



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:17 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

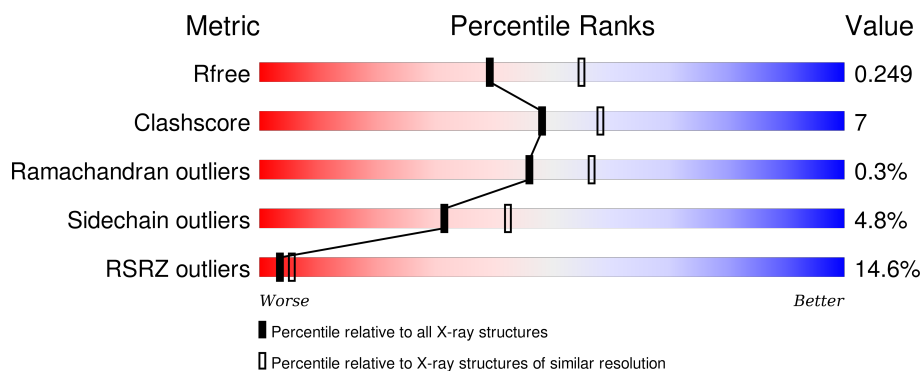
1 Overall quality at a glance

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	229	<div> <div>12%</div> <div>78%</div> <div>13%</div> <div>9%</div> </div>
1	B	229	<div> <div>19%</div> <div>76%</div> <div>12%</div> <div>•</div> <div>10%</div> </div>
1	C	229	<div> <div>13%</div> <div>73%</div> <div>14%</div> <div>•</div> <div>10%</div> </div>
1	D	229	<div> <div>8%</div> <div>73%</div> <div>14%</div> <div>•</div> <div>11%</div> </div>
1	E	229	<div> <div>17%</div> <div>72%</div> <div>17%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	229	

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

2 Entry composition

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



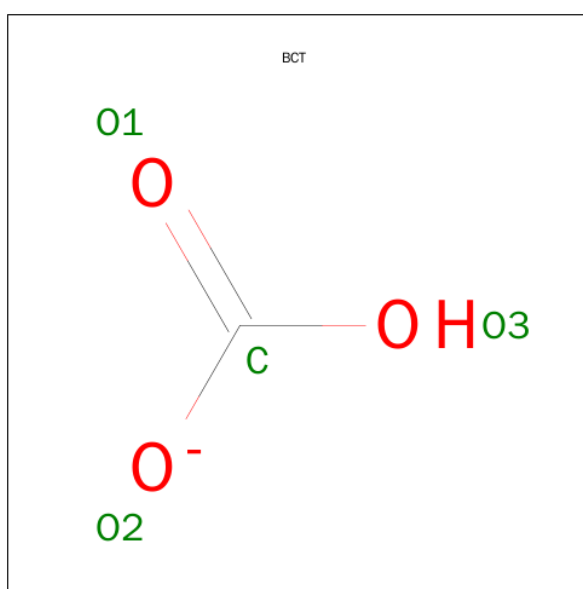
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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

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



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

- Molecule 5 is water.

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

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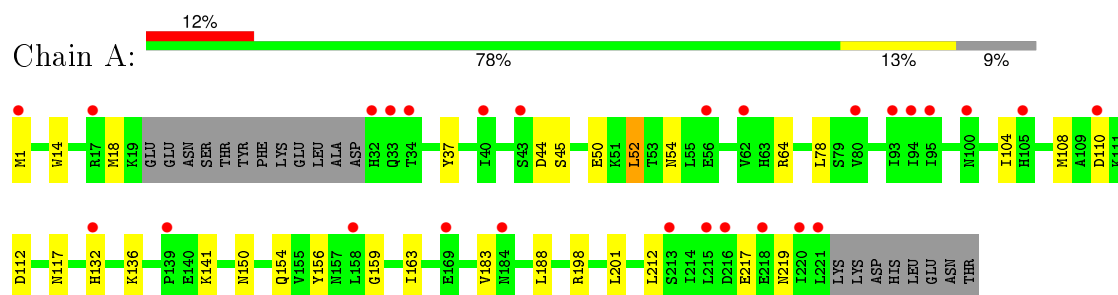
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	29	Total	O	0	0
			29	29		
5	F	29	Total	O	0	0
			29	29		

