WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 8, 2017 – 06:46 PM EST

PDB ID : 4LXA
Title : Crystal Structure of Human Beta Secretase in Complex with Compound 11a
Authors : Rondeau, J.M.; Bourgier, E.
Deposited on : unknown
Resolution : 1.95 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.
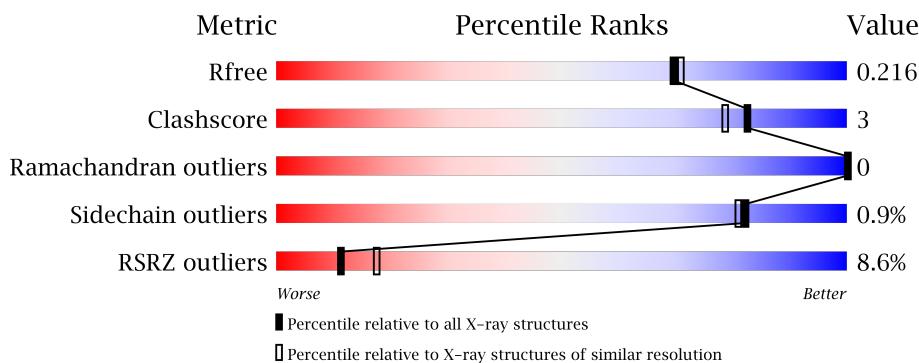
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
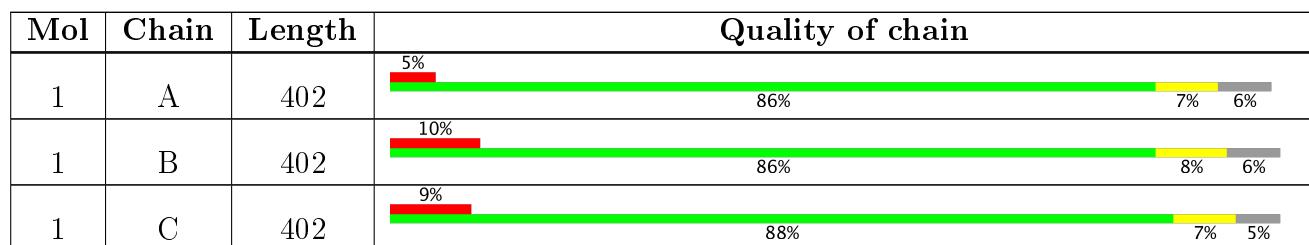
The reported resolution of this entry is 1.95 Å.

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	Percentile Ranks	Value
Rfree		0.216
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.9%
RSRZ outliers		8.6%

Worse   Better

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	402	5% 86% 7% 6%
1	B	402	10% 86% 8% 6%
1	C	402	9% 88% 7% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9566 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.
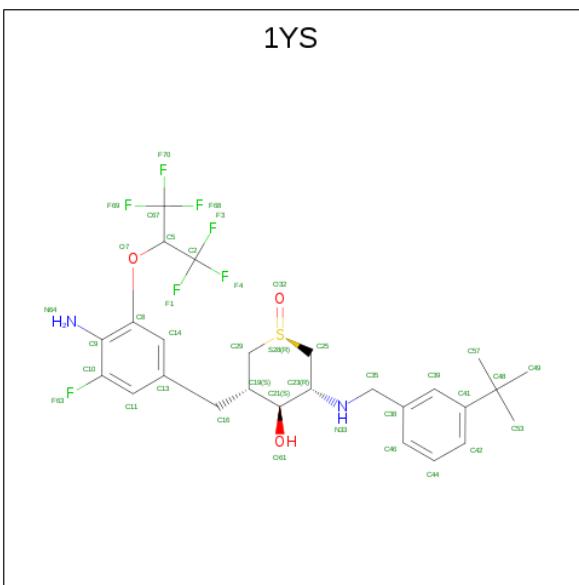
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2961	1895	492	560	14			
1	B	378	Total	C	N	O	S	0	0	0
			2971	1901	494	562	14			
1	C	381	Total	C	N	O	S	0	0	0
			2993	1917	497	565	14			

