



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:48 PM UTC

PDB ID : 3MSJ / pdb_00003msj
Title : Structure of bace (beta secretase) in complex with inhibitor
Authors : Madden, J.; Kramer, J.; Smith, M.A.; Barker, J.; Godemann, R.
Deposited on : 2010-04-29
Resolution : 1.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

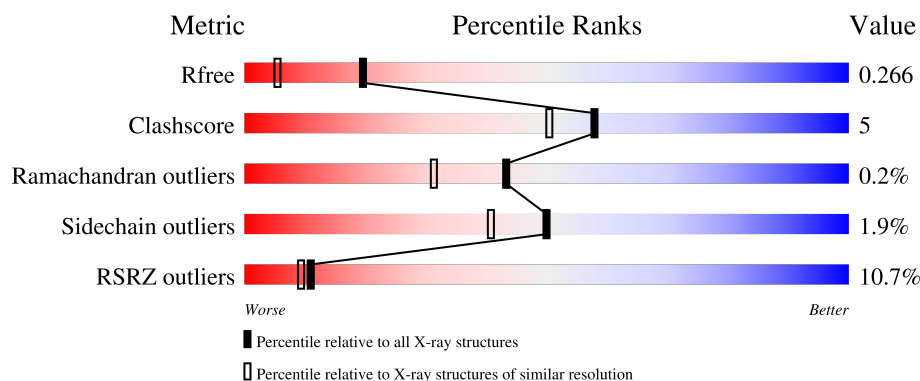
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	411	9% 78% 12% • 9%
1	B	411	9% 82% 9% 9%
1	C	411	11% 83% 6% • 9%

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	GOL	B	394	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9702 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.

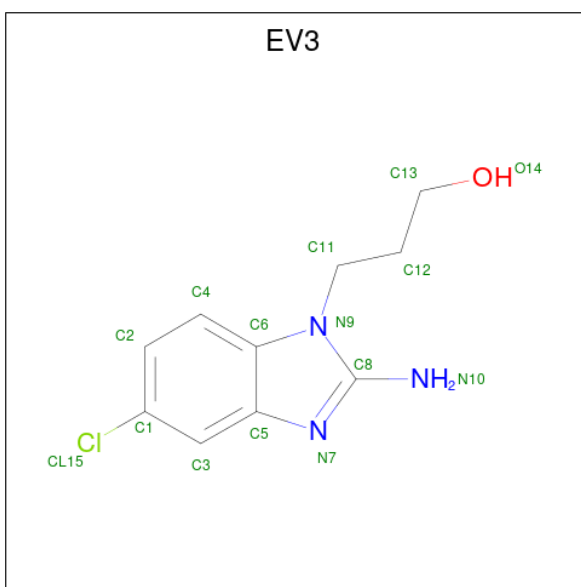
- Molecule 1 is a protein called BETA-SECRETASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	4	0
			2962	1897	493	558	14			
1	B	373	Total	C	N	O	S	0	4	0
			2956	1894	493	555	14			
1	C	375	Total	C	N	O	S	0	6	0
			2987	1912	494	567	14			

There are 6 discrepancies between the modelled and reference sequences:

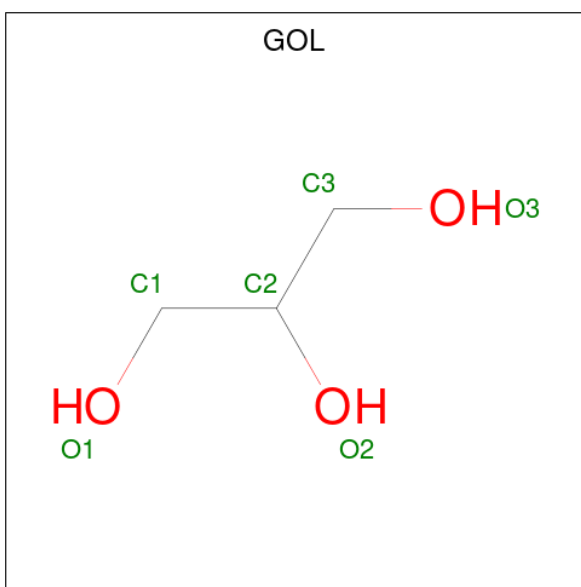
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LYS	ARG	engineered mutation	UNP P56817
A	-4	THR	ARG	engineered mutation	UNP P56817
B	-5	LYS	ARG	engineered mutation	UNP P56817
B	-4	THR	ARG	engineered mutation	UNP P56817
C	-5	LYS	ARG	engineered mutation	UNP P56817
C	-4	THR	ARG	engineered mutation	UNP P56817

