2	1.88	0.56
1:F:5:ARG:NH1	1:F:59:VAL:O	2.38	0.56
1:F:266:THR:OG1	1:F:321:GLY:N	2.37	0.56
1:J:14:ALA:HB2	1:J:301:ARG:HB2	1.88	0.55
1:B:207:GLU:HG2	1:B:208:LYS:HD2	1.88	0.55
1:C:14:ALA:HB2	1:C:301:ARG:HB2	1.88	0.55
1:K:220:ARG:NH2	1:K:240:THR:O	2.38	0.55
1:L:290:ASP:HB2	1:L:304:LYS:HD2	1.88	0.55
1:L:133:TYR:OH	1:L:165:ASN:ND2	2.39	0.55
1:F:243:THR:CG2	1:F:245:LEU:HG	2.36	0.55
1:I:81:ARG:NH1	4:I:508:HOH:O	2.39	0.55
1:L:14:ALA:HB2	1:L:301:ARG:HB2	1.89	0.54
1:D:253:ASN:ND2	1:D:256:GLY:H	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:248:TYR:HB3	1:I:264:ILE:HD11	1.89	0.53
1:D:76:ILE:HB	1:D:79:ALA:HB2	1.90	0.53
1:E:163:ARG:HG2	1:E:168:LEU:HD11	1.89	0.53
1:D:5:ARG:NH2	1:D:62:GLY:O	2.36	0.53
1:G:102:LYS:NZ	4:G:513:HOH:O	2.41	0.53
1:F:203:MET:HB3	1:F:211:LEU:HD21	1.91	0.53
1:F:242:ASP:N	1:F:242:ASP:OD1	2.42	0.53
1:I:97:MET:HB3	1:I:113:ALA:HB3	1.91	0.53
1:I:289:HIS:CE1	1:I:301:ARG:HD2	2.44	0.53
1:J:253:ASN:OD1	1:J:256:GLY:N	2.40	0.52
1:K:252:ASP:OD1	1:K:253:ASN:ND2	2.37	0.52
1:E:7:LEU:HD13	1:E:56:MET:HE2	1.90	0.52
1:A:253:ASN:HD21	1:A:256:GLY:HA3	1.74	0.52
1:H:8:VAL:HG23	1:H:303:LEU:HD11	1.92	0.52
1:H:14:ALA:HB2	1:H:301:ARG:HB2	1.92	0.52
1:K:113:ALA:HB1	1:K:122:PHE:HB3	1.91	0.52
1:G:263:VAL:HG13	1:G:265:LEU:O	2.10	0.52
1:E:200:ARG:NH2	4:E:530:HOH:O	2.43	0.52
1:B:219:ARG:HG2	1:B:260:TYR:CZ	2.45	0.51
1:F:15:ASP:H	1:F:289:HIS:CD2	2.28	0.51
1:H:113:ALA:HB1	1:H:122:PHE:HB3	1.92	0.51
1:I:5:ARG:NH2	1:I:62:GLY:O	2.29	0.51
1:J:113:ALA:HB1	1:J:122:PHE:HB3	1.92	0.51
1:F:242:ASP:O	1:F:244:HIS:NE2	2.43	0.51
1:H:51:TYR:OH	1:H:84:TRP:O	2.21	0.51
1:J:51:TYR:OH	1:J:84:TRP:O	2.23	0.51
1:G:268:VAL:HG13	1:G:290:ASP:OD1	2.11	0.51
1:I:14:ALA:HB2	1:I:301:ARG:HB2	1.92	0.51
1:K:1:MET:O	1:K:1:MET:HG2	2.11	0.50
1:L:55:SER:HB3	1:L:65:THR:HB	1.93	0.50
1:D:113:ALA:HB1	1:D:122:PHE:HB3	1.94	0.50
1:G:77:PRO:HG2	1:G:126:GLU:HA	1.93	0.50
1:F:289:HIS:CE1	1:F:301:ARG:HD2	2.47	0.50
1:E:76:ILE:HB	1:E:79:ALA:HB2	1.93	0.50
1:G:267:PRO:HB2	1:G:323:ALA:O	2.12	0.50
1:L:273:THR:HG23	1:L:273:THR:O	2.11	0.50
1:B:53:VAL:HG11	1:B:119:GLU:HA	1.94	0.50
1:K:77:PRO:HG2	1:K:126:GLU:HA	1.93	0.50
1:A:77:PRO:HG2	1:A:126:GLU:HA	1.94	0.49
1:J:8:VAL:HG23	1:J:303:LEU:HD11	1.94	0.49
1:K:180:ALA:HB2	1:K:214:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:MET:HB3	1:D:113:ALA:HB3	1.94	0.49
1:D:163:ARG:HG2	1:D:168:LEU:HD11	1.94	0.49
1:I:252:ASP:OD1	1:I:253:ASN:ND2	2.37	0.49
1:K:253:ASN:OD1	1:K:256:GLY:N	2.42	0.49
1:D:82:GLN:OE1	1:D:102:LYS:HD2	2.12	0.49
1:C:74:GLU:OE2	1:C:74:GLU:N	2.46	0.49
1:H:242:ASP:OD1	1:H:242:ASP:N	2.43	0.49
1:E:279:GLU:HB2	1:E:284:TRP:CE2	2.48	0.49
1:J:78:TRP:CG	1:J:128:PRO:HD3	2.48	0.49
1:L:183:PRO:HG2	1:L:202:LEU:HB3	1.95	0.49
1:D:14:ALA:HB2	1:D:301:ARG:HB2	1.95	0.48
