Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 04:45 PM EDT

PDB ID	:	3E2A
Title	:	H. influenzae beta-carbonic anhydrase, variant Y181F with 100 mM bicarbonate
Authors	:	Rowlett, R.S.; Lee, J.
Deposited on	:	2008-08-05
Resolution	:	2.30 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:

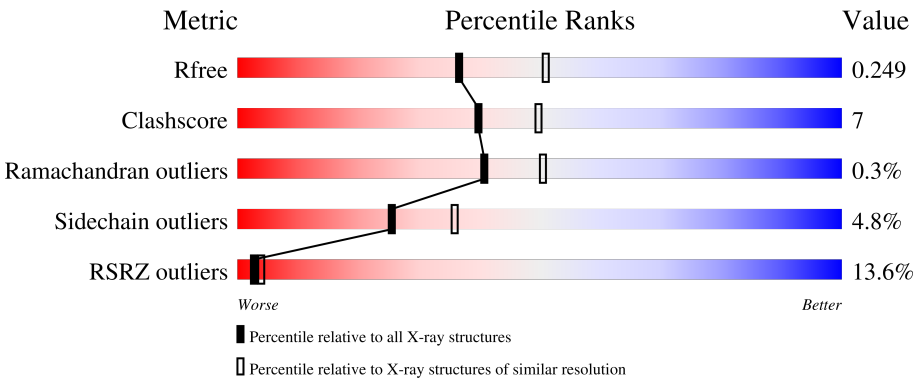
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	229	11% 78% 13% 9%
1	B	229	17% 76% 12% • 10%
1	C	229	13% 73% 14% • 10%
1	D	229	7% 73% 14% • 11%
1	E	229	16% 72% 17% 10%

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Mol	Chain	Length	Quality of chain
1	F	229	9% 79% 9% • 11%

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	232	-	-	X	-
3	SO4	B	232	-	-	X	-
3	SO4	C	232	-	-	X	-
3	SO4	D	232	-	-	X	-
3	SO4	E	233	-	-	X	-
3	SO4	F	231	-	-	X	-
4	BCT	F	232	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10134 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 Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	209	1677	1067	301	300	9	0	0	0
1	B	207	1659	1055	296	299	9	0	0	0
1	C	205	1643	1044	294	296	9	0	0	0
1	D	204	1632	1038	294	291	9	0	0	0
1	E	207	1661	1055	298	299	9	0	0	0
1	F	204	1634	1038	292	295	9	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	PHE	TYR	engineered mutation	UNP P45148
B	181	PHE	TYR	engineered mutation	UNP P45148
C	181	PHE	TYR	engineered mutation	UNP P45148
D	181	PHE	TYR	engineered mutation	UNP P45148
E	181	PHE	TYR	engineered mutation	UNP P45148
F	181	PHE	TYR	engineered mutation	UNP P45148

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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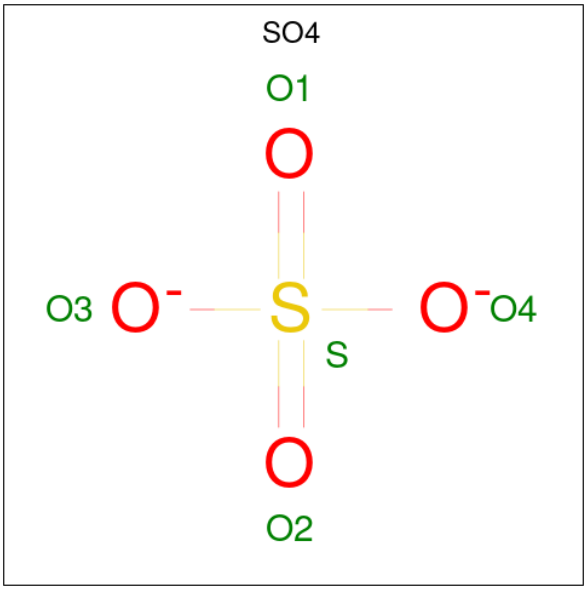
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- 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
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

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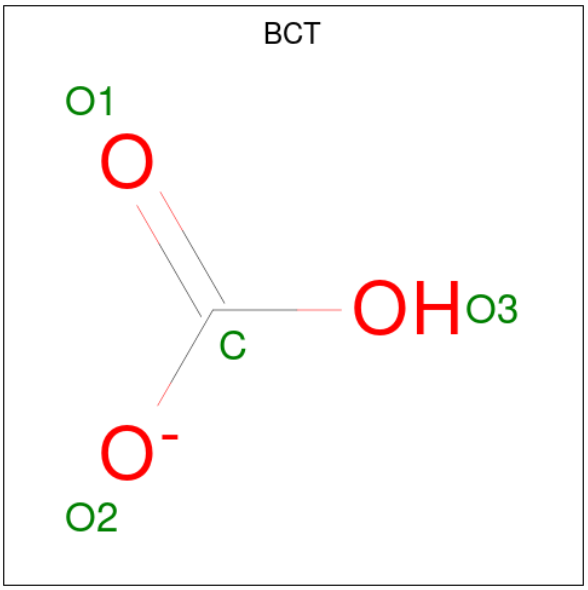
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 4 1 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	18	Total O 18 18	0	0
5	C	24	Total O 24 24	0	0
5	D	27	Total O 27 27	0	0

