Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 02:06 PM JST

PDB ID	:	5IFJ
Title	:	Crystal structure of anti-gliadin 1002-1E01 Fab fragment in complex of peptide PLQPEQPFP
Authors	:	Snir, O.; Chen, X.; Gidoni, M.; du Pre, M.F.; Zhao, Y.; Steinsbo, O.; Lundin, K.E.; Yaari, G.; Sollid, L.M.
Deposited on	:	2016-02-26
Resolution	:	2.35 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 (i) 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 (i)) were used in the production of this report:

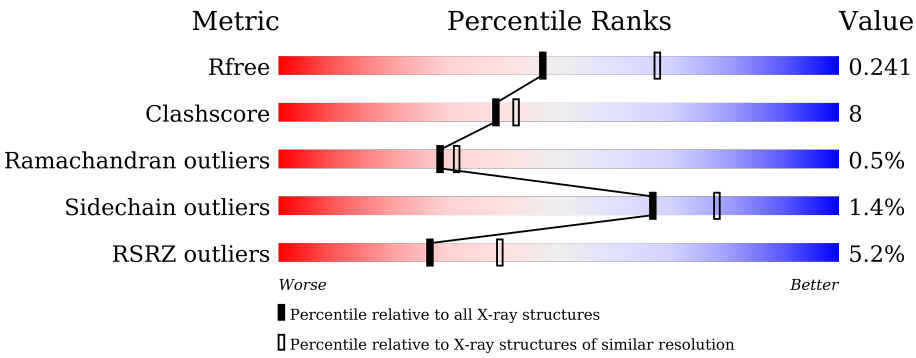
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	227	%, 85%, 9%, 5%
1	D	227	%, 85%, 10%, •
1	G	227	9%, 83%, 11%, 5%
1	J	227	3%, 83%, 13%, •, •
2	B	216	%, 89%, 9%, •
2	E	216	%, 87%, 11%, ••

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Mol	Chain	Length	Quality of chain
2	H	216	19% 75% 22%
2	K	216	6% 72% 25%
3	C	9	78% 22%
3	F	9	89% 11%
3	I	9	78% 22%
3	L	9	11% 67% 33%

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
4	SO4	A	301	-	-	-	X
4	SO4	B	301	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13491 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 1E01 Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1593	1000	267	318	8	0	0	0
1	D	217	1602	1006	269	319	8	0	0	0
1	G	215	1591	1000	267	316	8	0	0	0
1	J	219	1614	1012	271	322	9	0	0	0

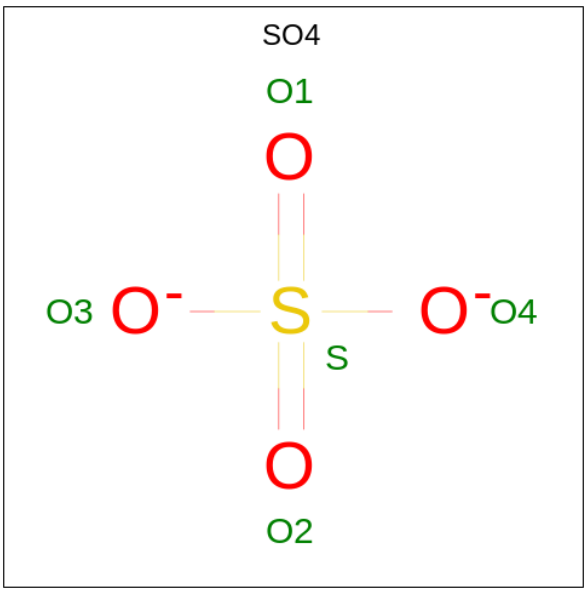
- Molecule 2 is a protein called 1E01 Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	1593	993	270	325	5	0	0	0
2	E	213	1593	993	270	325	5	0	0	0
2	H	213	1593	993	270	325	5	0	0	0
2	K	213	1593	993	270	325	5	0	0	0

- Molecule 3 is a protein called peptide PRO-LEU-GLN-PRO-GLU-GLN-PRO-PHE-PRO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	74	50	11	13	0	0	0
3	F	9	74	50	11	13	0	0	0
3	I	9	74	50	11	13	0	0	0
3	L	9	74	50	11	13	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
4	A	1	5	4	1		0	0
4	A	1	5	4	1		0	0
4	A	1	5	4	1		0	0
4	B	1	5	4	1		0	0
4	B	1	5	4	1		0	0
4	B	1	5	4	1		0	0
4	B	1	5	4	1		0	0
4	E	1	5	4	1		0	0
4	G	1	5	4	1		0	0
4	G	1	5	4	1		0	0
4	H	1	5	4	1		0	0
4	K	1	5	4	1		0	0

- Molecule 5 is water.

