



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 02:51 PM EST

PDB ID : 3QI0
Title : Structural, thermodynamic and kinetic analysis of the picomolar binding affinity interaction of the beta-lactamase inhibitor protein-II (BLIP-II) with class A beta-lactamases
Authors : Brown, N.G.; Chow, D.C.; Sankaran, B.; Zwart, P.; Prasad, B.V.V.; Palzkill, T.
Deposited on : 2011-01-26
Resolution : 2.80 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)
Xtrriage (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

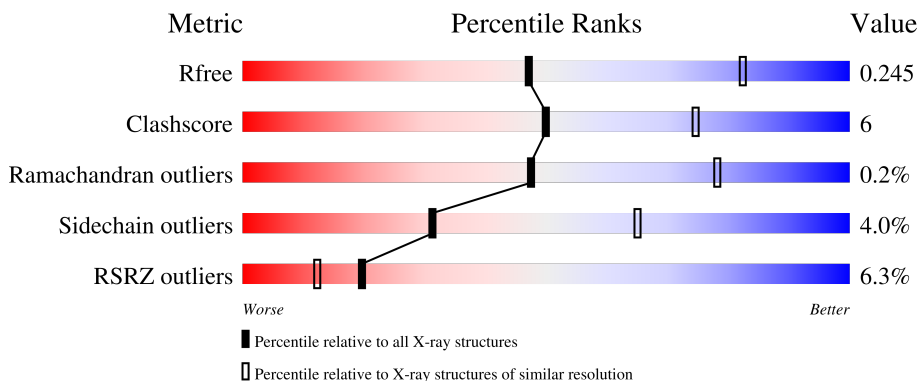
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



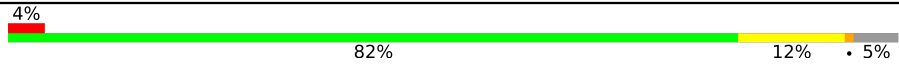

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	 83% 10% • 5%
1	B	282	 86% 8% • 5%
1	C	282	 89% 6% 5%
1	D	282	 87% 8% • 5%

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Mol	Chain	Length	Quality of chain
1	E	282	
1	F	282	

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
2	SO4	B	24	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11817 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-lactamase inhibitory protein II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	1904	1192	326	385	1	0	0	0
1	B	268	1904	1192	326	385	1	0	0	0
1	C	269	1911	1196	327	387	1	0	0	0
1	D	269	1911	1196	327	387	1	0	0	0
1	E	269	1911	1196	327	387	1	0	0	0
1	F	268	1902	1190	325	386	1	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	GLY	-	expression tag	UNP O87916
A	313	SER	-	expression tag	UNP O87916
A	314	GLY	-	expression tag	UNP O87916
A	315	SER	-	expression tag	UNP O87916
A	316	GLY	-	expression tag	UNP O87916
A	317	HIS	-	expression tag	UNP O87916
A	318	HIS	-	expression tag	UNP O87916
A	319	HIS	-	expression tag	UNP O87916
A	320	HIS	-	expression tag	UNP O87916
A	321	HIS	-	expression tag	UNP O87916
A	322	HIS	-	expression tag	UNP O87916
B	312	GLY	-	expression tag	UNP O87916
B	313	SER	-	expression tag	UNP O87916
B	314	GLY	-	expression tag	UNP O87916
B	315	SER	-	expression tag	UNP O87916
B	316	GLY	-	expression tag	UNP O87916
B	317	HIS	-	expression tag	UNP O87916

