Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2021 – 07:04 PM EDT

PDB ID	:	3E3G
Title	:	H. influenzae beta-carbonic anhydrase, variant G41A
Authors	:	Rowlett, R.S.; Failing, H.
Deposited on	:	2008-08-07
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 following versions of software and data (see references (i)) were used in the production of this report:

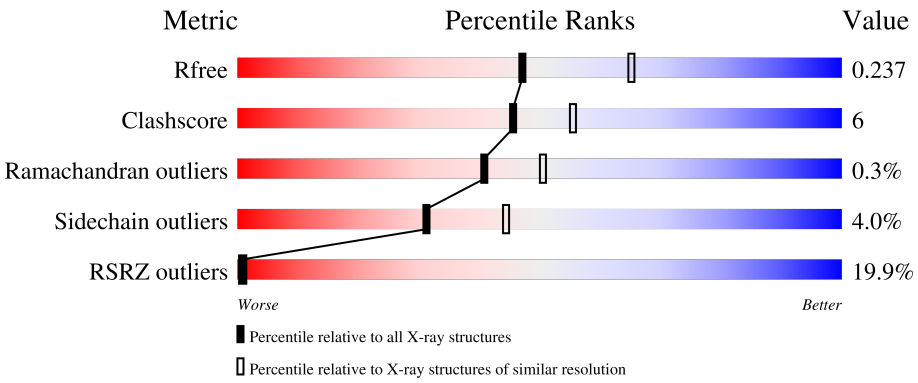
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	16% 75% 15% 10%
1	B	229	18% 75% 14% • 10%
1	C	229	18% 77% 11% • 11%
1	D	229	16% 74% 13% 13%
1	E	229	20% 74% 16% 10%

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Mol	Chain	Length	Quality of chain
1	F	229	19% 75% 14% • 10%

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	234	-	-	X	-
3	SO4	B	232	-	-	X	-
3	SO4	D	231	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10130 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	207	1669	1064	296	300	9	0	1	0
1	B	207	1669	1064	296	300	9	0	1	0
1	C	204	1644	1047	292	296	9	0	1	0
1	D	200	1610	1029	287	285	9	0	1	0
1	E	207	1671	1064	298	300	9	0	1	0
1	F	206	1663	1058	297	299	9	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	GLY	engineered mutation	UNP P45148
B	41	ALA	GLY	engineered mutation	UNP P45148
C	41	ALA	GLY	engineered mutation	UNP P45148
D	41	ALA	GLY	engineered mutation	UNP P45148
E	41	ALA	GLY	engineered mutation	UNP P45148
F	41	ALA	GLY	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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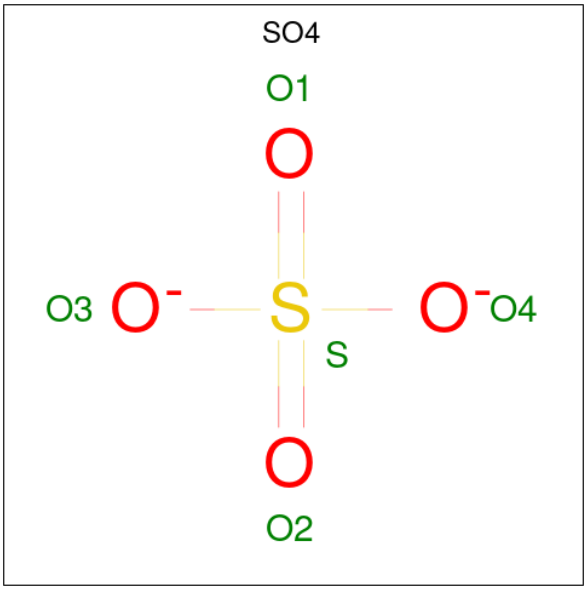
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- 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	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

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

- Molecule 4 is water.

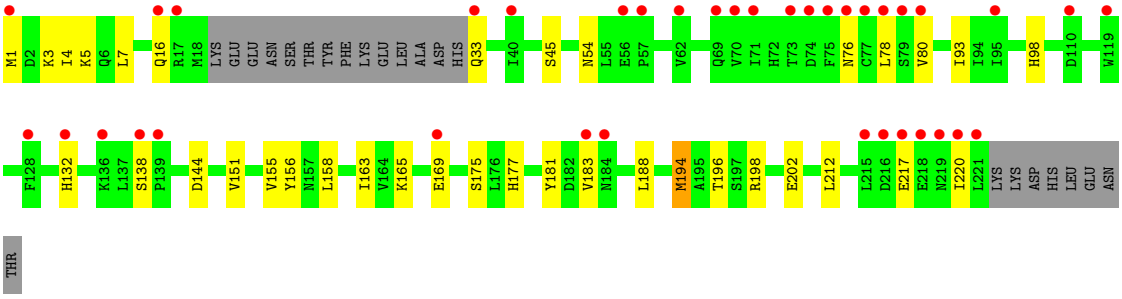
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	34	Total O 34 34	0	0
4	B	22	Total O 22 22	0	0
4	C	21	Total O 21 21	0	0
4	D	24	Total O 24 24	0	0
4	E	15	Total O 15 15	0	0
4	F	17	Total O 17 17	0	0

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.

