



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:07 am GMT

PDB ID : 2PR9
Title : Mu2 adaptin subunit (AP50) of AP2 adaptor (second domain), complexed with GABAA receptor-gamma2 subunit-derived internalization peptide DEEY-GYECL
Authors : Vahedi-Faridi, A.; Haucke, V.; Kittler, J.T.; Kukhtina, V.; Moss, S.J.; Saenger, W.; Chen, G.-J.; Tretter, V.; Smith, K.; Yan, Z.; McAinsh, K.; Arancibia-Carcamo, L.
Deposited on : 2007-05-04
Resolution : 2.51 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

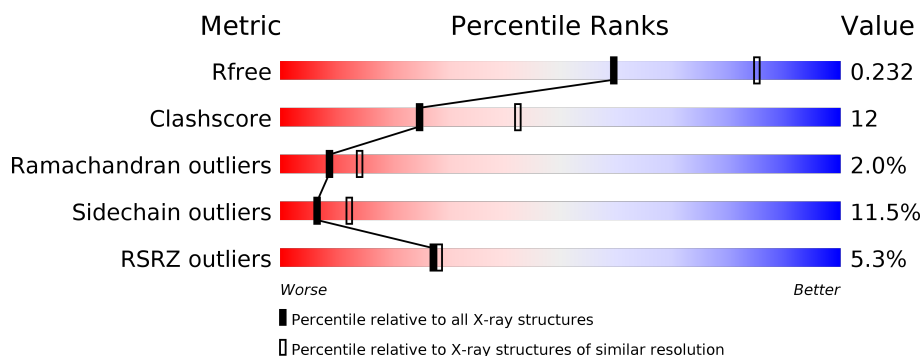
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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	299	<div> <div>4%</div> <div>60%</div> <div>19%</div> <div>• •</div> <div>15%</div> </div>
2	P	10	<div> <div>30%</div> <div>10%</div> <div>50%</div> <div>10%</div> <div>30%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2174 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 AP-2 complex subunit mu-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	2029	1305	353	357	14	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	MET	-	EXPRESSION TAG	UNP P84092
A	138	GLY	-	EXPRESSION TAG	UNP P84092
A	139	SER	-	EXPRESSION TAG	UNP P84092
A	140	SER	-	EXPRESSION TAG	UNP P84092
A	141	HIS	-	EXPRESSION TAG	UNP P84092
A	142	HIS	-	EXPRESSION TAG	UNP P84092
A	143	HIS	-	EXPRESSION TAG	UNP P84092
A	144	HIS	-	EXPRESSION TAG	UNP P84092
A	145	HIS	-	EXPRESSION TAG	UNP P84092
A	146	HIS	-	EXPRESSION TAG	UNP P84092
A	147	SER	-	EXPRESSION TAG	UNP P84092
A	148	SER	-	EXPRESSION TAG	UNP P84092
A	149	GLY	-	EXPRESSION TAG	UNP P84092
A	150	LEU	-	EXPRESSION TAG	UNP P84092
A	151	VAL	-	EXPRESSION TAG	UNP P84092
A	152	PRO	-	EXPRESSION TAG	UNP P84092
A	153	ARG	-	EXPRESSION TAG	UNP P84092
A	154	GLY	-	EXPRESSION TAG	UNP P84092
A	155	SER	-	EXPRESSION TAG	UNP P84092
A	156	HIS	-	EXPRESSION TAG	UNP P84092
A	157	MET	-	EXPRESSION TAG	UNP P84092

- Molecule 2 is a protein called GABA(A) receptor subunit gamma-2 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	S	0	0	0
			86	52	10	23	1			

