



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:13 PM GMT

PDB ID : 4BWB
Title : Structure of Evolved Agonist-bound Neurotensin Receptor 1 Mutant without
Lysozyme Fusion
Authors : Egloff, P.; Hillenbrand, M.; Scott, D.J.; Schlinkmann, K.M.; Heine, P.; Balada,
S.; Batyuk, A.; Mittl, P.; Plueckthun, A.
Deposited on : 2013-07-01
Resolution : 3.57 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

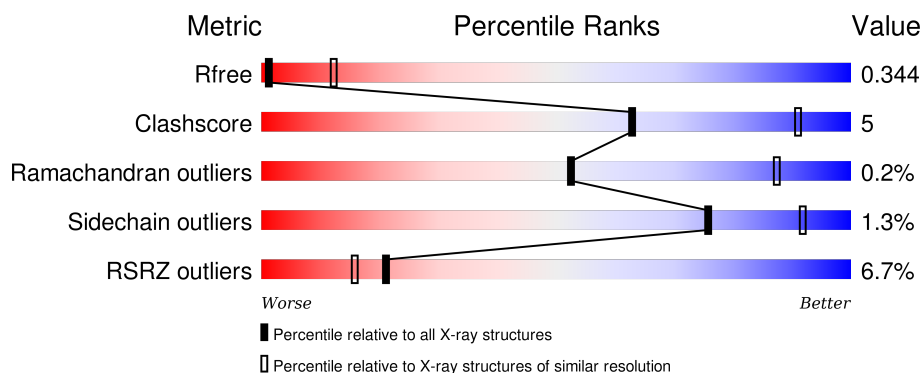
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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}	91344	1261 (3.76-3.40)
Clashscore	102246	1026 (3.72-3.44)
Ramachandran outliers	100387	1028 (3.74-3.42)
Sidechain outliers	100360	1028 (3.74-3.42)
RSRZ outliers	91569	1268 (3.76-3.40)

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	338	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>
1	B	338	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>11%</div> </div> </div>
2	C	10	<div> <div>20%</div> <div> <div></div> <div>30%</div> <div>20%</div> <div>50%</div> </div> </div>
2	D	10	<div> <div></div> <div> <div></div> <div>30%</div> <div>70%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4838 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 NEUROTENSIN RECEPTOR TYPE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2397	1585	388	409	15			
1	B	300	Total	C	N	O	S	0	0	0
			2365	1564	388	400	13			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLY	-	EXPRESSION TAG	UNP P20789
A	47	PRO	-	EXPRESSION TAG	UNP P20789
A	48	GLY	-	EXPRESSION TAG	UNP P20789
A	49	SER	-	EXPRESSION TAG	UNP P20789
A	391	THR	-	EXPRESSION TAG	UNP P20789
A	392	ARG	-	EXPRESSION TAG	UNP P20789
A	393	GLU	-	EXPRESSION TAG	UNP P20789
A	394	LEU	-	EXPRESSION TAG	UNP P20789
A	395	GLU	-	EXPRESSION TAG	UNP P20789
A	396	VAL	-	EXPRESSION TAG	UNP P20789
A	397	LEU	-	EXPRESSION TAG	UNP P20789
A	398	PHE	-	EXPRESSION TAG	UNP P20789
A	399	GLN	-	EXPRESSION TAG	UNP P20789
A	83	GLY	SER	ENGINEERED MUTATION	UNP P20789
A	86	LEU	ALA	ENGINEERED MUTATION	UNP P20789
A	101	ARG	THR	ENGINEERED MUTATION	UNP P20789
A	103	ASP	HIS	ENGINEERED MUTATION	UNP P20789
A	105	TYR	HIS	ENGINEERED MUTATION	UNP P20789
A	119	PHE	LEU	ENGINEERED MUTATION	UNP P20789
A	121	LEU	MET	ENGINEERED MUTATION	UNP P20789
A	124	ASP	GLU	ENGINEERED MUTATION	UNP P20789
A	143	LYS	ARG	ENGINEERED MUTATION	UNP P20789
A	150	GLU	ASP	ENGINEERED MUTATION	UNP P20789
A	161	VAL	ALA	ENGINEERED MUTATION	UNP P20789
A	167	LEU	ARG	ENGINEERED MUTATION	UNP P20789

