Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 06:48 am BST

PDB ID	:	5MXD
Title	:	BACE-1 IN COMPLEX WITH LIGAND 32397778
Authors	:	Alexander, R.
Deposited on	:	2017-01-23
Resolution	:	2.52 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

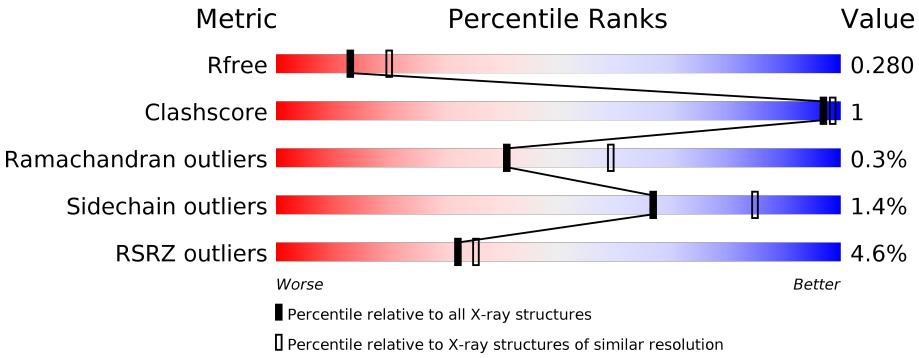
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 >=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 <=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	432	4% 85% 6% 10%
1	B	432	4% 83% 14%
1	C	432	4% 85% 12%

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
2	III	B	701	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9015 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	390	Total	C	N	O	S	0	0	0
			3059	1957	508	580	14			
1	B	370	Total	C	N	O	S	0	0	0
			2915	1868	486	547	14			
1	C	380	Total	C	N	O	S	0	0	0
			2984	1908	496	566	14			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-46	MET	-	initiating methionine	UNP P56817
A	-45	HIS	-	expression tag	UNP P56817
A	-44	HIS	-	expression tag	UNP P56817
A	-43	HIS	-	expression tag	UNP P56817
A	-42	HIS	-	expression tag	UNP P56817
A	-41	HIS	-	expression tag	UNP P56817
A	-40	HIS	-	expression tag	UNP P56817
A	-5	THR	ARG	conflict	UNP P56817
A	-4	THR	ARG	conflict	UNP P56817
B	-46	MET	-	initiating methionine	UNP P56817
B	-45	HIS	-	expression tag	UNP P56817
B	-44	HIS	-	expression tag	UNP P56817
B	-43	HIS	-	expression tag	UNP P56817
B	-42	HIS	-	expression tag	UNP P56817
B	-41	HIS	-	expression tag	UNP P56817
B	-40	HIS	-	expression tag	UNP P56817
B	-5	THR	ARG	conflict	UNP P56817
B	-4	THR	ARG	conflict	UNP P56817
C	-46	MET	-	initiating methionine	UNP P56817
C	-45	HIS	-	expression tag	UNP P56817
C	-44	HIS	-	expression tag	UNP P56817
C	-43	HIS	-	expression tag	UNP P56817
C	-42	HIS	-	expression tag	UNP P56817

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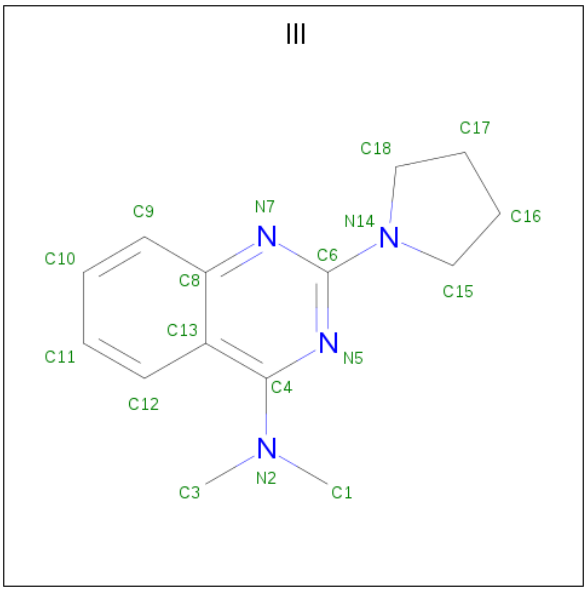
Chain	Residue	Modelled	Actual	Comment	Reference
C	-41	HIS	-	expression tag	UNP P56817
C	-40	HIS	-	expression tag	UNP P56817
C	-5	THR	ARG	conflict	UNP P56817
C	-4	THR	ARG	conflict	UNP P56817