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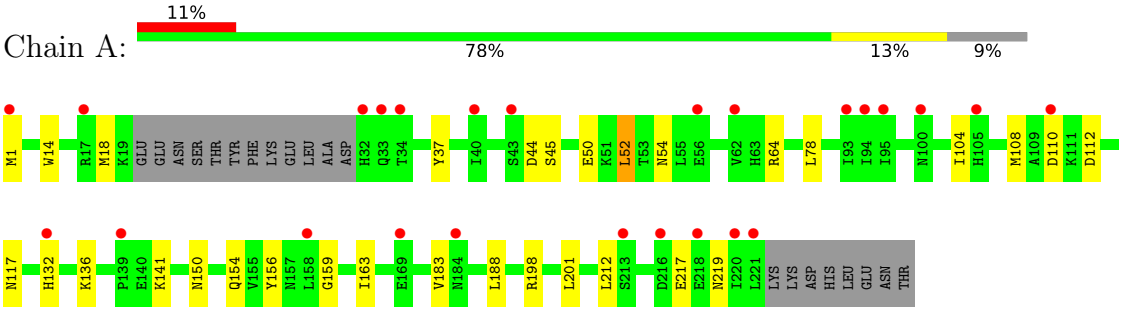
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	E	29	29	29	0	0
			Total	O		
5	F	29	29	29	0	0

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.

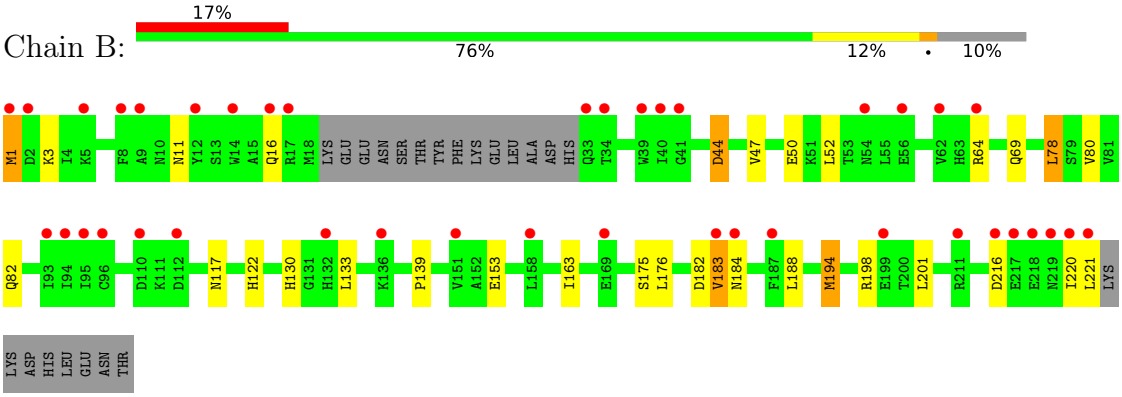
• Molecule 1: Carbonic anhydrase 2

Chain A:



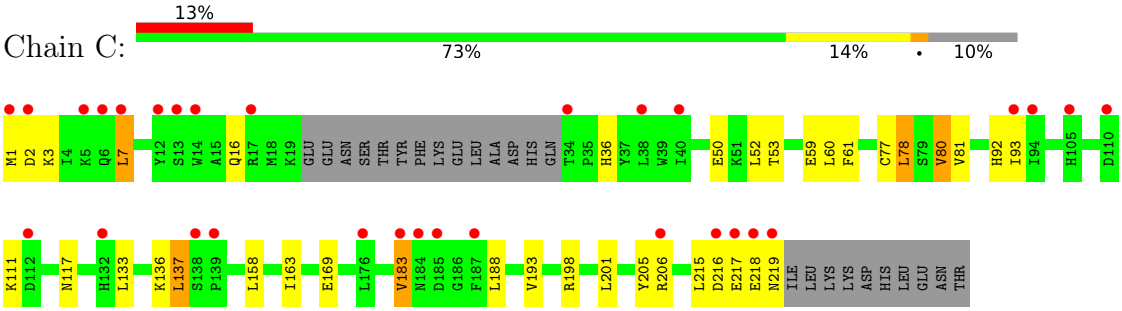
• Molecule 1: Carbonic anhydrase 2

Chain B:



