Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:49 PM GMT

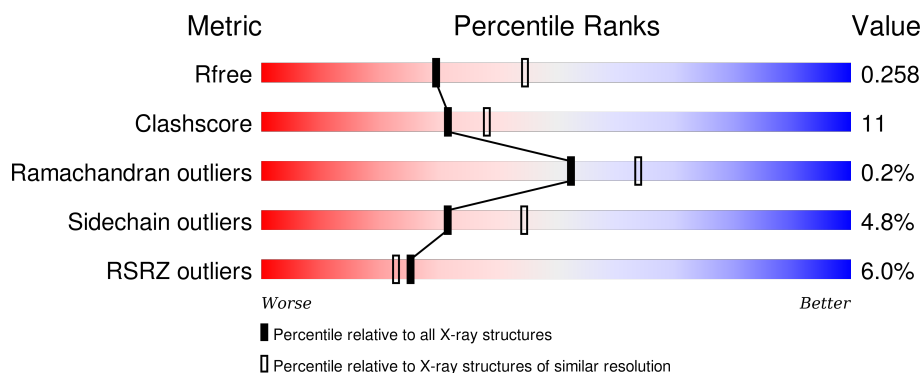|		
PDB ID	:	4GB9
Title	:	Potent and Highly Selective Benzimidazole Inhibitors of PI3K-delta
Authors	:	Murray, J.M.
Deposited on	:	2012-07-26
Resolution	:	2.44 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		11
Ramachandran outliers		0.2%
Sidechain outliers		4.8%
RSRZ outliers		6.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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 <=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	5% · 66% · 19% · 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6911 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
			Total	C	N	O	S			
1	A	840	6801	4365	1160	1241	35	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	INITIATING METHIONINE	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-[1-({2-[2-(DIMETHYLAMINO)-1H-BENZIMIDAZOL-1-YL]-9-METHYL-6-(MORPHOLIN-4-YL)-9H-PURIN-8-YL}METHYL)PIPERIDIN-4-YL]PROPAN-2-OL (three-letter code: 0WR) (formula: $C_{28}H_{39}N_9O_2$).
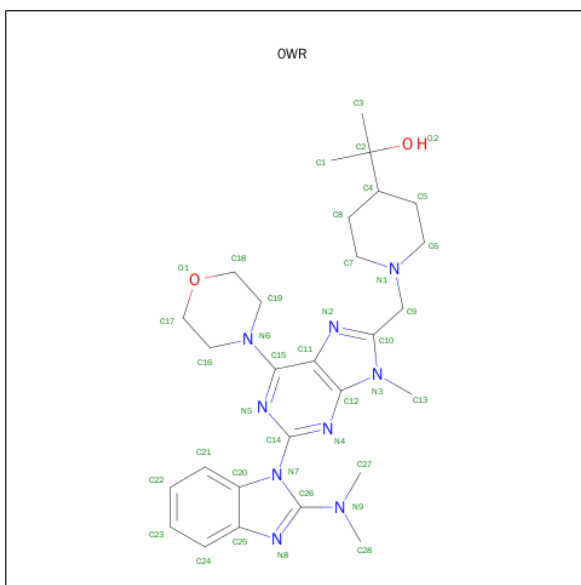
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 39	C 28	N 9	O 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total 71	O 71	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 subunit gamma isoform