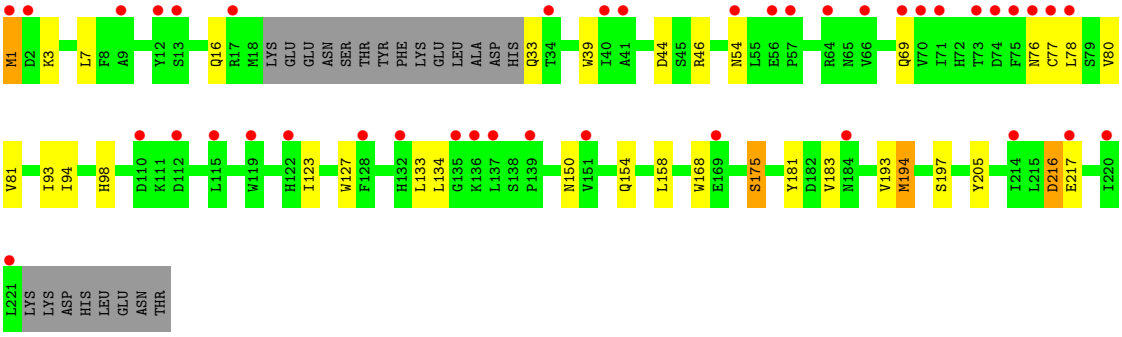
• Molecule 1: Carbonic anhydrase 2

Chain A:



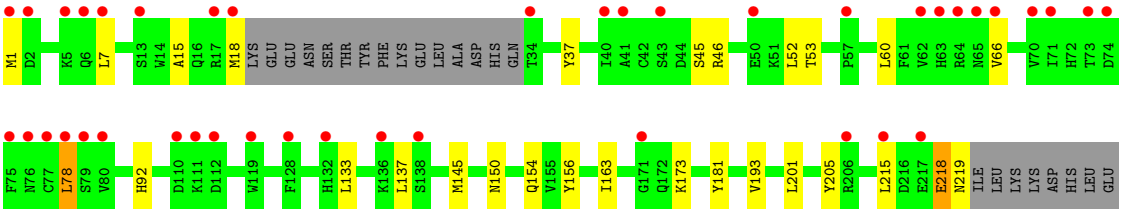
• Molecule 1: Carbonic anhydrase 2

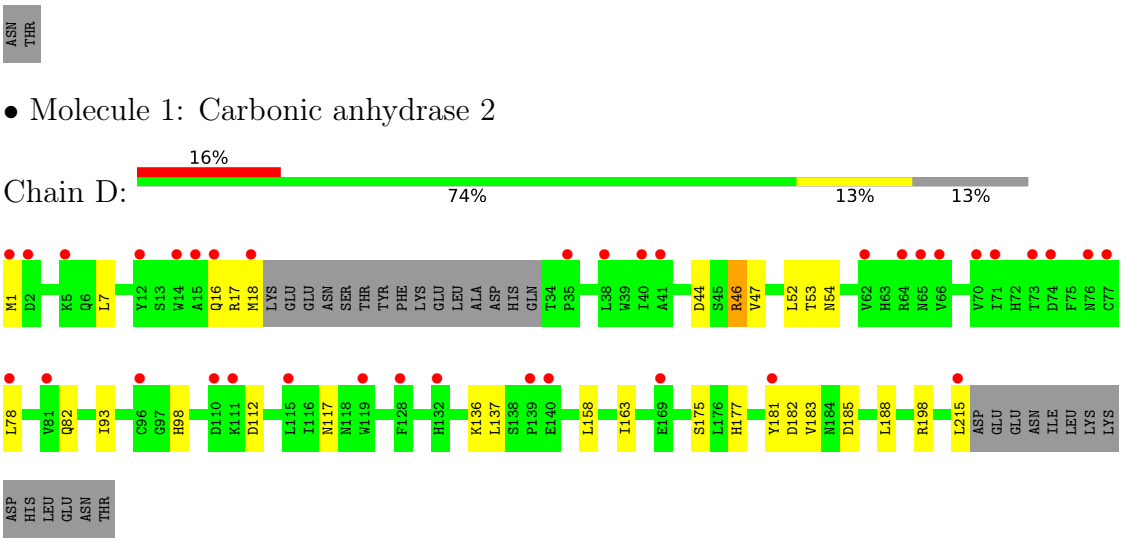
Chain B:

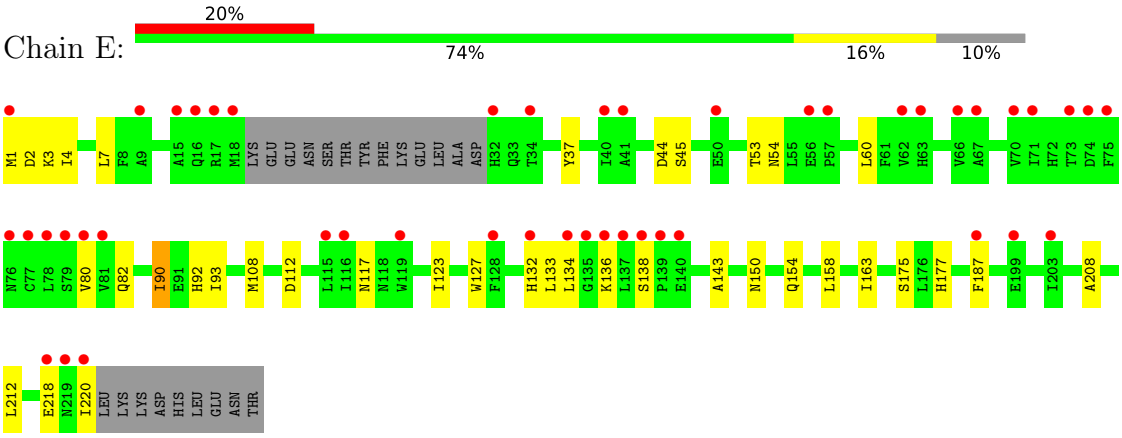


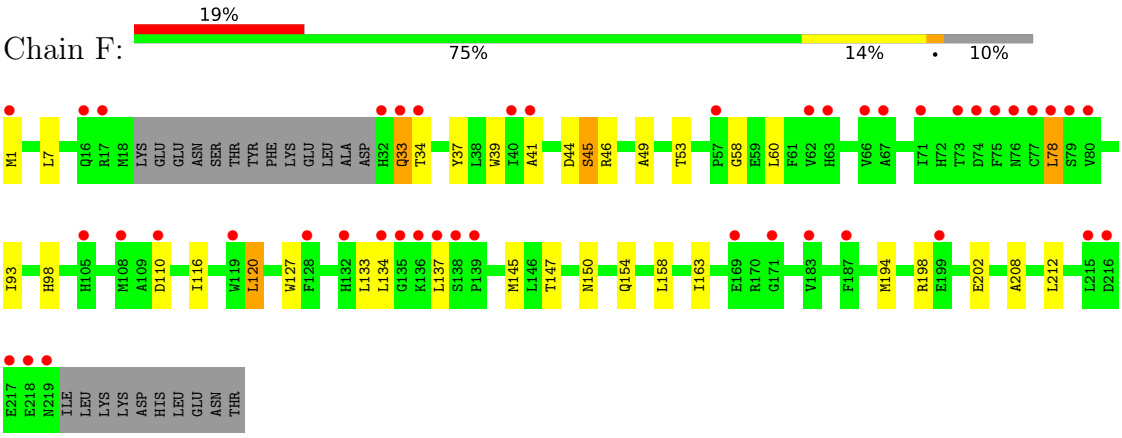
• Molecule 1: Carbonic anhydrase 2

Chain C:




ASN
THR
• Molecule 1: Carbonic anhydrase 2
Chain D:
16%
74%
13%
13%
M1 D2 K5 Q6 L7 Y12 S13 W14 A15 Q16 R17 M18 LYS GLU GLU ASN SER THR TYR PHE LYS GLU LEU ALA ASP HIS GLN T34 P35 L38 W39 I40 A41 D44 S45 R46 V47 L52 T53 N54 V62 H63 R64 N65 V66 V70 I71 H72 T73 D74 F75 N76 C77
L78 V81 Q82 I93 C96 G97 H98 D110 K111 D112 L115 I116 N117 N118 W119 F128 H132 K136 L137 S138 P139 E140 L158 I163 E169 S175 L176 H177 Y181 D182 V183 N184 D185 L188 R198 L215 ASP GLU GLU ASN ILE LEU LYS LYS
ASP HIS LEU GLU ASN THR


• Molecule 1: Carbonic anhydrase 2
Chain E:
20%
74%
16%
10%
M1 D2 K3 I4 L7 F8 A9 A15 Q16 R17 M18 LYS GLU GLU ASN SER THR TYR PHE LYS GLU LEU ALA ASP H32 Q33 T34 Y37 I40 A41 D44 S45 E50 T53 N54 L55 E56 P57 L60 F61 V62 H63 V66 A67 V70 I71 H72 T73 D74 F75
N76 C77 L78 S79 V80 V81 Q82 I90 E91 H92 I93 M108 D112 L115 I116 N117 N118 W119 I123 W127 F128 H132 L133 L134 G135 K136 L137 S138 P139 E140 A143 N150 Q154 L158 I163 S175 L176 H177 F187 E199 I203 A208
L212 E218 N219 I220 LEU LYS LYS ASP HIS LEU GLU ASN THR


• Molecule 1: Carbonic anhydrase 2
Chain F:
19%
75%
14%
10%
M1 L7 Q16 R17 M18 LYS GLU GLU ASN SER THR TYR PHE LYS GLU LEU ALA ASP H32 Q33 T34 Y37 L38 W39 I40 A41 D44 S45 R46 A49 T53 P57 G58 E59 L60 F61 V62 H63 V66 A67 I71 H72 T73 D74 F75 N76 C77 L78 S79 V80
I93 H98 H105 M108 A109 D110 I116 W119 L120 W127 F128 H132 L133 L134 G135 K136 L137 S138 P139 M145 L146 T147 N150 Q154 L158 I163 E169 R170 G171 V183 F187 M194 R198 E199 E202 A208 L212 L215 D216
E217 E218 N219 ILE LEU LYS LYS ASP HIS LEU GLU ASN THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	231.93Å 145.23Å 52.97Å 90.00° 93.82° 90.00°	Depositor
Resolution (Å)	39.41 – 2.30 39.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.41-2.30) 98.2 (39.40-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.234 0.201 , 0.237	Depositor DCC
R_{free} test set	3804 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.0	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	0.94	EDS
Total number of atoms	10130	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN

