



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WXI
Title : THE CRYSTAL STRUCTURE OF THE MURINE CLASS IA PI 3-KINASE P110DELTA IN COMPLEX WITH SW30.
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 : 2009-11-09
Resolution : 2.80 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

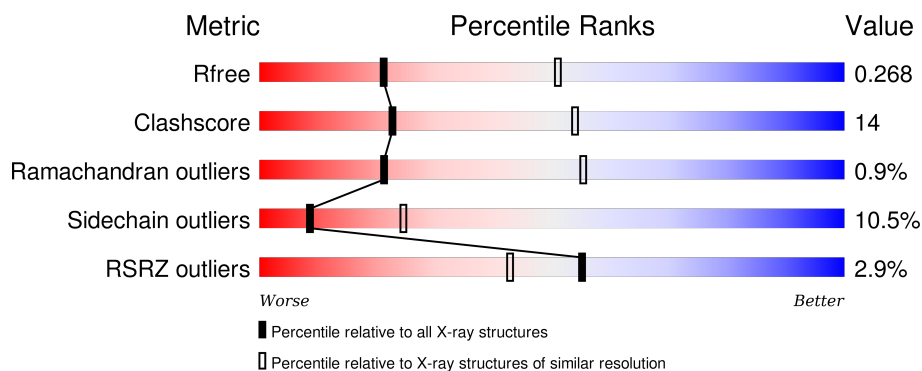
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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	940	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	2028	-	-	X	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6625 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.

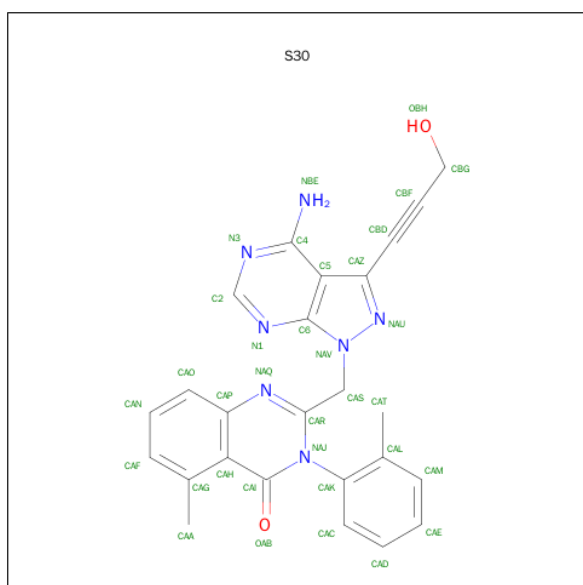
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	815	Total	C	N	O	S	0	0	0
			6569	4214	1113	1188	54			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	EXPRESSION TAG	UNP Q3UDT3

- Molecule 2 is 2-{[4-AMINO-3-(3-HYDROXYPROP-1-YN-1-YL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-1-YL]METHYL}-5-METHYL-3-(2-METHYLPHENYL)QUINAZOLIN-4(3H)-ONE (three-letter code: S30) (formula: C₂₅H₂₁N₇O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	25	7	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.96Å 64.67Å 116.51Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	34.54 – 2.80 34.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (34.54-2.80) 98.6 (34.54-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.32 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.201 , 0.264 0.202 , 0.268	Depositor DCC
R_{free} test set	796 reflections (3.26%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 68.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 25181 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6625	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: GOL, S30

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	0.75	3/6713 (0.0%)	0.80	4/9060 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	745	CYS	CB-SG	-5.65	1.72	1.81
1	A	320	GLU	C-O	5.33	1.33	1.23
1	A	687	GLU	CG-CD	5.31	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	902	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	986	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	423	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	603	LEU	CA-CB-CG	5.10	127.02	115.30

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	6569	0	6545	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	34	0	21	0	0
3	A	6	0	8	9	0
4	A	16	0	0	3	0
All	All	6625	0	6574	179	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 14.

