



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:39 PM UTC

PDB ID : 6BDL / pdb_00006bdl
Title : Crystal structure of cGMP-dependent protein kinase Ialpha (PKG Ialpha) catalytic domain in apo state
Authors : Qin, L.; Sankaran, B.; Kim, C.
Deposited on : 2017-10-23
Resolution : 1.96 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

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

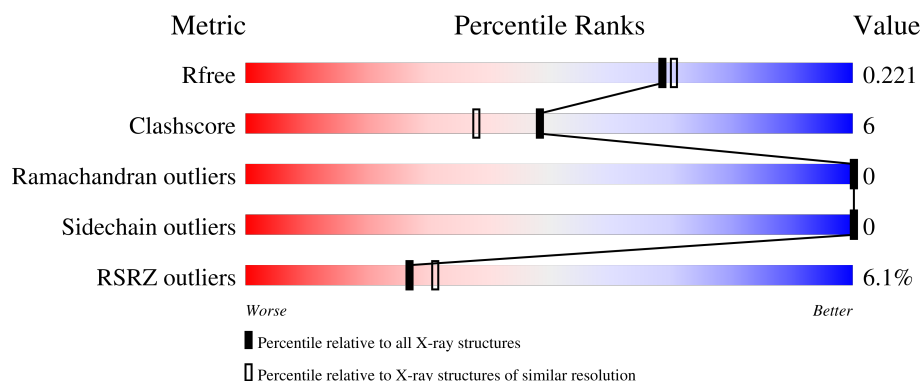
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 ≥ 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	347	
1	B	347	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5680 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.

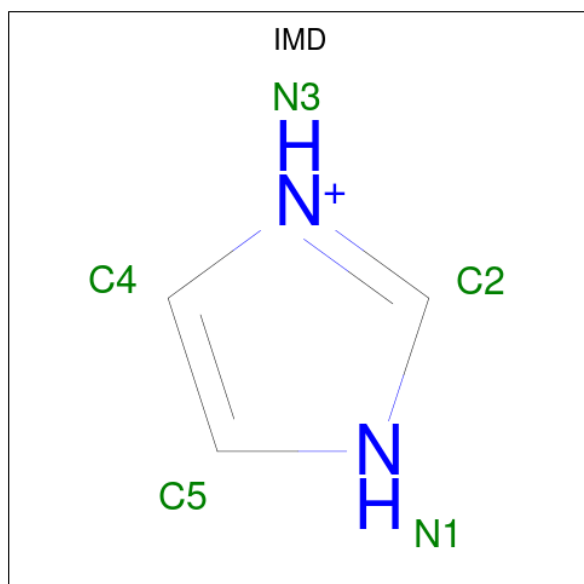
- Molecule 1 is a protein called cGMP-dependent protein kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	P	S	0	0	0
			2585	1668	424	482	1	10			
1	B	335	Total	C	N	O	P	S	0	0	0
			2616	1694	431	480	1	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	GLY	-	expression tag	UNP Q13976
A	326	SER	-	expression tag	UNP Q13976
B	325	GLY	-	expression tag	UNP Q13976
B	326	SER	-	expression tag	UNP Q13976

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		

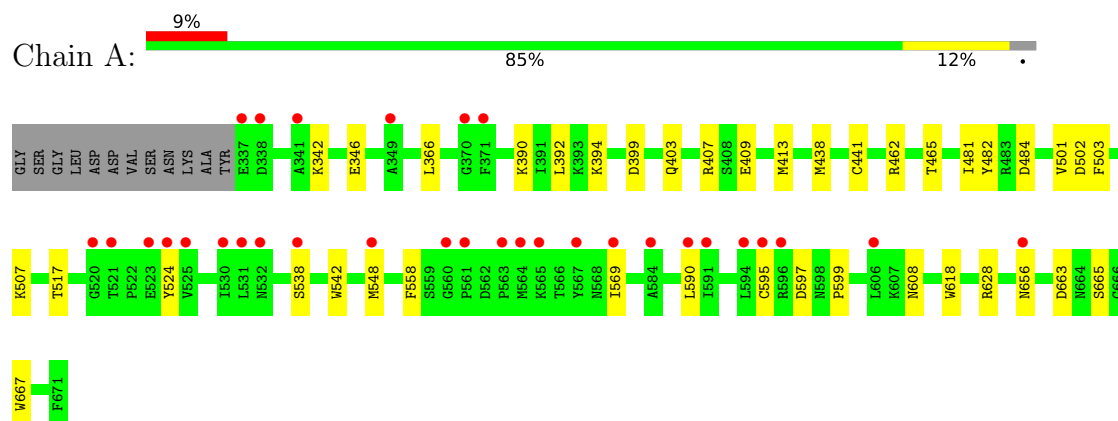
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	222	Total	O	0	0
			222	222		
3	B	246	Total	O	0	1
			247	247		

