



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:18 AM GMT

PDB ID : 3E2W  
Title : H. influenzae beta-carbonic anhydrase, variant Y181F with 1M bicarbonate  
Authors : Rowlett, R.S.; Lee, J.  
Deposited on : 2008-08-06  
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:

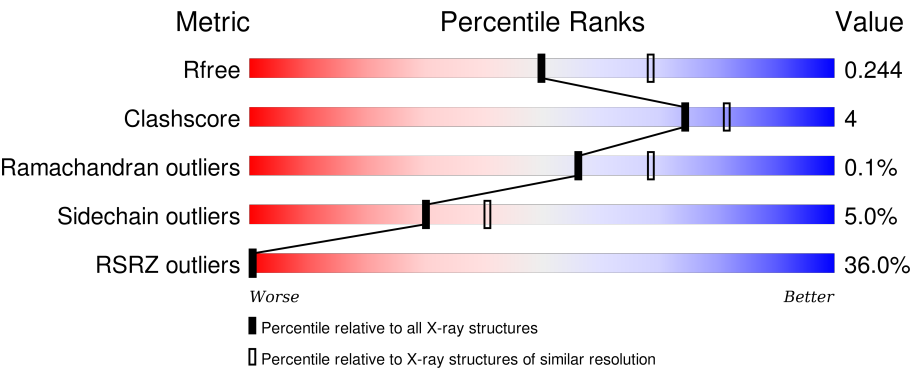
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance 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 <sub>free</sub>	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>25%</div><div><div></div><div>81%</div><div>9%</div><div>9%</div></div></div>
1	B	229	<div><div>32%</div><div><div></div><div>76%</div><div>10%</div><div>•</div><div>12%</div></div></div>
1	C	229	<div><div>38%</div><div><div></div><div>83%</div><div>5%</div><div>11%</div></div></div>
1	D	229	<div><div>33%</div><div><div></div><div>80%</div><div>8%</div><div>•</div><div>11%</div></div></div>
1	E	229	<div><div>32%</div><div><div></div><div>79%</div><div>10%</div><div>12%</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	231	-	-	-	X
3	SO4	A	233	-	-	X	-
3	SO4	C	231	-	-	-	X
3	SO4	E	232	-	-	X	-
3	SO4	F	233	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10077 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	208	Total	C	N	O	S	0	0	0
			1670	1059	298	304	9			
1	B	201	Total	C	N	O	S	0	0	0
			1609	1024	288	289	8			
1	C	203	Total	C	N	O	S	0	0	0
			1626	1035	292	290	9			
1	D	204	Total	C	N	O	S	0	0	0
			1636	1039	294	294	9			
1	E	202	Total	C	N	O	S	0	0	0
			1617	1029	290	289	9			
1	F	199	Total	C	N	O	S	0	0	0
			1592	1014	286	283	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).

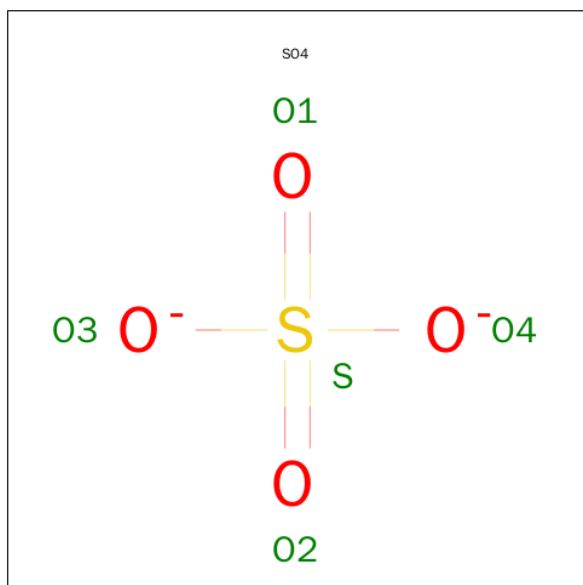
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

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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: O<sub>4</sub>S).



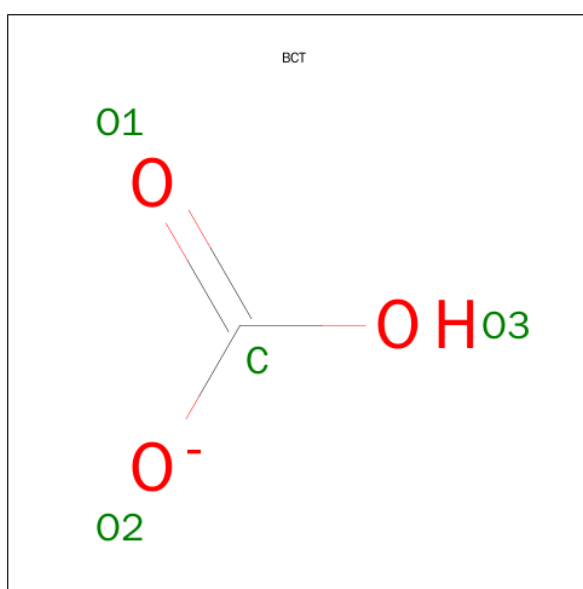
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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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	F	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:  $\text{CHO}_3$ ).