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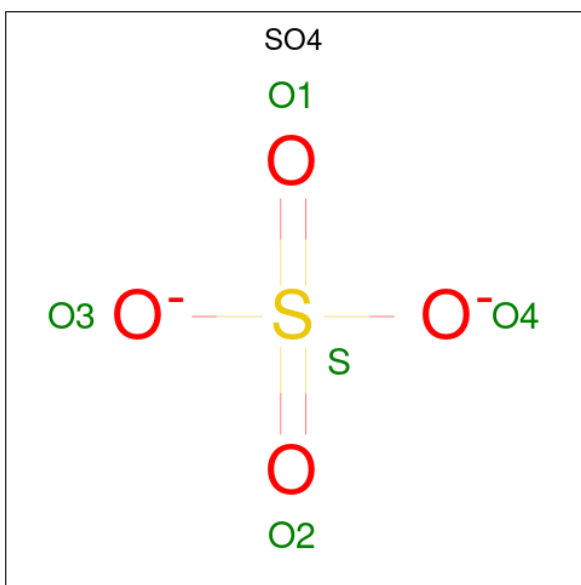
Chain	Residue	Modelled	Actual	Comment	Reference
B	318	HIS	-	expression tag	UNP O87916
B	319	HIS	-	expression tag	UNP O87916
B	320	HIS	-	expression tag	UNP O87916
B	321	HIS	-	expression tag	UNP O87916
B	322	HIS	-	expression tag	UNP O87916
C	312	GLY	-	expression tag	UNP O87916
C	313	SER	-	expression tag	UNP O87916
C	314	GLY	-	expression tag	UNP O87916
C	315	SER	-	expression tag	UNP O87916
C	316	GLY	-	expression tag	UNP O87916
C	317	HIS	-	expression tag	UNP O87916
C	318	HIS	-	expression tag	UNP O87916
C	319	HIS	-	expression tag	UNP O87916
C	320	HIS	-	expression tag	UNP O87916
C	321	HIS	-	expression tag	UNP O87916
C	322	HIS	-	expression tag	UNP O87916
D	312	GLY	-	expression tag	UNP O87916
D	313	SER	-	expression tag	UNP O87916
D	314	GLY	-	expression tag	UNP O87916
D	315	SER	-	expression tag	UNP O87916
D	316	GLY	-	expression tag	UNP O87916
D	317	HIS	-	expression tag	UNP O87916
D	318	HIS	-	expression tag	UNP O87916
D	319	HIS	-	expression tag	UNP O87916
D	320	HIS	-	expression tag	UNP O87916
D	321	HIS	-	expression tag	UNP O87916
D	322	HIS	-	expression tag	UNP O87916
E	312	GLY	-	expression tag	UNP O87916
E	313	SER	-	expression tag	UNP O87916
E	314	GLY	-	expression tag	UNP O87916
E	315	SER	-	expression tag	UNP O87916
E	316	GLY	-	expression tag	UNP O87916
E	317	HIS	-	expression tag	UNP O87916
E	318	HIS	-	expression tag	UNP O87916
E	319	HIS	-	expression tag	UNP O87916
E	320	HIS	-	expression tag	UNP O87916
E	321	HIS	-	expression tag	UNP O87916
E	322	HIS	-	expression tag	UNP O87916
F	312	GLY	-	expression tag	UNP O87916
F	313	SER	-	expression tag	UNP O87916
F	314	GLY	-	expression tag	UNP O87916
F	315	SER	-	expression tag	UNP O87916

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Chain	Residue	Modelled	Actual	Comment	Reference
F	316	GLY	-	expression tag	UNP O87916
F	317	HIS	-	expression tag	UNP O87916
F	318	HIS	-	expression tag	UNP O87916
F	319	HIS	-	expression tag	UNP O87916
F	320	HIS	-	expression tag	UNP O87916
F	321	HIS	-	expression tag	UNP O87916
F	322	HIS	-	expression tag	UNP O87916

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

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

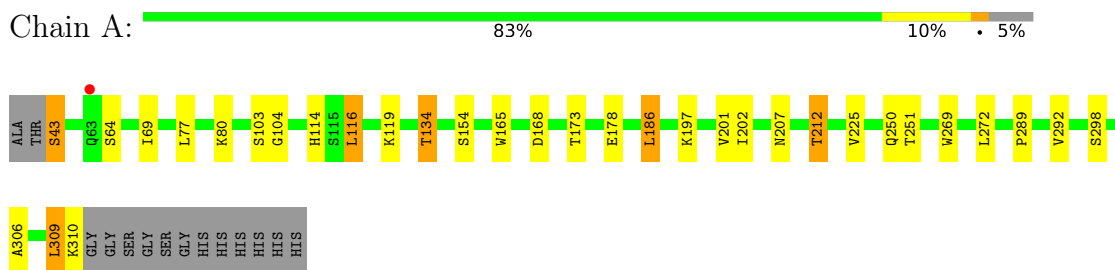
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	48	Total	O	0	0
			48	48		
3	C	37	Total	O	0	0
			37	37		
3	D	41	Total	O	0	0
			41	41		
3	E	19	Total	O	0	0
			19	19		
3	F	7	Total	O	0	0
			7	7		

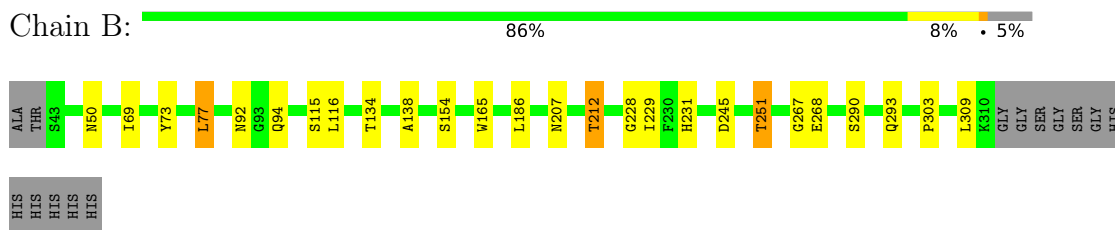
3 Residue-property plots [i](#)

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.

