Full wwPDB X-ray Structure Validation Report (i)

Mar 7, 2024 – 05:01 PM EST

PDB ID	:	6CBD
Title	:	Crystal Structure of Human Argonaute2 Bound to Three Tryptophans
Authors	:	Sheu-Gruttadauria, J.; MacRae, I.J.
Deposited on	:	2018-02-02
Resolution	:	2.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

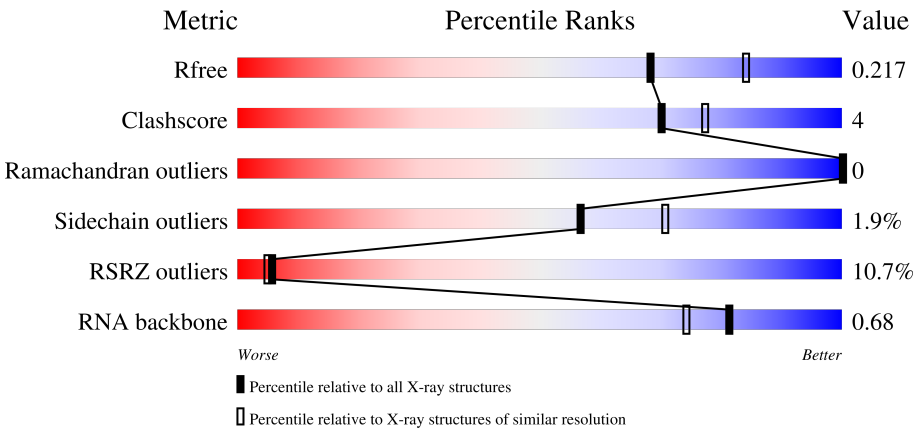
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

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 <=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	859	10% 83% 8% 8%
2	B	21	19% 62% 24% 5% 10%
3	C	11	9% 82% 9% 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7213 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 Protein argonaute-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	787	6299	4019	1126	1114	40	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	engineered mutation	UNP Q9UKV8

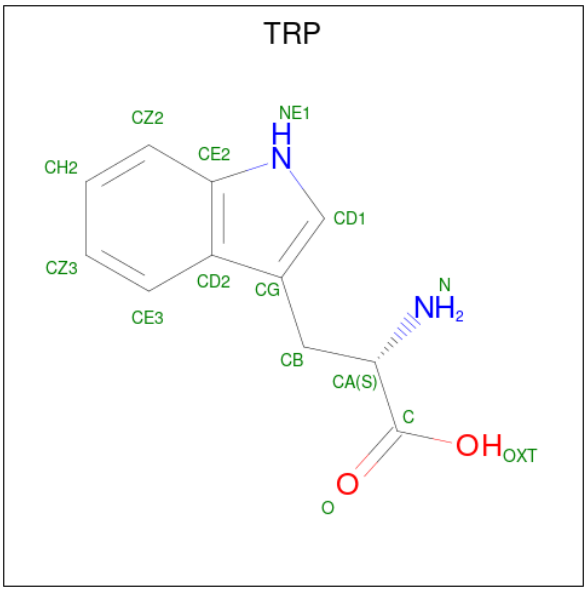
- Molecule 2 is a RNA chain called Guide RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	19	379	168	60	132	19	0	0	0

- Molecule 3 is a RNA chain called Target RNA.

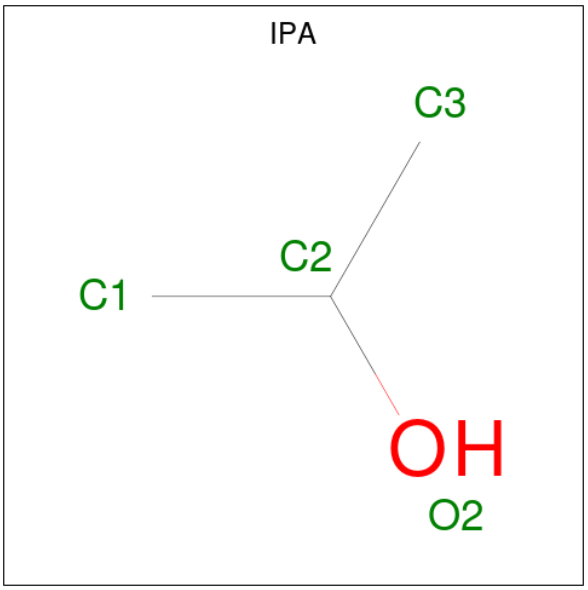
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	10	196	88	37	62	9	0	0	0

- Molecule 4 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	15	11	2	2	0	0
			Total	C	N	O		
4	A	1	15	11	2	2	0	0
			Total	C	N	O		
4	A	1	15	11	2	2	0	0

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is water.

