



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2018 – 01:17 PM EST

PDB ID : 5V54
Title : Crystal structure of 5-HT1B receptor in complex with methiothepin
Authors : Yin, W.C.; Zhou, X.E.; Yang, D.; de Waal, P.; Wang, M.T.; Dai, A.; Cai, X.; Huang, C.Y.; Liu, P.; Yin, Y.; Liu, B.; Caffrey, M.; Melcher, K.; Xu, Y.; Wang, M.W.; Xu, H.E.; Jiang, Y.
Deposited on : 2017-03-13
Resolution : 3.90 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

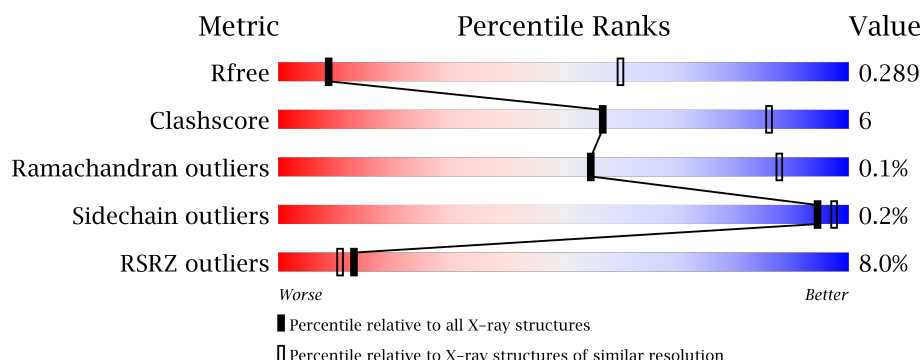
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	100719	1007 (4.20-3.60)
Clashscore	112137	1103 (4.20-3.60)
Ramachandran outliers	110173	1062 (4.20-3.60)
Sidechain outliers	110143	1053 (4.20-3.60)
RSRZ outliers	101464	1020 (4.20-3.60)

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 ≥ 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 $\leq 5\%$. 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	395	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div></div> </div> </div>
1	B	395	<div> <div>9%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div></div> </div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6180 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.

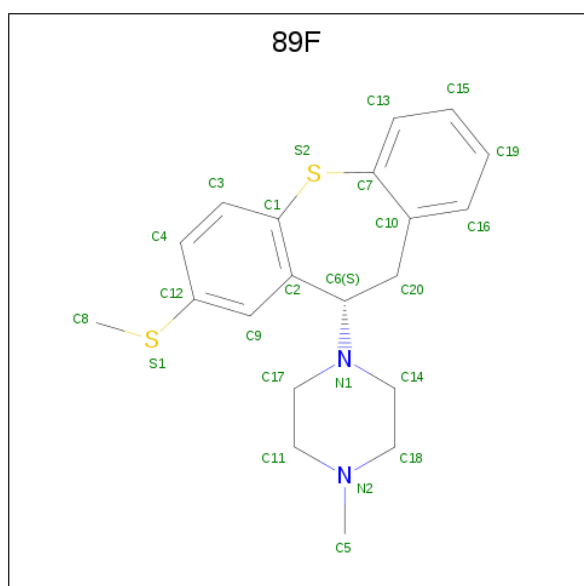
- Molecule 1 is a protein called 5-hydroxytryptamine receptor 1B,OB-1 fused 5-HT1b receptor,5-hydroxytryptamine receptor 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3063	1995	513	538	17			
1	B	383	Total	C	N	O	S	0	0	0
			3069	1998	511	543	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	TRP	LEU	engineered mutation	UNP P28222
B	138	TRP	LEU	engineered mutation	UNP P28222

- Molecule 2 is 1-methyl-4-[(5 {S})-3-methylsulfanyl-5,6-dihydrobenzo[b][1]benzothiepin-5-yl]piperazine (three-letter code: 89F) (formula: C₂₀H₂₄N₂S₂).