1:E:34:GLU:OE1	1:E:297:LYS:NZ	2.29	0.48
1:H:77:PRO:HG2	1:H:126:GLU:HA	1.94	0.48
1:I:216:ASP:OD2	1:I:219:ARG:NH1	2.45	0.48
1:F:135:MET:SD	1:F:153:GLY:HA3	2.54	0.48
1:I:253:ASN:HD21	1:I:256:GLY:HA3	1.79	0.48
1:A:56:MET:HE3	1:A:64:VAL:HG22	1.95	0.48
1:F:77:PRO:HG2	1:F:126:GLU:HA	1.95	0.48
1:C:119:GLU:OE1	1:C:119:GLU:N	2.43	0.48
1:C:27:ILE:HG22	1:C:29:PRO:HD3	1.95	0.48
1:J:269:VAL:HG23	1:J:322:THR:HB	1.96	0.48
1:L:299:TRP:CD1	1:L:300:LEU:HG	2.48	0.48
1:A:117:ARG:NH1	1:A:119:GLU:OE2	2.46	0.48
1:K:58:ASP:HB3	1:K:62:GLY:HA3	1.95	0.48
1:L:225:SER:HG	1:L:236:PHE:HE1	1.62	0.48
1:G:253:ASN:ND2	1:G:256:GLY:H	2.12	0.48
1:H:163:ARG:HG2	1:H:168:LEU:HD11	1.95	0.48
1:K:170:CYS:HA	1:L:170:CYS:HA	1.96	0.48
1:K:248:TYR:HB3	1:K:264:ILE:HD11	1.96	0.48
1:F:98:TYR:OH	1:F:192:MET:HB3	2.13	0.47
1:K:245:LEU:HD23	1:K:267:PRO:HD3	1.95	0.47
1:C:36:GLY:HA3	1:H:6:TYR:O	2.14	0.47
1:G:14:ALA:HB2	1:G:301:ARG:HB2	1.95	0.47
1:E:113:ALA:HB1	1:E:122:PHE:HB3	1.96	0.47
1:F:163:ARG:HG2	1:F:168:LEU:HD11	1.97	0.47
1:F:253:ASN:HD21	1:F:256:GLY:HA3	1.79	0.47
1:J:85:ASP:O	1:J:137:PRO:HD2	2.15	0.47
1:B:56:MET:SD	1:B:64:VAL:HG22	2.53	0.47
1:D:117:ARG:NH2	1:D:119:GLU:OE2	2.47	0.47
1:J:45:HIS:HD2	1:J:299:TRP:HB3	1.79	0.47
1:L:85:ASP:O	1:L:137:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ARG:HG2	1:C:168:LEU:HD11	1.96	0.47
1:F:153:GLY:O	1:F:159:LEU:HB2	2.14	0.47
1:A:5:ARG:NH1	1:A:59:VAL:O	2.46	0.47
1:G:265:LEU:CD1	1:G:266:THR:H	2.08	0.47
1:G:303:LEU:N	4:G:508:HOH:O	2.37	0.47
1:I:266:THR:HG1	1:I:321:GLY:H	1.59	0.47
1:A:113:ALA:HB1	1:A:122:PHE:HB3	1.95	0.47
1:F:290:ASP:OD2	1:F:322:THR:HG21	2.15	0.47
1:G:263:VAL:O	1:G:263:VAL:HG12	2.13	0.47
1:K:233:LYS:HD2	1:K:250:THR:HG23	1.97	0.46
1:F:233:LYS:HE2	1:F:314:GLY:HA3	1.98	0.46
1:G:42:ASN:ND2	1:G:44:ASP:OD2	2.48	0.46
1:G:265:LEU:CD1	1:G:266:THR:N	2.73	0.46
1:H:138:CYS:SG	1:H:150:TYR:HB2	2.56	0.46
1:I:39:GLU:O	1:I:39:GLU:HG3	2.15	0.46
1:D:34:GLU:OE1	1:D:299:TRP:NE1	2.34	0.46
1:G:40:ASN:H	1:G:45:HIS:CD2	2.33	0.46
1:H:97:MET:HB3	1:H:113:ALA:HB3	1.98	0.46
1:K:85:ASP:O	1:K:137:PRO:HD2	2.15	0.46
1:A:266:THR:HG1	1:A:321:GLY:H	1.57	0.46
1:G:266:THR:OG1	1:G:321:GLY:N	2.48	0.46
1:J:117:ARG:HB2	1:J:120:GLY:H	1.81	0.46
1:B:245:LEU:HD23	1:B:267:PRO:HD3	1.98	0.46
1:C:246:ILE:HB	1:C:265:LEU:HB3	1.98	0.46
1:G:266:THR:HB	1:G:267:PRO:CD	2.46	0.46
1:A:14:ALA:O	1:A:30:SER:N	2.45	0.46
1:C:31:HIS:ND1	1:C:50:ASP:OD1	2.46	0.46
1:E:58:ASP:HB3	1:E:62:GLY:HA3	1.98	0.46
1:C:218:LYS:HG2	1:C:243:THR:HG21	1.98	0.45
1:E:105:ASN:OD1	1:F:109:ARG:NH1	2.46	0.45
1:K:135:MET:SD	1:K:153:GLY:HA3	2.56	0.45
1:G:5:ARG:NH2	1:G:62:GLY:O	2.39	0.45
1:L:246:ILE:HB	1:L:265:LEU:HB3	1.98	0.45
1:H:187:ARG:HB2	1:H:255:TYR:OH	2.16	0.45
1:H:222:PHE:HD2	1:H:223:GLU:HG2	1.82	0.45