All (179) 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:830:HIS:HA	3:A:2028:GOL:H12	1.37	1.07
1:A:118:SER:HB3	1:A:124:GLY:HA2	1.36	1.07
1:A:837:ILE:CD1	1:A:901:ILE:HD11	1.86	1.06
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.24	1.01
1:A:335:ALA:C	1:A:365:VAL:HG21	1.82	0.99
1:A:830:HIS:HA	3:A:2028:GOL:H31	1.47	0.97
1:A:435:GLY:HA2	1:A:475:LEU:O	1.67	0.94
1:A:334:ASN:ND2	1:A:335:ALA:H	1.67	0.93
1:A:830:HIS:CA	3:A:2028:GOL:H31	2.01	0.91
1:A:549:LEU:HG	1:A:564:MET:HE3	1.54	0.90
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.52	0.90
1:A:436:GLU:O	1:A:437:ARG:HD2	1.73	0.89
1:A:830:HIS:H	3:A:2028:GOL:H31	1.38	0.88
1:A:329:GLU:HB2	1:A:369:PRO:O	1.73	0.87
1:A:830:HIS:N	3:A:2028:GOL:H31	1.89	0.86
1:A:837:ILE:HD12	1:A:901:ILE:HD11	1.56	0.84
1:A:145:GLN:O	1:A:149:GLU:HG3	1.81	0.81
1:A:982:ARG:NH2	1:A:991:CYS:HA	1.96	0.81
1:A:918:ASN:HB2	1:A:988:GLU:CG	2.15	0.77
1:A:830:HIS:H	3:A:2028:GOL:C3	1.98	0.75
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.69	0.74
1:A:432:LEU:HB3	1:A:483:VAL:HG23	1.70	0.74
1:A:846:ALA:HA	1:A:857:ASN:HB3	1.69	0.73
1:A:332:LYS:HE3	1:A:333:VAL:N	2.06	0.71
1:A:713:GLU:HA	1:A:713:GLU:OE1	1.92	0.70
1:A:914:HIS:HD2	1:A:918:ASN:O	1.74	0.70
1:A:698:PHE:HZ	1:A:714:MET:HG3	1.55	0.69
1:A:830:HIS:HA	3:A:2028:GOL:C1	2.17	0.69
1:A:387:MET:CE	1:A:590:CYS:HB3	2.23	0.68
1:A:319:LEU:O	1:A:382:CYS:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:THR:O	1:A:273:HIS:HD2	1.76	0.67
1:A:617:GLN:NE2	1:A:984:ALA:HA	2.09	0.67
1:A:962:ARG:HG2	1:A:962:ARG:NH1	2.04	0.67
1:A:549:LEU:HG	1:A:564:MET:CE	2.24	0.66
1:A:316:LEU:HD12	1:A:317:TRP:HD1	1.61	0.66
1:A:617:GLN:HE22	1:A:620:LYS:HZ2	1.44	0.65
1:A:553:THR:HG21	1:A:564:MET:HG2	1.79	0.64
1:A:256:LEU:O	1:A:262:ILE:HB	1.98	0.64
1:A:188:ARG:NH2	1:A:266:LEU:HD22	2.12	0.64
1:A:617:GLN:HE22	1:A:620:LYS:NZ	1.95	0.64
1:A:837:ILE:CD1	1:A:901:ILE:CD1	2.72	0.63
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.97	0.63
1:A:708:LYS:HD2	1:A:753:ASP:HB2	1.81	0.63
1:A:789:LEU:HD13	1:A:981:MET:HE2	1.81	0.63
1:A:984:ALA:HB3	1:A:986:LEU:HD13	1.80	0.63
1:A:765:SER:HB3	1:A:768:ALA:HB3	1.80	0.62
1:A:432:LEU:HB3	1:A:483:VAL:CG2	2.30	0.62
1:A:339:MET:O	1:A:365:VAL:HB	2.00	0.62
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.33	0.61
1:A:284:ALA:O	1:A:288:GLU:HG2	2.00	0.61
1:A:121:ILE:HG13	1:A:123:LYS:H	1.67	0.60
1:A:984:ALA:CB	1:A:986:LEU:HD13	2.31	0.60
1:A:962:ARG:CG	1:A:962:ARG:HH11	2.06	0.60
1:A:211:ASP:O	1:A:256:LEU:HG	2.01	0.59
1:A:334:ASN:CG	1:A:335:ALA:H	2.05	0.59
1:A:334:ASN:HD22	1:A:335:ALA:H	1.47	0.59
1:A:321:GLN:OE1	1:A:321:GLN:N	2.28	0.59
1:A:706:THR:CG2	1:A:711:THR:OG1	2.52	0.58
1:A:324:SER:HB3	1:A:376:GLU:HG3	1.85	0.58
1:A:735:LEU:HD13	1:A:826:GLU:HB2	1.86	0.58
1:A:858:TRP:CZ3	1:A:901:ILE:HD13	2.39	0.58
