



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:03 PM GMT

PDB ID : 4URK
Title : PI3Kg in complex with AZD6482
Authors : Giordanetto, F.; Barlaam, B.; Berglund, S.; Edman, K.; Karlsson, O.; Lindberg, J.; Nylander, S.; Inghardt, T.
Deposited on : 2014-06-30
Resolution : 2.90 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
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

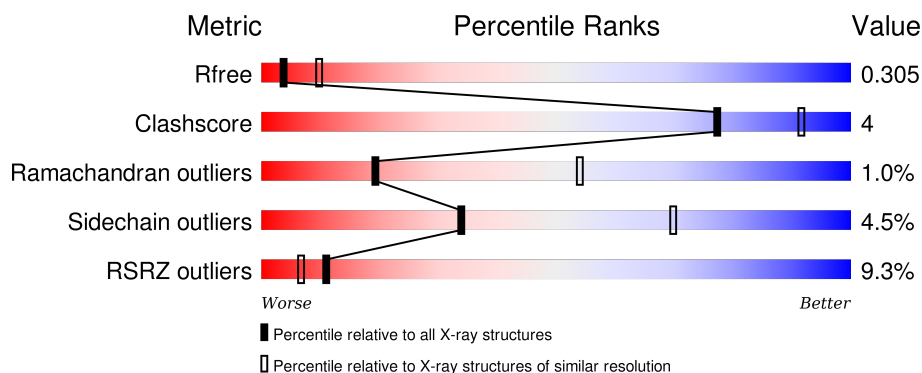
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	966	<div> <div>8%</div> <div>74%</div> <div>12%</div> <div>13%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6823 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.

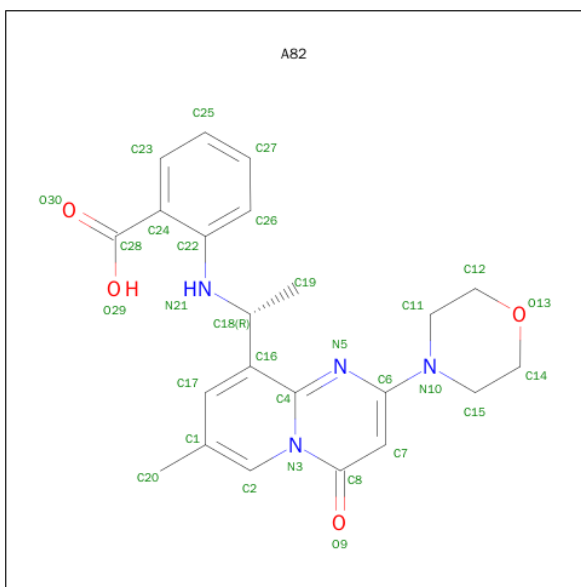
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	837	Total	C	N	O	S	0	0	0
			6793	4361	1159	1238	35			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is 2-[[[(1R)-1-(7-METHYL-2-MORPHOLIN-4-YL-4-OXIDANYLIDENE-PYRIDO[1,2-A]PYRIMIDIN-9-YL)ETHYL]AMINO]BENZOIC ACID (three-letter code: A82) (formula: C₂₂H₂₄N₄O₄).

