



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:40 am BST

PDB ID : 6RPS  
Title : X-ray crystal structure of carbonic anhydrase XII complexed with a theranostic monoclonal antibody fragment  
Authors : Alterio, V.; Esposito, D.; De Simone, G.  
Deposited on : 2019-05-14  
Resolution : 2.79 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

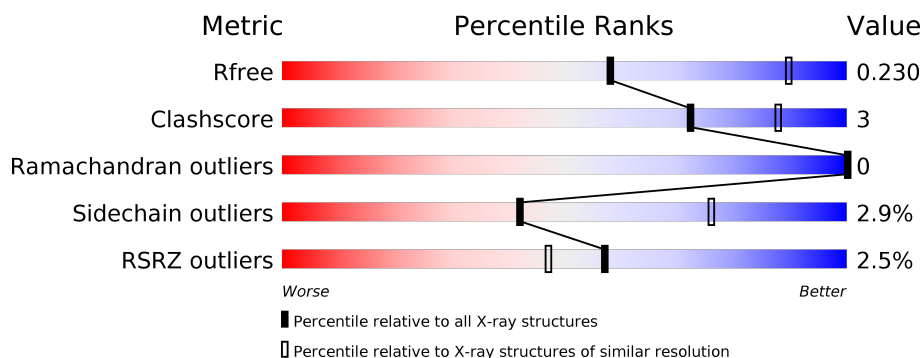
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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  $\leq 5\%$ . 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	283	<div> <div>80%</div> <div>12%</div> <div>7%</div> </div>
1	B	283	<div> <div>81%</div> <div>12%</div> <div>7%</div> </div>
2	L	216	<div> <div>13%</div> <div>88%</div> <div>10%</div> <div>•</div> </div>
2	M	216	<div> <div>2%</div> <div>90%</div> <div>9%</div> <div>•</div> </div>
3	H	229	<div> <div>88%</div> <div>6%</div> <div>5%</div> </div>
3	N	229	<div> <div>87%</div> <div>7%</div> <div>5%</div> </div>

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
5	ACT	A	302	-	-	X	-
5	ACT	B	302	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10838 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 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2105	1338	358	401	8			
1	B	262	Total	C	N	O	S	0	0	0
			2105	1338	358	401	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	initiating methionine	UNP O43570
A	263	GLY	-	expression tag	UNP O43570
A	264	GLY	-	expression tag	UNP O43570
A	265	GLY	-	expression tag	UNP O43570
A	266	GLY	-	expression tag	UNP O43570
A	267	SER	-	expression tag	UNP O43570
A	268	GLY	-	expression tag	UNP O43570
A	269	GLY	-	expression tag	UNP O43570
A	270	GLY	-	expression tag	UNP O43570
A	271	GLY	-	expression tag	UNP O43570
A	272	SER	-	expression tag	UNP O43570
A	273	GLY	-	expression tag	UNP O43570
A	274	GLY	-	expression tag	UNP O43570
A	275	GLY	-	expression tag	UNP O43570
A	276	GLY	-	expression tag	UNP O43570
A	277	SER	-	expression tag	UNP O43570
A	278	HIS	-	expression tag	UNP O43570
A	279	HIS	-	expression tag	UNP O43570
A	280	HIS	-	expression tag	UNP O43570
A	281	HIS	-	expression tag	UNP O43570
A	282	HIS	-	expression tag	UNP O43570
A	283	HIS	-	expression tag	UNP O43570
B	3	MET	-	initiating methionine	UNP O43570
B	263	GLY	-	expression tag	UNP O43570
B	264	GLY	-	expression tag	UNP O43570

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Chain	Residue	Modelled	Actual	Comment	Reference
B	265	GLY	-	expression tag	UNP O43570
B	266	GLY	-	expression tag	UNP O43570
B	267	SER	-	expression tag	UNP O43570
B	268	GLY	-	expression tag	UNP O43570
B	269	GLY	-	expression tag	UNP O43570
B	270	GLY	-	expression tag	UNP O43570
B	271	GLY	-	expression tag	UNP O43570
B	272	SER	-	expression tag	UNP O43570
B	273	GLY	-	expression tag	UNP O43570
B	274	GLY	-	expression tag	UNP O43570
B	275	GLY	-	expression tag	UNP O43570
B	276	GLY	-	expression tag	UNP O43570
B	277	SER	-	expression tag	UNP O43570
B	278	HIS	-	expression tag	UNP O43570
B	279	HIS	-	expression tag	UNP O43570
B	280	HIS	-	expression tag	UNP O43570
B	281	HIS	-	expression tag	UNP O43570
B	282	HIS	-	expression tag	UNP O43570
B	283	HIS	-	expression tag	UNP O43570

