



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:00 AM GMT

PDB ID : 2Z5K  
Title : Complex of Transportin 1 with TAP NLS  
Authors : Imasaki, T.; Shimizu, T.; Hashimoto, H.; Hidaka, Y.; Yamada, M.; Kose, S.;  
Imamoto, N.; Sato, M.  
Deposited on : 2007-07-14  
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  
<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

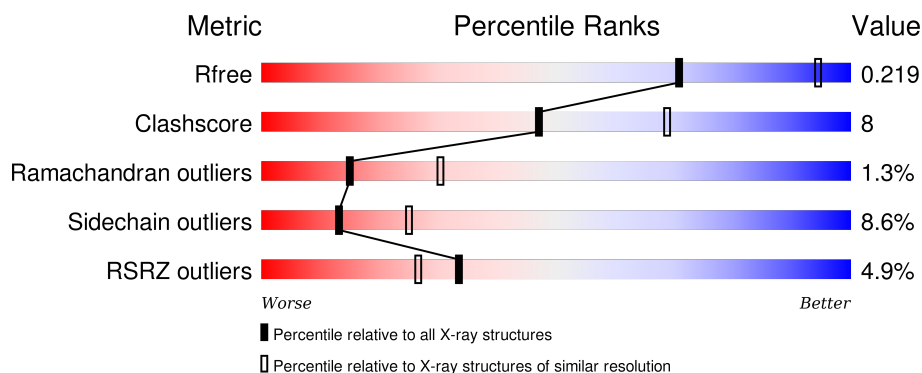
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	890	<div> <div>5%</div> <div>73%</div> <div>19%</div> <div>6%</div> </div>
2	B	30	<div> <div>3%</div> <div>30%</div> <div>10%</div> <div>60%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6831 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.

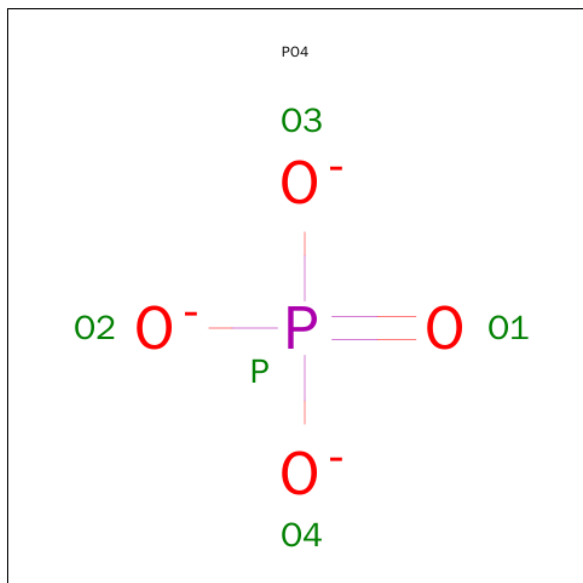
- Molecule 1 is a protein called Transportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	840	Total	C	N	O	S	0	0	0
			6691	4290	1114	1236	51			

- Molecule 2 is a protein called Nuclear RNA export factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	0	0	0
			107	68	22	17			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total 26	O 26	0	0
4	B	2	Total 2	O 2	0	0

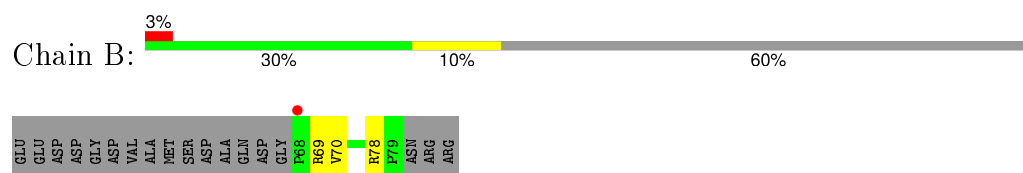
### 3 Residue-property plots

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: Transportin-1



#### • Molecule 2: Nuclear RNA export factor 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.64Å 119.74Å 147.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.40 – 2.60 43.40 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.40-2.60) 95.8 (43.40-2.59)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.99 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.221 , 0.268 0.219 , 0.219	Depositor DCC
$R_{free}$ test set	1861 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 80.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 37498 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4

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	0.56	6/6834 (0.1%)	0.58	2/9282 (0.0%)
2	B	0.46	0/111	0.64	0/151
All	All	0.56	6/6945 (0.1%)	0.58	2/9433 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	882	GLU	CD-OE2	23.39	1.51	1.25
1	A	80	PHE	CG-CD2	9.05	1.52	1.38
1	A	80	PHE	CE2-CZ	8.90	1.54	1.37
1	A	80	PHE	CG-CD1	8.45	1.51	1.38
1	A	80	PHE	CE1-CZ	5.65	1.48	1.37
1	A	866	ASP	CG-OD1	5.56	1.38	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	882	GLU	CG-CD-OE1	-5.30	107.71	118.30
1	A	80	PHE	CB-CG-CD2	-5.07	117.25	120.80

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	6691	0	6750	103	0
2	B	107	0	107	0	0
3	A	5	0	0	0	0
4	A	26	0	0	2	0
4	B	2	0	0	0	0
All	All	6831	0	6857	103	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 8.

