



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:12 AM UTC

PDB ID : 2WXI / pdb_00002wxi
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

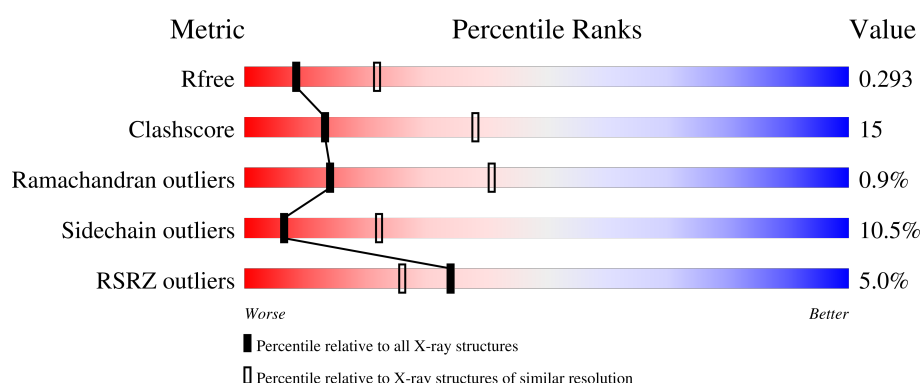
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	-

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.

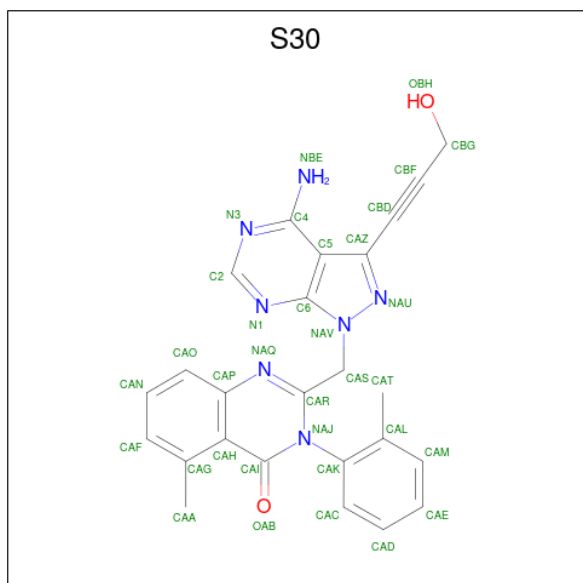
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

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

There is a discrepancy between the modelled and reference sequences:

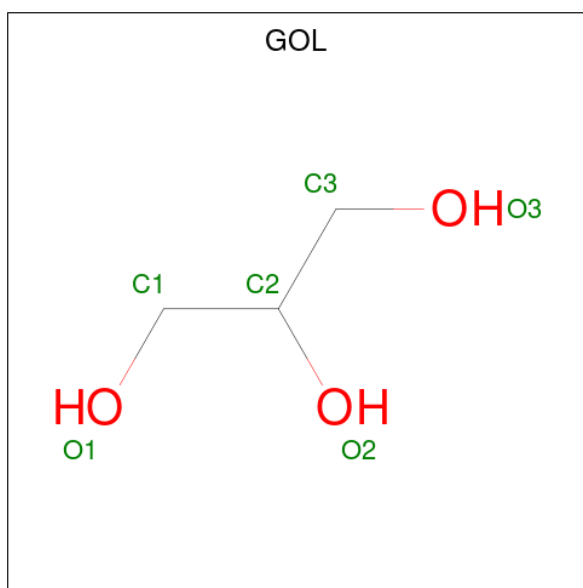
Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	expression tag	UNP Q3UDT3

- 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 (CCD ID: S30) (formula: C₂₅H₂₁N₇O₂).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

