



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:06 PM UTC

PDB ID : 2WXK / pdb_00002wxk
Title : The crystal structure of the murine class IA PI 3-kinase p110delta in complex with INK666.
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 : 2.90 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

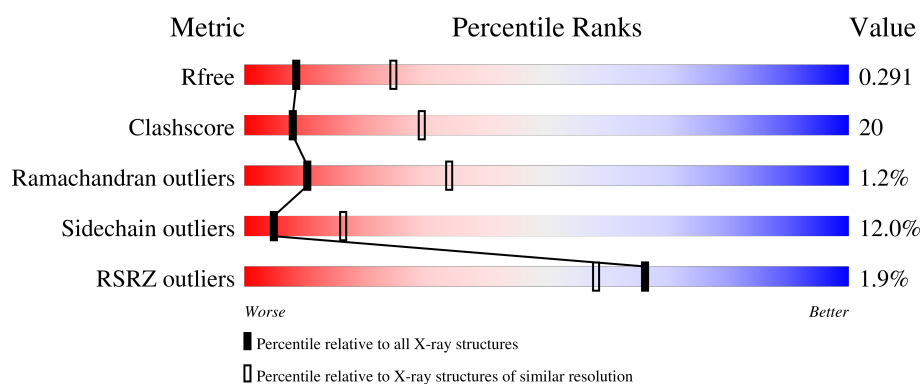
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	2% 53% 30% 6% 11%

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.

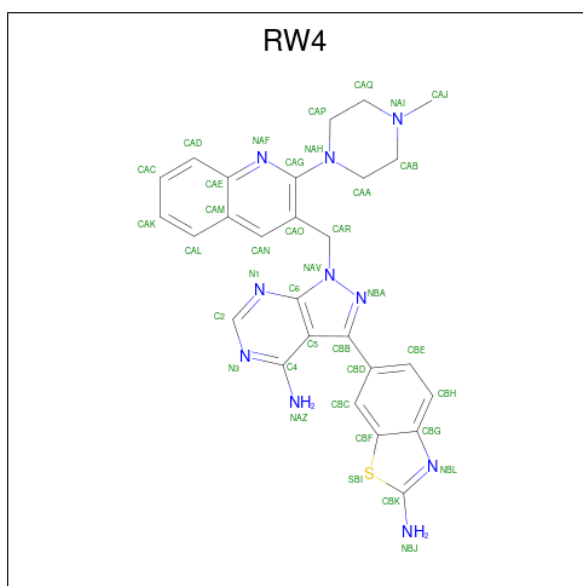
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total	C	N	O	S	0	0	0
			6739	4315	1144	1226	54			

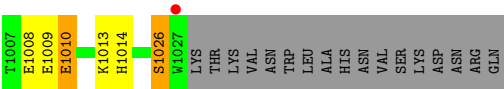
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is 3-(2-amino-1,3-benzothiazol-6-yl)-1-{[2-(4-methylpiperazin-1-yl)quinolin-3-yl]methyl}-1H-pyrazolo[3,4-d]pyrimidin-4-amine (CCD ID: RW4) (formula: C₂₇H₂₆N₁₀S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			38	27	10	1		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.36Å 143.67Å 223.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.36 – 2.90 68.36 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.36-2.90) 100.0 (68.36-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.213 , 0.287 0.213 , 0.291	Depositor DCC
R_{free} test set	733 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6777	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: RW4

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	0.89	4/6882 (0.1%)	1.11	32/9281 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	GLY	N-CA	5.94	1.51	1.45
1	A	730	HIS	CA-C	-5.85	1.48	1.53
1	A	930	VAL	CA-CB	5.55	1.61	1.54
1	A	661	ALA	CA-CB	-5.06	1.45	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ARG	N-CA-C	8.46	122.08	107.28
1	A	333	VAL	N-CA-C	8.10	119.78	108.12
1	A	442	TRP	CA-C-N	7.25	128.91	119.84
1	A	442	TRP	C-N-CA	7.25	128.91	119.84
1	A	334	ASN	N-CA-C	7.23	117.42	107.73
1	A	332	LYS	N-CA-C	6.78	117.44	107.88
1	A	991	CYS	N-CA-C	6.14	116.11	108.19
1	A	418	ILE	CB-CA-C	6.06	117.19	111.44