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Chain	Residue	Modelled	Actual	Comment	Reference
A	213	LEU	ARG	ENGINEERED MUTATION	UNP P20789
A	234	LEU	VAL	ENGINEERED MUTATION	UNP P20789
A	235	ARG	LYS	ENGINEERED MUTATION	UNP P20789
A	240	LEU	VAL	ENGINEERED MUTATION	UNP P20789
A	253	ALA	ILE	ENGINEERED MUTATION	UNP P20789
A	260	ALA	ILE	ENGINEERED MUTATION	UNP P20789
A	262	ARG	ASN	ENGINEERED MUTATION	UNP P20789
A	263	ARG	LYS	ENGINEERED MUTATION	UNP P20789
A	.	-	VAL	DELETION	UNP P20789
A	.	-	GLY	DELETION	UNP P20789
A	.	-	THR	DELETION	UNP P20789
A	.	-	HIS	DELETION	UNP P20789
A	.	-	ASN	DELETION	UNP P20789
A	.	-	GLY	DELETION	UNP P20789
A	.	-	LEU	DELETION	UNP P20789
A	.	-	GLU	DELETION	UNP P20789
A	.	-	HIS	DELETION	UNP P20789
A	.	-	SER	DELETION	UNP P20789
A	.	-	THR	DELETION	UNP P20789
A	.	-	PHE	DELETION	UNP P20789
A	.	-	ASN	DELETION	UNP P20789
A	.	-	MET	DELETION	UNP P20789
A	.	-	THR	DELETION	UNP P20789
A	.	-	ILE	DELETION	UNP P20789
A	305	ARG	HIS	ENGINEERED MUTATION	UNP P20789
A	332	VAL	CYS	ENGINEERED MUTATION	UNP P20789
A	342	ALA	PHE	ENGINEERED MUTATION	UNP P20789
A	354	SER	THR	ENGINEERED MUTATION	UNP P20789
A	358	VAL	PHE	ENGINEERED MUTATION	UNP P20789
A	362	ALA	SER	ENGINEERED MUTATION	UNP P20789
B	46	GLY	-	EXPRESSION TAG	UNP P20789
B	47	PRO	-	EXPRESSION TAG	UNP P20789
B	48	GLY	-	EXPRESSION TAG	UNP P20789
B	49	SER	-	EXPRESSION TAG	UNP P20789
B	391	THR	-	EXPRESSION TAG	UNP P20789
B	392	ARG	-	EXPRESSION TAG	UNP P20789
B	393	GLU	-	EXPRESSION TAG	UNP P20789
B	394	LEU	-	EXPRESSION TAG	UNP P20789
B	395	GLU	-	EXPRESSION TAG	UNP P20789
B	396	VAL	-	EXPRESSION TAG	UNP P20789
B	397	LEU	-	EXPRESSION TAG	UNP P20789
B	398	PHE	-	EXPRESSION TAG	UNP P20789

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Chain	Residue	Modelled	Actual	Comment	Reference
B	399	GLN	-	EXPRESSION TAG	UNP P20789
B	83	GLY	SER	ENGINEERED MUTATION	UNP P20789
B	86	LEU	ALA	ENGINEERED MUTATION	UNP P20789
B	101	ARG	THR	ENGINEERED MUTATION	UNP P20789
B	103	ASP	HIS	ENGINEERED MUTATION	UNP P20789
B	105	TYR	HIS	ENGINEERED MUTATION	UNP P20789
B	119	PHE	LEU	ENGINEERED MUTATION	UNP P20789
B	121	LEU	MET	ENGINEERED MUTATION	UNP P20789
B	124	ASP	GLU	ENGINEERED MUTATION	UNP P20789
B	143	LYS	ARG	ENGINEERED MUTATION	UNP P20789
B	150	GLU	ASP	ENGINEERED MUTATION	UNP P20789
B	161	VAL	ALA	ENGINEERED MUTATION	UNP P20789
B	167	LEU	ARG	ENGINEERED MUTATION	UNP P20789
B	213	LEU	ARG	ENGINEERED MUTATION	UNP P20789
B	234	LEU	VAL	ENGINEERED MUTATION	UNP P20789
B	235	ARG	LYS	ENGINEERED MUTATION	UNP P20789
B	240	LEU	VAL	ENGINEERED MUTATION	UNP P20789
B	253	ALA	ILE	ENGINEERED MUTATION	UNP P20789
B	260	ALA	ILE	ENGINEERED MUTATION	UNP P20789
B	262	ARG	ASN	ENGINEERED MUTATION	UNP P20789
B	263	ARG	LYS	ENGINEERED MUTATION	UNP P20789
B	.	-	VAL	DELETION	UNP P20789
B	.	-	GLY	DELETION	UNP P20789
B	.	-	THR	DELETION	UNP P20789
B	.	-	HIS	DELETION	UNP P20789
B	.	-	ASN	DELETION	UNP P20789
B	.	-	GLY	DELETION	UNP P20789
B	.	-	LEU	DELETION	UNP P20789
B	.	-	GLU	DELETION	UNP P20789
B	.	-	HIS	DELETION	UNP P20789
B	.	-	SER	DELETION	UNP P20789
B	.	-	THR	DELETION	UNP P20789
B	.	-	PHE	DELETION	UNP P20789
B	.	-	ASN	DELETION	UNP P20789
B	.	-	MET	DELETION	UNP P20789
B	.	-	THR	DELETION	UNP P20789
B	.	-	ILE	DELETION	UNP P20789
B	305	ARG	HIS	ENGINEERED MUTATION	UNP P20789
B	332	VAL	CYS	ENGINEERED MUTATION	UNP P20789
B	342	ALA	PHE	ENGINEERED MUTATION	UNP P20789
B	354	SER	THR	ENGINEERED MUTATION	UNP P20789
B	358	VAL	PHE	ENGINEERED MUTATION	UNP P20789