There are 6 discrepancies between the modelled and reference sequences:
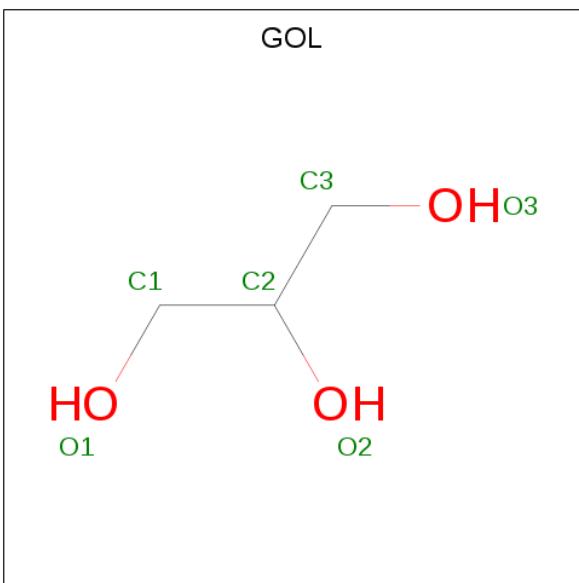
Chain	Residue	Modelled	Actual	Comment	Reference
A	33P	GLY	-	EXPRESSION TAG	UNP P56817
A	34P	PRO	-	EXPRESSION TAG	UNP P56817
B	33P	GLY	-	EXPRESSION TAG	UNP P56817
B	34P	PRO	-	EXPRESSION TAG	UNP P56817
C	33P	GLY	-	EXPRESSION TAG	UNP P56817
C	34P	PRO	-	EXPRESSION TAG	UNP P56817

- Molecule 2 is (1R,3S,4S,5R)-3-{4-amino-3-fluoro-5-[(1,1,1,3,3,3-hexafluoropropan-2-yl)oxy]benzyl}-5-[(3-tert-butylbenzyl)amino]tetrahydro-2H-thiopyran-4-ol 1-oxide (three-letter code: 1YS) (formula: $C_{26}H_{31}F_7N_2O_3S$).