1	A	444	SER	N-CA-C	6.03	118.44	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	GLY	N-CA-C	-6.03	105.35	112.64
1	A	656	HIS	N-CA-C	-5.93	105.90	113.02
1	A	329	GLU	N-CA-C	5.91	116.21	107.88
1	A	230	GLN	N-CA-C	5.78	117.98	109.42
1	A	417	PRO	CA-C-N	-5.63	117.39	123.08
1	A	417	PRO	C-N-CA	-5.63	117.39	123.08
1	A	590	CYS	N-CA-C	5.62	117.86	111.11
1	A	443	PRO	CA-C-N	-5.51	115.64	123.03
1	A	443	PRO	C-N-CA	-5.51	115.64	123.03
1	A	675	SER	N-CA-C	5.38	116.21	107.23
1	A	718	CYS	N-CA-C	-5.35	105.61	111.82
1	A	115	SER	CA-C-N	-5.32	112.74	120.29
1	A	115	SER	C-N-CA	-5.32	112.74	120.29
1	A	643	ILE	CB-CA-C	-5.29	104.92	111.70
1	A	330	GLY	N-CA-C	5.26	120.72	110.73
1	A	911	ASP	N-CA-C	5.25	117.59	111.02
1	A	197	GLU	N-CA-C	5.21	117.70	111.71
1	A	963	ALA	N-CA-C	-5.13	105.69	111.28
1	A	782	ASP	CA-C-N	-5.07	115.91	123.11
1	A	782	ASP	C-N-CA	-5.07	115.91	123.11
1	A	910	ILE	CB-CA-C	-5.01	104.32	111.34
1	A	708	LYS	CA-C-N	-5.01	113.49	119.05
1	A	708	LYS	C-N-CA	-5.01	113.49	119.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	GLN	Peptide

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	6739	0	6704	259	0
2	A	38	0	26	6	0
All	All	6777	0	6730	265	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 20.

All (265) 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:918:ASN:ND2	1:A:927:ARG:HG3	1.41	1.35
1:A:355:CYS:SG	1:A:379:ILE:HD12	1.88	1.12
1:A:549:LEU:HG	1:A:564:MET:HE1	1.13	1.11
1:A:231:PRO:HB2	1:A:232:LEU:HA	1.07	1.05
1:A:550:LEU:O	1:A:553:THR:HG22	1.57	1.01
1:A:918:ASN:ND2	1:A:927:ARG:CG	2.24	0.99
2:A:1500:RW4:HAZ2	2:A:1500:RW4:CBE	1.78	0.94
1:A:231:PRO:CB	1:A:232:LEU:HA	1.97	0.94
1:A:918:ASN:HD22	1:A:927:ARG:HG3	1.28	0.94
1:A:918:ASN:HD21	1:A:927:ARG:HG3	1.33	0.92
1:A:231:PRO:HB2	1:A:232:LEU:CA	2.00	0.91
1:A:512:ARG:O	1:A:515:LEU:HD12	1.71	0.91
2:A:1500:RW4:HAZ2	2:A:1500:RW4:HBE	1.34	0.90
1:A:901:ILE:HD13	1:A:901:ILE:N	1.88	0.87
1:A:929:ARG:O	1:A:929:ARG:HG3	1.73	0.87
1:A:982:ARG:HD2	1:A:995:ILE:HD11	1.56	0.85
1:A:512:ARG:HD3	1:A:534:MET:HG2	1.57	0.85
1:A:355:CYS:SG	1:A:379:ILE:CD1	2.64	0.84