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	0.56	0/1708	0.63	0/2314
1	B	0.51	0/1708	0.59	1/2314 (0.0%)
1	C	0.48	0/1683	0.56	0/2280
1	D	0.52	0/1649	0.64	1/2234 (0.0%)
1	E	0.49	0/1711	0.60	0/2318
1	F	0.52	0/1703	0.62	0/2307
All	All	0.51	0/10162	0.61	2/13767 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	44	ASP	CB-CA-C	-7.28	95.83	110.40
1	B	44	ASP	CB-CA-C	-5.24	99.92	110.40

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	1669	0	1662	21	0
1	B	1669	0	1662	25	0
1	C	1644	0	1632	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1610	0	1610	24	0
1	E	1671	0	1658	29	0
1	F	1663	0	1647	22	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	20	0	0	3	1
3	B	10	0	0	7	0
3	C	10	0	0	0	0
3	D	5	0	0	4	0
3	E	15	0	0	0	0
3	F	5	0	0	0	0
4	A	34	0	0	0	1
4	B	22	0	0	0	0
4	C	21	0	0	0	0
4	D	24	0	0	0	0
4	E	15	0	0	0	0
4	F	17	0	0	1	0
All	All	10130	0	9871	127	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 6.

All (127) 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:B:69:GLN:NE2	1:B:123:ILE:HD11	1.77	1.00
1:D:183:VAL:HG12	3:D:231:SO4:O4	1.77	0.85
1:D:112:ASP:HA	1:D:117:ASN:HD21	1.40	0.84
1:D:181:TYR:OH	3:D:231:SO4:O2	1.95	0.83
1:D:53:THR:HG22	1:F:7:LEU:HD21	1.61	0.82
1:D:98:HIS:HB3	1:D:181:TYR:CE2	2.16	0.80
1:E:90:ILE:HD12	1:E:92:HIS:H	1.48	0.79
1:B:183:VAL:HG12	3:B:232:SO4:O4	1.84	0.76
1:B:46:ARG:N	3:B:232:SO4:O3	2.17	0.76
1:F:78:LEU:HD13	1:F:163:ILE:HD12	1.71	0.73
1:B:69:GLN:HE22	1:B:123:ILE:HD11	1.51	0.73
1:B:69:GLN:HE22	1:B:123:ILE:CD1	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:SER:HB2	1:A:194:MET:HE3	1.72	0.70
1:D:136:LYS:O	1:D:137:LEU:HD12	1.92	0.70
1:A:181:TYR:OH	3:A:234:SO4:O2	2.06	0.69
1:C:78:LEU:HD13	1:C:163:ILE:HD12	1.73	0.69
1:D:112:ASP:HA	1:D:117:ASN:ND2	2.08	0.67
1:A:217:GLU:HA	1:A:220:ILE:HD12	1.77	0.67
1:C:53:THR:HG22	1:E:7:LEU:HD21	1.75	0.67
1:A:194:MET:HE1	1:A:196:THR:HG23	1.76	0.66
1:D:78:LEU:HD22	1:D:163:ILE:HD12	1.77	0.66
1:B:1:MET:HE2	1:B:3:LYS:H	1.64	0.62
1:F:116:ILE:HG13	1:F:120:LEU:HD22	1.81	0.62
1:C:7:LEU:HD21	1:E:53:THR:HG22	1.82	0.61
1:F:208:ALA:O	1:F:212:LEU:HD23	2.00	0.60
1:E:1:MET:HE3	1:E:3:LYS:HD2	1.84	0.58
1:C:53:THR:CG2	1:E:7:LEU:HD21	2.32	0.58
1:D:78:LEU:HD22	1:D:163:ILE:CD1	2.32	0.58
1:F:37:TYR:HB2	1:F:60:LEU:HD23	1.85	0.58
1:B:93:ILE:HG21	1:B:158:LEU:HD21	1.85	0.57
1:D:93:ILE:HG21	1:D:158:LEU:HD21	1.86	0.57
1:E:1:MET:O	1:E:4:ILE:N	2.27	0.57
1:D:181:TYR:OH	3:D:231:SO4:S	2.59	0.57
1:E:108:MET:HE1	1:E:143:ALA:HB2	1.87	0.57
1:E:112:ASP:HA	1:E:117:ASN:OD1	2.05	0.56
1:A:78:LEU:HD22	1:A:163:ILE:HD12	1.86	0.56
1:A:78:LEU:CD2	1:A:163:ILE:HD12	2.35	0.56
1:A:1:MET:O	1:A:5:LYS:NZ	2.38	0.56
1:C:37:TYR:HB2	1:C:60:LEU:HD23	1.86	0.56
1:F:33:GLN:HG3	1:F:34:THR:N	2.21	0.56
1:D:7:LEU:HD21	1:F:53:THR:HG22	1.88	0.55
1:B:98:HIS:ND1	3:B:232:SO4:O1	2.40	0.55
1:E:93:ILE:HG21	1:E:158:LEU:HD21	1.89	0.55
1:A:183:VAL:HG12	3:A:234:SO4:O4	2.06	0.54
1:F:110:ASP:OD1	1:F:110:ASP:C	2.45	0.54
1:B:76:ASN:O	1:B:80:VAL:HG23	2.09	0.53
1:D:136:LYS:C	1:D:137:LEU:HD12	2.28	0.53
1:F:78:LEU:HD13	1:F:163:ILE:CD1	2.39	0.53
1:C:137:LEU:CD1	1:C:215:LEU:HD22	2.39	0.52
1:C:150:ASN:O	1:C:154:GLN:HG2	2.09	0.52
1:E:133:LEU:C	1:E:133:LEU:HD23	2.30	0.52
1:E:208:ALA:O	1:E:212:LEU:HD23	2.09	0.52