1:F:7:LEU:HB3	1:F:64:VAL:HG21	1.98	0.45
1:L:222:PHE:HD2	1:L:223:GLU:HG2	1.82	0.45
1:B:25:LEU:HD22	1:B:59:VAL:HG22	1.97	0.45
1:F:53:VAL:HG13	1:F:67:HIS:HB2	1.98	0.45
1:A:85:ASP:O	1:A:137:PRO:HD2	2.16	0.45
1:C:222:PHE:HD2	1:C:223:GLU:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:ASP:O	1:F:244:HIS:CD2	2.70	0.45
1:A:245:LEU:HD23	1:A:267:PRO:HD3	1.99	0.44
1:C:78:TRP:CG	1:C:128:PRO:HD3	2.53	0.44
1:C:219:ARG:HG2	1:C:260:TYR:CZ	2.52	0.44
1:F:51:TYR:OH	1:F:84:TRP:O	2.28	0.44
1:D:222:PHE:HD2	1:D:223:GLU:HG2	1.82	0.44
1:F:78:TRP:CG	1:F:128:PRO:HD3	2.52	0.44
1:H:266:THR:HG1	1:H:321:GLY:H	1.61	0.44
1:G:45:HIS:CD2	1:G:45:HIS:H	2.34	0.44
1:D:268:VAL:HB	1:D:290:ASP:HB3	1.99	0.44
1:F:151:PHE:CE1	1:F:184:LYS:HB2	2.53	0.44
1:G:51:TYR:OH	1:G:84:TRP:O	2.25	0.44
1:L:242:ASP:OD1	1:L:242:ASP:N	2.48	0.44
1:H:19:HIS:NE2	1:H:87:ASP:OD1	2.40	0.44
1:F:317:GLN:HA	1:F:318:PRO:HD3	1.89	0.44
1:H:135:MET:SD	1:H:153:GLY:HA3	2.58	0.44
1:J:253:ASN:HD21	1:J:256:GLY:HA3	1.82	0.44
1:D:260:TYR:O	1:E:117:ARG:NH1	2.44	0.44
1:K:5:ARG:NH1	1:K:59:VAL:O	2.43	0.44
1:C:95:TYR:CE1	1:C:118:PRO:HG3	2.53	0.43
1:H:56:MET:HE3	1:H:64:VAL:HG22	1.99	0.43
1:I:135:MET:SD	1:I:153:GLY:HA3	2.58	0.43
1:H:219:ARG:HG2	1:H:260:TYR:CZ	2.53	0.43
1:J:39:GLU:HG3	1:J:45:HIS:CE1	2.53	0.43
1:J:227:MET:HE1	1:J:236:PHE:HB2	2.00	0.43
1:B:40:ASN:ND2	1:B:42:ASN:OD1	2.50	0.43
1:J:219:ARG:O	1:J:238:TYR:OH	2.30	0.43
1:L:184:LYS:NZ	1:L:201:ASP:OD1	2.35	0.43
1:F:151:PHE:CZ	1:F:184:LYS:HB2	2.53	0.43
1:G:244:HIS:ND1	1:G:271:TRP:O	2.44	0.43
1:B:113:ALA:HB1	1:B:122:PHE:HB3	1.99	0.43
1:C:78:TRP:HA	1:D:130:LYS:HD3	2.00	0.43
1:H:44:ASP:OD1	1:H:81:ARG:NH1	2.40	0.43
1:J:292:VAL:HG21	1:J:322:THR:HG21	1.99	0.43
1:D:139:ILE:HD12	1:D:188:LEU:HD11	2.00	0.43
1:G:7:LEU:HB3	1:G:64:VAL:HG21	2.01	0.43
1:I:245:LEU:HD23	1:I:267:PRO:HD3	2.00	0.43
1:K:130:LYS:NZ	4:K:511:HOH:O	2.45	0.43
1:J:117:ARG:NE	1:J:119:GLU:OE2	2.52	0.43
1:D:103:ASP:OD1	1:D:107:ILE:O	2.37	0.43
1:G:269:VAL:H	1:G:322:THR:HB	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:ASP:HB3	1:J:144:ASP:OD1	2.19	0.43
1:L:79:ALA:HA	1:L:101:LEU:HD21	2.01	0.43
1:B:78:TRP:CG	1:B:128:PRO:HD3	2.54	0.43
1:E:78:TRP:CG	1:E:128:PRO:HD3	2.54	0.43
1:J:119:GLU:H	1:J:119:GLU:CD	2.22	0.43
1:C:43:GLY:HA2	1:C:45:HIS:CE1	2.53	0.42
1:E:161:ARG:NH2	4:E:533:HOH:O	2.52	0.42
1:D:77:PRO:HG2	1:D:126:GLU:HA	2.00	0.42
1:F:240:THR:HG21	1:F:243:THR:HB	1.99	0.42
1:E:85:ASP:O	1:E:137:PRO:HD2	2.20	0.42
1:G:266:THR:HB	1:G:267:PRO:HD2	2.01	0.42
1:H:253:ASN:HB2	1:H:254:PRO:HD2	2.01	0.42
1:J:119:GLU:CD	1:J:119:GLU:N	2.73	0.42
1:A:58:ASP:O	1:A:62:GLY:HA3	2.19	0.42
1:B:242:ASP:OD1	1:B:242:ASP:N	2.51	0.42
1:C:294:SER:HB3	1:C:297:LYS:HB2	2.01	0.42
1:D:58:ASP:HB3	1:D:62:GLY:HA3	2.01	0.42