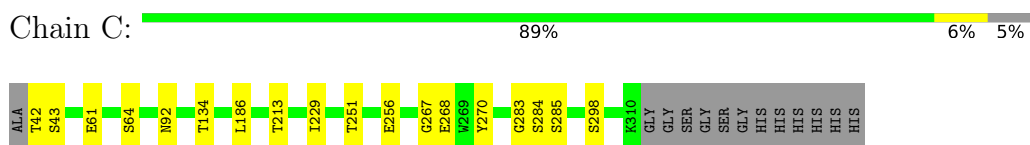
- Molecule 1: Beta-lactamase inhibitory protein II



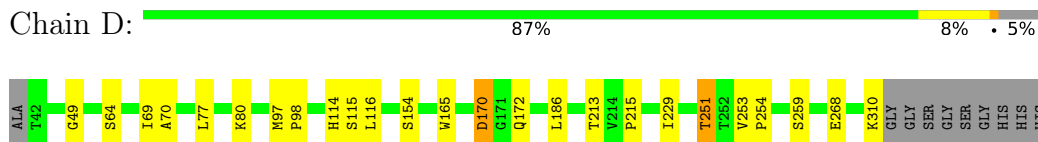
- Molecule 1: Beta-lactamase inhibitory protein II



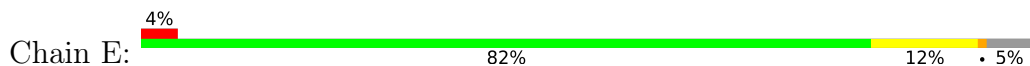
- Molecule 1: Beta-lactamase inhibitory protein II