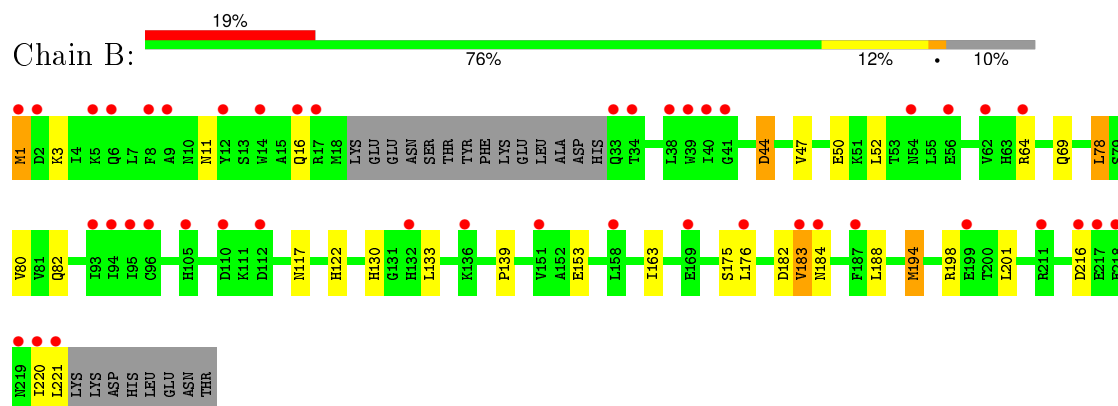
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