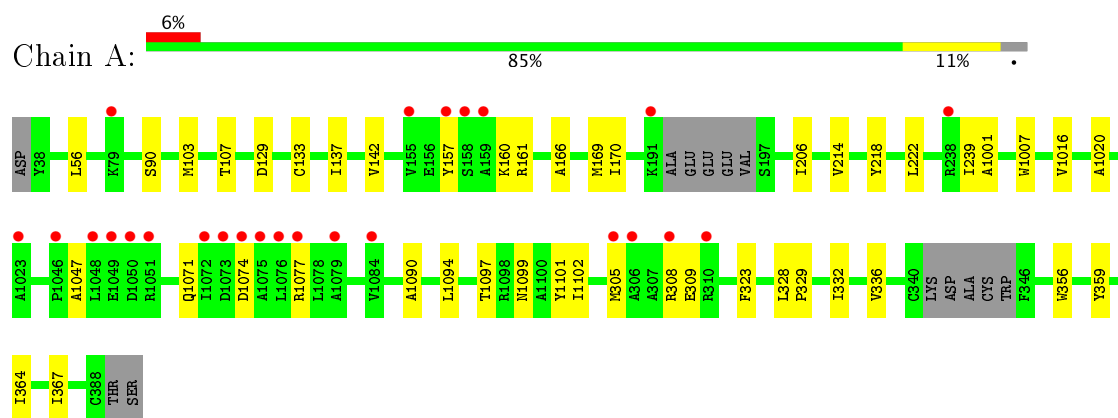


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			24	20	2	2		
2	B	1	Total	C	N	S	0	0
			24	20	2	2		

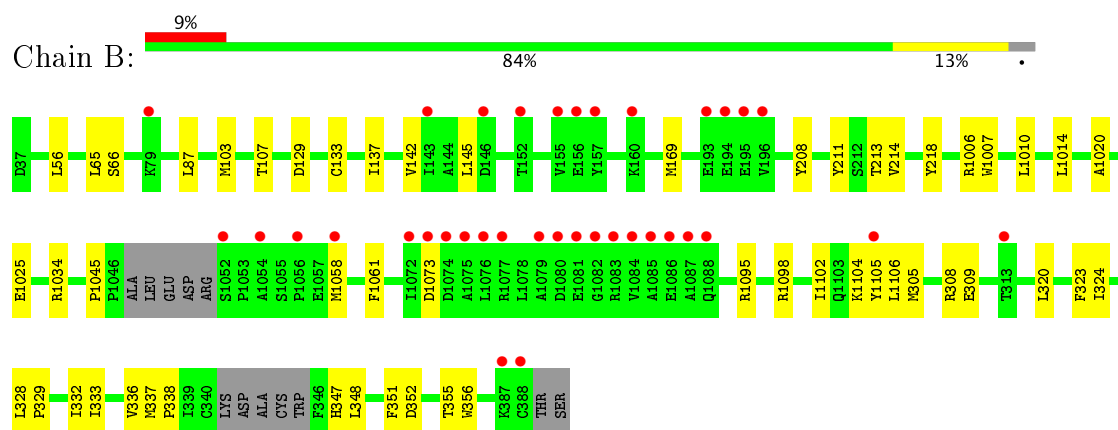
3 Residue-property plots [i](#)

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: 5-hydroxytryptamine receptor 1B,OB-1 fused 5-HT1b receptor,5-hydroxytryptamine receptor 1B



- Molecule 1: 5-hydroxytryptamine receptor 1B,OB-1 fused 5-HT1b receptor,5-hydroxytryptamine receptor 1B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.20 Å 48.83 Å 139.22 Å 90.00° 124.07° 90.00°	Depositor
Resolution (Å)	45.51 – 3.90 47.37 – 3.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (45.51-3.90) 97.8 (47.37-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.88 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.272 , 0.288 0.272 , 0.289	Depositor DCC
R_{free} test set	858 reflections (7.15%)	DCC
Wilson B-factor (Å ²)	152.1	Xtriage
Anisotropy	0.846	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 148.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.107 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6180	wwPDB-VP
Average B, all atoms (Å ²)	201.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.55% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 89F