1:A:365:VAL:O	1:A:365:VAL:HG13	1.77	0.82
1:A:842:SER:O	1:A:844:MET:HE2	1.78	0.81
1:A:234:GLU:OE2	1:A:239:TYR:OH	1.97	0.81
2:A:1500:RW4:HBE	2:A:1500:RW4:NAZ	1.95	0.80
1:A:959:TYR:HD1	1:A:959:TYR:H	1.29	0.80
1:A:394:LEU:HD23	1:A:418:ILE:HD12	1.63	0.80
1:A:550:LEU:O	1:A:553:THR:CG2	2.32	0.78
1:A:317:TRP:HA	1:A:382:CYS:HB2	1.65	0.77
1:A:699:VAL:O	1:A:703:SER:OG	2.03	0.77
1:A:191:LEU:CD2	1:A:204:THR:HG22	2.15	0.76
1:A:332:LYS:HE3	1:A:332:LYS:O	1.85	0.76
1:A:343:VAL:H	1:A:360:SER:HB3	1.51	0.76
1:A:332:LYS:HB2	1:A:332:LYS:HZ2	1.53	0.73
1:A:434:THR:HA	1:A:475:LEU:HB3	1.71	0.72
1:A:507:GLU:CG	1:A:511:LEU:HD23	2.19	0.72
1:A:841:LYS:NZ	1:A:844:MET:HE3	2.05	0.72
1:A:762:MET:HE2	1:A:775:GLY:HA3	1.73	0.71
1:A:365:VAL:O	1:A:365:VAL:CG1	2.38	0.71
1:A:345:ALA:O	1:A:357:THR:HB	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:MET:HE3	1:A:978:PHE:CE1	2.27	0.69
1:A:928:GLU:HG3	1:A:929:ARG:N	2.07	0.69
1:A:379:ILE:N	1:A:379:ILE:HD13	2.07	0.69
1:A:507:GLU:HG2	1:A:511:LEU:HD23	1.73	0.69
1:A:918:ASN:HD21	1:A:927:ARG:CG	1.94	0.69
1:A:154:ARG:HD2	1:A:165:TYR:CE2	2.28	0.68
1:A:901:ILE:HD13	1:A:901:ILE:H	1.58	0.68
1:A:193:ASN:HD21	1:A:202:SER:HB2	1.59	0.68
1:A:435:GLY:HA2	1:A:475:LEU:O	1.94	0.68
1:A:841:LYS:HZ2	1:A:844:MET:HE3	1.59	0.68
1:A:395:TYR:HA	1:A:418:ILE:HG22	1.77	0.67
1:A:841:LYS:O	1:A:844:MET:HG2	1.95	0.66
1:A:841:LYS:HG3	1:A:844:MET:HG3	1.78	0.66
1:A:173:PRO:HG2	1:A:802:LYS:HD3	1.76	0.66
1:A:332:LYS:HE3	1:A:332:LYS:C	2.21	0.66
1:A:116:GLN:HE21	1:A:679:MET:HE3	1.62	0.65
1:A:515:LEU:C	1:A:515:LEU:HD13	2.22	0.64
1:A:513:GLU:HG2	1:A:542:PHE:CZ	2.32	0.64
1:A:428:TYR:CE2	1:A:429:LYS:HD3	2.32	0.64
1:A:395:TYR:HB2	1:A:416:CYS:O	1.98	0.64
1:A:325:ILE:HD11	1:A:375:LEU:HD12	1.79	0.63
1:A:914:HIS:HB3	1:A:918:ASN:O	1.99	0.63
1:A:918:ASN:HD21	1:A:927:ARG:CD	2.12	0.63
1:A:957:ARG:O	1:A:961:GLU:HG3	1.99	0.63
1:A:539:GLN:HG3	1:A:571:TRP:CE3	2.35	0.62
1:A:762:MET:HE1	1:A:827:VAL:HG11	1.82	0.62
1:A:935:THR:HG22	1:A:937:ASP:H	1.64	0.62
1:A:494:LEU:HD11	1:A:559:GLU:HG2	1.81	0.62
1:A:550:LEU:C	1:A:553:THR:HG22	2.24	0.62
