



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:18 AM GMT

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](mailto: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.

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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

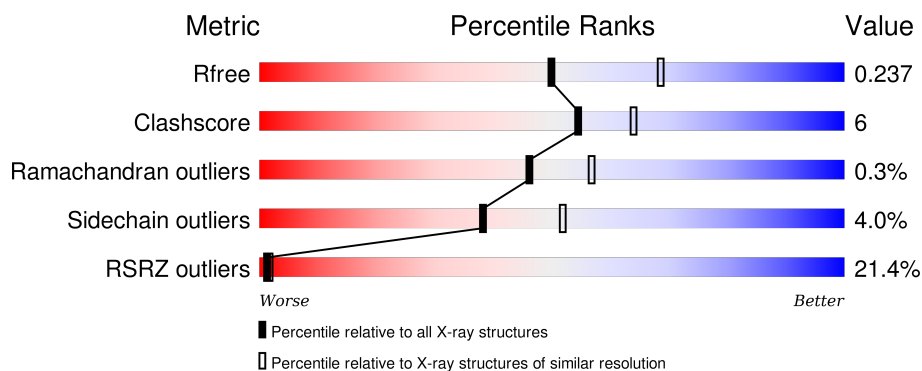
# 1 Overall quality at a glance

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  $\geq 3$ , 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>17%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>10%</div> </div> </div>
1	B	229	<div> <div>20%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>• 10%</div> </div> </div>
1	C	229	<div> <div>21%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>• 11%</div> </div> </div>
1	D	229	<div> <div>16%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>13%</div> </div> </div>
1	E	229	<div> <div>21%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>10%</div> </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	234	-	-	X	X
3	SO4	B	232	-	-	X	X
3	SO4	D	231	-	-	X	-

## 2 Entry composition

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
1	A	207	Total	C	N	O	S	0	1	0
			1669	1064	296	300	9			
1	B	207	Total	C	N	O	S	0	1	0
			1669	1064	296	300	9			
1	C	204	Total	C	N	O	S	0	1	0
			1644	1047	292	296	9			
1	D	200	Total	C	N	O	S	0	1	0
			1610	1029	287	285	9			
1	E	207	Total	C	N	O	S	0	1	0
			1671	1064	298	300	9			
1	F	206	Total	C	N	O	S	0	1	0
			1663	1058	297	299	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	GLY	ENGINEERED	UNP P45148
B	41	ALA	GLY	ENGINEERED	UNP P45148
C	41	ALA	GLY	ENGINEERED	UNP P45148
D	41	ALA	GLY	ENGINEERED	UNP P45148
E	41	ALA	GLY	ENGINEERED	UNP P45148
F	41	ALA	GLY	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: O<sub>4</sub>S).



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	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		

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

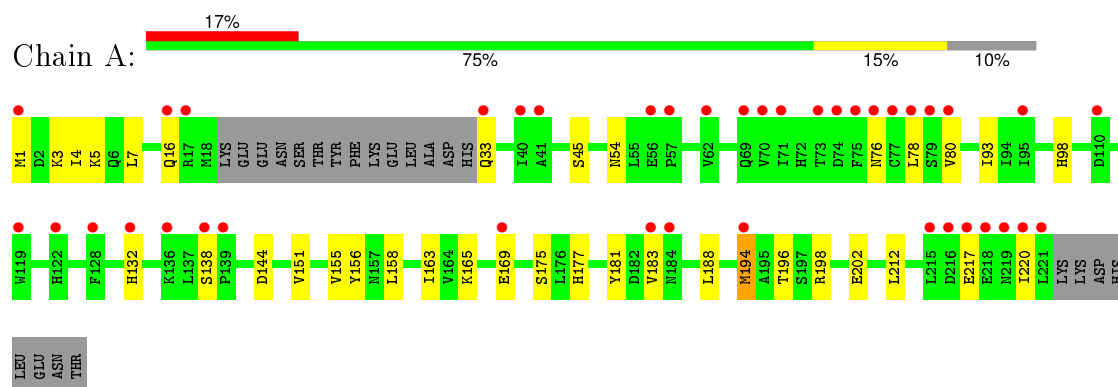
- Molecule 4 is water.