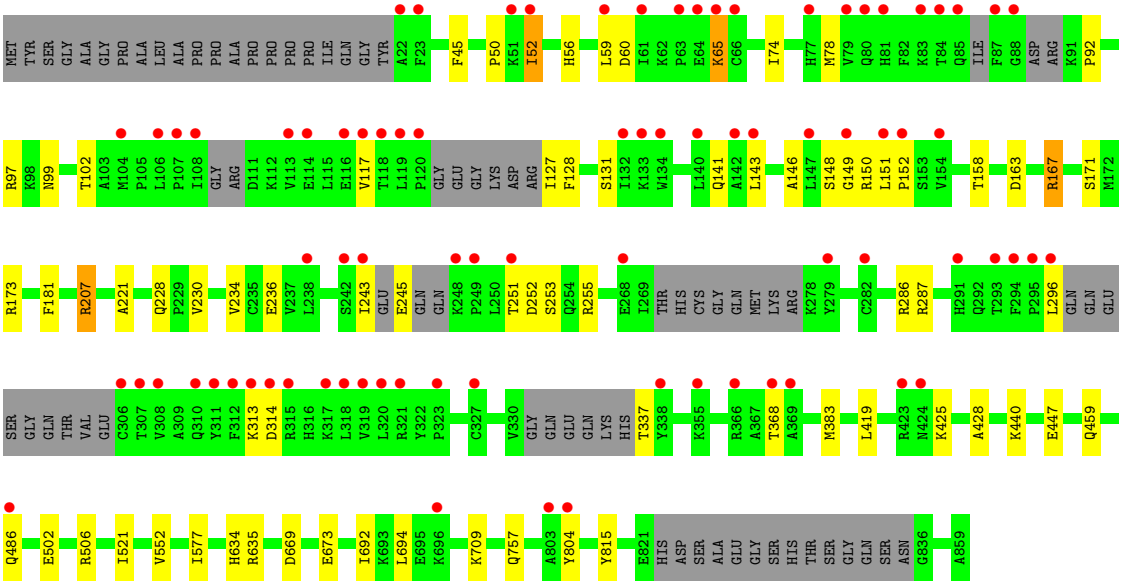
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	229	229	229	0	0
			Total	O		
7	B	31	31	31	0	0
			Total	O		
7	C	19	19	19	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

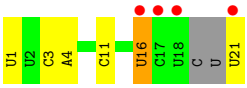
- Molecule 1: Protein argonaute-2

Chain A:



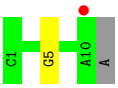
- Molecule 2: Guide RNA

Chain B:



- Molecule 3: Target RNA

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.83Å 117.00Å 70.25Å 90.00° 92.64° 90.00°	Depositor
Resolution (Å)	35.50 – 2.20 35.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (35.50-2.20) 98.2 (35.51-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.176 , 0.215 0.178 , 0.217	Depositor DCC
R_{free} test set	2174 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7213	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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 (i)

5.1 Standard geometry (i)

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

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	0.25	0/6444	0.43	0/8716
2	B	0.57	1/419 (0.2%)	0.73	0/645
3	C	0.30	0/219	0.79	0/340
All	All	0.28	1/7082 (0.0%)	0.47	0/9701

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.69	1.48	1.61

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	6299	0	6362	47	0
2	B	379	0	193	4	0
3	C	196	0	98	2	0
4	A	45	0	27	2	0
5	A	8	0	16	0	0
5	B	4	0	8	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	229	0	0	4	0
7	B	31	0	0	0	0
7	C	19	0	0	0	0
All	All	7213	0	6704	49	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 4.