- Molecule 2 is 3-(2-amino-5-chloro-1H-benzimidazol-1-yl)propan-1-ol (CCD ID: EV3) (formula: C₁₀H₁₂ClN₃O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			15	10	1	3	1		
2	B	1	Total	C	Cl	N	O	0	0
			15	10	1	3	1		
2	C	1	Total	C	Cl	N	O	0	0
			15	10	1	3	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

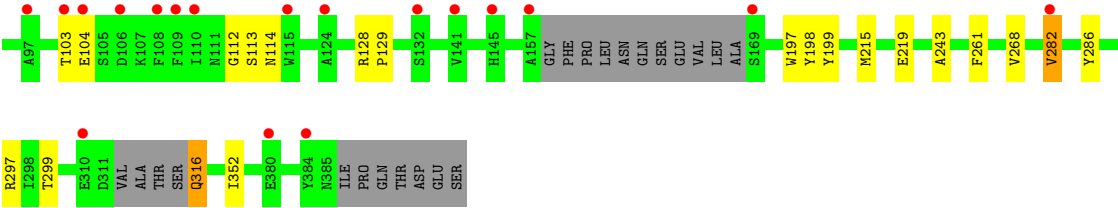
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	236	Total O 236 236	0	0
4	B	243	Total O 246 246	0	3
4	C	167	Total O 168 168	0	1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.20Å 98.83Å 63.13Å 90.00° 103.36° 90.00°	Depositor
Resolution (Å)	111.80 – 1.80 111.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (111.80-1.80) 94.4 (111.50-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.177 , 0.208 0.247 , 0.266	Depositor DCC
R_{free} test set	1212 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9702	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, EV3

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	0.66	0/3046	0.76	0/4136
1	B	0.69	0/3039	0.79	3/4127 (0.1%)
1	C	0.62	0/3077	0.74	0/4179
All	All	0.66	0/9162	0.76	3/12442 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	THR	CA-C-N	-7.22	112.56	119.85
1	B	191	THR	C-N-CA	-7.22	112.56	119.85
1	B	67	VAL	CB-CA-C	-6.88	99.90	110.50

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	2962	0	2875	39	0
1	B	2956	0	2882	26	0
1	C	2987	0	2897	18	0
2	A	15	0	12	3	0
2	B	15	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	12	0	0
3	A	42	0	56	2	0
3	B	48	0	64	7	0
3	C	12	0	16	0	0
4	A	236	0	0	3	0
4	B	246	0	0	0	0
4	C	168	0	0	0	0
All	All	9702	0	8826	81	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 5.