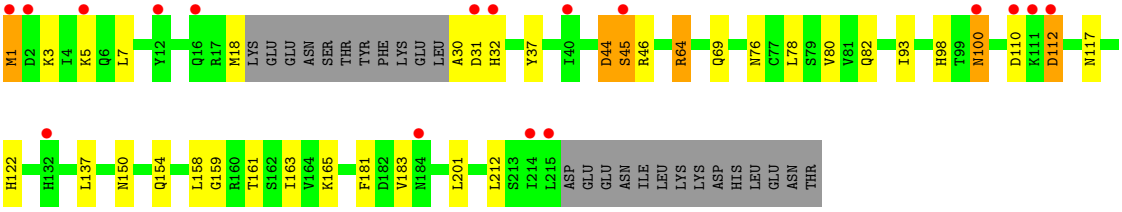
• Molecule 1: Carbonic anhydrase 2

Chain C:



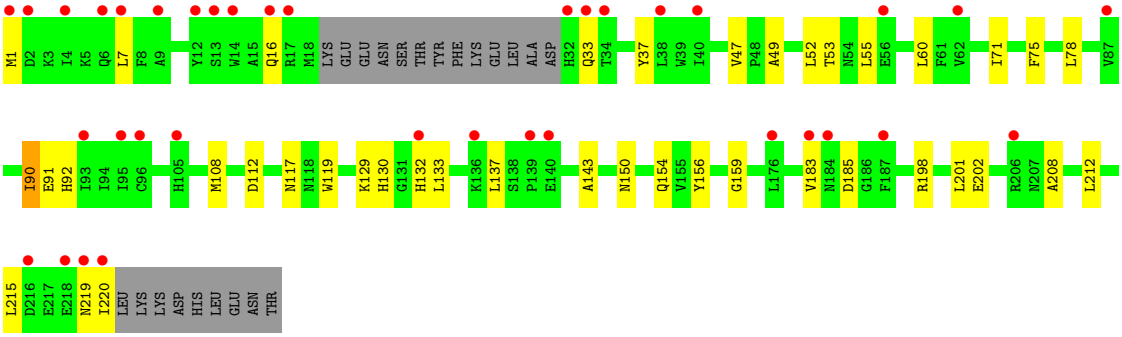
• Molecule 1: Carbonic anhydrase 2

Chain D:



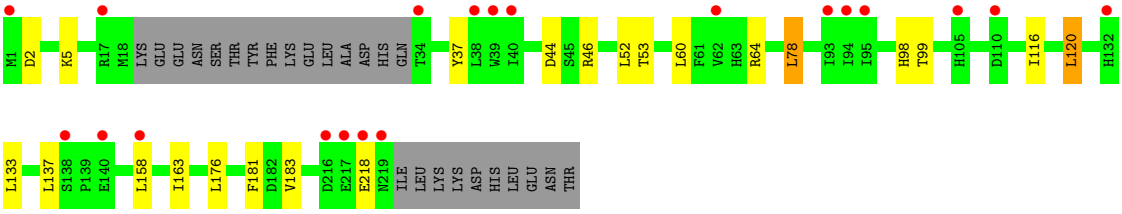
- Molecule 1: Carbonic anhydrase 2

Chain E:



- Molecule 1: Carbonic anhydrase 2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	230.61Å 145.51Å 53.23Å 90.00° 93.78° 90.00°	Depositor
Resolution (Å)	24.78 – 2.30 24.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.78-2.30) 99.9 (24.77-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.244 0.207 , 0.249	Depositor DCC
R_{free} test set	7808 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10134	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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: BCT, ZN, 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	0.54	0/1713	0.69	3/2318 (0.1%)
1	B	0.55	1/1694 (0.1%)	0.62	1/2294 (0.0%)
1	C	0.51	0/1678	0.61	0/2271
1	D	0.58	0/1668	0.68	2/2259 (0.1%)
1	E	0.53	0/1697	0.63	0/2298
1	F	0.58	0/1669	0.67	3/2260 (0.1%)
All	All	0.55	1/10119 (0.0%)	0.65	9/13700 (0.1%)

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	B	11	ASN	CG-ND2	5.55	1.46	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	44	ASP	CB-CA-C	-6.88	96.64	110.40
1	F	64	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	64	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	52	LEU	CA-CB-CG	5.70	128.41	115.30
1	F	64	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	64	ARG	NE-CZ-NH2	-5.50	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	32	HIS	N-CA-C	5.28	125.25	111.00
1	D	64	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	44	ASP	CB-CA-C	-5.11	100.18	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	31	ASP	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	1677	0	1671	20	1
1	B	1659	0	1651	23	0
1	C	1643	0	1634	29	0
1	D	1632	0	1623	30	0
1	E	1661	0	1647	37	0
1	F	1634	0	1621	15	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
3	A	10	0	0	3	0
3	B	10	0	0	2	0
3	C	10	0	0	3	0
3	D	10	0	0	3	0
3	E	15	0	0	3	0
3	F	5	0	0	2	0
4	F	4	0	1	2	0
5	A	31	0	0	0	1
5	B	18	0	0	0	0
5	C	24	0	0	2	0
5	D	27	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	29	0	0	0	0
5	F	29	0	0	0	0
All	All	10134	0	9848	145	1

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 7.