2:A:1500:RW4:CBE	2:A:1500:RW4:NAZ	2.56	0.61
1:A:162:TRP:CE3	1:A:286:ARG:HG3	2.36	0.61
1:A:512:ARG:HD3	1:A:534:MET:CG	2.31	0.60
1:A:155:GLN:HE21	1:A:290:SER:HB3	1.67	0.60
1:A:435:GLY:O	1:A:475:LEU:N	2.21	0.60
1:A:246:ARG:NH1	1:A:248:GLU:OE2	2.33	0.60
1:A:385:PRO:HD2	1:A:388:ALA:HB2	1.83	0.60
1:A:335:ALA:O	1:A:365:VAL:HG11	2.02	0.60
1:A:762:MET:CE	1:A:827:VAL:HG11	2.32	0.60
1:A:793:MET:HE3	1:A:978:PHE:CD1	2.37	0.60
1:A:901:ILE:N	1:A:901:ILE:CD1	2.65	0.59
1:A:335:ALA:C	1:A:365:VAL:HG11	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:TRP:CZ3	1:A:286:ARG:HG3	2.36	0.59
1:A:397:VAL:CG2	1:A:398:VAL:H	2.16	0.59
1:A:959:TYR:HD1	1:A:959:TYR:N	1.97	0.59
1:A:507:GLU:C	1:A:511:LEU:N	2.61	0.58
1:A:855:LEU:O	1:A:859:LEU:HD12	2.03	0.58
1:A:213:PRO:HD3	1:A:254:TYR:O	2.03	0.58
1:A:214:LEU:HD11	1:A:237:GLU:HG3	1.85	0.58
1:A:788:MET:HG3	1:A:815:CYS:O	2.03	0.58
1:A:390:LEU:HB2	1:A:425:LEU:HD21	1.86	0.57
1:A:707:THR:HB	1:A:709:PRO:HD2	1.86	0.57
1:A:936:TYR:HB2	1:A:1026:SER:OG	2.04	0.57
1:A:833:THR:OG1	1:A:836:ASN:HB2	2.05	0.57
1:A:191:LEU:CD2	1:A:204:THR:CG2	2.82	0.57
1:A:154:ARG:HD2	1:A:165:TYR:CZ	2.39	0.56
1:A:1006:LYS:HB3	1:A:1010:GLU:OE1	2.05	0.56
1:A:820:ASP:O	1:A:821:ARG:C	2.47	0.56
1:A:397:VAL:HG22	1:A:398:VAL:N	2.21	0.55
1:A:142:LYS:HG2	1:A:143:MET:HE2	1.88	0.55
1:A:918:ASN:HD21	1:A:927:ARG:HD3	1.71	0.55
1:A:319:LEU:N	1:A:319:LEU:HD12	2.22	0.55
1:A:278:HIS:CD2	1:A:280:SER:H	2.25	0.55
1:A:955:ARG:O	1:A:958:GLY:N	2.40	0.55
1:A:895:HIS:HB2	1:A:897:ASP:OD1	2.07	0.55
1:A:110:LYS:HE3	1:A:144:ARG:HH22	1.72	0.54
1:A:378:ASP:CG	1:A:378:ASP:O	2.49	0.54
1:A:907:LEU:HD23	1:A:907:LEU:C	2.33	0.54
1:A:316:LEU:HB3	1:A:318:SER:OG	2.07	0.54
1:A:431:GLN:NE2	1:A:482:PRO:HB3	2.23	0.54
1:A:556:ASN:O	1:A:557:LYS:HD3	2.07	0.54
1:A:898:ASN:C	1:A:898:ASN:HD22	2.15	0.54
1:A:842:SER:O	1:A:844:MET:CE	2.54	0.54
1:A:225:ALA:HB1	1:A:230:GLN:HB3	1.89	0.54
1:A:397:VAL:CG2	1:A:398:VAL:N	2.71	0.54
1:A:317:TRP:CD1	1:A:317:TRP:C	2.87	0.53
1:A:332:LYS:HB3	1:A:469:ALA:HB2	1.90	0.53
1:A:511:LEU:HD12	1:A:511:LEU:O	2.09	0.53
1:A:145:GLN:O	1:A:149:GLU:HG3	2.09	0.53