All (49) 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:502:GLU:O	1:A:506:ARG:HG3	1.89	0.72
1:A:167:ARG:HG2	1:A:181:PHE:HZ	1.55	0.70
4:A:902:TRP:N	7:A:1003:HOH:O	2.27	0.68
1:A:286:ARG:NH2	1:A:287:ARG:HH12	1.91	0.67
1:A:757:GLN:HG3	3:C:5:G:N2	2.08	0.66
1:A:521:ILE:HD12	1:A:552:VAL:HG21	1.79	0.65
1:A:313:LYS:NZ	7:A:1008:HOH:O	2.33	0.61
1:A:228:GLN:NE2	1:A:236:GLU:OE2	2.30	0.61
1:A:286:ARG:CZ	1:A:287:ARG:HH12	2.17	0.57
1:A:65:LYS:NZ	2:B:16:U:O2'	2.20	0.55
2:B:3:C:H2'	2:B:4:A:C8	2.42	0.54
1:A:148:SER:OG	1:A:150:ARG:NH1	2.39	0.54
1:A:252:ASP:OD1	1:A:255:ARG:NH1	2.31	0.54
1:A:428:ALA:HB2	1:A:440:LYS:HE2	1.89	0.54
1:A:56:HIS:NE2	1:A:99:ASN:OD1	2.37	0.53
1:A:296:LEU:HD12	1:A:296:LEU:H	1.73	0.53
1:A:207:ARG:NH2	1:A:673:GLU:OE1	2.40	0.52
1:A:146:ALA:HA	1:A:151:LEU:HB2	1.92	0.51
1:A:143:LEU:HB2	1:A:158:THR:HG21	1.92	0.51
1:A:50:PRO:HB2	1:A:52:ILE:HG13	1.93	0.51
1:A:148:SER:OG	1:A:149:GLY:N	2.44	0.50
1:A:337:THR:HA	2:B:21:U:H1'	1.94	0.49
1:A:45:PHE:CZ	1:A:383:MET:HG3	2.47	0.49
1:A:757:GLN:HG3	3:C:5:G:H21	1.75	0.49
1:A:251:THR:HG22	1:A:253:SER:H	1.78	0.48
1:A:74:ILE:HG23	1:A:117:VAL:HG21	1.95	0.48
1:A:287:ARG:HG3	1:A:287:ARG:HH11	1.79	0.48
1:A:221:ALA:HB3	1:A:368:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:HG23	1:A:128:PHE:HB2	1.95	0.47
1:A:59:LEU:HA	1:A:131:SER:O	2.15	0.47
1:A:167:ARG:HG2	1:A:181:PHE:CZ	2.44	0.46
1:A:92:PRO:HB3	1:A:102:THR:HG22	1.98	0.45
1:A:709:LYS:HG3	7:A:1083:HOH:O	2.17	0.45
1:A:245:GLU:N	1:A:245:GLU:OE1	2.50	0.45
1:A:692:ILE:HD11	4:A:903:TRP:HZ3	1.82	0.45
1:A:60:ASP:HB2	1:A:131:SER:HB2	1.99	0.44
1:A:78:MET:HB2	1:A:117:VAL:HG11	1.99	0.44
1:A:243:ILE:O	1:A:245:GLU:N	2.50	0.44
1:A:419:LEU:HD23	1:A:577:ILE:HD11	2.00	0.44
1:A:634:HIS:CD2	1:A:635:ARG:HG3	2.54	0.43
1:A:447:GLU:OE2	1:A:486:GLN:NE2	2.53	0.42
1:A:669:ASP:OD1	7:A:1001:HOH:O	2.21	0.42
1:A:230:VAL:O	1:A:234:VAL:HG23	2.20	0.42
1:A:151:LEU:HA	1:A:152:PRO:HD3	1.83	0.41
1:A:117:VAL:O	1:A:127:ILE:N	2.54	0.41
1:A:635:ARG:HD3	2:B:11:C:OP1	2.21	0.41
1:A:163:ASP:O	1:A:167:ARG:HB2	2.21	0.41
1:A:425:LYS:HE3	1:A:425:LYS:HB3	1.92	0.40
1:A:694:LEU:HD23	1:A:694:LEU:HA	1.98	0.40

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	766/859 (89%)	743 (97%)	23 (3%)	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	696/752 (93%)	684 (98%)	12 (2%)	60 74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ILE
1	A	65	LYS
1	A	97	ARG
1	A	141	GLN
1	A	167	ARG
1	A	171	SER
1	A	173	ARG
1	A	207	ARG
1	A	314	ASP
1	A	459	GLN
1	A	804	TYR
1	A	815	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	16/21 (76%)	1 (6%)	0
3	C	8/11 (72%)	0	0
All	All	24/32 (75%)	1 (4%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	16	U

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
5	IPA	B	101	-	3,3,3	0.55	0	3,3,3	0.31	0
5	IPA	A	905	-	3,3,3	0.52	0	3,3,3	0.34	0
4	TRP	A	901	-	14,16,16	0.84	1 (7%)	16,22,22	1.16	2 (12%)
5	IPA	A	904	-	3,3,3	0.52	0	3,3,3	0.33	0
4	TRP	A	902	-	14,16,16	0.85	1 (7%)	16,22,22	1.18	2 (12%)
4	TRP	A	903	-	14,16,16	0.85	1 (7%)	16,22,22	1.12	2 (12%)