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	56	Total	O	0	0
			56	56		
5	B	33	Total	O	0	0
			33	33		
5	C	37	Total	O	0	0
			37	37		
5	D	51	Total	O	0	0
			51	51		

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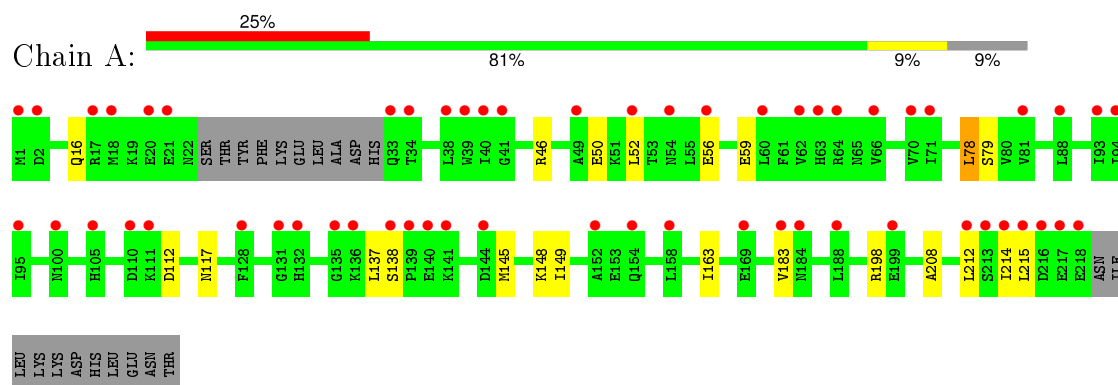
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	40	Total	O	0	0
			40	40		
5	F	40	Total	O	0	0
			40	40		

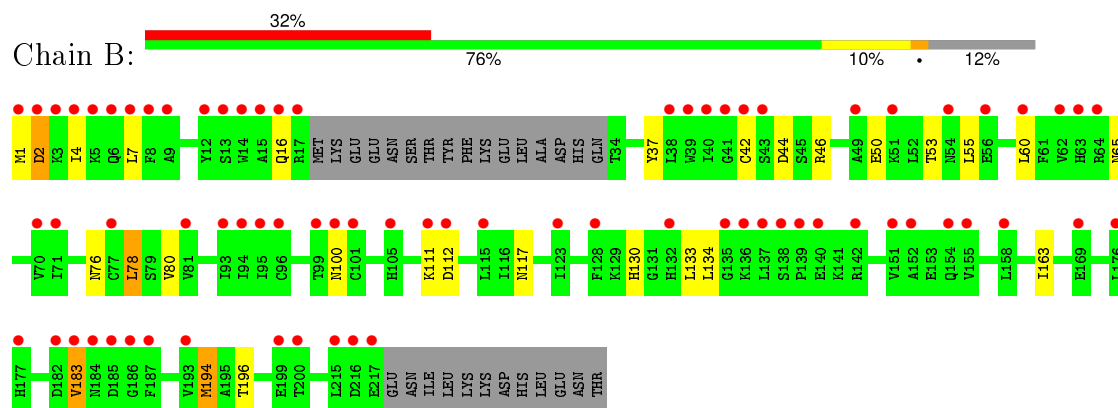
### 3 Residue-property plots

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.

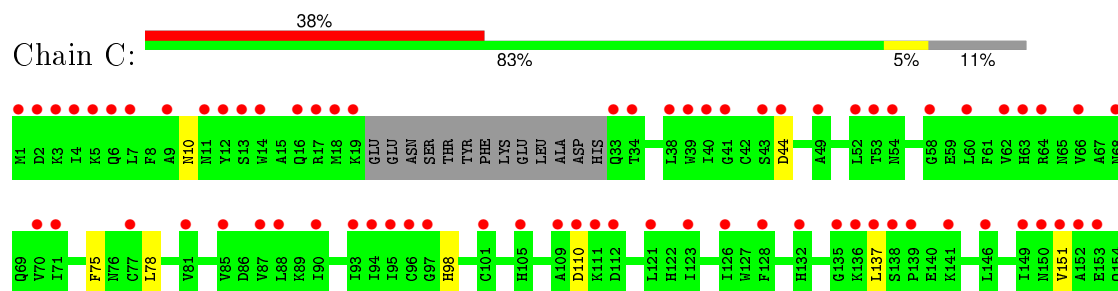
#### • Molecule 1: Carbonic anhydrase 2

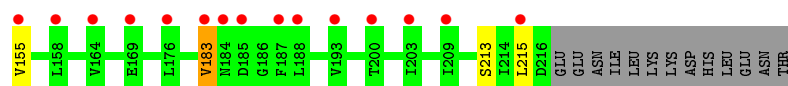


#### • Molecule 1: Carbonic anhydrase 2

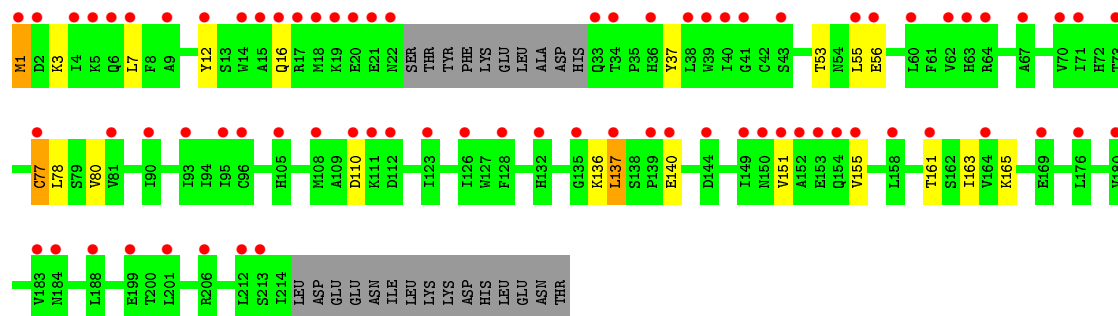
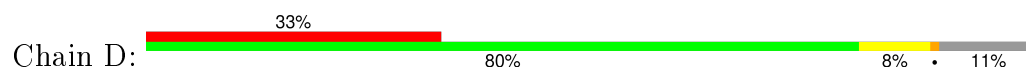