1:A:332:LYS:HB3	1:A:469:ALA:CB	2.39	0.53
1:A:904:SER:OG	1:A:906:GLN:NE2	2.40	0.52
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.91	0.52
1:A:895:HIS:N	1:A:898:ASN:HD21	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLU:HB3	1:A:474:TYR:HB3	1.92	0.52
1:A:507:GLU:HG3	1:A:511:LEU:HB3	1.91	0.52
2:A:1500:RW4:NBA	2:A:1500:RW4:HAN	2.23	0.52
1:A:553:THR:HG23	1:A:555:TRP:NE1	2.25	0.52
1:A:155:GLN:NE2	1:A:290:SER:HA	2.25	0.51
1:A:242:GLN:HG3	1:A:249:TYR:CE1	2.45	0.51
1:A:379:ILE:HD13	1:A:379:ILE:H	1.76	0.51
1:A:527:GLU:O	1:A:531:VAL:HG23	2.10	0.51
1:A:793:MET:CE	1:A:978:PHE:CE1	2.92	0.51
1:A:512:ARG:HH11	1:A:534:MET:CG	2.24	0.51
1:A:244:ASN:ND2	1:A:273:HIS:HB3	2.26	0.51
1:A:291:ASN:ND2	1:A:676:THR:H	2.09	0.51
1:A:528:LYS:HB3	1:A:552:VAL:HB	1.91	0.51
1:A:841:LYS:HZ2	1:A:844:MET:CE	2.24	0.51
1:A:488:LEU:HG	1:A:492:LEU:HD22	1.93	0.51
1:A:208:SER:OG	1:A:210:LYS:HG3	2.11	0.51
1:A:434:THR:HA	1:A:475:LEU:CB	2.40	0.51
1:A:708:LYS:HG3	1:A:751:PHE:CZ	2.46	0.51
1:A:353:MET:HG2	1:A:355:CYS:O	2.12	0.50
1:A:938:PHE:CD1	1:A:938:PHE:N	2.78	0.50
1:A:645:HIS:CG	1:A:737:PRO:HG3	2.47	0.50
1:A:512:ARG:HH11	1:A:534:MET:HG2	1.76	0.50
1:A:394:LEU:HD22	1:A:441:MET:HE1	1.92	0.50
1:A:752:MET:HE3	1:A:754:SER:OG	2.12	0.50
1:A:191:LEU:HD22	1:A:204:THR:CG2	2.42	0.49
1:A:809:ARG:HG3	1:A:874:GLU:OE2	2.11	0.49
1:A:208:SER:OG	1:A:210:LYS:CG	2.60	0.49
1:A:291:ASN:HD21	1:A:676:THR:H	1.61	0.49
1:A:394:LEU:CD2	1:A:418:ILE:HD12	2.36	0.49
1:A:550:LEU:HA	1:A:564:MET:HE3	1.94	0.49
1:A:135:GLU:HG3	1:A:428:TYR:CG	2.47	0.49
1:A:225:ALA:HB2	1:A:232:LEU:HD22	1.94	0.49
1:A:419:ALA:HB3	1:A:441:MET:HE3	1.94	0.49
1:A:754:SER:O	1:A:755:LYS:HB2	2.12	0.49
1:A:1002:LEU:O	1:A:1003:ALA:C	2.55	0.49
1:A:418:ILE:C	1:A:444:SER:HB2	2.37	0.49
1:A:157:LEU:O	1:A:286:ARG:NH1	2.46	0.49
1:A:191:LEU:HD23	1:A:204:THR:HG22	1.92	0.49
1:A:982:ARG:HD2	1:A:995:ILE:CD1	2.38	0.49
1:A:574:LEU:O	1:A:602:LYS:NZ	2.30	0.49
1:A:425:LEU:O	1:A:432:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:LYS:NZ	1:A:844:MET:CE	2.76	0.48
1:A:958:GLY:O	1:A:959:TYR:C	2.54	0.48