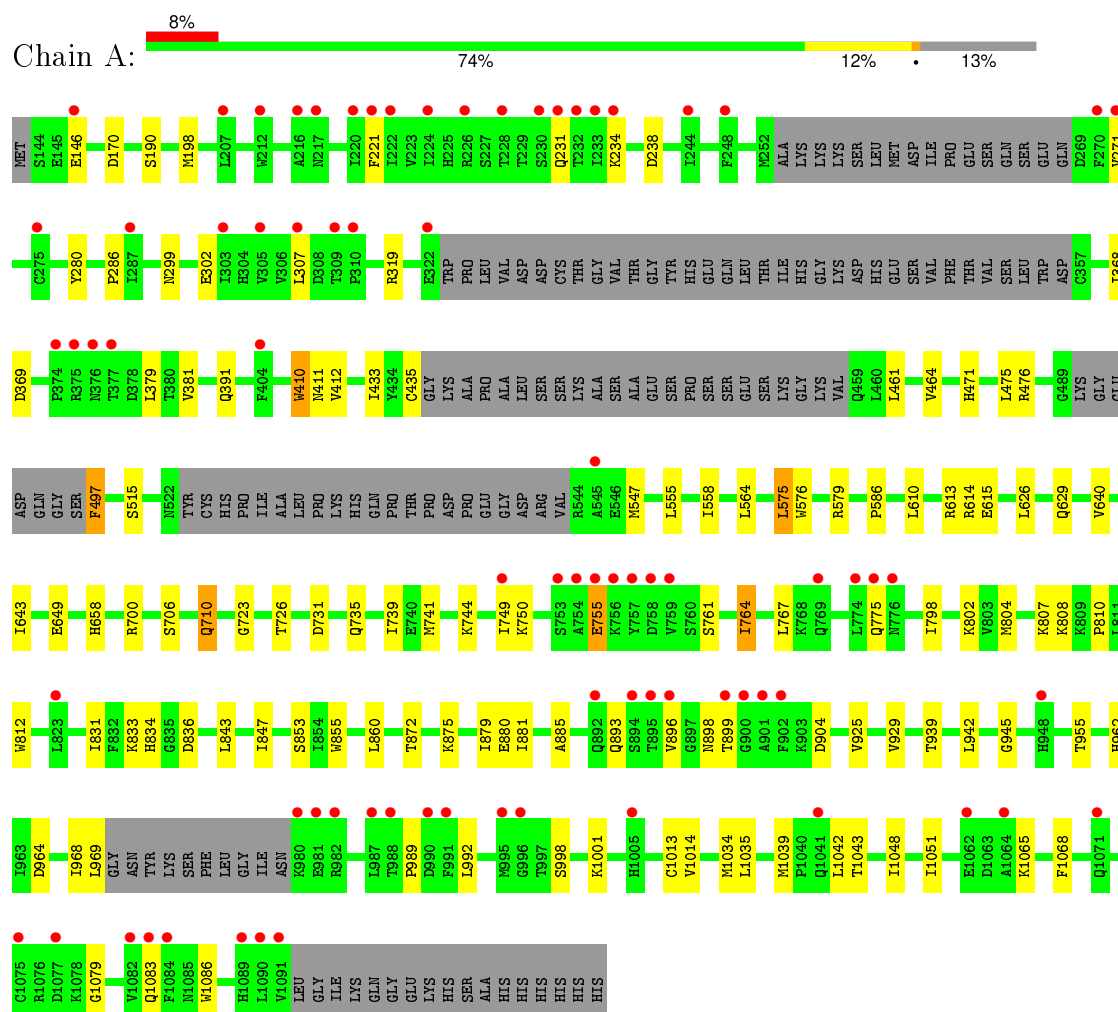


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	22	4	4	0	0

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: PHOSPHATIDYLINOSITOL 4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUB-UNIT GAMMA ISOFORM



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.18Å 67.52Å 106.17Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	40.80 – 2.90 40.54 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.80-2.90) 95.8 (40.54-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.250 , 0.309 0.243 , 0.305	Depositor DCC
R_{free} test set	1111 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 21691 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6823	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A82

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	0.44	0/6938	0.67	0/9384

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	6793	0	6841	51	0
2	A	30	0	23	2	0
All	All	6823	0	6864	51	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 4.