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

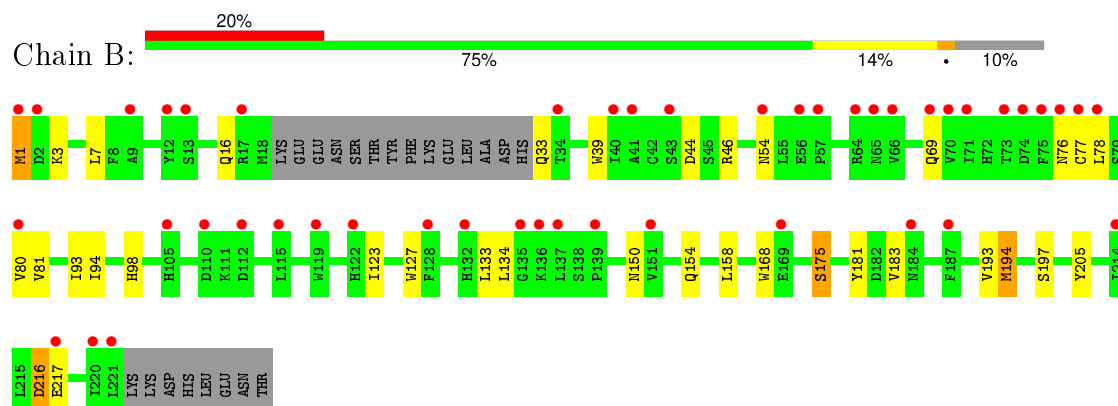
### 3 Residue-property plots [i](#)

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.

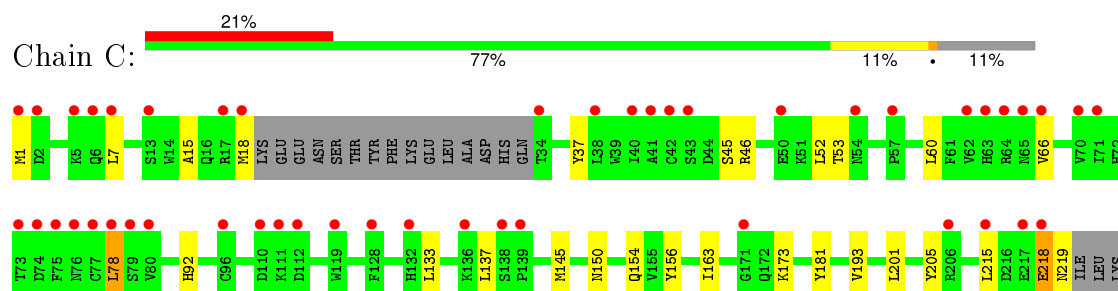
#### • Molecule 1: Carbonic anhydrase 2



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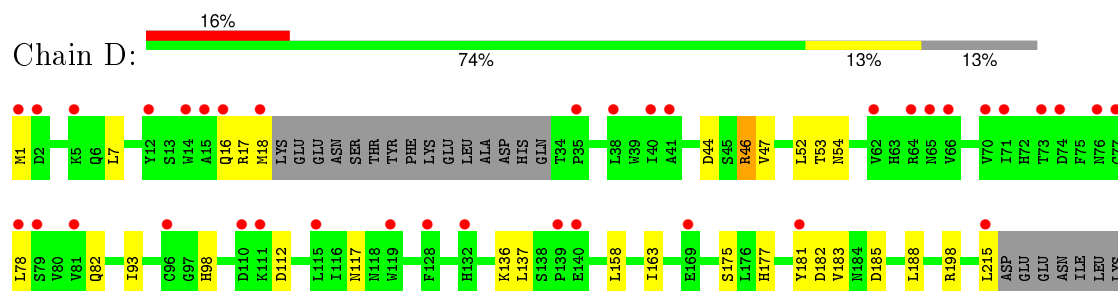


