



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:56 AM GMT

PDB ID : 3DM6  
Title : Beta-secretase 1 complexed with statine-based inhibitor  
Authors : Lindberg, J.; Borkakoti, N.; Nystrom, S.  
Deposited on : 2008-06-30  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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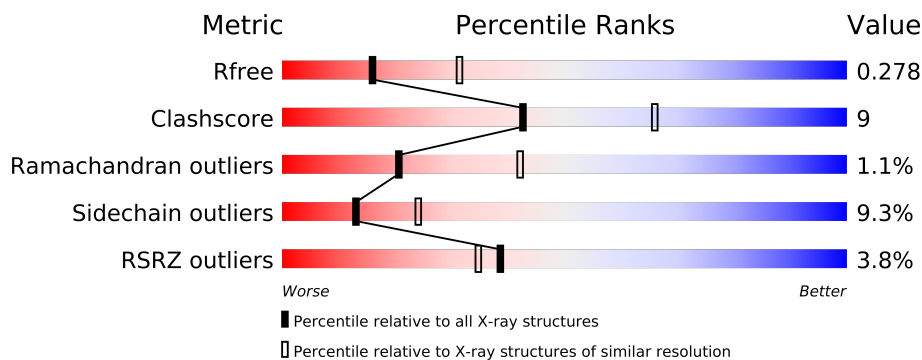
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	
1	C	406	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8934 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

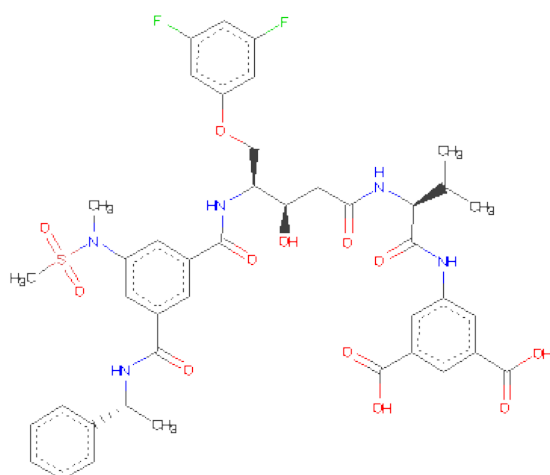
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2909	1865	485	546	13			
1	B	368	Total	C	N	O	S	0	0	0
			2902	1860	484	545	13			
1	C	367	Total	C	N	O	S	0	0	0
			2893	1855	483	542	13			

There are 3 discrepancies between the modelled and reference sequences:

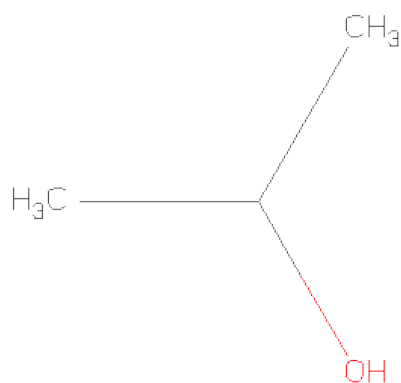
Chain	Residue	Modelled	Actual	Comment	Reference
A	28P	MET	-	INITIATING METHIONINE	UNP P56817
B	28P	MET	-	INITIATING METHIONINE	UNP P56817
C	28P	MET	-	INITIATING METHIONINE	UNP P56817

- Molecule 2 is 5-[[[(2S)-2-[[[(3R,4S)-5-(3,5-DIFLUOROPHENOXY)-3-HYDROXY-4-[[3-(METHYL-METHYLSULFONYL-AMINO)-5-[[[(1R)-1-PHENYLETHYL]CARBAMOYL]PHENYL]CARBOXYLAMINO]PENTANOYL]AMINO]-3-METHYL-BUTANOYL]AMINO]BENZENE-1,3-DICARBOXYLICACID (three-letter code: 757) (formula: C<sub>42</sub>H<sub>45</sub>F<sub>2</sub>N<sub>5</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			62	42	2	5	12	1		
2	B	1	Total	C	F	N	O	S	0	0
			62	42	2	5	12	1		
2	C	1	Total	C	F	N	O	S	0	0
			62	42	2	5	12	1		