#### • Molecule 1: Carbonic anhydrase 2

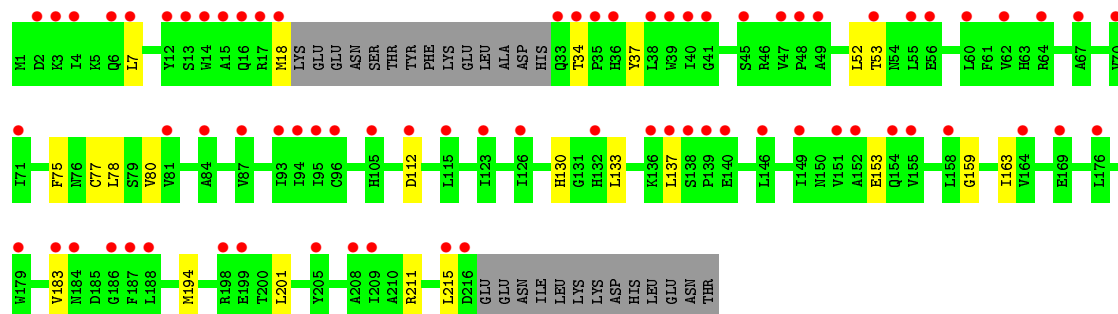
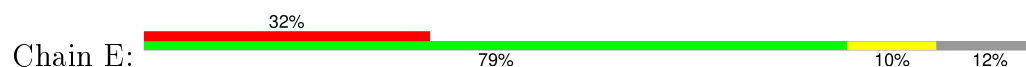




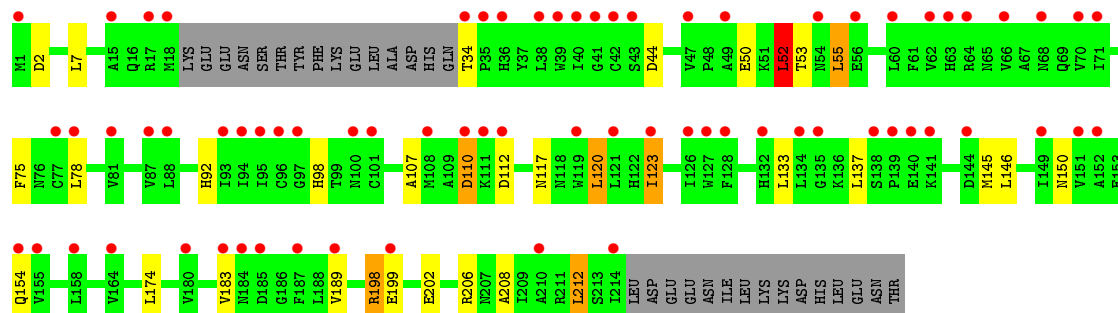
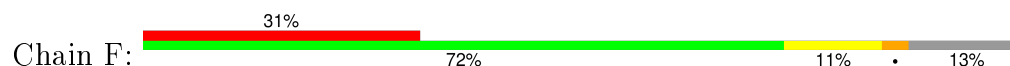
• Molecule 1: Carbonic anhydrase 2



• 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, $\alpha$ , $\beta$ , $\gamma$	250.14Å 145.22Å 53.50Å 90.00° 93.78° 90.00°	Depositor
Resolution (Å)	26.20 – 2.30 26.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.5 (26.20-2.30) 91.5 (26.19-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.205 , 0.242 0.210 , 0.244	Depositor DCC
$R_{free}$ test set	3911 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 82.0	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	0 of 77675 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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: 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	0.61	0/1705	0.68	1/2307 (0.0%)
1	B	0.59	0/1644	0.66	1/2227 (0.0%)
1	C	0.62	0/1661	0.69	0/2248
1	D	0.66	1/1671 (0.1%)	0.66	0/2261
1	E	0.63	0/1652	0.63	0/2237
1	F	0.64	0/1627	0.70	1/2203 (0.0%)
All	All	0.63	1/9960 (0.0%)	0.67	3/13483 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	CYS	CB-SG	6.24	1.92	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	52	LEU	CA-CB-CG	7.19	131.84	115.30
1	B	44	ASP	CB-CA-C	-7.09	96.23	110.40
1	A	52	LEU	CA-CB-CG	5.46	127.86	115.30