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	0/3135	0.53	0/4271
1	B	0.28	0/3141	0.53	0/4280
All	All	0.28	0/6276	0.53	0/8551

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

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	3063	0	3109	32	0
1	B	3069	0	3106	40	0
2	A	24	0	0	2	0
2	B	24	0	0	2	0
All	All	6180	0	6215	71	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 6.

All (71) 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:1061:PHE:HE1	1:B:1104:LYS:HE2	1.57	0.69
1:B:1045:PRO:HG2	1:B:1058:MET:CE	2.24	0.68
1:B:1105:TYR:C	1:B:305:MET:H	1.96	0.68
1:A:305:MET:HG2	1:A:308:ARG:CZ	2.26	0.65
1:A:1016:VAL:O	1:A:1020:ALA:N	2.32	0.62
1:A:305:MET:HB3	1:A:308:ARG:HD2	1.80	0.62
1:A:1090:ALA:O	1:A:1094:LEU:HG	2.01	0.61
1:B:348:LEU:HA	1:B:351:PHE:HD2	1.68	0.59
1:B:137:ILE:HG12	1:B:323:PHE:HE2	1.68	0.58
1:B:1045:PRO:HG2	1:B:1058:MET:HE1	1.85	0.58
1:B:337:MET:HB3	1:B:338:PRO:HD3	1.85	0.57
1:A:305:MET:O	1:A:308:ARG:HB2	2.05	0.57
1:B:1102:ILE:HA	1:B:1105:TYR:HB3	1.87	0.56
1:B:352:ASP:O	1:B:355:THR:OG1	2.25	0.54
1:B:145:LEU:HD23	1:B:169:MET:HE3	1.89	0.54
1:A:1097:THR:O	1:A:1101:TYR:HD2	1.90	0.54
1:A:157:TYR:HD1	1:A:160:LYS:HE3	1.73	0.54
1:A:142:VAL:HG22	1:A:169:MET:HE3	1.89	0.54
1:B:103:MET:HG2	1:B:356:TRP:CZ3	2.44	0.53
1:B:333:ILE:HG22	1:B:351:PHE:CE1	2.44	0.53
1:A:166:ALA:O	1:A:170:ILE:HG12	2.09	0.52
1:B:305:MET:HG2	1:B:308:ARG:CZ	2.40	0.51
1:B:1061:PHE:CE1	1:B:1104:LYS:HB3	2.45	0.51
1:B:133:CYS:HB3	2:B:1201:89F:C19	2.41	0.51
1:A:1047:ALA:N	1:A:309:GLU:HG2	2.26	0.50
1:B:208:TYR:HA	1:B:211:TYR:HB3	1.93	0.50
1:B:1098:ARG:HG3	1:B:1102:ILE:HD12	1.94	0.49
1:A:214:VAL:HA	1:A:218:TYR:HB2	1.94	0.49
1:B:87:LEU:HD13	1:B:142:VAL:HG12	1.93	0.49
1:A:56:LEU:HD22	1:A:356:TRP:CD2	2.48	0.49
1:B:137:ILE:HG12	1:B:323:PHE:CE2	2.48	0.49
1:B:1034:ARG:NH1	1:B:1073:ASP:OD1	2.46	0.48
1:B:213:THR:HG22	1:B:218:TYR:CE2	2.48	0.48
1:B:1105:TYR:O	1:B:305:MET:N	2.47	0.48
1:B:329:PRO:HA	1:B:332:ILE:HD12	1.96	0.48
1:B:1007:TRP:NE1	1:B:1102:ILE:HG21	2.28	0.48
1:A:137:ILE:HG12	1:A:323:PHE:CE2	2.49	0.47
1:A:1074:ASP:OD1	1:A:1077:ARG:NH2	2.47	0.47
1:B:1014:LEU:HD21	1:B:1095:ARG:HB2	1.95	0.47
1:B:56:LEU:HB2	1:B:107:THR:HG23	1.96	0.47