1:A:390:LEU:HB2	1:A:425:LEU:HD21	1.87	0.57
1:A:347:LEU:HD22	1:A:425:LEU:HD11	1.85	0.57
1:A:365:VAL:O	1:A:366:CYS:O	2.22	0.56
1:A:343:VAL:H	1:A:360:SER:HB2	1.70	0.56
1:A:256:LEU:HB3	1:A:262:ILE:HG13	1.88	0.56
1:A:866:GLU:HA	4:A:2012:HOH:O	2.05	0.56
1:A:488:LEU:HD22	1:A:591:TYR:CE1	2.40	0.56
1:A:344:GLN:HG3	1:A:359:SER:OG	2.06	0.55
1:A:367:SER:C	1:A:369:PRO:HD3	2.25	0.55
1:A:918:ASN:CB	1:A:988:GLU:HG3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:HIS:HA	1:A:988:GLU:OE1	2.05	0.55
1:A:188:ARG:HH21	1:A:266:LEU:HD22	1.69	0.55
1:A:278:HIS:HD2	1:A:280:SER:H	1.54	0.55
1:A:842:SER:O	1:A:844:MET:HG2	2.05	0.55
1:A:341:LEU:HD11	1:A:365:VAL:O	2.07	0.54
1:A:344:GLN:HB2	1:A:395:TYR:OH	2.07	0.54
1:A:328:ILE:HG22	1:A:329:GLU:HG2	1.90	0.54
1:A:1002:LEU:O	1:A:1003:ALA:C	2.46	0.54
1:A:245:GLY:HA3	1:A:768:ALA:CB	2.34	0.53
1:A:110:LYS:HZ2	1:A:144:ARG:HH12	1.56	0.53
1:A:568:LEU:O	1:A:568:LEU:HD12	2.09	0.53
1:A:278:HIS:CD2	1:A:280:SER:H	2.26	0.53
1:A:247:HIS:O	1:A:738:SER:HB2	2.08	0.53
1:A:873:GLU:OE1	1:A:873:GLU:HA	2.09	0.53
1:A:330:GLY:HA2	1:A:470:ALA:O	2.09	0.53
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.90	0.52
1:A:247:HIS:HB2	1:A:738:SER:HA	1.91	0.52
1:A:285:MET:O	1:A:289:GLN:HG3	2.10	0.52
1:A:368:GLU:N	1:A:369:PRO:HD3	2.23	0.52
1:A:786:GLN:HG2	1:A:913:GLY:HA2	1.92	0.52
1:A:366:CYS:SG	1:A:367:SER:N	2.83	0.52
1:A:918:ASN:HB2	1:A:988:GLU:OE1	2.10	0.52
1:A:331:ARG:HG3	1:A:470:ALA:HB3	1.91	0.52
1:A:488:LEU:HD12	1:A:488:LEU:O	2.09	0.52
1:A:902:ARG:HD2	4:A:2010:HOH:O	2.09	0.51
1:A:799:VAL:O	1:A:803:GLN:HG3	2.10	0.51
1:A:735:LEU:HD12	1:A:776:ILE:HG22	1.92	0.51
1:A:213:PRO:HD3	1:A:254:TYR:O	2.11	0.51
1:A:217:MET:HG2	1:A:276:MET:SD	2.50	0.50
1:A:342:VAL:HB	1:A:395:TYR:CE1	2.47	0.50
1:A:436:GLU:O	1:A:437:ARG:CD	2.54	0.50
1:A:698:PHE:CZ	1:A:714:MET:HG3	2.42	0.49
1:A:902:ARG:CD	4:A:2010:HOH:O	2.60	0.49
1:A:617:GLN:NE2	1:A:984:ALA:CA	2.75	0.49
1:A:581:GLU:HB2	1:A:976:HIS:CE1	2.48	0.49
1:A:332:LYS:C	1:A:332:LYS:HE3	2.33	0.49
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.78	0.49
1:A:618:VAL:HG12	1:A:629:LEU:CD2	2.43	0.49
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.49	0.48
1:A:329:GLU:HB3	1:A:370:VAL:HA	1.95	0.48
1:A:430:ASP:O	1:A:484:TYR:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:MET:HE2	1:A:590:CYS:HB3	1.93	0.48
1:A:150:ALA:O	1:A:153:HIS:HB3	2.14	0.48
1:A:1010:GLU:O	1:A:1013:LYS:HB3	2.13	0.47
1:A:386:ARG:NH2	1:A:430:ASP:OD1	2.45	0.47
1:A:895:HIS:H	1:A:898:ASN:HD21	1.63	0.47
1:A:255:PRO:HG2	1:A:258:HIS:CD2	2.50	0.47
1:A:323:PHE:O	1:A:377:PHE:N	2.33	0.46
1:A:171:LEU:O	1:A:260:GLN:NE2	2.40	0.46
1:A:154:ARG:HD2	1:A:165:TYR:CE2	2.51	0.46
1:A:693:LYS:NZ	1:A:697:ASP:OD2	2.44	0.46
1:A:316:LEU:HD12	1:A:317:TRP:CD1	2.47	0.46