- Molecule 2 is {N}, {N}-dimethyl-2-pyrrolidin-1-yl-quinazolin-4-amine (three-letter code: III) (formula: $C_{14}H_{18}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 18 14 4	0	0
2	B	1	Total C N 18 14 4	0	0
2	C	1	Total C N 18 14 4	0	0

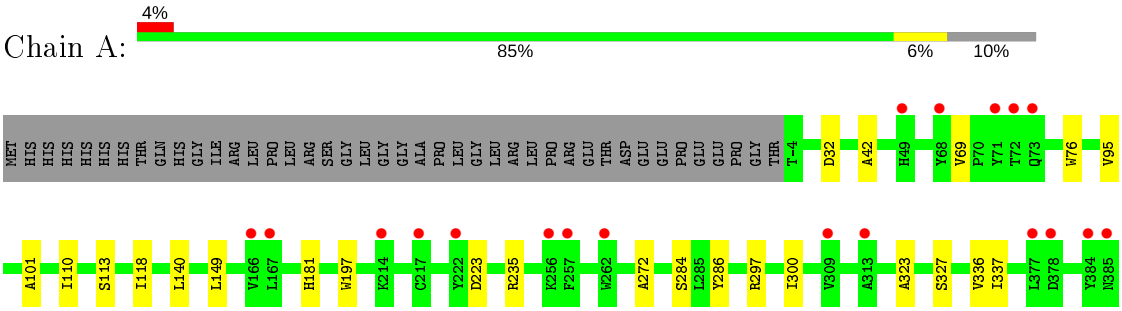
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

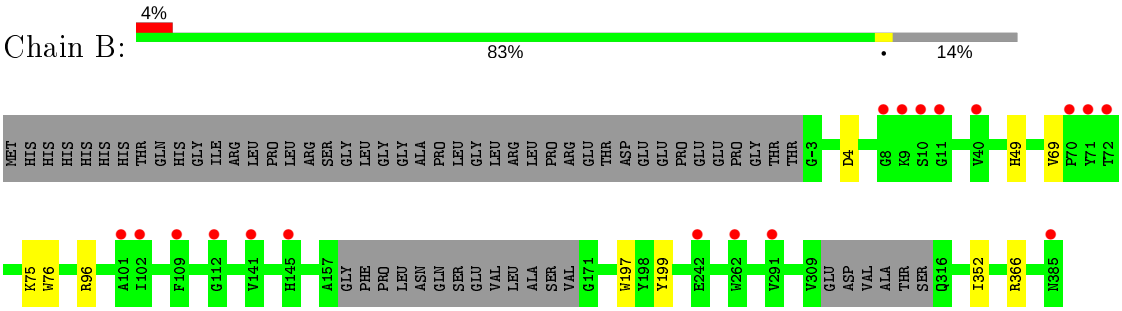
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

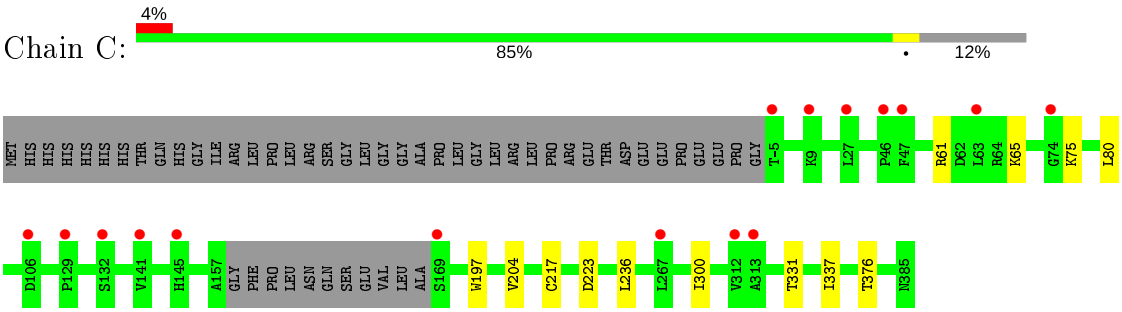
- Molecule 1: Beta-secretase 1



- Molecule 1: Beta-secretase 1



- Molecule 1: Beta-secretase 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	232.91Å 100.74Å 59.05Å 90.00° 102.03° 90.00°	Depositor
Resolution (Å)	113.90 – 2.52 47.66 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.6 (113.90-2.52) 96.6 (47.66-2.52)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.227 , 0.281 0.242 , 0.280	Depositor DCC
R_{free} test set	991 reflections (2.27%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.033 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9015	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: III, 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	0.40	0/3137	0.63	0/4266
1	B	0.39	0/2989	0.63	1/4059 (0.0%)
1	C	0.41	0/3059	0.62	0/4158
All	All	0.40	0/9185	0.63	1/12483 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	366	ARG	NE-CZ-NH1	5.57	123.08	120.30

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	3059	0	2969	9	0
1	B	2915	0	2830	2	0
1	C	2984	0	2895	5	0
2	A	18	0	0	1	0
2	B	18	0	0	0	0
2	C	18	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	9015	0	8694	16	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 1.