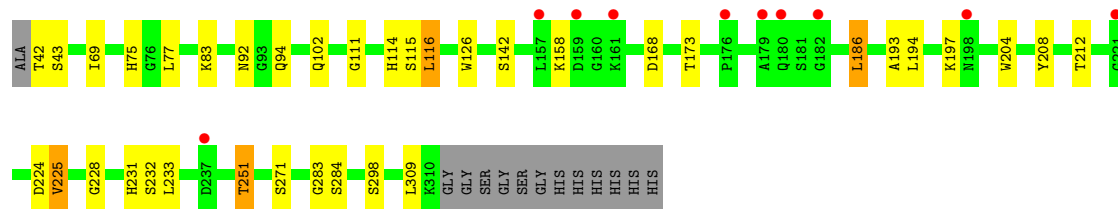


- Molecule 1: Beta-lactamase inhibitory protein II

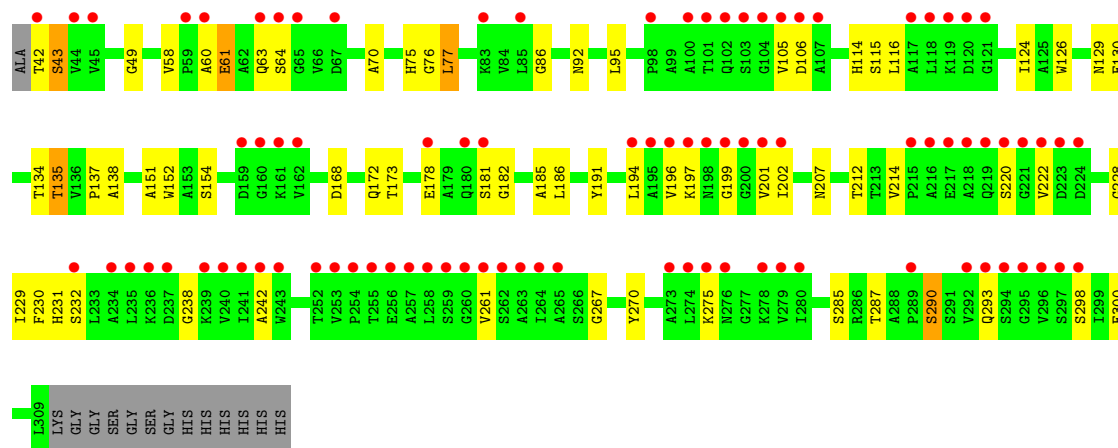


- Molecule 1: Beta-lactamase inhibitory protein II





• Molecule 1: Beta-lactamase inhibitory protein II



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.61Å 114.74Å 173.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.17 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.80) 99.3 (49.17-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.15 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.195 , 0.243 0.198 , 0.245	Depositor DCC
R_{free} test set	2898 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtrriage
Anisotropy	0.089	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.011 for k,h,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11817	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.85	0/1945	0.81	2/2656 (0.1%)
1	B	0.84	0/1945	0.79	3/2656 (0.1%)
1	C	0.86	0/1952	0.77	0/2666
1	D	0.88	0/1952	0.80	1/2666 (0.0%)
1	E	0.85	0/1952	0.81	2/2666 (0.1%)
1	F	1.07	0/1943	0.80	0/2655
All	All	0.90	0/11689	0.80	8/15965 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	170	ASP	CB-CG-OD1	-7.45	111.59	118.30
1	E	168	ASP	CB-CG-OD1	6.84	124.45	118.30
1	B	245	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	B	267	GLY	N-CA-C	-5.58	99.15	113.10
1	E	116	LEU	CB-CG-CD1	-5.40	101.82	111.00
1	B	245	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	168	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	116	LEU	CB-CG-CD1	-5.08	102.37	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1904	0	1820	23	0
1	B	1904	0	1820	15	0
1	C	1911	0	1827	7	0
1	D	1911	0	1827	14	0
1	E	1911	0	1827	24	0
1	F	1902	0	1814	51	0
2	A	35	0	0	0	0
2	B	40	0	0	1	0
2	C	20	0	0	0	0
2	D	30	0	0	1	0
2	E	40	0	0	0	0
2	F	10	0	0	1	0
3	A	47	0	0	0	0
3	B	48	0	0	0	0
3	C	37	0	0	0	0
3	D	41	0	0	0	0
3	E	19	0	0	0	0
3	F	7	0	0	0	0
All	All	11817	0	10935	130	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 6.