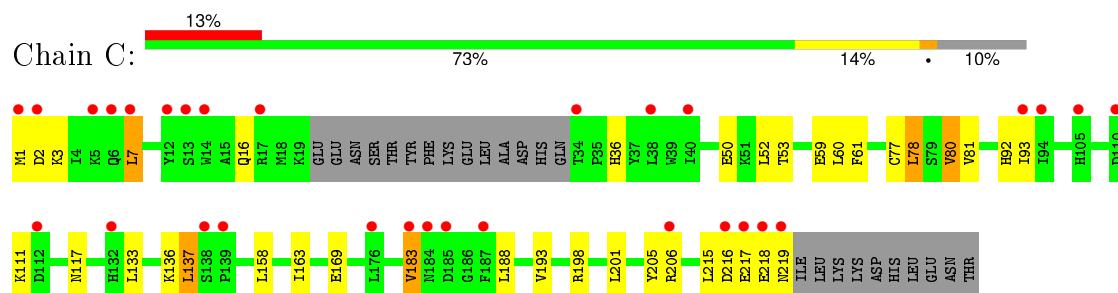
• Molecule 1: Carbonic anhydrase 2



• Molecule 1: Carbonic anhydrase 2

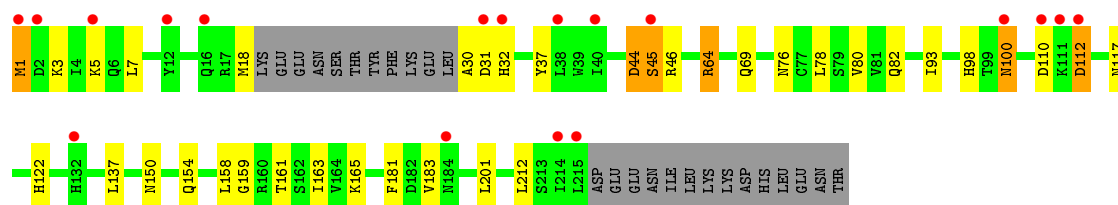


• Molecule 1: Carbonic anhydrase 2

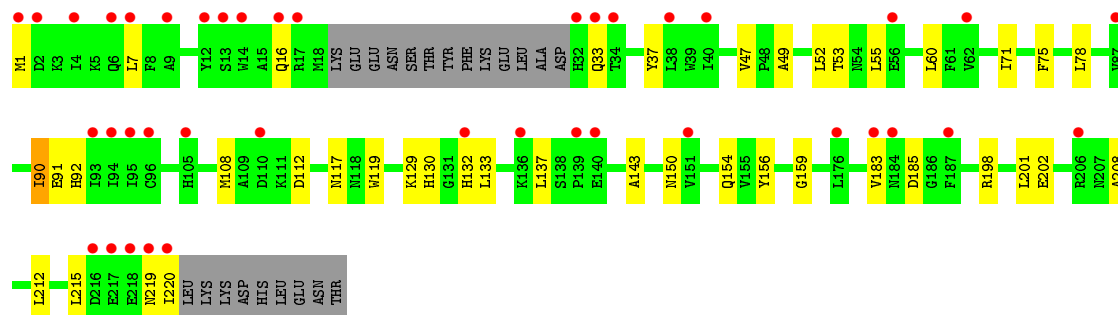


• Molecule 1: Carbonic anhydrase 2

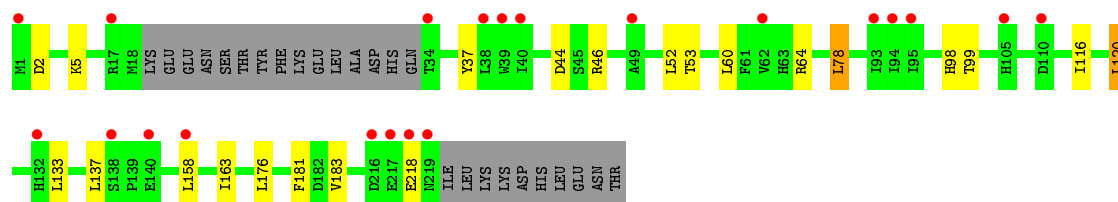
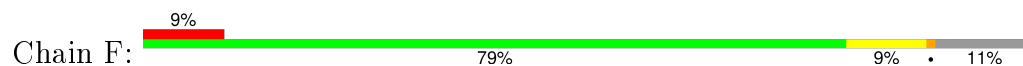




• Molecule 1: Carbonic anhydrase 2



• Molecule 1: Carbonic anhydrase 2



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.201 , 0.244 0.207 , 0.249	Depositor DCC
R_{free} test set	7808 reflections (11.22%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 77404 reflections (0.001%)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	Ideal(°)
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(°)	Ideal(°)
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

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:HE2	1:B:1:MET:H1	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:N	1:B:1:MET:HE2	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:D:1:MET:C	1:D:5:LYS:NZ	2.63	0.52
1:C:137:LEU:CD1	1:C:215:LEU:HD13	2.39	0.52
1:C:50:GLU:HG3	1:C:60:LEU:HD12	1.90	0.52
1:D:100:ASN:HD22	1:D:100:ASN:C	2.13	0.52
1:D:69:GLN:HE22	1:D:122:HIS:HB2	1.73	0.52
1:B:1:MET:CE	1:B:1:MET:N	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:F:52:LEU:HD21	1:F:181:PHE:CZ	2.46	0.50
1:D:161:THR:O	1:D:165:LYS:HG3	2.10	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:CE	1:B:1:MET:H1	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:D:44:ASP:O	1:D:46:ARG:N	2.46	0.48
1:C:136:LYS:O	1:C:219:ASN:ND2	2.42	0.48
1:D:78:LEU:HD12	1:E:75:PHE:CE1	2.49	0.48