All (81) 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:2:MET:HE3	1:A:90:GLY:HA2	1.56	0.86
1:A:215:MET:HE1	1:A:240:VAL:HA	1.61	0.82
1:A:267:LEU:HD23	1:A:321:LYS:HG3	1.60	0.82
1:C:282:VAL:HG13	1:C:299:THR:HG23	1.68	0.75
1:B:0:VAL:H	3:B:394:GOL:H31	1.63	0.63
1:A:309:VAL:HG21	1:A:321:LYS:HD2	1.83	0.61
1:B:0:VAL:HG22	3:B:394:GOL:H32	1.81	0.60
1:C:199:TYR:HB3	1:C:352:ILE:HD11	1.84	0.59
1:A:267:LEU:CD2	1:A:321:LYS:HG3	2.31	0.59
1:C:286:TYR:CZ	1:C:297:ARG:HD3	2.38	0.58
1:A:213:LEU:HD23	1:A:215:MET:HE3	1.86	0.57
1:A:199:TYR:HB3	1:A:352:ILE:HD11	1.87	0.56
1:A:197:TRP:CG	1:A:198:TYR:H	2.24	0.56
1:C:282:VAL:HG13	1:C:299:THR:CG2	2.34	0.55
1:A:69:VAL:HG21	1:A:76:TRP:CZ2	2.41	0.55
1:B:205:ARG:HA	3:B:400:GOL:H32	1.89	0.55
1:C:67:VAL:HG22	1:C:80:LEU:HD22	1.90	0.54
1:B:199:TYR:HB3	1:B:352:ILE:HD11	1.91	0.52
1:C:69:VAL:HG21	1:C:76:TRP:CZ2	2.45	0.51
1:A:17:GLU:HB3	4:A:607:HOH:O	2.11	0.51
1:A:134:GLU:OE2	1:B:1:GLU:OE2	2.28	0.51
1:A:2:MET:HE1	1:A:176:ILE:HB	1.94	0.50
1:A:1:GLU:H	1:A:1:GLU:CD	2.21	0.49
1:A:92:ASN:HD22	1:A:92:ASN:C	2.21	0.48
1:A:111:ASN:HD22	1:A:112:GLY:N	2.12	0.47
1:A:215:MET:CE	1:A:243:ALA:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASP:OD2	1:A:118:ILE:HD11	2.13	0.47
1:B:0:VAL:HG22	3:B:394:GOL:C3	2.45	0.47
2:A:393:EV3:C3	3:A:398:GOL:H2	2.45	0.47
1:A:357:SER:HB3	1:A:360:HIS:HB3	1.97	0.46
1:C:112:GLY:O	1:C:114:ASN:N	2.48	0.46
1:B:95:VAL:HG11	1:B:140:LEU:HD12	1.98	0.46
1:B:156:GLY:O	1:B:157:ALA:CB	2.64	0.46
1:A:364:GLU:HB3	4:A:499:HOH:O	2.16	0.45
1:C:215:MET:HE1	1:C:243:ALA:HB3	1.97	0.45
1:A:32:ASP:OD2	2:A:393:EV3:N7	2.49	0.45
1:C:77:GLU:HG3	1:C:104:GLU:CG	2.47	0.45
1:A:154:LEU:O	1:A:339:GLU:HA	2.18	0.44
1:B:261:PHE:CD1	1:B:268:VAL:HG23	2.52	0.44
1:C:69:VAL:HG22	1:C:128:ARG:HG3	1.98	0.44
1:C:197:TRP:CG	1:C:198:TYR:H	2.35	0.44
1:A:222:TYR:HA	1:A:223:ASP:HA	1.74	0.44