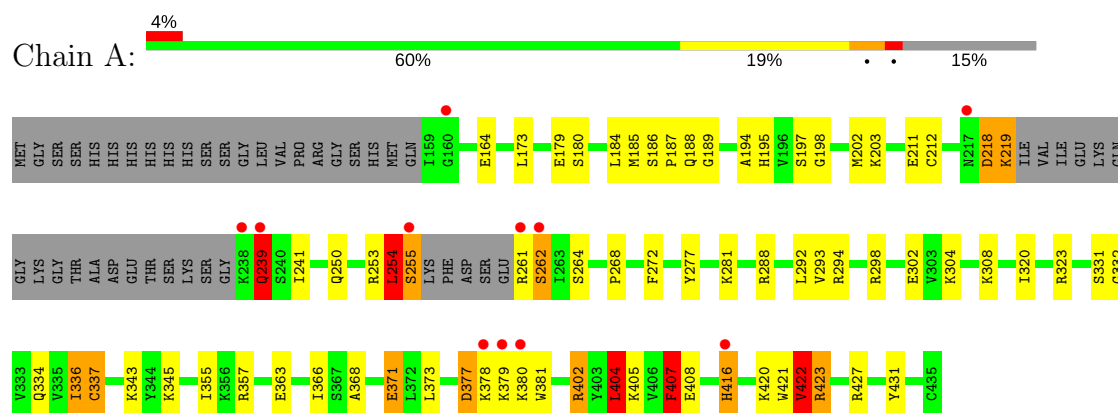
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	P	5	Total	O	0	0
			5	5		

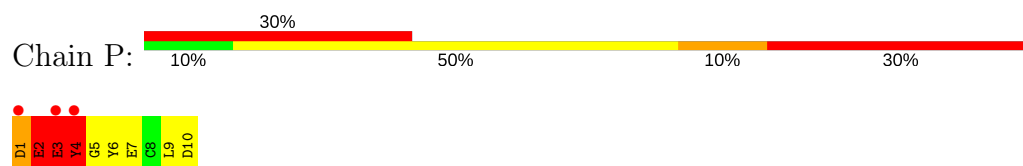
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: AP-2 complex subunit mu-1



- Molecule 2: GABA(A) receptor subunit gamma-2 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	126.30Å 126.30Å 74.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.97 – 2.51 9.97 – 2.51	Depositor EDS
% Data completeness (in resolution range)	100.0 (9.97-2.51) 99.7 (9.97-2.51)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.240 0.195 , 0.232	Depositor DCC
R_{free} test set	913 reflections (4.17%)	DCC
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2174	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

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	1.75	27/2070 (1.3%)	1.29	17/2786 (0.6%)
2	P	1.92	1/87 (1.1%)	1.66	1/115 (0.9%)
All	All	1.75	28/2157 (1.3%)	1.30	18/2901 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	P	0	2
All	All	0	4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	SER	C-O	31.73	1.83	1.23
1	A	219	LYS	C-O	21.06	1.63	1.23
1	A	261	ARG	NE-CZ	11.54	1.48	1.33
1	A	261	ARG	CZ-NH2	10.54	1.46	1.33
1	A	255	SER	CA-C	9.48	1.77	1.52
1	A	261	ARG	CG-CD	8.67	1.73	1.51
1	A	431	TYR	CD2-CE2	8.06	1.51	1.39
1	A	261	ARG	CZ-NH1	8.03	1.43	1.33
1	A	211	GLU	CB-CG	-7.14	1.38	1.52
1	A	323	ARG	CB-CG	-6.75	1.34	1.52
1	A	254	LEU	C-O	6.50	1.35	1.23
1	A	381	TRP	CB-CG	6.20	1.61	1.50
2	P	4	TYR	CD2-CE2	6.07	1.48	1.39
1	A	407	PHE	CG-CD1	5.93	1.47	1.38
1	A	323	ARG	CG-CD	5.91	1.66	1.51
1	A	343	LYS	CD-CE	5.90	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	PHE	CE1-CZ	5.87	1.48	1.37
1	A	211	GLU	CD-OE1	5.86	1.32	1.25
1	A	261	ARG	CD-NE	5.83	1.56	1.46
1	A	179	GLU	CD-OE1	5.66	1.31	1.25
1	A	304	LYS	CD-CE	5.47	1.65	1.51
1	A	337	CYS	CB-SG	-5.45	1.73	1.81
1	A	180	SER	CB-OG	-5.42	1.35	1.42
1	A	427	ARG	NE-CZ	5.36	1.40	1.33
1	A	407	PHE	CB-CG	5.29	1.60	1.51
1	A	427	ARG	CZ-NH1	5.24	1.39	1.33
1	A	407	PHE	CD1-CE1	5.21	1.49	1.39
1	A	239	GLN	CB-CG	5.14	1.66	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	SER	CA-C-O	-12.71	93.40	120.10
1	A	261	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	A	427	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	219	LYS	CA-C-O	-8.54	102.17	120.10
2	P	3	GLU	N-CA-C	8.27	133.32	111.00
1	A	404	LEU	CA-CB-CG	-7.80	97.36	115.30
1	A	336	ILE	CG1-CB-CG2	-7.70	94.47	111.40
1	A	422	VAL	CB-CA-C	-7.10	97.91	111.40
1	A	241	ILE	N-CA-C	6.48	128.49	111.00
1	A	261	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	211	GLU	OE1-CD-OE2	6.08	130.59	123.30
1	A	218	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	253	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	189	GLY	N-CA-C	5.63	127.18	113.10
1	A	323	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	402	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	202	MET	CG-SD-CE	5.18	108.49	100.20
1	A	423	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	ASP	Peptide
1	A	262	SER	Peptide
2	P	2	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	P	3	GLU	Peptide