1:A:549:LEU:CG	1:A:564:MET:HE1	2.09	0.48
1:A:542:PHE:O	1:A:544:GLU:N	2.47	0.48
1:A:698:PHE:HZ	1:A:714:MET:HB3	1.79	0.48
1:A:332:LYS:HB2	1:A:332:LYS:NZ	2.27	0.48
1:A:116:GLN:HE21	1:A:679:MET:CE	2.25	0.48
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.94	0.48
1:A:224:LYS:HD3	1:A:228:PHE:HD1	1.78	0.48
1:A:155:GLN:HE21	1:A:290:SER:CB	2.26	0.48
1:A:512:ARG:NH2	1:A:542:PHE:CE2	2.82	0.47
1:A:959:TYR:N	1:A:959:TYR:CD1	2.66	0.47
1:A:895:HIS:O	1:A:898:ASN:ND2	2.48	0.47
1:A:331:ARG:HA	1:A:367:SER:O	2.15	0.47
1:A:418:ILE:O	1:A:444:SER:HB2	2.15	0.47
1:A:317:TRP:CA	1:A:382:CYS:HB2	2.39	0.46
1:A:350:GLY:N	1:A:588:PRO:HG3	2.30	0.46
1:A:321:GLN:O	1:A:381:VAL:HG23	2.15	0.46
1:A:720:ARG:HH22	1:A:747:GLU:HG2	1.81	0.46
1:A:1009:GLU:OE2	1:A:1009:GLU:HA	2.15	0.46
1:A:155:GLN:NE2	1:A:290:SER:CA	2.78	0.46
1:A:434:THR:C	1:A:437:ARG:HH12	2.24	0.46
1:A:225:ALA:O	1:A:230:GLN:HB3	2.15	0.46
1:A:975:LEU:HD23	1:A:975:LEU:HA	1.73	0.46
1:A:838:GLN:NE2	1:A:937:ASP:OD2	2.49	0.46
1:A:944:GLN:HE22	1:A:952:LYS:HE2	1.80	0.46
1:A:139:PHE:CE2	1:A:666:LEU:HB3	2.51	0.46
1:A:394:LEU:HD23	1:A:418:ILE:HG23	1.97	0.46
1:A:285:MET:O	1:A:288:GLU:HG2	2.16	0.46
1:A:488:LEU:HD22	1:A:591:TYR:CE1	2.51	0.46
1:A:553:THR:HB	1:A:564:MET:HE2	1.98	0.45
1:A:379:ILE:CD1	1:A:379:ILE:N	2.79	0.45
1:A:971:GLY:HA3	1:A:1004:LEU:HD11	1.99	0.45
1:A:856:LEU:HG	1:A:860:LYS:HE3	1.99	0.45
1:A:708:LYS:O	1:A:709:PRO:C	2.56	0.45
1:A:394:LEU:HD23	1:A:418:ILE:CD1	2.39	0.45
1:A:135:GLU:HG3	1:A:428:TYR:CD1	2.52	0.45
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.82	0.44
1:A:285:MET:O	1:A:289:GLN:HG3	2.17	0.44
1:A:478:VAL:O	1:A:479:ALA:HB2	2.17	0.44
1:A:321:GLN:N	1:A:321:GLN:OE1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLY:CA	1:A:588:PRO:HG3	2.47	0.44
1:A:1010:GLU:H	1:A:1010:GLU:HG3	1.33	0.44
1:A:137:ASN:O	1:A:141:THR:HG23	2.18	0.44
1:A:914:HIS:NE2	1:A:920:LYS:HB3	2.32	0.44
1:A:436:GLU:O	1:A:437:ARG:HD3	2.18	0.44
1:A:944:GLN:NE2	1:A:952:LYS:HE2	2.33	0.44
1:A:195:LYS:HB3	1:A:202:SER:HB3	2.00	0.44
1:A:377:PHE:HB3	1:A:379:ILE:CD1	2.48	0.44