1YS
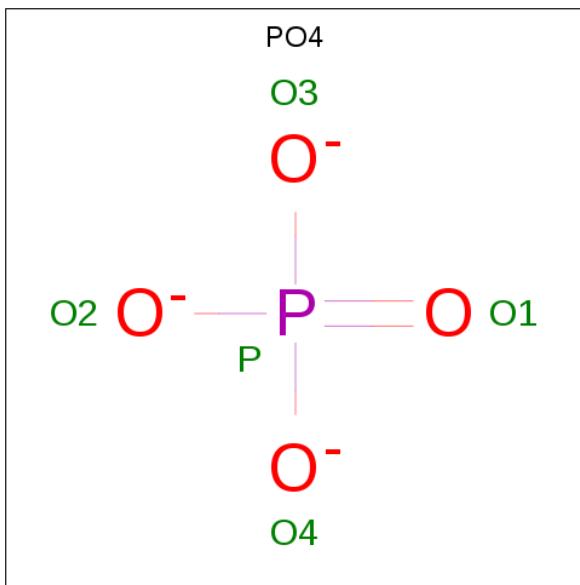
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S		0	0
			39	26	7	2	3	1			
2	B	1	Total	C	F	N	O	S		0	0
			39	26	7	2	3	1			
2	C	1	Total	C	F	N	O	S		0	0
			39	26	7	2	3	1			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 5	O 4	P 1	0	0
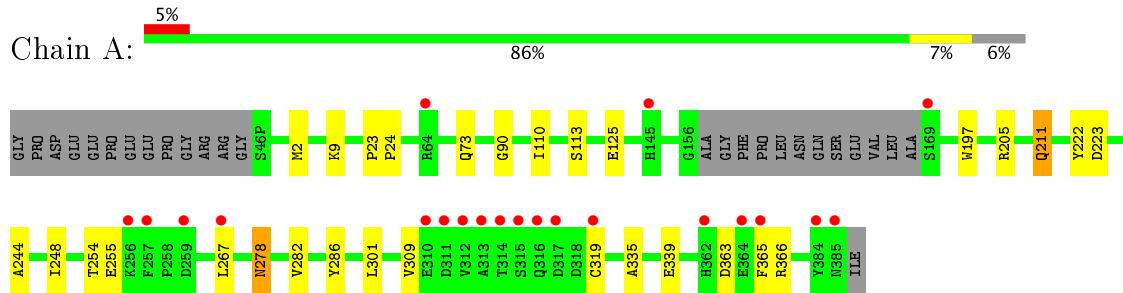
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total 172	O 172	0	0
5	B	168	Total 168	O 168	0	0
5	C	173	Total 173	O 173	0	0
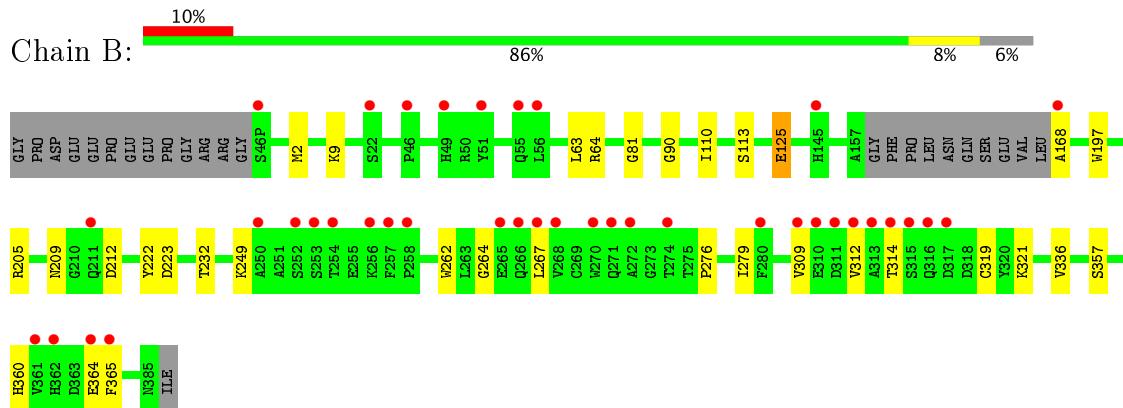
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.
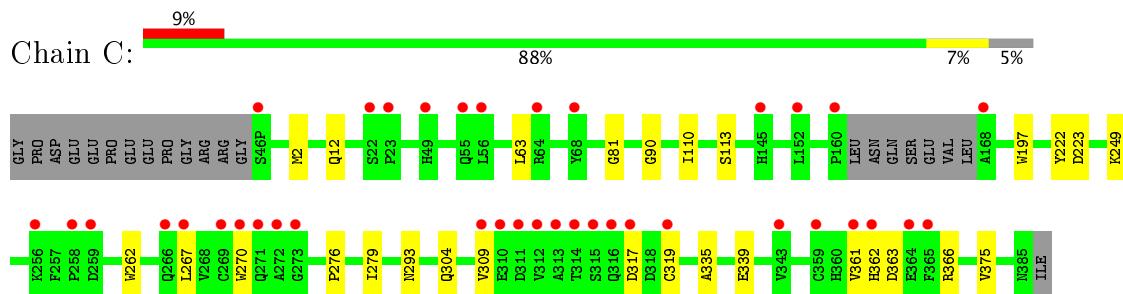
- Molecule 1: Beta-secretase 1

- Molecule 1: Beta-secretase 1

- Molecule 1: Beta-secretase 1

4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.93Å　　103.07Å　　100.23Å 90.00°　　104.33°　　90.00°	Depositor
Resolution (Å)	37.65　–　1.95	Depositor
	37.65　–　1.95	EDS
% Data completeness	99.4 (37.65-1.95)	Depositor
(in resolution range)	99.6 (37.65-1.95)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.24 (at 1.95Å)	Xtriage
Refinement program	CNS, CNX	Depositor
R, R_{free}	0.199　,　0.222	Depositor
	0.194　,　0.216	DCC
R_{free} test set	5880 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.6	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9566	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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, PO4, 1YS

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	0.27	0/3036	0.46	0/4126
1	B	0.27	0/3046	0.46	0/4140
1	C	0.26	0/3070	0.46	0/4173
All	All	0.27	0/9152	0.46	0/12439

