



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 09:11 AM EDT

PDB ID : 3H85  
Title : Molecular basis for the association of PIPKI gamma-p90 with the clathrin adaptor AP-2  
Authors : Vahedi-Faridi, A.; Kahlfeldt, N.; Schaefer, J.G.; Haucke, V.  
Deposited on : 2009-04-28  
Resolution : 2.60 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](mailto: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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
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

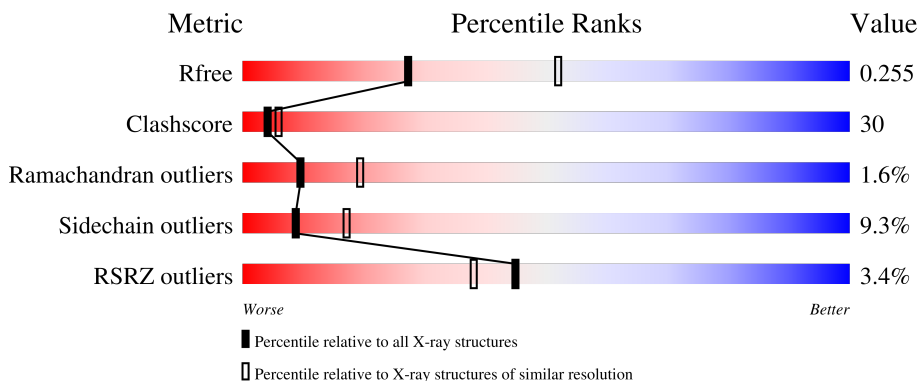
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	
2	P	8	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2142 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	253	2039	1311	359	355	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 Phosphatidylinositol-4-phosphate 5-kinase type-1 gamma.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	0	0	0
			71	48	11	12			

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

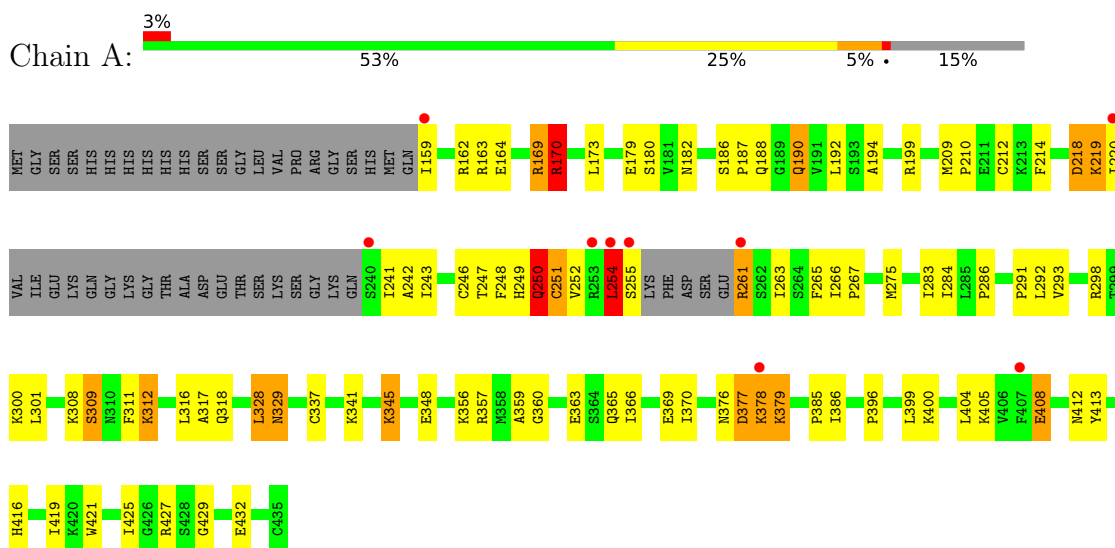
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		

### 3 Residue-property plots

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: AP-2 complex subunit mu-1



- Molecule 2: Phosphatidylinositol-4-phosphate 5-kinase type-1 gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.30Å 125.30Å 74.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.01 – 2.60 43.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.6 (41.01-2.60) 92.6 (43.87-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.61Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.231 , 0.263 0.233 , 0.255	Depositor DCC
$R_{free}$ test set	792 reflections (4.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.43	1/2080 (0.0%)	0.58	0/2796
2	P	0.55	0/75	0.62	0/102
All	All	0.44	1/2155 (0.0%)	0.58	0/2898

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	CYS	CB-SG	-5.38	1.73	1.81

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	2039	0	2132	126	0
2	P	71	0	65	5	0
3	A	1	0	0	0	0
4	A	31	0	0	9	0
All	All	2142	0	2197	128	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 30.