1:D:175:SER:OG	1:D:177:HIS:NE2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:ILE:HG21	1:F:158:LEU:HD21	1.91	0.52
1:E:138:SER:N	1:E:220:ILE:HG22	2.24	0.51
1:B:69:GLN:NE2	1:B:123:ILE:CD1	2.56	0.51
1:F:127:TRP:HD1	1:F:134:LEU:HD13	1.75	0.51
1:B:193:VAL:HG22	1:B:205:TYR:HA	1.92	0.50
1:E:127:TRP:CD1	1:E:134:LEU:HD13	2.48	0.49
1:E:175:SER:OG	1:E:177:HIS:NE2	2.43	0.49
1:F:127:TRP:CD1	1:F:134:LEU:HD13	2.48	0.48
1:B:183:VAL:HG12	3:B:232:SO4:S	2.53	0.48
1:B:127:TRP:CD1	1:B:134:LEU:HD13	2.49	0.48
1:E:136:LYS:O	1:E:220:ILE:HG23	2.13	0.48
1:D:182:ASP:OD1	1:D:183:VAL:N	2.47	0.48
1:B:183:VAL:CG1	3:B:232:SO4:O4	2.57	0.48
1:D:78:LEU:CD2	1:D:163:ILE:HD12	2.44	0.48
1:E:127:TRP:HD1	1:E:134:LEU:HD13	1.79	0.47
1:C:92:HIS:NE2	1:E:1:MET:HE2	2.29	0.47
1:A:76:ASN:O	1:A:80:VAL:HG23	2.15	0.47
1:A:1:MET:HE3	1:A:3:LYS:CG	2.45	0.47
1:A:156:TYR:OH	1:A:202:GLU:OE2	2.25	0.47
1:A:175:SER:HG	1:A:177:HIS:HE2	1.63	0.47
1:B:46:ARG:HG2	3:B:232:SO4:O2	2.15	0.47
1:A:198:ARG:NH2	3:A:232:SO4:O1	2.48	0.47
1:A:1:MET:HE3	1:A:3:LYS:HG3	1.96	0.47
1:F:49:ALA:CB	1:F:60:LEU:HD13	2.45	0.46
1:D:183:VAL:CG1	3:D:231:SO4:O4	2.58	0.46
1:B:1:MET:HE1	1:B:3:LYS:HG3	1.97	0.46
1:B:175:SER:HB2	1:B:194:MET:CE	2.45	0.46
1:D:181:TYR:HB3	1:D:188:LEU:HD23	1.97	0.46
1:F:145:MET:SD	1:F:212:LEU:HD12	2.56	0.46
1:F:150:ASN:O	1:F:154:GLN:HG2	2.15	0.46
1:D:47:VAL:HG12	1:D:52:LEU:HG	1.98	0.46
1:A:78:LEU:HD22	1:A:163:ILE:CD1	2.45	0.46
1:B:150:ASN:O	1:B:154:GLN:HG2	2.16	0.45
1:D:137:LEU:HD11	1:D:215:LEU:HD12	1.98	0.45
1:F:49:ALA:HB3	1:F:60:LEU:HD13	1.99	0.45
1:A:93:ILE:HG21	1:A:158:LEU:HD21	1.99	0.45
1:C:218:GLU:O	1:C:219:ASN:C	2.55	0.45
1:E:1:MET:O	1:E:3:LYS:N	2.50	0.44
1:E:90:ILE:CD1	1:E:92:HIS:O	2.65	0.44
1:B:181:TYR:OH	3:B:232:SO4:O3	2.25	0.44
1:D:16:GLN:C	1:D:18:MET:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:HB3	1:A:98:HIS:CD2	2.53	0.44
1:E:37:TYR:HB2	1:E:60:LEU:HD23	2.00	0.44
1:B:1:MET:HE1	1:B:3:LYS:CG	2.47	0.43
1:C:52:LEU:HD11	1:C:181:TYR:CE2	2.54	0.43
1:E:90:ILE:HD11	1:E:92:HIS:O	2.18	0.43
1:E:150:ASN:O	1:E:154:GLN:HG2	2.19	0.43
1:B:7:LEU:HD12	1:B:7:LEU:HA	1.81	0.43
1:F:44:ASP:O	1:F:45:SER:C	2.55	0.43
1:B:216:ASP:O	1:B:217:GLU:HB3	2.18	0.43
1:D:82:GLN:HA	1:D:163:ILE:HG21	2.01	0.42
1:F:39:TRP:NE1	1:F:41:ALA:HB2	2.34	0.42
1:D:93:ILE:CG2	1:D:158:LEU:HD21	2.50	0.42
1:A:1:MET:H2	1:A:4:ILE:HB	1.85	0.42
1:C:156:TYR:HA	1:C:201:LEU:HD11	2.02	0.42
1:C:173:LYS:HZ1	1:E:1:MET:HE2	1.84	0.42
1:B:77:CYS:O	1:B:81:VAL:HG23	2.20	0.42
1:E:123:ILE:CD1	1:E:150:ASN:OD1	2.67	0.42
1:C:193:VAL:HG22	1:C:205:TYR:HA	2.01	0.42
1:A:7:LEU:C	1:A:7:LEU:HD23	2.41	0.41
1:C:15:ALA:HB3	1:E:187:PHE:CE2	2.55	0.41
1:A:151:VAL:O	1:A:155:VAL:HG23	2.21	0.41
1:C:133:LEU:HD21	1:C:145:MET:HE3	2.01	0.41
1:A:181:TYR:HB3	1:A:188:LEU:HD23	2.02	0.41
1:C:66:VAL:HG23	1:E:80:VAL:HG22	2.02	0.41
1:F:98:HIS:O	1:F:147:THR:HG21	2.21	0.41
1:E:82:GLN:HA	1:E:163:ILE:HG21	2.03	0.41
1:E:123:ILE:HD12	1:E:150:ASN:OD1	2.21	0.41
1:F:46:ARG:HG2	4:F:237:HOH:O	2.19	0.40
1:C:173:LYS:NZ	1:E:1:MET:HE2	2.36	0.40
1:B:168:TRP:CD2	1:B:197:SER:HA	2.56	0.40
1:F:137:LEU:HD12	1:F:137:LEU:HA	1.90	0.40
1:B:39:TRP:CZ3	1:B:94:ILE:HD13	2.57	0.40
1:D:46:ARG:HG2	1:F:58:GLY:N	2.37	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)
3:A:233:SO4:O4	4:A:267:HOH:O[2_556]	1.94	0.26