All (103) 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:791:GLN:H	1:A:791:GLN:HE21	1.02	0.98
1:A:700:GLN:HE21	1:A:700:GLN:H	1.17	0.88
1:A:534:GLN:HB3	4:A:904:HOH:O	1.73	0.87
1:A:869:TRP:HE1	1:A:890:VAL:HG12	1.44	0.82
1:A:115:THR:CG2	1:A:154:LYS:HG2	2.13	0.78
1:A:115:THR:HG21	1:A:154:LYS:HG2	1.68	0.75
1:A:587:LEU:HD12	1:A:643:VAL:HG23	1.71	0.73
1:A:534:GLN:H	1:A:534:GLN:CD	1.93	0.71
1:A:51:ILE:O	1:A:55:THR:HG22	1.92	0.68
1:A:123:LEU:HG	1:A:168:LEU:HD22	1.78	0.66
1:A:498:GLU:HG3	1:A:540:ILE:CD1	2.26	0.66
1:A:6:LYS:HD3	1:A:6:LYS:H	1.61	0.66
1:A:791:GLN:NE2	1:A:791:GLN:H	1.86	0.65
1:A:5:TRP:HH2	1:A:56:LYS:HE2	1.59	0.65
1:A:168:LEU:O	1:A:169:ASP:HB3	1.97	0.64
1:A:122:GLU:O	1:A:123:LEU:HB2	1.98	0.62
1:A:168:LEU:HG	1:A:168:LEU:O	1.98	0.62
1:A:255:HIS:ND1	1:A:296:HIS:HE1	1.97	0.62
1:A:869:TRP:NE1	1:A:890:VAL:HG12	2.13	0.61
1:A:858:HIS:HE1	1:A:888:TYR:O	1.84	0.60
1:A:185:HIS:HD2	1:A:187:SER:H	1.50	0.60
1:A:512:CYS:HA	1:A:551:SER:HB3	1.85	0.59
1:A:415:GLU:OE2	1:A:457:ILE:HG12	2.03	0.59
1:A:168:LEU:O	1:A:169:ASP:CB	2.50	0.59
1:A:55:THR:HG21	1:A:94:GLU:HB3	1.87	0.57
1:A:578:ASP:OD2	1:A:611:ARG:HD2	2.06	0.56
1:A:164:ASP:OD2	1:A:206:THR:HG22	2.07	0.55
1:A:460:TRP:CZ2	1:A:464:ARG:HD2	2.42	0.55
1:A:115:THR:HG23	1:A:154:LYS:HG2	1.88	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:ILE:HG21	1:A:785:GLU:HB3	1.88	0.54
1:A:739:MET:HB2	1:A:743:MET:HG2	1.88	0.54
1:A:570:ILE:HD11	1:A:604:TYR:CE2	2.42	0.54
1:A:885:ALA:HA	1:A:890:VAL:H	1.73	0.53
1:A:165:SER:HB3	1:A:167:VAL:HG22	1.90	0.53
1:A:70:LEU:HD13	1:A:109:THR:HG23	1.92	0.51
1:A:374:ASN:HD22	1:A:377:LYS:HD2	1.74	0.51
1:A:33:VAL:O	1:A:37:LEU:HB2	2.10	0.51
1:A:301:ILE:HB	1:A:302:PRO:HD3	1.93	0.51
1:A:498:GLU:HG3	1:A:540:ILE:HD13	1.91	0.51
1:A:5:TRP:CH2	1:A:56:LYS:HE2	2.44	0.51
1:A:868:ASN:H	1:A:868:ASN:HD22	1.58	0.51
1:A:318:LEU:HG	1:A:370:ILE:HD11	1.93	0.51
1:A:415:GLU:HG2	1:A:457:ILE:HD11	1.94	0.49
1:A:38:GLU:O	1:A:41:ASN:HB2	2.13	0.49
1:A:245:VAL:HG12	1:A:246:ARG:HG2	1.96	0.48
1:A:859:GLY:O	1:A:863:GLN:HB2	2.14	0.48
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.79	0.48
1:A:647:LEU:O	1:A:651:LEU:HB2	2.13	0.48
1:A:700:GLN:NE2	1:A:700:GLN:H	1.97	0.48
1:A:48:ASN:HD21	1:A:87:VAL:HA	1.79	0.47
1:A:183:PHE:CD1	1:A:219:ASN:HB3	2.50	0.47
1:A:318:LEU:O	1:A:319:LYS:HD3	2.15	0.47
1:A:254:MET:O	1:A:258:VAL:HG12	2.15	0.47