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	2961	0	2870	17	0
1	B	2971	0	2880	19	0
1	C	2993	0	2899	16	0
2	A	39	0	31	0	0
2	B	39	0	31	0	0
2	C	39	0	31	0	0
3	B	6	0	8	0	0
4	C	5	0	0	0	0
5	A	172	0	0	2	0
5	B	168	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	173	0	0	0	0
All	All	9566	0	8750	52	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 (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LEU:HD13	1:B:319:CYS:HB3	1.71	0.71
1:A:267:LEU:HD13	1:A:319:CYS:HB3	1.75	0.67
1:A:254:THR:HG23	1:A:255:GLU:HG3	1.81	0.62
1:B:267:LEU:HD22	1:B:309:VAL:HG21	1.82	0.62
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.83	0.61
1:B:357:SER:O	1:B:360:HIS:HB3	2.01	0.60
1:B:9:LYS:HZ1	1:B:168:ALA:N	1.99	0.60
1:C:335:ALA:O	1:C:339:GLU:HG3	2.02	0.60
1:B:264:GLY:O	1:B:321:LYS:HE3	2.03	0.58
1:B:232:THR:O	1:B:336:VAL:HG13	2.03	0.58
1:B:64:ARG:HH11	1:B:64:ARG:HB3	1.69	0.58
1:A:278:ASN:H	1:A:278:ASN:HD22	1.52	0.57
1:A:125:GLU:HG3	5:A:744:HOH:O	2.05	0.56
1:B:276:PRO:O	1:B:279:ILE:HG12	2.06	0.56
1:C:249:LYS:HE2	1:C:262:TRP:CD1	2.41	0.55
1:C:267:LEU:HD13	1:C:319:CYS:HB3	1.88	0.55
1:C:363:ASP:HB3	1:C:366:ARG:O	2.05	0.55
1:A:335:ALA:O	1:A:339:GLU:HG3	2.08	0.54
1:C:267:LEU:HD22	1:C:309:VAL:HG21	1.89	0.54
1:B:63:LEU:HG	1:B:81:GLY:HA2	1.92	0.52
1:A:365:PHE:HB2	5:A:768:HOH:O	2.08	0.52
1:C:63:LEU:HG	1:C:81:GLY:HA2	1.93	0.50
1:A:267:LEU:HD22	1:A:309:VAL:HG21	1.94	0.49
1:B:205:ARG:NH2	1:B:212:ASP:HB2	2.28	0.49
1:C:110:ILE:HB	1:C:113:SER:HB3	1.94	0.49
1:B:267:LEU:HD21	1:B:312:VAL:HG13	1.94	0.49
1:C:304:GLN:HG3	1:C:361:VAL:HG21	1.94	0.49
1:B:267:LEU:HD22	1:B:309:VAL:CG2	2.42	0.48
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.96	0.48
1:A:363:ASP:HB3	1:A:366:ARG:O	2.14	0.48
1:B:110:ILE:HB	1:B:113:SER:HB3	1.96	0.47
1:C:12:GLN:OE1	1:C:113:SER:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:HD22	1:C:309:VAL:CG2	2.44	0.47
1:A:205:ARG:HB3	1:A:286:TYR:HB2	1.98	0.46
1:B:222:TYR:HA	1:B:223:ASP:HA	1.62	0.45
1:C:276:PRO:O	1:C:279:ILE:HG12	2.17	0.45
1:A:282:VAL:HG12	1:A:301:LEU:HD23	1.99	0.44
1:A:244:ALA:O	1:A:248:ILE:HG13	2.17	0.44
1:C:293:ASN:HA	1:C:375:VAL:HA	1.99	0.43
1:A:110:ILE:HB	1:A:113:SER:HB3	2.01	0.43
1:A:211:GLN:HB2	1:A:211:GLN:HE21	1.62	0.43
1:C:222:TYR:HA	1:C:223:ASP:HA	1.65	0.43
1:C:2:MET:HG2	1:C:90:GLY:HA2	2.00	0.43
1:A:222:TYR:HA	1:A:223:ASP:HA	1.70	0.43
1:A:9:LYS:HE2	1:A:9:LYS:HB3	1.83	0.42
1:B:249:LYS:HE2	1:B:262:TRP:CD1	2.54	0.42
1:B:364:GLU:HG3	1:B:365:PHE:CD2	2.55	0.42
1:B:314:THR:O	1:B:314:THR:HG23	2.20	0.41
1:C:304:GLN:CG	1:C:361:VAL:HG21	2.50	0.41
1:C:270:TRP:O	1:C:317:ASP:HB3	2.21	0.41
1:A:23:PRO:HA	1:A:24:PRO:HD3	1.93	0.40