All (128) 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:261:ARG:O	1:A:261:ARG:HD3	1.45	1.16
1:A:248:PHE:HB3	1:A:252:VAL:HG11	1.19	1.14
1:A:399:LEU:HD23	1:A:400:LYS:N	1.67	1.09
1:A:425:ILE:HG12	2:P:1:SER:HA	1.35	1.05
1:A:399:LEU:HD23	1:A:399:LEU:C	1.77	1.05
1:A:312:LYS:N	1:A:312:LYS:HD3	1.69	1.04
1:A:248:PHE:CB	1:A:252:VAL:HG11	1.88	1.03
1:A:312:LYS:H	1:A:312:LYS:CD	1.71	1.00
1:A:248:PHE:HB3	1:A:252:VAL:CG1	1.91	0.99
1:A:169:ARG:CB	1:A:169:ARG:HH11	1.76	0.98
1:A:169:ARG:HH11	1:A:169:ARG:CG	1.78	0.95
1:A:214:PHE:HE2	1:A:275:MET:CE	1.80	0.94
1:A:379:LYS:H	1:A:379:LYS:HD3	1.34	0.91
1:A:254:LEU:HD23	1:A:254:LEU:H	1.36	0.90
1:A:312:LYS:N	1:A:312:LYS:CD	2.34	0.84
4:A:31:HOH:O	2:P:8:HIS:HE1	1.60	0.84
1:A:400:LYS:CE	4:A:24:HOH:O	2.24	0.84
1:A:329:ASN:HD22	1:A:329:ASN:H	1.28	0.81
1:A:186:SER:HB3	1:A:192:LEU:HD11	1.65	0.79
1:A:328:LEU:H	1:A:328:LEU:CD2	1.96	0.78
1:A:400:LYS:HE2	4:A:24:HOH:O	1.83	0.78
1:A:261:ARG:HD3	1:A:261:ARG:C	2.03	0.78
1:A:169:ARG:HH11	1:A:169:ARG:HG2	1.47	0.78
1:A:180:SER:HA	1:A:427:ARG:O	1.84	0.77
1:A:328:LEU:H	1:A:328:LEU:HD22	1.49	0.77
1:A:311:PHE:HB2	1:A:312:LYS:HE3	1.67	0.76
1:A:399:LEU:C	1:A:399:LEU:CD2	2.50	0.76
1:A:328:LEU:HD22	1:A:328:LEU:N	2.02	0.75
1:A:164:GLU:HA	1:A:209:MET:CE	2.17	0.74
1:A:255:SER:CB	1:A:261:ARG:HB2	2.18	0.74
1:A:400:LYS:HE3	4:A:24:HOH:O	1.87	0.74
1:A:169:ARG:CB	1:A:169:ARG:NH1	2.50	0.74
1:A:218:ASP:CG	1:A:218:ASP:O	2.25	0.74
1:A:214:PHE:HE2	1:A:275:MET:HE2	1.53	0.72
1:A:219:LYS:NZ	1:A:219:LYS:HB3	2.07	0.69
1:A:169:ARG:O	1:A:170:ARG:CB	2.41	0.69
1:A:214:PHE:CE2	1:A:275:MET:CE	2.71	0.68
1:A:292:LEU:HD23	1:A:292:LEU:C	2.15	0.67
1:A:249:HIS:O	1:A:252:VAL:HG12	1.94	0.67
1:A:219:LYS:NZ	1:A:219:LYS:CB	2.57	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LYS:NZ	1:A:363:GLU:OE1	2.28	0.67
1:A:169:ARG:NH1	1:A:169:ARG:HB2	2.10	0.66
1:A:214:PHE:CE2	1:A:275:MET:HE2	2.30	0.66
1:A:309:SER:HB2	1:A:360:GLY:HA2	1.78	0.66
1:A:214:PHE:HE2	1:A:275:MET:HE1	1.58	0.66
1:A:219:LYS:HB3	1:A:219:LYS:HZ3	1.59	0.66
1:A:169:ARG:HG2	1:A:169:ARG:NH1	2.11	0.65
1:A:312:LYS:H	1:A:312:LYS:CE	2.09	0.65
1:A:254:LEU:HD23	1:A:254:LEU:N	2.08	0.64
1:A:248:PHE:CB	1:A:252:VAL:CG1	2.64	0.64
1:A:210:PRO:O	1:A:266:ILE:HG12	1.98	0.63
1:A:399:LEU:HD23	1:A:400:LYS:CA	2.28	0.63
1:A:170:ARG:HH21	1:A:419:ILE:HD13	1.62	0.62
1:A:377:ASP:OD1	1:A:377:ASP:N	2.33	0.61
1:A:291:PRO:HB3	1:A:386:ILE:HD12	1.83	0.60
1:A:163:ARG:O	1:A:209:MET:CE	2.49	0.60
1:A:249:HIS:O	1:A:251:CYS:N	2.34	0.60
1:A:365:GLN:O	1:A:365:GLN:HG3	2.01	0.60
1:A:252:VAL:HG21	1:A:263:ILE:HG23	1.85	0.59
1:A:163:ARG:O	1:A:209:MET:HE1	2.04	0.58
1:A:248:PHE:CG	1:A:252:VAL:HG11	2.40	0.57
1:A:220:ILE:HG12	1:A:242:ALA:HA	1.88	0.56
1:A:261:ARG:C	1:A:261:ARG:CD	2.72	0.56
1:A:179:GLU:OE1	1:A:396:PRO:HD2	2.06	0.56
1:A:427:ARG:HD3	4:A:25:HOH:O	2.05	0.56
1:A:255:SER:HB3	1:A:261:ARG:HB2	1.87	0.55
1:A:164:GLU:HA	1:A:209:MET:HE3	1.90	0.54
