



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:18 pm BST

PDB ID : 3TPL  
Title : APO Structure of BACE1  
Authors : Xu, Y.C.; Li, M.J.; Greenblatt, H.; Chen, T.T.; Silman, I.; Sussman, J.L.  
Deposited on : 2011-09-08  
Resolution : 2.50 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

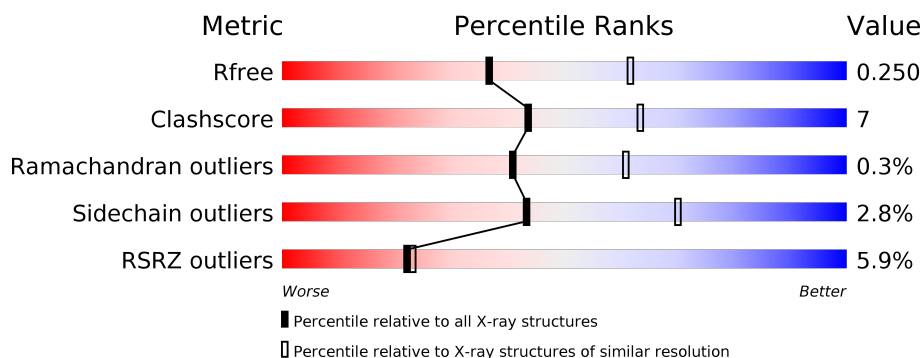
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	433	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>14%</div> </div> </div>
1	B	433	<div> <div>9%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>• 13%</div> </div> </div>
1	C	433	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>11%</div> <div>• 15%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8617 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	1	0
			2841	1831	467	530	13			
1	B	377	Total	C	N	O	S	0	0	0
			2852	1846	465	527	14			
1	C	370	Total	C	N	O	S	0	0	0
			2810	1810	464	522	14			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	EXPRESSION TAG	UNP P56817
A	-38	GLY	-	EXPRESSION TAG	UNP P56817
A	-37	SER	-	EXPRESSION TAG	UNP P56817
A	-36	SER	-	EXPRESSION TAG	UNP P56817
A	-35	HIS	-	EXPRESSION TAG	UNP P56817
A	-34	HIS	-	EXPRESSION TAG	UNP P56817
A	-33	HIS	-	EXPRESSION TAG	UNP P56817
A	-32	HIS	-	EXPRESSION TAG	UNP P56817
A	-31	HIS	-	EXPRESSION TAG	UNP P56817
A	-30	HIS	-	EXPRESSION TAG	UNP P56817
A	-29	SER	-	EXPRESSION TAG	UNP P56817
A	-28	ALA	-	EXPRESSION TAG	UNP P56817
A	-27	GLY	-	EXPRESSION TAG	UNP P56817
A	-26	GLU	-	EXPRESSION TAG	UNP P56817
A	-25	ASN	-	EXPRESSION TAG	UNP P56817
A	-24	LEU	-	EXPRESSION TAG	UNP P56817
A	-23	TYR	-	EXPRESSION TAG	UNP P56817
A	-22	PHE	-	EXPRESSION TAG	UNP P56817
A	-21	GLN	-	EXPRESSION TAG	UNP P56817
A	-20	GLY	-	EXPRESSION TAG	UNP P56817
A	-19	THR	-	EXPRESSION TAG	UNP P56817
A	75	ALA	LYS	ENGINEERED MUTATION	UNP P56817
A	77	ALA	GLU	ENGINEERED MUTATION	UNP P56817