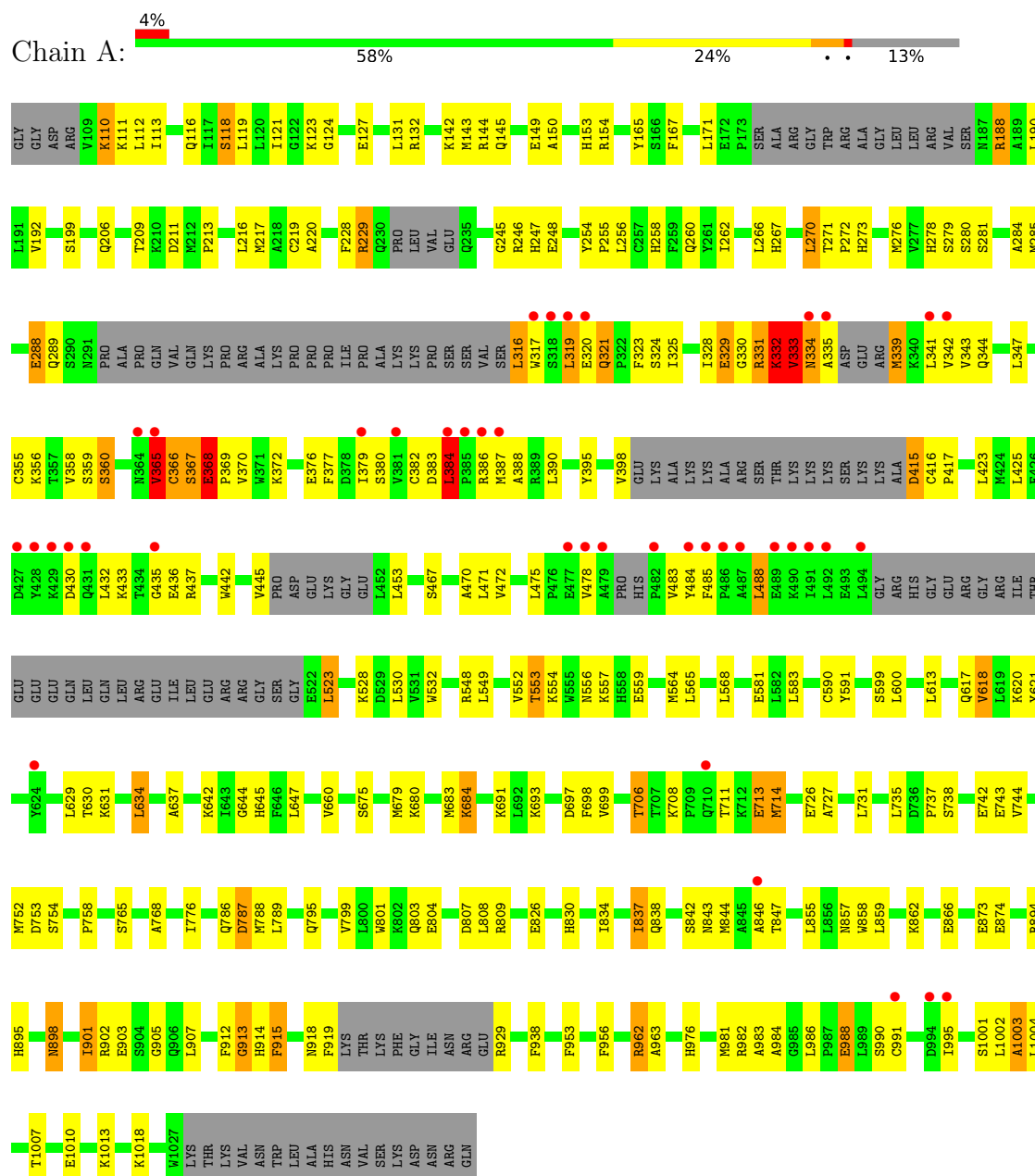
- Molecule 4 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



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) 98.5 (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 (Not available) , 0.293	Depositor DCC
R_{free} test set	796 reflections (3.16%)	wwPDB-VP
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 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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, 0.333 respectively for untwinned datasets, and 0.375, 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: S30, GOL

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	0.90	2/6713 (0.0%)	1.08	23/9060 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	GLU	C-O	6.80	1.33	1.24
1	A	320	GLU	CA-C	5.98	1.60	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ASN	N-CA-C	9.24	120.11	108.19
1	A	332	LYS	N-CA-C	6.78	117.00	108.45
1	A	837	ILE	N-CA-C	-6.67	104.26	110.53
1	A	329	GLU	N-CA-C	6.61	117.20	107.88
1	A	333	VAL	N-CA-C	6.13	116.91	107.78
1	A	368	GLU	CA-C-N	6.07	126.03	119.78
1	A	368	GLU	C-N-CA	6.07	126.03	119.78
1	A	321	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	A	630	THR	N-CA-C	-5.95	104.14	111.40
1	A	384	LEU	CA-C-N	-5.93	114.52	120.21
1	A	384	LEU	C-N-CA	-5.93	114.52	120.21
1	A	485	PHE	CA-C-N	5.88	125.88	119.89
1	A	485	PHE	C-N-CA	5.88	125.88	119.89
1	A	699	VAL	N-CA-C	5.76	116.41	110.36
1	A	675	SER	N-CA-C	5.61	117.87	107.60
1	A	442	TRP	CA-C-N	5.57	125.88	119.92
1	A	442	TRP	C-N-CA	5.57	125.88	119.92
1	A	270	LEU	N-CA-C	5.53	117.43	110.24
1	A	647	LEU	N-CA-C	-5.49	105.20	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	VAL	N-CA-C	5.37	116.75	110.62
1	A	795	GLN	N-CA-C	-5.29	105.59	111.36
1	A	915	PHE	N-CA-C	5.15	117.24	109.41
1	A	523	LEU	N-CA-C	5.07	116.77	108.76