1:A:345:LYS:HD3	1:A:348:GLU:OE1	2.07	0.54
1:A:284:ILE:O	1:A:286:PRO:HD3	2.08	0.53
1:A:218:ASP:O	1:A:220:ILE:HG13	2.09	0.53
1:A:249:HIS:ND1	1:A:251:CYS:HB3	2.23	0.53
1:A:328:LEU:CD2	1:A:328:LEU:N	2.62	0.51
1:A:214:PHE:CE2	1:A:275:MET:HE1	2.42	0.51
1:A:169:ARG:O	1:A:170:ARG:HB3	2.12	0.50
1:A:170:ARG:HE	1:A:419:ILE:HD12	1.77	0.50
1:A:421:TRP:HB3	2:P:4:TYR:HB3	1.93	0.50
1:A:159:ILE:HG23	1:A:159:ILE:O	2.11	0.50
1:A:190:GLN:O	1:A:192:LEU:HD13	2.11	0.50
1:A:318:GLN:NE2	2:P:2:TRP:CZ2	2.79	0.50
1:A:241:ILE:HD11	1:A:243:ILE:HD11	1.93	0.50
1:A:300:LYS:HD2	1:A:369:GLU:HG2	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASN:OD1	1:A:378:LYS:HB2	2.12	0.49
1:A:219:LYS:CB	1:A:219:LYS:HZ2	2.23	0.49
1:A:404:LEU:C	1:A:404:LEU:HD23	2.32	0.49
1:A:379:LYS:HD3	1:A:379:LYS:N	2.16	0.49
1:A:317:ALA:O	1:A:357:ARG:HA	2.13	0.48
1:A:164:GLU:HA	1:A:209:MET:HE2	1.97	0.47
1:A:163:ARG:O	1:A:209:MET:HE2	2.13	0.47
1:A:173:LEU:C	1:A:173:LEU:HD12	2.35	0.47
1:A:212:CYS:HA	1:A:405:LYS:O	2.14	0.47
1:A:329:ASN:H	1:A:329:ASN:ND2	2.05	0.47
1:A:218:ASP:C	1:A:220:ILE:N	2.67	0.47
1:A:412:ASN:OD1	1:A:413:TYR:N	2.48	0.47
1:A:376:ASN:HB3	1:A:379:LYS:NZ	2.31	0.46
1:A:292:LEU:HD23	1:A:293:VAL:N	2.31	0.46
1:A:252:VAL:HA	1:A:265:PHE:HB3	1.98	0.45
1:A:292:LEU:C	1:A:292:LEU:CD2	2.84	0.45
1:A:241:ILE:HD12	1:A:243:ILE:HD12	1.98	0.45
1:A:219:LYS:HZ2	1:A:219:LYS:HB2	1.81	0.45
1:A:408:GLU:O	4:A:3:HOH:O	2.21	0.45
1:A:190:GLN:O	1:A:192:LEU:CD1	2.65	0.45
1:A:192:LEU:CD1	1:A:192:LEU:N	2.80	0.44
1:A:298:ARG:NH1	1:A:377:ASP:HB3	2.32	0.44
1:A:301:LEU:HB2	1:A:370:ILE:HB	1.98	0.44
1:A:316:LEU:HD21	1:A:357:ARG:HD2	2.00	0.44
1:A:169:ARG:O	1:A:170:ARG:HB2	2.18	0.43
1:A:311:PHE:HB2	1:A:312:LYS:CE	2.42	0.43
1:A:316:LEU:HD12	1:A:359:ALA:HA	2.01	0.43
1:A:283:ILE:HG22	1:A:284:ILE:N	2.33	0.43
1:A:329:ASN:HD22	1:A:329:ASN:N	2.04	0.43
1:A:173:LEU:HD12	1:A:173:LEU:O	2.19	0.43
1:A:429:GLY:HA2	4:A:26:HOH:O	2.18	0.43
1:A:162:ARG:HD2	1:A:267:PRO:O	2.18	0.42
1:A:283:ILE:CG2	1:A:284:ILE:N	2.81	0.42
1:A:190:GLN:HG2	1:A:192:LEU:CD1	2.49	0.42
1:A:385:PRO:HB2	1:A:432:GLU:HB3	2.02	0.42
1:A:376:ASN:HB3	1:A:379:LYS:HZ1	1.85	0.42
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.79	0.42
1:A:247:THR:HG22	4:A:436:HOH:O	2.20	0.42
1:A:169:ARG:C	1:A:169:ARG:HD3	2.41	0.41
1:A:255:SER:OG	1:A:261:ARG:HB2	2.19	0.41
1:A:199:ARG:HA	1:A:275:MET:O	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:CYS:HB3	1:A:366:ILE:HG13	2.03	0.41
1:A:312:LYS:H	1:A:312:LYS:HE3	1.84	0.41
1:A:182:ASN:O	1:A:194:ALA:HA	2.20	0.40
1:A:187:PRO:HD2	1:A:188:GLN:OE1	2.21	0.40
1:A:250:GLN:N	4:A:12:HOH:O	2.36	0.40
2:P:7:LEU:HA	2:P:7:LEU:HD12	1.74	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	247/299 (83%)	229 (93%)	14 (6%)	4 (2%)	9	19
2	P	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	253/307 (82%)	234 (92%)	15 (6%)	4 (2%)	9	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	LEU
1	A	250	GLN
1	A	378	LYS
1	A	170	ARG