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		

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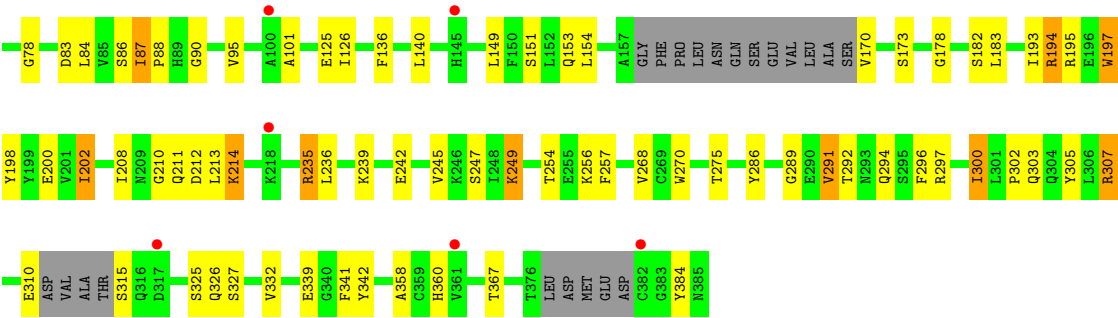
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	3	1		
3	C	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	12	Total	O	0	0
			12	12		
4	C	9	Total	O	0	0
			9	9		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.44Å 103.02Å 103.11Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	63.76 – 2.60 63.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (63.76-2.60) 97.6 (63.74-2.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.50 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.223 , 0.281 0.221 , 0.278	Depositor DCC
$R_{free}$ test set	2605 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 51026 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8934	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, 757

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	0.64	0/2982	0.70	0/4048
1	B	0.60	1/2975 (0.0%)	0.70	0/4038
1	C	0.60	0/2966	0.69	0/4026
All	All	0.62	1/8923 (0.0%)	0.70	0/12112

