Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:26 AM GMT

PDB ID	:	2X38
Title	:	THE CRYSTAL STRUCTURE OF THE MURINE CLASS IA PI 3-KINASE P110DELTA IN COMPLEX WITH IC87114.
Authors	:	Berndt, A.; Miller, S.; Williams, O.; Lee, D.D.; Houseman, B.T.; Pacold, J.I.; Gorrec, F.; Hon, W.-C.; Liu, Y.; Rommel, C.; Gaillard, P.; Ruckle, T.; Schwarz, M.K.; Shokat, K.M.; Shaw, J.P.; Williams, R.L.
Deposited on	:	2010-01-22
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

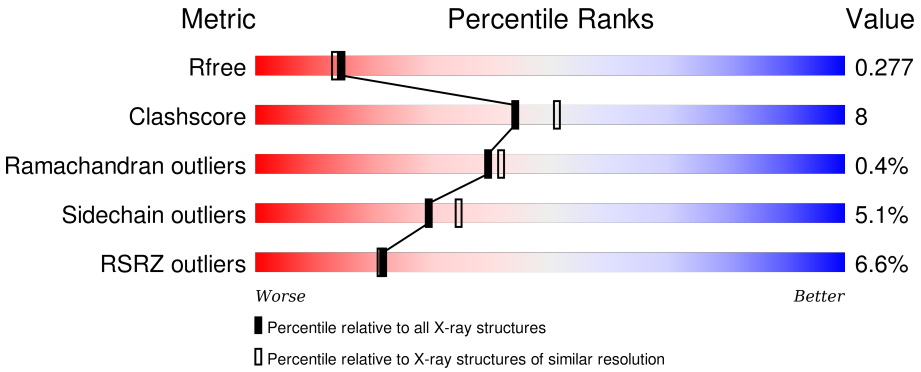
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	940	6%, 71%, 15%, 13%

2 Entry composition

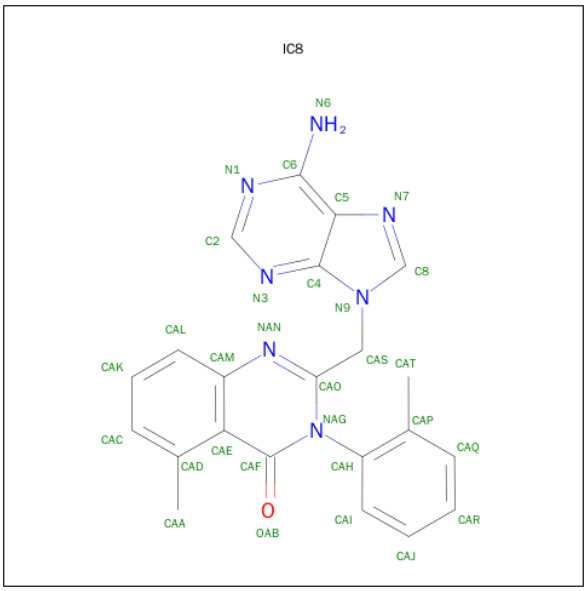
There are 3 unique types of molecules in this entry. The entry contains 6709 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	822	6639	4257	1127	1200	55	0	1	0

- Molecule 2 is 2-[(6-AMINO-9H-PURIN-9-YL)METHYL]-5-METHYL-3-(2-METHYLPHENYL)QUINAZOLIN-4(3H)-ONE (three-letter code: IC8) (formula: $C_{22}H_{19}N_7O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	22	7	1	0	0

- Molecule 3 is water.