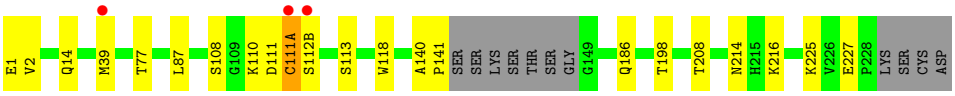
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	56	56	56	0	0
			Total	O		
5	B	67	67	67	0	0
			Total	O		
5	C	2	2	2	0	0
			Total	O		
5	D	53	53	53	0	0
			Total	O		
5	E	69	69	69	0	0
			Total	O		
5	F	1	1	1	0	0
			Total	O		
5	G	50	50	50	0	0
			Total	O		
5	H	35	35	35	0	0
			Total	O		
5	I	1	1	1	0	0
			Total	O		
5	J	22	22	22	0	0
			Total	O		
5	K	5	5	5	0	0
			Total	O		
5	L	2	2	2	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.

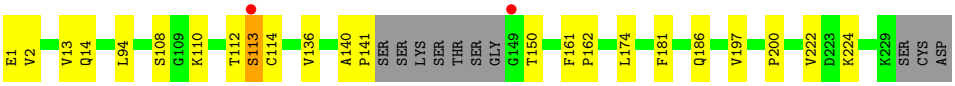
• Molecule 1: 1E01 Fab fragment heavy chain

Chain A:



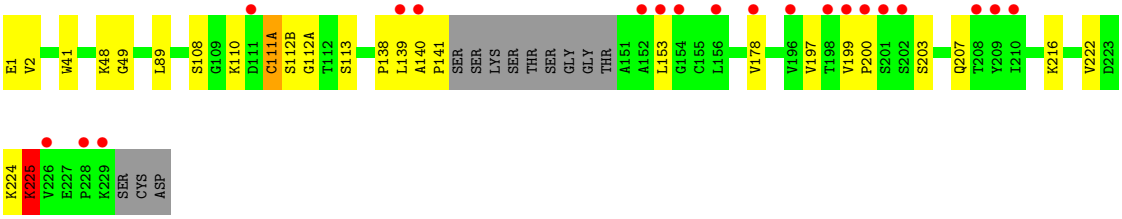
• Molecule 1: 1E01 Fab fragment heavy chain

Chain D:



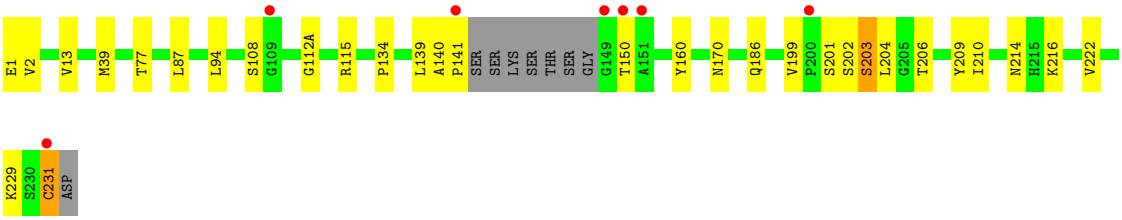
• Molecule 1: 1E01 Fab fragment heavy chain

Chain G:



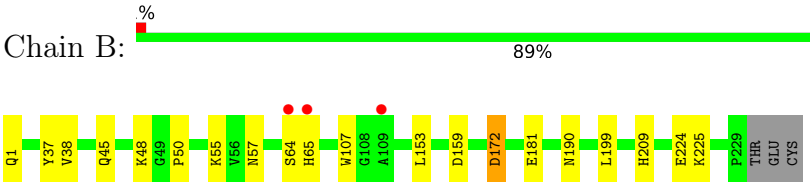
• Molecule 1: 1E01 Fab fragment heavy chain

Chain J:



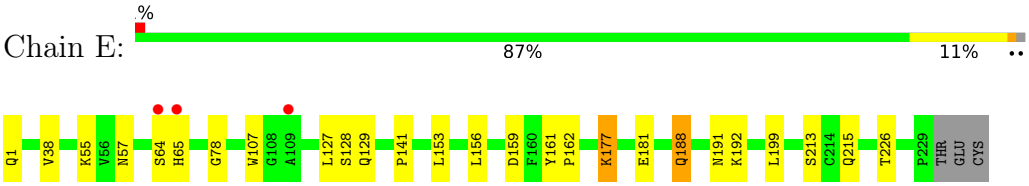
• Molecule 2: 1E01 Fab fragment light chain

Chain B:



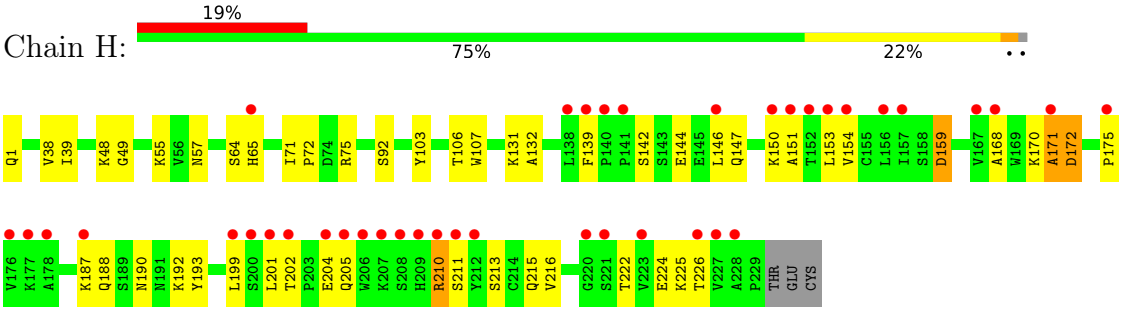
• Molecule 2: 1E01 Fab fragment light chain