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	CYS	CB-SG	-5.02	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2909	0	2824	49	0
1	B	2902	0	2815	52	0
1	C	2893	0	2809	54	0
2	A	62	0	43	4	0
2	B	62	0	43	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	62	0	43	1	0
3	A	4	0	8	0	0
3	B	4	0	8	0	0
3	C	4	0	8	1	0
4	A	11	0	0	0	0
4	B	12	0	0	0	0
4	C	9	0	0	0	0
All	All	8934	0	8601	155	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (155) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:THR:HG22	1:B:50:ARG:HH12	0.97	1.12
1:C:194:ARG:HH22	1:C:384:TYR:H	1.08	0.97
1:B:26:THR:HG22	1:B:50:ARG:NH1	1.80	0.96
1:C:291:VAL:HG22	1:C:294:GLN:HB2	1.49	0.94
1:C:26:THR:HG22	1:C:50:ARG:HH12	1.34	0.91
1:C:26:THR:HG22	1:C:50:ARG:NH1	1.89	0.87
1:C:194:ARG:HH22	1:C:384:TYR:N	1.81	0.76
1:B:307:ARG:HH11	1:B:307:ARG:HG2	1.53	0.73
1:A:301:LEU:H	1:A:304:GLN:NE2	1.86	0.73
1:A:257:PHE:HD2	1:A:268:VAL:HG11	1.55	0.71
1:A:82:THR:OG1	1:A:96:ARG:NH1	2.22	0.70
1:A:46(P):SER:O	1:A:47(P):PHE:HB2	1.91	0.69
1:B:307:ARG:CG	1:B:307:ARG:HH11	2.06	0.69
1:C:291:VAL:HG22	1:C:294:GLN:CB	2.21	0.69
1:C:194:ARG:HB3	1:C:200:GLU:HG2	1.76	0.67
1:C:235:ARG:HG3	1:C:332:VAL:HB	1.75	0.67
1:A:3:VAL:HG22	1:A:183:LEU:HD11	1.79	0.65
1:C:21:GLY:O	1:C:24:PRO:HA	1.97	0.65
1:C:291:VAL:CG2	1:C:294:GLN:HB2	2.24	0.65
1:B:272:ALA:HB2	1:B:316:GLN:O	1.99	0.63
1:B:208:ILE:HD12	1:B:213:LEU:HD11	1.80	0.63
1:B:307:ARG:NH2	1:B:339:GLU:OE2	2.32	0.63
1:B:307:ARG:NH1	1:B:307:ARG:HG2	2.12	0.63
1:B:98:ASN:ND2	1:B:134:GLU:O	2.32	0.62
1:B:26:THR:O	1:B:50:ARG:NH1	2.32	0.61
1:B:47:PHE:CD2	1:B:111:ASN:HB2	2.35	0.61
1:C:194:ARG:NH2	1:C:384:TYR:H	1.90	0.61
1:B:360:HIS:CE1	1:B:368:ALA:H	2.20	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:26:THR:O	1:C:50:ARG:NH1	2.36	0.57
1:A:300:ILE:HD13	1:A:337:ILE:CD1	2.34	0.57
1:A:256:LYS:HZ3	1:A:256:LYS:H	1.51	0.57
1:A:300:ILE:HD13	1:A:337:ILE:HD12	1.87	0.56
1:A:253:SER:C	1:A:255:GLU:H	2.08	0.56
1:B:44:PRO:HD3	1:B:51:TYR:CZ	2.41	0.56
1:A:300:ILE:HD11	1:A:337:ILE:HG23	1.88	0.55
1:C:95:VAL:HG11	1:C:140:LEU:HA	1.89	0.55
1:C:194:ARG:HG3	1:C:202:ILE:CD1	2.37	0.55
1:C:17:GLU:HG2	1:C:88:PRO:HG2	1.87	0.55
1:B:20:VAL:HG12	1:B:85:VAL:HG22	1.88	0.55
1:A:209:ASN:ND2	1:A:281:PRO:HB3	2.21	0.55
1:B:70:PRO:HA	1:B:75:LYS:HB3	1.88	0.55
1:C:300:ILE:HD11	1:C:341:PHE:HE1	1.72	0.54
1:B:5:ASN:OD1	1:B:173:SER:HA	2.08	0.54
1:C:257:PHE:HD2	1:C:268:VAL:HG11	1.74	0.54
1:C:198:TYR:CE1	3:C:1139:IPA:H13	2.43	0.53
1:B:84:LEU:HA	1:B:95:VAL:O	2.09	0.53
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.91	0.53