1:A:150:ASN:O	1:A:154:GLN:HG2	2.13	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:E:47:VAL:O	1:E:52:LEU:HD11	2.14	0.47
1:A:132:HIS:O	1:A:136:LYS:HG3	2.13	0.47
1:E:220:ILE:CD1	1:E:220:ILE:O	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:D:183:VAL:CG2	3:D:232:SO4:O1	2.51	0.46
1:B:1:MET:HE1	1:B:3:LYS:HB2	1.98	0.46
1:C:198:ARG:NH1	1:C:201:LEU:HD23	2.31	0.46
1:E:7:LEU:HD23	1:E:7:LEU:O	2.17	0.45
1:F:52:LEU:HD22	1:F:181:PHE:CD1	2.50	0.45
1:B:139:PRO:HD3	1:B:221:LEU:HD13	1.98	0.45
1:F:52:LEU:CD2	1:F:181:PHE:CZ	3.00	0.45
1:E:198:ARG:O	1:E:198:ARG:HD2	2.17	0.45
1:E:137:LEU:HD21	1:E:215:LEU:HD22	1.97	0.45
1:D:82:GLN:HA	1:D:163:ILE:HG21	1.99	0.45
1:D:30:ALA:HB1	1:F:183:VAL:CG2	2.46	0.45
1:B:82:GLN:HA	1:B:163:ILE:HG21	1.99	0.44
1:E:129:LYS:O	1:E:132:HIS:HE1	2.00	0.44
1:D:80:VAL:HG22	5:D:233:HOH:O	2.17	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:F:98:HIS:ND1	3:F:231:SO4:O4	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:HD23	1:B:133:LEU:C	2.38	0.44
1:C:193:VAL:HG22	1:C:205:TYR:HA	2.00	0.44
1:C:77:CYS:O	1:C:81:VAL:HG23	2.19	0.43
1:E:156:TYR:OH	1:E:202:GLU:OE2	2.32	0.43
1:A:156:TYR:HA	1:A:201:LEU:HD11	2.00	0.43
1:C:133:LEU:HD23	1:C:133:LEU:C	2.38	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:E:90:ILE:HD12	1:E:92:HIS:N	2.29	0.43
1:B:52:LEU:HD21	1:B:188:LEU:HD11	2.00	0.43
1:E:47:VAL:HG12	1:E:52:LEU:CD1	2.35	0.43
1:A:159:GLY:HA3	1:A:201:LEU:HD22	2.00	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:E:108:MET:CE	1:E:143:ALA:HB2	2.49	0.41
1:D:159:GLY:HA3	1:D:201:LEU:HD22	2.00	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:D:78:LEU:HD12	1:E:75:PHE:HE1	1.84	0.41
1:C:1:MET:HG3	1:C:2:ASP:N	2.35	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