- Molecule 2 is a protein called Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	214	Total	C	N	O	S	0	0	0
			1644	1029	275	336	4			
2	L	214	Total	C	N	O	S	0	0	0
			1644	1029	275	336	4			

- Molecule 3 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	217	Total	C	N	O	S	0	0	0
			1646	1041	268	329	8			
3	H	217	Total	C	N	O	S	0	0	0
			1646	1041	268	329	8			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cd	0	0
			1	1		
7	A	3	Total	Cd	0	0
			3	3		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	9	Total	O	0	0
			9	9		
9	B	5	Total	O	0	0
			5	5		

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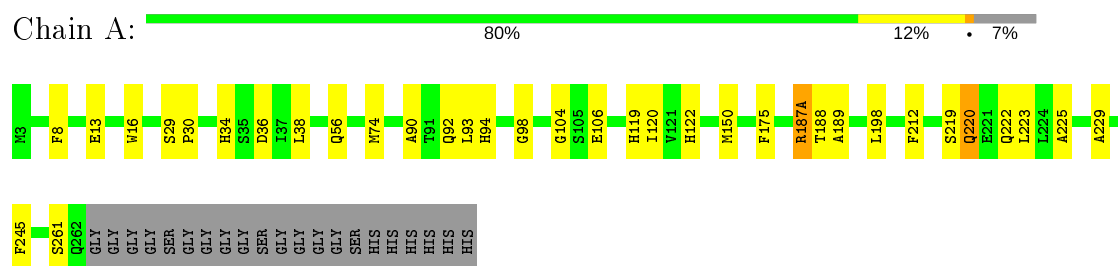
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	2	Total	O	0	0
			2	2		
9	N	3	Total	O	0	0
			3	3		
9	L	4	Total	O	0	0
			4	4		



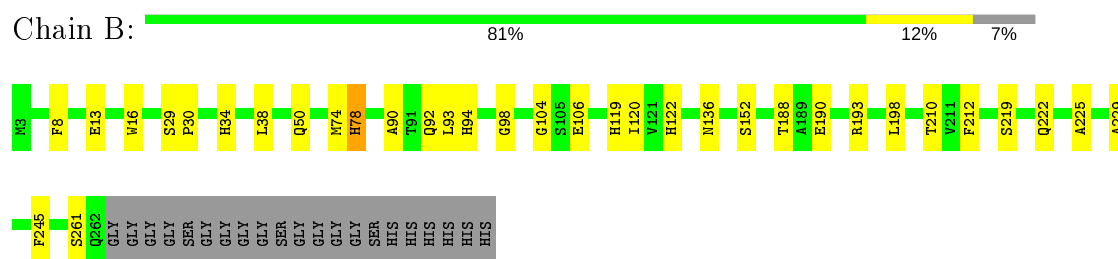
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

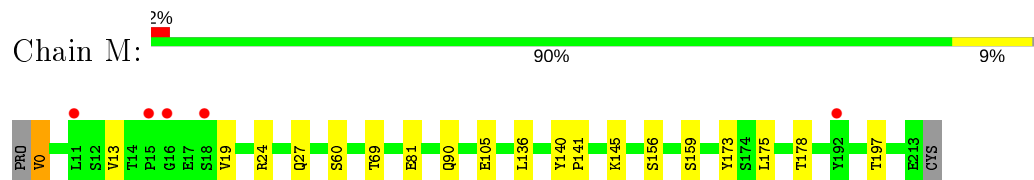
#### • Molecule 1: Carbonic anhydrase 12



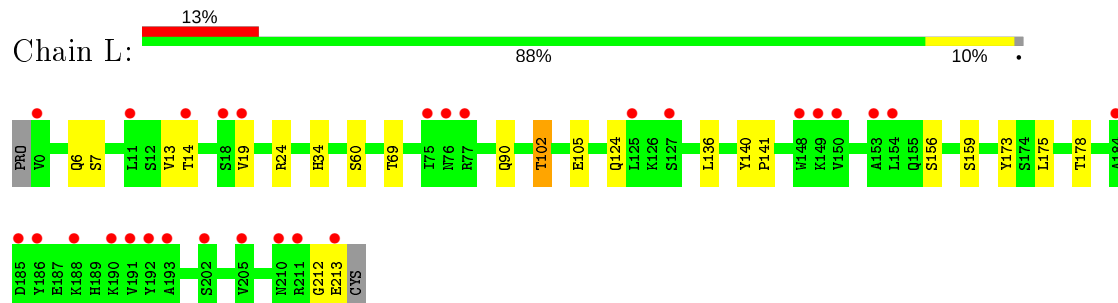
#### • Molecule 1: Carbonic anhydrase 12