1:B:258:PRO:HB2	1:B:266:GLN:HE21	1.74	0.52
1:C:358:ALA:O	1:C:360:HIS:HD2	1.92	0.52
1:A:256:LYS:NZ	1:A:256:LYS:H	2.07	0.52
1:B:32:ASP:OD2	2:B:1000:757:H31A	2.10	0.52
1:C:208:ILE:HD12	1:C:213:LEU:HD13	1.90	0.52
1:B:291:VAL:O	1:B:294:GLN:HB3	2.10	0.51
1:B:47:PHE:CE2	1:B:111:ASN:HB2	2.45	0.51
1:B:29:ILE:CG2	1:B:119:LEU:HB2	2.41	0.51
1:C:125:GLU:OE2	1:C:195:ARG:NH2	2.43	0.51
1:A:149:LEU:HD13	1:A:178:GLY:HA2	1.93	0.51
1:B:29:ILE:HG21	1:B:119:LEU:HB2	1.93	0.50
1:B:258:PRO:HB2	1:B:266:GLN:NE2	2.27	0.49
1:C:197:TRP:CD1	1:C:197:TRP:N	2.80	0.49
1:A:340:GLY:O	1:A:357:SER:HB3	2.12	0.49
1:C:47(P):PHE:CZ	1:C:178:GLY:HA3	2.47	0.49
1:A:126:ILE:HD12	2:A:1000:757:C50	2.43	0.49
1:A:261:PHE:CE1	1:A:268:VAL:HG22	2.47	0.49
1:C:286:TYR:HA	1:C:296:PHE:O	2.11	0.49
1:B:289:GLY:HA3	1:B:294:GLN:O	2.13	0.49
1:A:153:GLN:NE2	1:A:183:LEU:HD22	2.27	0.48
1:C:126:ILE:HG23	1:C:197:TRP:HB2	1.95	0.48
1:A:33:THR:OG1	1:A:228:ASP:HA	2.13	0.48
1:C:289:GLY:HA3	1:C:294:GLN:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14:TYR:CG	1:A:154:LEU:HD22	2.49	0.48
1:C:212:ASP:C	1:C:214:LYS:H	2.17	0.48
1:A:54:ARG:HD2	1:A:60:TYR:CZ	2.48	0.48
1:C:302:PRO:HA	1:C:305:TYR:CE2	2.48	0.48
1:A:270:TRP:CE3	1:A:275:THR:HG23	2.49	0.47
1:B:209:ASN:HB2	1:B:281:PRO:CB	2.44	0.47
1:C:78:GLY:HA3	1:C:101:ALA:O	2.14	0.47
1:C:194:ARG:HG3	1:C:202:ILE:HD11	1.95	0.47
1:A:20:VAL:HG12	1:A:85:VAL:HG22	1.96	0.47
1:C:307:ARG:HH12	1:C:339:GLU:CD	2.18	0.47
1:B:59:THR:HB	1:B:96:ARG:HH22	1.80	0.47
1:A:6:LEU:O	1:A:171:GLY:HA2	2.15	0.47
1:B:149:LEU:C	1:B:149:LEU:HD23	2.36	0.46
1:A:371:GLU:O	1:A:374:PHE:HE1	1.98	0.46
1:A:126:ILE:HD12	2:A:1000:757:H50A	1.99	0.45
1:A:363:ASP:C	1:A:363:ASP:OD1	2.54	0.45
1:B:69:VAL:HG22	1:B:128:ARG:HB2	1.97	0.45
1:C:193:ILE:O	1:C:194:ARG:C	2.55	0.45
1:B:150:PHE:CE2	1:B:345:PHE:CD2	3.05	0.45
1:A:257:PHE:CD2	1:A:268:VAL:HG11	2.44	0.45
1:A:92:ASN:HD22	1:A:92:ASN:C	2.20	0.45
1:A:153:GLN:HE22	1:A:183:LEU:HD22	1.81	0.45
1:B:307:ARG:HH22	1:B:339:GLU:CD	2.19	0.45
1:B:244:ALA:O	1:B:248:ILE:HG13	2.16	0.44
1:A:35:SER:CB	2:A:1000:757:H50B	2.48	0.44
1:C:54:ARG:HD2	1:C:60:TYR:CE1	2.52	0.44
1:B:302:PRO:HA	1:B:305:TYR:CE2	2.52	0.44
1:B:307:ARG:CG	1:B:307:ARG:NH1	2.71	0.44
1:C:235:ARG:HA	1:C:325:SER:O	2.18	0.44
1:B:8:GLY:HA2	1:B:15:TYR:CE2	2.53	0.44
1:B:271:GLN:O	1:B:273:GLY:N	2.51	0.44
1:A:78:GLY:HA3	1:A:101:ALA:O	2.18	0.44
1:C:194:ARG:CB	1:C:200:GLU:HG2	2.45	0.44
1:A:180:ASP:HB3	1:A:183:LEU:HD12	1.99	0.44
1:C:83:ASP:OD1	1:C:84:LEU:N	2.42	0.44
1:A:301:LEU:H	1:A:304:GLN:HE21	1.62	0.43
1:B:208:ILE:CD1	1:B:213:LEU:HD11	2.48	0.43