1:G:180:ALA:HB2	1:G:214:ALA:HA	2.01	0.42
1:B:135:MET:SD	1:B:153:GLY:HA3	2.59	0.42
1:D:78:TRP:CG	1:D:128:PRO:HD3	2.55	0.42
1:G:216:ASP:OD2	1:G:219:ARG:HD3	2.18	0.42
1:H:269:VAL:O	1:H:291:CYS:N	2.49	0.42
1:K:44:ASP:OD1	1:K:81:ARG:NH1	2.52	0.42
1:K:113:ALA:HA	1:K:124:PRO:HA	2.02	0.42
1:K:222:PHE:HD2	1:K:223:GLU:HG2	1.84	0.42
1:D:78:TRP:CH2	1:D:101:LEU:HB3	2.54	0.42
1:E:286:LEU:HD22	1:E:319:ILE:HD12	2.02	0.42
1:G:166:LYS:NZ	1:H:104:GLN:O	2.36	0.42
1:I:85:ASP:O	1:I:137:PRO:HD2	2.19	0.42
1:I:233:LYS:HE3	1:I:233:LYS:HB2	1.90	0.42
1:E:51:TYR:OH	1:E:84:TRP:O	2.22	0.42
1:E:245:LEU:HD22	1:E:263:VAL:HG11	2.01	0.42
1:A:158:GLN:HB3	1:A:161:ARG:HD2	2.01	0.42
1:E:130:LYS:HD3	1:F:78:TRP:HA	2.01	0.42
1:J:76:ILE:HA	1:J:77:PRO:HD3	1.93	0.42
1:J:163:ARG:HG2	1:J:168:LEU:HD11	2.02	0.42
1:J:242:ASP:OD1	1:J:242:ASP:N	2.52	0.42
1:A:78:TRP:CG	1:A:128:PRO:HD3	2.54	0.42
1:A:163:ARG:HG2	1:A:168:LEU:HD11	2.01	0.42
1:B:98:TYR:OH	1:B:192:MET:HB3	2.20	0.42
1:D:12:TYR:CE1	1:D:300:LEU:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:PRO:HB3	1:G:303:LEU:HD13	2.01	0.42
1:I:5:ARG:HH12	1:I:62:GLY:H	1.66	0.42
1:G:299:TRP:CD1	1:G:300:LEU:HG	2.55	0.41
1:I:27:ILE:HG21	1:I:303:LEU:HD21	2.02	0.41
1:I:78:TRP:CG	1:I:128:PRO:HD3	2.55	0.41
1:C:76:ILE:HA	1:C:77:PRO:HD3	1.92	0.41
1:F:219:ARG:O	1:F:238:TYR:OH	2.32	0.41
1:E:229:TYR:OH	1:E:232:GLY:HA2	2.20	0.41
1:F:59:VAL:HG11	1:F:285:TYR:CZ	2.55	0.41
1:L:78:TRP:CG	1:L:128:PRO:HD3	2.55	0.41
1:E:288:HIS:NE2	1:E:304:LYS:HD2	2.35	0.41
1:L:150:TYR:CD1	1:L:202:LEU:HD22	2.55	0.41
1:L:165:ASN:ND2	1:L:199:PRO:HB2	2.35	0.41
1:B:76:ILE:HB	1:B:79:ALA:HB2	2.02	0.41
1:D:235:TYR:OH	1:D:314:GLY:O	2.31	0.41
1:D:244:HIS:HB2	1:D:267:PRO:HB3	2.01	0.41
1:I:320:LYS:HB2	1:I:320:LYS:HE3	1.86	0.41
1:A:40:ASN:OD1	1:A:41:ASP:N	2.54	0.41
1:H:85:ASP:O	1:H:137:PRO:HD2	2.20	0.41
1:K:98:TYR:OH	1:K:192:MET:HB3	2.21	0.41
1:C:163:ARG:NH2	1:C:172:LEU:O	2.44	0.41
1:F:208:LYS:HE2	1:F:208:LYS:HB3	1.91	0.41
1:K:78:TRP:CG	1:K:128:PRO:HD3	2.56	0.41
1:F:233:LYS:NZ	1:F:235:TYR:OH	2.29	0.41
1:H:245:LEU:HD22	1:H:263:VAL:HG11	2.03	0.41
1:K:227:MET:HE2	1:K:227:MET:HB2	1.94	0.41
1:L:309:LYS:HE2	1:L:309:LYS:HB3	1.87	0.41
1:A:140:TRP:HA	1:A:141:PRO:HD3	1.93	0.41
1:D:150:TYR:CD1	1:D:202:LEU:HD22	2.56	0.41
1:E:227:MET:HB2	1:E:227:MET:HE2	1.95	0.41
1:G:183:PRO:HG2	1:G:202:LEU:HB3	2.03	0.41
1:B:224:ALA:O	1:B:238:TYR:HA	2.21	0.40
1:C:113:ALA:HA	1:C:124:PRO:HA	2.03	0.40
1:E:180:ALA:HB2	1:E:214:ALA:HA	2.03	0.40
1:F:58:ASP:HB3	1:F:62:GLY:HA3	2.04	0.40
1:H:12:TYR:HE1	1:H:294:SER:HB3	1.86	0.40
1:I:76:ILE:HB	1:I:79:ALA:HB2	2.02	0.40
1:A:222:PHE:HD2	1:A:223:GLU:HG2	1.86	0.40
1:B:117:ARG:HG3	1:B:120:GLY:H	1.87	0.40
1:H:198:GLU:HA	1:H:199:PRO:HD3	1.95	0.40