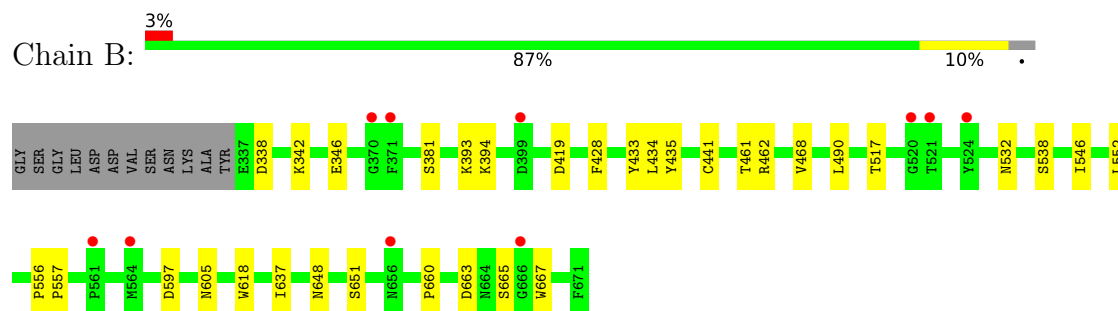
3 Residue-property plots

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: cGMP-dependent protein kinase 1



- Molecule 1: cGMP-dependent protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	85.11Å 50.88Å 85.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.10 – 1.96 38.10 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.10-1.96) 99.6 (38.10-1.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.209 , 0.222 0.209 , 0.221	Depositor DCC
R_{free} test set	2017 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.050 for l,k,-h 0.024 for h,-k,-l 0.023 for l,-k,h	Xtriage
F_o , F_c correlation	0.95	EDS
Total number of atoms	5680	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.20	0/2637	0.41	0/3568
1	B	0.19	0/2670	0.39	0/3609
All	All	0.20	0/5307	0.40	0/7177

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	2585	0	2412	32	0
1	B	2616	0	2500	24	0
2	A	5	0	5	2	0
2	B	5	0	5	1	0
3	A	222	0	0	14	0
3	B	247	0	0	10	0
All	All	5680	0	4922	56	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 (56) 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:597:ASP:OD2	3:A:801:HOH:O	1.89	0.89
1:B:338:ASP:OD1	3:B:801:HOH:O	1.90	0.89
1:A:409:GLU:OE2	3:A:803:HOH:O	1.97	0.82
1:B:651:SER:OG	3:B:802:HOH:O	1.99	0.81
1:A:465:THR:HG21	1:A:548:MET:HE3	1.69	0.74
1:A:399:ASP:OD2	3:A:804:HOH:O	2.10	0.68
1:A:595:CYS:SG	3:A:1013:HOH:O	2.52	0.67
1:A:441:CYS:H	2:A:700:IMD:HN1	1.41	0.65
1:A:502:ASP:HA	3:A:803:HOH:O	2.00	0.61
1:A:390:LYS:HB2	1:A:438:MET:HE2	1.84	0.60
1:A:628:ARG:NH1	3:A:809:HOH:O	2.22	0.59
1:A:542:TRP:NE1	3:A:805:HOH:O	2.12	0.59
1:B:648:ASN:OD1	3:B:805:HOH:O	2.16	0.59
1:A:342:LYS:O	1:A:346:GLU:HG2	2.05	0.57
1:A:462:ARG:HA	1:A:618:TRP:CH2	2.39	0.57
1:A:484:ASP:OD2	3:A:807:HOH:O	2.17	0.57
1:A:665:SER:HB2	1:A:667:TRP:HD1	1.70	0.56
1:A:524:TYR:O	3:A:808:HOH:O	2.18	0.56
1:A:413:MET:HE1	3:A:803:HOH:O	2.06	0.55
1:A:413:MET:HE2	1:A:503:PHE:CD1	2.42	0.54
1:B:538:SER:HB3	1:B:605:ASN:ND2	2.23	0.54
1:B:419:ASP:OD2	3:B:807:HOH:O	2.19	0.52
1:A:548:MET:HE2	1:A:618:TRP:CZ3	2.45	0.52
1:A:558:PHE:HD1	1:A:569:ILE:HG22	1.76	0.51
1:A:366:LEU:HD13	2:A:700:IMD:H2	1.92	0.51
1:B:441:CYS:H	2:B:700:IMD:HN1	1.57	0.51
1:B:538:SER:HB3	1:B:605:ASN:HD21	1.75	0.51
1:B:665:SER:HB2	1:B:667:TRP:HD1	1.76	0.50
1:B:462:ARG:HA	1:B:618:TRP:CH2	2.47	0.48
1:A:481:ILE:HG22	1:A:507:LYS:O	2.13	0.48
1:B:393:LYS:HG2	1:B:660:PRO:HG3	1.96	0.48
1:B:433:TYR:OH	3:B:803:HOH:O	2.07	0.47
1:B:532:ASN:OD1	3:B:809:HOH:O	2.20	0.47
1:B:597:ASP:OD1	3:B:808:HOH:O	2.20	0.47
1:B:637:ILE:O	3:B:810:HOH:O	2.21	0.46
1:B:468:VAL:HG22	1:B:490:LEU:HD21	1.99	0.45
1:A:608:ASN:ND2	3:A:834:HOH:O	2.50	0.45
1:B:434:LEU:HD11	1:B:667:TRP:CH2	2.52	0.44
1:A:390:LYS:HG2	1:A:392:LEU:HD11	1.98	0.44
1:B:342:LYS:O	1:B:346:GLU:HG2	2.18	0.44
1:B:461:THR:HG21	1:B:552:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:PHE:HB2	1:B:435:TYR:HB2	2.00	0.44
1:B:546:ILE:HG23	1:B:557:PRO:HD2	2.00	0.44
1:A:403:GLN:O	1:A:407:ARG:HG3	2.17	0.43
1:B:394:LYS:HE3	1:B:663:ASP:HB3	2.01	0.42
1:B:381:SER:OG	3:B:806:HOH:O	2.17	0.42
1:A:628:ARG:HD2	3:A:809:HOH:O	2.20	0.42
1:A:394:LYS:HE2	1:A:663:ASP:HB3	2.00	0.42
1:A:656:ASN:ND2	3:A:838:HOH:O	2.53	0.42
1:B:556:PRO:HB2	3:B:840:HOH:O	2.19	0.42
1:A:482:TYR:OH	1:A:501:VAL:O	2.38	0.41
1:A:413:MET:HE2	1:A:503:PHE:HD1	1.83	0.41
1:B:394:LYS:HG2	1:B:434:LEU:HG	2.02	0.41
1:A:538:SER:OG	1:A:599:PRO:HB3	2.21	0.40
1:A:548:MET:HE1	1:A:590:LEU:CD2	2.51	0.40
1:A:608:ASN:CG	3:A:834:HOH:O	2.65	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	332/347 (96%)	325 (98%)	7 (2%)	0	100	100
1	B	332/347 (96%)	325 (98%)	7 (2%)	0	100	100
All	All	664/694 (96%)	650 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	247/297 (83%)	247 (100%)	0	100	100
1	B	255/297 (86%)	255 (100%)	0	100	100
All	All	502/594 (84%)	502 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	361	ASN
1	A	648	ASN
1	B	396	HIS
1	B	568	ASN
1	B	608	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	B	517	1	8,10,11	1.66	1 (12%)	10,14,16	1.96	2 (20%)
1	TPO	A	517	1	8,10,11	1.59	1 (12%)	10,14,16	2.12	1 (10%)