1:B:3:VAL:HG13	1:B:183:LEU:HD21	2.01	0.43
1:A:134:GLU:HA	1:A:135:PRO:HD3	1.66	0.43
1:C:8:GLY:HA2	1:C:15:TYR:CE2	2.53	0.43
1:C:35:SER:HA	2:C:1000:757:H50B	2.00	0.43
1:A:222:TYR:HA	1:A:223:ASP:HA	1.72	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:ARG:HG3	1:A:332:VAL:HB	2.00	0.43
1:C:245:VAL:O	1:C:249:LYS:HB2	2.19	0.43
1:C:136:PHE:C	1:C:136:PHE:CD2	2.91	0.43
1:A:372:GLY:HA2	1:A:374:PHE:CE1	2.54	0.43
1:A:280:PHE:HA	1:A:281:PRO:HD3	1.87	0.42
1:B:209:ASN:HB2	1:B:281:PRO:HB2	2.01	0.42
1:B:326:GLN:HE21	1:B:326:GLN:HB2	1.60	0.42
1:A:253:SER:C	1:A:255:GLU:N	2.72	0.42
1:A:244:ALA:O	1:A:248:ILE:HG13	2.19	0.42
1:C:210:GLY:O	1:C:211:GLN:HG2	2.19	0.42
1:B:222:TYR:HA	1:B:223:ASP:HA	1.74	0.42
1:C:197:TRP:HD1	1:C:197:TRP:H	1.67	0.42
1:B:67:VAL:HG23	1:B:129:PRO:HG3	2.00	0.42
1:B:44:PRO:HD3	1:B:51:TYR:OH	2.20	0.42
1:B:35:SER:HA	2:B:1000:757:H50B	2.01	0.42
1:A:9:LYS:O	1:A:10:SER:C	2.58	0.42
1:B:59:THR:HB	1:B:96:ARG:NH2	2.34	0.42
1:A:59:THR:HG21	1:A:84:LEU:HD12	2.01	0.42
1:C:28:ASN:HD22	1:C:28:ASN:HA	1.68	0.42
1:C:151:SER:HB2	1:C:342:TYR:CE1	2.55	0.41
1:C:270:TRP:CE3	1:C:275:THR:HG23	2.55	0.41
1:C:2:MET:CG	1:C:90:GLY:HA2	2.50	0.41
1:A:83:ASP:O	1:A:96:ARG:HA	2.20	0.41
1:B:63:LEU:C	1:B:65:LYS:H	2.24	0.41
1:B:270:TRP:CE3	1:B:275:THR:HG23	2.56	0.41
1:A:234:LEU:HD13	1:A:337:ILE:HD11	2.03	0.41
1:A:35:SER:HB2	2:A:1000:757:H50B	2.03	0.41
1:A:59:THR:HG21	1:A:84:LEU:CD1	2.50	0.41
1:B:194:ARG:NH1	1:B:200:GLU:OE2	2.54	0.41
1:C:154:LEU:O	1:C:339:GLU:HA	2.21	0.41
1:B:283:ILE:HB	1:B:300:ILE:HG22	2.03	0.41
1:C:236:LEU:O	1:C:327:SER:N	2.44	0.41
1:C:153:GLN:OE1	1:C:183:LEU:HD22	2.21	0.41
1:C:87:ILE:O	1:C:88:PRO:C	2.59	0.41
1:B:38:PHE:HE1	1:B:85:VAL:HG21	1.86	0.41
1:C:70:PRO:HA	1:C:75:LYS:HB3	2.02	0.41
1:A:69:VAL:HG22	1:A:128:ARG:HB2	2.02	0.41
1:A:252:SER:HA	1:A:279:ILE:HD12	2.03	0.41
1:A:110:ILE:HB	1:A:113:SER:HB3	2.03	0.41
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.50	0.40
1:B:154:LEU:O	1:B:339:GLU:HA	2.20	0.40
1:B:184:TYR:CD1	1:B:342:TYR:CD2	3.10	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:286:TYR:CE2	1:C:297:ARG:HB3	2.56	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	361/406 (89%)	333 (92%)	26 (7%)	2 (1%)	33	63
1	B	360/406 (89%)	327 (91%)	25 (7%)	8 (2%)	10	18
1	C	359/406 (88%)	325 (90%)	32 (9%)	2 (1%)	33	63
All	All	1080/1218 (89%)	985 (91%)	83 (8%)	12 (1%)	21	42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47(P)	PHE
1	B	47(P)	PHE
1	B	272	ALA
1	C	214	LYS
1	A	254	THR
1	B	209	ASN
1	B	292	THR
1	B	10	SER
1	B	251	ALA
1	B	259	ASP
1	C	303	GLN
1	B	260	GLY