#### • Molecule 1: Carbonic anhydrase 2



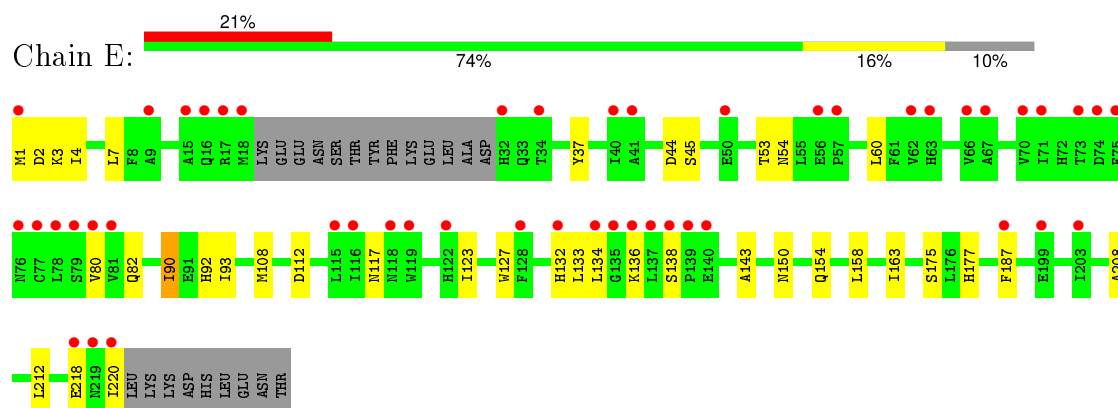
LYS  
ASP  
HIS  
LEU  
GLU  
ASN  
THR

• Molecule 1: Carbonic anhydrase 2

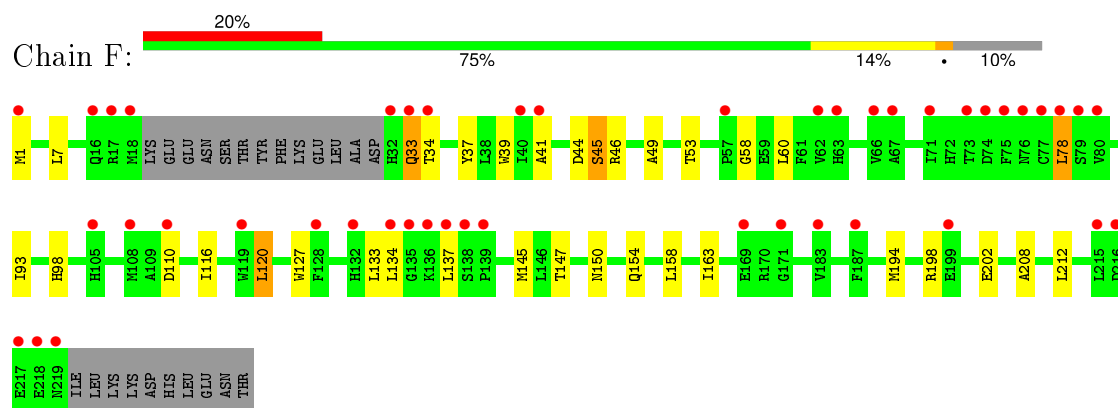


LYS  
ASP  
HIS  
LEU  
GLU  
ASN  
THR

• 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, $\alpha$ , $\beta$ , $\gamma$	231.93 Å   145.23 Å   52.97 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.197   ,   0.234 0.201   ,   0.237	Depositor DCC
$R_{free}$ test set	3804 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.2	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 76058 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10130	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.56	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(°)	Ideal(°)
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:C:53:THR:HG22	1:E:7:LEU:HD21	1.75	0.67
1:A:217:GLU:HA	1:A:220:ILE:HD12	1.77	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:F:116:ILE:HG13	1:F:120:LEU:HD22	1.81	0.62
1:B:1:MET:HE2	1:B:3:LYS:H	1.64	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:C	1:F:110:ASP:OD1	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:E:136:LYS:O	1:E:220:ILE:HG23	2.13	0.48
1:B:127:TRP:CD1	1:B:134:LEU:HD13	2.49	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:175:SER:HG	1:A:177:HIS:HE2	1.63	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: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:D:181:TYR:HB3	1:D:188:LEU:HD23	1.97	0.46
1:B:175:SER:HB2	1:B:194:MET:CE	2.45	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:D:137:LEU:HD11	1:D:215:LEU:HD12	1.98	0.45
1:B:150:ASN:O	1:B:154:GLN:HG2	2.16	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:90:ILE:CD1	1:E:92:HIS:O	2.65	0.44
1:E:1:MET:O	1:E:3:LYS:N	2.50	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:E:90:ILE:HD11	1:E:92:HIS:O	2.18	0.43
1:C:52:LEU:HD11	1:C:181:TYR:CE2	2.54	0.43
1:E:150:ASN:O	1:E:154:GLN:HG2	2.19	0.43
1:F:44:ASP:O	1:F:45:SER:C	2.55	0.43