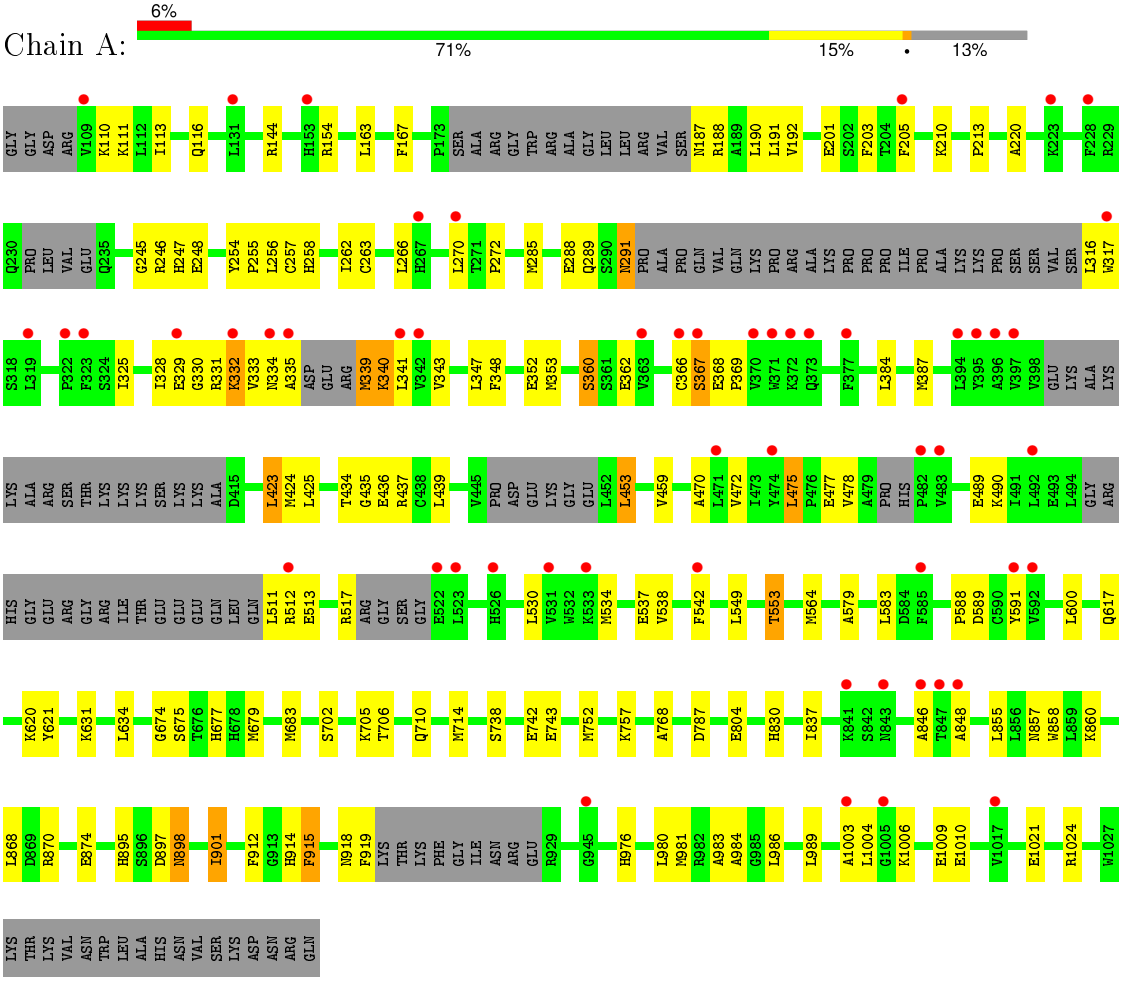
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	40	40	40	0	0

3 Residue-property plots (i)

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 DELTA ISOFORM

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.42Å 64.66Å 116.90Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	56.89 – 2.20 56.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (56.89-2.20) 98.1 (56.86-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.239 , 0.277 0.238 , 0.277	Depositor DCC
R_{free} test set	1578 reflections (3.14%)	DCC
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 51811 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6709	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IC8