### 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	315/347 (91%)	290 (92%)	25 (8%)	18	34
1	B	314/347 (90%)	282 (90%)	32 (10%)	11	19
1	C	313/347 (90%)	282 (90%)	31 (10%)	11	21
All	All	942/1041 (90%)	854 (91%)	88 (9%)	13	24

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48(P)	VAL
1	A	9	LYS
1	A	12	GLN
1	A	19	THR
1	A	22	SER
1	A	65	LYS
1	A	92	ASN
1	A	125	GLU
1	A	149	LEU
1	A	151	SER
1	A	173	SER
1	A	197	TRP
1	A	202	ILE
1	A	215	MET
1	A	256	LYS
1	A	259	ASP
1	A	300	ILE
1	A	307	ARG
1	A	321	LYS
1	A	327	SER
1	A	360	HIS
1	A	361	VAL
1	A	363	ASP
1	A	377	LEU
1	A	385	ASN
1	B	1	GLU
1	B	20	VAL
1	B	26	THR
1	B	53	GLN
1	B	55	GLN
1	B	59	THR
1	B	65	LYS

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Mol	Chain	Res	Type
1	B	73	GLN
1	B	75	LYS
1	B	82	THR
1	B	145	HIS
1	B	173	SER
1	B	187	SER
1	B	194	ARG
1	B	197	TRP
1	B	209	ASN
1	B	212	ASP
1	B	214	LYS
1	B	218	LYS
1	B	254	THR
1	B	256	LYS
1	B	259	ASP
1	B	261	PHE
1	B	271	GLN
1	B	292	THR
1	B	307	ARG
1	B	315	SER
1	B	316	GLN
1	B	326	GLN
1	B	356	VAL
1	B	364	GLU
1	B	385	ASN
1	C	48(P)	VAL
1	C	9	LYS
1	C	59	THR
1	C	61	ARG
1	C	65	LYS
1	C	73	GLN
1	C	75	LYS
1	C	86	SER
1	C	87	ILE
1	C	149	LEU
1	C	170	VAL
1	C	173	SER
1	C	182	SER
1	C	194	ARG
1	C	197	TRP
1	C	202	ILE
1	C	235	ARG

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Mol	Chain	Res	Type
1	C	239	LYS
1	C	242	GLU
1	C	247	SER
1	C	249	LYS
1	C	254	THR
1	C	256	LYS
1	C	291	VAL
1	C	292	THR
1	C	300	ILE
1	C	307	ARG
1	C	310	GLU
1	C	315	SER
1	C	326	GLN
1	C	367	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	92	ASN
1	A	114	ASN
1	A	293	ASN
1	A	304	GLN
1	A	326	GLN
1	B	28	ASN
1	B	53	GLN
1	B	55	GLN
1	B	266	GLN
1	B	271	GLN
1	B	326	GLN
1	B	360	HIS
1	B	385	ASN
1	C	28	ASN
1	C	53	GLN
1	C	73	GLN
1	C	89	HIS
1	C	294	GLN
1	C	360	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 ligands are modelled in this entry.

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	757	A	1000	-	65,65,65	1.27	6 (9%)	93,93,93	2.01	22 (23%)
3	IPA	A	1137	-	3,3,3	0.58	0	3,3,3	0.46	0
2	757	B	1000	-	65,65,65	1.15	3 (4%)	93,93,93	1.81	23 (24%)
3	IPA	B	1138	-	3,3,3	0.54	0	3,3,3	0.45	0
2	757	C	1000	-	65,65,65	1.13	3 (4%)	93,93,93	1.96	23 (24%)
3	IPA	C	1139	-	3,3,3	0.50	0	3,3,3	0.77	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
2	757	A	1000	-	1/1/13/17	0/67/67/67	0/4/4/4
3	IPA	A	1137	-	-	0/0/0/0	0/0/0/0
2	757	B	1000	-	1/1/13/17	0/67/67/67	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IPA	B	1138	-	-	0/0/0/0	0/0/0/0
2	757	C	1000	-	1/1/13/17	0/67/67/67	0/4/4/4
3	IPA	C	1139	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	757	C24-S23	-4.11	1.67	1.75
2	A	1000	757	C54-N53	-4.06	1.33	1.41
2	B	1000	757	C24-S23	-4.05	1.67	1.75
2	B	1000	757	S23-N21	-4.03	1.54	1.64
2	A	1000	757	C24-S23	-3.95	1.67	1.75
2	C	1000	757	S23-N21	-3.94	1.54	1.64
2	A	1000	757	S23-N21	-3.70	1.55	1.64
2	B	1000	757	C54-N53	-3.67	1.34	1.41
2	A	1000	757	O26-S23	3.10	1.46	1.43
2	C	1000	757	C54-N53	-2.65	1.36	1.41
2	A	1000	757	C14-N21	-2.20	1.41	1.44
2	A	1000	757	C38-C37	2.04	1.41	1.37