1:A:534:MET:HG3	1:A:537:GLU:HB2	1.99	0.44
1:A:981:MET:C	1:A:983:ALA:N	2.73	0.43
1:A:982:ARG:CD	1:A:995:ILE:HD11	2.40	0.43
1:A:515:LEU:C	1:A:515:LEU:CD1	2.90	0.43
1:A:346:GLY:HA3	1:A:357:THR:HG22	2.01	0.43
1:A:386:ARG:HB2	1:A:485:PHE:CE1	2.53	0.43
1:A:387:MET:HG3	1:A:589:ASP:HA	1.99	0.43
1:A:383:ASP:O	1:A:384:LEU:C	2.62	0.43
1:A:219:CYS:SG	1:A:222:ARG:NH2	2.91	0.43
1:A:385:PRO:O	1:A:387:MET:N	2.52	0.43
1:A:426:PHE:CE1	1:A:485:PHE:HB2	2.53	0.43
1:A:439:LEU:N	1:A:471:LEU:O	2.49	0.43
1:A:915:PHE:O	1:A:918:ASN:HB2	2.19	0.43
1:A:741:LEU:HB3	1:A:763:TYR:CD1	2.54	0.43
1:A:167:PHE:HE1	1:A:247:HIS:CD2	2.37	0.42
1:A:716:HIS:O	1:A:720:ARG:HG3	2.18	0.42
1:A:1006:LYS:HE3	1:A:1014:HIS:CD2	2.54	0.42
1:A:165:TYR:OH	1:A:641:ARG:HG3	2.20	0.42
1:A:589:ASP:OD2	1:A:591:TYR:N	2.53	0.42
1:A:618:VAL:O	1:A:619:LEU:C	2.62	0.42
1:A:426:PHE:CZ	1:A:485:PHE:HD2	2.37	0.42
1:A:512:ARG:HG3	1:A:530:LEU:HG	2.01	0.42
1:A:117:ILE:O	1:A:121:ILE:HG23	2.19	0.42
1:A:796:LEU:O	1:A:797:MET:C	2.63	0.42
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.94	0.42
1:A:895:HIS:H	1:A:898:ASN:HD21	1.66	0.42
1:A:199:SER:OG	1:A:201:GLU:HB2	2.19	0.42
1:A:245:GLY:HA3	1:A:768:ALA:HB2	2.02	0.42
1:A:488:LEU:HD22	1:A:591:TYR:HE1	1.85	0.42
1:A:810:MET:HE3	1:A:882:TYR:CZ	2.55	0.42
1:A:442:TRP:HA	1:A:443:PRO:HD3	1.94	0.41
1:A:809:ARG:O	1:A:906:GLN:HG2	2.20	0.41
1:A:940:HIS:CE1	1:A:945:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ARG:NH2	1:A:542:PHE:CD2	2.85	0.41
1:A:142:LYS:HG2	1:A:143:MET:CE	2.49	0.41
1:A:538:VAL:HG13	1:A:545:ALA:HB3	2.02	0.41
1:A:395:TYR:HB3	1:A:417:PRO:HA	2.02	0.41
1:A:638:LEU:HD23	1:A:638:LEU:HA	1.77	0.41
1:A:525:GLU:O	1:A:526:HIS:C	2.64	0.41
1:A:796:LEU:HD23	1:A:974:PHE:CE1	2.55	0.41
1:A:561:VAL:O	1:A:565:LEU:CD1	2.69	0.41
1:A:801:TRP:CZ2	1:A:963:ALA:HB1	2.56	0.41
1:A:1004:LEU:HD22	1:A:1004:LEU:HA	1.89	0.41
2:A:1500:RW4:HAP1	2:A:1500:RW4:CAR	2.50	0.41
1:A:563:GLN:O	1:A:566:TYR:HB3	2.21	0.41
1:A:545:ALA:O	1:A:546:LEU:C	2.63	0.41
1:A:762:MET:CE	1:A:775:GLY:HA3	2.46	0.41
1:A:188:ARG:HB3	1:A:188:ARG:NH1	2.36	0.41