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-39	MET	-	EXPRESSION TAG	UNP P56817
B	-38	GLY	-	EXPRESSION TAG	UNP P56817
B	-37	SER	-	EXPRESSION TAG	UNP P56817
B	-36	SER	-	EXPRESSION TAG	UNP P56817
B	-35	HIS	-	EXPRESSION TAG	UNP P56817
B	-34	HIS	-	EXPRESSION TAG	UNP P56817
B	-33	HIS	-	EXPRESSION TAG	UNP P56817
B	-32	HIS	-	EXPRESSION TAG	UNP P56817
B	-31	HIS	-	EXPRESSION TAG	UNP P56817
B	-30	HIS	-	EXPRESSION TAG	UNP P56817
B	-29	SER	-	EXPRESSION TAG	UNP P56817
B	-28	ALA	-	EXPRESSION TAG	UNP P56817
B	-27	GLY	-	EXPRESSION TAG	UNP P56817
B	-26	GLU	-	EXPRESSION TAG	UNP P56817
B	-25	ASN	-	EXPRESSION TAG	UNP P56817
B	-24	LEU	-	EXPRESSION TAG	UNP P56817
B	-23	TYR	-	EXPRESSION TAG	UNP P56817
B	-22	PHE	-	EXPRESSION TAG	UNP P56817
B	-21	GLN	-	EXPRESSION TAG	UNP P56817
B	-20	GLY	-	EXPRESSION TAG	UNP P56817
B	-19	THR	-	EXPRESSION TAG	UNP P56817
B	75	ALA	LYS	ENGINEERED MUTATION	UNP P56817
B	77	ALA	GLU	ENGINEERED MUTATION	UNP P56817
C	-39	MET	-	EXPRESSION TAG	UNP P56817
C	-38	GLY	-	EXPRESSION TAG	UNP P56817
C	-37	SER	-	EXPRESSION TAG	UNP P56817
C	-36	SER	-	EXPRESSION TAG	UNP P56817
C	-35	HIS	-	EXPRESSION TAG	UNP P56817
C	-34	HIS	-	EXPRESSION TAG	UNP P56817
C	-33	HIS	-	EXPRESSION TAG	UNP P56817
C	-32	HIS	-	EXPRESSION TAG	UNP P56817
C	-31	HIS	-	EXPRESSION TAG	UNP P56817
C	-30	HIS	-	EXPRESSION TAG	UNP P56817
C	-29	SER	-	EXPRESSION TAG	UNP P56817
C	-28	ALA	-	EXPRESSION TAG	UNP P56817
C	-27	GLY	-	EXPRESSION TAG	UNP P56817
C	-26	GLU	-	EXPRESSION TAG	UNP P56817
C	-25	ASN	-	EXPRESSION TAG	UNP P56817
C	-24	LEU	-	EXPRESSION TAG	UNP P56817
C	-23	TYR	-	EXPRESSION TAG	UNP P56817
C	-22	PHE	-	EXPRESSION TAG	UNP P56817
C	-21	GLN	-	EXPRESSION TAG	UNP P56817

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	GLY	-	EXPRESSION TAG	UNP P56817
C	-19	THR	-	EXPRESSION TAG	UNP P56817
C	75	ALA	LYS	ENGINEERED MUTATION	UNP P56817
C	77	ALA	GLU	ENGINEERED MUTATION	UNP P56817

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0

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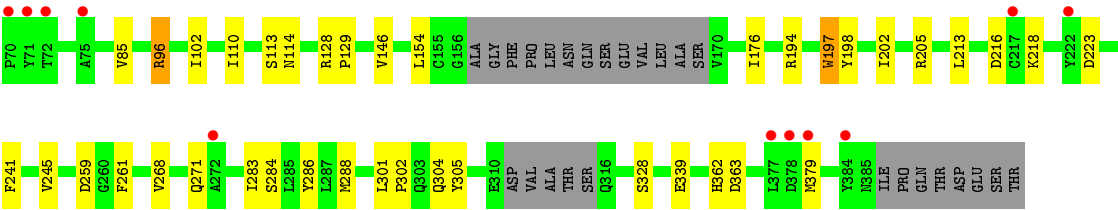
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	22	Total	O	0	0
			22	22		
4	C	30	Total	O	0	0
			30	30		



- Molecule 1: Beta-secretase 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.10 Å   105.17 Å   65.14 Å 90.00°   102.05°   90.00°	Depositor
Resolution (Å)	46.76 – 2.50 47.45 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.76-2.50) 99.0 (47.45-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.91 (at 2.51 Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, $R_{free}$	0.215   ,   0.264 0.206   ,   0.250	Depositor DCC
$R_{free}$ test set	1528 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8617	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.48	0/2917	0.62	0/3974
1	B	0.45	0/2924	0.59	0/3987
1	C	0.44	0/2882	0.59	0/3932
All	All	0.46	0/8723	0.60	0/11893

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

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	2841	0	2681	31	0
1	B	2852	0	2693	50	0
1	C	2810	0	2641	31	0
2	A	5	0	0	0	0
2	C	10	0	0	0	0
3	B	1	0	0	0	0
4	A	46	0	0	0	0
4	B	22	0	0	0	0
4	C	30	0	0	1	0
All	All	8617	0	8015	111	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 7.