1:B:11:GLY:N	3:B:397:GOL:H2	2.32	0.44
2:A:393:EV3:C5	3:A:398:GOL:H2	2.48	0.44
1:B:197:TRP:CG	1:B:198:TYR:H	2.36	0.44
1:B:32:ASP:OD2	2:B:393:EV3:N7	2.51	0.44
1:B:222:TYR:OH	1:C:219:GLU:OE1	2.26	0.44
1:A:333:MET:HE3	1:A:337:ILE:HG21	2.00	0.43
1:B:149:LEU:C	1:B:149:LEU:HD23	2.43	0.43
1:A:238:LYS:NZ	1:A:242:GLU:OE2	2.49	0.43
1:B:110:ILE:HB	1:B:113:SER:HB3	2.01	0.43
1:B:293:ASN:HA	1:B:376:THR:O	2.19	0.42
1:A:8:GLY:C	1:A:170:VAL:HG22	2.44	0.42
1:A:134:GLU:HB2	3:B:394:GOL:H2	2.01	0.42
1:A:333:MET:CE	1:A:337:ILE:HG21	2.50	0.42
1:B:67:VAL:HG13	1:B:129:PRO:HD3	2.01	0.42
1:A:197:TRP:CG	1:A:198:TYR:N	2.88	0.42
1:C:71:TYR:CE1	1:C:75:LYS:HA	2.55	0.42
1:A:211:GLN:NE2	4:A:483:HOH:O	2.53	0.42
1:B:-1:PHE:HB3	1:B:2:MET:HE3	2.01	0.42
1:B:92:ASN:HD22	3:B:395:GOL:H31	1.85	0.42
1:A:2:MET:CE	1:A:176:ILE:H	2.33	0.41
1:A:2:MET:HE2	1:A:174:MET:O	2.20	0.41
1:A:95:VAL:HG11	1:A:140:LEU:HA	2.02	0.41
1:A:238:LYS:HE2	1:A:326:GLN:HE22	1.84	0.41
1:A:82:THR:HG21	1:B:0:VAL:HG12	2.02	0.41
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:O	1:B:181:HIS:HD2	2.04	0.41
1:C:65:LYS:NZ	1:C:129:PRO:HG3	2.35	0.41
1:C:316:GLN:N	1:C:316:GLN:CD	2.78	0.41
1:A:215:MET:HE2	1:A:243:ALA:CB	2.51	0.41
1:B:267:LEU:HD21	1:B:309:VAL:HG21	2.02	0.41
1:B:32:ASP:OD2	1:B:118:ILE:HD11	2.21	0.41
1:B:215:MET:HE1	1:B:239:LYS:O	2.20	0.41
1:C:78:GLY:HA2	1:C:103:THR:HG22	2.03	0.41
1:B:201:VAL:O	1:B:225[B]:SER:OG	2.39	0.41
1:C:63:LEU:HD12	1:C:80:LEU:HB3	2.02	0.41
1:B:215:MET:HE3	1:B:243:ALA:HB2	2.03	0.40
1:A:293:ASN:HA	1:A:376:THR:O	2.21	0.40
1:C:261:PHE:CD1	1:C:268:VAL:HG23	2.57	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	371/411 (90%)	362 (98%)	9 (2%)	0	100	100
1	B	371/411 (90%)	364 (98%)	7 (2%)	0	100	100
1	C	375/411 (91%)	364 (97%)	9 (2%)	2 (0%)	24	14
All	All	1117/1233 (91%)	1090 (98%)	25 (2%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-3	GLY
1	C	113	SER