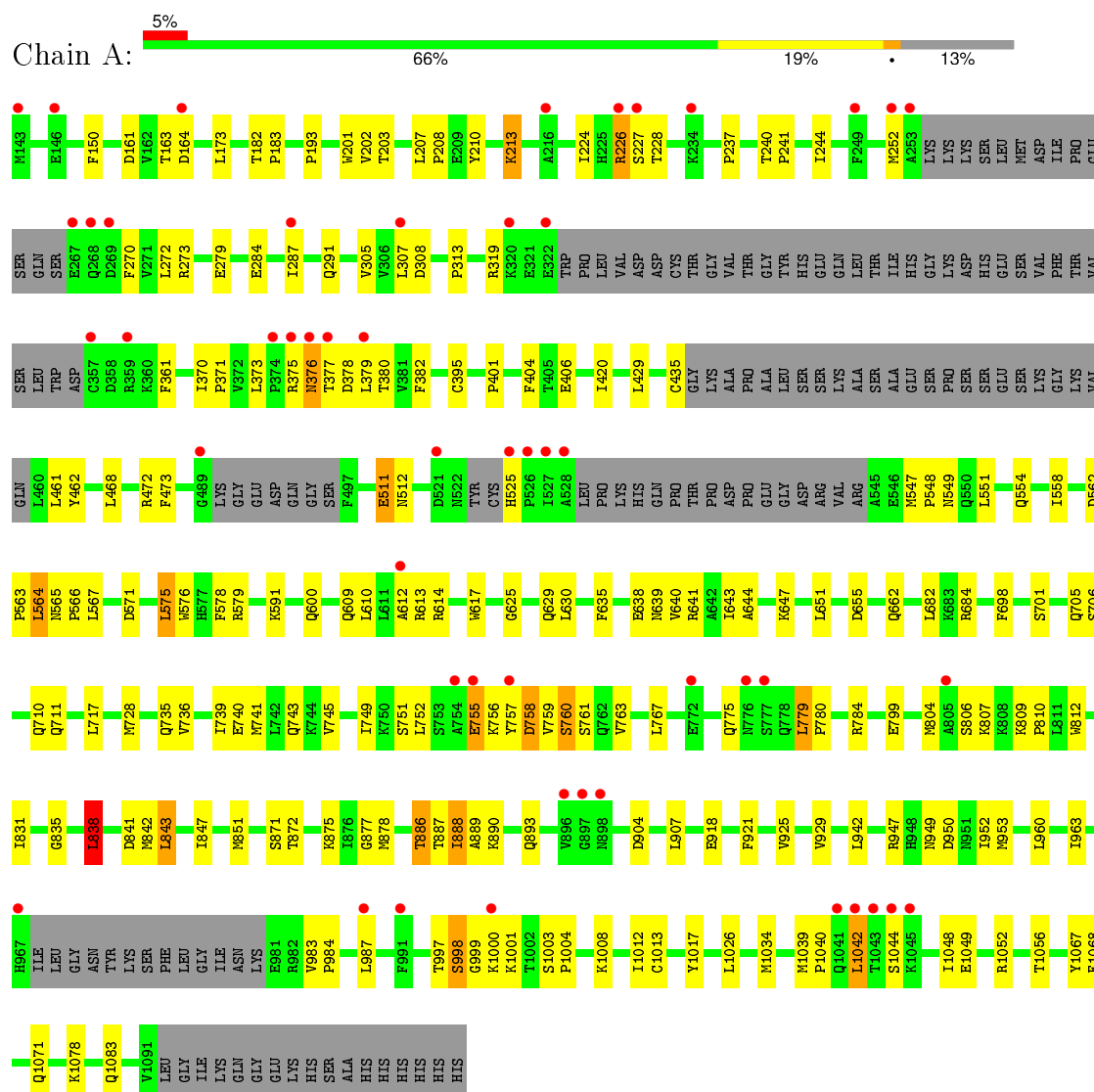
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.35Å 66.02Å 102.28Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	53.65 – 2.44 61.12 – 2.44	Depositor EDS
% Data completeness (in resolution range)	97.2 (53.65-2.44) 97.2 (61.12-2.44)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1066)	Depositor
R, R_{free}	0.203 , 0.248 0.215 , 0.258	Depositor DCC
R_{free} test set	1705 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	1 of 33607 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6911	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 0WR

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	0.55	0/6947	0.83	8/9398 (0.1%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	838	LEU	CB-CG-CD2	-9.25	95.27	111.00
1	A	373	LEU	CA-CB-CG	8.88	135.73	115.30
1	A	779	LEU	CA-CB-CG	7.95	133.58	115.30
1	A	749	ILE	CG1-CB-CG2	-6.91	96.20	111.40
1	A	1042	LEU	CA-CB-CG	6.88	131.14	115.30
1	A	888	ILE	CG1-CB-CG2	-6.38	97.37	111.40
1	A	987	LEU	CA-CB-CG	6.20	129.55	115.30
1	A	525	HIS	C-N-CD	5.16	139.24	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	998	SER	Peptide

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	6801	0	6830	146	0
2	A	39	0	39	1	0
3	A	71	0	0	1	0
All	All	6911	0	6869	146	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 11.