All (145) 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:C:78:LEU:HD22	1:C:163:ILE:CD1	1.80	1.11
1:C:78:LEU:HD22	1:C:163:ILE:HD12	1.31	1.07
1:A:183:VAL:HG11	3:A:232:SO4:O1	1.53	1.07
1:D:78:LEU:HD22	1:D:163:ILE:HD12	1.44	0.98
1:E:220:ILE:HD12	1:E:220:ILE:O	1.64	0.96
1:D:183:VAL:HG21	3:D:232:SO4:O1	1.68	0.93
1:E:47:VAL:HG12	1:E:52:LEU:HD12	1.52	0.92
1:A:78:LEU:HD22	1:A:163:ILE:HD12	1.58	0.86
1:C:78:LEU:CD2	1:C:163:ILE:HD12	2.05	0.86
1:C:80:VAL:HG21	5:C:240:HOH:O	1.78	0.81
1:F:52:LEU:HD22	1:F:181:PHE:CE1	2.15	0.81
1:D:78:LEU:HD22	1:D:163:ILE:CD1	2.17	0.74
1:E:90:ILE:HD11	1:E:92:HIS:O	1.87	0.74
1:D:1:MET:O	1:D:5:LYS:NZ	2.22	0.72
1:C:183:VAL:CG1	3:C:232:SO4:O3	2.39	0.71
1:A:112:ASP:HA	1:A:117:ASN:ND2	2.06	0.69
1:A:183:VAL:CG1	3:A:232:SO4:O1	2.35	0.69
1:B:1:MET:H1	1:B:1:MET:HE2	1.58	0.69
1:B:52:LEU:HD21	1:B:188:LEU:HD21	1.75	0.69
1:E:90:ILE:HD12	1:E:92:HIS:H	1.56	0.68
1:D:45:SER:OG	5:D:249:HOH:O	2.10	0.68
1:A:78:LEU:HD22	1:A:163:ILE:CD1	2.25	0.67
1:D:44:ASP:O	1:D:45:SER:C	2.34	0.66
1:C:53:THR:HG22	1:E:7:LEU:HD21	1.78	0.65
1:E:90:ILE:CD1	1:E:92:HIS:O	2.45	0.65
1:F:52:LEU:CD2	1:F:181:PHE:CE1	2.79	0.64
1:B:1:MET:HE2	1:B:1:MET:N	2.11	0.63
1:C:7:LEU:CD2	1:E:55:LEU:HD11	2.29	0.62
1:E:208:ALA:O	1:E:212:LEU:HD23	1.99	0.62
1:E:108:MET:HE1	1:E:143:ALA:HB2	1.82	0.62
1:F:116:ILE:HG13	1:F:120:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLU:OE2	1:B:50:GLU:N	2.31	0.61
1:A:141:LYS:NZ	1:A:219:ASN:ND2	2.49	0.61
1:A:141:LYS:HZ2	1:A:219:ASN:HD22	1.48	0.60
1:B:78:LEU:HD13	1:B:163:ILE:HD12	1.84	0.59
1:A:44:ASP:O	1:A:45:SER:C	2.41	0.59
1:E:47:VAL:CG1	1:E:52:LEU:HD12	2.32	0.58
1:B:183:VAL:CG1	3:B:232:SO4:O4	2.51	0.58
1:D:1:MET:HE3	1:D:3:LYS:HD2	1.85	0.58
1:A:112:ASP:HA	1:A:117:ASN:HD21	1.69	0.57
1:B:176:LEU:O	1:B:194:MET:HE2	2.04	0.57
1:F:37:TYR:HB2	1:F:60:LEU:HD23	1.84	0.57
1:E:130:HIS:HA	1:E:132:HIS:CE1	2.40	0.57
1:D:112:ASP:HA	1:D:117:ASN:HD21	1.70	0.56
1:B:198:ARG:NH1	1:B:201:LEU:HD23	2.20	0.56
1:C:217:GLU:O	1:C:219:ASN:N	2.39	0.56
1:E:183:VAL:HG13	3:E:233:SO4:O2	2.06	0.56
1:C:61:PHE:CE2	1:C:80:VAL:HG12	2.41	0.55
1:C:137:LEU:HD13	1:C:215:LEU:HD13	1.88	0.55
1:D:76:ASN:O	1:D:80:VAL:HG23	2.06	0.55
1:E:183:VAL:HG12	3:E:233:SO4:O3	2.07	0.55
1:A:141:LYS:NZ	1:A:219:ASN:HD22	2.04	0.55
1:B:175:SER:HB2	1:B:194:MET:HE1	1.88	0.55
1:D:64:ARG:HH21	4:F:232:BCT:C	2.19	0.55
1:A:52:LEU:HD21	1:A:188:LEU:HD21	1.89	0.54
1:C:183:VAL:HG12	3:C:232:SO4:O3	2.07	0.54
1:E:49:ALA:HA	1:E:52:LEU:HD13	1.89	0.54
1:C:183:VAL:HG13	3:C:232:SO4:O4	2.08	0.53
1:C:7:LEU:HD21	1:E:55:LEU:HD11	1.91	0.53
1:D:112:ASP:HA	1:D:117:ASN:ND2	2.24	0.53
1:C:80:VAL:CG2	5:C:240:HOH:O	2.44	0.53
1:D:7:LEU:HD21	1:F:53:THR:HG22	1.90	0.53
1:C:137:LEU:CD1	1:C:215:LEU:HD13	2.39	0.52
1:D:1:MET:C	1:D:5:LYS:NZ	2.63	0.52
1:C:50:GLU:HG3	1:C:60:LEU:HD12	1.90	0.52
1:D:100:ASN:C	1:D:100:ASN:HD22	2.13	0.52
1:D:69:GLN:HE22	1:D:122:HIS:HB2	1.73	0.52
1:B:1:MET:N	1:B:1:MET:CE	2.73	0.51
1:C:7:LEU:HD11	1:E:53:THR:HG22	1.91	0.51
1:B:130:HIS:NE2	1:B:153:GLU:OE2	2.34	0.50
1:D:161:THR:O	1:D:165:LYS:HG3	2.10	0.50
1:F:52:LEU:HD21	1:F:181:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CE	1:B:3:LYS:HB2	2.41	0.50