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	2029	0	2095	42	0
2	P	86	0	65	14	0
3	A	54	0	0	13	1
3	P	5	0	0	0	0
All	All	2174	0	2160	52	1

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 12.

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:A:255:SER:C	1:A:255:SER:CA	1.77	1.49
1:A:255:SER:C	1:A:255:SER:O	1.83	1.14
1:A:185:MET:HE2	3:A:479:HOH:O	1.68	0.91
2:P:5:GLY:H	2:P:6:TYR:HA	1.37	0.90
1:A:402:ARG:HD2	3:A:474:HOH:O	1.78	0.80
2:P:2:GLU:O	2:P:3:GLU:HG3	1.87	0.75
2:P:4:TYR:HB3	2:P:5:GLY:HA3	1.67	0.74
1:A:185:MET:CE	3:A:479:HOH:O	2.32	0.73
1:A:254:LEU:H	1:A:254:LEU:HD22	1.53	0.72
1:A:345:LYS:HD2	3:A:453:HOH:O	1.88	0.72
1:A:173:LEU:HD22	1:A:404:LEU:HD22	1.69	0.71
2:P:5:GLY:N	2:P:6:TYR:HA	2.02	0.71
1:A:173:LEU:CD2	1:A:404:LEU:HD22	2.22	0.70
1:A:416:HIS:HB3	3:A:446:HOH:O	1.92	0.69
2:P:5:GLY:H	2:P:6:TYR:CA	2.09	0.65
1:A:421:TRP:HB3	2:P:6:TYR:HB3	1.79	0.65
2:P:5:GLY:N	2:P:6:TYR:CA	2.62	0.62
1:A:294:ARG:NH1	1:A:302:GLU:HG3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:CYS:HA	1:A:405:LYS:O	2.00	0.60
2:P:4:TYR:CB	2:P:5:GLY:HA3	2.33	0.57
1:A:422:VAL:HG22	2:P:9:LEU:HB2	1.86	0.57
1:A:255:SER:CB	1:A:255:SER:C	2.72	0.52
1:A:308:LYS:HG2	1:A:363:GLU:HG3	1.92	0.51
1:A:377:ASP:CB	3:A:472:HOH:O	2.59	0.51
1:A:281:LYS:CG	3:A:466:HOH:O	2.58	0.51
2:P:1:ASP:O	2:P:2:GLU:HG3	2.11	0.51
1:A:194:ALA:O	1:A:195:HIS:HB3	2.11	0.50
1:A:332:GLY:O	1:A:371:GLU:HG3	2.12	0.50
2:P:1:ASP:O	2:P:2:GLU:CG	2.60	0.49
1:A:268:PRO:HD2	1:A:272:PHE:CE1	2.48	0.49
1:A:239:GLN:CG	1:A:402:ARG:HH22	2.25	0.49
1:A:239:GLN:HG2	1:A:402:ARG:HH22	1.78	0.48
1:A:337:CYS:HB3	1:A:366:ILE:HG13	1.94	0.48
1:A:407:PHE:HB3	3:A:455:HOH:O	2.12	0.48
1:A:186:SER:HB2	1:A:187:PRO:CD	2.44	0.47
1:A:255:SER:O	1:A:255:SER:CA	2.62	0.47
1:A:334:GLN:O	1:A:368:ALA:HA	2.15	0.47
1:A:377:ASP:HB3	3:A:472:HOH:O	2.14	0.47
1:A:423:ARG:HG2	2:P:6:TYR:CE1	2.50	0.46
1:A:423:ARG:HD3	2:P:5:GLY:HA2	1.97	0.46
3:A:478:HOH:O	2:P:7:GLU:HG3	2.17	0.45
1:A:377:ASP:HB2	3:A:472:HOH:O	2.19	0.43
1:A:239:GLN:HG2	1:A:402:ARG:HH12	1.84	0.43
1:A:404:LEU:O	1:A:420:LYS:HE2	2.19	0.43
1:A:198:GLY:HA3	1:A:277:TYR:CZ	2.54	0.42
1:A:173:LEU:HD21	1:A:404:LEU:HD22	1.98	0.42
1:A:357:ARG:HB3	3:A:485:HOH:O	2.19	0.42
1:A:331:SER:HB3	1:A:373:LEU:HG	2.01	0.42
1:A:250:GLN:HB2	3:A:442:HOH:O	2.19	0.42
1:A:268:PRO:HD2	1:A:272:PHE:CD1	2.56	0.41
1:A:336:ILE:HD13	1:A:336:ILE:HG21	1.64	0.41
1:A:320:ILE:HB	1:A:355:ILE:HB	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:463:HOH:O	3:A:463:HOH:O[4_565]	2.08	0.12