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	322/352 (92%)	315 (98%)	7 (2%)	45	34
1	B	322/352 (92%)	317 (98%)	5 (2%)	55	47
1	C	326/352 (93%)	320 (98%)	6 (2%)	51	43
All	All	970/1056 (92%)	952 (98%)	18 (2%)	50	41

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	72	THR
1	A	169	SER
1	A	213	LEU
1	A	259	ASP
1	A	364	GLU
1	A	367	THR
1	B	67	VAL
1	B	69	VAL
1	B	73	GLN
1	B	149	LEU
1	B	239	LYS
1	C	65	LYS
1	C	67	VAL
1	C	75	LYS
1	C	80	LEU
1	C	282	VAL
1	C	316	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	73	GLN
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	111	ASN
1	A	211	GLN
1	A	266	GLN
1	A	316	GLN
1	A	326	GLN
1	A	362	HIS
1	B	28	ASN
1	B	53	GLN
1	B	73	GLN
1	B	92	ASN
1	B	111	ASN
1	B	181	HIS
1	B	278	ASN
1	B	362	HIS
1	C	28	ASN
1	C	53	GLN
1	C	92	ASN
1	C	111	ASN
1	C	294	GLN
1	C	316	GLN
1	C	362	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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
3	GOL	B	397	-	5,5,5	0.31	0	5,5,5	0.41	0
2	EV3	A	393	-	16,16,16	1.68	3 (18%)	19,22,22	1.14	2 (10%)
3	GOL	A	400	-	5,5,5	0.39	0	5,5,5	0.18	0
2	EV3	B	393	-	16,16,16	1.74	3 (18%)	19,22,22	1.18	3 (15%)
3	GOL	A	399	-	5,5,5	0.41	0	5,5,5	0.77	0
3	GOL	B	400	-	5,5,5	0.34	0	5,5,5	0.59	0
3	GOL	B	395	-	5,5,5	0.37	0	5,5,5	0.29	0
3	GOL	C	394	-	5,5,5	0.45	0	5,5,5	0.47	0
3	GOL	A	394	-	5,5,5	0.39	0	5,5,5	0.27	0
3	GOL	B	398	-	5,5,5	0.39	0	5,5,5	0.39	0
3	GOL	B	394	-	5,5,5	0.73	0	5,5,5	1.63	2 (40%)
3	GOL	A	398	-	5,5,5	0.38	0	5,5,5	0.38	0
2	EV3	C	393	-	16,16,16	1.73	3 (18%)	19,22,22	1.23	3 (15%)
3	GOL	C	395	-	5,5,5	0.41	0	5,5,5	0.35	0
3	GOL	A	395	-	5,5,5	0.64	0	5,5,5	0.46	0
3	GOL	A	396	-	5,5,5	0.56	0	5,5,5	0.58	0
3	GOL	B	401	-	5,5,5	0.36	0	5,5,5	0.50	0
3	GOL	B	396	-	5,5,5	0.45	0	5,5,5	0.56	0
3	GOL	A	397	-	5,5,5	0.32	0	5,5,5	0.36	0
3	GOL	B	399	-	5,5,5	0.39	0	5,5,5	0.53	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	GOL	B	397	-	-	2/4/4/4	-
2	EV3	A	393	-	-	1/4/4/4	0/2/2/2
3	GOL	A	400	-	-	0/4/4/4	-
2	EV3	B	393	-	-	1/4/4/4	0/2/2/2
3	GOL	A	399	-	-	2/4/4/4	-
3	GOL	B	400	-	-	1/4/4/4	-
3	GOL	B	395	-	-	2/4/4/4	-
3	GOL	C	394	-	-	2/4/4/4	-
3	GOL	A	394	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	398	-	-	4/4/4/4	-
3	GOL	B	394	-	-	2/4/4/4	-
3	GOL	A	398	-	-	3/4/4/4	-
2	EV3	C	393	-	-	1/4/4/4	0/2/2/2
3	GOL	C	395	-	-	1/4/4/4	-
3	GOL	A	395	-	-	4/4/4/4	-
3	GOL	A	396	-	-	0/4/4/4	-
3	GOL	B	401	-	-	0/4/4/4	-
3	GOL	B	396	-	-	2/4/4/4	-
3	GOL	A	397	-	-	0/4/4/4	-
3	GOL	B	399	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	393	EV3	C8-N10	3.70	1.40	1.34
2	C	393	EV3	C8-N10	3.57	1.40	1.34
2	C	393	EV3	C5-N7	-3.39	1.33	1.39
2	A	393	EV3	C8-N10	3.37	1.40	1.34
2	B	393	EV3	C5-N7	-3.31	1.33	1.39
2	A	393	EV3	C6-N9	-3.19	1.33	1.39
2	A	393	EV3	C5-N7	-3.11	1.33	1.39
2	C	393	EV3	C6-N9	-2.93	1.34	1.39
2	B	393	EV3	C6-N9	-2.88	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	393	EV3	N10-C8-N7	-3.01	122.17	124.78
2	C	393	EV3	N10-C8-N7	-2.93	122.24	124.78
3	B	394	GOL	O1-C1-C2	2.49	121.57	110.38
2	B	393	EV3	C5-C6-N9	2.45	107.49	105.55
2	C	393	EV3	C5-C6-N9	2.42	107.46	105.55
2	A	393	EV3	C5-C6-N9	2.30	107.37	105.55
3	B	394	GOL	O3-C3-C2	2.26	120.56	110.38
2	B	393	EV3	N10-C8-N7	-2.18	122.89	124.78
2	C	393	EV3	C3-C5-C6	2.17	122.15	120.16
2	B	393	EV3	C3-C5-C6	2.08	122.08	120.16