1:B:125:GLU:O	1:B:125:GLU:HG3	2.21	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	372/402 (92%)	366 (98%)	6 (2%)	0	100	100
1	B	374/402 (93%)	366 (98%)	8 (2%)	0	100	100
1	C	377/402 (94%)	368 (98%)	9 (2%)	0	100	100
All	All	1123/1206 (93%)	1100 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	322/342 (94%)	318 (99%)	4 (1%)	75	72
1	B	322/342 (94%)	319 (99%)	3 (1%)	82	81
1	C	324/342 (95%)	322 (99%)	2 (1%)	89	88
All	All	968/1026 (94%)	959 (99%)	9 (1%)	82	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	197	TRP
1	A	211	GLN
1	A	278	ASN
1	B	125	GLU
1	B	197	TRP
1	B	209	ASN
1	C	197	TRP
1	C	362	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	278	ASN
1	A	326	GLN
1	B	114	ASN
1	B	278	ASN
1	B	293	ASN
1	B	326	GLN
1	C	114	ASN
1	C	326	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	1YS	A	501	-	37,41,41	1.51	5 (13%)	54,63,63	1.26	7 (12%)
3	GOL	B	501	-	5,5,5	0.70	0	5,5,5	0.46	0
2	1YS	B	502	-	37,41,41	1.55	5 (13%)	54,63,63	1.20	6 (11%)
2	1YS	C	501	-	37,41,41	1.52	5 (13%)	54,63,63	1.20	6 (11%)
4	PO4	C	502	-	4,4,4	1.32	0	6,6,6	0.39	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	1YS	A	501	-	-	0/31/47/47	0/3/3/3
3	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	1YS	B	502	-	-	0/31/47/47	0/3/3/3
2	1YS	C	501	-	-	0/31/47/47	0/3/3/3
4	PO4	C	502	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	1YS	C11-C10	2.26	1.41	1.37
2	C	501	1YS	C39-C41	2.30	1.43	1.39
2	B	502	1YS	C39-C41	2.30	1.43	1.39
2	A	501	1YS	C39-C41	2.32	1.43	1.39
2	B	502	1YS	C42-C41	2.48	1.43	1.39
2	A	501	1YS	C42-C41	2.49	1.43	1.39
2	C	501	1YS	C42-C41	2.50	1.43	1.39
2	B	502	1YS	C16-C19	2.53	1.57	1.53
2	C	501	1YS	C16-C19	2.56	1.57	1.53
2	C	501	1YS	C11-C10	2.59	1.42	1.37
2	B	502	1YS	C11-C10	2.62	1.42	1.37
2	A	501	1YS	C19-C21	2.67	1.56	1.53
2	A	501	1YS	C16-C19	2.77	1.57	1.53
2	C	501	1YS	C19-C21	2.91	1.56	1.53
2	B	502	1YS	C19-C21	2.97	1.56	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	1YS	C13-C16-C19	-3.05	108.58	113.77
2	B	502	1YS	C13-C16-C19	-2.64	109.27	113.77
2	C	501	1YS	C13-C16-C19	-2.53	109.47	113.77
2	C	501	1YS	C11-C10-C9	-2.09	120.34	123.37
2	A	501	1YS	C11-C10-C9	-2.03	120.42	123.37
2	B	502	1YS	C2-C5-C67	2.07	116.37	112.55
2	A	501	1YS	C2-C5-C67	2.07	116.38	112.55
2	B	502	1YS	C53-C48-C41	2.10	115.36	110.35
2	C	501	1YS	C53-C48-C41	2.19	115.58	110.35
2	A	501	1YS	C53-C48-C41	2.47	116.25	110.35
2	B	502	1YS	O7-C8-C9	2.47	117.93	114.64
2	C	501	1YS	O7-C8-C9	2.97	118.58	114.64
2	C	501	1YS	C35-N33-C23	3.00	121.32	114.95
2	A	501	1YS	O7-C8-C9	3.17	118.85	114.64
2	A	501	1YS	C8-C9-C10	3.27	119.24	116.03
2	A	501	1YS	C35-N33-C23	3.37	122.10	114.95
2	B	502	1YS	C35-N33-C23	3.45	122.27	114.95
2	C	501	1YS	C8-C9-C10	3.46	119.42	116.03
2	B	502	1YS	C8-C9-C10	3.50	119.46	116.03

