



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:09 PM GMT

PDB ID : 3DBS
Title : Structure of PI3K gamma in complex with GDC0941
Authors : Wiesmann, C.; Ultsch, M.
Deposited on : 2008-06-02
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

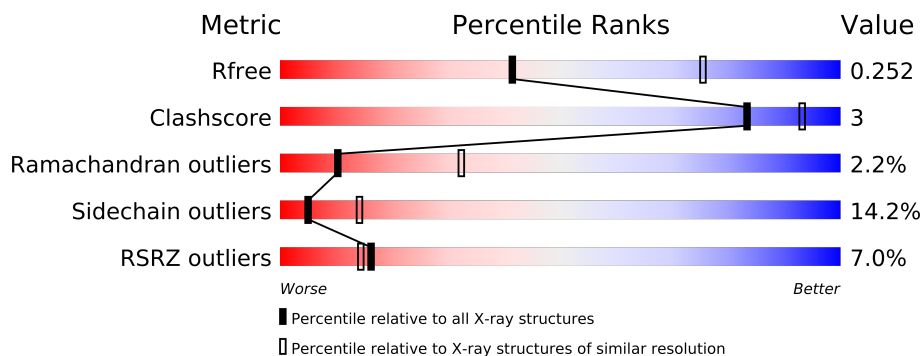
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	960	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 6847 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

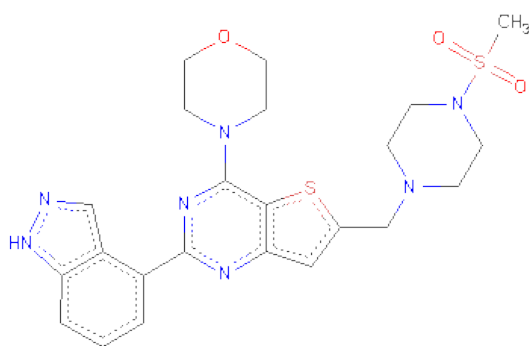
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6812	4371	1164	1242	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	INITIATING METHIONINE	UNP P48736

- Molecule 2 is 2-(1H-INDAZOL-4-YL)-6-{[4-(METHYLSULFONYL)PIPERAZIN-1-YL]METHYL}-4-MORPHOLIN-4-YL-THIENO[3,2-D]PYRIMIDINE (three-letter code: GD9) (formula: C₂₃H₂₇N₇O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	23	7	3	2		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.28Å 67.76Å 106.97Å 90.00° 95.31° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 44.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.80) 99.7 (44.81-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.219 , 0.262 0.218 , 0.252	Depositor DCC
R_{free} test set	1317 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25552 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6847	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GD9

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	0.51	1/6958 (0.0%)	0.77	28/9412 (0.3%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	904	ASP	CG-OD1	7.57	1.42	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	632	ASP	CB-CG-OD2	7.32	124.89	118.30
1	A	1011	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	874	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	278	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	1070	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	378	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	837	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	521	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	192	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	238	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	358	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	637	ASP	CB-CG-OD2	5.79	123.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	841	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	312	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	964	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	164	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	171	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	369	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	836	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	470	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	422	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	861	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	819	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	1077	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	674	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	884	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	1053	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	562	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	756	LYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6812	0	6843	40	0
2	A	35	0	27	2	0
All	All	6847	0	6870	41	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (41) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:802:LYS:NZ	2:A:1:GD9:O1	2.14	0.80
1:A:576:TRP:O	1:A:579:ARG:HD3	1.96	0.66
1:A:743:GLN:HE21	1:A:876:ILE:HG12	1.61	0.66
1:A:606:LYS:HA	1:A:609:GLN:HE21	1.63	0.64
1:A:731:ASP:OD2	1:A:784:ARG:NE	2.35	0.60
1:A:527:ILE:HG23	1:A:601:GLN:HE22	1.70	0.57
1:A:905:GLU:HA	1:A:993:PHE:CD2	2.41	0.55
1:A:734:GLN:HE21	1:A:734:GLN:HA	1.72	0.54
1:A:204:SER:OG	1:A:652:GLU:OE2	2.18	0.53
1:A:576:TRP:O	1:A:579:ARG:CD	2.57	0.52
1:A:182:THR:HB	1:A:183:PRO:HD3	1.92	0.52
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.92	0.51
1:A:743:GLN:NE2	1:A:876:ILE:HG23	2.26	0.50
1:A:624:VAL:O	1:A:628:MET:HG2	2.11	0.50
1:A:935:TYR:O	1:A:939:THR:HB	2.10	0.50
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.92	0.50
1:A:181:VAL:O	1:A:185:MET:HG3	2.11	0.50
1:A:743:GLN:HE22	1:A:876:ILE:HG23	1.77	0.48
1:A:807:LYS:O	1:A:833:LYS:NZ	2.37	0.48
1:A:895:THR:O	1:A:897:GLY:N	2.45	0.48
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.96	0.48
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.95	0.48
1:A:373:LEU:N	1:A:374:PRO:CD	2.77	0.47
1:A:498:ASN:C	1:A:498:ASN:OD1	2.53	0.47
1:A:743:GLN:NE2	1:A:876:ILE:HG12	2.28	0.46
1:A:775:GLN:HE22	1:A:795:ALA:HB1	1.80	0.46
1:A:395:CYS:SG	1:A:418:ILE:HG12	2.56	0.45
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	1.98	0.45
1:A:359:ARG:O	1:A:420:ILE:HG12	2.16	0.45
1:A:888:ILE:HD13	1:A:952:ILE:HG22	1.99	0.44
1:A:632:ASP:C	1:A:632:ASP:OD1	2.56	0.44
1:A:476:ARG:HG2	1:A:520:LEU:HD23	2.00	0.43
1:A:734:GLN:HA	1:A:734:GLN:NE2	2.34	0.43
1:A:212:TRP:CE3	1:A:215:ILE:HD12	2.54	0.42
1:A:685:GLY:HA2	1:A:691:ILE:HG22	2.02	0.42
2:A:1:GD9:S1	2:A:1:GD9:H17A	2.60	0.42
1:A:895:THR:O	1:A:896:VAL:C	2.58	0.41
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.66	0.41
1:A:887:THR:HG22	1:A:890:LYS:H	1.85	0.41
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.56	0.41
1:A:483:HIS:CD2	1:A:510:LYS:HE3	2.57	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	825/960 (86%)	757 (92%)	50 (6%)	18 (2%)	10	32