#### • Molecule 2: Fab Light chain



#### • Molecule 2: Fab Light chain



● Molecule 3: Fab Heavy chain

Chain N: 

87%

7%

5%



● Molecule 3: Fab Heavy chain

Chain H: 

88%

6%

5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.33Å 222.16Å 266.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 2.79 49.65 – 2.79	Depositor EDS
% Data completeness (in resolution range)	92.4 (49.65-2.79) 92.4 (49.65-2.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.203 , 0.231 0.203 , 0.230	Depositor DCC
$R_{free}$ test set	1116 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 27.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, 0.333 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: ACT, ZN, CD, SO4, CL

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	0.31	0/2168	0.56	0/2952
1	B	0.32	0/2168	0.56	0/2952
2	L	0.30	0/1678	0.53	0/2277
2	M	0.30	0/1678	0.53	0/2277
3	H	0.32	0/1688	0.57	0/2300
3	N	0.32	0/1688	0.57	0/2300
All	All	0.31	0/11068	0.55	0/15058

There are no bond length outliers.

There are no bond angle outliers.

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	2105	0	1996	21	0
1	B	2105	0	1996	17	0
2	L	1644	0	1602	12	0
2	M	1644	0	1602	12	0
3	H	1646	0	1598	7	0
3	N	1646	0	1598	6	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	4	0	3	2	0
5	B	4	0	3	2	0
6	A	5	0	0	0	0
6	N	5	0	0	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
9	A	9	0	0	0	0
9	B	5	0	0	0	0
9	L	4	0	0	0	0
9	M	2	0	0	0	0
9	N	3	0	0	0	0
All	All	10838	0	10398	73	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 3.