All (111) 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:A:241:PHE:O	1:A:245:VAL:HG23	1.76	0.83
1:B:95:VAL:HG11	1:B:140:LEU:HA	1.64	0.79
1:C:301:LEU:H	1:C:304:GLN:NE2	1.84	0.76
1:A:297:ARG:HH21	1:A:371:GLU:HG3	1.51	0.75
1:C:47:PHE:O	1:C:48:LEU:HB2	1.89	0.71
1:A:203:ILE:H	1:A:221:ASN:HD21	1.37	0.70
1:B:385:ASN:O	1:B:386:ILE:HB	1.90	0.69
1:B:238:LYS:HD3	1:B:326:GLN:NE2	2.07	0.68
1:B:283:ILE:HD12	1:B:305:TYR:CD2	2.32	0.65
1:C:261:PHE:CD1	1:C:268:VAL:HG23	2.33	0.63
1:C:271:GLN:HB2	4:C:410:HOH:O	1.97	0.63
1:C:47:PHE:N	1:C:47:PHE:CD2	2.67	0.61
1:B:378:ASP:O	1:B:381:ASP:HB2	2.02	0.60
1:B:310:GLU:HG3	1:B:311:ASP:CB	2.31	0.60
1:A:297:ARG:NH2	1:A:371:GLU:HG3	2.18	0.59
1:B:238:LYS:HD3	1:B:326:GLN:HE21	1.66	0.58
1:A:68:TYR:OH	1:B:128:ARG:HG3	2.04	0.57
1:B:362:HIS:CD2	1:B:367:THR:HG22	2.40	0.57
1:A:249:LYS:HE2	1:A:262:TRP:CD1	2.40	0.57
1:B:110:ILE:HB	1:B:113:SER:HB3	1.87	0.57
1:B:45:HIS:CG	1:B:46:PRO:HD2	2.40	0.56
1:B:42:ALA:CB	1:B:101:ALA:HB1	2.36	0.55
1:B:378:ASP:HB3	1:B:381:ASP:OD2	2.06	0.55
1:A:45:HIS:HB3	1:A:48:LEU:HD12	1.89	0.54
1:A:71:TYR:HE2	1:A:76:TRP:HE1	1.56	0.54
1:B:255:GLU:HG3	1:B:279:ILE:CD1	2.38	0.54
1:C:301:LEU:H	1:C:304:GLN:HE21	1.55	0.53
1:A:71:TYR:HE2	1:A:76:TRP:NE1	2.05	0.53
1:B:310:GLU:CG	1:B:311:ASP:CB	2.87	0.52
1:A:12:GLN:OE1	1:A:113:SER:HA	2.09	0.52
1:C:59:THR:O	1:C:96:ARG:NH2	2.34	0.52
1:A:357:SER:HB3	1:A:360:HIS:HB3	1.92	0.52
1:B:82:THR:HG22	1:B:98:ASN:HD22	1.75	0.52
1:B:54:ARG:HG2	1:B:60:TYR:CD1	2.46	0.51
1:C:45:HIS:O	1:C:47:PHE:O	2.29	0.50
1:C:194:ARG:HD2	1:C:202:ILE:HD11	1.93	0.50
1:C:216:ASP:OD1	1:C:218:LYS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:PHE:O	1:C:245:VAL:HG23	2.11	0.50
1:B:39:ALA:HB2	1:B:100:ALA:HB3	1.93	0.50
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.93	0.49
1:B:255:GLU:HG3	1:B:279:ILE:HD12	1.94	0.49
1:C:362:HIS:HD2	1:C:363:ASP:O	1.95	0.49
1:C:20:VAL:HG12	1:C:85:VAL:HG22	1.93	0.49
1:A:222:TYR:HA	1:A:223:ASP:HA	1.64	0.48
1:B:245:VAL:HG12	1:B:249:LYS:HD2	1.95	0.48
1:C:259:ASP:O	1:C:259:ASP:OD1	2.31	0.48
1:C:301:LEU:HB3	1:C:302:PRO:HD2	1.94	0.48
1:C:176:ILE:HD12	1:C:176:ILE:N	2.29	0.48
1:B:45:HIS:CE1	1:B:47:PHE:HB2	2.48	0.48
1:B:45:HIS:HB3	1:B:48:LEU:HG	1.95	0.47
1:B:54:ARG:HD2	1:B:60:TYR:CZ	2.49	0.47
1:A:267:LEU:HD13	1:A:319:CYS:HB3	1.96	0.47
1:B:217:CYS:HA	1:B:220:TYR:CD1	2.49	0.47
1:B:376:THR:O	1:B:377:LEU:HD23	2.15	0.47
1:B:205:ARG:HB3	1:B:286:TYR:HB2	1.97	0.46
1:C:61:ARG:HG3	1:C:96:ARG:NH2	2.30	0.46
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.97	0.46
1:B:195:ARG:HB3	1:B:197:TRP:CD1	2.51	0.46
1:B:69:VAL:HG22	1:B:128:ARG:HG2	1.97	0.46
1:C:154:LEU:O	1:C:339:GLU:HA	2.16	0.46
1:A:17:GLU:HG2	1:A:88:PRO:HG2	1.97	0.46