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	1670	0	1654	10	0
1	B	1609	0	1600	18	0
1	C	1626	0	1624	6	0
1	D	1636	0	1627	13	0
1	E	1617	0	1611	10	0
1	F	1592	0	1588	25	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	15	0	0	2	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
3	D	15	0	0	0	0
3	E	10	0	0	2	0
3	F	10	0	0	0	0
4	F	4	0	0	1	0
5	A	56	0	0	1	0
5	B	33	0	0	2	0
5	C	37	0	0	0	0
5	D	51	0	0	0	0
5	E	40	0	0	0	0
5	F	40	0	0	0	0
All	All	10077	0	9704	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (78) 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:133:LEU:HD22	1:B:134:LEU:HD12	1.49	0.94
1:F:208:ALA:O	1:F:212:LEU:HD23	1.72	0.89
1:B:80:VAL:HG21	5:B:263:HOH:O	1.80	0.80
1:A:50:GLU:OE1	5:A:268:HOH:O	2.07	0.72
1:A:112:ASP:HA	1:A:117:ASN:HD21	1.57	0.69
1:D:137:LEU:HD13	1:D:137:LEU:N	2.11	0.66
1:A:137:LEU:HD13	1:A:215:LEU:HD22	1.77	0.66
1:A:208:ALA:O	1:A:212:LEU:HD23	1.97	0.65
1:B:1:MET:O	1:B:4:ILE:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:ASP:N	1:F:110:ASP:OD2	2.32	0.62
1:F:50:GLU:OE1	4:F:231:BCT:O3	2.18	0.62
1:C:183:VAL:HG13	3:C:231:SO4:O3	2.00	0.61
1:E:137:LEU:HD21	1:E:215:LEU:HD22	1.82	0.60
1:B:78:LEU:HD13	1:B:163:ILE:HD12	1.83	0.60
1:C:213:SER:O	1:C:215:LEU:HD22	2.01	0.60
1:D:77:CYS:O	1:D:80:VAL:HG12	2.02	0.59
1:A:112:ASP:HA	1:A:117:ASN:ND2	2.19	0.57
1:A:183:VAL:HG11	3:A:233:SO4:O4	2.05	0.57
1:F:183:VAL:HG22	1:F:183:VAL:O	2.05	0.56
1:A:78:LEU:HD23	1:A:163:ILE:HD12	1.86	0.56
1:B:194:MET:HE1	1:B:196:THR:HG23	1.89	0.54
1:F:112:ASP:HA	1:F:117:ASN:ND2	2.22	0.54
1:B:133:LEU:HD23	1:B:133:LEU:C	2.29	0.53
1:D:7:LEU:HD21	1:F:55:LEU:HD21	1.91	0.52
1:B:76:ASN:O	1:B:80:VAL:HG23	2.09	0.52
1:B:80:VAL:CG2	5:B:263:HOH:O	2.45	0.52
1:C:137:LEU:HD21	1:C:215:LEU:HD12	1.92	0.52
1:F:112:ASP:HA	1:F:117:ASN:HD21	1.74	0.52
1:E:78:LEU:CD2	1:E:163:ILE:HD12	2.40	0.51
1:A:183:VAL:CG1	3:A:233:SO4:O2	2.59	0.51
1:F:198:ARG:NH1	1:F:202:GLU:HG2	2.25	0.51
1:D:53:THR:HG22	1:F:7:LEU:HD21	1.93	0.51
1:C:151:VAL:O	1:C:155:VAL:HG23	2.11	0.51
1:F:133:LEU:C	1:F:133:LEU:HD23	2.31	0.50
1:F:137:LEU:HD11	1:F:145:MET:HG2	1.93	0.50
1:F:52:LEU:HD22	1:F:53:THR:HG23	1.94	0.49
1:E:52:LEU:HD12	1:E:53:THR:HG23	1.95	0.49
1:B:183:VAL:CG1	3:B:231:SO4:O4	2.62	0.48
1:B:112:ASP:HA	1:B:117:ASN:ND2	2.28	0.47
1:D:1:MET:HE3	1:F:92:HIS:HE1	1.79	0.47
1:B:112:ASP:HA	1:B:117:ASN:HD21	1.79	0.47
1:B:50:GLU:HG3	1:B:60:LEU:HD12	1.96	0.47
1:C:137:LEU:HD21	1:C:215:LEU:CD1	2.45	0.46
1:A:148:LYS:HZ2	1:A:212:LEU:HD11	1.81	0.46
1:F:53:THR:OG1	1:F:55:LEU:HD22	2.15	0.46
1:B:37:TYR:HB2	1:B:60:LEU:HD23	1.97	0.46
1:F:150:ASN:O	1:F:154:GLN:HG2	2.16	0.46
1:D:151:VAL:O	1:D:155:VAL:HG23	2.16	0.46
1:B:130:HIS:O	1:B:134:LEU:HD13	2.16	0.45
1:D:78:LEU:CD1	1:D:163:ILE:HD12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:HIS:HE1	1:E:153:GLU:OE2	2.00	0.45
1:E:183:VAL:HG11	3:E:232:SO4:O2	2.17	0.45
1:F:123:ILE:HD11	1:F:146:LEU:HD21	1.99	0.45
1:F:212:LEU:CD2	1:F:212:LEU:N	2.79	0.44
1:F:107:ALA:HB2	1:F:120:LEU:HG	1.99	0.43
1:F:198:ARG:O	1:F:198:ARG:HD2	2.17	0.43
1:D:1:MET:HE3	1:D:3:LYS:HG3	2.00	0.43
1:F:52:LEU:CD2	1:F:53:THR:HG23	2.49	0.43
1:D:56:GLU:OE1	1:D:56:GLU:N	2.51	0.43
1:F:212:LEU:HD22	1:F:212:LEU:N	2.33	0.43
1:B:78:LEU:HD13	1:B:163:ILE:CD1	2.47	0.43
1:A:145:MET:HG3	1:A:149:ILE:HD12	2.01	0.43
1:E:159:GLY:HA3	1:E:201:LEU:HD22	2.01	0.43
1:B:53:THR:OG1	1:B:55:LEU:HD23	2.17	0.42
1:E:77:CYS:O	1:E:80:VAL:HG12	2.19	0.42
1:D:136:LYS:HB2	1:D:137:LEU:HD13	2.01	0.42
1:D:1:MET:CE	1:F:92:HIS:HE1	2.32	0.42
1:E:130:HIS:CE1	1:E:153:GLU:OE2	2.72	0.42
1:D:78:LEU:HD12	1:D:163:ILE:HD12	2.01	0.42
1:E:133:LEU:C	1:E:133:LEU:HD23	2.39	0.42
1:F:199:GLU:N	1:F:199:GLU:OE1	2.47	0.42
1:D:161:THR:O	1:D:165:LYS:HG3	2.20	0.41
1:E:183:VAL:CG1	3:E:232:SO4:O2	2.69	0.41
1:B:133:LEU:CD2	1:B:133:LEU:C	2.89	0.41
1:F:123:ILE:CD1	1:F:146:LEU:HD21	2.51	0.41
1:F:44:ASP:OD2	1:F:98:HIS:CE1	2.73	0.40
1:C:44:ASP:HB2	1:C:98:HIS:CE1	2.56	0.40
1:B:42:CYS:HA	1:B:65:ASN:O	2.22	0.40

There are no symmetry-related clashes.