All (146) 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:757:TYR:HA	1:A:758:ASP:CB	1.44	1.36
1:A:757:TYR:CA	1:A:758:ASP:HB2	1.57	1.28
1:A:756:LYS:HA	1:A:758:ASP:CA	1.97	0.95
1:A:756:LYS:HA	1:A:758:ASP:N	1.82	0.94
1:A:565:ASN:OD1	1:A:566:PRO:HD2	1.74	0.87
1:A:759:VAL:HA	1:A:760:SER:CB	2.05	0.86
1:A:757:TYR:CA	1:A:758:ASP:CB	2.30	0.82
1:A:564:LEU:HD12	1:A:1048:ILE:HG21	1.61	0.80
1:A:564:LEU:HD12	1:A:1048:ILE:CG2	2.13	0.77
1:A:757:TYR:CD1	1:A:758:ASP:HB3	2.20	0.77
1:A:576:TRP:CZ3	1:A:579:ARG:HD2	2.25	0.71
1:A:759:VAL:HA	1:A:760:SER:HB2	1.71	0.70
1:A:756:LYS:HA	1:A:757:TYR:C	2.10	0.65
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.79	0.65
1:A:564:LEU:HD21	1:A:1052:ARG:CD	2.27	0.64
1:A:889:ALA:CB	1:A:950:ASP:OD1	2.46	0.64
1:A:999:GLY:O	1:A:1000:LYS:HB2	1.97	0.64
1:A:759:VAL:HA	1:A:760:SER:HB3	1.78	0.63
1:A:706:SER:O	1:A:710:GLN:HB3	2.01	0.60
1:A:562:ASP:OD2	1:A:564:LEU:HD22	2.01	0.60
1:A:228:THR:HG22	1:A:228:THR:O	2.02	0.60
1:A:564:LEU:CD1	1:A:1048:ILE:CG2	2.80	0.59
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.84	0.59
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:HD23	1:A:564:LEU:C	2.25	0.58
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.39	0.57
1:A:564:LEU:CD2	1:A:1052:ARG:HD2	2.35	0.57
1:A:947:ARG:NH2	1:A:963:ILE:O	2.36	0.57
1:A:461:LEU:HB3	1:A:462:TYR:CD1	2.40	0.57
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.87	0.56
1:A:838:LEU:O	1:A:842:MET:HG3	2.05	0.56
1:A:564:LEU:CD1	1:A:1048:ILE:HG22	2.35	0.56
1:A:226:ARG:HH21	1:A:270:PHE:HE2	1.54	0.56
1:A:163:THR:O	1:A:163:THR:HG22	2.05	0.56
1:A:635:PHE:O	1:A:641:ARG:HD2	2.07	0.54
1:A:564:LEU:HD21	1:A:1052:ARG:HD3	1.90	0.54
1:A:1017:TYR:OH	1:A:1056:THR:HG23	2.07	0.54
1:A:376:ASN:HD22	1:A:377:THR:HA	1.73	0.54
1:A:925:VAL:O	1:A:929:VAL:HG23	2.08	0.54
1:A:173:LEU:HD11	1:A:711:GLN:HB3	1.89	0.54
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.08	0.53
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.08	0.53
1:A:1044:SER:O	1:A:1048:ILE:HD12	2.09	0.53
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.90	0.53
1:A:756:LYS:HA	1:A:758:ASP:HA	1.85	0.52
1:A:380:THR:O	1:A:435:CYS:HA	2.09	0.52
1:A:240:THR:CG2	1:A:241:PRO:HD2	2.39	0.52
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.90	0.52
1:A:756:LYS:HA	1:A:758:ASP:CB	2.40	0.52
1:A:997:THR:HG23	1:A:1001:LYS:O	2.10	0.52
1:A:755:GLU:O	1:A:756:LYS:C	2.48	0.51
1:A:751:SER:O	1:A:752:LEU:HD23	2.11	0.51
1:A:547:MET:HG2	1:A:578:PHE:CD1	2.45	0.51