All (130) 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:F:207:ASN:CG	1:F:212:THR:HG22	1.85	0.97
1:E:212:THR:O	1:E:212:THR:HG22	1.78	0.81
1:C:213:THR:HG22	1:C:213:THR:O	1.82	0.80
1:F:207:ASN:CB	1:F:212:THR:HG22	2.15	0.76
1:A:69:ILE:HG13	1:A:309:LEU:HD11	1.68	0.74
1:B:207:ASN:CG	1:B:212:THR:HG22	2.10	0.72
1:F:42:THR:O	1:F:64:SER:HA	1.91	0.70
1:E:212:THR:O	1:E:212:THR:CG2	2.39	0.69
1:F:207:ASN:HB2	1:F:212:THR:HG22	1.74	0.68
1:F:182:GLY:O	1:F:197:LYS:HG3	1.95	0.67
1:F:172:GLN:OE1	1:F:191:TYR:HA	1.95	0.66
1:F:290:SER:HA	1:F:293:GLN:HG2	1.76	0.66
1:F:267:GLY:HA3	1:F:270:TYR:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:ASN:HB2	1:F:212:THR:CG2	2.27	0.65
1:B:77:LEU:HD21	1:B:115:SER:HB3	1.77	0.65
1:E:208:TYR:HE1	1:F:130:GLU:HG2	1.61	0.64
1:F:186:LEU:O	1:F:186:LEU:HD12	1.99	0.63
1:C:42:THR:O	1:C:64:SER:HA	1.98	0.62
1:B:69:ILE:HG13	1:B:309:LEU:HD11	1.82	0.62
1:F:70:ALA:HB3	1:F:77:LEU:HB2	1.81	0.61
1:F:181:SER:O	1:F:197:LYS:HE3	2.02	0.60
1:A:114:HIS:CD2	1:A:116:LEU:HD11	2.37	0.59
1:A:250:GLN:NE2	1:A:269:TRP:HE3	2.00	0.59
1:F:129:ASN:HB2	1:F:134:THR:OG1	2.03	0.58
1:B:154:SER:HB2	1:B:165:TRP:CE2	2.38	0.58
1:E:208:TYR:CE1	1:F:130:GLU:HG2	2.38	0.58
1:C:42:THR:HG22	1:C:43:SER:H	1.68	0.58
1:E:224:ASP:CG	1:E:225:VAL:H	2.07	0.58
1:A:250:GLN:HE21	1:A:269:TRP:HE3	1.52	0.57
1:B:92:ASN:HD22	1:B:94:GLN:HE22	1.52	0.57
1:F:49:GLY:N	2:F:30:SO4:O1	2.36	0.57
1:C:283:GLY:O	1:C:284:SER:HB2	2.06	0.56
1:F:178:GLU:HB3	1:F:202:ILE:HD13	1.87	0.55
1:F:42:THR:HA	1:F:64:SER:HB2	1.87	0.55
1:E:77:LEU:HD21	1:E:115:SER:HB3	1.89	0.54
1:F:201:VAL:HB	1:F:214:VAL:CG1	2.38	0.54
1:C:42:THR:HG22	1:C:43:SER:N	2.22	0.54
1:E:75:HIS:CD2	1:E:77:LEU:HD13	2.43	0.54
1:E:173:THR:HG22	1:E:173:THR:O	2.08	0.53
1:F:116:LEU:HD21	1:F:154:SER:HB3	1.89	0.53
1:F:168:ASP:OD1	1:F:173:THR:HB	2.08	0.53
1:F:77:LEU:HD21	1:F:115:SER:HB3	1.91	0.53
1:F:228:GLY:HA3	1:F:231:HIS:CE1	2.44	0.52
1:E:142:SER:O	1:E:158:LYS:HE3	2.10	0.52
1:D:229:ILE:HG22	1:D:268:GLU:O	2.10	0.52
1:D:115:SER:O	1:D:116:LEU:HD12	2.08	0.52
1:E:116:LEU:HD12	1:E:116:LEU:N	2.25	0.51
1:F:201:VAL:HB	1:F:214:VAL:HG11	1.92	0.51
1:F:60:ALA:HA	1:F:63:GLN:HG2	1.92	0.51
1:E:83:LYS:HE3	1:E:102:GLN:NE2	2.25	0.51
1:D:154:SER:HB2	1:D:165:TRP:CE2	2.45	0.51
1:F:151:ALA:HB3	1:F:152:TRP:CE3	2.46	0.51
1:E:92:ASN:HD22	1:E:94:GLN:HE22	1.60	0.50
1:A:207:ASN:CG	1:A:212:THR:HG22	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:HB2	1:A:165:TRP:CE2	2.47	0.50
1:A:64:SER:O	1:A:80:LYS:HE3	2.12	0.49
1:A:103:SER:O	1:A:119:LYS:HE3	2.11	0.49
1:C:267:GLY:HA3	1:C:270:TYR:CE2	2.47	0.49
1:F:116:LEU:HD12	1:F:116:LEU:N	2.27	0.49
1:A:201:VAL:HG12	1:A:202:ILE:N	2.27	0.49
1:E:194:LEU:HD11	1:E:232:SER:HB3	1.94	0.49
1:A:201:VAL:CG1	1:A:202:ILE:N	2.76	0.49
1:F:173:THR:CG2	1:F:173:THR:O	2.60	0.49
1:B:290:SER:HA	1:B:293:GLN:HG2	1.94	0.48
1:B:116:LEU:HD12	1:B:116:LEU:N	2.28	0.48
1:E:228:GLY:HA3	1:E:231:HIS:CE1	2.48	0.48
1:D:69:ILE:HG22	1:D:70:ALA:N	2.28	0.48
1:A:178:GLU:O	1:A:197:LYS:HD2	2.13	0.48
1:B:138:ALA:HB2	2:B:31:SO4:O3	2.14	0.48