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Chain	Residue	Modelled	Actual	Comment	Reference
B	362	ALA	SER	ENGINEERED MUTATION	UNP P20789

- Molecule 2 is a protein called NEUROTENSIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			49	32	11	6			
2	D	3	Total	C	N	O	0	0	0
			27	20	3	4			

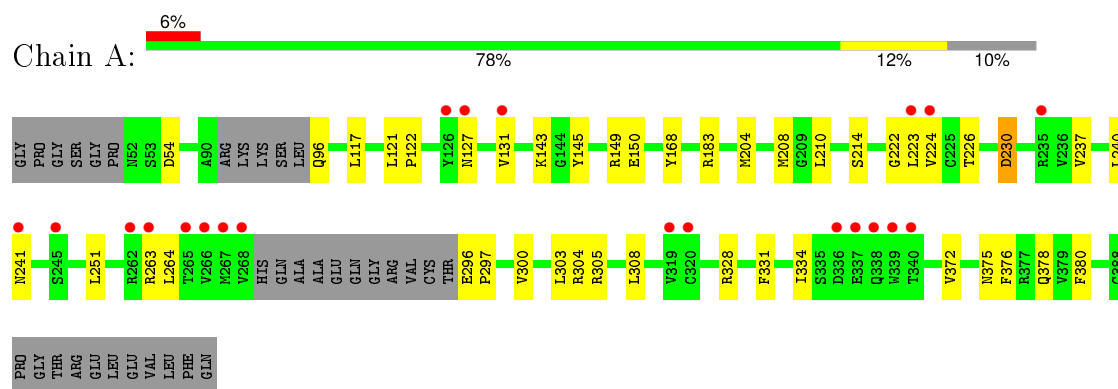
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	GLY	-	EXPRESSION TAG	UNP P20068
C	5	PRO	-	EXPRESSION TAG	UNP P20068
C	6	GLY	-	EXPRESSION TAG	UNP P20068
C	7	GLY	-	EXPRESSION TAG	UNP P20068
D	4	GLY	-	EXPRESSION TAG	UNP P20068
D	5	PRO	-	EXPRESSION TAG	UNP P20068
D	6	GLY	-	EXPRESSION TAG	UNP P20068
D	7	GLY	-	EXPRESSION TAG	UNP P20068

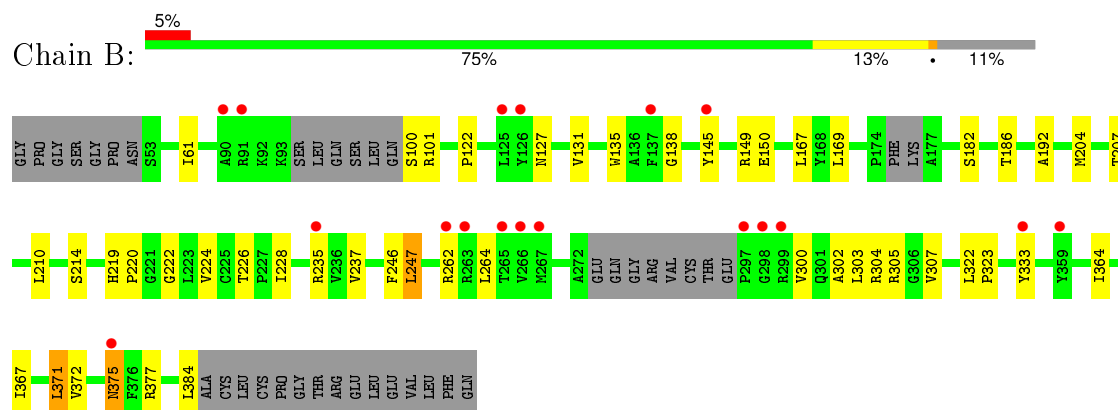
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