All (73) 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)
2:M:0:VAL:HG12	2:M:27:GLN:HE22	1.34	0.92
1:A:150:MET:CE	1:A:223:LEU:HD22	2.18	0.72
1:A:198:LEU:HD23	5:A:302:ACT:H2	1.71	0.71
2:M:0:VAL:HG12	2:M:27:GLN:NE2	2.05	0.71
2:M:13:VAL:HG11	2:M:19:VAL:HG12	1.72	0.70
2:L:13:VAL:HG11	2:L:19:VAL:HG12	1.75	0.69
1:B:50:GLN:HB2	1:B:78:HIS:CD2	2.27	0.68
1:B:198:LEU:HD23	5:B:302:ACT:H2	1.79	0.64
1:A:150:MET:HG2	1:A:220:GLN:CD	2.22	0.59
2:L:212:GLY:O	2:L:213:GLU:HB3	2.03	0.57
2:L:6:GLN:HB3	2:L:102:THR:HG22	1.85	0.57
1:B:219:SER:HB3	1:B:222:GLN:HG3	1.87	0.56
1:A:150:MET:HE1	1:A:223:LEU:HD22	1.88	0.56
1:A:219:SER:HB3	1:A:222:GLN:HG3	1.87	0.56
2:L:34:HIS:CE1	3:H:100(D):PRO:HG3	2.44	0.53
3:N:97:GLY:HA3	3:N:100:ASP:O	2.09	0.53
1:A:34:HIS:O	1:A:38:LEU:HG	2.10	0.52
3:H:97:GLY:HA3	3:H:100:ASP:O	2.09	0.52
3:N:100(C):SER:N	3:N:100(D):PRO:CD	2.74	0.51
1:B:34:HIS:O	1:B:38:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:GLN:HB3	2:L:102:THR:CG2	2.41	0.50
2:M:24:ARG:HA	2:M:69:THR:O	2.12	0.50
3:H:100(C):SER:N	3:H:100(D):PRO:CD	2.74	0.50
2:M:0:VAL:CG1	2:M:27:GLN:HE22	2.16	0.50
2:L:24:ARG:HA	2:L:69:THR:O	2.12	0.50
1:A:150:MET:HE3	1:A:223:LEU:CD2	2.42	0.49
2:L:105:GLU:HG3	2:L:173:TYR:OH	2.13	0.49
2:M:105:GLU:HG3	2:M:173:TYR:OH	2.13	0.49
1:B:193:ARG:NH1	1:B:210:THR:OG1	2.46	0.48
1:A:150:MET:HG2	1:A:220:GLN:NE2	2.29	0.48
1:A:98:GLY:N	1:A:104:GLY:HA3	2.30	0.47
1:B:94:HIS:CE1	5:B:302:ACT:OXT	2.69	0.46
1:B:120:ILE:HG22	1:B:122:HIS:CE1	2.50	0.46
1:A:120:ILE:HG22	1:A:122:HIS:CE1	2.51	0.46
3:N:48:MET:HB3	3:N:67:LEU:HD11	1.97	0.46
3:H:48:MET:HB3	3:H:67:LEU:HD11	1.98	0.45
1:A:187(A):ARG:HH21	1:A:189:ALA:HB2	1.81	0.45
2:M:13:VAL:HG11	2:M:19:VAL:CG1	2.43	0.45
1:B:98:GLY:N	1:B:104:GLY:HA3	2.32	0.44
1:A:93:LEU:HA	1:A:119:HIS:O	2.17	0.44
2:L:136:LEU:HB2	2:L:175:LEU:HB3	1.99	0.44
2:L:159:SER:HA	2:L:178:THR:O	2.18	0.44
2:M:105:GLU:HG3	2:M:173:TYR:HH	1.83	0.44
1:B:106:GLU:HG2	1:B:245:PHE:HB2	1.99	0.44
1:B:29:SER:HB3	1:B:30:PRO:HA	2.00	0.43
1:A:29:SER:HB3	1:A:30:PRO:HA	1.99	0.43
1:A:150:MET:HE3	1:A:223:LEU:HD22	1.94	0.43
1:B:30:PRO:HG3	1:B:106:GLU:HB3	2.00	0.43
3:H:100(B):SER:HB2	3:H:100(D):PRO:HD2	2.00	0.43
1:B:93:LEU:HA	1:B:119:HIS:O	2.18	0.43
1:A:74:MET:HB3	1:A:90:ALA:HB3	2.00	0.43
2:M:136:LEU:HB2	2:M:175:LEU:HB3	2.00	0.43
1:B:13:GLU:HA	1:B:16:TRP:CE2	2.54	0.43
1:A:56:GLN:HE21	1:A:175:PHE:HB3	1.84	0.43
2:L:140:TYR:CG	2:L:141:PRO:HA	2.54	0.42
1:A:188:THR:HB	1:A:212:PHE:CE1	2.54	0.42
2:M:159:SER:HA	2:M:178:THR:O	2.19	0.42
3:N:39:GLN:HB3	3:N:45:PRO:HA	2.01	0.42
1:B:74:MET:HB3	1:B:90:ALA:HB3	2.00	0.42
3:H:39:GLN:HB3	3:H:45:PRO:HA	2.01	0.42
1:A:225:ALA:O	1:A:229:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:140:TYR:CG	2:M:141:PRO:HA	2.54	0.42
2:M:145:LYS:HB3	2:M:197:THR:HB	2.02	0.41
1:A:13:GLU:HA	1:A:16:TRP:CE2	2.55	0.41
1:A:106:GLU:HG2	1:A:245:PHE:HB2	2.01	0.41
1:B:188:THR:HB	1:B:212:PHE:CE1	2.56	0.41
2:L:124:GLN:HG3	3:H:122:PHE:CE2	2.55	0.41
2:L:105:GLU:HG3	2:L:173:TYR:HH	1.84	0.41
1:B:225:ALA:O	1:B:229:ALA:HB2	2.21	0.41
3:N:150:VAL:HG12	3:N:200:HIS:HB2	2.03	0.41
3:N:123:PRO:HD3	3:N:209:LYS:HE3	2.03	0.40
1:B:50:GLN:HB2	1:B:78:HIS:HD2	1.81	0.40
1:A:94:HIS:CE1	5:A:302:ACT:OXT	2.74	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	260/283 (92%)	254 (98%)	6 (2%)	0	100	100
1	B	260/283 (92%)	251 (96%)	9 (4%)	0	100	100
2	L	212/216 (98%)	203 (96%)	9 (4%)	0	100	100
2	M	212/216 (98%)	204 (96%)	8 (4%)	0	100	100
3	H	213/229 (93%)	207 (97%)	6 (3%)	0	100	100
3	N	213/229 (93%)	206 (97%)	7 (3%)	0	100	100
All	All	1370/1456 (94%)	1325 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	234/243 (96%)	228 (97%)	6 (3%)	46	79
1	B	234/243 (96%)	227 (97%)	7 (3%)	41	75
2	L	191/193 (99%)	185 (97%)	6 (3%)	40	74
2	M	191/193 (99%)	186 (97%)	5 (3%)	46	79
3	H	191/202 (95%)	185 (97%)	6 (3%)	40	74
3	N	191/202 (95%)	185 (97%)	6 (3%)	40	74
All	All	1232/1276 (97%)	1196 (97%)	36 (3%)	42	76