All (51) 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:1014:VAL:HG11	1:A:1065:LYS:HG3	1.76	0.67
1:A:706:SER:O	1:A:710:GLN:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.65	0.62
1:A:576:TRP:O	1:A:579:ARG:HG3	2.00	0.62
1:A:735:GLN:O	1:A:739:ILE:HG12	2.00	0.61
1:A:804:MET:HB2	1:A:810:PRO:HD2	1.83	0.61
1:A:579:ARG:HB3	1:A:610:LEU:HD21	1.84	0.60
1:A:880:GLU:O	2:A:2092:A82:H122	2.04	0.57
1:A:739:ILE:HG21	1:A:872:THR:HG21	1.87	0.56
1:A:146:GLU:HB3	1:A:319:ARG:HH22	1.71	0.55
1:A:833:LYS:HE3	1:A:836:ASP:HB2	1.89	0.55
1:A:640:VAL:O	1:A:643:ILE:HG12	2.07	0.54
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.90	0.54
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.90	0.54
1:A:775:GLN:HE21	1:A:798:ILE:HD11	1.72	0.53
1:A:238:ASP:HA	1:A:286:PRO:HB3	1.92	0.52
1:A:804:MET:HE1	1:A:808:LYS:HB2	1.90	0.52
1:A:750:LYS:HE2	1:A:834:HIS:HD2	1.75	0.52
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.91	0.52
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.92	0.52
1:A:497:PHE:O	1:A:1043:THR:HB	2.12	0.50
1:A:881:ILE:HA	2:A:2092:A82:H142	1.94	0.49
1:A:804:MET:CB	1:A:810:PRO:HD2	2.44	0.48
1:A:1039:MET:HB3	1:A:1042:LEU:HD23	1.96	0.48
1:A:435:CYS:HB3	1:A:461:LEU:HD11	1.96	0.47
1:A:893:GLN:HG2	1:A:898:ASN:H	1.79	0.47
1:A:613:ARG:O	1:A:615:GLU:N	2.47	0.46
1:A:989:PRO:HA	1:A:992:LEU:HB2	1.97	0.46
1:A:1083:GLN:HA	1:A:1086:TRP:HD1	1.81	0.46
1:A:741:MET:HA	1:A:744:LYS:HE3	1.99	0.45
1:A:831:ILE:HB	1:A:879:ILE:HB	1.99	0.44
1:A:471:HIS:H	1:A:471:HIS:CD2	2.34	0.44
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.50	0.43
1:A:807:LYS:HE3	1:A:808:LYS:HE3	1.99	0.43
1:A:586:PRO:O	1:A:626:LEU:HD21	2.19	0.43
1:A:855:TRP:HB3	1:A:860:LEU:HB2	2.01	0.42
1:A:198:MET:HG2	1:A:280:TYR:CG	2.55	0.42
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	2.02	0.42
1:A:834:HIS:HA	1:A:875:LYS:O	2.20	0.42
1:A:1083:GLN:HA	1:A:1086:TRP:CD1	2.55	0.42
1:A:802:LYS:HG2	1:A:812:TRP:HB3	2.01	0.42
1:A:221:PHE:CE1	1:A:234:LYS:HG2	2.55	0.42
1:A:998:SER:H	1:A:1001:LYS:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:VAL:O	1:A:929:VAL:HG23	2.20	0.41
1:A:847:ILE:HG21	1:A:942:LEU:HD21	2.02	0.41
1:A:939:THR:HB	1:A:945:GLY:HA2	2.01	0.41
1:A:939:THR:HG21	1:A:962:HIS:CE1	2.55	0.41
1:A:761:SER:HA	1:A:764:ILE:HD12	2.02	0.41
1:A:885:ALA:HB2	1:A:955:THR:HG22	2.03	0.40
1:A:843:LEU:HD13	1:A:1034:MET:HG3	2.02	0.40
1:A:968:ILE:HD12	1:A:969:LEU:HG	2.03	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	823/966 (85%)	761 (92%)	54 (7%)	8 (1%)	19	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	ARG
1	A	755	GLU
1	A	190	SER
1	A	649	GLU
1	A	896	VAL
1	A	964	ASP
1	A	1079	GLY
1	A	723	GLY

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	754/864 (87%)	720 (96%)	34 (4%)	34 70

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	ASP
1	A	231	GLN
1	A	271	VAL
1	A	299	ASN
1	A	302	GLU
1	A	307	LEU
1	A	369	ASP
1	A	379	LEU
1	A	381	VAL
1	A	391	GLN
1	A	410	TRP
1	A	411	ASN
1	A	464	VAL
1	A	475	LEU
1	A	476	ARG
1	A	497	PHE
1	A	515	SER
1	A	547	MET
1	A	555	LEU
1	A	575	LEU
1	A	629	GLN
1	A	658	HIS
1	A	700	ARG
1	A	710	GLN
1	A	726	THR
1	A	731	ASP
1	A	749	ILE
1	A	755	GLU
1	A	764	ILE
1	A	767	LEU

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Mol	Chain	Res	Type
1	A	853	SER
1	A	899	THR
1	A	904	ASP
1	A	1051	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	GLN
1	A	585	HIS
1	A	734	GLN
1	A	775	GLN
1	A	834	HIS
1	A	892	GLN
1	A	908	ASN
1	A	948	HIS
1	A	962	HIS
1	A	1005	HIS
1	A	1007	GLN
1	A	1023	HIS