### 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	229/268 (85%)	209 (91%)	20 (9%)	10	20
2	P	8/8 (100%)	6 (75%)	2 (25%)	0	1
All	All	237/276 (86%)	215 (91%)	22 (9%)	9	17

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	170	ARG
1	A	190	GLN
1	A	218	ASP
1	A	219	LYS
1	A	250	GLN
1	A	251	CYS
1	A	254	LEU
1	A	261	ARG
1	A	309	SER
1	A	312	LYS
1	A	328	LEU
1	A	329	ASN
1	A	341	LYS
1	A	345	LYS
1	A	356	LYS
1	A	377	ASP
1	A	379	LYS
1	A	408	GLU
1	A	416	HIS
2	P	2	TRP
2	P	3	VAL

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

Mol	Chain	Res	Type
1	A	329	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	253/299 (84%)	0.19	9 (3%) 42 35	46, 62, 82, 92	0
2	P	8/8 (100%)	0.26	0 100 100	57, 63, 67, 67	0
All	All	261/307 (85%)	0.19	9 (3%) 45 38	46, 63, 82, 92	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ILE	3.9
1	A	220	ILE	3.8
1	A	240	SER	2.7
1	A	253	ARG	2.6
1	A	254	LEU	2.5
1	A	378	LYS	2.4
1	A	255	SER	2.2
1	A	261	ARG	2.1
1	A	407	PHE	2.1

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NI	A	1	1/1	0.89	0.28	98,98,98,98	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.