1:A:182:THR:HB	1:A:183:PRO:HD3	1.92	0.51
1:A:308:ASP:N	1:A:308:ASP:OD1	2.43	0.51
1:A:757:TYR:CG	1:A:758:ASP:HB3	2.46	0.51
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.46	0.50
1:A:949:ASN:N	1:A:1083:GLN:OE1	2.45	0.50
1:A:799:GLU:N	1:A:799:GLU:OE1	2.42	0.50
1:A:150:PHE:CE1	1:A:319:ARG:HD3	2.46	0.50
1:A:739:ILE:HG13	1:A:740:GLU:H	1.77	0.49
1:A:565:ASN:OD1	1:A:566:PRO:CD	2.52	0.49
1:A:379:LEU:HG	1:A:380:THR:H	1.76	0.49
1:A:376:ASN:HD22	1:A:378:ASP:N	2.11	0.49
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:ILE:HG13	1:A:740:GLU:N	2.28	0.49
1:A:567:LEU:HD21	1:A:591:LYS:HG2	1.94	0.48
1:A:779:LEU:HG	1:A:780:PRO:HD2	1.95	0.48
1:A:736:VAL:HA	1:A:739:ILE:HG12	1.95	0.48
1:A:757:TYR:HA	1:A:758:ASP:HB2	0.60	0.48
1:A:842:MET:HE1	1:A:871:SER:HB3	1.96	0.48
1:A:564:LEU:HD22	1:A:1052:ARG:HD2	1.97	0.47
1:A:739:ILE:O	1:A:743:GLN:HG3	2.14	0.47
1:A:887:THR:HG22	1:A:889:ALA:N	2.30	0.47
1:A:210:TYR:O	1:A:213:LYS:HD3	2.15	0.47
1:A:564:LEU:HD21	1:A:1052:ARG:HD2	1.96	0.47
1:A:640:VAL:O	1:A:643:ILE:HG12	2.14	0.47
1:A:564:LEU:HD23	1:A:564:LEU:O	2.15	0.46
1:A:571:ASP:O	1:A:575:LEU:HD23	2.15	0.46
1:A:953:MET:O	1:A:960:LEU:HD12	2.16	0.46
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.98	0.46
1:A:886:THR:HG22	1:A:887:THR:H	1.81	0.46
1:A:625:GLY:O	1:A:629:GLN:HG3	2.16	0.46
1:A:576:TRP:O	1:A:579:ARG:HD3	2.15	0.46
1:A:757:TYR:CG	1:A:758:ASP:CB	2.99	0.46
1:A:999:GLY:O	1:A:1000:LYS:CB	2.64	0.46
1:A:240:THR:O	1:A:244:ILE:HG23	2.16	0.46
1:A:890:LYS:HA	1:A:893:GLN:HG2	1.97	0.46
1:A:701:SER:O	1:A:705:GLN:HG2	2.16	0.45
1:A:842:MET:HE2	1:A:871:SER:HB2	1.97	0.45
1:A:921:PHE:O	1:A:925:VAL:HG23	2.16	0.45
1:A:639:ASN:O	1:A:643:ILE:HG23	2.16	0.45
1:A:564:LEU:CD2	1:A:564:LEU:C	2.85	0.45
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.99	0.45
1:A:759:VAL:CA	1:A:760:SER:CB	2.84	0.45
1:A:376:ASN:HB2	1:A:377:THR:C	2.37	0.45
1:A:804:MET:HB2	1:A:810:PRO:HG2	1.98	0.45
1:A:698:PHE:O	1:A:701:SER:OG	2.29	0.44
1:A:847:ILE:O	1:A:851:MET:HG3	2.17	0.44
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.83	0.44
1:A:562:ASP:HB2	1:A:563:PRO:HD2	1.99	0.44
1:A:630:LEU:HB2	1:A:644:ALA:HB2	2.00	0.44
1:A:273:ARG:HG3	1:A:279:GLU:O	2.17	0.44
1:A:759:VAL:HG12	1:A:763:VAL:HG21	1.99	0.44
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.82	0.44
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:ASP:OD1	1:A:904:ASP:N	2.52	0.43
1:A:193:PRO:HB2	1:A:313:PRO:HB3	2.01	0.43
1:A:887:THR:HG22	1:A:889:ALA:H	1.84	0.42
1:A:842:MET:CE	1:A:871:SER:HB3	2.49	0.42