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
2	A82	A	2092	-	26,33,33	1.60	6 (23%)	34,47,47	1.71	8 (23%)

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	A82	A	2092	-	-	0/12/24/24	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2092	A82	C4-N5	-3.95	1.29	1.35
2	A	2092	A82	C7-C6	-3.32	1.34	1.40
2	A	2092	A82	C2-C1	-2.72	1.33	1.39
2	A	2092	A82	C17-C16	-2.23	1.34	1.37
2	A	2092	A82	C17-C1	2.76	1.43	1.38
2	A	2092	A82	C6-N5	3.32	1.37	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2092	A82	C22-N21-C18	-4.71	115.44	124.71
2	A	2092	A82	C23-C24-C28	-2.41	116.52	120.23
2	A	2092	A82	C20-C1-C17	-2.37	117.35	120.95
2	A	2092	A82	O13-C14-C15	-2.03	107.18	111.84
2	A	2092	A82	C8-C7-C6	2.51	119.47	116.33
2	A	2092	A82	C17-C16-C18	2.69	124.45	120.63
2	A	2092	A82	C2-C1-C17	2.88	120.47	117.29
2	A	2092	A82	C23-C24-C22	3.84	121.46	117.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2092	A82	2	0

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, 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	837/966 (86%)	0.59	78 (9%) 11 7	23, 66, 116, 141	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1089	HIS	6.8
1	A	901	ALA	6.1
1	A	270	PHE	5.8
1	A	895	THR	5.7
1	A	1075	CYS	5.4
1	A	307	LEU	4.6
1	A	404	PHE	4.6
1	A	1090	LEU	4.5
1	A	892	GLN	4.4
1	A	988	THR	4.4
1	A	545	ALA	3.8
1	A	990	ASP	3.8
1	A	248	PHE	3.8
1	A	271	VAL	3.8
1	A	220	ILE	3.8
1	A	377	THR	3.7
1	A	823	LEU	3.7
1	A	981	GLU	3.7
1	A	757	TYR	3.7
1	A	375	ARG	3.6
1	A	980	LYS	3.5
1	A	900	GLY	3.5
1	A	995	MET	3.4
1	A	212	TRP	3.3
1	A	228	THR	3.3
1	A	991	PHE	3.3
1	A	275	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	987	LEU	3.2
1	A	756	LYS	3.2
1	A	216	ALA	3.2
1	A	231	GLN	3.1
1	A	755	GLU	3.0
1	A	1005	HIS	2.9
1	A	1082	VAL	2.9
1	A	207	LEU	2.8
1	A	982	ARG	2.8
1	A	234	LYS	2.7
1	A	902	PHE	2.7
1	A	1062	GLU	2.7
1	A	374	PRO	2.7
1	A	233	ILE	2.7
1	A	230	SER	2.7
1	A	948	HIS	2.7
1	A	775	GLN	2.6
1	A	996	GLY	2.6
1	A	754	ALA	2.6
1	A	1091	VAL	2.6
1	A	232	THR	2.6
1	A	1084	PHE	2.6
1	A	226	ARG	2.5
1	A	287	ILE	2.5
1	A	1041	GLN	2.5
1	A	1077	ASP	2.5
1	A	310	PRO	2.4
1	A	376	ASN	2.4
1	A	1064	ALA	2.4
1	A	758	ASP	2.3
1	A	769	GLN	2.3
1	A	753	SER	2.3
1	A	322	GLU	2.3
1	A	244	ILE	2.3
1	A	894	SER	2.3
1	A	305	VAL	2.3
1	A	896	VAL	2.3
1	A	776	ASN	2.3
1	A	759	VAL	2.3
1	A	774	LEU	2.2
1	A	1083	GLN	2.2
1	A	222	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	221	PHE	2.2
1	A	899	THR	2.2
1	A	146	GLU	2.2
1	A	224	ILE	2.1
1	A	303	ILE	2.1
1	A	749	ILE	2.1
1	A	217	ASN	2.1
1	A	1071	GLN	2.0
1	A	309	THR	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	A82	A	2092	30/30	0.92	0.19	-0.90	64,66,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.