1:F:133:LEU:O	1:F:137:LEU:HD13	2.12	0.50
1:B:1:MET:H1	1:B:1:MET:CE	2.24	0.49
1:D:181:PHE:CE2	1:D:183:VAL:HG22	2.48	0.49
1:E:183:VAL:CG1	3:E:233:SO4:O3	2.61	0.49
1:A:141:LYS:HZ3	1:A:219:ASN:ND2	2.10	0.49
1:F:99:THR:O	3:F:231:SO4:O3	2.32	0.48
1:B:69:GLN:HE22	1:B:122:HIS:HB2	1.78	0.48
1:C:136:LYS:O	1:C:219:ASN:ND2	2.42	0.48
1:D:44:ASP:O	1:D:46:ARG:N	2.46	0.48
1:A:150:ASN:O	1:A:154:GLN:HG2	2.13	0.48
1:D:78:LEU:HD12	1:E:75:PHE:CE1	2.49	0.48
1:E:37:TYR:HB2	1:E:60:LEU:HD23	1.94	0.47
1:C:93:ILE:HG21	1:C:158:LEU:HD21	1.97	0.47
1:A:132:HIS:O	1:A:136:LYS:HG3	2.13	0.47
1:E:47:VAL:O	1:E:52:LEU:HD11	2.14	0.47
1:E:220:ILE:O	1:E:220:ILE:CD1	2.52	0.47
1:A:14:TRP:O	1:A:18:MET:HG2	2.14	0.47
1:C:78:LEU:HD22	1:C:163:ILE:HD11	1.87	0.47
1:E:71:ILE:HD12	1:E:119:TRP:CH2	2.50	0.47
1:C:52:LEU:HD21	1:C:188:LEU:HD11	1.95	0.46
1:B:183:VAL:HG13	3:B:232:SO4:O4	2.15	0.46
1:E:159:GLY:HA3	1:E:201:LEU:HD22	1.98	0.46
1:B:1:MET:HE1	1:B:3:LYS:HB2	1.98	0.46
1:D:183:VAL:CG2	3:D:232:SO4:O1	2.51	0.46
1:C:198:ARG:NH1	1:C:201:LEU:HD23	2.31	0.46
1:E:7:LEU:O	1:E:7:LEU:HD23	2.17	0.45
1:B:139:PRO:HD3	1:B:221:LEU:HD13	1.98	0.45
1:F:52:LEU:HD22	1:F:181:PHE:CD1	2.50	0.45
1:E:198:ARG:HD2	1:E:198:ARG:O	2.17	0.45
1:F:52:LEU:CD2	1:F:181:PHE:CZ	3.00	0.45
1:E:137:LEU:HD21	1:E:215:LEU:HD22	1.97	0.45
1:D:30:ALA:HB1	1:F:183:VAL:CG2	2.46	0.45
1:D:82:GLN:HA	1:D:163:ILE:HG21	1.99	0.45
1:B:82:GLN:HA	1:B:163:ILE:HG21	1.99	0.44
1:D:80:VAL:HG22	5:D:233:HOH:O	2.17	0.44
1:E:129:LYS:O	1:E:132:HIS:HE1	2.00	0.44
1:D:93:ILE:HG21	1:D:158:LEU:HD21	2.00	0.44
1:B:52:LEU:CD2	1:B:188:LEU:HD11	2.48	0.44
1:F:158:LEU:CD2	1:F:176:LEU:HD22	2.48	0.44
1:B:133:LEU:C	1:B:133:LEU:HD23	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:HIS:ND1	3:F:231:SO4:O4	2.51	0.44
1:C:193:VAL:HG22	1:C:205:TYR:HA	2.00	0.44
1:A:156:TYR:HA	1:A:201:LEU:HD11	2.00	0.43
1:C:77:CYS:O	1:C:81:VAL:HG23	2.19	0.43
1:C:133:LEU:C	1:C:133:LEU:HD23	2.38	0.43
1:E:156:TYR:OH	1:E:202:GLU:OE2	2.32	0.43
1:F:78:LEU:HD13	1:F:163:ILE:HD12	2.00	0.43
1:A:183:VAL:CG1	3:A:232:SO4:S	3.06	0.43
1:E:132:HIS:CD2	1:E:133:LEU:H	2.36	0.43
1:B:52:LEU:HD21	1:B:188:LEU:HD11	2.00	0.43
1:E:90:ILE:HD12	1:E:92:HIS:N	2.29	0.43
1:A:159:GLY:HA3	1:A:201:LEU:HD22	2.00	0.43
1:E:47:VAL:HG12	1:E:52:LEU:CD1	2.35	0.43
1:B:175:SER:HB2	1:B:194:MET:CE	2.47	0.43
1:D:150:ASN:O	1:D:154:GLN:HG2	2.19	0.43
1:B:182:ASP:OD1	1:B:184:ASN:ND2	2.48	0.43
1:E:90:ILE:HD12	1:E:91:GLU:N	2.34	0.42
1:E:150:ASN:O	1:E:154:GLN:HG2	2.19	0.42
1:F:183:VAL:HG22	1:F:183:VAL:O	2.20	0.42
1:E:37:TYR:HA	1:E:90:ILE:HD13	2.01	0.41
1:D:159:GLY:HA3	1:D:201:LEU:HD22	2.00	0.41
1:E:108:MET:CE	1:E:143:ALA:HB2	2.49	0.41
1:C:92:HIS:NE2	1:E:1:MET:CE	2.83	0.41
1:D:183:VAL:HG21	3:D:232:SO4:S	2.58	0.41
1:C:1:MET:HG3	1:C:2:ASP:N	2.35	0.41
1:D:78:LEU:HD12	1:E:75:PHE:HE1	1.84	0.41
1:A:104:ILE:O	1:A:108:MET:HG3	2.20	0.41
1:D:44:ASP:HB2	1:D:98:HIS:CE1	2.56	0.41
1:C:1:MET:HG2	1:C:3:LYS:HB2	2.03	0.40
1:D:64:ARG:NH2	4:F:232:BCT:O3	2.55	0.40
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.96	0.40
1:C:36:HIS:HD2	1:C:59:GLU:OE1	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:OE1	5:A:246:HOH:O[2_556]	1.92	0.28