5.3.1 Protein backbone

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%)	34	41
1	D	200/229 (87%)	195 (98%)	4 (2%)	1 (0%)	34	41
1	E	203/229 (89%)	197 (97%)	6 (3%)	0	100	100
1	F	200/229 (87%)	193 (96%)	5 (2%)	2 (1%)	19	21
All	All	1212/1374 (88%)	1174 (97%)	34 (3%)	4 (0%)	46	57

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

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%)	40	54
1	B	180/201 (90%)	168 (93%)	12 (7%)	20	26
1	C	178/201 (89%)	167 (94%)	11 (6%)	23	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	176/201 (88%)	167 (95%)	9 (5%)	29	39
1	E	180/201 (90%)	172 (96%)	8 (4%)	35	46
1	F	177/201 (88%)	173 (98%)	4 (2%)	58	75
All	All	1073/1206 (89%)	1022 (95%)	51 (5%)	31	42

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

Some 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 carbohydrates 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	A	231	-	4,4,4	0.37	0	6,6,6	0.29	0
3	SO4	A	232	-	4,4,4	0.20	0	6,6,6	0.36	0
3	SO4	B	231	-	4,4,4	0.33	0	6,6,6	0.50	0
3	SO4	B	232	-	4,4,4	0.17	0	6,6,6	0.17	0
3	SO4	C	231	-	4,4,4	0.33	0	6,6,6	0.28	0
3	SO4	C	232	-	4,4,4	0.23	0	6,6,6	0.32	0
3	SO4	D	231	-	4,4,4	0.34	0	6,6,6	0.28	0
3	SO4	D	232	-	4,4,4	0.17	0	6,6,6	0.30	0
3	SO4	E	231	-	4,4,4	0.43	0	6,6,6	0.43	0
3	SO4	E	232	-	4,4,4	0.20	0	6,6,6	0.48	0
3	SO4	E	233	-	4,4,4	0.27	0	6,6,6	0.46	0
3	SO4	F	231	-	4,4,4	0.31	0	6,6,6	0.45	0
4	BCT	F	232	-	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	231	-	-	0/0/0/0	0/0/0/0
3	SO4	A	232	-	-	0/0/0/0	0/0/0/0
3	SO4	B	231	-	-	0/0/0/0	0/0/0/0
3	SO4	B	232	-	-	0/0/0/0	0/0/0/0
3	SO4	C	231	-	-	0/0/0/0	0/0/0/0
3	SO4	C	232	-	-	0/0/0/0	0/0/0/0
3	SO4	D	231	-	-	0/0/0/0	0/0/0/0
3	SO4	D	232	-	-	0/0/0/0	0/0/0/0
3	SO4	E	231	-	-	0/0/0/0	0/0/0/0
3	SO4	E	232	-	-	0/0/0/0	0/0/0/0
3	SO4	E	233	-	-	0/0/0/0	0/0/0/0
3	SO4	F	231	-	-	0/0/0/0	0/0/0/0
4	BCT	F	232	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	232	SO4	3	0
3	B	232	SO4	2	0
3	C	232	SO4	3	0
3	D	232	SO4	3	0
3	E	233	SO4	3	0
3	F	231	SO4	2	0
4	F	232	BCT	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.84	27 (12%) 5 7	23, 42, 54, 63	0
1	B	207/229 (90%)	1.17	44 (21%) 1 2	38, 45, 60, 63	0
1	C	205/229 (89%)	0.79	30 (14%) 3 5	36, 42, 55, 65	0
1	D	204/229 (89%)	0.67	18 (8%) 12 18	33, 40, 51, 59	0
1	E	207/229 (90%)	0.94	40 (19%) 2 2	37, 43, 55, 62	0
1	F	204/229 (89%)	0.70	21 (10%) 9 13	33, 41, 52, 65	0
All	All	1236/1374 (89%)	0.85	180 (14%) 3 5	23, 42, 55, 65	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ILE	7.5
1	D	215	LEU	6.3
1	B	1	MET	6.0
1	C	5	LYS	6.0
1	A	32	HIS	5.9
1	E	219	ASN	5.6
1	B	2	ASP	5.6
1	D	1	MET	5.3
1	B	221	LEU	5.3
1	A	132	HIS	5.3
1	C	183	VAL	5.1
1	E	132	HIS	5.0
1	E	218	GLU	5.0
1	C	1	MET	5.0
1	E	13	SER	4.8
1	B	40	ILE	4.8
1	B	184	ASN	4.6
1	B	187	PHE	4.6
1	E	93	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	16	GLN	4.4
1	B	136	LYS	4.4
1	A	110	ASP	4.3
1	B	54	ASN	4.3
1	D	2	ASP	4.3
1	B	183	VAL	4.3
1	A	1	MET	4.1
1	D	16	GLN	4.1
1	B	217	GLU	4.0
1	C	2	ASP	4.0
1	E	220	ILE	4.0
1	F	40	ILE	4.0
1	E	34	THR	3.9
1	D	31	ASP	3.9
1	C	217	GLU	3.9
1	B	220	ILE	3.9
1	B	12	TYR	3.8
1	E	16	GLN	3.8
1	A	93	ILE	3.8
1	B	219	ASN	3.8
1	F	110	ASP	3.8
1	E	32	HIS	3.8
1	C	219	ASN	3.8
1	B	218	GLU	3.7
1	B	132	HIS	3.7