1:I:76:ILE:HA	1:I:77:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:51:TYR:OH	1:K:84:TRP:O	2.25	0.40
1:K:289:HIS:NE2	1:K:301:ARG:HD2	2.36	0.40
1:L:163:ARG:HG2	1:L:168:LEU:HD11	2.02	0.40
1:B:85:ASP:O	1:B:137:PRO:HD2	2.21	0.40
1:B:163:ARG:HG2	1:B:168:LEU:HD11	2.03	0.40
1:C:13:MET:HB2	1:C:303:LEU:HG	2.03	0.40
1:I:279:GLU:HB2	1:I:284:TRP:CE2	2.57	0.40
1:K:37:ILE:HG21	1:K:44:ASP:HB3	2.04	0.40
1:K:87:ASP:OD1	1:K:88:VAL:N	2.52	0.40
1:F:15:ASP:H	1:F:289:HIS:HD2	1.68	0.40
1:I:229:TYR:OH	1:I:232:GLY:HA2	2.20	0.40
1:B:25:LEU:HD21	1:B:287:PHE:CZ	2.56	0.40
1:L:198:GLU:HA	1:L:199:PRO:HD3	1.91	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	321/324 (99%)	302 (94%)	19 (6%)	0	100	100
1	B	321/324 (99%)	303 (94%)	18 (6%)	0	100	100
1	C	321/324 (99%)	303 (94%)	18 (6%)	0	100	100
1	D	320/324 (99%)	304 (95%)	16 (5%)	0	100	100
1	E	321/324 (99%)	304 (95%)	17 (5%)	0	100	100
1	F	321/324 (99%)	300 (94%)	21 (6%)	0	100	100
1	G	322/324 (99%)	298 (92%)	24 (8%)	0	100	100
1	H	322/324 (99%)	304 (94%)	18 (6%)	0	100	100
1	I	319/324 (98%)	296 (93%)	23 (7%)	0	100	100
1	J	321/324 (99%)	300 (94%)	21 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	322/324 (99%)	302 (94%)	20 (6%)	0	100	100
1	L	320/324 (99%)	301 (94%)	19 (6%)	0	100	100
All	All	3851/3888 (99%)	3617 (94%)	234 (6%)	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	280/281 (100%)	276 (99%)	4 (1%)	67	86
1	B	280/281 (100%)	275 (98%)	5 (2%)	59	83
1	C	279/281 (99%)	276 (99%)	3 (1%)	73	90
1	D	280/281 (100%)	274 (98%)	6 (2%)	53	80
1	E	280/281 (100%)	278 (99%)	2 (1%)	84	94
1	F	279/281 (99%)	277 (99%)	2 (1%)	84	94
1	G	279/281 (99%)	275 (99%)	4 (1%)	67	86
1	H	280/281 (100%)	277 (99%)	3 (1%)	73	90
1	I	276/281 (98%)	273 (99%)	3 (1%)	73	90
1	J	279/281 (99%)	276 (99%)	3 (1%)	73	90
1	K	280/281 (100%)	273 (98%)	7 (2%)	47	76
1	L	279/281 (99%)	273 (98%)	6 (2%)	52	79
All	All	3351/3372 (99%)	3303 (99%)	48 (1%)	67	86

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	108	PHE
1	A	135	MET
1	A	220	ARG

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Mol	Chain	Res	Type
1	B	108	PHE
1	B	135	MET
1	B	220	ARG
1	B	233	LYS
1	B	297	LYS
1	C	135	MET
1	C	220	ARG
1	C	303	LEU
1	D	11	ASP
1	D	49	LYS
1	D	108	PHE
1	D	135	MET
1	D	220	ARG
1	D	303	LEU
1	E	135	MET
1	E	220	ARG
1	F	135	MET
1	F	220	ARG
1	G	108	PHE
1	G	135	MET
1	G	220	ARG
1	G	266	THR
1	H	135	MET
1	H	200	ARG
1	H	220	ARG
1	I	135	MET
1	I	220	ARG
1	I	231	ASN
1	J	108	PHE
1	J	135	MET
1	J	220	ARG
1	K	108	PHE
1	K	135	MET
1	K	220	ARG
1	K	266	THR
1	K	294	SER
1	K	322	THR
1	K	324	GLU
1	L	135	MET
1	L	220	ARG
1	L	269	VAL
1	L	290	ASP

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Mol	Chain	Res	Type
1	L	301	ARG
1	L	322	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	289	HIS