Chain E:



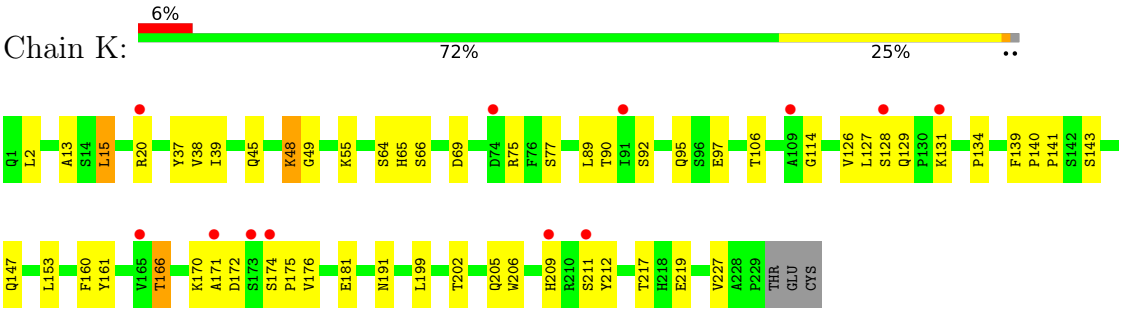
• Molecule 2: 1E01 Fab fragment light chain

Chain H:



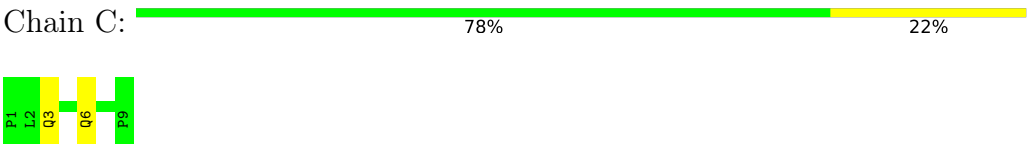
• Molecule 2: 1E01 Fab fragment light chain

Chain K:



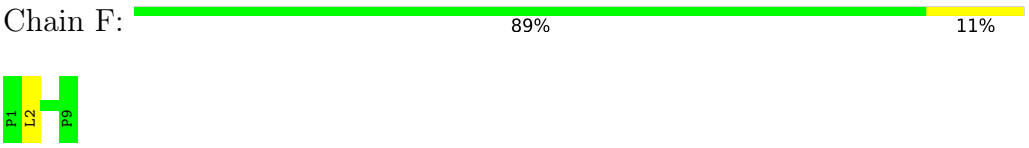
• Molecule 3: peptide PRO-LEU-GLN-PRO-GLU-GLN-PRO-PHE-PRO

Chain C:



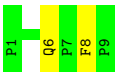
• Molecule 3: peptide PRO-LEU-GLN-PRO-GLU-GLN-PRO-PHE-PRO

Chain F:



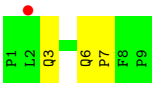
• Molecule 3: peptide PRO-LEU-GLN-PRO-GLU-GLN-PRO-PHE-PRO

Chain I:



- Molecule 3: peptide PRO-LEU-GLN-PRO-GLU-GLN-PRO-PHE-PRO

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.45Å 141.28Å 177.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.53 – 2.35 110.43 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (88.53-2.35) 93.2 (110.43-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.205 , 0.241 0.204 , 0.241	Depositor DCC
R_{free} test set	5828 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13491	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.33	0/1629	0.56	0/2215
1	D	0.30	0/1638	0.56	0/2226
1	G	0.36	1/1627 (0.1%)	0.58	0/2211
1	J	0.28	0/1650	0.55	0/2242
2	B	0.29	0/1630	0.52	0/2219
2	E	0.29	0/1630	0.54	0/2219
2	H	0.29	0/1630	0.59	0/2219
2	K	0.27	0/1630	0.57	1/2219 (0.0%)
3	C	0.28	0/78	0.54	0/107
3	F	0.33	0/78	0.48	0/107
3	I	0.31	0/78	0.46	0/107
3	L	0.27	0/78	0.50	0/107
All	All	0.30	1/13376 (0.0%)	0.56	1/18198 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	225	LYS	CD-CE	-5.08	1.38	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	15	LEU	CA-CB-CG	5.54	128.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	113	SER	Peptide

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	1593	0	1550	15	0
1	D	1602	0	1563	16	0
1	G	1591	0	1553	23	0
1	J	1614	0	1573	23	0
2	B	1593	0	1546	17	0
2	E	1593	0	1546	20	0
2	H	1593	0	1546	42	0
2	K	1593	0	1546	53	0
3	C	74	0	72	2	0
3	F	74	0	72	1	0
3	I	74	0	72	1	0
3	L	74	0	72	3	0
4	A	15	0	0	0	0
4	B	20	0	0	1	0
4	E	5	0	0	0	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
4	K	5	0	0	1	0
5	A	56	0	0	0	0
5	B	67	0	0	2	0
5	C	2	0	0	0	0
5	D	53	0	0	0	0
5	E	69	0	0	0	0
5	F	1	0	0	0	0
5	G	50	0	0	0	0
5	H	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	1	0	0	0	0
5	J	22	0	0	0	0
5	K	5	0	0	0	0
5	L	2	0	0	0	0
All	All	13491	0	12711	194	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 8.