1:A:691:LYS:HG3	1:A:727:ALA:CB	2.46	0.46
1:A:801:TRP:CE2	1:A:963:ALA:HB1	2.51	0.46
1:A:123:LYS:NZ	1:A:127:GLU:OE1	2.44	0.46
1:A:801:TRP:CE3	1:A:808:LEU:HD12	2.51	0.46
1:A:898:ASN:C	1:A:898:ASN:HD22	2.19	0.45
1:A:982:ARG:CZ	1:A:991:CYS:HA	2.46	0.45
1:A:953:PHE:O	1:A:956:PHE:HB3	2.17	0.45
1:A:379:ILE:HD12	1:A:556:ASN:HB2	1.99	0.45
1:A:830:HIS:HA	3:A:2028:GOL:C3	2.33	0.45
1:A:837:ILE:HD11	1:A:901:ILE:HD11	1.91	0.45
1:A:435:GLY:CA	1:A:475:LEU:O	2.53	0.45
1:A:192:VAL:HG22	1:A:272:PRO:HG2	1.99	0.45
1:A:634:LEU:HA	1:A:634:LEU:HD12	1.83	0.45
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.99	0.44
1:A:894:ARG:HA	1:A:898:ASN:HD21	1.81	0.44
1:A:131:LEU:O	1:A:132:ARG:C	2.55	0.44
1:A:787:ASP:OD1	1:A:912:PHE:HD2	2.01	0.44
1:A:862:LYS:HG3	1:A:903:GLU:HG2	2.00	0.44
1:A:433:LYS:HB2	1:A:475:LEU:HD13	1.99	0.44
1:A:918:ASN:HB2	1:A:988:GLU:CD	2.37	0.44
1:A:437:ARG:O	1:A:472:VAL:HA	2.18	0.44
1:A:1010:GLU:O	1:A:1013:LYS:N	2.51	0.44
1:A:528:LYS:HG2	1:A:552:VAL:HG12	2.00	0.43
1:A:387:MET:HE2	1:A:590:CYS:CB	2.49	0.43
1:A:219:CYS:O	1:A:220:ALA:C	2.57	0.43
1:A:370:VAL:HG11	1:A:372:LYS:HE2	2.00	0.43
1:A:901:ILE:O	1:A:901:ILE:HD12	2.18	0.43
1:A:436:GLU:HG2	1:A:437:ARG:H	1.84	0.42
1:A:319:LEU:O	1:A:382:CYS:N	2.50	0.42
1:A:347:LEU:HD23	1:A:390:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:LYS:HE3	1:A:557:LYS:HG3	2.01	0.42
1:A:387:MET:HE3	1:A:590:CYS:HB3	2.00	0.42
1:A:329:GLU:CB	1:A:370:VAL:HA	2.49	0.42
1:A:929:ARG:HH22	1:A:1001:SER:CB	2.32	0.42
1:A:859:LEU:HD21	1:A:905:GLY:HA2	2.01	0.42
1:A:691:LYS:HG3	1:A:727:ALA:HB3	2.02	0.42
1:A:645:HIS:CG	1:A:737:PRO:HG3	2.54	0.42
1:A:834:ILE:HG22	1:A:838:GLN:OE1	2.20	0.42
1:A:416:CYS:HA	1:A:417:PRO:HD3	1.69	0.42
1:A:383:ASP:O	1:A:384:LEU:C	2.58	0.41
1:A:617:GLN:HE21	1:A:984:ALA:CA	2.34	0.41
1:A:192:VAL:HG13	1:A:272:PRO:HB2	2.02	0.41
1:A:830:HIS:N	3:A:2028:GOL:C3	2.66	0.41
1:A:433:LYS:CB	1:A:475:LEU:HD13	2.50	0.41
1:A:387:MET:CE	1:A:590:CYS:CB	2.97	0.41
1:A:918:ASN:HB2	1:A:988:GLU:HG2	1.99	0.41
1:A:752:MET:HB3	1:A:758:PRO:HG2	2.02	0.41
1:A:388:ALA:HB1	1:A:425:LEU:HD12	2.03	0.41
1:A:380:SER:HB3	1:A:383:ASP:OD1	2.20	0.41
1:A:356:LYS:HG2	1:A:356:LYS:H	1.63	0.41
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.79	0.40
1:A:938:PHE:N	1:A:938:PHE:CD1	2.88	0.40
1:A:380:SER:O	1:A:383:ASP:HB2	2.22	0.40
1:A:229:ARG:HA	1:A:229:ARG:NE	2.34	0.40
1:A:684:LYS:HD2	1:A:684:LYS:HA	1.67	0.40
1:A:415:ASP:N	1:A:415:ASP:OD2	2.54	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	795/940 (85%)	746 (94%)	42 (5%)	7 (1%)	21	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	CYS
1	A	355	CYS
1	A	478	VAL
1	A	1003	ALA
1	A	384	LEU
1	A	742	GLU
1	A	913	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	721/827 (87%)	645 (90%)	76 (10%)	8	24