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	6569	0	6545	195	0
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	195	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 15.

All (195) 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:335:ALA:C	1:A:365:VAL:HG21	1.82	1.03
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.24	1.01
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: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:549:LEU:HG	1:A:564:MET:HE1	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:549:LEU:CG	1:A:564:MET:HE1	2.12	0.80
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
1:A:271:THR:O	1:A:273:HIS:HD2	1.76	0.67
1:A:142:LYS:HG2	1:A:143:MET:HE2	1.77	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:789:LEU:HD13	1:A:981:MET:HE2	1.79	0.65
1:A:256:LEU:O	1:A:262:ILE:HB	1.98	0.64
1:A:553:THR:HG21	1:A:564:MET:HG2	1.79	0.64
1:A:188:ARG:NH2	1:A:266:LEU:HD22	2.12	0.64
1:A:334:ASN:CG	1:A:335:ALA:H	2.05	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:387:MET:HE3	1:A:590:CYS:HB3	1.80	0.63
1:A:708:LYS:HD2	1:A:753:ASP:HB2	1.81	0.63
1:A:617:GLN:HE22	1:A:620:LYS:HZ2	1.47	0.63
1:A:984:ALA:HB3	1:A:986:LEU:HD13	1.80	0.63
1:A:167:PHE:HZ	1:A:285:MET:HE1	1.64	0.62
1:A:432:LEU:HB3	1:A:483:VAL:CG2	2.30	0.62
1:A:765:SER:HB3	1:A:768:ALA:HB3	1.80	0.62
1:A:339:MET:O	1:A:365:VAL:HB	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:367:SER:C	1:A:369:PRO:HD3	2.25	0.60
1:A:984:ALA:CB	1:A:986:LEU:HD13	2.31	0.60
1:A:962:ARG:HH11	1:A:962:ARG:CG	2.06	0.60
1:A:211:ASP:O	1:A:256:LEU:HG	2.01	0.59
1:A:116:GLN:HE21	1:A:679:MET:HE3	1.67	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:387:MET:HE2	1:A:590:CYS:SG	2.43	0.58
1:A:1002:LEU:O	1:A:1003:ALA:C	2.46	0.58
1:A:324:SER:HB3	1:A:376:GLU:HG3	1.85	0.58
1:A:706:THR:CG2	1:A:711:THR:OG1	2.52	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:842:SER:O	1:A:844:MET:HE2	2.06	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:914:HIS:HA	1:A:988:GLU:OE1	2.05	0.55
1:A:918:ASN:CB	1:A:988:GLU:HG3	2.36	0.55
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.71	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:110:LYS:HZ2	1:A:144:ARG:HH12	1.55	0.54
1:A:116:GLN:HG2	1:A:683:MET:HE1	1.89	0.54
1:A:328:ILE:HG22	1:A:329:GLU:HG2	1.90	0.54
1:A:245:GLY:HA3	1:A:768:ALA:CB	2.34	0.53
1:A:332:LYS:HE3	1:A:332:LYS:C	2.33	0.53
1:A:568:LEU:HD12	1:A:568:LEU:O	2.09	0.53
1:A:247:HIS:O	1:A:738:SER:HB2	2.08	0.53
1:A:278:HIS:CD2	1:A:280:SER:H	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:GLU:HA	1:A:873:GLU:OE1	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:331:ARG:HG3	1:A:470:ALA:HB3	1.91	0.52
1:A:918:ASN:HB2	1:A:988:GLU:OE1	2.10	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:898:ASN:HD22	1:A:898:ASN:C	2.19	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:131:LEU:O	1:A:132:ARG:C	2.55	0.49
1:A:918:ASN:HB2	1:A:988:GLU:CD	2.37	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
1:A:150:ALA:O	1:A:153:HIS:HB3	2.14	0.48
1:A:553:THR:CG2	1:A:564:MET:HE3	2.44	0.48
1:A:219:CYS:O	1:A:220:ALA:C	2.57	0.47