All (16) 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:323:ALA:HB1	1:A:336:VAL:HG21	1.91	0.52
1:C:204:VAL:CG1	1:C:376:THR:HG21	2.41	0.51
1:C:204:VAL:HG11	1:C:376:THR:HG21	1.94	0.50
1:A:110:ILE:HD11	2:A:701:III:N5	2.26	0.50
1:B:69:VAL:HG21	1:B:76:TRP:CZ2	2.47	0.49
1:B:199:TYR:HB3	1:B:352:ILE:HD11	1.95	0.48
1:A:286:TYR:CZ	1:A:297:ARG:HD3	2.49	0.48
1:A:69:VAL:HG21	1:A:76:TRP:CZ2	2.51	0.46
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.47	0.45
1:C:236:LEU:HD23	1:C:331:THR:HG23	2.00	0.44
1:A:235:ARG:HB3	1:A:327:SER:HB2	1.99	0.43
1:A:32:ASP:OD2	1:A:118:ILE:HD11	2.18	0.42
1:C:65:LYS:HB3	1:C:80:LEU:HD12	2.01	0.42
1:A:300:ILE:HD13	1:A:337:ILE:HD13	2.02	0.41
1:A:95:VAL:HG11	1:A:140:LEU:HD12	2.02	0.41
1:C:300:ILE:HD13	1:C:337:ILE:HD13	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	388/432 (90%)	371 (96%)	15 (4%)	2 (0%)	29 47
1	B	364/432 (84%)	354 (97%)	10 (3%)	0	100 100
1	C	376/432 (87%)	361 (96%)	14 (4%)	1 (0%)	41 59
All	All	1128/1296 (87%)	1086 (96%)	39 (4%)	3 (0%)	41 59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	C	223	ASP
1	A	272	ALA

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	332/367 (90%)	327 (98%)	5 (2%)	65 83
1	B	315/367 (86%)	310 (98%)	5 (2%)	62 82
1	C	324/367 (88%)	320 (99%)	4 (1%)	71 87
All	All	971/1101 (88%)	957 (99%)	14 (1%)	67 85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	A	149	LEU
1	A	181	HIS
1	A	197	TRP
1	A	284	SER
1	B	4	ASP
1	B	49	HIS
1	B	75	LYS
1	B	96	ARG
1	B	197	TRP

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Mol	Chain	Res	Type
1	C	61	ARG
1	C	75	LYS
1	C	197	TRP
1	C	217	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	GLN

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 6 ligands modelled in this entry, 3 are 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	III	B	701	-	19,20,20	0.96	1 (5%)	25,28,28	2.16	9 (36%)
2	III	A	701	-	19,20,20	0.93	1 (5%)	25,28,28	2.14	8 (32%)
2	III	C	701	-	19,20,20	0.95	1 (5%)	25,28,28	2.17	9 (36%)