1:A:319:LYS:HA	4:A:900:HOH:O	2.15	0.47
1:A:130:LEU:HB2	1:A:131:PRO:HD3	1.97	0.47
1:A:243:LEU:HD11	1:A:279:PHE:CE1	2.50	0.46
1:A:191:ARG:HD2	1:A:223:LEU:HD21	1.96	0.46
1:A:203:ILE:C	1:A:205:ARG:H	2.18	0.46
1:A:37:LEU:HD21	1:A:71:ILE:HD13	1.98	0.46
1:A:370:ILE:HG22	1:A:371:SER:N	2.31	0.45
1:A:27:THR:HA	1:A:30:GLN:HB2	1.99	0.45
1:A:869:TRP:HE1	1:A:890:VAL:CG1	2.24	0.45
1:A:47:ASN:HD22	1:A:50:LEU:HD22	1.81	0.45
1:A:376:ARG:CZ	1:A:419:LEU:HD22	2.46	0.45
1:A:395:LEU:HD11	1:A:431:GLY:HA3	1.99	0.45
1:A:159:SER:HB3	1:A:162:ILE:HB	1.97	0.45
1:A:236:CYS:O	1:A:240:VAL:HG23	2.17	0.45
1:A:66:SER:O	1:A:70:LEU:HD22	2.17	0.45
1:A:6:LYS:HD3	1:A:6:LYS:N	2.28	0.44
1:A:811:ASP:O	1:A:815:ARG:HG3	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ARG:NH1	1:A:170:ARG:HB2	2.32	0.44
1:A:226:ASP:O	1:A:232:ARG:HG3	2.17	0.44
1:A:6:LYS:CD	1:A:6:LYS:H	2.28	0.44
1:A:787:ALA:O	1:A:790:LEU:HB2	2.16	0.44
1:A:470:VAL:HG11	1:A:511:ALA:HA	2.00	0.44
1:A:185:HIS:CD2	1:A:187:SER:H	2.32	0.44
1:A:672:MET:HE1	1:A:694:LEU:HD12	2.00	0.44
1:A:128:ASP:OD1	1:A:128:ASP:N	2.51	0.44
1:A:842:TRP:HB3	1:A:845:PRO:HG3	1.98	0.44
1:A:153:GLN:OE1	1:A:193:HIS:HD2	2.01	0.43
1:A:170:ARG:HH11	1:A:170:ARG:HB2	1.82	0.43
1:A:253:HIS:O	1:A:257:ILE:HG12	2.18	0.43
1:A:457:ILE:HG13	1:A:457:ILE:H	1.61	0.43
1:A:201:PHE:HB3	1:A:206:THR:OG1	2.19	0.43
1:A:856:ILE:O	1:A:860:PHE:HD1	2.02	0.43
1:A:790:LEU:HB3	1:A:827:GLY:HA3	2.01	0.43
1:A:430:GLN:HA	1:A:433:ILE:HD12	1.99	0.43
1:A:868:ASN:H	1:A:868:ASN:ND2	2.16	0.43
1:A:540:ILE:O	1:A:543:ASP:HB3	2.18	0.42
1:A:169:ASP:OD2	1:A:170:ARG:N	2.49	0.42
1:A:504:PHE:O	1:A:508:GLU:HG3	2.19	0.42
1:A:264:ARG:O	1:A:267:ASP:HB2	2.20	0.41
1:A:726:ASN:ND2	1:A:770:ASN:HD22	2.17	0.41
1:A:700:GLN:N	1:A:700:GLN:HE21	1.98	0.41
1:A:50:LEU:HB3	1:A:72:LEU:HB2	2.01	0.41
1:A:319:LYS:HE3	1:A:493:ASN:HD21	1.85	0.41
1:A:255:HIS:ND1	1:A:296:HIS:CE1	2.84	0.41
1:A:264:ARG:HD3	1:A:264:ARG:HA	1.89	0.41
1:A:401:LEU:O	1:A:405:LEU:HG	2.21	0.41
1:A:422:GLY:O	1:A:464:ARG:HD3	2.20	0.40
1:A:262:LEU:HD13	1:A:299:LYS:HD3	2.03	0.40
1:A:646:ASP:O	1:A:649:SER:HB2	2.21	0.40
1:A:238:ALA:O	1:A:242:LEU:HB2	2.21	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	836/890 (94%)	793 (95%)	33 (4%)	10 (1%)	16	33
2	B	10/30 (33%)	9 (90%)	0	1 (10%)	1	0
All	All	846/920 (92%)	802 (95%)	33 (4%)	11 (1%)	15	30