1:B:7:LEU:HA	1:B:7:LEU:HD12	1.81	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:173:LYS:HZ1	1:E:1:MET:HE2	1.84	0.42
1:C:156:TYR:HA	1:C:201:LEU:HD11	2.02	0.42
1:E:123:ILE:CD1	1:E:150:ASN:OD1	2.67	0.42
1:B:77:CYS:O	1:B:81:VAL:HG23	2.20	0.42
1:C:193:VAL:HG22	1:C:205:TYR:HA	2.01	0.42
1:A:7:LEU:HD23	1:A:7:LEU:C	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:123:ILE:HD12	1:E:150:ASN:OD1	2.21	0.41
1:E:82:GLN:HA	1:E:163:ILE:HG21	2.03	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:D:46:ARG:HG2	1:F:58:GLY:N	2.37	0.40
1:B:39:TRP:CZ3	1:B:94:ILE:HD13	2.57	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

### 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	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%)	34	41
1	D	197/229 (86%)	190 (96%)	6 (3%)	1 (0%)	34	41
1	E	204/229 (89%)	197 (97%)	5 (2%)	2 (1%)	19	21
1	F	203/229 (89%)	199 (98%)	4 (2%)	0	100	100
All	All	1213/1374 (88%)	1178 (97%)	31 (3%)	4 (0%)	46	57

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

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%)	27	36
1	B	181/201 (90%)	172 (95%)	9 (5%)	30	41
1	C	178/201 (89%)	173 (97%)	5 (3%)	51	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	174/201 (87%)	169 (97%)	5 (3%)	50	66
1	E	181/201 (90%)	176 (97%)	5 (3%)	51	68
1	F	180/201 (90%)	171 (95%)	9 (5%)	30	41
All	All	1075/1206 (89%)	1032 (96%)	43 (4%)	38	52

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

Some 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 ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	0.41	0	6,6,6	0.61	0
3	SO4	A	232	-	4,4,4	0.44	0	6,6,6	0.56	0
3	SO4	A	233	-	4,4,4	0.78	0	6,6,6	0.59	0
3	SO4	A	234	-	4,4,4	0.37	0	6,6,6	0.32	0
3	SO4	B	231	-	4,4,4	0.20	0	6,6,6	0.22	0
3	SO4	B	232	-	4,4,4	0.41	0	6,6,6	0.24	0
3	SO4	C	231	-	4,4,4	0.28	0	6,6,6	0.18	0
3	SO4	C	232	-	4,4,4	0.38	0	6,6,6	0.52	0
3	SO4	D	231	-	4,4,4	0.48	0	6,6,6	0.22	0
3	SO4	E	231	-	4,4,4	0.09	0	6,6,6	0.21	0
3	SO4	E	232	-	4,4,4	0.31	0	6,6,6	0.28	0
3	SO4	E	233	-	4,4,4	0.33	0	6,6,6	0.51	0
3	SO4	F	231	-	4,4,4	0.24	0	6,6,6	0.40	0