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
4	TRP	A	903	-	-	6/7/8/8	0/2/2/2
4	TRP	A	902	-	-	4/7/8/8	0/2/2/2
4	TRP	A	901	-	-	0/7/8/8	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	TRP	OXT-C	-2.15	1.23	1.30
4	A	901	TRP	OXT-C	-2.09	1.23	1.30
4	A	902	TRP	OXT-C	-2.09	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	TRP	OXT-C-O	-2.69	117.99	124.09
4	A	902	TRP	OXT-C-O	-2.63	118.11	124.09
4	A	903	TRP	OXT-C-O	-2.59	118.21	124.09
4	A	902	TRP	OXT-C-CA	2.31	121.27	113.38
4	A	901	TRP	OXT-C-CA	2.31	121.25	113.38
4	A	903	TRP	OXT-C-CA	2.11	120.58	113.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	TRP	O-C-CA-N
4	A	902	TRP	C-CA-CB-CG
4	A	903	TRP	CA-CB-CG-CD1
4	A	902	TRP	OXT-C-CA-N
4	A	903	TRP	OXT-C-CA-CB
4	A	903	TRP	O-C-CA-CB
4	A	903	TRP	OXT-C-CA-N
4	A	903	TRP	N-CA-CB-CG
4	A	903	TRP	O-C-CA-N
4	A	902	TRP	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	TRP	1	0
4	A	903	TRP	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 (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(Å^2)	Q<0.9
1	A	787/859 (91%)	0.34	82 (10%)	6	5	19, 39, 90, 112	0
2	B	19/21 (90%)	0.49	4 (21%)	1	0	24, 42, 107, 120	0
3	C	10/11 (90%)	-0.23	1 (10%)	7	6	37, 40, 55, 82	0
All	All	816/891 (91%)	0.34	87 (10%)	6	5	19, 39, 91, 120	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	LEU	7.8
1	A	108	ILE	7.0
1	A	319	VAL	6.2
1	A	120	PRO	6.1
1	A	279	TYR	5.7
1	A	64	GLU	5.2
1	A	84	THR	5.1
1	A	134	TRP	5.0
1	A	308	VAL	4.9
1	A	23	PHE	4.9
1	A	296	LEU	4.8
1	A	66	CYS	4.5
1	A	151	LEU	4.4
1	A	65	LYS	4.3
1	A	113	VAL	4.1
1	A	311	TYR	4.0
1	A	52	ILE	4.0
1	A	59	LEU	4.0
1	A	61	ILE	3.8
1	A	152	PRO	3.8
1	A	77	HIS	3.7
1	A	249	PRO	3.7
1	A	104	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	248	LYS	3.6
1	A	238	LEU	3.6
1	A	79	VAL	3.5
1	A	318	LEU	3.5
1	A	22	ALA	3.4
1	A	149	GLY	3.4
1	A	107	PRO	3.4
1	A	294	PHE	3.4
1	A	63	PRO	3.3
1	A	368	THR	3.3
1	A	315	ARG	3.3
1	A	423	ARG	3.2
1	A	310	GLN	3.1
1	A	313	LYS	3.1
1	A	293	THR	3.1
2	B	21	U	3.1
1	A	327	CYS	3.1
2	B	17	C	3.1
1	A	80	GLN	3.0
1	A	147	LEU	3.0
1	A	291	HIS	3.0
1	A	314	ASP	3.0
1	A	323	PRO	2.9
1	A	242	SER	2.9
1	A	317	LYS	2.9
1	A	142	ALA	2.9
1	A	88	GLY	2.8
1	A	132	ILE	2.8
1	A	87	PHE	2.8
1	A	366	ARG	2.8
2	B	18	U	2.8
1	A	306	CYS	2.8
1	A	114	GLU	2.7
1	A	83	LYS	2.6
1	A	243	ILE	2.6
1	A	369	ALA	2.6
1	A	106	LEU	2.5
1	A	312	PHE	2.5
1	A	424	ASN	2.4
1	A	154	VAL	2.4
1	A	268	GLU	2.4
1	A	282	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	295	PRO	2.4
1	A	133	LYS	2.3
1	A	338	TYR	2.3
2	B	16	U	2.3
1	A	143	LEU	2.3
1	A	320	LEU	2.3
1	A	85	GLN	2.3
1	A	307	THR	2.2
1	A	696	LYS	2.2
1	A	804	TYR	2.2
1	A	118	THR	2.1
1	A	81	HIS	2.1
1	A	116	GLU	2.1
1	A	251	THR	2.1
1	A	321	ARG	2.1
1	A	117	VAL	2.1
1	A	51	LYS	2.1
1	A	355	LYS	2.1
3	C	10	A	2.1
1	A	486	GLN	2.0
1	A	140	LEU	2.0
1	A	803	ALA	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 monosaccharides 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
4	TRP	A	902	15/15	0.80	0.20	35,41,73,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TRP	A	903	15/15	0.80	0.18	39,45,62,67	15
5	IPA	A	904	4/4	0.81	0.22	48,56,62,67	0
6	MG	B	102	1/1	0.82	0.05	60,60,60,60	0
5	IPA	B	101	4/4	0.84	0.20	35,44,48,51	0
4	TRP	A	901	15/15	0.86	0.24	36,47,73,77	0
5	IPA	A	905	4/4	0.87	0.21	38,42,44,51	0
6	MG	C	101	1/1	0.95	0.04	38,38,38,38	0
6	MG	A	906	1/1	0.98	0.08	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.