1:A:41:GLY:HA2	1:A:102:ILE:HB	1.97	0.46
1:B:260:GLY:HA2	1:B:263:LEU:HD12	1.98	0.46
1:B:288:MET:HE2	1:B:379:MET:HB3	1.97	0.46
1:B:238:LYS:CD	1:B:326:GLN:NE2	2.78	0.46
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.51	0.45
1:B:301:LEU:H	1:B:304:GLN:NE2	2.14	0.45
1:C:41:GLY:HA2	1:C:102:ILE:HB	1.97	0.45
1:B:59:THR:HG21	1:B:84:LEU:CD1	2.46	0.45
1:A:292:THR:HG22	1:A:293:ASN:ND2	2.31	0.45
1:A:19:THR:HA	1:A:25:GLN:O	2.17	0.45
1:B:137:PHE:O	1:B:141:VAL:HG23	2.17	0.45
1:B:39:ALA:CB	1:B:100:ALA:HB3	2.47	0.45
1:C:9:LYS:O	1:C:12:GLN:HB2	2.17	0.45
1:B:26:THR:HG22	1:B:50:ARG:NH2	2.32	0.44
1:B:301:LEU:H	1:B:304:GLN:HE21	1.66	0.44
1:C:45:HIS:CG	1:C:46:PRO:HD2	2.52	0.44
1:A:301:LEU:H	1:A:304:GLN:NE2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLN:HG2	1:C:110:ILE:HG21	1.99	0.44
1:B:283:ILE:HD12	1:B:305:TYR:CE2	2.53	0.44
1:B:69:VAL:HA	1:B:70:PRO:HD3	1.80	0.43
1:C:283:ILE:HD12	1:C:305:TYR:CD2	2.53	0.43
1:B:222:TYR:O	1:B:223:ASP:CB	2.66	0.43
1:B:235:ARG:HA	1:B:325:SER:O	2.18	0.43
1:C:113:SER:O	1:C:114:ASN:HB3	2.17	0.43
1:A:45:HIS:CG	1:A:46:PRO:HD2	2.54	0.43
1:B:69:VAL:HG22	1:B:128:ARG:CB	2.49	0.43
1:B:269:CYS:HA	1:B:318:ASP:O	2.19	0.43
1:A:307:ARG:HA	1:A:308:PRO:HD3	1.87	0.43
1:B:26:THR:HG22	1:B:50:ARG:HH21	1.84	0.43
1:B:55:GLN:HG2	1:B:56:LEU:H	1.83	0.43
1:C:197:TRP:N	1:C:197:TRP:CD1	2.87	0.43
1:C:205:ARG:HB3	1:C:286:TYR:HB2	2.01	0.42
1:B:29:ILE:HG21	1:B:119:LEU:HB2	2.02	0.42
1:A:301:LEU:H	1:A:304:GLN:HE21	1.68	0.42
1:C:197:TRP:CG	1:C:198:TYR:N	2.87	0.42
1:A:69:VAL:HG22	1:A:128:ARG:HG3	2.02	0.41
1:B:310:GLU:HA	1:B:311:ASP:HA	1.47	0.41
1:A:258:PRO:HB2	1:A:266:GLN:OE1	2.21	0.41
1:A:244:ALA:O	1:A:248:ILE:HG13	2.20	0.41
1:A:276:PRO:O	1:A:279:ILE:HG12	2.21	0.41
1:A:286:TYR:CZ	1:A:297:ARG:HD3	2.56	0.41
1:A:151:SER:OG	1:A:175:ILE:HB	2.21	0.41
1:A:9:LYS:O	1:A:12:GLN:HB2	2.20	0.41
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.92	0.41
1:B:71:TYR:HE2	1:B:76:TRP:HE1	1.69	0.41
1:C:128:ARG:HA	1:C:129:PRO:C	2.42	0.41
1:C:288:MET:HG3	1:C:379:MET:HE3	2.03	0.41
1:A:17:GLU:O	1:A:88:PRO:HD2	2.21	0.40
1:B:300:ILE:HD13	1:B:337:ILE:HD13	2.03	0.40
1:C:146:VAL:HG11	1:C:176:ILE:HG22	2.03	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	364/433 (84%)	344 (94%)	19 (5%)	1 (0%)	41	61
1	B	371/433 (86%)	353 (95%)	17 (5%)	1 (0%)	41	61
1	C	364/433 (84%)	353 (97%)	10 (3%)	1 (0%)	41	61
All	All	1099/1299 (85%)	1050 (96%)	46 (4%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	B	223	ASP
1	C	223	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	291/368 (79%)	283 (97%)	8 (3%)	44	71
1	B	283/368 (77%)	273 (96%)	10 (4%)	36	62
1	C	283/368 (77%)	277 (98%)	6 (2%)	53	78
All	All	857/1104 (78%)	833 (97%)	24 (3%)	43	70