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:613:LEU:HD22	1:A:788:MET:HE3	1.96	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:549:LEU:CD1	1:A:564:MET:HE1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:HD2	1:A:165:TYR:CE2	2.51	0.46
1:A:383:ASP:O	1:A:384:LEU:C	2.58	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:953:PHE:O	1:A:956:PHE:HB3	2.17	0.45
1:A:982:ARG:CZ	1:A:991:CYS:HA	2.46	0.45
1:A:116:GLN:NE2	1:A:679:MET:HE3	2.30	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:HD12	1:A:634:LEU:HA	1.83	0.45
1:A:334:ASN:CG	1:A:335:ALA:N	2.75	0.44
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.99	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:894:ARG:HA	1:A:898:ASN:HD21	1.81	0.44
1:A:433:LYS:HB2	1:A:475:LEU:HD13	1.99	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:807:ASP:OD1	1:A:807:ASP:C	2.60	0.43
1:A:809:ARG:HE	1:A:874:GLU:CD	2.26	0.43
1:A:528:LYS:HG2	1:A:552:VAL:HG12	2.00	0.43
1:A:370:VAL:HG11	1:A:372:LYS:HE2	2.00	0.43
1:A:901:ILE:HD12	1:A:901:ILE:O	2.18	0.43
1:A:907:LEU:C	1:A:907:LEU:HD23	2.44	0.43
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
1:A:436:GLU:HG2	1:A:437:ARG:H	1.84	0.42
1:A:554:LYS:HE3	1:A:557:LYS:HG3	2.01	0.42
1:A:329:GLU:CB	1:A:370:VAL:HA	2.49	0.42
1:A:808:LEU:O	1:A:809:ARG:C	2.61	0.42
1:A:859:LEU:HD21	1:A:905:GLY:HA2	2.01	0.42
1:A:929:ARG:HH22	1:A:1001:SER:CB	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:192:VAL:HG13	1:A:272:PRO:HB2	2.02	0.41
1:A:617:GLN:HE21	1:A:984:ALA:CA	2.34	0.41
1:A:387:MET:CE	1:A:590:CYS:CB	2.97	0.41
1:A:433:LYS:CB	1:A:475:LEU:HD13	2.50	0.41
1:A:830:HIS:N	3:A:2028:GOL:C3	2.66	0.41
1:A:981:MET:C	1:A:983:ALA:N	2.78	0.41
1:A:752:MET:HB3	1:A:758:PRO:HG2	2.02	0.41
1:A:918:ASN:HB2	1:A:988:GLU:HG2	1.99	0.41
1:A:356:LYS:H	1:A:356:LYS:HG2	1.63	0.41
1:A:380:SER:HB3	1:A:383:ASP:OD1	2.20	0.41
1:A:388:ALA:HB1	1:A:425:LEU:HD12	2.03	0.41
1:A:859:LEU:HA	1:A:859:LEU:HD23	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:NE	1:A:229:ARG:HA	2.34	0.40
1:A:415:ASP:OD2	1:A:415:ASP:N	2.54	0.40
1:A:684:LYS:HD2	1:A:684:LYS:HA	1.67	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%)	14 41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	CYS
1	A	355	CYS

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Mol	Chain	Res	Type
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%)	6 22

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	113	ILE
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
1	A	270	LEU
1	A	279	SER
1	A	281	SER
1	A	288	GLU
1	A	316	LEU
1	A	319	LEU

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Mol	Chain	Res	Type
1	A	325	ILE
1	A	331	ARG
1	A	332	LYS
1	A	333	VAL
1	A	339	MET
1	A	358	VAL
1	A	360	SER
1	A	365	VAL
1	A	367	SER
1	A	368	GLU
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	530	LEU
1	A	548	ARG
1	A	553	THR
1	A	559	GLU
1	A	565	LEU
1	A	599	SER
1	A	618	VAL
1	A	631	LYS
1	A	634	LEU
1	A	642	LYS
1	A	680	LYS
1	A	684	LYS
1	A	706	THR
1	A	713	GLU
1	A	714	MET
1	A	726	GLU
1	A	731	LEU
1	A	743	GLU
1	A	744	VAL
1	A	754	SER
1	A	787	ASP
1	A	804	GLU
1	A	843	ASN