All (194) 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:48:LYS:HD2	1:G:49:GLY:H	1.22	1.01
2:H:187:LYS:HE2	2:H:193:TYR:CZ	2.07	0.90
2:K:170:LYS:HD2	2:K:171:ALA:H	1.36	0.90
1:G:111(A):CYS:HB3	1:G:113:SER:HB2	1.52	0.90
2:E:177:LYS:HD3	2:E:177:LYS:H	1.37	0.88
1:G:138:PRO:HD3	1:G:224:LYS:HE3	1.57	0.86
1:G:225:LYS:HD2	1:G:225:LYS:H	1.41	0.85
1:J:150:THR:HA	1:J:201:SER:OG	1.78	0.84
1:A:111(A):CYS:H	1:A:112(B):SER:HA	1.43	0.81
2:H:168:ALA:HB3	2:H:215:GLN:HB2	1.64	0.79
2:B:45:GLN:HB2	2:B:48:LYS:HD3	1.64	0.79
2:H:187:LYS:CE	2:H:193:TYR:CZ	2.67	0.78
3:I:6:GLN:HE21	3:I:8:PHE:H	1.33	0.76
2:K:45:GLN:HB2	2:K:48:LYS:HE3	1.67	0.75
2:B:64:SER:O	2:B:65:HIS:ND1	2.21	0.72
2:H:159:ASP:HA	2:H:192:LYS:HG2	1.70	0.72
2:E:64:SER:O	2:E:65:HIS:ND1	2.23	0.72
1:G:178:VAL:HG12	1:G:197:VAL:HG22	1.71	0.71
2:K:170:LYS:HD2	2:K:171:ALA:N	2.05	0.71
2:H:64:SER:O	2:H:65:HIS:ND1	2.25	0.70
1:G:48:LYS:CD	1:G:49:GLY:H	2.01	0.70
2:B:65:HIS:NE2	5:B:403:HOH:O	2.24	0.70
2:K:20:ARG:HH22	2:K:90:THR:HA	1.56	0.69
2:H:144:GLU:O	2:H:147:GLN:NE2	2.25	0.69
2:K:64:SER:O	2:K:65:HIS:ND1	2.27	0.68
2:H:187:LYS:HE2	2:H:193:TYR:CE2	2.30	0.67
2:H:172:ASP:O	2:H:210:ARG:NH2	2.27	0.66
2:E:153:LEU:HD12	2:E:199:LEU:HD23	1.78	0.65
2:B:38:VAL:HG22	2:B:57:ASN:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:GLN:OE1	2:E:1:GLN:N	2.28	0.64
1:A:111(A):CYS:H	1:A:112(B):SER:CA	2.11	0.64
2:B:153:LEU:HD12	2:B:199:LEU:HD23	1.80	0.64
2:H:170:LYS:HG3	2:H:213:SER:HB2	1.80	0.64
1:J:214:ASN:HD21	1:J:216:LYS:HE3	1.62	0.63
2:K:171:ALA:HA	2:K:212:TYR:HA	1.79	0.63
2:H:170:LYS:HA	2:H:175:PRO:HA	1.83	0.61
2:K:202:THR:HG23	2:K:205:GLN:H	1.64	0.61
2:K:20:ARG:HH12	2:K:90:THR:HA	1.64	0.61
2:H:187:LYS:CE	2:H:193:TYR:CE2	2.85	0.59
2:K:20:ARG:NH2	2:K:90:THR:HG23	2.17	0.59
2:H:48:LYS:HD2	2:H:49:GLY:H	1.68	0.59
2:E:127:LEU:O	2:E:128:SER:OG	2.14	0.59
2:K:37:TYR:CE2	3:L:3:GLN:HB3	2.38	0.59
1:A:1:GLU:HG2	1:A:2:VAL:H	1.68	0.59
2:H:144:GLU:N	2:H:144:GLU:OE2	2.35	0.58
1:J:1:GLU:HG2	1:J:2:VAL:H	1.69	0.58
1:A:186:GLN:HG2	2:B:181:GLU:HG3	1.86	0.57
1:J:202:SER:C	1:J:204:LEU:H	2.08	0.57
2:E:38:VAL:HG22	2:E:57:ASN:HB3	1.85	0.57
2:K:170:LYS:HB2	2:K:175:PRO:HA	1.86	0.57
2:K:206:TRP:HH2	2:K:227:VAL:HG13	1.70	0.56
2:H:142:SER:O	2:H:146:LEU:HD12	2.05	0.56
2:K:170:LYS:HE3	2:K:174:SER:O	2.05	0.56
2:E:177:LYS:H	2:E:177:LYS:CD	2.14	0.56
1:A:14:GLN:HG3	1:J:222:VAL:HG22	1.87	0.56
1:J:170:ASN:ND2	1:J:210:ILE:H	2.03	0.56
2:K:38:VAL:HG13	3:L:3:GLN:OE1	2.06	0.55
1:J:108:SER:OG	2:K:55:LYS:NZ	2.39	0.55
1:D:14:GLN:HG3	1:G:222:VAL:HG22	1.87	0.55
1:D:1:GLU:HG2	1:D:2:VAL:H	1.71	0.55
1:J:229:LYS:NZ	1:J:231:CYS:O	2.38	0.55
2:H:132:ALA:CB	2:H:192:LYS:HE3	2.37	0.54
1:J:202:SER:O	1:J:204:LEU:N	2.40	0.54
1:J:214:ASN:ND2	1:J:216:LYS:HE3	2.23	0.54
1:G:111(A):CYS:HA	1:G:112(B):SER:OG	2.08	0.53
2:H:210:ARG:NH1	2:H:211:SER:O	2.41	0.53
2:H:213:SER:OG	2:H:226:THR:HG22	2.09	0.53
1:D:108:SER:OG	2:E:55:LYS:NZ	2.42	0.53
4:B:301:SO4:O3	5:B:401:HOH:O	2.19	0.53