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LYS
1	A	111	LYS
1	A	112	LEU
1	A	118	SER
1	A	119	LEU
1	A	188	ARG
1	A	190	LEU
1	A	199	SER
1	A	206	GLN
1	A	209	THR
1	A	216	LEU
1	A	228	PHE
1	A	229	ARG
1	A	267	HIS

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Mol	Chain	Res	Type
1	A	270	LEU
1	A	279	SER
1	A	281	SER
1	A	316	LEU
1	A	317	TRP
1	A	319	LEU
1	A	325	ILE
1	A	331	ARG
1	A	332	LYS
1	A	339	MET
1	A	340	LYS
1	A	352	GLU
1	A	358	VAL
1	A	360	SER
1	A	365	VAL
1	A	367	SER
1	A	368	GLU
1	A	382	CYS
1	A	394	LEU
1	A	398	VAL
1	A	415	ASP
1	A	423	LEU
1	A	445	VAL
1	A	453	LEU
1	A	467	SER
1	A	471	LEU
1	A	488	LEU
1	A	523	LEU
1	A	529	ASP
1	A	530	LEU
1	A	548	ARG
1	A	553	THR
1	A	560	ASP
1	A	565	LEU
1	A	594	SER
1	A	599	SER
1	A	631	LYS
1	A	634	LEU
1	A	680	LYS
1	A	684	LYS
1	A	713	GLU
1	A	714	MET