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Mol	Chain	Res	Type
1	A	847	THR
1	A	855	LEU
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	995	ILE
1	A	1004	LEU
1	A	1007	THR
1	A	1018	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	156	GLN
1	A	193	ASN
1	A	258	HIS
1	A	273	HIS
1	A	278	HIS
1	A	334	ASN
1	A	422	ASN
1	A	526	HIS
1	A	558	HIS
1	A	617	GLN
1	A	780	ASN
1	A	786	GLN
1	A	851	ASN
1	A	895	HIS
1	A	898	ASN
1	A	906	GLN
1	A	914	HIS
1	A	970	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 oligosaccharides 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	-	36,38,38	2.20	9 (25%)	47,55,55	2.97	20 (42%)
3	GOL	A	2028	-	5,5,5	0.64	0	5,5,5	1.31	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	-	-	0/6/12/12	0/5/5/5
3	GOL	A	2028	-	-	4/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	S30	NAV-NAU	-7.13	1.23	1.36
2	A	1500	S30	CAS-CAR	5.43	1.54	1.49
2	A	1500	S30	CBD-CBF	-3.99	1.16	1.19
2	A	1500	S30	CAR-NAQ	3.57	1.35	1.29
2	A	1500	S30	CAK-NAJ	-3.26	1.40	1.44
2	A	1500	S30	CAA-CAG	3.18	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	S30	CAH-CAI	-2.96	1.40	1.47
2	A	1500	S30	C5-C6	-2.49	1.37	1.40
2	A	1500	S30	CAS-NAV	2.02	1.49	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	S30	C5-C6-N1	-9.07	117.35	126.97
2	A	1500	S30	N1-C6-NAV	6.53	135.53	125.34
2	A	1500	S30	CAZ-NAU-NAV	6.11	109.62	103.83
2	A	1500	S30	N3-C2-N1	-5.52	120.22	128.58
2	A	1500	S30	C2-N1-C6	5.13	124.36	111.83
2	A	1500	S30	CAS-NAV-C6	4.44	130.63	127.81
2	A	1500	S30	OAB-CAI-NAJ	-4.15	114.86	120.38
2	A	1500	S30	CAH-CAI-NAJ	3.93	119.51	115.14
2	A	1500	S30	CAL-CAK-NAJ	3.80	123.48	118.69
2	A	1500	S30	CAR-CAS-NAV	-3.67	107.04	112.14
2	A	1500	S30	CAE-CAM-CAL	-3.54	115.58	121.14
2	A	1500	S30	CAD-CAE-CAM	3.48	124.54	120.24
2	A	1500	S30	C4-C5-C6	3.33	118.24	115.74
2	A	1500	S30	CAM-CAL-CAK	3.16	121.35	117.42
2	A	1500	S30	C6-C5-CAZ	-3.10	102.59	104.74
2	A	1500	S30	CAS-NAV-NAU	-3.06	117.58	120.01
2	A	1500	S30	C5-CAZ-CBD	2.60	129.85	123.49
3	A	2028	GOL	O3-C3-C2	2.34	120.92	110.38
2	A	1500	S30	C5-C4-N3	2.29	120.69	118.64
2	A	1500	S30	CAC-CAK-NAJ	-2.23	114.18	118.61
2	A	1500	S30	CAA-CAG-CAF	-2.16	116.11	120.28

There are no chirality outliers.

All (4) torsion outliers are listed below:

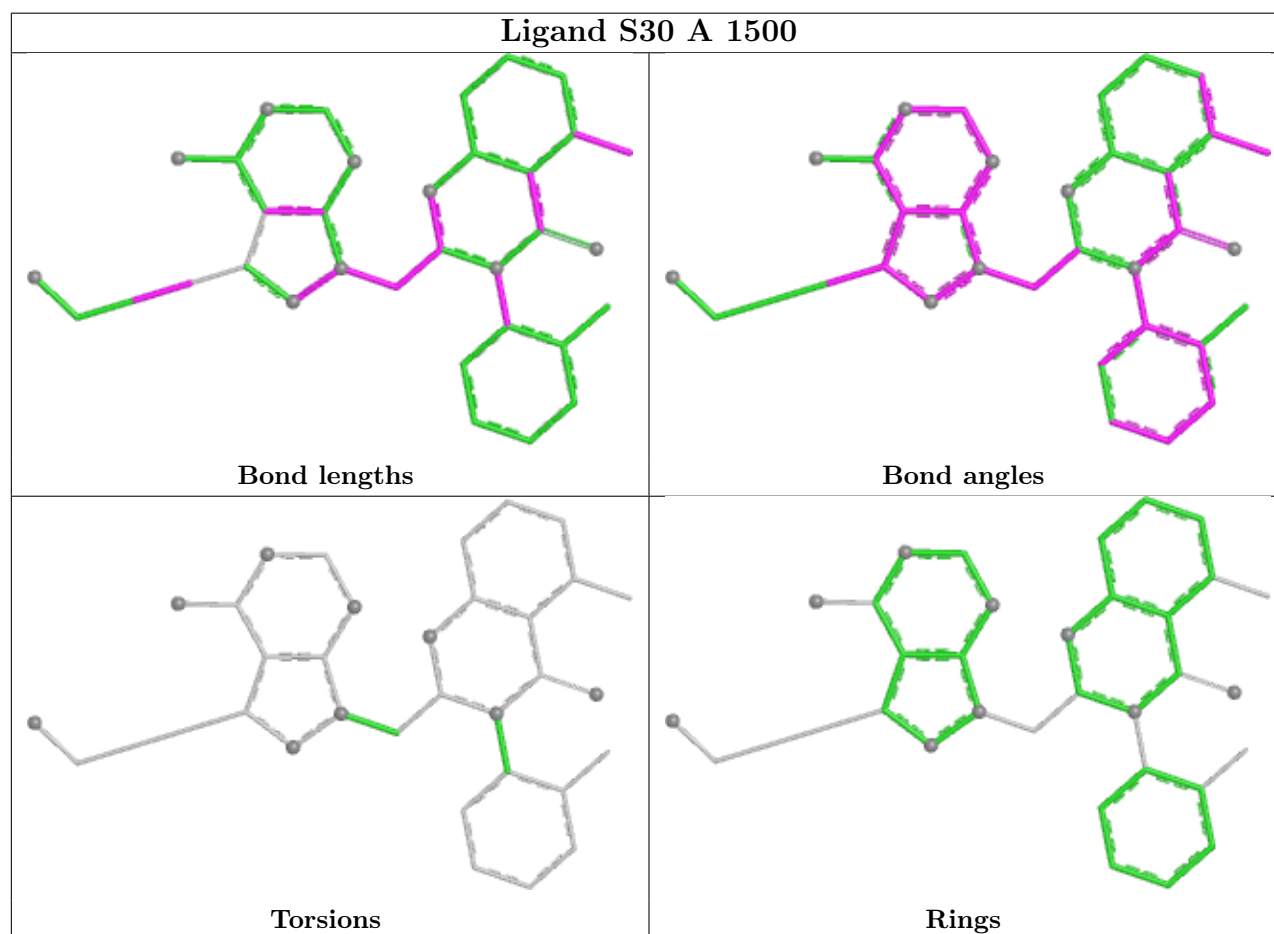
Mol	Chain	Res	Type	Atoms
3	A	2028	GOL	C1-C2-C3-O3
3	A	2028	GOL	O2-C2-C3-O3
3	A	2028	GOL	O1-C1-C2-C3
3	A	2028	GOL	O1-C1-C2-O2

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

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	815/940 (86%)	0.23	41 (5%) 34 26	6, 19, 33, 47	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	ALA	6.1
1	A	487	ALA	5.4
1	A	494	LEU	5.4
1	A	318	SER	4.7
1	A	428	TYR	4.7
1	A	482	PRO	4.6
1	A	334	ASN	4.2
1	A	486	PRO	4.0
1	A	846	ALA	3.8
1	A	484	TYR	3.6
1	A	491	ILE	3.6
1	A	478	VAL	3.5
1	A	341	LEU	3.4
1	A	317	TRP	3.3
1	A	319	LEU	3.2
1	A	386	ARG	3.2
1	A	320	GLU	3.1
1	A	489	GLU	3.1
1	A	490	LYS	3.0
1	A	429	LYS	2.9
1	A	485	PHE	2.8
1	A	430	ASP	2.8
1	A	387	MET	2.7
1	A	991	CYS	2.6
1	A	384	LEU	2.5
1	A	381	VAL	2.5
1	A	364	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	994	ASP	2.4
1	A	624	TYR	2.4
1	A	379	ILE	2.3
1	A	477	GLU	2.3
1	A	365	VAL	2.3
1	A	427	ASP	2.3
1	A	435	GLY	2.3
1	A	995	ILE	2.2
1	A	431	GLN	2.2
1	A	492	LEU	2.1
1	A	335	ALA	2.1
1	A	710	GLN	2.0
1	A	342	VAL	2.0
1	A	385	PRO	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](#)