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	204/229 (89%)	201 (98%)	3 (2%)	0	100	100
1	B	204/229 (89%)	198 (97%)	6 (3%)	0	100	100
1	C	201/229 (88%)	193 (96%)	7 (4%)	1 (0%)	29	35
1	D	197/229 (86%)	190 (96%)	6 (3%)	1 (0%)	29	35
1	E	204/229 (89%)	197 (97%)	5 (2%)	2 (1%)	15	17
1	F	203/229 (89%)	199 (98%)	4 (2%)	0	100	100
All	All	1213/1374 (88%)	1178 (97%)	31 (3%)	4 (0%)	41	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	ASP
1	E	45	SER
1	D	17	ARG
1	C	46	ARG

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	181/201 (90%)	171 (94%)	10 (6%)	21	30
1	B	181/201 (90%)	172 (95%)	9 (5%)	24	34
1	C	178/201 (89%)	173 (97%)	5 (3%)	43	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	174/201 (87%)	169 (97%)	5 (3%)	42	58
1	E	181/201 (90%)	176 (97%)	5 (3%)	43	60
1	F	180/201 (90%)	171 (95%)	9 (5%)	24	34
All	All	1075/1206 (89%)	1032 (96%)	43 (4%)	31	44

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	33	GLN
1	A	54	ASN
1	A	132	HIS
1	A	138	SER
1	A	144	ASP
1	A	165	LYS
1	A	169	GLU
1	A	194	MET
1	A	212	LEU
1	B	1	MET
1	B	16	GLN
1	B	33	GLN
1	B	54	ASN
1	B	78	LEU
1	B	133	LEU
1	B	175	SER
1	B	194	MET
1	B	216	ASP
1	C	1	MET
1	C	18	MET
1	C	45	SER
1	C	78	LEU
1	C	218	GLU
1	D	1	MET
1	D	46	ARG
1	D	54	ASN
1	D	185	ASP
1	D	198	ARG
1	E	44	ASP
1	E	54	ASN
1	E	90	ILE
1	E	132	HIS