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	248/299 (83%)	237 (96%)	8 (3%)	3 (1%)	15	27
2	P	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0	0
All	All	256/309 (83%)	241 (94%)	10 (4%)	5 (2%)	9	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	3	GLU
1	A	254	LEU
1	A	239	GLN
1	A	378	LYS
2	P	2	GLU

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	225/268 (84%)	202 (90%)	23 (10%)	8	16
2	P	9/9 (100%)	5 (56%)	4 (44%)	0	0
All	All	234/277 (84%)	207 (88%)	27 (12%)	6	12

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	GLU

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Mol	Chain	Res	Type
1	A	184	LEU
1	A	188	GLN
1	A	197	SER
1	A	203	LYS
1	A	219	LYS
1	A	239	GLN
1	A	254	LEU
1	A	262	SER
1	A	264	SER
1	A	288	ARG
1	A	292	LEU
1	A	293	VAL
1	A	298	ARG
1	A	371	GLU
1	A	377	ASP
1	A	379	LYS
1	A	380	LYS
1	A	404	LEU
1	A	407	PHE
1	A	408	GLU
1	A	416	HIS
1	A	422	VAL
2	P	1	ASP
2	P	3	GLU
2	P	4	TYR
2	P	10	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	250	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 [i](#)

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	254/299 (84%)	-0.22	11 (4%) 36 38	36, 49, 67, 94	0
2	P	10/10 (100%)	1.10	3 (30%) 1 0	46, 56, 70, 72	0
All	All	264/309 (85%)	-0.17	14 (5%) 27 28	36, 50, 67, 94	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	LYS	4.8
1	A	239	GLN	3.9
1	A	416	HIS	3.2
1	A	378	LYS	3.2
1	A	255	SER	2.9
1	A	261	ARG	2.8
1	A	379	LYS	2.8
2	P	4	TYR	2.8
1	A	160	GLY	2.6
2	P	3	GLU	2.5
1	A	262	SER	2.2
1	A	217	ASN	2.2
1	A	380	LYS	2.1
2	P	1	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.