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	A	233	-	-	0/0/0/0	0/0/0/0
3	SO4	A	234	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	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

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	A	232	SO4	1	0
3	A	233	SO4	0	1
3	A	234	SO4	2	0
3	B	232	SO4	7	0
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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	207/229 (90%)	1.04	40 (19%) 2 2	34, 42, 55, 67	0
1	B	207/229 (90%)	1.09	46 (22%) 1 1	37, 46, 66, 81	0
1	C	204/229 (89%)	1.20	47 (23%) 1 1	40, 49, 75, 89	0
1	D	200/229 (87%)	1.03	37 (18%) 2 2	35, 46, 66, 88	0
1	E	207/229 (90%)	1.23	48 (23%) 1 1	40, 51, 71, 90	0
1	F	206/229 (89%)	1.05	45 (21%) 1 1	38, 47, 62, 76	0
All	All	1231/1374 (89%)	1.11	263 (21%) 1 2	34, 47, 68, 90	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ILE	7.2
1	E	132	HIS	6.5
1	D	215	LEU	6.3
1	A	217	GLU	5.9
1	C	5	LYS	5.6
1	F	32	HIS	5.5
1	C	132	HIS	5.3
1	E	34	THR	5.3
1	D	1	MET	5.2
1	F	128[A]	PHE	5.0
1	A	71	ILE	5.0
1	C	34	THR	4.9
1	B	221	LEU	4.9
1	C	17	ARG	4.9
1	E	32	HIS	4.9
1	B	71	ILE	4.8
1	A	221	LEU	4.8
1	D	5	LYS	4.8
1	C	128[A]	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	2	ASP	4.6
1	A	110	ASP	4.6
1	F	1	MET	4.5
1	E	1	MET	4.5
1	F	34	THR	4.5
1	F	138	SER	4.5
1	B	220	ILE	4.4
1	F	71	ILE	4.4
1	C	71	ILE	4.3
1	A	56	GLU	4.3
1	F	110	ASP	4.3
1	F	216	ASP	4.2
1	E	40	ILE	4.2
1	D	110	ASP	4.1
1	D	181	TYR	4.1
1	A	139	PRO	4.1
1	D	71	ILE	4.0
1	F	132	HIS	4.0
1	B	1	MET	4.0
1	B	135	GLY	4.0
1	E	71	ILE	4.0
1	F	218	GLU	4.0
1	D	18	MET	4.0
1	A	1	MET	3.9
1	B	73	THR	3.9
1	A	218	GLU	3.9
1	E	140	GLU	3.8
1	C	78	LEU	3.8
1	C	50	GLU	3.8
1	A	77	CYS	3.8
1	A	17	ARG	3.8
1	E	73	THR	3.7
1	D	40	ILE	3.7
1	F	217	GLU	3.7
1	C	40	ILE	3.7
1	C	70	VAL	3.7
1	C	41	ALA	3.7
1	C	73	THR	3.7
1	E	187	PHE	3.7
1	D	16	GLN	3.6
1	A	132	HIS	3.6
1	B	66	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	80	VAL	3.6
1	B	2	ASP	3.6
1	F	17	ARG	3.6
1	B	132	HIS	3.6
1	F	135	GLY	3.6
1	C	57	PRO	3.5
1	C	77	CYS	3.5
1	B	41	ALA	3.5
1	F	183	VAL	3.5
1	B	17	ARG	3.5
1	E	17	ARG	3.5
1	A	40	ILE	3.5
1	B	214	ILE	3.5
1	E	66	VAL	3.5
1	B	56	GLU	3.5
1	B	217	GLU	3.5
1	E	77	CYS	3.5
1	E	135	GLY	3.4
1	E	15	ALA	3.4
1	B	77	CYS	3.4
1	A	219	ASN	3.4
1	E	41	ALA	3.4
1	B	9	ALA	3.4
1	E	119	TRP	3.4
1	B	112	ASP	3.3
1	B	40	ILE	3.3
1	A	70	VAL	3.3
1	B	54	ASN	3.3
1	A	75	PHE	3.3
1	E	128[A]	PHE	3.3
1	D	14	TRP	3.2
1	A	169	GLU	3.2
1	E	134	LEU	3.2
1	C	66	VAL	3.2
1	A	216	ASP	3.2
1	F	62	VAL	3.2
1	C	111	LYS	3.2
1	E	16	GLN	3.2
1	F	77	CYS	3.2
1	B	70	VAL	3.2
1	A	62	VAL	3.1
1	E	75	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	75	PHE	3.1
1	C	75	PHE	3.1
1	E	220	ILE	3.1