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	0.53	0/6782	0.62	2/9150 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	423	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	384	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	6639	0	6619	105	0
2	A	30	0	19	1	0
3	A	40	0	0	3	0
All	All	6709	0	6638	106	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 (106) 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:837:ILE:CD1	1:A:901:ILE:HD11	1.73	1.18
1:A:366:CYS:O	1:A:367:SER:HB2	1.67	0.94
1:A:837:ILE:HD11	1:A:901:ILE:HD11	1.49	0.92
1:A:549:LEU:HG	1:A:564:MET:CE	2.01	0.91
1:A:837:ILE:HD12	1:A:901:ILE:HD11	1.54	0.87
1:A:367:SER:HB3	1:A:369:PRO:N	1.91	0.85
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.59	0.84
1:A:549:LEU:HG	1:A:564:MET:HE1	1.59	0.84
1:A:830:HIS:HD2	3:A:2033:HOH:O	1.64	0.81
1:A:367:SER:HB3	1:A:368:GLU:C	2.00	0.81
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.63	0.79
1:A:617:GLN:NE2	1:A:984:ALA:HA	1.98	0.78
1:A:553:THR:CG2	1:A:564:MET:HE2	2.14	0.77
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.68	0.74
1:A:553:THR:HG21	1:A:564:MET:HE2	1.69	0.73
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.88	0.72
1:A:366:CYS:O	1:A:367:SER:CB	2.40	0.69
1:A:549:LEU:HG	1:A:564:MET:HE3	1.74	0.67
1:A:848:ALA:HB2	1:A:857:ASN:ND2	2.09	0.67
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.58	0.66
1:A:895:HIS:H	1:A:898:ASN:HD21	1.45	0.65
1:A:588:PRO:HB3	3:A:2004:HOH:O	1.96	0.64
1:A:192:VAL:HG13	1:A:272:PRO:HB2	1.80	0.62
1:A:113:ILE:HA	1:A:116:GLN:HE21	1.65	0.62
1:A:870:ARG:NH2	1:A:874:GLU:OE2	2.32	0.61
1:A:914:HIS:HB3	1:A:918:ASN:O	2.01	0.61
1:A:110:LYS:HZ1	1:A:144:ARG:HH12	1.49	0.60
1:A:710:GLN:O	1:A:714:MET:HG2	2.02	0.59
1:A:285:MET:O	1:A:288:GLU:HG2	2.03	0.58
1:A:187:ASN:N	1:A:210:LYS:HD3	2.19	0.58
1:A:256:LEU:O	1:A:262:ILE:HB	2.04	0.58
1:A:837:ILE:CD1	1:A:901:ILE:CD1	2.67	0.57
1:A:706:THR:OG1	1:A:710:GLN:OE1	2.23	0.56
1:A:860:LYS:HG2	1:A:868:LEU:HD22	1.88	0.56
1:A:387:MET:HG3	1:A:589:ASP:HA	1.88	0.56
1:A:787:ASP:OD1	1:A:912:PHE:O	2.23	0.55
1:A:334:ASN:ND2	1:A:335:ALA:H	2.05	0.55
1:A:328:ILE:HG22	1:A:329:GLU:HG2	1.89	0.55
1:A:553:THR:HG22	1:A:564:MET:HE2	1.87	0.55
1:A:436:GLU:O	1:A:437:ARG:HD2	2.06	0.54
1:A:549:LEU:CG	1:A:564:MET:HE1	2.34	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:SER:O	1:A:706:THR:HG22	2.08	0.54
1:A:191:LEU:O	1:A:272:PRO:HD2	2.09	0.53
1:A:332:LYS:NZ	1:A:341:LEU:HD21	2.23	0.53
1:A:617:GLN:HE22	1:A:620:LYS:NZ	2.08	0.52
1:A:329:GLU:HB2	1:A:369:PRO:O	2.10	0.52
1:A:858:TRP:CZ3	1:A:901:ILE:HD13	2.45	0.51
1:A:255:PRO:HG2	1:A:258:HIS:CD2	2.46	0.51
1:A:915:PHE:CD2	1:A:915:PHE:C	2.84	0.50