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	20	VAL
1	A	197	TRP
1	A	238	LYS
1	A	259	ASP
1	A	359	CYS
1	A	367	THR
1	A	371	GLU
1	B	0	VAL
1	B	50	ARG
1	B	59	THR
1	B	106	ASP
1	B	132	SER
1	B	181	HIS
1	B	197	TRP
1	B	213	LEU
1	B	254	THR
1	B	309	VAL
1	C	4	ASP
1	C	47	PHE
1	C	96	ARG
1	C	197	TRP
1	C	284	SER
1	C	328	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	221	ASN
1	A	293	ASN
1	A	294	GLN
1	A	304	GLN
1	A	362	HIS
1	B	28	ASN
1	B	98	ASN
1	B	304	GLN
1	B	326	GLN
1	B	362	HIS
1	C	28	ASN
1	C	114	ASN
1	C	304	GLN
1	C	362	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z  > 2$
2	SO4	C	394	-	4,4,4	0.22	0	6,6,6	0.23	0
2	SO4	A	394	-	4,4,4	0.21	0	6,6,6	0.17	0
2	SO4	C	395	-	4,4,4	0.28	0	6,6,6	0.27	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.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	371/433 (85%)	0.33	13 (3%) 44 47	36, 48, 77, 91	0
1	B	377/433 (87%)	0.51	39 (10%) 6 6	37, 55, 86, 102	0
1	C	370/433 (85%)	0.27	14 (3%) 40 43	40, 54, 84, 97	0
All	All	1118/1299 (86%)	0.37	66 (5%) 22 23	36, 53, 82, 102	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	VAL	7.9
1	B	379	MET	5.2
1	C	-2	SER	4.4
1	B	47	PHE	4.4
1	A	272	ALA	4.4
1	B	377	LEU	4.2
1	C	379	MET	4.2
1	A	319	CYS	4.0
1	A	257	PHE	3.9
1	C	384	TYR	3.9
1	A	46	PRO	3.6
1	B	60	TYR	3.4
1	C	377	LEU	3.4
1	C	71	TYR	3.3
1	C	378	ASP	3.2
1	B	258	PRO	3.2
1	B	311	ASP	3.2
1	B	157	ALA	3.1
1	B	309	VAL	3.1
1	B	71	TYR	3.1
1	B	380	GLU	3.1
1	B	138	ASP	3.0
1	A	267	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	49	HIS	3.0
1	B	70	PRO	3.0
1	C	75	ALA	3.0
1	B	272	ALA	2.9
1	B	319	CYS	2.9
1	C	217	CYS	2.9
1	A	47	PHE	2.8
1	C	-1	PHE	2.8
1	B	81	GLY	2.7
1	C	69	VAL	2.7
1	C	222	TYR	2.7
1	A	378	ASP	2.7
1	C	72	THR	2.6
1	B	84	LEU	2.6
1	B	263	LEU	2.6
1	C	70	PRO	2.6
1	B	265	GLU	2.6
1	A	262	TRP	2.6
1	B	51	TYR	2.6
1	B	69	VAL	2.5
1	B	56	LEU	2.5
1	A	265	GLU	2.5
1	B	378	ASP	2.5
1	B	110	ILE	2.5
1	B	46	PRO	2.5
1	B	22	SER	2.4
1	B	93	VAL	2.4
1	A	256	LYS	2.4
1	B	73	GLN	2.4
1	B	257	PHE	2.3
1	B	170	VAL	2.3
1	B	85	VAL	2.2
1	B	262	TRP	2.2
1	B	133	LEU	2.2
1	B	145	HIS	2.1
1	B	268	VAL	2.1
1	B	310	GLU	2.1
1	B	61	ARG	2.1
1	C	272	ALA	2.1
1	B	269	CYS	2.1
1	A	332	VAL	2.0
1	B	111	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	268	VAL	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
2	SO4	C	395	5/5	0.68	0.22	84,86,93,114	0
3	CL	B	394	1/1	0.90	0.31	87,87,87,87	0
2	SO4	C	394	5/5	0.92	0.19	78,79,95,103	0
2	SO4	A	394	5/5	0.93	0.11	72,75,96,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.