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	36	ASP
1	A	92	GLN
1	A	187(A)	ARG
1	A	220	GLN
1	A	261	SER
1	B	8	PHE
1	B	78	HIS
1	B	92	GLN
1	B	136	ASN
1	B	152	SER
1	B	190	GLU
1	B	261	SER
2	M	0	VAL
2	M	60	SER
2	M	81	GLU
2	M	90	GLN
2	M	156	SER
3	N	17	THR
3	N	24	VAL
3	N	58	VAL
3	N	67	LEU

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Mol	Chain	Res	Type
3	N	127	SER
3	N	179	SER
2	L	7	SER
2	L	14	THR
2	L	60	SER
2	L	90	GLN
2	L	102	THR
2	L	156	SER
3	H	17	THR
3	H	24	VAL
3	H	58	VAL
3	H	67	LEU
3	H	179	SER
3	H	187	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	101	ASN
1	A	112	GLN
1	B	56	GLN
1	B	78	HIS
1	B	101	ASN
1	B	262	GLN
2	M	27	GLN
2	M	138	ASN
3	N	199	ASN
2	L	27	GLN
3	H	199	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 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	$\# Z  > 2$
5	ACT	B	302	4	1,3,3	0.24	0	0,3,3	0.00	-
5	ACT	A	302	4	1,3,3	0.52	0	0,3,3	0.00	-
6	SO4	N	601	-	4,4,4	0.38	0	6,6,6	0.06	0
6	SO4	A	303	-	4,4,4	0.40	0	6,6,6	0.06	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	302	ACT	2	0
5	A	302	ACT	2	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	262/283 (92%)	-0.07	0 100 100	17, 32, 54, 73	0
1	B	262/283 (92%)	-0.15	0 100 100	15, 27, 49, 85	0
2	L	214/216 (99%)	0.75	28 (13%) 3 2	30, 49, 78, 105	0
2	M	214/216 (99%)	0.17	5 (2%) 60 51	23, 34, 56, 72	0
3	H	217/229 (94%)	0.02	1 (0%) 91 88	24, 36, 56, 77	0
3	N	217/229 (94%)	-0.11	0 100 100	18, 28, 45, 74	0
All	All	1386/1456 (95%)	0.09	34 (2%) 57 47	15, 33, 63, 105	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	191	VAL	4.8
2	L	213	GLU	4.6
2	L	76	ASN	4.1
2	L	0	VAL	3.9
2	L	186	TYR	3.8
2	L	154	LEU	3.5
2	L	190	LYS	3.3
2	L	193	ALA	3.2
2	L	192	TYR	3.1
2	L	210	ASN	2.9
2	L	19	VAL	2.9
2	L	77	ARG	2.9
2	L	125	LEU	2.8
2	L	185	ASP	2.8
2	L	184	ALA	2.8
2	L	18	SER	2.7
2	L	14	THR	2.7
2	L	153	ALA	2.7
2	M	15	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	150	VAL	2.6
2	L	205	VAL	2.5
2	L	149	LYS	2.5
2	L	11	LEU	2.5
2	M	18	SER	2.5
2	L	75	ILE	2.4
2	L	148	TRP	2.4
2	M	16	GLY	2.2
2	M	11	LEU	2.2
2	L	188	LYS	2.1
2	M	192	TYR	2.1
2	L	127	SER	2.1
2	L	202	SER	2.1
2	L	211	ARG	2.0
3	H	204	ASN	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
7	CD	A	306	1/1	0.95	0.07	50,50,50,50	1
7	CD	A	304	1/1	0.96	0.04	88,88,88,88	0
7	CD	A	307	1/1	0.97	0.17	35,35,35,35	1
6	SO4	A	303	5/5	0.98	0.14	31,34,36,37	0
5	ACT	A	302	4/4	0.98	0.22	22,24,25,25	0
8	CL	A	305	1/1	0.99	0.13	26,26,26,26	0
6	SO4	N	601	5/5	0.99	0.13	30,30,33,33	0
5	ACT	B	302	4/4	0.99	0.21	21,26,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	A	301	1/1	0.99	0.17	17,17,17,17	0
7	CD	B	303	1/1	0.99	0.04	64,64,64,64	0
4	ZN	B	301	1/1	0.99	0.15	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.