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
1	TPO	B	517	1	-	1/9/11/13	-
1	TPO	A	517	1	-	0/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	517	TPO	P-O1P	3.41	1.61	1.50
1	A	517	TPO	P-O1P	3.40	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	TPO	P-OG1-CB	-6.12	106.71	123.33
1	B	517	TPO	P-OG1-CB	-5.29	108.95	123.33
1	B	517	TPO	CG2-CB-CA	-2.23	108.92	113.26

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	517	TPO	CB-OG1-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	IMD	B	700	-	5,5,5	0.68	0	5,5,5	0.45	0
2	IMD	A	700	-	5,5,5	0.69	0	5,5,5	0.37	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
2	IMD	B	700	-	-	-	0/1/1/1
2	IMD	A	700	-	-	-	0/1/1/1

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	700	IMD	1	0
2	A	700	IMD	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	334/347 (96%)	0.70	31 (9%) 14 16	24, 40, 62, 75	0
1	B	334/347 (96%)	0.35	10 (2%) 52 59	24, 36, 55, 67	0
All	All	668/694 (96%)	0.53	41 (6%) 27 31	24, 38, 59, 75	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	521	THR	4.6
1	A	567	TYR	4.5
1	A	606	LEU	4.2
1	A	337	GLU	4.0
1	A	565	LYS	4.0
1	A	371	PHE	4.0
1	A	531	LEU	3.5
1	A	532	ASN	3.3
1	A	564	MET	3.1
1	A	538	SER	3.0
1	A	521	THR	3.0
1	A	524	TYR	2.9
1	A	595	CYS	2.9
1	A	656	ASN	2.9
1	A	560	GLY	2.9
1	A	530	ILE	2.9
1	B	371	PHE	2.9
1	B	520	GLY	2.8
1	A	596	ARG	2.7
1	A	561	PRO	2.7
1	A	569	ILE	2.7
1	B	370	GLY	2.6
1	B	524	TYR	2.6
1	B	399	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	563	PRO	2.5
1	A	594	LEU	2.5
1	B	656	ASN	2.5
1	A	341	ALA	2.4
1	B	561	PRO	2.4
1	A	548	MET	2.4
1	A	349	ALA	2.4
1	B	564	MET	2.4
1	A	590	LEU	2.3
1	A	523	GLU	2.3
1	A	520	GLY	2.3
1	A	584	ALA	2.2
1	B	666	GLY	2.2
1	A	591	ILE	2.1
1	A	338	ASP	2.1
1	A	525	VAL	2.0
1	A	370	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å ²)	Q<0.9
1	TPO	B	517	11/12	0.96	0.08	25,26,30,31	0
1	TPO	A	517	11/12	0.98	0.06	28,30,38,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	IMD	B	700	5/5	0.71	0.25	57,57,58,58	0
2	IMD	A	700	5/5	0.85	0.13	45,45,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.