1:A:202:VAL:CG1	1:A:203:THR:N	2.81	0.42
1:A:741:MET:O	1:A:745:VAL:HG23	2.20	0.42
1:A:888:ILE:HD13	1:A:952:ILE:HG22	2.01	0.42
1:A:705:GLN:HG2	1:A:705:GLN:H	1.70	0.42
1:A:429:LEU:HB2	1:A:468:LEU:HD21	2.01	0.42
1:A:812:TRP:CH2	2:A:1201:0WR:H17	2.54	0.42
1:A:161:ASP:OD2	1:A:164:ASP:HB2	2.20	0.42
1:A:952:ILE:CG2	1:A:960:LEU:HD11	2.50	0.42
1:A:735:GLN:NE2	1:A:784:ARG:HB2	2.35	0.42
1:A:1003:SER:HB2	1:A:1004:PRO:CD	2.50	0.42
1:A:835:GLY:HA3	1:A:875:LYS:O	2.21	0.41
1:A:227:SER:O	1:A:228:THR:HB	2.19	0.41
1:A:838:LEU:HB2	3:A:1322:HOH:O	2.20	0.41
1:A:240:THR:CG2	1:A:284:GLU:HA	2.50	0.41
1:A:843:LEU:HD23	1:A:1034:MET:HG3	2.02	0.41
1:A:554:GLN:O	1:A:558:ILE:HG13	2.20	0.41
1:A:224:ILE:HA	1:A:305:VAL:O	2.20	0.41
1:A:609:GLN:O	1:A:612:ALA:HB3	2.21	0.41
1:A:807:LYS:HD3	1:A:807:LYS:HA	1.90	0.41
1:A:511:GLU:HG2	1:A:512:ASN:CG	2.40	0.41
1:A:361:PHE:HA	1:A:420:ILE:HD11	2.02	0.41
1:A:804:MET:HE1	1:A:831:ILE:HG23	2.03	0.41
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.19	0.41
1:A:736:VAL:O	1:A:739:ILE:HG13	2.21	0.41
1:A:240:THR:HG22	1:A:241:PRO:HD2	2.02	0.41
1:A:207:LEU:HA	1:A:208:PRO:HD3	1.81	0.41
1:A:613:ARG:H	1:A:613:ARG:HG2	1.74	0.41
1:A:370:ILE:HG13	1:A:371:PRO:HD2	2.03	0.41
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.51	0.41
1:A:684:ARG:HA	1:A:684:ARG:HD2	1.88	0.41
1:A:472:ARG:O	1:A:473:PHE:HB2	2.20	0.41
1:A:406:GLU:N	1:A:406:GLU:OE1	2.52	0.41
1:A:376:ASN:H	1:A:377:THR:HA	1.85	0.40
1:A:756:LYS:HA	1:A:758:ASP:HB2	2.02	0.40
1:A:806:SER:O	1:A:809:LYS:HD3	2.21	0.40
1:A:382:PHE:HB3	1:A:401:PRO:HA	2.02	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	824/966 (85%)	798 (97%)	24 (3%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	758	ASP
1	A	760	SER

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	753/864 (87%)	717 (95%)	36 (5%)	31	44

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	LYS
1	A	226	ARG
1	A	252	MET
1	A	307	LEU
1	A	375	ARG
1	A	376	ASN
1	A	395	CYS
1	A	404	PHE
1	A	511	GLU

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Mol	Chain	Res	Type
1	A	549	ASN
1	A	564	LEU
1	A	575	LEU
1	A	600	GLN
1	A	610	LEU
1	A	638	GLU
1	A	647	LYS
1	A	662	GLN
1	A	682	LEU
1	A	717	LEU
1	A	728	MET
1	A	755	GLU
1	A	761	SER
1	A	767	LEU
1	A	775	GLN
1	A	838	LEU
1	A	841	ASP
1	A	843	LEU
1	A	878	MET
1	A	886	THR
1	A	907	LEU
1	A	918	GLU
1	A	998	SER
1	A	1026	LEU
1	A	1042	LEU
1	A	1049	GLU
1	A	1078	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	762	GLN
1	A	949	ASN
1	A	959	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	#$|Z| > 2$