1:B:328:LEU:HB3	1:B:329:PRO:HD3	1.95	0.47
1:A:328:LEU:HB3	1:A:329:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:SER:OG	1:A:170:ILE:HD12	2.15	0.47
1:A:1071:GLN:HB3	1:A:1094:LEU:HD21	1.96	0.46
1:B:214:VAL:HA	1:B:218:TYR:HB2	1.97	0.46
1:A:133:CYS:HB3	2:A:1201:89F:C19	2.46	0.45
1:B:320:LEU:O	1:B:324:ILE:HG12	2.15	0.45
1:B:65:LEU:HD12	1:B:66:SER:N	2.31	0.45
1:A:129:ASP:OD2	2:A:1201:89F:N2	2.48	0.45
1:A:305:MET:SD	1:A:308:ARG:NH1	2.90	0.45
1:A:157:TYR:CE2	1:A:161:ARG:HB2	2.52	0.45
1:B:129:ASP:OD2	2:B:1201:89F:N2	2.50	0.44
1:B:1105:TYR:C	1:B:305:MET:N	2.65	0.44
1:B:1020:ALA:HB1	1:B:1025:GLU:HB2	1.99	0.43
1:A:137:ILE:HG12	1:A:323:PHE:HE2	1.83	0.43
1:A:332:ILE:O	1:A:336:VAL:HG23	2.18	0.43
1:A:56:LEU:HB2	1:A:107:THR:HG23	1.99	0.43
1:A:364:ILE:HA	1:A:367:ILE:HG12	2.01	0.43
1:A:103:MET:HE2	1:A:359:TYR:HB3	2.01	0.43
1:B:1006:ARG:O	1:B:1010:LEU:HG	2.18	0.42
1:A:1099:ASN:HA	1:A:1102:ILE:HG22	2.01	0.42
1:A:1007:TRP:HD1	1:A:1102:ILE:HG12	1.84	0.42
1:A:222:LEU:HD13	1:B:218:TYR:CE2	2.55	0.42
1:A:239:ILE:HG13	1:A:1001:ALA:N	2.34	0.42
1:B:333:ILE:HA	1:B:336:VAL:HG22	2.02	0.42
1:B:347:HIS:O	1:B:351:PHE:CD2	2.72	0.42
1:B:1045:PRO:HB2	1:B:309:GLU:HG3	2.02	0.41
1:B:1007:TRP:CD1	1:B:1102:ILE:HG21	2.56	0.41
1:A:305:MET:HG2	1:A:308:ARG:NH1	2.35	0.41
1:B:1061:PHE:CE1	1:B:1104:LYS:HE2	2.47	0.41
1:A:1047:ALA:HB2	1:A:309:GLU:HB2	2.03	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	376/395 (95%)	369 (98%)	7 (2%)	0	100	100
1	B	377/395 (95%)	371 (98%)	5 (1%)	1 (0%)	44	80
All	All	753/790 (95%)	740 (98%)	12 (2%)	1 (0%)	55	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1106	LEU

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	326/337 (97%)	325 (100%)	1 (0%)	94	97
1	B	327/337 (97%)	327 (100%)	0	100	100
All	All	653/674 (97%)	652 (100%)	1 (0%)	94	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ILE

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

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

2 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	89F	A	1201	-	26,27,27	2.79	4 (15%)	30,38,38	1.29	4 (13%)
2	89F	B	1201	-	26,27,27	2.63	4 (15%)	30,38,38	1.29	2 (6%)