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	205/229 (90%)	199 (97%)	6 (3%)	0	100	100
1	B	203/229 (89%)	197 (97%)	6 (3%)	0	100	100
1	C	201/229 (88%)	193 (96%)	7 (4%)	1 (0%)	29	35
1	D	200/229 (87%)	195 (98%)	4 (2%)	1 (0%)	29	35
1	E	203/229 (89%)	197 (97%)	6 (3%)	0	100	100
1	F	200/229 (87%)	193 (96%)	5 (2%)	2 (1%)	15	17
All	All	1212/1374 (88%)	1174 (97%)	34 (3%)	4 (0%)	41	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	45	SER
1	F	2	ASP
1	C	218	GLU
1	F	218	GLU

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	182/201 (90%)	175 (96%)	7 (4%)	33	47
1	B	180/201 (90%)	168 (93%)	12 (7%)	16	21
1	C	178/201 (89%)	167 (94%)	11 (6%)	18	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	176/201 (88%)	167 (95%)	9 (5%)	24	33
1	E	180/201 (90%)	172 (96%)	8 (4%)	28	39
1	F	177/201 (88%)	173 (98%)	4 (2%)	50	67
All	All	1073/1206 (89%)	1022 (95%)	51 (5%)	25	36

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	37	TYR
1	A	54	ASN
1	A	110	ASP
1	A	198	ARG
1	A	212	LEU
1	A	217	GLU
1	B	1	MET
1	B	16	GLN
1	B	44	ASP
1	B	47	VAL
1	B	64	ARG
1	B	78	LEU
1	B	80	VAL
1	B	117	ASN
1	B	183	VAL
1	B	194	MET
1	B	216	ASP
1	B	220	ILE
1	C	7	LEU
1	C	16	GLN
1	C	78	LEU
1	C	80	VAL
1	C	111	LYS
1	C	117	ASN
1	C	137	LEU
1	C	169	GLU
1	C	183	VAL
1	C	206	ARG
1	C	216	ASP
1	D	1	MET
1	D	18	MET
1	D	37	TYR