2	0WR	A	1201	-	38,44,44	1.83	12 (31%)	43,66,66	1.94	10 (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	0WR	A	1201	-	-	0/16/40/40	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	0WR	C16-N6	-3.56	1.41	1.46
2	A	1201	0WR	C8-C4	-3.52	1.43	1.53
2	A	1201	0WR	C19-N6	-3.35	1.41	1.46
2	A	1201	0WR	O2-C2	-3.31	1.38	1.44
2	A	1201	0WR	C15-N6	2.11	1.43	1.36
2	A	1201	0WR	C9-N1	2.14	1.51	1.47
2	A	1201	0WR	C2-C4	2.29	1.58	1.55
2	A	1201	0WR	C12-N4	2.73	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	0WR	C11-N2	2.78	1.41	1.38
2	A	1201	0WR	C15-N5	2.86	1.36	1.32
2	A	1201	0WR	C14-N5	2.99	1.36	1.32
2	A	1201	0WR	C10-N2	3.55	1.41	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	0WR	C12-C11-N2	-2.85	107.04	109.55
2	A	1201	0WR	N4-C14-N5	-2.40	122.25	126.37
2	A	1201	0WR	C3-C2-C4	-2.27	107.46	111.81
2	A	1201	0WR	C13-N3-C10	2.20	129.37	125.22
2	A	1201	0WR	C16-N6-C19	2.22	116.26	111.59
2	A	1201	0WR	C26-N8-C25	2.30	109.89	106.64
2	A	1201	0WR	C14-N5-C15	2.92	120.30	115.25
2	A	1201	0WR	C16-N6-C15	3.45	126.18	117.56
2	A	1201	0WR	C14-N4-C12	3.82	119.69	115.09
2	A	1201	0WR	C9-N1-C7	7.91	128.73	111.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	0WR	1	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 (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, 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	840/966 (86%)	0.28	50 (5%)	25	23	28, 54, 110, 169	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ALA	33.0
1	A	528	ALA	11.6
1	A	1044	SER	9.9
1	A	1041	GLN	7.5
1	A	527	ILE	7.2
1	A	269	ASP	6.9
1	A	268	GLN	6.5
1	A	1042	LEU	6.0
1	A	757	TYR	5.3
1	A	216	ALA	4.6
1	A	252	MET	4.3
1	A	227	SER	4.2
1	A	755	GLU	4.1
1	A	322	GLU	4.0
1	A	249	PHE	3.9
1	A	377	THR	3.9
1	A	776	ASN	3.8
1	A	359	ARG	3.8
1	A	1045	LYS	3.8
1	A	376	ASN	3.4
1	A	772	GLU	3.3
1	A	1000	LYS	3.1
1	A	1043	THR	3.0
1	A	375	ARG	3.0
1	A	525	HIS	2.9
1	A	379	LEU	2.9
1	A	754	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	898	ASN	2.8
1	A	897	GLY	2.8
1	A	805	ALA	2.8
1	A	489	GLY	2.7
1	A	146	GLU	2.7
1	A	267	GLU	2.7
1	A	287	ILE	2.6
1	A	143	MET	2.6
1	A	164	ASP	2.6
1	A	226	ARG	2.6
1	A	320	LYS	2.6
1	A	612	ALA	2.6
1	A	526	PRO	2.5
1	A	307	LEU	2.5
1	A	967	HIS	2.4
1	A	357	CYS	2.4
1	A	896	VAL	2.2
1	A	374	PRO	2.1
1	A	234	LYS	2.1
1	A	521	ASP	2.1
1	A	987	LEU	2.1
1	A	777	SER	2.1
1	A	991	PHE	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	0WR	A	1201	39/39	0.95	0.19	0.85	34,44,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.