1	G	45	HIS
1	I	52	HIS
1	K	274	HIS
1	L	165	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	J	402	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	L	402	-	4,4,4	0.14	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	C	403	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	L	403	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	K	402	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	J	403	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	E	403	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	E	402	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	K	403	-	4,4,4	0.13	0	6,6,6	0.05	0
3	SO4	H	403	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	D	403	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	F	402	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	G	402	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	402	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	I	402	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	A	403	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	F	403	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	G	403	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	H	402	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	C	402	-	4,4,4	0.15	0	6,6,6	0.04	0
3	SO4	D	402	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	I	403	-	4,4,4	0.14	0	6,6,6	0.04	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	323/324 (99%)	0.27	10 (3%) 49 49	43, 60, 88, 99	0
1	B	323/324 (99%)	0.40	13 (4%) 38 37	45, 67, 86, 105	0
1	C	323/324 (99%)	0.55	25 (7%) 13 11	50, 78, 112, 146	0
1	D	322/324 (99%)	0.31	7 (2%) 62 63	43, 65, 91, 121	0
1	E	323/324 (99%)	0.38	18 (5%) 24 23	48, 66, 91, 120	0
1	F	323/324 (99%)	0.67	28 (8%) 10 8	49, 75, 104, 131	0
1	G	324/324 (100%)	0.57	17 (5%) 27 25	46, 78, 117, 183	0
1	H	324/324 (100%)	0.55	25 (7%) 13 11	51, 75, 105, 159	0
1	I	321/324 (99%)	0.76	29 (9%) 9 7	53, 76, 109, 148	0
1	J	323/324 (99%)	0.47	14 (4%) 35 33	50, 69, 99, 118	0
1	K	324/324 (100%)	0.70	18 (5%) 24 23	54, 77, 103, 140	0
1	L	322/324 (99%)	0.97	45 (13%) 2 1	58, 89, 123, 151	0
All	All	3875/3888 (99%)	0.55	249 (6%) 19 18	43, 72, 107, 183	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	323	ALA	9.0
1	H	324	GLU	6.6
1	L	42	ASN	5.4
1	J	322	THR	4.9
1	K	177	ASP	4.7
1	F	120	GLY	4.5
1	B	136	ASP	4.3
1	L	138	CYS	4.2
1	I	320	LYS	4.2
1	F	137	PRO	4.1
1	B	138	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	225	SER	4.0
1	I	275	HIS	3.9
1	I	17	ALA	3.9
1	J	175	GLU	3.9
1	F	136	ASP	3.9
1	I	86	SER	3.9
1	G	23	ASP	3.9
1	H	322	THR	3.8
1	F	85	ASP	3.8
1	G	138	CYS	3.8
1	I	23	ASP	3.8
1	A	136	ASP	3.8
1	K	225	SER	3.7
1	E	36	GLY	3.7
1	C	138	CYS	3.6
1	L	215	GLY	3.6
1	K	2	LYS	3.6