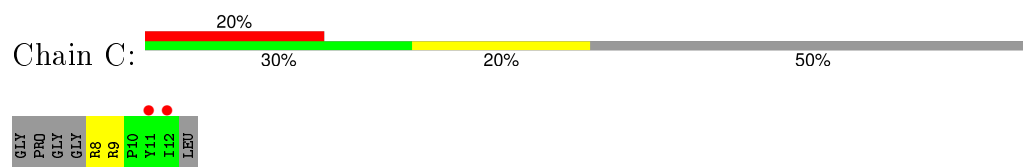
• Molecule 1: NEUROTENSIN RECEPTOR TYPE 1



• Molecule 1: NEUROTENSIN RECEPTOR TYPE 1



• Molecule 2: NEUROTENSIN



• Molecule 2: NEUROTENSIN



GLY	PRO	GLY	GLY	ARG	P10	Y11	I12	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.88Å 90.89Å 211.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.88 – 3.57 49.19 – 3.57	Depositor EDS
% Data completeness (in resolution range)	89.4 (21.88-3.57) 89.6 (49.19-3.57)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.309 , 0.345 0.317 , 0.344	Depositor DCC
R_{free} test set	649 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	174.9	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 124.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 13044 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	4838	wwPDB-VP
Average B, all atoms (Å ²)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.22	0/2455	0.41	0/3352
1	B	0.23	0/2422	0.41	0/3303
2	C	0.17	0/50	0.40	0/66
2	D	0.19	0/28	0.35	0/37
All	All	0.22	0/4955	0.41	0/6758

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	2397	0	2455	27	0
1	B	2365	0	2433	28	0
2	C	49	0	52	3	0
2	D	27	0	27	0	0
All	All	4838	0	4967	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 5.

The worst 5 of 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:150:GLU:HG3	1:B:204:MET:HG3	1.66	0.77
1:A:150:GLU:HG3	1:A:204:MET:HG3	1.76	0.68
1:B:167:LEU:HD21	1:B:307:VAL:HG22	1.77	0.67
1:A:264:LEU:HD21	1:A:304:ARG:HG2	1.78	0.65
1:A:168:TYR:OH	1:A:263:ARG:NH1	2.34	0.61

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	299/338 (88%)	287 (96%)	12 (4%)	0	100	100
1	B	292/338 (86%)	286 (98%)	5 (2%)	1 (0%)	46	83
2	C	3/10 (30%)	3 (100%)	0	0	100	100
2	D	1/10 (10%)	1 (100%)	0	0	100	100
All	All	595/696 (86%)	577 (97%)	17 (3%)	1 (0%)	52	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	247	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	261/288 (91%)	258 (99%)	3 (1%)	80	92
1	B	256/288 (89%)	252 (98%)	4 (2%)	70	90
2	C	5/7 (71%)	5 (100%)	0	100	100
2	D	3/7 (43%)	3 (100%)	0	100	100
All	All	525/590 (89%)	518 (99%)	7 (1%)	76	92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	122	PRO
1	B	384	LEU
1	B	371	LEU
1	A	230	ASP
1	B	375	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	159	ASN
1	A	239	GLN
1	A	365	ASN
1	B	133	HIS

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 [i](#)

There are no ligands in this entry.

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	305/338 (90%)	-0.02	21 (6%) 20 15	97, 175, 288, 472	0
1	B	300/338 (88%)	-0.20	18 (6%) 25 19	109, 175, 294, 381	0
2	C	5/10 (50%)	1.73	2 (40%) 0 1	146, 158, 208, 215	0
2	D	3/10 (30%)	-0.51	0 100 100	140, 140, 175, 202	0
All	All	613/696 (88%)	-0.10	41 (6%) 21 16	97, 175, 294, 472	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	VAL	5.7
1	A	337	GLU	5.2
2	C	11	TYR	5.0
1	A	265	THR	4.8
1	A	338	GLN	4.5

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.