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	376/402 (93%)	0.30	21 (5%)	25	35	24, 38, 71, 106	0
1	B	378/402 (94%)	0.49	39 (10%)	7	12	23, 39, 76, 110	0
1	C	381/402 (94%)	0.53	38 (9%)	8	13	26, 40, 73, 105	0
All	All	1135/1206 (94%)	0.44	98 (8%)	11	17	23, 39, 74, 110	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	VAL	12.6
1	B	314	THR	12.5
1	A	312	VAL	11.3
1	C	312	VAL	9.7
1	A	314	THR	9.7
1	C	313	ALA	9.4
1	C	315	SER	9.3
1	B	313	ALA	8.9
1	C	314	THR	8.2
1	A	313	ALA	8.1
1	A	311	ASP	6.9
1	B	311	ASP	6.8
1	A	316	GLN	6.3
1	B	310	GLU	6.2
1	B	365	PHE	6.0
1	A	315	SER	5.8
1	B	315	SER	5.6
1	C	310	GLU	5.6
1	B	316	GLN	5.2
1	C	311	ASP	4.9
1	C	272	ALA	4.9
1	C	316	GLN	4.7
1	A	310	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	256	LYS	4.7
1	C	168	ALA	4.6
1	C	259	ASP	4.4
1	B	364	GLU	4.4
1	A	256	LYS	4.3
1	C	160	PRO	3.8
1	B	309	VAL	3.8
1	C	309	VAL	3.7
1	B	254	THR	3.6
1	C	267	LEU	3.6
1	C	273	GLY	3.6
1	B	253	SER	3.5
1	B	317	ASP	3.5
1	B	168	ALA	3.4
1	A	145	HIS	3.2
1	B	274	THR	3.2
1	C	145	HIS	3.1
1	A	317	ASP	3.1
1	C	269	CYS	3.1
1	C	56	LEU	3.1
1	B	145	HIS	3.1
1	B	51	TYR	3.1
1	B	267	LEU	3.1
1	C	49	HIS	3.0
1	B	268	VAL	3.0
1	B	266	GLN	3.0
1	B	250	ALA	3.0
1	A	364	GLU	2.9
1	C	271	GLN	2.9
1	C	317	ASP	2.9
1	B	272	ALA	2.9
1	B	252	SER	2.8
1	A	384	TYR	2.8
1	B	55	GLN	2.8
1	A	259	ASP	2.8
1	C	64	ARG	2.8
1	C	270	TRP	2.8
1	B	257	PHE	2.8
1	B	361	VAL	2.8
1	B	270	TRP	2.7
1	A	267	LEU	2.7
1	C	46(P)	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	55	GLN	2.7
1	C	365	PHE	2.7
1	A	319	CYS	2.6
1	A	365	PHE	2.6
1	B	49	HIS	2.6
1	B	46	PRO	2.6
1	C	343	VAL	2.6
1	B	56	LEU	2.6
1	C	256	LYS	2.5
1	B	271	GLN	2.5
1	C	23	PRO	2.5
1	A	385	ASN	2.4
1	C	152	LEU	2.3
1	B	280	PHE	2.3
1	B	362	HIS	2.3
1	C	266	GLN	2.3
1	A	362	HIS	2.3
1	A	64	ARG	2.3
1	C	22	SER	2.3
1	C	361	VAL	2.2
1	A	169	SER	2.1
1	C	68	TYR	2.1
1	B	46(P)	SER	2.1
1	C	258	PRO	2.1
1	C	362	HIS	2.1
1	B	211	GLN	2.1
1	C	364	GLU	2.1
1	C	359	CYS	2.1
1	B	258	PRO	2.1
1	A	257	PHE	2.1
1	B	22	SER	2.1
1	C	319	CYS	2.1
1	B	265	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
2	1YS	A	501	39/39	0.95	0.14	0.38	27,33,41,44	0
3	GOL	B	501	6/6	0.95	0.10	0.16	40,43,44,46	0
2	1YS	C	501	39/39	0.96	0.12	-0.12	28,34,44,46	0
2	1YS	B	502	39/39	0.96	0.10	-0.40	26,32,44,46	0
4	PO4	C	502	5/5	0.99	0.12	-	45,46,47,49	0

6.5 Other polymers (i)

There are no such residues in this entry.