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Mol	Chain	Res	Type
1	D	44	ASP
1	D	100	ASN
1	D	110	ASP
1	D	112	ASP
1	D	137	LEU
1	D	212	LEU
1	E	16	GLN
1	E	33	GLN
1	E	78	LEU
1	E	90	ILE
1	E	112	ASP
1	E	117	ASN
1	E	185	ASP
1	E	219	ASN
1	F	5	LYS
1	F	46	ARG
1	F	78	LEU
1	F	120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	117	ASN
1	A	219	ASN
1	B	16	GLN
1	B	54	ASN
1	B	69	GLN
1	B	117	ASN
1	B	132	HIS
1	C	36	HIS
1	C	54	ASN
1	D	36	HIS
1	D	54	ASN
1	D	69	GLN
1	D	100	ASN
1	D	117	ASN
1	E	6	GLN
1	E	36	HIS
1	E	92	HIS
1	E	117	ASN
1	E	132	HIS

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Mol	Chain	Res	Type
1	F	54	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 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	D	231	-	4,4,4	0.17	0	6,6,6	0.34	0
3	SO4	B	232	-	4,4,4	0.14	0	6,6,6	0.27	0
3	SO4	B	231	-	4,4,4	0.17	0	6,6,6	0.27	0
3	SO4	F	231	-	4,4,4	0.28	0	6,6,6	0.40	0
3	SO4	D	232	-	4,4,4	0.16	0	6,6,6	0.40	0
3	SO4	C	232	-	4,4,4	0.14	0	6,6,6	0.33	0
3	SO4	A	232	-	4,4,4	0.14	0	6,6,6	0.45	0
3	SO4	C	231	-	4,4,4	0.23	0	6,6,6	0.41	0
3	SO4	A	231	-	4,4,4	0.21	0	6,6,6	0.28	0
4	BCT	F	232	-	2,3,3	0.63	0	2,3,3	0.94	0
3	SO4	E	233	-	4,4,4	0.17	0	6,6,6	0.51	0
3	SO4	E	232	-	4,4,4	0.13	0	6,6,6	0.49	0
3	SO4	E	231	-	4,4,4	0.18	0	6,6,6	0.54	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.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	232	SO4	2	0
3	F	231	SO4	2	0
3	D	232	SO4	3	0
3	C	232	SO4	3	0
3	A	232	SO4	3	0
4	F	232	BCT	2	0
3	E	233	SO4	3	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	209/229 (91%)	0.76	25 (11%) 4 6	23, 42, 54, 63	0
1	B	207/229 (90%)	1.09	40 (19%) 1 1	38, 45, 60, 63	0
1	C	205/229 (89%)	0.71	30 (14%) 2 3	36, 42, 55, 65	0
1	D	204/229 (89%)	0.60	17 (8%) 11 15	33, 40, 51, 59	0
1	E	207/229 (90%)	0.86	36 (17%) 1 1	37, 43, 55, 62	0
1	F	204/229 (89%)	0.63	20 (9%) 7 10	33, 41, 52, 65	0
All	All	1236/1374 (89%)	0.78	168 (13%) 3 4	23, 42, 55, 65	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ILE	7.2
1	D	215	LEU	6.2
1	C	5	LYS	5.9
1	B	1	MET	5.9
1	A	32	HIS	5.7
1	B	2	ASP	5.4
1	E	219	ASN	5.4
1	D	1	MET	5.2
1	A	132	HIS	5.1
1	B	221	LEU	5.0
1	C	183	VAL	4.9
1	E	132	HIS	4.9
1	E	218	GLU	4.9
1	C	1	MET	4.8
1	E	13	SER	4.7
1	B	40	ILE	4.5
1	B	187	PHE	4.4
1	B	184	ASN	4.4
1	E	93	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	136	LYS	4.3
1	B	16	GLN	4.3
1	A	110	ASP	4.2
1	D	2	ASP	4.2
1	B	54	ASN	4.1
1	B	183	VAL	4.1
1	A	1	MET	3.9
1	D	16	GLN	3.9
1	B	217	GLU	3.9
1	C	2	ASP	3.9
1	C	217	GLU	3.8
1	D	31	ASP	3.8
1	E	220	ILE	3.8
1	F	40	ILE	3.8
1	B	12	TYR	3.8
1	E	34	THR	3.8
1	E	16	GLN	3.7
1	B	220	ILE	3.7
1	F	110	ASP	3.7
1	A	93	ILE	3.7
1	B	219	ASN	3.6
1	B	218	GLU	3.6
1	C	219	ASN	3.6
1	E	32	HIS	3.6
1	B	132	HIS	3.6
1	D	132	HIS	3.5
1	F	93	ILE	3.5
1	C	184	ASN	3.5
1	A	56	GLU	3.5
1	B	33	GLN	3.5
1	A	218	GLU	3.5
1	B	56	GLU	3.4