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	757	O25-S23-O26	-7.84	107.73	118.68
2	A	1000	757	C43-C44-N46	6.30	124.29	116.25
2	A	1000	757	C14-N21-S23	6.12	126.02	118.45
2	B	1000	757	O25-S23-O26	-5.55	110.94	118.68
2	A	1000	757	O26-S23-N21	5.19	112.89	107.07
2	A	1000	757	O25-S23-O26	-5.11	111.54	118.68
2	B	1000	757	C14-N21-S23	5.05	124.69	118.45
2	C	1000	757	O25-S23-N21	4.82	112.48	107.07
2	C	1000	757	C24-S23-N21	4.53	112.64	105.95
2	A	1000	757	C48-C47-C51	-4.49	99.91	111.39
2	A	1000	757	O32-C31-C30	4.33	116.33	108.33
2	A	1000	757	C41-C30-N29	4.24	117.16	109.61
2	C	1000	757	C14-N21-S23	4.16	123.59	118.45
2	B	1000	757	C41-C30-N29	4.12	116.95	109.61
2	B	1000	757	C43-C44-N46	4.06	121.44	116.25
2	A	1000	757	C31-O32-C33	3.91	126.21	117.91
2	B	1000	757	C48-C47-C51	-3.87	101.50	111.39
2	B	1000	757	O26-S23-N21	3.85	111.39	107.07
2	C	1000	757	C41-C30-N29	3.74	116.27	109.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	757	O32-C31-C30	3.56	114.92	108.33
2	C	1000	757	C16-C18-N29	3.56	122.82	116.89
2	C	1000	757	C48-C47-C51	-3.55	102.30	111.39
2	C	1000	757	C9-C7-C6	-3.55	104.87	112.11
2	C	1000	757	C31-C30-C41	-3.49	104.73	112.48
2	B	1000	757	O25-S23-N21	3.47	110.97	107.07
2	C	1000	757	C31-O32-C33	3.47	125.27	117.91
2	C	1000	757	C43-C44-N46	3.35	120.53	116.25
2	B	1000	757	C48-C47-N46	3.34	119.85	111.37
2	C	1000	757	C22-N21-C14	3.33	120.19	116.88
2	B	1000	757	O32-C31-C30	3.25	114.33	108.33
2	A	1000	757	C54-N53-C51	-3.23	121.30	127.29
2	A	1000	757	C48-C47-N46	3.10	119.25	111.37
2	A	1000	757	O45-C44-N46	-3.09	117.71	123.08
2	B	1000	757	C31-O32-C33	3.07	124.43	117.91
2	A	1000	757	C31-C30-C41	-2.90	106.05	112.48
2	C	1000	757	C12-C10-N8	2.89	121.70	116.89
2	C	1000	757	O19-C18-C16	-2.88	115.95	121.01
2	A	1000	757	C55-C56-C60	-2.85	115.27	119.97
2	A	1000	757	C57-C58-C63	2.77	124.54	119.97
2	B	1000	757	C22-N21-C14	2.72	119.58	116.88
2	B	1000	757	C47-C51-N53	-2.68	111.86	115.19
2	A	1000	757	C33-C34-C35	2.67	121.46	117.61
2	B	1000	757	C33-C34-C35	2.60	121.36	117.61
2	B	1000	757	C31-C30-C41	-2.52	106.89	112.48
2	C	1000	757	C6-C7-N8	2.50	116.18	111.46
2	B	1000	757	C24-S23-N21	2.48	109.61	105.95
2	B	1000	757	O61-C60-C56	2.48	121.56	115.01
2	C	1000	757	C54-N53-C51	2.43	131.79	127.29
2	C	1000	757	C33-C38-C37	2.41	121.09	117.61
2	A	1000	757	C47-C51-N53	2.41	118.18	115.19
2	C	1000	757	C48-C47-N46	2.40	117.46	111.37
2	A	1000	757	C12-C10-N8	2.36	120.83	116.89
2	B	1000	757	C57-C58-C63	2.31	123.79	119.97
2	B	1000	757	C9-C7-C6	-2.30	107.41	112.11
2	C	1000	757	C33-C34-C35	2.30	120.92	117.61
2	B	1000	757	C36-C35-C34	-2.28	120.25	123.48
2	B	1000	757	O61-C60-O62	-2.28	118.17	123.35
2	A	1000	757	O45-C44-C43	-2.27	118.00	121.24
2	B	1000	757	O45-C44-C43	-2.26	118.01	121.24
2	A	1000	757	F39-C37-C38	2.26	121.70	118.22
2	B	1000	757	C59-C58-C63	-2.25	116.26	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1000	757	O25-S23-C24	-2.17	105.66	108.77
2	A	1000	757	C33-C38-C37	2.15	120.70	117.61
2	A	1000	757	C30-N29-C18	2.12	127.51	122.92
2	C	1000	757	C12-C13-C14	2.12	121.95	119.89
2	A	1000	757	O65-C63-C58	2.10	120.58	115.01
2	C	1000	757	O65-C63-O64	-2.03	118.74	123.35
2	B	1000	757	C57-C56-C60	2.01	123.30	119.97