## 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%)	198 (97%)	6 (3%)	0	100	100
1	B	197/229 (86%)	189 (96%)	7 (4%)	1 (0%)	34	41
1	C	199/229 (87%)	194 (98%)	5 (2%)	0	100	100
1	D	200/229 (87%)	194 (97%)	6 (3%)	0	100	100
1	E	198/229 (86%)	194 (98%)	4 (2%)	0	100	100
1	F	195/229 (85%)	192 (98%)	3 (2%)	0	100	100
All	All	1193/1374 (87%)	1161 (97%)	31 (3%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ASP

### 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%)	172 (95%)	9 (5%)	30	41
1	B	174/201 (87%)	165 (95%)	9 (5%)	29	38
1	C	176/201 (88%)	171 (97%)	5 (3%)	51	68
1	D	177/201 (88%)	169 (96%)	8 (4%)	34	46
1	E	175/201 (87%)	167 (95%)	8 (5%)	33	44
1	F	172/201 (86%)	158 (92%)	14 (8%)	15	18
All	All	1055/1206 (88%)	1002 (95%)	53 (5%)	30	41

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	46	ARG
1	A	56	GLU
1	A	59	GLU

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Mol	Chain	Res	Type
1	A	78	LEU
1	A	79	SER
1	A	138	SER
1	A	198	ARG
1	A	214	ILE
1	B	2	ASP
1	B	7	LEU
1	B	16	GLN
1	B	46	ARG
1	B	78	LEU
1	B	100	ASN
1	B	111	LYS
1	B	183	VAL
1	B	194	MET
1	C	10	ASN
1	C	75	PHE
1	C	78	LEU
1	C	110	ASP
1	C	183	VAL
1	D	1	MET
1	D	12	TYR
1	D	16	GLN
1	D	37	TYR
1	D	55	LEU
1	D	110	ASP
1	D	137	LEU
1	D	140	GLU
1	E	7	LEU
1	E	18	MET
1	E	34	THR
1	E	37	TYR
1	E	75	PHE
1	E	112	ASP
1	E	194	MET
1	E	211	ARG
1	F	2	ASP
1	F	34	THR
1	F	52	LEU
1	F	55	LEU
1	F	75	PHE
1	F	78	LEU
1	F	110	ASP

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Mol	Chain	Res	Type
1	F	120	LEU
1	F	123	ILE
1	F	174	LEU
1	F	189	VAL
1	F	198	ARG
1	F	206	ARG
1	F	212	LEU

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	117	ASN
1	A	132	HIS
1	B	117	ASN
1	B	184	ASN
1	C	6	GLN
1	C	10	ASN
1	C	54	ASN
1	C	105	HIS
1	D	100	ASN
1	D	105	HIS
1	D	132	HIS
1	E	100	ASN
1	E	130	HIS
1	E	184	ASN
1	F	92	HIS
1	F	130	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	0.25	0	6,6,6	0.21	0
3	SO4	A	232	-	4,4,4	0.28	0	6,6,6	0.29	0
3	SO4	A	233	-	4,4,4	0.30	0	6,6,6	0.28	0
3	SO4	B	231	-	4,4,4	0.29	0	6,6,6	0.15	0
3	SO4	C	231	-	4,4,4	0.30	0	6,6,6	0.19	0
3	SO4	D	231	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	D	232	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	D	233	-	4,4,4	0.28	0	6,6,6	0.17	0
3	SO4	E	231	-	4,4,4	0.19	0	6,6,6	0.39	0
3	SO4	E	232	-	4,4,4	0.33	0	6,6,6	0.07	0
4	BCT	F	231	-	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	F	232	-	4,4,4	0.27	0	6,6,6	0.17	0
3	SO4	F	233	-	4,4,4	0.27	0	6,6,6	0.18	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	B	231	-	-	0/0/0/0	0/0/0/0
3	SO4	C	231	-	-	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	D	233	-	-	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
4	BCT	F	231	-	-	0/0/0/0	0/0/0/0
3	SO4	F	232	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	F	233	-	-	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 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	233	SO4	2	0
3	B	231	SO4	1	0
3	C	231	SO4	1	0
3	E	232	SO4	2	0
4	F	231	BCT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	208/229 (90%)	1.61	57 (27%) <b>1</b> <b>1</b>	56, 65, 75, 83	0
1	B	201/229 (87%)	1.94	74 (36%) <b>0</b> <b>0</b>	60, 66, 79, 83	0
1	C	203/229 (88%)	1.96	86 (42%) <b>0</b> <b>0</b>	61, 67, 77, 80	0
1	D	204/229 (89%)	1.78	76 (37%) <b>0</b> <b>0</b>	59, 66, 76, 82	0
1	E	202/229 (88%)	1.90	74 (36%) <b>0</b> <b>0</b>	59, 66, 75, 82	0
1	F	199/229 (86%)	1.71	71 (35%) <b>0</b> <b>0</b>	51, 66, 76, 80	0
All	All	1217/1374 (88%)	1.82	438 (35%) <b>0</b> <b>0</b>	51, 66, 77, 83	0