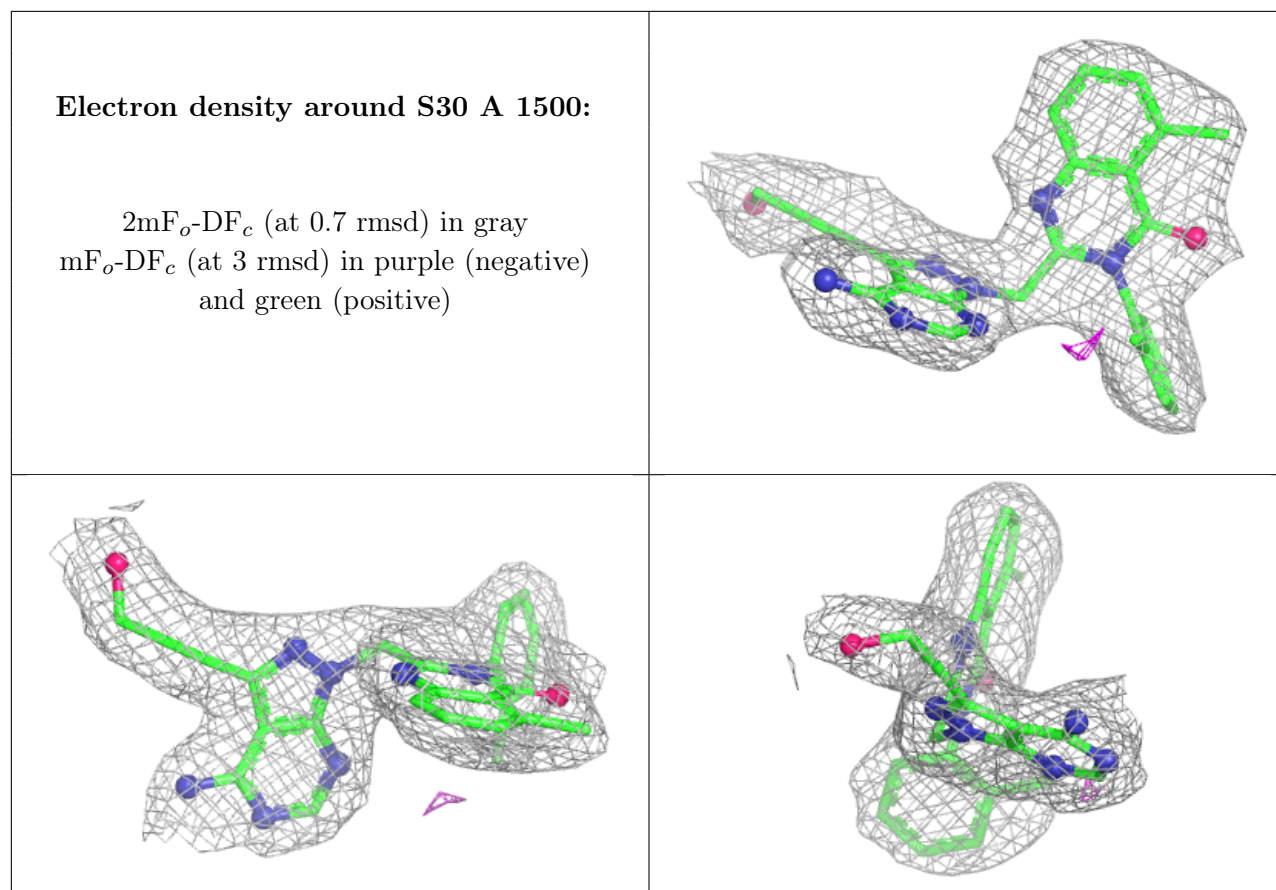
There are no oligosaccharides in this entry.

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	2028	6/6	0.68	0.18	49,52,52,54	0
2	S30	A	1500	34/34	0.96	0.07	20,25,29,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.