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Mol	Chain	Res	Type
1	A	726	GLU
1	A	731	LEU
1	A	743	GLU
1	A	744	VAL
1	A	754	SER
1	A	757	LYS
1	A	787	ASP
1	A	804	GLU
1	A	836	ASN
1	A	843	ASN
1	A	855	LEU
1	A	895	HIS
1	A	898	ASN
1	A	901	ILE
1	A	915	PHE
1	A	919	PHE
1	A	962	ARG
1	A	988	GLU
1	A	990	SER
1	A	1004	LEU

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	116	GLN
1	A	258	HIS
1	A	273	HIS
1	A	278	HIS
1	A	334	ASN
1	A	558	HIS
1	A	617	GLN
1	A	780	ASN
1	A	786	GLN
1	A	895	HIS
1	A	898	ASN
1	A	914	HIS

5.3.3 RNA ⓘ

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](#)

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	S30	A	1500	-	33,38,38	1.70	6 (18%)	28,55,55	2.77	7 (25%)
3	GOL	A	2028	-	5,5,5	0.57	0	5,5,5	1.21	1 (20%)

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	S30	A	1500	-	-	0/8/12/12	0/5/5/5
3	GOL	A	2028	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	S30	CAK-NAJ	-4.58	1.40	1.45
2	A	1500	S30	CBD-CBF	-2.98	1.16	1.19
2	A	1500	S30	C5-C6	-2.03	1.37	1.43
2	A	1500	S30	CAF-CAG	2.03	1.42	1.37
2	A	1500	S30	CAA-CAG	3.01	1.57	1.51
2	A	1500	S30	CAS-CAR	5.14	1.54	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	S30	N1-C2-N3	-11.32	120.22	128.89
2	A	1500	S30	CAC-CAK-NAJ	-3.35	114.18	118.50
2	A	1500	S30	CAE-CAM-CAL	-3.12	115.58	121.09
2	A	1500	S30	CAZ-C5-C6	-2.10	102.59	106.55
3	A	2028	GOL	O3-C3-C2	2.21	120.92	110.18
2	A	1500	S30	CAD-CAE-CAM	2.97	124.54	120.19
2	A	1500	S30	CAM-CAL-CAK	3.35	121.35	116.13
2	A	1500	S30	CAS-CAR-NAQ	4.80	122.94	116.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2028	GOL	9	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	815/940 (86%)	-0.04	24 (2%) 55 43	6, 19, 33, 47	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ASN	6.1
1	A	341	LEU	5.8
1	A	846	ALA	4.8
1	A	364	ASN	3.5
1	A	524	TYR	3.3
1	A	317	TRP	3.1
1	A	534	MET	3.1
1	A	913	GLY	3.1
1	A	847	THR	2.9
1	A	361	SER	2.9
1	A	529	ASP	2.8
1	A	842	SER	2.7
1	A	329	GLU	2.7
1	A	474	TYR	2.7
1	A	843	ASN	2.6
1	A	360	SER	2.5
1	A	342	VAL	2.5
1	A	540	GLU	2.3
1	A	339	MET	2.3
1	A	483	VAL	2.2
1	A	840	ASN	2.1
1	A	319	LEU	2.1
1	A	492	LEU	2.1
1	A	526	HIS	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(\AA^2)	Q<0.9
3	GOL	A	2028	6/6	0.74	0.28	6.38	49,52,52,54	0
2	S30	A	1500	34/34	0.97	0.14	-1.00	20,25,29,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.