1	A	184	ASN	3.1
1	B	137	LEU	3.1
1	B	119	TRP	3.1
1	A	78	LEU	3.0
1	A	33	GLN	3.0
1	D	128[A]	PHE	3.0
1	E	137	LEU	3.0
1	C	6	GLN	3.0
1	F	119	TRP	3.0
1	C	2	ASP	3.0
1	A	73	THR	3.0
1	E	78	LEU	3.0
1	B	110	ASP	2.9
1	C	171	GLY	2.9
1	A	128[A]	PHE	2.9
1	F	40	ILE	2.9
1	F	73	THR	2.9
1	F	57	PRO	2.9
1	A	183	VAL	2.9
1	E	9	ALA	2.9
1	F	66	VAL	2.9
1	D	65	ASN	2.9
1	B	76	ASN	2.9
1	E	199	GLU	2.9
1	A	136	LYS	2.9
1	E	63	HIS	2.9
1	B	12	TYR	2.8
1	C	1	MET	2.8
1	C	7	LEU	2.8
1	D	132	HIS	2.8
1	B	74	ASP	2.8
1	D	66	VAL	2.8
1	E	62	VAL	2.8
1	D	115	LEU	2.8
1	E	115	LEU	2.8
1	C	79	SER	2.8
1	D	78	LEU	2.8
1	F	80	VAL	2.8
1	B	184	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	78	LEU	2.7
1	D	76	ASN	2.7
1	F	136	LYS	2.7
1	B	34	THR	2.7
1	E	138	SER	2.7
1	F	79	SER	2.7
1	D	119	TRP	2.7
1	A	215	LEU	2.7
1	F	215	LEU	2.7
1	E	74	ASP	2.7
1	C	65	ASN	2.7
1	A	119	TRP	2.7
1	E	139	PRO	2.7
1	F	139	PRO	2.7
1	F	105	HIS	2.6
1	D	139	PRO	2.6
1	D	96	CYS	2.6
1	A	79	SER	2.6
1	B	122	HIS	2.6
1	D	15	ALA	2.6
1	C	119	TRP	2.6
1	E	203	ILE	2.6
1	A	57	PRO	2.6
1	E	67	ALA	2.6
1	C	217	GLU	2.6
1	A	16	GLN	2.6
1	C	76	ASN	2.6
1	F	76	ASN	2.6
1	F	219	ASN	2.6
1	C	138	SER	2.6
1	F	78	LEU	2.6
1	A	76	ASN	2.6
1	D	77	CYS	2.6
1	E	218	GLU	2.5
1	B	69	GLN	2.5
1	D	169	GLU	2.5
1	E	18	MET	2.5
1	C	64	ARG	2.5
1	D	73	THR	2.5
1	B	151	VAL	2.5
1	C	13	SER	2.5
1	D	38	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	57	PRO	2.5
1	E	116	ILE	2.5
1	E	76	ASN	2.5
1	E	219	ASN	2.4
1	E	56	GLU	2.4
1	E	70	VAL	2.4
1	E	80	VAL	2.4
1	A	95	ILE	2.4
1	C	136	LYS	2.4
1	C	63	HIS	2.4
1	D	41	ALA	2.4
1	D	74	ASP	2.4
1	F	41	ALA	2.4
1	B	169	GLU	2.4
1	A	80	VAL	2.3
1	B	139	PRO	2.3
1	D	140	GLU	2.3
1	F	63	HIS	2.3
1	B	128[A]	PHE	2.3
1	E	50	GLU	2.3
1	E	136	LYS	2.3
1	C	62	VAL	2.3
1	F	75	PHE	2.3
1	C	43	SER	2.3
1	D	64	ARG	2.3
1	F	67	ALA	2.3
1	F	137	LEU	2.3
1	A	74	ASP	2.2
1	D	12	TYR	2.2
1	F	199	GLU	2.2
1	D	70	VAL	2.2
1	F	16	GLN	2.2
1	F	108	MET	2.2
1	B	57	PRO	2.2
1	C	110	ASP	2.2
1	B	13	SER	2.2
1	D	62	VAL	2.2
1	D	81	VAL	2.2
1	F	187	PHE	2.2
1	F	169	GLU	2.2
1	C	74	ASP	2.2
1	F	74	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	69	GLN	2.2
1	F	171	GLY	2.2
1	D	35	PRO	2.2
1	F	134	LEU	2.2
1	B	136	LYS	2.2
1	D	111	LYS	2.2
1	F	33	GLN	2.2
1	E	81	VAL	2.2
1	C	206	ARG	2.2
1	C	18	MET	2.2
1	A	138	SER	2.2
1	B	115	LEU	2.1
1	C	215	LEU	2.1
1	C	42	CYS	2.1
1	B	105	HIS	2.1
1	E	79	SER	2.1
1	B	187	PHE	2.1
1	C	112	ASP	2.1
1	C	54	ASN	2.1
1	B	43	SER	2.1
1	B	64	ARG	2.1
1	E	122	HIS	2.1
1	C	38	LEU	2.1
1	C	96	CYS	2.1
1	E	118	ASN	2.1
1	A	122	HIS	2.1
1	C	218	GLU	2.0
1	A	41	ALA	2.0
1	D	79	SER	2.0
1	C	139	PRO	2.0
1	B	65	ASN	2.0
1	B	80	VAL	2.0
1	A	194	MET	2.0
1	F	18	MET	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 [i](#)