2:K:20:ARG:NH2	2:K:90:THR:HA	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:SER:OG	2:H:55:LYS:NZ	2.42	0.52
2:K:166:THR:HG23	2:K:217:THR:HB	1.90	0.52
2:B:37:TYR:CE2	3:C:3:GLN:HB3	2.43	0.52
2:K:129:GLN:HB2	2:K:161:TYR:CE1	2.44	0.52
2:H:150:LYS:HD2	2:H:151:ALA:H	1.74	0.52
2:K:202:THR:HG22	2:K:205:GLN:OE1	2.08	0.52
1:A:111:ASP:CB	1:A:111(A):CYS:HA	2.39	0.52
1:J:13:VAL:HG11	1:J:94:LEU:HD13	1.91	0.52
1:A:39:MET:HB3	1:A:87:LEU:HD22	1.93	0.51
2:K:77:SER:OG	2:K:90:THR:HB	2.11	0.51
2:H:187:LYS:HE2	2:H:193:TYR:CE1	2.46	0.50
1:A:110:LYS:HG3	2:B:107:TRP:HZ2	1.77	0.50
1:D:186:GLN:HG2	2:E:181:GLU:HG3	1.94	0.50
2:H:38:VAL:HG22	2:H:57:ASN:HB3	1.93	0.50
2:K:20:ARG:NH1	2:K:90:THR:HA	2.27	0.49
2:H:170:LYS:CG	2:H:213:SER:HB2	2.42	0.49
2:H:187:LYS:NZ	2:H:193:TYR:CE2	2.80	0.49
1:J:115:ARG:NH1	2:K:69:ASP:HB2	2.27	0.49
2:K:170:LYS:HA	2:K:176:VAL:HG12	1.94	0.49
2:H:159:ASP:HA	2:H:192:LYS:CG	2.42	0.49
1:D:13:VAL:HG11	1:D:94:LEU:HD13	1.96	0.48
1:G:1:GLU:HG2	1:G:2:VAL:H	1.77	0.48
1:G:48:LYS:HD2	1:G:49:GLY:N	2.08	0.48
1:G:110:LYS:HG3	2:H:107:TRP:HZ2	1.78	0.48
1:D:112:THR:H	1:D:114:CYS:H	1.62	0.47
2:H:39:ILE:HG22	2:H:106:THR:HB	1.97	0.47
1:A:225:LYS:HE2	1:A:227:GLU:OE1	2.13	0.47
2:E:213:SER:HG	2:E:226:THR:HG1	1.59	0.47
2:K:140:PRO:HG3	2:K:227:VAL:HG21	1.97	0.47
1:J:140:ALA:HB1	1:J:141:PRO:HA	1.97	0.47
2:B:1:GLN:OE1	2:B:1:GLN:N	2.40	0.46
2:H:139:PHE:HB2	2:H:154:VAL:HG13	1.97	0.46
2:H:168:ALA:N	2:H:215:GLN:O	2.47	0.46
1:D:174:LEU:HD21	1:D:197:VAL:HG21	1.97	0.46
2:K:127:LEU:O	2:K:128:SER:HB3	2.14	0.46
2:H:210:ARG:HD2	2:H:211:SER:HB2	1.98	0.46
2:K:206:TRP:CH2	2:K:227:VAL:HG13	2.51	0.46
2:B:159:ASP:OD1	2:B:190:ASN:ND2	2.49	0.46
1:J:150:THR:HA	1:J:201:SER:HG	1.81	0.46
2:E:65:HIS:CE1	2:E:78:GLY:H	2.34	0.45
1:D:110:LYS:HG3	2:E:107:TRP:HZ2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:134:PRO:HB3	1:J:160:TYR:HB3	1.99	0.45
1:J:202:SER:OG	1:J:203:SER:N	2.33	0.45
2:K:15:LEU:HD13	2:K:126:VAL:HG11	1.98	0.45
2:K:131:LYS:HZ1	2:K:219:GLU:HG3	1.80	0.45
2:K:45:GLN:H	2:K:48:LYS:HE3	1.82	0.45
1:A:208:THR:HG23	1:A:225:LYS:HE3	1.99	0.45
2:B:172:ASP:OD2	2:B:209:HIS:HB3	2.17	0.45
2:K:143:SER:O	2:K:147:GLN:HG3	2.17	0.45
1:G:41:TRP:NE1	1:G:89:LEU:HB2	2.32	0.45
2:K:140:PRO:HA	2:K:153:LEU:HD13	1.99	0.45
2:K:141:PRO:HD3	2:K:153:LEU:HD13	1.99	0.44
1:A:108:SER:OG	2:B:55:LYS:NZ	2.51	0.44
2:H:202:THR:N	2:H:205:GLN:OE1	2.50	0.44
1:A:140:ALA:HB1	1:A:141:PRO:HA	1.99	0.44
2:H:216:VAL:O	2:H:222:THR:HA	2.18	0.44
2:K:153:LEU:HB2	2:K:199:LEU:HB3	2.00	0.44
2:H:153:LEU:HD12	2:H:199:LEU:HD12	2.00	0.44
1:A:214:ASN:OD1	1:A:216:LYS:NZ	2.50	0.44
1:D:1:GLU:CG	1:D:2:VAL:H	2.29	0.44
1:D:140:ALA:HB1	1:D:141:PRO:HA	1.99	0.44
1:D:150:THR:HG21	1:D:200:PRO:HA	2.00	0.44
1:J:39:MET:HB3	1:J:87:LEU:HD22	1.99	0.44
2:K:20:ARG:NH1	2:K:89:LEU:O	2.49	0.44
1:A:111:ASP:HB3	1:A:111(A):CYS:HA	1.99	0.43
1:G:49:GLY:HA2	2:H:103:TYR:OH	2.18	0.43
2:K:114:GLY:HA2	3:L:7:PRO:O	2.18	0.43
1:J:170:ASN:HD21	1:J:210:ILE:H	1.63	0.43
1:J:216:LYS:HA	1:J:216:LYS:HE2	2.00	0.43
2:B:64:SER:OG	2:B:65:HIS:N	2.52	0.43
2:H:215:GLN:HG2	2:H:224:GLU:CG	2.48	0.43