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	776	ASN
1	A	896	VAL
1	A	898	ASN
1	A	805	ALA
1	A	1040	PRO
1	A	1087	PHE
1	A	227	SER
1	A	252	MET
1	A	376	ASN
1	A	545	ALA
1	A	778	GLN
1	A	899	THR
1	A	228	THR
1	A	527	ILE
1	A	999	GLY
1	A	526	PRO
1	A	1079	GLY
1	A	374	PRO

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	754/858 (88%)	647 (86%)	107 (14%)	5	14

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	153	GLN
1	A	168	VAL
1	A	185	MET
1	A	204	SER
1	A	207	LEU
1	A	213	LYS
1	A	215	ILE
1	A	219	CYS
1	A	226	ARG
1	A	231	GLN
1	A	247	SER
1	A	250	THR
1	A	252	MET
1	A	271	VAL
1	A	281	LEU
1	A	282	VAL
1	A	306	VAL
1	A	362	ARG
1	A	366	ARG
1	A	372	VAL
1	A	375	ARG
1	A	376	ASN
1	A	377	THR
1	A	379	LEU
1	A	380	THR
1	A	388	GLN
1	A	391	GLN
1	A	395	CYS
1	A	470	ASP
1	A	472	ARG
1	A	477	ARG
1	A	511	GLU
1	A	515	SER
1	A	520	LEU
1	A	525	HIS
1	A	527	ILE
1	A	544	ARG
1	A	549	ASN
1	A	550	GLN
1	A	554	GLN
1	A	570	GLU

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Mol	Chain	Res	Type
1	A	574	LEU
1	A	575	LEU
1	A	591	LYS
1	A	610	LEU
1	A	619	GLN
1	A	626	LEU
1	A	638	GLU
1	A	647	LYS
1	A	650	SER
1	A	662	GLN
1	A	682	LEU
1	A	701	SER
1	A	717	LEU
1	A	728	MET
1	A	731	ASP
1	A	749	ILE
1	A	756	LYS
1	A	760	SER
1	A	761	SER
1	A	764	ILE
1	A	766	GLN
1	A	767	LEU
1	A	770	LYS
1	A	778	GLN
1	A	779	LEU
1	A	782	SER
1	A	792	LYS
1	A	819	ASP
1	A	823	LEU
1	A	833	LYS
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	871	SER
1	A	875	LYS
1	A	883	LYS
1	A	887	THR
1	A	888	ILE
1	A	895	THR
1	A	899	THR

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Mol	Chain	Res	Type
1	A	907	LEU
1	A	926	GLU
1	A	939	THR
1	A	946	ASP
1	A	982	ARG
1	A	988	THR
1	A	1001	LYS
1	A	1002	THR
1	A	1008	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1032	SER
1	A	1042	LEU
1	A	1043	THR
1	A	1044	SER
1	A	1046	GLU
1	A	1048	ILE
1	A	1049	GLU
1	A	1052	ARG
1	A	1053	ASP
1	A	1087	PHE
1	A	1088	LEU
1	A	1089	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	231	GLN
1	A	391	GLN
1	A	483	HIS
1	A	601	GLN
1	A	609	GLN
1	A	646	GLN
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	778	GLN
1	A	825	ASN
1	A	908	ASN
1	A	959	ASN
1	A	1083	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	GD9	A	1	-	40,40,40	2.32	14 (35%)	54,59,59	3.90	20 (37%)