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	III	B	701	-	-	4/8/15/15	0/3/3/3
2	III	A	701	-	-	5/8/15/15	0/3/3/3
2	III	C	701	-	-	4/8/15/15	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	III	C6-N14	2.42	1.40	1.35
2	C	701	III	C6-N14	2.40	1.40	1.35
2	A	701	III	C6-N14	2.19	1.39	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	III	C18-N14-C6	-5.87	113.17	123.48
2	A	701	III	C15-N14-C6	-5.57	113.69	123.48
2	C	701	III	C15-N14-C6	-4.75	115.13	123.48
2	C	701	III	C18-N14-C6	-4.43	115.69	123.48
2	A	701	III	C6-N5-C4	4.17	123.48	115.20
2	B	701	III	C6-N5-C4	3.82	122.78	115.20
2	C	701	III	C6-N5-C4	3.80	122.73	115.20
2	A	701	III	C18-N14-C15	-3.62	104.89	111.46
2	B	701	III	C15-N14-C6	-3.60	117.15	123.48
2	C	701	III	N5-C4-N2	3.59	121.34	115.67
2	A	701	III	N5-C4-N2	3.54	121.26	115.67
2	B	701	III	C13-C8-N7	-3.50	119.10	122.81
2	C	701	III	C18-N14-C15	-3.48	105.14	111.46
2	C	701	III	C13-C8-N7	-3.08	119.55	122.81
2	A	701	III	C18-N14-C6	-3.04	118.13	123.48
2	B	701	III	N5-C4-N2	3.01	120.43	115.67
2	A	701	III	C13-C8-N7	-3.01	119.62	122.81
2	B	701	III	C17-C18-N14	2.89	107.11	103.45
2	B	701	III	C18-N14-C15	-2.76	106.45	111.46
2	C	701	III	N5-C6-N14	2.72	120.46	117.11
2	A	701	III	C13-C4-N5	-2.49	117.35	122.66
2	A	701	III	C1-N2-C4	-2.38	112.32	119.51
2	C	701	III	C13-C4-N5	-2.26	117.85	122.66
2	B	701	III	C13-C4-N5	-2.18	118.03	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	III	C1-N2-C4	-2.13	113.08	119.51
2	B	701	III	C1-N2-C4	-2.04	113.35	119.51

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	III	N5-C4-N2-C1
2	C	701	III	N5-C6-N14-C15
2	C	701	III	N7-C6-N14-C15
2	B	701	III	N5-C4-N2-C1
2	B	701	III	N5-C6-N14-C18
2	B	701	III	N7-C6-N14-C18
2	A	701	III	N5-C6-N14-C15
2	A	701	III	N7-C6-N14-C15
2	C	701	III	N5-C4-N2-C3
2	B	701	III	N5-C4-N2-C3
2	A	701	III	N5-C4-N2-C1
2	A	701	III	N5-C4-N2-C3
2	A	701	III	C13-C4-N2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	III	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	390/432 (90%)	0.40	19 (4%)	29	32	34, 69, 135, 208	0
1	B	370/432 (85%)	0.46	18 (4%)	29	32	45, 78, 137, 183	0
1	C	380/432 (87%)	0.43	16 (4%)	36	40	40, 79, 119, 174	0
All	All	1140/1296 (87%)	0.43	53 (4%)	32	35	34, 75, 133, 208	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	GLY	6.2
1	C	132	SER	5.4
1	A	71	TYR	5.0
1	A	313	ALA	4.8
1	B	72	THR	4.5
1	B	10	SER	4.3
1	A	378	ASP	4.2
1	A	72	THR	4.1
1	A	73	GLN	4.0
1	B	9	LYS	4.0
1	A	377	LEU	3.7
1	B	102	ILE	3.7
1	B	11	GLY	3.4
1	C	313	ALA	3.3
1	B	262	TRP	3.3
1	C	-5	THR	3.2
1	A	256	LYS	3.2
1	A	257	PHE	2.9
1	A	166	VAL	2.8
1	B	40	VAL	2.8
1	B	71	TYR	2.8
1	C	27	LEU	2.7
1	A	309	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	217	CYS	2.6
1	B	385	ASN	2.5
1	B	8	GLY	2.5
1	C	129	PRO	2.5
1	B	101	ALA	2.4
1	C	312	VAL	2.4
1	B	141	VAL	2.4
1	A	385	ASN	2.3
1	B	109	PHE	2.3
1	A	262	TRP	2.3
1	A	384	TYR	2.3
1	C	47	PHE	2.3
1	C	106	ASP	2.3
1	A	167	LEU	2.3
1	B	112	GLY	2.2
1	B	291	VAL	2.2
1	C	169	SER	2.2
1	A	222	TYR	2.2
1	B	242	GLU	2.1
1	A	214	LYS	2.1
1	B	70	PRO	2.1
1	C	63	LEU	2.1
1	C	267	LEU	2.1
1	A	49	HIS	2.1
1	B	145	HIS	2.1
1	C	46	PRO	2.1
1	A	68	TYR	2.1
1	C	141	VAL	2.0
1	C	9	LYS	2.0
1	C	145	HIS	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

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^{th} 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
2	III	B	701	18/18	0.75	0.45	77,112,122,129	0
3	CL	B	702	1/1	0.86	0.11	70,70,70,70	0
2	III	C	701	18/18	0.87	0.42	59,72,92,94	0
2	III	A	701	18/18	0.89	0.23	46,59,69,71	0
3	CL	A	702	1/1	0.92	0.20	64,64,64,64	0
3	CL	C	702	1/1	0.96	0.10	63,63,63,63	0

6.5 Other polymers

There are no such residues in this entry.