1	E	136	LYS	3.4
1	F	219	ASN	3.4
1	D	32	HIS	3.4
1	C	17	ARG	3.4
1	B	158	LEU	3.4
1	E	2	ASP	3.4
1	E	183	VAL	3.4
1	E	40	ILE	3.4
1	B	62	VAL	3.3
1	F	1	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	9	ALA	3.3
1	E	1	MET	3.3
1	F	216	ASP	3.2
1	F	95	ILE	3.2
1	F	140	GLU	3.2
1	F	94	ILE	3.2
1	B	17	ARG	3.2
1	A	221	LEU	3.2
1	E	38	LEU	3.2
1	F	38	LEU	3.1
1	D	12	TYR	3.1
1	F	218	GLU	3.1
1	A	17	ARG	3.0
1	A	40	ILE	3.0
1	B	216	ASP	3.0
1	F	105	HIS	3.0
1	E	187	PHE	3.0
1	B	34	THR	3.0
1	E	140	GLU	3.0
1	A	105	HIS	2.9
1	E	17	ARG	2.9
1	C	40	ILE	2.9
1	A	216	ASP	2.9
1	E	206	ARG	2.9
1	E	62	VAL	2.9
1	C	13	SER	2.8
1	F	62	VAL	2.8
1	D	110	ASP	2.8
1	B	95	ILE	2.8
1	C	187	PHE	2.8
1	E	56	GLU	2.8
1	C	139	PRO	2.8
1	E	6	GLN	2.8
1	C	38	LEU	2.8
1	D	40	ILE	2.7
1	A	34	THR	2.7
1	C	94	ILE	2.7
1	A	62	VAL	2.7
1	D	5	LYS	2.7
1	C	110	ASP	2.7
1	A	184	ASN	2.6
1	A	139	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	111	LYS	2.6
1	C	34	THR	2.6
1	C	112	ASP	2.6
1	A	158	LEU	2.6
1	C	176	LEU	2.6
1	C	12	TYR	2.6
1	C	132	HIS	2.6
1	F	138	SER	2.5
1	B	14	TRP	2.5
1	D	100	ASN	2.5
1	A	213	SER	2.5
1	C	206	ARG	2.5
1	E	105	HIS	2.5
1	B	5	LYS	2.5
1	D	45	SER	2.4
1	D	112	ASP	2.4
1	E	96	CYS	2.4
1	C	218	GLU	2.4
1	A	33	GLN	2.4
1	D	184	ASN	2.4
1	C	7	LEU	2.4
1	E	9	ALA	2.4
1	F	34	THR	2.4
1	E	95	ILE	2.4
1	B	64	ARG	2.4
1	C	216	ASP	2.3
1	C	14	TRP	2.3
1	F	132	HIS	2.3
1	B	94	ILE	2.3
1	A	169	GLU	2.3
1	F	17	ARG	2.3
1	B	93	ILE	2.3
1	E	184	ASN	2.3
1	A	95	ILE	2.3
1	C	93	ILE	2.3
1	C	138	SER	2.3
1	B	211	ARG	2.3
1	F	217	GLU	2.2
1	E	139	PRO	2.2
1	E	4	ILE	2.2
1	B	169	GLU	2.2
1	F	39	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	41	GLY	2.2
1	B	199	GLU	2.2
1	B	96	CYS	2.2
1	E	7	LEU	2.2
1	B	151	VAL	2.2
1	B	8	PHE	2.2
1	C	6	GLN	2.2
1	B	39	TRP	2.1
1	E	87	VAL	2.1
1	C	185	ASP	2.1
1	E	33	GLN	2.1
1	A	94	ILE	2.1
1	E	176	LEU	2.1
1	C	105	HIS	2.1
1	B	110	ASP	2.1
1	E	216	ASP	2.0
1	D	214	ILE	2.0
1	F	158	LEU	2.0
1	A	100	ASN	2.0
1	B	112	ASP	2.0
1	E	12	TYR	2.0
1	E	14	TRP	2.0
1	A	43	SER	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	F	231	5/5	0.83	0.53	103,103,104,104	0
3	SO4	B	232	5/5	0.88	0.34	81,81,82,82	0
3	SO4	C	231	5/5	0.94	0.20	64,64,66,66	0
3	SO4	E	233	5/5	0.94	0.39	76,76,78,78	0
3	SO4	A	231	5/5	0.94	0.21	60,63,63,63	0
4	BCT	F	232	4/4	0.94	0.12	42,42,43,43	0
3	SO4	E	232	5/5	0.96	0.21	60,62,63,63	0
2	ZN	A	230	1/1	0.96	0.06	48,48,48,48	0
3	SO4	A	232	5/5	0.96	0.39	54,56,58,58	0
3	SO4	C	232	5/5	0.96	0.47	83,83,83,84	0
3	SO4	B	231	5/5	0.97	0.15	53,55,57,58	0
3	SO4	E	231	5/5	0.98	0.17	56,58,58,59	0
2	ZN	C	230	1/1	0.98	0.04	42,42,42,42	0
2	ZN	D	230	1/1	0.98	0.04	41,41,41,41	0
3	SO4	D	231	5/5	0.98	0.23	56,58,59,59	0
3	SO4	D	232	5/5	0.98	0.20	45,45,48,49	0
2	ZN	E	230	1/1	0.99	0.07	41,41,41,41	0
2	ZN	F	230	1/1	0.99	0.05	44,44,44,44	0
2	ZN	B	230	1/1	0.99	0.05	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.