1:A:837:ILE:HD11	1:A:901:ILE:CD1	2.32	0.50
1:A:617:GLN:HE21	1:A:984:ALA:CA	2.25	0.50
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.45	0.50
1:A:513:GLU:OE1	1:A:542:PHE:HZ	1.95	0.49
1:A:343:VAL:H	1:A:360:SER:HB2	1.77	0.49
1:A:553:THR:CG2	1:A:564:MET:CE	2.88	0.48
1:A:589:ASP:OD2	1:A:591:TYR:HB2	2.13	0.48
1:A:110:LYS:HZ3	1:A:144:ARG:HH12	1.61	0.47
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.49	0.47
1:A:679:MET:O	1:A:683:MET:HG3	2.13	0.47
1:A:489:GLU:HG3	1:A:490:LYS:HE2	1.97	0.47
1:A:984:ALA:HB1	1:A:986:LEU:HD13	1.96	0.47
1:A:213:PRO:HD3	1:A:254:TYR:O	2.14	0.47
1:A:579:ALA:HB1	1:A:600:LEU:HG	1.97	0.46
1:A:330:GLY:HA2	1:A:470:ALA:O	2.16	0.46
1:A:367:SER:HB3	1:A:369:PRO:CA	2.46	0.46
1:A:367:SER:CB	1:A:368:GLU:C	2.80	0.45
1:A:291:ASN:HD21	1:A:675:SER:HA	1.80	0.45
1:A:205:PHE:CZ	1:A:220:ALA:HA	2.51	0.45
1:A:513:GLU:HG2	1:A:542:PHE:CZ	2.52	0.45
1:A:205:PHE:HZ	1:A:220:ALA:HA	1.81	0.45
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.51	0.45
1:A:154:ARG:NH2	1:A:674:GLY:O	2.50	0.45
1:A:247:HIS:HB2	1:A:738:SER:HA	1.97	0.45
1:A:1021:GLU:HA	1:A:1024:ARG:HH11	1.82	0.45
1:A:846:ALA:HA	1:A:857:ASN:HB3	1.98	0.45
2:A:2028:IC8:CAA	2:A:2028:IC8:OAB	2.65	0.44
1:A:332:LYS:HZ2	1:A:341:LEU:HD21	1.83	0.44
1:A:976:HIS:O	1:A:980:LEU:HG	2.18	0.43
1:A:583:LEU:HD11	1:A:600:LEU:CD1	2.44	0.43
1:A:332:LYS:C	1:A:332:LYS:HE3	2.38	0.43
1:A:348:PHE:CE1	1:A:353:MET:HG2	2.53	0.43
1:A:981:MET:HB3	1:A:989:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:HIS:H	1:A:898:ASN:ND2	2.15	0.43
1:A:915:PHE:HD2	1:A:915:PHE:C	2.20	0.43
1:A:163:LEU:HD23	1:A:167:PHE:HD2	1.83	0.43
1:A:435:GLY:HA2	1:A:475:LEU:O	2.19	0.43
1:A:553:THR:HG21	1:A:564:MET:CE	2.43	0.43
1:A:1006:LYS:HB3	1:A:1010:GLU:HB2	2.00	0.43
1:A:1003:ALA:HB1	1:A:1006:LYS:HD2	2.01	0.43
1:A:257:CYS:O	1:A:263:CYS:HB2	2.18	0.42
1:A:553:THR:HG22	1:A:564:MET:CE	2.48	0.42
1:A:424:MET:SD	1:A:459:VAL:HG11	2.60	0.42
1:A:895:HIS:CE1	1:A:897:ASP:HB2	2.55	0.42
1:A:870:ARG:HD2	1:A:870:ARG:HA	1.96	0.41
1:A:347:LEU:HD22	1:A:425:LEU:HD11	2.02	0.41
1:A:534:MET:O	1:A:538:VAL:HG23	2.20	0.41
1:A:439:LEU:O	1:A:470:ALA:HA	2.21	0.41
1:A:434:THR:HG21	1:A:477:GLU:HA	2.03	0.41
1:A:534:MET:SD	1:A:537:GLU:HG3	2.61	0.41
1:A:339:MET:N	3:A:2002:HOH:O	2.53	0.41
1:A:490:LYS:HA	1:A:490:LYS:HD3	1.96	0.41
1:A:340:LYS:HG2	1:A:362:GLU:HB3	2.03	0.41
1:A:325:ILE:HG22	1:A:475:LEU:HD12	2.03	0.40
1:A:453:LEU:HA	1:A:453:LEU:HD12	1.92	0.40
1:A:860:LYS:HG2	1:A:868:LEU:CD2	2.51	0.40
1:A:752:MET:O	1:A:757:LYS:HA	2.21	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	801/940 (85%)	774 (97%)	24 (3%)	3 (0%)	39 42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	SER
1	A	742	GLU
1	A	478	VAL