All (438) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	34	THR	9.2
1	A	215	LEU	8.9
1	C	19	LYS	8.0
1	B	1	MET	7.9
1	B	216	ASP	7.7
1	D	22	ASN	7.6
1	D	1	MET	7.0
1	E	18	MET	6.5
1	B	183	VAL	6.4
1	E	17	ARG	6.1
1	E	4	ILE	5.8
1	E	140	GLU	5.8
1	C	33	GLN	5.6
1	F	214	ILE	5.6
1	C	215	LEU	5.6
1	C	5	LYS	5.6
1	D	19	LYS	5.5
1	F	95	ILE	5.5
1	D	2	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	139	PRO	5.5
1	C	6	GLN	5.4
1	B	40	ILE	5.4
1	A	40	ILE	5.4
1	A	110	ASP	5.3
1	B	12	TYR	5.3
1	F	40	ILE	5.3
1	E	15	ALA	5.3
1	E	16	GLN	5.3
1	C	34	THR	5.3
1	E	13	SER	5.3
1	F	128	PHE	5.2
1	B	139	PRO	5.2
1	B	2	ASP	5.2
1	A	132	HIS	5.1
1	C	138	SER	5.1
1	A	56	GLU	5.1
1	E	132	HIS	5.1
1	B	187	PHE	5.1
1	B	136	LYS	5.0
1	E	7	LEU	5.0
1	B	184	ASN	4.9
1	B	9	ALA	4.8
1	B	94	ILE	4.8
1	A	20	GLU	4.8
1	E	12	TYR	4.8
1	C	1	MET	4.8
1	D	21	GLU	4.8
1	D	34	THR	4.7
1	C	3	LYS	4.7
1	C	40	ILE	4.7
1	D	16	GLN	4.6
1	E	40	ILE	4.6
1	D	20	GLU	4.6
1	D	56	GLU	4.6
1	F	141	LYS	4.6
1	A	34	THR	4.6
1	C	139	PRO	4.6
1	E	152	ALA	4.5
1	F	138	SER	4.5
1	A	21	GLU	4.5
1	E	139	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	56	GLU	4.4
1	C	187	PHE	4.4
1	D	40	ILE	4.4
1	C	17	ARG	4.4
1	F	132	HIS	4.4
1	F	38	LEU	4.3
1	B	169	GLU	4.3
1	C	95	ILE	4.3
1	B	17	ARG	4.3
1	A	141	LYS	4.3
1	F	158	LEU	4.3
1	E	187	PHE	4.2
1	B	39	TRP	4.2
1	C	112	ASP	4.2
1	C	137	LEU	4.2
1	C	135	GLY	4.1
1	A	216	ASP	4.1
1	A	213	SER	4.1
1	A	95	ILE	4.1
1	D	12	TYR	4.1
1	D	132	HIS	4.0
1	E	6	GLN	4.0
1	B	38	LEU	4.0
1	D	70	VAL	4.0
1	E	38	LEU	4.0
1	F	94	ILE	4.0
1	A	218	GLU	3.9
1	C	12	TYR	3.9
1	D	139	PRO	3.9
1	E	183	VAL	3.9
1	B	132	HIS	3.9
1	F	135	GLY	3.8
1	E	184	ASN	3.8
1	B	62	VAL	3.8
1	B	112	ASP	3.8
1	D	55	LEU	3.8
1	F	34	THR	3.8
1	B	93	ILE	3.8
1	D	126	ILE	3.8
1	E	95	ILE	3.8
1	C	183	VAL	3.8
1	F	187	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	6	GLN	3.8
1	E	33	GLN	3.8
1	D	38	LEU	3.8
1	E	199	GLU	3.8
1	B	51	LYS	3.8
1	C	38	LEU	3.8
1	B	185	ASP	3.8
1	B	200	THR	3.7
1	A	105	HIS	3.7
1	A	131	GLY	3.7
1	C	126	ILE	3.7
1	F	41	GLY	3.7
1	F	93	ILE	3.7
1	E	3	LYS	3.7
1	D	112	ASP	3.7
1	C	149	ILE	3.7
1	E	93	ILE	3.7
1	B	54	ASN	3.7
1	D	201	LEU	3.7
1	A	199	GLU	3.7
1	E	155	VAL	3.7
1	A	2	ASP	3.6
1	B	135	GLY	3.6
1	F	62	VAL	3.6
1	B	4	ILE	3.6
1	C	110	ASP	3.6
1	C	70	VAL	3.6
1	F	70	VAL	3.6
1	B	215	LEU	3.6
1	E	136	LYS	3.5
1	C	158	LEU	3.5
1	E	14	TRP	3.5
1	B	158	LEU	3.5
1	E	216	ASP	3.5
1	A	33	GLN	3.5
1	F	151	VAL	3.5
1	A	70	VAL	3.5
1	A	140	GLU	3.5
1	A	38	LEU	3.5
1	C	18	MET	3.5
1	E	215	LEU	3.5
1	C	128	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	2	ASP	3.4
1	E	2	ASP	3.4
1	E	81	VAL	3.4
1	A	1	MET	3.4
1	A	212	LEU	3.4
1	D	18	MET	3.4
1	F	112	ASP	3.4
1	D	140	GLU	3.4
1	A	169	GLU	3.4
1	E	96	CYS	3.4
1	E	137	LEU	3.4
1	D	71	ILE	3.4
1	A	62	VAL	3.3
1	B	5	LYS	3.3
1	F	63	HIS	3.3
1	B	128	PHE	3.3
1	B	95	ILE	3.3
1	D	111	LYS	3.3
1	A	71	ILE	3.3
1	C	54	ASN	3.3