1:F:105:VAL:HG12	1:F:106:ASP:N	2.28	0.48
1:F:114:HIS:CD2	1:F:116:LEU:HD11	2.49	0.48
1:F:173:THR:O	1:F:173:THR:HG22	2.14	0.48
1:E:69:ILE:HG12	1:E:309:LEU:HD11	1.96	0.47
1:A:114:HIS:CD2	1:A:116:LEU:CD1	2.97	0.47
1:F:186:LEU:HD12	1:F:186:LEU:C	2.34	0.47
1:F:199:GLY:O	1:F:222:VAL:HB	2.15	0.47
1:B:229:ILE:HG22	1:B:268:GLU:O	2.14	0.47
1:A:250:GLN:NE2	1:A:269:TRP:CE3	2.80	0.47
1:F:232:SER:O	1:F:242:ALA:HA	2.16	0.46
1:A:272:LEU:HD11	1:A:306:ALA:HB1	1.97	0.45
1:F:238:GLY:HA2	1:F:261:VAL:O	2.16	0.45
1:A:69:ILE:CG1	1:A:309:LEU:HD11	2.44	0.45
1:B:73:TYR:HA	1:B:303:PRO:HG2	1.99	0.45
1:D:213:THR:O	1:D:215:PRO:HD3	2.17	0.45
1:F:137:PRO:O	1:F:138:ALA:C	2.56	0.44
1:F:194:LEU:HD11	1:F:232:SER:HB3	2.00	0.44
1:A:104:GLY:O	1:A:119:LYS:HG3	2.17	0.44
1:A:289:PRO:HD2	1:A:292:VAL:CG2	2.48	0.44
1:A:116:LEU:HD21	1:A:154:SER:HB3	1.98	0.44
1:B:212:THR:HG23	1:B:212:THR:O	2.18	0.44
1:D:116:LEU:HD21	1:D:154:SER:HB3	2.00	0.44
1:E:224:ASP:CG	1:E:225:VAL:N	2.71	0.44
1:F:70:ALA:HA	1:F:300:GLU:OE2	2.17	0.44
1:F:75:HIS:HD2	1:F:77:LEU:HD13	1.83	0.44
1:E:115:SER:HB2	1:E:126:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:HIS:CD2	1:F:77:LEU:HD13	2.53	0.43
1:A:289:PRO:HD2	1:A:292:VAL:HG21	2.00	0.43
1:D:49:GLY:N	2:D:14:SO4:O1	2.52	0.43
1:E:193:ALA:HB3	1:E:204:TRP:CE2	2.54	0.43
1:F:75:HIS:HB2	1:F:95:LEU:HD21	2.00	0.43
1:D:253:VAL:HA	1:D:254:PRO:HD3	1.93	0.43
1:E:111:GLY:HA3	1:E:114:HIS:CE1	2.53	0.43
1:F:42:THR:HG22	1:F:43:SER:N	2.33	0.43
1:F:124:ILE:HG22	1:F:126:TRP:CE3	2.53	0.43
1:A:298:SER:HB2	1:A:309:LEU:HD22	2.00	0.43
1:F:115:SER:HB2	1:F:126:TRP:CE2	2.54	0.43
1:F:70:ALA:HB3	1:F:77:LEU:CB	2.48	0.43
1:A:43:SER:HB3	1:A:310:LYS:HB2	2.00	0.42
1:F:76:GLY:O	1:F:86:GLY:HA2	2.19	0.42
1:F:114:HIS:NE2	1:F:116:LEU:HD11	2.34	0.42
1:B:228:GLY:HA3	1:B:231:HIS:CE1	2.54	0.42
1:E:233:LEU:HD11	1:E:271:SER:HB3	2.02	0.42
1:E:186:LEU:HD12	1:E:186:LEU:O	2.20	0.42
1:F:261:VAL:HG22	1:F:275:LYS:HB2	2.01	0.42
1:F:185:ALA:HB3	1:F:196:VAL:CG2	2.49	0.42
1:A:186:LEU:HD12	1:A:186:LEU:O	2.20	0.41
1:B:69:ILE:CG1	1:B:309:LEU:HD11	2.49	0.41
1:D:310:LYS:HD3	1:F:135:THR:HG21	2.01	0.41
1:E:283:GLY:O	1:E:284:SER:HB2	2.19	0.41
1:D:114:HIS:CD2	1:D:116:LEU:HD11	2.55	0.41
1:B:251:THR:O	1:B:251:THR:CG2	2.68	0.41
1:A:134:THR:O	1:A:134:THR:HG23	2.21	0.41
1:D:64:SER:O	1:D:80:LYS:HE3	2.21	0.41
1:E:251:THR:O	1:E:251:THR:CG2	2.69	0.41
1:C:229:ILE:HG22	1:C:268:GLU:O	2.21	0.41
1:D:97:MET:HA	1:D:98:PRO:HD3	1.97	0.41
1:D:115:SER:C	1:D:116:LEU:HD12	2.42	0.41
1:E:173:THR:O	1:E:173:THR:CG2	2.68	0.40
1:F:229:ILE:HG23	1:F:230:PHE:N	2.36	0.40
1:B:50:ASN:HD21	1:D:251:THR:HG23	1.86	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	266/282 (94%)	260 (98%)	6 (2%)	0	100	100
1	B	266/282 (94%)	263 (99%)	3 (1%)	0	100	100
1	C	267/282 (95%)	263 (98%)	3 (1%)	1 (0%)	34	66
1	D	267/282 (95%)	260 (97%)	7 (3%)	0	100	100
1	E	267/282 (95%)	264 (99%)	3 (1%)	0	100	100
1	F	266/282 (94%)	248 (93%)	16 (6%)	2 (1%)	19	49
All	All	1599/1692 (94%)	1558 (97%)	38 (2%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	285	SER
1	F	61	GLU
1	F	220	SER