1	F	93	ILE	3.7
1	C	184	ASN	3.7
1	D	132	HIS	3.7
1	B	33	GLN	3.6
1	A	56	GLU	3.6
1	A	218	GLU	3.6
1	E	183	VAL	3.6
1	D	32	HIS	3.6
1	E	2	ASP	3.6
1	B	62	VAL	3.5
1	B	158	LEU	3.5
1	B	56	GLU	3.5
1	E	136	LYS	3.5
1	F	219	ASN	3.5
1	C	17	ARG	3.5
1	E	40	ILE	3.5
1	F	1	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	9	ALA	3.4
1	E	1	MET	3.4
1	F	95	ILE	3.4
1	F	216	ASP	3.3
1	F	94	ILE	3.3
1	F	140	GLU	3.3
1	A	221	LEU	3.3
1	E	38	LEU	3.3
1	B	17	ARG	3.2
1	F	38	LEU	3.2
1	A	40	ILE	3.2
1	F	218	GLU	3.2
1	D	12	TYR	3.2
1	E	187	PHE	3.1
1	B	216	ASP	3.1
1	F	105	HIS	3.1
1	A	17	ARG	3.1
1	B	34	THR	3.1
1	E	140	GLU	3.1
1	A	105	HIS	3.1
1	E	62	VAL	3.1
1	C	40	ILE	3.0
1	A	216	ASP	3.0
1	F	62	VAL	3.0
1	E	17	ARG	3.0
1	E	206	ARG	3.0
1	B	95	ILE	3.0
1	C	187	PHE	3.0
1	C	139	PRO	2.9
1	D	110	ASP	2.9
1	C	13	SER	2.9
1	E	6	GLN	2.9
1	C	38	LEU	2.9
1	A	62	VAL	2.9
1	A	34	THR	2.9
1	C	94	ILE	2.9
1	D	40	ILE	2.9
1	E	56	GLU	2.9
1	C	110	ASP	2.8
1	D	5	LYS	2.8
1	A	184	ASN	2.7
1	A	139	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	34	THR	2.7
1	D	111	LYS	2.7
1	C	112	ASP	2.7
1	A	158	LEU	2.7
1	C	176	LEU	2.7
1	C	132	HIS	2.7
1	F	138	SER	2.7
1	B	14	TRP	2.7
1	D	100	ASN	2.6
1	C	12	TYR	2.6
1	E	96	CYS	2.6
1	A	213	SER	2.6
1	E	105	HIS	2.6
1	C	206	ARG	2.6
1	B	5	LYS	2.6
1	D	45	SER	2.5
1	C	218	GLU	2.5
1	D	112	ASP	2.5
1	E	9	ALA	2.5
1	A	33	GLN	2.5
1	F	34	THR	2.5
1	D	184	ASN	2.5
1	C	7	LEU	2.5
1	E	95	ILE	2.5
1	B	64	ARG	2.4
1	B	94	ILE	2.4
1	C	216	ASP	2.4
1	B	93	ILE	2.4
1	A	95	ILE	2.4
1	C	14	TRP	2.4
1	E	184	ASN	2.4
1	C	138	SER	2.4
1	F	132	HIS	2.4
1	A	169	GLU	2.4
1	B	96	CYS	2.4
1	E	139	PRO	2.4
1	B	41	GLY	2.4
1	C	93	ILE	2.4
1	E	4	ILE	2.4
1	F	17	ARG	2.4
1	F	217	GLU	2.3
1	B	211	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	39	TRP	2.3
1	B	151	VAL	2.3
1	B	169	GLU	2.3
1	B	8	PHE	2.3
1	B	199	GLU	2.3
1	E	7	LEU	2.3
1	B	39	TRP	2.3
1	C	185	ASP	2.2
1	E	176	LEU	2.2
1	A	94	ILE	2.2
1	C	105	HIS	2.2
1	C	6	GLN	2.2
1	E	87	VAL	2.2
1	E	216	ASP	2.2
1	E	33	GLN	2.2
1	A	100	ASN	2.2
1	F	158	LEU	2.2
1	B	110	ASP	2.1
1	D	214	ILE	2.1
1	B	112	ASP	2.1
1	A	80	VAL	2.1
1	A	43	SER	2.1
1	E	12	TYR	2.1
1	E	14	TRP	2.1
1	B	38	LEU	2.1
1	B	105	HIS	2.1
1	E	151	VAL	2.1
1	A	215	LEU	2.1
1	D	38	LEU	2.1
1	E	94	ILE	2.1
1	B	176	LEU	2.0
1	B	6	GLN	2.0
1	E	110	ASP	2.0
1	E	217	GLU	2.0
1	F	49	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	F	231	5/5	0.83	0.53	12.05	103,103,104,104	0
3	SO4	A	232	5/5	0.96	0.39	5.54	54,56,58,58	0
3	SO4	E	233	5/5	0.94	0.39	3.48	76,76,78,78	0
3	SO4	C	232	5/5	0.96	0.48	3.30	83,83,83,84	0
3	SO4	D	231	5/5	0.98	0.23	2.88	56,58,59,59	0
3	SO4	B	232	5/5	0.88	0.34	2.22	81,81,82,82	0
3	SO4	C	231	5/5	0.94	0.20	1.25	64,64,66,66	0
3	SO4	A	231	5/5	0.94	0.21	1.23	60,63,63,63	0
3	SO4	E	232	5/5	0.96	0.21	0.92	60,62,63,63	0
3	SO4	D	232	5/5	0.98	0.20	0.39	45,45,48,49	0
3	SO4	E	231	5/5	0.98	0.17	0.01	56,58,58,59	0
3	SO4	B	231	5/5	0.97	0.15	-0.84	53,55,57,58	0
4	BCT	F	232	4/4	0.94	0.12	-1.40	42,42,43,43	0
2	ZN	E	230	1/1	0.99	0.08	-1.91	41,41,41,41	0
2	ZN	D	230	1/1	0.98	0.04	-2.41	41,41,41,41	0
2	ZN	A	230	1/1	0.96	0.06	-3.64	48,48,48,48	0
2	ZN	C	230	1/1	0.98	0.04	-4.64	42,42,42,42	0
2	ZN	F	230	1/1	0.99	0.05	-4.67	44,44,44,44	0
2	ZN	B	230	1/1	0.99	0.05	-4.91	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.