1	K	323	ALA	3.6
1	J	177	ASP	3.6
1	D	23	ASP	3.5
1	I	274	HIS	3.5
1	H	214	ALA	3.4
1	L	210	LYS	3.4
1	H	207	GLU	3.4
1	C	225	SER	3.4
1	G	320	LYS	3.4
1	B	225	SER	3.4
1	I	322	THR	3.3
1	A	322	THR	3.3
1	G	225	SER	3.3
1	C	121	PRO	3.3
1	K	120	GLY	3.3
1	L	85	ASP	3.3
1	I	136	ASP	3.2
1	L	144	ASP	3.2
1	L	217	THR	3.2
1	G	74	GLU	3.2
1	I	138	CYS	3.2
1	B	145	GLY	3.2
1	B	16	PRO	3.2
1	F	276	SER	3.1
1	L	276	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	37	ILE	3.1
1	I	39	GLU	3.1
1	F	2	LYS	3.1
1	L	224	ALA	3.1
1	B	86	SER	3.1
1	B	137	PRO	3.1
1	L	176	GLY	3.0
1	I	239	SER	3.0
1	F	17	ALA	3.0
1	I	64	VAL	3.0
1	E	41	ASP	3.0
1	K	224	ALA	3.0
1	L	86	SER	3.0
1	H	138	CYS	2.9
1	J	138	CYS	2.9
1	J	36	GLY	2.9
1	K	80	GLY	2.9
1	L	137	PRO	2.9
1	I	87	ASP	2.9
1	C	269	VAL	2.9
1	J	1	MET	2.9
1	I	137	PRO	2.9
1	I	63	GLU	2.9
1	H	225	SER	2.9
1	L	274	HIS	2.9
1	G	268	VAL	2.9
1	L	305	VAL	2.9
1	C	20	VAL	2.9
1	E	138	CYS	2.9
1	L	172	LEU	2.8
1	J	40	ASN	2.8
1	F	170	CYS	2.8
1	L	1	MET	2.8
1	C	226	TRP	2.8
1	I	55	SER	2.8
1	L	136	ASP	2.8
1	I	224	ALA	2.8
1	F	225	SER	2.8
1	H	94	LYS	2.8
1	C	275	HIS	2.7
1	A	62	GLY	2.7
1	C	291	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	120	GLY	2.7
1	F	307	GLU	2.7
1	E	10	GLY	2.7
1	D	224	ALA	2.7
1	B	275	HIS	2.7
1	H	274	HIS	2.7
1	J	176	GLY	2.7
1	H	137	PRO	2.6
1	L	121	PRO	2.6
1	E	177	ASP	2.6
1	I	85	ASP	2.6
1	C	86	SER	2.6
1	I	225	SER	2.6
1	F	232	GLY	2.6
1	H	136	ASP	2.6
1	C	322	THR	2.6
1	J	41	ASP	2.6
1	A	275	HIS	2.6
1	G	274	HIS	2.6
1	C	63	GLU	2.6
1	G	120	GLY	2.6
1	H	275	HIS	2.6
1	C	85	ASP	2.6
1	F	23	ASP	2.6
1	K	137	PRO	2.5
1	A	224	ALA	2.5
1	C	67	HIS	2.5
1	D	138	CYS	2.5
1	I	291	CYS	2.5
1	H	231	ASN	2.5
1	F	77	PRO	2.5
1	K	87	ASP	2.5
1	L	177	ASP	2.5
1	L	216	ASP	2.5
1	K	38	PRO	2.5
1	E	61	GLN	2.5
1	H	120	GLY	2.5
1	E	86	SER	2.5
1	K	42	ASN	2.5
1	C	120	GLY	2.5
1	F	61	GLN	2.5
1	D	87	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	323	ALA	2.4
1	G	269	VAL	2.4
1	G	292	VAL	2.4
1	K	23	ASP	2.4
1	C	268	VAL	2.4
1	L	53	VAL	2.4
1	I	68	GLY	2.4
1	F	231	ASN	2.4
1	A	63	GLU	2.4
1	L	40	ASN	2.4
1	H	209	GLY	2.4
1	J	63	GLU	2.4
1	H	312	PRO	2.4
1	E	224	ALA	2.4
1	L	168	LEU	2.4
1	B	55	SER	2.4
1	H	177	ASP	2.4
1	H	237	SER	2.4
1	K	138	CYS	2.4
1	J	86	SER	2.3
1	L	242	ASP	2.3
1	B	36	GLY	2.3
1	L	38	PRO	2.3
1	L	313	ASP	2.3
1	G	53	VAL	2.3
1	G	85	ASP	2.3
1	G	177	ASP	2.3
1	K	15	ASP	2.3
1	B	276	SER	2.3
1	B	226	TRP	2.3
1	E	3	GLU	2.3
1	I	15	ASP	2.3
1	F	286	LEU	2.3
1	H	224	ALA	2.3
1	I	292	VAL	2.3
1	L	20	VAL	2.3
1	H	249	ALA	2.3
1	L	214	ALA	2.3
1	B	85	ASP	2.3
1	E	225	SER	2.3
1	F	1	MET	2.3
1	G	323	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	57	ASP	2.3
1	L	19	HIS	2.2
1	K	240	THR	2.2
1	A	30	SER	2.2
1	C	29	PRO	2.2
1	L	71	LEU	2.2
1	K	176	GLY	2.2
1	G	299	TRP	2.2
1	K	320	LYS	2.2