2:K:170:LYS:HZ3	2:K:172:ASP:H	1.66	0.43
2:K:2:LEU:HD21	2:K:106:THR:HG23	2.00	0.43
1:D:161:PHE:HA	1:D:162:PRO:HA	1.84	0.43
2:E:161:TYR:CG	2:E:162:PRO:HA	2.54	0.43
1:G:203:SER:O	1:G:207:GLN:HB3	2.18	0.43
1:D:181:PHE:CZ	2:E:156:LEU:HB3	2.54	0.43
1:G:141:PRO:C	1:G:153:LEU:HB3	2.39	0.43
1:J:186:GLN:HG2	2:K:181:GLU:HG3	1.99	0.43
1:G:139:LEU:HB3	2:H:139:PHE:CD2	2.54	0.43
1:G:199:VAL:HG12	1:G:200:PRO:O	2.18	0.42
1:G:199:VAL:HG13	1:G:200:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:139:LEU:HB3	2:K:139:PHE:CD1	2.54	0.42
1:J:199:VAL:HG11	1:J:209:TYR:CE2	2.54	0.42
2:K:97:GLU:HG3	2:K:191:ASN:HD21	1.84	0.42
2:K:170:LYS:NZ	2:K:172:ASP:H	2.16	0.42
2:K:48:LYS:HD2	2:K:49:GLY:O	2.19	0.42
2:B:37:TYR:CD2	3:C:3:GLN:HB3	2.54	0.42
2:E:159:ASP:OD1	2:E:192:LYS:HD2	2.20	0.42
1:G:216:LYS:HB3	1:G:216:LYS:HE2	1.93	0.42
2:H:75:ARG:HB3	2:H:92:SER:O	2.20	0.42
1:G:140:ALA:HB1	1:G:141:PRO:HA	2.01	0.42
2:K:39:ILE:HG22	2:K:106:THR:HB	2.01	0.42
2:E:65:HIS:HE1	2:E:78:GLY:O	2.02	0.42
2:E:129:GLN:HB2	2:E:161:TYR:CE1	2.54	0.42
2:K:75:ARG:HG3	2:K:92:SER:O	2.20	0.42
2:H:188:GLN:HB2	2:H:190:ASN:OD1	2.19	0.41
1:D:136:VAL:HB	1:D:222:VAL:HG11	2.01	0.41
2:K:66:SER:HA	4:K:301:SO4:O1	2.19	0.41
2:H:215:GLN:HG2	2:H:224:GLU:HG3	2.03	0.41
1:D:112:THR:HA	1:D:113:SER:HA	1.55	0.41
2:H:139:PHE:HB2	2:H:154:VAL:CG1	2.51	0.41
1:J:203:SER:HA	1:J:206:THR:OG1	2.20	0.41
1:D:224:LYS:HD2	1:D:224:LYS:HA	1.93	0.41
2:H:171:ALA:O	2:H:210:ARG:NH1	2.36	0.41
2:K:75:ARG:NH1	2:K:95:GLN:OE1	2.52	0.41
2:E:141:PRO:HD3	2:E:153:LEU:HD23	2.03	0.41
2:E:188:GLN:O	2:E:191:ASN:N	2.46	0.41
2:H:150:LYS:HD2	2:H:201:LEU:O	2.21	0.41
2:B:153:LEU:HB2	2:B:199:LEU:HB3	2.03	0.41
2:K:20:ARG:CZ	2:K:20:ARG:HA	2.50	0.41
2:K:45:GLN:CB	2:K:48:LYS:HE3	2.45	0.41
2:K:129:GLN:HB2	2:K:161:TYR:CZ	2.56	0.41
2:K:172:ASP:CG	2:K:209:HIS:HE1	2.23	0.41
2:K:170:LYS:HG3	2:K:172:ASP:H	1.85	0.41
1:G:48:LYS:CG	1:G:49:GLY:N	2.84	0.40
2:K:134:PRO:HA	2:K:160:PHE:HB3	2.03	0.40
1:G:225:LYS:H	1:G:225:LYS:CD	2.18	0.40
2:H:71:ILE:HA	2:H:72:PRO:HD3	1.98	0.40
2:K:13:ALA:O	2:K:126:VAL:HA	2.21	0.40
1:A:118:TRP:CE2	2:B:50:PRO:HB2	2.56	0.40
2:B:224:GLU:O	2:B:225:LYS:HD2	2.21	0.40
2:E:153:LEU:HB2	2:E:199:LEU:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:LEU:HD23	3:F:2:LEU:HA	1.88	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	212/227 (93%)	209 (99%)	3 (1%)	0	100	100
1	D	213/227 (94%)	208 (98%)	5 (2%)	0	100	100
1	G	211/227 (93%)	204 (97%)	6 (3%)	1 (0%)	29	32
1	J	215/227 (95%)	207 (96%)	6 (3%)	2 (1%)	17	17
2	B	211/216 (98%)	199 (94%)	11 (5%)	1 (0%)	29	32
2	E	211/216 (98%)	197 (93%)	13 (6%)	1 (0%)	29	32
2	H	211/216 (98%)	199 (94%)	10 (5%)	2 (1%)	17	17
2	K	211/216 (98%)	199 (94%)	11 (5%)	1 (0%)	29	32
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	I	7/9 (78%)	7 (100%)	0	0	100	100
3	L	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1723/1808 (95%)	1650 (96%)	65 (4%)	8 (0%)	29	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	215	GLN
2	H	171	ALA
2	H	172	ASP