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Mol	Chain	Res	Type
1	E	218	GLU
1	F	1	MET
1	F	33	GLN
1	F	45	SER
1	F	78	LEU
1	F	120	LEU
1	F	133	LEU
1	F	194	MET
1	F	198	ARG
1	F	202	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	33	GLN
1	A	36	HIS
1	A	54	ASN
1	A	117	ASN
1	B	33	GLN
1	B	54	ASN
1	B	69	GLN
1	B	132	HIS
1	B	219	ASN
1	C	54	ASN
1	C	219	ASN
1	D	54	ASN
1	D	117	ASN
1	E	54	ASN
1	F	105	HIS
1	F	219	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	E	233	-	4,4,4	0.17	0	6,6,6	0.33	0
3	SO4	C	231	-	4,4,4	0.20	0	6,6,6	0.28	0
3	SO4	B	232	-	4,4,4	0.20	0	6,6,6	0.32	0
3	SO4	A	234	-	4,4,4	0.16	0	6,6,6	0.27	0
3	SO4	A	232	-	4,4,4	0.19	0	6,6,6	0.46	0
3	SO4	E	232	-	4,4,4	0.15	0	6,6,6	0.36	0
3	SO4	C	232	-	4,4,4	0.22	0	6,6,6	0.26	0
3	SO4	B	231	-	4,4,4	0.10	0	6,6,6	0.22	0
3	SO4	A	233	-	4,4,4	0.42	0	6,6,6	0.82	0
3	SO4	F	231	-	4,4,4	0.21	0	6,6,6	0.37	0
3	SO4	D	231	-	4,4,4	0.21	0	6,6,6	0.29	0
3	SO4	A	231	-	4,4,4	0.21	0	6,6,6	0.58	0
3	SO4	E	231	-	4,4,4	0.15	0	6,6,6	0.24	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.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	232	SO4	7	0
3	A	234	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	232	SO4	1	0
3	A	233	SO4	0	1
3	D	231	SO4	4	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	207/229 (90%)	0.96	37 (17%)	1	1	34, 42, 55, 67	0
1	B	207/229 (90%)	1.01	41 (19%)	1	1	37, 46, 66, 81	0
1	C	204/229 (89%)	1.12	41 (20%)	1	1	40, 49, 75, 89	0
1	D	200/229 (87%)	0.95	36 (18%)	1	1	35, 46, 66, 88	0
1	E	207/229 (90%)	1.15	46 (22%)	0	1	40, 51, 71, 90	0
1	F	206/229 (89%)	0.97	44 (21%)	0	1	38, 47, 62, 76	0
All	All	1231/1374 (89%)	1.03	245 (19%)	1	1	34, 47, 68, 90	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ILE	6.9
1	E	132	HIS	6.3
1	D	215	LEU	6.1
1	A	217	GLU	5.8
1	C	5	LYS	5.5
1	F	32	HIS	5.3
1	C	132	HIS	5.1
1	E	34	THR	5.1
1	D	1	MET	5.1
1	F	128[A]	PHE	4.8
1	A	71	ILE	4.8
1	C	17	ARG	4.8
1	C	34	THR	4.7
1	B	221	LEU	4.7
1	E	32	HIS	4.7
1	D	5	LYS	4.7
1	B	71	ILE	4.6
1	A	221	LEU	4.6
1	C	128[A]	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	2	ASP	4.4
1	A	110	ASP	4.4
1	F	1	MET	4.4
1	E	1	MET	4.4
1	F	138	SER	4.3
1	F	34	THR	4.3
1	B	220	ILE	4.2
1	F	71	ILE	4.2
1	A	56	GLU	4.2
1	C	71	ILE	4.2
1	F	110	ASP	4.1
1	F	216	ASP	4.1
1	E	40	ILE	4.0
1	D	181	TYR	4.0
1	D	110	ASP	4.0
1	A	139	PRO	3.9
1	F	218	GLU	3.9
1	D	71	ILE	3.9
1	B	1	MET	3.9
1	F	132	HIS	3.8
1	D	18	MET	3.8
1	B	135	GLY	3.8
1	E	71	ILE	3.8
1	A	1	MET	3.8
1	A	218	GLU	3.8
1	B	73	THR	3.7
1	E	140	GLU	3.7
1	C	50	GLU	3.7
1	A	17	ARG	3.7
1	C	78	LEU	3.6
1	F	217	GLU	3.6
1	E	73	THR	3.6
1	D	40	ILE	3.6
1	A	77	CYS	3.6
1	C	40	ILE	3.5
1	E	187	PHE	3.5
1	C	70	VAL	3.5
1	C	41	ALA	3.5
1	C	73	THR	3.5
1	D	16	GLN	3.5
1	F	17	ARG	3.5
1	A	132	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	2	ASP	3.5
1	B	66	VAL	3.4
1	B	132	HIS	3.4
1	B	17	ARG	3.4
1	C	80	VAL	3.4
1	E	17	ARG	3.4
1	F	135	GLY	3.4
1	C	57	PRO	3.4
1	B	41	ALA	3.4
1	B	56	GLU	3.4
1	B	217	GLU	3.4
1	A	40	ILE	3.4
1	C	77	CYS	3.4
1	F	183	VAL	3.3
1	B	214	ILE	3.3
1	E	135	GLY	3.3
1	E	66	VAL	3.3
1	E	15	ALA	3.3
1	A	219	ASN	3.3
1	E	77	CYS	3.3
1	E	41	ALA	3.2
1	B	9	ALA	3.2
1	B	77	CYS	3.2
1	E	119	TRP	3.2
1	B	112	ASP	3.2
1	B	54	ASN	3.2
1	B	40	ILE	3.2
1	A	75	PHE	3.2
1	A	70	VAL	3.2
1	A	169	GLU	3.1
1	E	128[A]	PHE	3.1
1	C	111	LYS	3.1
1	E	16	GLN	3.1
1	D	14	TRP	3.1
1	E	134	LEU	3.1
1	A	216	ASP	3.1
1	C	66	VAL	3.1
1	F	62	VAL	3.0