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	729/827 (88%)	692 (95%)	37 (5%)	29 34

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	188	ARG
1	A	190	LEU
1	A	201	GLU
1	A	203	PHE
1	A	266	LEU
1	A	270	LEU
1	A	291	ASN
1	A	316	LEU
1	A	317	TRP
1	A	331	ARG
1	A	332	LYS
1	A	333	VAL
1	A	339	MET
1	A	340	LYS
1	A	352	GLU
1	A	360	SER
1	A	423	LEU
1	A	453	LEU
1	A	475	LEU
1	A	511	LEU
1	A	512	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	517	ARG
1	A	530	LEU
1	A	553	THR
1	A	631	LYS
1	A	634	LEU
1	A	705	LYS
1	A	743	GLU
1	A	804	GLU
1	A	855	LEU
1	A	898	ASN
1	A	901	ILE
1	A	915	PHE
1	A	919	PHE
1	A	1004	LEU
1	A	1009	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	HIS
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	334	ASN
1	A	344	GLN
1	A	431	GLN
1	A	536	HIS
1	A	617	GLN
1	A	780	ASN
1	A	830	HIS
1	A	898	ASN
1	A	918	ASN

5.3.3 RNA

There are no RNA molecules 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 (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	IC8	A	2028	-	30,34,34	1.78	3 (10%)	24,50,50	2.58	4 (16%)

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	IC8	A	2028	-	-	0/7/8/8	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2028	IC8	CAH-NAG	-3.91	1.40	1.45
2	A	2028	IC8	CAF-NAG	2.68	1.42	1.37
2	A	2028	IC8	CAS-CAO	6.74	1.56	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2028	IC8	N3-C2-N1	-11.29	120.25	128.89
2	A	2028	IC8	CAQ-CAP-CAH	2.02	119.27	116.13
2	A	2028	IC8	CAE-CAF-NAG	2.35	121.14	119.47
2	A	2028	IC8	CAS-CAO-NAN	2.83	120.12	116.09

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	2028	IC8	1	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, 95^{th} 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	822/940 (87%)	0.55	54 (6%)	22	21	8, 21, 35, 53	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ASN	8.6
1	A	341	LEU	7.1
1	A	846	ALA	5.2
1	A	366	CYS	5.0
1	A	228	PHE	4.8
1	A	373	GLN	4.6
1	A	319	LEU	4.6
1	A	370	VAL	4.5
1	A	317	TRP	4.2
1	A	591	TYR	4.1
1	A	372	LYS	4.0
1	A	363	VAL	3.7
1	A	396	ALA	3.7
1	A	394	LEU	3.4
1	A	342	VAL	3.4
1	A	367	SER	3.4
1	A	377	PHE	3.3
1	A	397	VAL	3.2
1	A	270	LEU	3.0
1	A	522	GLU	3.0
1	A	474	TYR	3.0
1	A	131	LEU	3.0
1	A	847	THR	2.9
1	A	945	GLY	2.9
1	A	322	PRO	2.8
1	A	471	LEU	2.8
1	A	371	TRP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	841	LYS	2.8
1	A	323	PHE	2.7
1	A	109	VAL	2.6
1	A	531	VAL	2.6
1	A	205	PHE	2.6
1	A	1003	ALA	2.6
1	A	523	LEU	2.5
1	A	848	ALA	2.5
1	A	329	GLU	2.5
1	A	483	VAL	2.4
1	A	592	VAL	2.4
1	A	332	LYS	2.4
1	A	1017	VAL	2.3
1	A	153	HIS	2.3
1	A	512	ARG	2.3
1	A	335	ALA	2.3
1	A	526	HIS	2.3
1	A	482	PRO	2.3
1	A	267	HIS	2.2
1	A	542	PHE	2.2
1	A	843	ASN	2.1
1	A	533	LYS	2.1
1	A	1005	GLY	2.1
1	A	223	LYS	2.0
1	A	492	LEU	2.0
1	A	585	PHE	2.0
1	A	395	TYR	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^{th} 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	IC8	A	2028	30/30	0.96	0.15	-0.70	23,27,32,34	0

6.5 Other polymers (i)

There are no such residues in this entry.