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	393	EV3	N9-C11-C12-C13
3	A	395	GOL	O1-C1-C2-C3
3	B	394	GOL	O1-C1-C2-C3
3	B	396	GOL	O1-C1-C2-C3
3	B	397	GOL	O1-C1-C2-C3
3	B	398	GOL	C1-C2-C3-O3
3	A	394	GOL	O1-C1-C2-O2
2	B	393	EV3	C11-C12-C13-O14
3	A	394	GOL	O1-C1-C2-C3
3	A	398	GOL	C1-C2-C3-O3
3	A	399	GOL	C1-C2-C3-O3
3	B	398	GOL	O1-C1-C2-C3
3	B	399	GOL	C1-C2-C3-O3
3	A	395	GOL	O1-C1-C2-O2
3	B	396	GOL	O1-C1-C2-O2
3	B	397	GOL	O1-C1-C2-O2
3	B	398	GOL	O1-C1-C2-O2
3	B	398	GOL	O2-C2-C3-O3
3	B	394	GOL	O1-C1-C2-O2
3	A	398	GOL	O2-C2-C3-O3
3	A	399	GOL	O2-C2-C3-O3
3	B	400	GOL	O2-C2-C3-O3
3	C	394	GOL	O1-C1-C2-O2
3	A	395	GOL	O2-C2-C3-O3
3	A	395	GOL	C1-C2-C3-O3
3	B	395	GOL	O1-C1-C2-C3
3	C	394	GOL	O1-C1-C2-C3
3	A	398	GOL	O1-C1-C2-O2
3	C	395	GOL	O1-C1-C2-O2
3	B	395	GOL	O1-C1-C2-O2
3	B	399	GOL	O2-C2-C3-O3
2	A	393	EV3	N9-C11-C12-C13