1	F	39	TRP	3.3
1	A	52	LEU	3.3
1	B	70	VAL	3.3
1	F	64	ARG	3.3
1	F	144	ASP	3.3
1	B	101	CYS	3.3
1	F	81	VAL	3.2
1	B	8	PHE	3.2
1	F	60	LEU	3.2
1	B	56	GLU	3.2
1	D	199	GLU	3.2
1	B	71	ILE	3.2
1	C	111	LYS	3.2
1	B	138	SER	3.2
1	D	150	ASN	3.2
1	C	49	ALA	3.2
1	B	14	TRP	3.1
1	D	144	ASP	3.1
1	F	139	PRO	3.1
1	D	158	LEU	3.1
1	C	151	VAL	3.1
1	A	158	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	140	GLU	3.1
1	B	41	GLY	3.1
1	C	7	LEU	3.1
1	E	186	GLY	3.1
1	F	96	CYS	3.1
1	F	43	SER	3.1
1	B	15	ALA	3.0
1	E	94	ILE	3.0
1	A	184	ASN	3.0
1	C	109	ALA	3.0
1	E	149	ILE	3.0
1	C	14	TRP	3.0
1	A	135	GLY	3.0
1	F	155	VAL	3.0
1	C	94	ILE	3.0
1	B	60	LEU	3.0
1	B	100	ASN	3.0
1	B	151	VAL	3.0
1	A	39	TRP	3.0
1	F	68	ASN	3.0
1	D	5	LYS	3.0
1	E	62	VAL	3.0
1	E	87	VAL	3.0
1	C	71	ILE	3.0
1	F	71	ILE	3.0
1	D	212	LEU	3.0
1	C	136	LYS	2.9
1	F	185	ASP	2.9
1	E	151	VAL	2.9
1	C	9	ALA	2.9
1	B	3	LYS	2.9
1	C	93	ILE	2.9
1	D	4	ILE	2.9
1	C	132	HIS	2.9
1	A	188	LEU	2.9
1	C	62	VAL	2.9
1	E	126	ILE	2.9
1	A	217	GLU	2.9
1	C	169	GLU	2.9
1	C	184	ASN	2.9
1	A	183	VAL	2.9
1	B	96	CYS	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	155	VAL	2.9
1	B	105	HIS	2.9
1	D	137	LEU	2.9
1	D	15	ALA	2.9
1	D	151	VAL	2.9
1	E	39	TRP	2.9
1	D	81	VAL	2.8
1	D	135	GLY	2.8
1	D	149	ILE	2.8
1	C	60	LEU	2.8
1	F	66	VAL	2.8
1	F	189	VAL	2.8
1	C	123	ILE	2.8
1	D	95	ILE	2.8
1	D	152	ALA	2.8
1	B	199	GLU	2.8
1	C	13	SER	2.8
1	F	42	CYS	2.8
1	D	169	GLU	2.8
1	E	169	GLU	2.8
1	C	43	SER	2.8
1	D	108	MET	2.8
1	D	176	LEU	2.8
1	A	64	ARG	2.8
1	F	77	CYS	2.8
1	A	138	SER	2.7
1	A	18	MET	2.7
1	A	111	LYS	2.7
1	D	110	ASP	2.7
1	F	183	VAL	2.7
1	E	60	LEU	2.7
1	C	141	LYS	2.7
1	D	96	CYS	2.7
1	F	18	MET	2.7
1	F	149	ILE	2.7
1	F	152	ALA	2.7
1	C	63	HIS	2.7
1	A	154	GLN	2.7
1	E	55	LEU	2.7
1	B	186	GLY	2.7
1	A	81	VAL	2.7
1	F	140	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	93	ILE	2.7
1	D	9	ALA	2.7
1	C	96	CYS	2.7
1	C	200	THR	2.7
1	F	36	HIS	2.7
1	A	136	LYS	2.7
1	B	182	ASP	2.6
1	F	119	TRP	2.6
1	A	94	ILE	2.6
1	F	54	ASN	2.6
1	A	17	ARG	2.6
1	B	13	SER	2.6
1	D	7	LEU	2.6
1	C	53	THR	2.6
1	A	100	ASN	2.6
1	C	77	CYS	2.6
1	C	85	VAL	2.6
1	C	176	LEU	2.6
1	B	99	THR	2.6
1	E	176	LEU	2.6
1	C	4	ILE	2.6
1	D	93	ILE	2.6
1	E	70	VAL	2.6
1	A	63	HIS	2.5
1	C	152	ALA	2.5
1	C	188	LEU	2.5
1	F	17	ARG	2.5
1	E	53	THR	2.5
1	D	64	ARG	2.5
1	F	56	GLU	2.5
1	D	39	TRP	2.5
1	C	44	ASP	2.5
1	F	199	GLU	2.5
1	A	144	ASP	2.5
1	D	77	CYS	2.5
1	C	155	VAL	2.5
1	C	68	ASN	2.5
1	B	217	GLU	2.5
1	B	7	LEU	2.5
1	C	88	LEU	2.4
1	E	188	LEU	2.4
1	F	78	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	142	ARG	2.4
1	E	64	ARG	2.4
1	D	123	ILE	2.4
1	D	63	HIS	2.4
1	E	154	GLN	2.4
1	C	66	VAL	2.4
1	F	126	ILE	2.4
1	D	154	GLN	2.4
1	D	184	ASN	2.4
1	A	88	LEU	2.4
1	C	146	LEU	2.4
1	F	1	MET	2.4
1	B	77	CYS	2.4
1	D	41	GLY	2.4
1	C	185	ASP	2.4
1	A	60	LEU	2.4
1	B	64	ARG	2.4
1	D	17	ARG	2.4
1	A	66	VAL	2.4