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	89F	A	1201	-	-	0/6/28/28	0/3/4/4
2	89F	B	1201	-	-	0/6/28/28	0/3/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	89F	C1-C2	-2.67	1.36	1.40
2	B	1201	89F	C1-C2	-2.29	1.37	1.40
2	B	1201	89F	C12-S1	2.86	1.83	1.76
2	A	1201	89F	C12-S1	2.88	1.83	1.76
2	B	1201	89F	C1-S2	6.35	1.83	1.78
2	A	1201	89F	C1-S2	6.46	1.83	1.78
2	B	1201	89F	C7-S2	10.76	1.87	1.78
2	A	1201	89F	C7-S2	11.47	1.88	1.78

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	89F	C13-C7-S2	-2.15	114.00	118.68
2	B	1201	89F	C13-C7-S2	-2.15	114.00	118.68
2	A	1201	89F	C17-N1-C6	-2.08	109.74	113.28
2	A	1201	89F	C9-C2-C1	2.25	120.49	118.31
2	A	1201	89F	C1-S2-C7	3.79	109.72	99.09
2	B	1201	89F	C1-S2-C7	3.87	109.93	99.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	89F	2	0
2	B	1201	89F	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	382/395 (96%)	-0.06	25 (6%)	20 14	116, 202, 274, 290	0
1	B	383/395 (96%)	0.06	36 (9%)	9 8	116, 190, 270, 291	0
All	All	765/790 (96%)	0.00	61 (7%)	13 11	116, 196, 271, 291	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1049	GLU	8.1
1	B	1075	ALA	6.2
1	A	1050	ASP	6.0
1	B	1080	ASP	5.7
1	A	1048	LEU	5.5
1	A	1076	LEU	5.5
1	B	1084	VAL	5.4
1	B	388	CYS	5.3
1	B	1085	ALA	5.0
1	B	1076	LEU	4.9
1	B	195	GLU	4.9
1	B	193	GLU	4.7
1	B	194	GLU	4.6
1	B	1079	ALA	4.6
1	A	157	TYR	4.5
1	A	191	LYS	4.5
1	A	1072	ILE	4.3
1	B	1074	ASP	4.2
1	A	1046	PRO	4.2
1	A	310	ARG	4.2
1	A	1084	VAL	4.2
1	A	1074	ASP	4.1
1	B	1081	GLU	4.0
1	A	305	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	155	VAL	4.0
1	B	1072	ILE	4.0
1	A	1075	ALA	3.6
1	A	238	ARG	3.4
1	A	159	ALA	3.4
1	B	1082	GLY	3.4
1	B	1056	PRO	3.3
1	B	156	GLU	3.1
1	B	1058	MET	2.9
1	B	160	LYS	2.8
1	B	1073	ASP	2.7
1	A	1077	ARG	2.7
1	B	1083	ARG	2.7
1	A	306	ALA	2.7
1	A	158	SER	2.7
1	A	308	ARG	2.7
1	A	79	LYS	2.6
1	B	146	ASP	2.6
1	A	1023	ALA	2.6
1	B	152	THR	2.5
1	B	1086	GLU	2.5
1	B	157	TYR	2.5
1	B	1077	ARG	2.5
1	B	196	VAL	2.5
1	B	1088	GLN	2.4
1	A	1051	ARG	2.4
1	A	1079	ALA	2.3
1	B	387	LYS	2.3
1	B	79	LYS	2.2
1	B	313	THR	2.2
1	B	1052	SER	2.2
1	A	155	VAL	2.1
1	B	1087	ALA	2.1
1	B	143	ILE	2.1
1	B	1105	TYR	2.1
1	B	1054	ALA	2.0
1	A	1073	ASP	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 [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(\AA^2)	Q<0.9
2	89F	A	1201	24/24	0.88	0.26	0.38	110,154,236,298	0
2	89F	B	1201	24/24	0.87	0.24	0.04	92,163,228,250	0

6.5 Other polymers [i](#)

There are no such residues in this entry.