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1000	757	C41
2	A	1000	757	C41
2	B	1000	757	C41

There are no torsion outliers.

There are no ring outliers.

## 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	369/406 (90%)	0.49	11 (2%) 48 45	37, 60, 85, 98	3 (0%)
1	B	368/406 (90%)	0.59	18 (4%) 28 25	46, 64, 95, 105	3 (0%)
1	C	367/406 (90%)	0.56	13 (3%) 42 38	45, 66, 88, 99	3 (0%)
All	All	1104/1218 (90%)	0.55	42 (3%) 38 35	37, 64, 89, 105	9 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	LYS	5.7
1	B	10	SER	4.6
1	B	107	LYS	3.6
1	A	315	SER	3.2
1	B	316	GLN	3.0
1	B	56	LEU	2.9
1	C	21	GLY	2.9
1	A	267	LEU	2.8
1	C	145	HIS	2.8
1	B	49	HIS	2.7
1	A	256	LYS	2.6
1	B	46(P)	SER	2.6
1	B	8	GLY	2.5
1	C	218	LYS	2.4
1	A	259	ASP	2.4
1	C	27	LEU	2.4
1	C	41	GLY	2.4
1	A	310	GLU	2.3
1	B	84	LEU	2.3
1	C	317	ASP	2.3
1	A	377	LEU	2.3
1	C	100	ALA	2.2
1	C	59	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	316	GLN	2.2
1	B	60	TYR	2.2
1	A	268	VAL	2.2
1	B	272	ALA	2.2
1	C	20	VAL	2.2
1	C	361	VAL	2.2
1	B	101	ALA	2.2
1	B	310	GLU	2.1
1	A	48	LEU	2.1
1	B	52	TYR	2.1
1	B	54	ARG	2.1
1	B	375	VAL	2.1
1	A	374	PHE	2.1
1	C	9	LYS	2.1
1	A	47	PHE	2.1
1	B	55	GLN	2.1
1	B	365	PHE	2.1
1	C	42	ALA	2.0
1	C	382	CYS	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	757	C	1000	62/62	0.23	-	38,50,60,61	12
2	757	A	1000	62/62	0.26	-	38,54,64,65	12

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	IPA	A	1137	4/4	0.18	-	42,44,45,47	0
3	IPA	B	1138	4/4	0.30	-	54,55,56,56	0
2	757	B	1000	62/62	0.24	-	49,58,67,69	12
3	IPA	C	1139	4/4	0.38	-	62,62,63,66	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.