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	GD9	A	1	-	-	0/18/36/36	0/2/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	GD9	C8-C3	-6.92	1.39	1.48
2	A	1	GD9	S2-N5	6.32	1.72	1.63
2	A	1	GD9	C22-C21	-3.64	1.34	1.41
2	A	1	GD9	O2-S2	3.62	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	GD9	O1-S2	3.53	1.47	1.43
2	A	1	GD9	C13-S2	3.37	1.82	1.75
2	A	1	GD9	N6-N7	3.22	1.43	1.37
2	A	1	GD9	C1-S1	-3.15	1.70	1.74
2	A	1	GD9	C5-S1	-2.88	1.68	1.73
2	A	1	GD9	C11-N5	-2.74	1.44	1.47
2	A	1	GD9	C4-N2	2.51	1.36	1.32
2	A	1	GD9	C6-C5	-2.46	1.33	1.35
2	A	1	GD9	C2-N1	-2.14	1.33	1.37
2	A	1	GD9	C8-C22	-2.09	1.37	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	GD9	C23-N7-N6	19.09	109.62	104.27
2	A	1	GD9	C11-N5-S2	-9.52	106.75	116.13
2	A	1	GD9	C8-C22-C21	8.04	124.03	118.32
2	A	1	GD9	N1-C3-N2	-7.47	121.12	126.10
2	A	1	GD9	O1-S2-O2	-6.05	110.24	118.68
2	A	1	GD9	C12-C11-N5	-5.43	104.72	109.02
2	A	1	GD9	C6-C5-S1	5.03	116.14	111.87
2	A	1	GD9	C11-C12-N4	-4.47	101.81	110.61
2	A	1	GD9	C8-C3-N2	3.59	122.67	116.97
2	A	1	GD9	C4-N2-C3	3.58	122.14	116.16
2	A	1	GD9	C10-N5-S2	-3.51	112.67	116.13
2	A	1	GD9	O1-S2-N5	3.14	110.17	106.98
2	A	1	GD9	C7-C5-C6	-3.06	121.36	126.87
2	A	1	GD9	C3-N1-C2	2.83	118.37	116.25
2	A	1	GD9	C6-C2-C1	2.65	112.19	110.48
2	A	1	GD9	C16-C17-N3	-2.33	105.58	110.05
2	A	1	GD9	C23-C22-C8	-2.21	129.36	134.55
2	A	1	GD9	C17-N3-C14	2.16	116.11	111.67
2	A	1	GD9	C17-N3-C4	2.05	123.56	118.10
2	A	1	GD9	O2-S2-C13	2.02	111.65	108.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	841/960 (87%)	0.30	59 (7%) 16 14	31, 48, 62, 88	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ASN	12.5
1	A	1044	SER	9.4
1	A	528	ALA	9.1
1	A	896	VAL	6.6
1	A	899	THR	5.5
1	A	374	PRO	5.3
1	A	907	LEU	5.2
1	A	377	THR	5.1
1	A	220	ILE	5.1
1	A	1088	LEU	4.9
1	A	221	PHE	4.9
1	A	143	MET	4.9
1	A	212	TRP	4.7
1	A	527	ILE	4.3
1	A	253	ALA	4.2
1	A	222	ILE	4.2
1	A	544	ARG	4.2
1	A	895	THR	4.1
1	A	375	ARG	4.0
1	A	281	LEU	3.8
1	A	987	LEU	3.8
1	A	1089	HIS	3.7
1	A	1091	VAL	3.7
1	A	234	LYS	3.5
1	A	489	GLY	3.4
1	A	378	ASP	3.3
1	A	248	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	373	LEU	3.3
1	A	766	GLN	3.2
1	A	1041	GLN	3.2
1	A	898	ASN	3.1
1	A	272	LEU	3.1
1	A	1068	PHE	3.1
1	A	988	THR	3.0
1	A	404	PHE	3.0
1	A	320	LYS	3.0
1	A	216	ALA	2.9
1	A	1043	THR	2.9
1	A	1045	LYS	2.8
1	A	900	GLY	2.8
1	A	232	THR	2.7
1	A	233	ILE	2.6
1	A	282	VAL	2.6
1	A	303	ILE	2.5
1	A	403	PRO	2.5
1	A	995	MET	2.5
1	A	251	LYS	2.5
1	A	948	HIS	2.4
1	A	991	PHE	2.4
1	A	1075	CYS	2.3
1	A	902	PHE	2.3
1	A	823	LEU	2.2
1	A	1086	TRP	2.2
1	A	250	THR	2.2
1	A	321	GLU	2.2
1	A	994	VAL	2.2
1	A	244	ILE	2.0
1	A	215	ILE	2.0
1	A	153	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GD9	A	1	35/35	0.16	-0.62	86,91,95,97	0

6.5 Other polymers

There are no such residues in this entry.