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLU
1	A	123	LEU
1	A	534	GLN
1	A	169	ASP
1	A	289	CYS
1	A	7	PRO
1	A	456	SER
1	A	8	ASP
1	A	79	HIS
2	B	70	VAL
1	A	318	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	755/802 (94%)	691 (92%)	64 (8%)	13	25
2	B	12/26 (46%)	10 (83%)	2 (17%)	3	4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	767/828 (93%)	701 (91%)	66 (9%)	13	25

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TRP
1	A	6	LYS
1	A	27	THR
1	A	38	GLU
1	A	41	ASN
1	A	70	LEU
1	A	96	LEU
1	A	123	LEU
1	A	128	ASP
1	A	136	LEU
1	A	149	PHE
1	A	205	ARG
1	A	211	LEU
1	A	247	MET
1	A	251	LEU
1	A	258	VAL
1	A	259	GLU
1	A	264	ARG
1	A	283	LEU
1	A	288	ILE
1	A	292	VAL
1	A	300	LEU
1	A	304	LEU
1	A	309	LYS
1	A	313	ILE
1	A	319	LYS
1	A	391	ARG
1	A	394	LEU
1	A	421	LEU
1	A	451	LYS
1	A	456	SER
1	A	457	ILE
1	A	475	ASP
1	A	485	LEU
1	A	488	ARG
1	A	490	LEU
1	A	501	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	525	THR
1	A	534	GLN
1	A	539	LEU
1	A	548	LEU
1	A	575	MET
1	A	592	SER
1	A	610	GLN
1	A	648	LEU
1	A	651	LEU
1	A	700	GLN
1	A	717	LEU
1	A	760	ARG
1	A	768	LEU
1	A	789	MET
1	A	791	GLN
1	A	801	LEU
1	A	805	ARG
1	A	826	SER
1	A	829	ILE
1	A	833	ILE
1	A	850	ARG
1	A	855	LYS
1	A	863	GLN
1	A	878	LEU
1	A	884	LEU
1	A	887	PHE
1	A	890	VAL
2	B	69	ARG
2	B	78	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	47	ASN
1	A	48	ASN
1	A	81	GLN
1	A	173	ASN
1	A	185	HIS
1	A	193	HIS
1	A	207	GLN
1	A	296	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	374	ASN
1	A	534	GLN
1	A	574	ASN
1	A	627	ASN
1	A	700	GLN
1	A	726	ASN
1	A	759	ASN
1	A	770	ASN
1	A	791	GLN
1	A	844	ASN
1	A	858	HIS
1	A	868	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
3	PO4	A	891	-	4,4,4	0.39	0	6,6,6	0.28	0

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
3	PO4	A	891	-	-	0/0/0/0	0/0/0/0

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 ⓘ

### 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, 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	840/890 (94%)	0.45	41 (4%) 33 26	76, 86, 96, 121	0
2	B	12/30 (40%)	1.20	1 (8%) 14 9	83, 88, 94, 96	0
All	All	852/920 (92%)	0.46	42 (4%) 33 26	76, 86, 96, 121	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	68	PRO	9.8
1	A	5	TRP	7.7
1	A	366	ASP	4.9
1	A	631	ASP	4.3
1	A	633	TYR	4.2
1	A	52	PHE	4.1
1	A	367	ASP	4.0
1	A	407	PHE	3.9
1	A	632	GLN	3.9
1	A	203	ILE	3.7
1	A	369	THR	3.5
1	A	97	ASN	3.4
1	A	124	GLN	3.4
1	A	28	THR	3.3
1	A	402	LEU	3.3
1	A	624	MET	3.2
1	A	123	LEU	3.0
1	A	173	ASN	2.9
1	A	137	LEU	2.9
1	A	521	TYR	2.8
1	A	875	GLN	2.8
1	A	161	GLU	2.8
1	A	142	TYR	2.7
1	A	288	ILE	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	679	LYS	2.6
1	A	872	PHE	2.6
1	A	577	LYS	2.6
1	A	227	GLU	2.6
1	A	315	ILE	2.5
1	A	406	LEU	2.4
1	A	167	VAL	2.4
1	A	7	PRO	2.4
1	A	874	ASP	2.3
1	A	117	ILE	2.3
1	A	237	ARG	2.2
1	A	186	SER	2.2
1	A	370	ILE	2.1
1	A	263	GLN	2.1
1	A	99	ILE	2.1
1	A	625	LEU	2.0
1	A	368	ASP	2.0
1	A	244	GLU	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](#)

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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	891	5/5	0.78	0.32	-	124,125,125,125	0

## 6.5 Other polymers

There are no such residues in this entry.