1	F	77	CYS	3.0
1	B	70	VAL	3.0
1	C	75	PHE	3.0
1	E	75	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	62	VAL	3.0
1	A	33	GLN	3.0
1	B	75	PHE	3.0
1	A	184	ASN	3.0
1	E	220	ILE	2.9
1	B	137	LEU	2.9
1	B	119	TRP	2.9
1	A	78	LEU	2.9
1	C	6	GLN	2.9
1	D	128[A]	PHE	2.9
1	E	137	LEU	2.9
1	C	2	ASP	2.9
1	F	119	TRP	2.9
1	A	73	THR	2.8
1	B	110	ASP	2.8
1	E	78	LEU	2.8
1	C	171	GLY	2.8
1	A	128[A]	PHE	2.8
1	A	136	LYS	2.8
1	F	73	THR	2.8
1	F	40	ILE	2.8
1	E	199	GLU	2.8
1	F	57	PRO	2.8
1	D	65	ASN	2.8
1	B	76	ASN	2.8
1	E	9	ALA	2.8
1	B	12	TYR	2.8
1	A	183	VAL	2.7
1	F	66	VAL	2.7
1	E	63	HIS	2.7
1	C	1	MET	2.7
1	C	7	LEU	2.7
1	B	74	ASP	2.7
1	D	132	HIS	2.7
1	D	115	LEU	2.7
1	E	115	LEU	2.7
1	C	79	SER	2.7
1	B	184	ASN	2.7
1	D	66	VAL	2.7
1	D	78	LEU	2.7
1	E	62	VAL	2.7
1	F	136	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	76	ASN	2.6
1	B	78	LEU	2.6
1	F	80	VAL	2.6
1	E	138	SER	2.6
1	F	79	SER	2.6
1	D	119	TRP	2.6
1	B	34	THR	2.6
1	A	215	LEU	2.6
1	E	74	ASP	2.6
1	C	65	ASN	2.6
1	A	119	TRP	2.5
1	E	139	PRO	2.5
1	F	215	LEU	2.5
1	F	139	PRO	2.5
1	F	105	HIS	2.5
1	D	139	PRO	2.5
1	A	79	SER	2.5
1	C	217	GLU	2.5
1	A	16	GLN	2.5
1	A	57	PRO	2.5
1	B	122	HIS	2.5
1	C	76	ASN	2.5
1	C	119	TRP	2.5
1	D	15	ALA	2.5
1	E	203	ILE	2.5
1	F	76	ASN	2.5
1	F	219	ASN	2.5
1	C	138	SER	2.5
1	E	67	ALA	2.5
1	E	218	GLU	2.5
1	D	96	CYS	2.5
1	B	69	GLN	2.5
1	F	78	LEU	2.5
1	D	169	GLU	2.4
1	A	76	ASN	2.4
1	C	64	ARG	2.4
1	E	18	MET	2.4
1	D	77	CYS	2.4
1	D	73	THR	2.4
1	C	13	SER	2.4
1	C	136	LYS	2.4
1	E	116	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	38	LEU	2.4
1	E	57	PRO	2.4
1	B	151	VAL	2.4
1	E	56	GLU	2.4
1	E	76	ASN	2.4
1	E	219	ASN	2.3
1	E	70	VAL	2.3
1	A	95	ILE	2.3
1	D	74	ASP	2.3
1	E	80	VAL	2.3
1	C	63	HIS	2.3
1	B	169	GLU	2.3
1	D	41	ALA	2.3
1	F	41	ALA	2.3
1	D	140	GLU	2.2
1	E	136	LYS	2.2
1	B	128[A]	PHE	2.2
1	B	139	PRO	2.2
1	E	50	GLU	2.2
1	F	63	HIS	2.2
1	A	80	VAL	2.2
1	D	64	ARG	2.2
1	C	43	SER	2.2
1	F	75	PHE	2.2
1	F	199	GLU	2.2
1	D	12	TYR	2.1
1	C	62	VAL	2.1
1	F	67	ALA	2.1
1	A	74	ASP	2.1
1	F	137	LEU	2.1
1	F	16	GLN	2.1
1	F	169	GLU	2.1
1	C	110	ASP	2.1
1	F	108	MET	2.1
1	B	136	LYS	2.1
1	D	70	VAL	2.1
1	A	69	GLN	2.1
1	B	13	SER	2.1
1	B	57	PRO	2.1
1	D	111	LYS	2.1
1	C	74	ASP	2.1
1	F	33	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	74	ASP	2.1
1	C	206	ARG	2.1
1	F	187	PHE	2.1
1	D	62	VAL	2.1
1	D	81	VAL	2.1
1	A	138	SER	2.1
1	F	171	GLY	2.1
1	D	35	PRO	2.1
1	F	134	LEU	2.1
1	C	18	MET	2.1
1	E	81	VAL	2.0
1	B	115	LEU	2.0
1	C	215	LEU	2.0
1	B	64	ARG	2.0
1	C	112	ASP	2.0
1	E	79	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	232	5/5	0.81	0.43	63,64,65,65	5
3	SO4	E	231	5/5	0.89	0.23	88,89,89,90	0
3	SO4	D	231	5/5	0.92	0.19	50,50,51,53	5
3	SO4	A	234	5/5	0.94	0.36	45,46,46,48	5
3	SO4	C	231	5/5	0.94	0.20	66,67,68,69	0
3	SO4	E	233	5/5	0.96	0.12	63,63,66,66	0
2	ZN	E	230	1/1	0.97	0.06	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	231	5/5	0.97	0.13	64,64,65,65	5
3	SO4	E	232	5/5	0.97	0.22	74,74,74,74	0
3	SO4	C	232	5/5	0.97	0.18	63,63,64,67	0
2	ZN	B	230	1/1	0.98	0.03	42,42,42,42	0
3	SO4	A	231	5/5	0.98	0.14	59,60,60,61	0
3	SO4	A	233	5/5	0.98	0.12	44,44,46,47	5
2	ZN	C	230	1/1	0.98	0.04	46,46,46,46	0
3	SO4	F	231	5/5	0.98	0.10	61,62,63,64	0
3	SO4	A	232	5/5	0.99	0.16	55,55,56,56	0
2	ZN	A	230	1/1	0.99	0.02	38,38,38,38	0
2	ZN	F	230	1/1	0.99	0.03	42,42,42,42	0
2	ZN	D	230	1/1	0.99	0.02	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.