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Mol	Chain	Res	Type
1	J	203	SER
1	G	112(A)	GLY
1	J	112(A)	GLY
2	K	211	SER
2	B	172	ASP

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	178/188 (95%)	174 (98%)	4 (2%)	52	63
1	D	179/188 (95%)	179 (100%)	0	100	100
1	G	178/188 (95%)	176 (99%)	2 (1%)	73	84
1	J	181/188 (96%)	179 (99%)	2 (1%)	73	84
2	B	179/182 (98%)	179 (100%)	0	100	100
2	E	179/182 (98%)	177 (99%)	2 (1%)	73	84
2	H	179/182 (98%)	173 (97%)	6 (3%)	37	46
2	K	179/182 (98%)	177 (99%)	2 (1%)	73	84
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	5
3	F	9/9 (100%)	9 (100%)	0	100	100
3	I	9/9 (100%)	9 (100%)	0	100	100
3	L	9/9 (100%)	8 (89%)	1 (11%)	6	5
All	All	1468/1516 (97%)	1448 (99%)	20 (1%)	67	78

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	111(A)	CYS
1	A	113	SER
1	A	198	THR
3	C	6	GLN

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Mol	Chain	Res	Type
2	E	177	LYS
2	E	188	GLN
1	G	111(A)	CYS
1	G	225	LYS
2	H	1	GLN
2	H	131	LYS
2	H	159	ASP
2	H	204	GLU
2	H	210	ARG
2	H	225	LYS
1	J	77	THR
1	J	231	CYS
2	K	48	LYS
2	K	166	THR
3	L	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	29	HIS
2	B	215	GLN
2	E	191	ASN
1	G	3	GLN
1	G	170	ASN
3	I	6	GLN
1	J	170	ASN
2	K	209	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)