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	182/191 (95%)	173 (95%)	9 (5%)	25	57
1	B	182/191 (95%)	177 (97%)	5 (3%)	44	78
1	C	183/191 (96%)	176 (96%)	7 (4%)	33	67
1	D	183/191 (96%)	177 (97%)	6 (3%)	38	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	183/191 (96%)	176 (96%)	7 (4%)	33	67
1	F	182/191 (95%)	172 (94%)	10 (6%)	21	52
All	All	1095/1146 (96%)	1051 (96%)	44 (4%)	31	65

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	77	LEU
1	A	134	THR
1	A	173	THR
1	A	186	LEU
1	A	212	THR
1	A	225	VAL
1	A	251	THR
1	A	309	LEU
1	B	77	LEU
1	B	134	THR
1	B	186	LEU
1	B	212	THR
1	B	251	THR
1	C	61	GLU
1	C	92	ASN
1	C	134	THR
1	C	186	LEU
1	C	251	THR
1	C	256	GLU
1	C	298	SER
1	D	77	LEU
1	D	170	ASP
1	D	172	GLN
1	D	186	LEU
1	D	251	THR
1	D	259	SER
1	E	42	THR
1	E	43	SER
1	E	186	LEU
1	E	197	LYS
1	E	225	VAL
1	E	251	THR
1	E	298	SER

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Mol	Chain	Res	Type
1	F	43	SER
1	F	58	VAL
1	F	61	GLU
1	F	77	LEU
1	F	92	ASN
1	F	135	THR
1	F	285	SER
1	F	287	THR
1	F	290	SER
1	F	298	SER

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

Mol	Chain	Res	Type
1	B	50	ASN
1	B	92	ASN
1	C	92	ASN
1	D	92	ASN
1	D	293	GLN
1	E	92	ASN
1	E	102	GLN
1	F	92	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](#)