There are no carbohydrates 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	B	232	5/5	0.81	0.43	5.43	63,64,65,65	5
3	SO4	A	234	5/5	0.94	0.36	2.66	45,46,46,48	5
3	SO4	E	232	5/5	0.97	0.22	0.37	74,74,74,74	0
3	SO4	E	231	5/5	0.89	0.23	0.27	88,89,89,90	0
3	SO4	C	231	5/5	0.94	0.20	0.14	66,67,68,69	0
3	SO4	D	231	5/5	0.92	0.19	0.13	50,50,51,53	5
3	SO4	C	232	5/5	0.97	0.18	-0.07	63,63,64,67	0
3	SO4	E	233	5/5	0.96	0.12	-0.78	63,63,66,66	0
3	SO4	A	232	5/5	0.99	0.16	-0.81	55,55,56,56	0
3	SO4	A	231	5/5	0.98	0.14	-1.10	59,60,60,61	0
3	SO4	F	231	5/5	0.98	0.10	-1.64	61,62,63,64	0
2	ZN	F	230	1/1	0.99	0.03	-2.68	42,42,42,42	0
2	ZN	E	230	1/1	0.97	0.06	-3.45	50,50,50,50	0
2	ZN	C	230	1/1	0.98	0.04	-3.75	46,46,46,46	0
2	ZN	D	230	1/1	0.99	0.02	-3.80	40,40,40,40	0
2	ZN	B	230	1/1	0.98	0.03	-5.04	42,42,42,42	0
2	ZN	A	230	1/1	0.99	0.02	-7.97	38,38,38,38	0
3	SO4	A	233	5/5	0.98	0.12	-	44,44,46,47	5
3	SO4	B	231	5/5	0.97	0.13	-	64,64,65,65	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.