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	397	GOL	1	0
2	A	393	EV3	3	0
2	B	393	EV3	1	0
3	B	400	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	395	GOL	1	0
3	B	394	GOL	4	0
3	A	398	GOL	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, 95th 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 ²)	Q<0.9
1	A	373/411 (90%)	0.77	39 (10%) 11 10	9, 20, 34, 179	9 (2%)
1	B	373/411 (90%)	0.35	35 (9%) 14 12	6, 24, 74, 100	8 (2%)
1	C	375/411 (91%)	1.08	46 (12%) 8 6	11, 20, 37, 618	10 (2%)
All	All	1121/1233 (90%)	0.74	120 (10%) 11 9	6, 20, 58, 618	27 (2%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	LEU	16.7
1	C	46	PRO	12.2
1	C	47	PHE	11.9
1	C	45	HIS	11.3
1	A	47	PHE	10.2
1	C	44	PRO	9.3
1	A	44	PRO	9.3
1	A	48	LEU	8.7
1	A	46	PRO	8.2
1	A	45	HIS	6.0
1	C	80	LEU	5.3
1	B	384	TYR	4.9
1	B	157	ALA	4.9
1	A	73	GLN	4.3
1	A	72	THR	4.2
1	A	-2	SER	4.2
1	C	70	PRO	4.1
1	B	272	ALA	3.8
1	A	43	ALA	3.7
1	C	73	GLN	3.7
1	C	103	THR	3.7
1	A	111	ASN	3.6
1	A	49	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	109	PHE	3.6
1	C	71	TYR	3.4
1	B	385	ASN	3.4
1	C	145	HIS	3.3
1	B	377	LEU	3.3
1	A	10	SER	3.3
1	C	42	ALA	3.3
1	C	84	LEU	3.2
1	B	379	MET	3.2
1	B	309	VAL	3.2
1	B	376	THR	3.1
1	C	60	TYR	3.1
1	A	106	ASP	3.1
1	B	267	LEU	3.1
1	C	157	ALA	3.0
1	A	68	TYR	3.0
1	C	132	SER	3.0
1	A	42	ALA	3.0
1	C	109	PHE	2.9
1	A	110	ILE	2.9
1	C	68	TYR	2.9
1	B	380	GLU	2.9
1	A	117	GLY	2.9
1	A	157	ALA	2.9
1	B	316	GLN	2.9
1	C	75	LYS	2.8
1	C	384	TYR	2.8
1	A	-1	PHE	2.8
1	B	73	GLN	2.8
1	C	74	GLY	2.8
1	C	64	ARG	2.8
1	C	110	ILE	2.8
1	C	72	THR	2.8
1	A	112	GLY	2.8
1	B	317	ASP	2.8
1	B	217	CYS	2.7
1	A	9	LYS	2.7
1	C	21	GLY	2.6
1	A	51	TYR	2.6
1	B	-4	THR	2.6
1	A	74	GLY	2.6
1	C	25	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	328	SER	2.6
1	C	76	TRP	2.6
1	B	156	GLY	2.6
1	C	104	GLU	2.5
1	A	56	LEU	2.5
1	B	145	HIS	2.5
1	B	256	LYS	2.5
1	B	382	CYS	2.5
1	A	104	GLU	2.5
1	B	364	GLU	2.5
1	C	82	THR	2.5
1	C	51	TYR	2.4
1	A	298	ILE	2.4
1	C	97	ALA	2.4
1	C	380	GLU	2.4
1	B	271	GLN	2.4
1	A	4	ASP	2.4
1	A	116	GLU	2.4
1	B	265	GLU	2.4
1	B	266	GLN	2.4
1	C	52	TYR	2.3
1	B	74	GLY	2.3
1	B	383	GLY	2.3
1	A	267	LEU	2.3
1	A	145	HIS	2.3
1	A	337	ILE	2.3
1	A	55	GLN	2.3
1	C	55	GLN	2.3
1	C	115	TRP	2.2
1	C	43	ALA	2.2
1	C	108	PHE	2.2
1	C	124	ALA	2.2
1	C	310	GLU	2.2
1	C	169	SER	2.2
1	A	15	TYR	2.2
1	B	375	VAL	2.2
1	C	141	VAL	2.2
1	B	319	CYS	2.2
1	A	263	LEU	2.2
1	B	263	LEU	2.2
1	C	81	GLY	2.2
1	A	-3	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	24	PRO	2.1
1	B	68	TYR	2.1
1	B	72	THR	2.1
1	A	1	GLU	2.1
1	A	20	VAL	2.1
1	B	268	VAL	2.1
1	C	282	VAL	2.1
1	B	273	GLY	2.0
1	A	23	PRO	2.0
1	B	258	PRO	2.0
1	C	20	VAL	2.0
1	B	269	CYS	2.0
1	C	106	ASP	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
3	GOL	A	399	6/6	0.60	0.17	51,56,57,58	0
3	GOL	A	396	6/6	0.61	0.19	22,40,41,45	0
3	GOL	A	394	6/6	0.68	0.13	46,51,52,53	0
3	GOL	C	395	6/6	0.72	0.16	43,47,49,52	0
3	GOL	B	395	6/6	0.74	0.15	36,41,44,44	0
3	GOL	B	401	6/6	0.75	0.17	51,54,56,58	0
2	EV3	C	393	15/15	0.76	0.20	62,72,72,72	0
3	GOL	A	397	6/6	0.76	0.16	47,47,48,49	0
3	GOL	B	400	6/6	0.79	0.12	35,42,43,46	0
3	GOL	A	400	6/6	0.80	0.13	51,52,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	398	6/6	0.81	0.13	19,39,42,44	0
2	EV3	B	393	15/15	0.81	0.12	38,42,44,44	0
3	GOL	A	398	6/6	0.83	0.12	50,53,55,58	0
3	GOL	B	394	6/6	0.83	0.22	5,19,31,38	0
3	GOL	B	399	6/6	0.83	0.10	31,40,42,43	0
3	GOL	B	396	6/6	0.84	0.14	11,37,42,42	0
3	GOL	A	395	6/6	0.85	0.15	21,31,34,42	0
2	EV3	A	393	15/15	0.85	0.10	27,31,34,36	0
3	GOL	C	394	6/6	0.88	0.14	21,34,35,43	0
3	GOL	B	397	6/6	0.88	0.12	29,33,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.