1	L	41	ASP	2.2
1	J	225	SER	2.2
1	F	138	CYS	2.2
1	K	45	HIS	2.2
1	E	322	THR	2.2
1	F	65	THR	2.2
1	C	276	SER	2.2
1	F	121	PRO	2.2
1	A	85	ASP	2.2
1	I	276	SER	2.2
1	L	16	PRO	2.2
1	C	93	GLY	2.2
1	L	226	TRP	2.2
1	C	274	HIS	2.1
1	F	16	PRO	2.1
1	J	312	PRO	2.1
1	E	137	PRO	2.1
1	L	145	GLY	2.1
1	L	318	PRO	2.1
1	L	263	VAL	2.1
1	A	137	PRO	2.1
1	L	66	ASP	2.1
1	H	70	VAL	2.1
1	I	74	GLU	2.1
1	H	196	ALA	2.1
1	L	55	SER	2.1
1	A	116	ASP	2.1
1	E	136	ASP	2.1
1	H	145	GLY	2.1
1	C	224	ALA	2.1
1	G	14	ALA	2.1
1	C	68	GLY	2.1
1	E	85	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	85	ASP	2.1
1	D	193	LEU	2.1
1	J	293	PRO	2.1
1	F	266	THR	2.1
1	E	44	ASP	2.1
1	C	137	PRO	2.1
1	F	277	ILE	2.1
1	G	137	PRO	2.1
1	C	196	ALA	2.1
1	L	196	ALA	2.1
1	I	34	GLU	2.1
1	L	310	TYR	2.0
1	E	17	ALA	2.0
1	C	292	VAL	2.0
1	L	275	HIS	2.0
1	H	139	ILE	2.0
1	L	3	GLU	2.0
1	F	224	ALA	2.0
1	L	291	CYS	2.0
1	I	226	TRP	2.0
1	F	274	HIS	2.0
1	F	312	PRO	2.0
1	L	51	TYR	2.0
1	D	86	SER	2.0
1	F	226	TRP	2.0
1	D	71	LEU	2.0
1	H	211	LEU	2.0
1	C	24	LYS	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, 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	B-factors(Å^2)	Q<0.9
3	SO4	K	403	5/5	0.11	0.69	161,161,161,161	0
3	SO4	G	403	5/5	0.54	0.43	148,149,149,149	0
3	SO4	F	402	5/5	0.60	0.52	106,106,107,107	0
3	SO4	L	403	5/5	0.60	0.53	152,153,153,153	0
3	SO4	E	403	5/5	0.64	0.27	131,131,131,131	0
3	SO4	J	403	5/5	0.66	0.48	153,154,154,154	0
3	SO4	B	403	5/5	0.70	0.18	116,116,116,116	0
3	SO4	F	403	5/5	0.71	0.29	136,136,137,137	0
3	SO4	C	403	5/5	0.72	0.29	137,137,137,137	0
3	SO4	A	403	5/5	0.72	0.34	123,123,124,124	0
3	SO4	K	402	5/5	0.73	0.49	110,110,111,111	0
3	SO4	I	403	5/5	0.73	0.45	162,162,163,163	0
3	SO4	A	402	5/5	0.73	0.57	109,109,109,109	0
3	SO4	J	402	5/5	0.76	0.32	101,101,102,102	0
3	SO4	H	403	5/5	0.77	0.25	113,113,114,114	0
3	SO4	C	402	5/5	0.78	0.35	103,103,104,104	0
3	SO4	G	402	5/5	0.78	0.51	126,126,126,126	0
2	CA	B	401	1/1	0.80	0.51	73,73,73,73	0
3	SO4	D	403	5/5	0.80	0.27	113,113,113,114	0
3	SO4	I	402	5/5	0.81	0.41	105,105,105,106	0
2	CA	K	401	1/1	0.82	0.54	81,81,81,81	0
3	SO4	E	402	5/5	0.83	0.41	105,105,105,105	0
2	CA	H	401	1/1	0.84	0.49	71,71,71,71	0
2	CA	G	401	1/1	0.84	0.43	77,77,77,77	0
3	SO4	L	402	5/5	0.85	0.36	111,111,111,111	0
3	SO4	H	402	5/5	0.87	0.30	94,94,94,95	0
2	CA	J	401	1/1	0.88	0.37	70,70,70,70	0
2	CA	F	401	1/1	0.89	0.53	84,84,84,84	0
3	SO4	B	402	5/5	0.89	0.35	85,85,86,86	0
3	SO4	D	402	5/5	0.91	0.36	92,93,93,93	0
2	CA	D	401	1/1	0.91	0.35	65,65,65,65	0
2	CA	A	401	1/1	0.91	0.50	62,62,62,62	0
2	CA	C	401	1/1	0.92	0.49	77,77,77,77	0
2	CA	L	401	1/1	0.92	0.49	80,80,80,80	0
2	CA	E	401	1/1	0.95	0.48	70,70,70,70	0
2	CA	I	401	1/1	0.96	0.61	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.