1	D	213	SER	2.4
1	B	176	LEU	2.4
1	D	183	VAL	2.4
1	C	64	ARG	2.4
1	E	198	ARG	2.4
1	B	81	VAL	2.3
1	E	209	ILE	2.3
1	B	152	ALA	2.3
1	D	67	ALA	2.3
1	C	90	ILE	2.3
1	D	155	VAL	2.3
1	D	73	THR	2.3
1	F	127	TRP	2.3
1	F	101	CYS	2.3
1	E	115	LEU	2.3
1	D	164	VAL	2.3
1	A	49	ALA	2.3
1	F	134	LEU	2.3
1	B	111	LYS	2.3
1	F	210	ALA	2.3
1	D	105	HIS	2.3
1	C	87	VAL	2.3
1	F	123	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	67	ALA	2.3
1	B	63	HIS	2.3
1	F	184	ASN	2.3
1	F	87	VAL	2.2
1	B	177	HIS	2.2
1	F	110	ASP	2.2
1	B	16	GLN	2.2
1	C	121	LEU	2.2
1	D	33	GLN	2.2
1	A	41	GLY	2.2
1	F	111	LYS	2.2
1	D	90	ILE	2.2
1	E	208	ALA	2.2
1	C	11	ASN	2.2
1	C	101	CYS	2.2
1	C	52	LEU	2.2
1	F	49	ALA	2.2
1	B	193	VAL	2.2
1	B	137	LEU	2.2
1	B	43	SER	2.2
1	B	154	GLN	2.2
1	C	105	HIS	2.2
1	F	100	ASN	2.2
1	D	14	TRP	2.2
1	E	47	VAL	2.2
1	F	164	VAL	2.2
1	F	180	VAL	2.2
1	E	48	PRO	2.2
1	F	108	MET	2.2
1	A	54	ASN	2.2
1	C	150	ASN	2.2
1	D	36	HIS	2.2
1	E	105	HIS	2.2
1	E	138	SER	2.2
1	A	152	ALA	2.2
1	F	15	ALA	2.2
1	C	39	TRP	2.2
1	C	81	VAL	2.2
1	E	112	ASP	2.2
1	A	128	PHE	2.2
1	E	35	PRO	2.2
1	C	153	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	128	PHE	2.1
1	E	205	TYR	2.1
1	D	43	SER	2.1
1	D	60	LEU	2.1
1	E	146	LEU	2.1
1	E	49	ALA	2.1
1	E	84	ALA	2.1
1	B	6	GLN	2.1
1	C	209	ILE	2.1
1	D	62	VAL	2.1
1	E	164	VAL	2.1
1	B	115	LEU	2.1
1	C	97	GLY	2.1
1	F	97	GLY	2.1
1	D	180	VAL	2.1
1	E	36	HIS	2.1
1	E	45	SER	2.1
1	C	16	GLN	2.1
1	E	158	LEU	2.1
1	C	41	GLY	2.1
1	D	153	GLU	2.1
1	F	154	GLN	2.1
1	E	41	GLY	2.1
1	A	214	ILE	2.1
1	E	71	ILE	2.1
1	F	35	PRO	2.1
1	C	58	GLY	2.1
1	E	123	ILE	2.1
1	E	179	TRP	2.0
1	B	123	ILE	2.0
1	D	206	ARG	2.0
1	C	164	VAL	2.0
1	C	193	VAL	2.0
1	F	47	VAL	2.0
1	D	161	THR	2.0
1	B	49	ALA	2.0
1	D	188	LEU	2.0
1	B	42	CYS	2.0
1	C	203	ILE	2.0
1	F	88	LEU	2.0
1	F	121	LEU	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 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	F	233	5/5	0.70	0.42	5.27	96,96,96,96	5
3	SO4	A	231	5/5	0.70	0.41	4.54	120,120,121,121	0
3	SO4	C	231	5/5	0.84	0.40	2.61	95,95,96,96	5
3	SO4	D	232	5/5	0.81	0.31	1.89	127,127,127,127	0
3	SO4	E	231	5/5	0.75	0.27	1.52	110,111,112,112	0
3	SO4	B	231	5/5	0.77	0.34	1.05	95,95,95,95	5
3	SO4	D	231	5/5	0.82	0.26	1.03	113,113,113,114	0
3	SO4	A	233	5/5	0.94	0.24	0.50	53,55,56,58	5
3	SO4	E	232	5/5	0.89	0.26	0.44	74,75,75,75	5
3	SO4	D	233	5/5	0.96	0.14	-1.80	52,53,54,55	5
4	BCT	F	231	4/4	0.97	0.08	-2.52	61,62,62,62	0
2	ZN	E	230	1/1	0.99	0.08	-3.91	64,64,64,64	0
2	ZN	C	230	1/1	0.98	0.05	-4.07	66,66,66,66	0
2	ZN	B	230	1/1	0.97	0.06	-4.29	65,65,65,65	0
2	ZN	A	230	1/1	0.98	0.05	-4.32	67,67,67,67	0
2	ZN	F	230	1/1	0.97	0.05	-5.35	68,68,68,68	0
2	ZN	D	230	1/1	0.98	0.04	-7.87	66,66,66,66	0
3	SO4	F	232	5/5	0.89	0.26	-	98,99,99,101	0
3	SO4	A	232	5/5	0.68	0.39	-	110,111,112,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.