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)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	301	-	4,4,4	0.16	0	6,6,6	0.04	0
4	SO4	B	304	2	4,4,4	0.16	0	6,6,6	0.06	0
4	SO4	K	301	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	302	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	G	301	-	4,4,4	0.16	0	6,6,6	0.08	0
4	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	B	303	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	E	301	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	H	301	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	G	302	-	4,4,4	0.13	0	6,6,6	0.07	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	SO4	1	0
4	K	301	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	216/227 (95%)	0.27	3 (1%)	75	83	37, 54, 89, 101	0
1	D	217/227 (95%)	0.20	2 (0%)	84	90	45, 56, 88, 110	0
1	G	215/227 (94%)	0.66	20 (9%)	8	14	39, 62, 138, 168	0
1	J	219/227 (96%)	0.31	7 (3%)	47	59	48, 68, 110, 143	0
2	B	213/216 (98%)	0.16	3 (1%)	75	83	39, 58, 91, 106	0
2	E	213/216 (98%)	0.15	3 (1%)	75	83	43, 57, 93, 101	0
2	H	213/216 (98%)	0.92	40 (18%)	1	2	40, 76, 169, 200	0
2	K	213/216 (98%)	0.38	12 (5%)	24	35	70, 101, 125, 140	0
3	C	9/9 (100%)	0.22	0	100	100	47, 59, 82, 84	0
3	F	9/9 (100%)	0.14	0	100	100	53, 64, 82, 84	0
3	I	9/9 (100%)	0.21	0	100	100	48, 57, 86, 87	0
3	L	9/9 (100%)	0.62	1 (11%)	5	8	63, 80, 102, 114	0
All	All	1755/1808 (97%)	0.38	91 (5%)	27	39	37, 64, 124, 200	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	209	TYR	8.1
1	G	152	ALA	6.1
2	K	20	ARG	5.2
2	H	175	PRO	5.2
2	H	227	VAL	5.0
1	G	200	PRO	4.8
2	H	140	PRO	4.7
2	H	152	THR	4.7
1	G	199	VAL	4.5
2	H	210	ARG	4.4
1	G	140	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	J	231	CYS	4.4
1	G	154	GLY	4.2
2	H	153	LEU	4.2
2	H	212	TYR	4.1
2	H	205	GLN	4.1
1	G	153	LEU	4.0
2	H	178	ALA	3.8
1	G	198	THR	3.8
1	J	149	GLY	3.7
2	H	176	VAL	3.7
2	H	211	SER	3.6
2	H	167	VAL	3.6
2	H	150	LYS	3.6
1	G	210	ILE	3.5
2	H	228	ALA	3.5
2	H	207	LYS	3.5
2	H	201	LEU	3.5
1	G	208	THR	3.4
1	J	151	ALA	3.4
2	B	64	SER	3.4
2	K	174	SER	3.4
1	J	200	PRO	3.4
2	H	139	PHE	3.3
2	H	138	LEU	3.3
2	H	208	SER	3.3
1	G	226	VAL	3.2
2	K	131	LYS	3.2
2	H	209	HIS	3.1
2	H	221	SER	3.1
2	H	154	VAL	3.0
2	K	171	ALA	3.0
2	H	204	GLU	3.0
1	G	139	LEU	3.0
1	J	141	PRO	3.0
2	E	65	HIS	3.0
2	B	65	HIS	3.0
2	K	91	ILE	2.9
1	G	111	ASP	2.9
2	H	177	LYS	2.8
1	G	178	VAL	2.8
2	H	146	LEU	2.8
2	E	64	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	206	TRP	2.7
1	G	156	LEU	2.6
2	K	173	SER	2.6
2	H	141	PRO	2.6
2	H	65	HIS	2.6
2	H	200	SER	2.6
2	H	187	LYS	2.6
1	A	112(B)	SER	2.5
2	B	109	ALA	2.5
2	K	128	SER	2.5
2	H	171	ALA	2.5
2	H	199	LEU	2.4
1	J	109	GLY	2.4
1	G	229	LYS	2.4
2	H	168	ALA	2.4
3	L	2	LEU	2.3
2	H	202	THR	2.3
1	G	228	PRO	2.3
2	K	74	ASP	2.3
2	H	151	ALA	2.3
1	G	196	VAL	2.3
1	A	111(A)	CYS	2.2
2	H	220	GLY	2.2
1	J	150	THR	2.2
2	K	209	HIS	2.2
1	G	202	SER	2.2
2	H	223	VAL	2.1
2	K	211	SER	2.1
1	D	113	SER	2.1
1	A	39	MET	2.1
1	D	149	GLY	2.1
2	H	157	ILE	2.1
2	H	226	THR	2.1
2	E	109	ALA	2.0
2	K	109	ALA	2.0
1	G	201	SER	2.0
2	K	165	VAL	2.0
2	H	156	LEU	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	SO4	A	303	5/5	0.54	0.31	166,168,169,169	0
4	SO4	B	304	5/5	0.56	0.21	107,136,137,139	0
4	SO4	A	301	5/5	0.67	0.46	165,172,176,176	0
4	SO4	B	303	5/5	0.71	0.20	138,139,142,142	0
4	SO4	B	301	5/5	0.74	0.57	164,167,169,170	0
4	SO4	A	302	5/5	0.75	0.37	153,158,160,162	0
4	SO4	G	302	5/5	0.77	0.29	161,161,162,166	0
4	SO4	K	301	5/5	0.79	0.18	132,133,138,143	0
4	SO4	B	302	5/5	0.81	0.23	148,150,152,153	0
4	SO4	E	301	5/5	0.82	0.17	120,123,129,129	0
4	SO4	H	301	5/5	0.86	0.19	140,140,143,145	0
4	SO4	G	301	5/5	0.87	0.23	118,128,131,138	0

6.5 Other polymers (i)

There are no such residues in this entry.