35 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	E	2	-	4,4,4	0.23	0	6,6,6	0.54	0
2	SO4	D	9	-	4,4,4	0.30	0	6,6,6	0.42	0
2	SO4	F	32	-	4,4,4	0.44	0	6,6,6	0.23	0
2	SO4	E	5	-	4,4,4	0.16	0	6,6,6	0.40	0
2	SO4	B	2	-	4,4,4	0.38	0	6,6,6	0.90	0
2	SO4	E	29	-	4,4,4	0.27	0	6,6,6	0.51	0
2	SO4	C	3	-	4,4,4	0.12	0	6,6,6	0.56	0
2	SO4	E	18	-	4,4,4	0.23	0	6,6,6	0.53	0
2	SO4	C	6	-	4,4,4	0.32	0	6,6,6	0.31	0
2	SO4	F	30	-	4,4,4	0.31	0	6,6,6	1.25	1 (16%)
2	SO4	B	7	-	4,4,4	0.27	0	6,6,6	0.53	0
2	SO4	D	1	-	4,4,4	0.19	0	6,6,6	0.07	0
2	SO4	B	19	-	4,4,4	0.13	0	6,6,6	0.36	0
2	SO4	D	13	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	A	1	-	4,4,4	0.43	0	6,6,6	0.94	0
2	SO4	D	16	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	A	4	-	4,4,4	0.38	0	6,6,6	0.89	0
2	SO4	A	11	-	4,4,4	0.22	0	6,6,6	0.40	0
2	SO4	B	24	-	4,4,4	0.15	0	6,6,6	0.29	0
2	SO4	C	8	-	4,4,4	0.21	0	6,6,6	0.30	0
2	SO4	A	15	-	4,4,4	0.19	0	6,6,6	0.42	0
2	SO4	C	12	-	4,4,4	0.26	0	6,6,6	0.43	0
2	SO4	B	21	-	4,4,4	0.21	0	6,6,6	0.46	0
2	SO4	B	3	-	4,4,4	0.21	0	6,6,6	0.49	0
2	SO4	E	22	-	4,4,4	0.17	0	6,6,6	0.29	0
2	SO4	A	23	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	E	17	-	4,4,4	0.22	0	6,6,6	0.24	0
2	SO4	A	25	-	4,4,4	0.18	0	6,6,6	0.43	0
2	SO4	B	31	-	4,4,4	0.42	0	6,6,6	0.57	0
2	SO4	D	14	-	4,4,4	0.09	0	6,6,6	0.36	0
2	SO4	D	27	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	A	26	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	B	10	-	4,4,4	0.16	0	6,6,6	0.46	0
2	SO4	E	28	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	E	20	-	4,4,4	0.29	0	6,6,6	0.34	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	F	30	SO4	O4-S-O3	-2.59	98.01	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	30	SO4	1	0
2	B	31	SO4	1	0
2	D	14	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	268/282 (95%)	-0.25	1 (0%) 92 91	12, 20, 37, 69	0
1	B	268/282 (95%)	-0.38	0 100 100	13, 20, 36, 57	0
1	C	269/282 (95%)	-0.36	0 100 100	13, 20, 35, 62	0
1	D	269/282 (95%)	-0.44	0 100 100	14, 21, 38, 64	0
1	E	269/282 (95%)	0.28	10 (3%) 41 31	15, 24, 43, 62	0
1	F	268/282 (95%)	1.33	90 (33%) 0 0	25, 39, 64, 87	0
All	All	1611/1692 (95%)	0.03	101 (6%) 20 12	12, 23, 52, 87	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	237	ASP	6.7
1	F	255	THR	5.7
1	F	257	ALA	5.5
1	F	221	GLY	5.3
1	F	258	LEU	5.2
1	F	297	SER	5.2
1	F	216	ALA	5.0
1	F	261	VAL	4.9
1	F	276	ASN	4.8
1	F	259	SER	4.8
1	F	240	VAL	4.8
1	F	219	GLN	4.7
1	F	104	GLY	4.6
1	F	236	LYS	4.6
1	F	294	SER	4.6
1	F	220	SER	4.5
1	F	120	ASP	4.5
1	F	223	ASP	4.4
1	F	260	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	241	ILE	4.4
1	F	118	LEU	4.3
1	F	218	ALA	4.0
1	F	239	LYS	4.0
1	A	63	GLN	3.9
1	F	234	ALA	3.8
1	F	42	THR	3.8
1	F	292	VAL	3.7
1	F	159	ASP	3.7
1	F	217	GLU	3.6
1	F	274	LEU	3.6
1	F	279	VAL	3.6
1	F	263	ALA	3.6
1	F	199	GLY	3.6
1	F	280	ILE	3.5
1	F	293	GLN	3.5
1	F	262	SER	3.5
1	F	254	PRO	3.4
1	F	100	ALA	3.4
1	F	273	ALA	3.4
1	F	107	ALA	3.4
1	F	198	ASN	3.4
1	F	242	ALA	3.4
1	F	222	VAL	3.4
1	F	119	LYS	3.4
1	F	215	PRO	3.3
1	F	201	VAL	3.3
1	F	253	VAL	3.3
1	F	67	ASP	3.3
1	F	59	PRO	3.2
1	F	103	SER	3.2
1	F	181	SER	3.2
1	F	106	ASP	3.1
1	F	298	SER	3.1
1	F	296	VAL	3.1
1	F	235	LEU	3.0
1	F	180	GLN	3.0
1	F	256	GLU	3.0
1	F	64	SER	2.9
1	F	101	THR	2.9
1	F	44	VAL	2.8
1	F	200	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	182	GLY	2.8
1	E	198	ASN	2.8
1	F	105	VAL	2.8
1	F	243	TRP	2.8
1	E	180	GLN	2.8
1	F	63	GLN	2.8
1	F	289	PRO	2.7
1	F	295	GLY	2.7
1	F	224	ASP	2.7
1	F	60	ALA	2.7
1	F	65	GLY	2.6
1	F	275	LYS	2.6
1	E	237	ASP	2.6
1	F	83	LYS	2.6
1	F	252	THR	2.5
1	F	117	ALA	2.5
1	F	265	ALA	2.5
1	F	278	LYS	2.5
1	E	221	GLY	2.5
1	F	102	GLN	2.4
1	F	196	VAL	2.4
1	E	157	LEU	2.4
1	F	160	GLY	2.3
1	E	161	LYS	2.3
1	F	195	ALA	2.3
1	F	197	LYS	2.2
1	F	162	VAL	2.2
1	E	176	PRO	2.2
1	F	85	LEU	2.2
1	F	202	ILE	2.2
1	F	121	GLY	2.2
1	E	179	ALA	2.2
1	F	178	GLU	2.2
1	F	194	LEU	2.1
1	F	232	SER	2.1
1	F	98	PRO	2.1
1	E	159	ASP	2.1
1	F	161	LYS	2.0
1	F	264	ILE	2.0
1	F	45	VAL	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
2	SO4	A	23	5/5	0.72	0.32	114,114,114,114	0
2	SO4	B	24	5/5	0.72	0.49	115,116,116,116	0
2	SO4	D	9	5/5	0.78	0.30	80,80,82,84	0
2	SO4	A	15	5/5	0.82	0.29	89,89,90,90	0
2	SO4	D	27	5/5	0.85	0.34	116,117,117,117	0
2	SO4	E	17	5/5	0.85	0.26	98,98,99,99	0
2	SO4	F	32	5/5	0.86	0.45	78,78,80,81	0
2	SO4	D	14	5/5	0.87	0.24	84,84,84,86	0
2	SO4	E	22	5/5	0.87	0.41	92,92,93,93	0
2	SO4	A	25	5/5	0.87	0.26	76,79,80,80	0
2	SO4	E	20	5/5	0.88	0.33	73,74,75,75	0
2	SO4	C	6	5/5	0.88	0.31	75,75,77,78	0
2	SO4	C	12	5/5	0.88	0.26	82,83,83,84	0
2	SO4	E	28	5/5	0.89	0.27	80,81,82,82	0
2	SO4	D	13	5/5	0.89	0.28	94,95,95,96	0
2	SO4	E	18	5/5	0.90	0.20	86,87,87,87	0
2	SO4	B	10	5/5	0.90	0.25	66,69,69,70	0
2	SO4	D	16	5/5	0.90	0.27	81,81,82,82	0
2	SO4	B	31	5/5	0.90	0.26	71,73,75,76	0
2	SO4	B	19	5/5	0.90	0.39	96,97,97,98	0
2	SO4	A	26	5/5	0.91	0.28	85,85,85,86	0
2	SO4	E	29	5/5	0.91	0.29	81,81,82,83	0
2	SO4	A	11	5/5	0.91	0.48	76,77,78,79	0
2	SO4	B	3	5/5	0.92	0.23	55,55,59,61	0
2	SO4	A	4	5/5	0.93	0.17	59,59,60,60	0
2	SO4	C	8	5/5	0.93	0.22	66,66,67,67	0
2	SO4	F	30	5/5	0.93	0.17	56,60,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	21	5/5	0.93	0.34	72,72,73,74	0
2	SO4	B	7	5/5	0.94	0.26	66,67,68,69	0
2	SO4	B	2	5/5	0.94	0.17	33,34,39,43	0
2	SO4	D	1	5/5	0.95	0.29	62,64,65,66	0
2	SO4	C	3	5/5	0.95	0.20	47,48,50,52	0
2	SO4	E	2	5/5	0.95	0.17	53,54,56,57	0
2	SO4	E	5	5/5	0.95	0.24	68,70,71,71	0
2	SO4	A	1	5/5	0.97	0.14	36,38,41,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.