1:A:998:LEU:HD23	1:A:998:LEU:HA	1.86	0.41
1:A:222:ARG:O	1:A:226:THR:HG23	2.21	0.40
1:A:324:SER:HA	1:A:375:LEU:O	2.21	0.40
1:A:839:LEU:O	1:A:840:ASN:C	2.64	0.40
1:A:154:ARG:NH2	1:A:674:GLY:O	2.54	0.40
1:A:645:HIS:CE1	1:A:734:PRO:HA	2.56	0.40
1:A:488:LEU:HD12	1:A:491:ILE:HB	2.04	0.40
1:A:523:LEU:HB2	1:A:527:GLU:OE1	2.22	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	811/940 (86%)	741 (91%)	60 (7%)	10 (1%)	10 34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	LEU
1	A	365	VAL
1	A	755	LYS
1	A	847	THR
1	A	1026	SER
1	A	231	PRO
1	A	366	CYS
1	A	386	ARG
1	A	1008	GLU
1	A	227	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	740/827 (90%)	651 (88%)	89 (12%)	5 16

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ILE
1	A	141	THR
1	A	156	GLN
1	A	172	GLU
1	A	188	ARG
1	A	191	LEU
1	A	195	LYS
1	A	203	PHE
1	A	206	GLN
1	A	210	LYS
1	A	224	LYS
1	A	230	GLN
1	A	247	HIS
1	A	262	ILE
1	A	263	CYS
1	A	267	HIS
1	A	285	MET

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Mol	Chain	Res	Type
1	A	317	TRP
1	A	318	SER
1	A	331	ARG
1	A	332	LYS
1	A	352	GLU
1	A	353	MET
1	A	363	VAL
1	A	365	VAL
1	A	368	GLU
1	A	374	ARG
1	A	379	ILE
1	A	397	VAL
1	A	418	ILE
1	A	423	LEU
1	A	429	LYS
1	A	430	ASP
1	A	444	SER
1	A	451	GLU
1	A	453	LEU
1	A	466	GLU
1	A	471	LEU
1	A	472	VAL
1	A	475	LEU
1	A	483	VAL
1	A	491	ILE
1	A	492	LEU
1	A	505	GLU
1	A	511	LEU
1	A	512	ARG
1	A	514	ILE
1	A	515	LEU
1	A	517	ARG
1	A	525	GLU
1	A	548	ARG
1	A	574	LEU
1	A	586	SER
1	A	594	SER
1	A	617	GLN
1	A	618	VAL
1	A	634	LEU
1	A	641	ARG
1	A	703	SER

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Mol	Chain	Res	Type
1	A	710	GLN
1	A	736	ASP
1	A	757	LYS
1	A	788	MET
1	A	793	MET
1	A	795	GLN
1	A	834	ILE
1	A	841	LYS
1	A	852	LYS
1	A	855	LEU
1	A	859	LEU
1	A	898	ASN
1	A	901	ILE
1	A	902	ARG
1	A	906	GLN
1	A	907	LEU
1	A	915	PHE
1	A	927	ARG
1	A	930	VAL
1	A	933	ILE
1	A	947	THR
1	A	948	ASN
1	A	951	GLU
1	A	959	TYR
1	A	962	ARG
1	A	975	LEU
1	A	992	SER
1	A	1004	LEU
1	A	1010	GLU
1	A	1013	LYS

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

Mol	Chain	Res	Type
1	A	116	GLN
1	A	155	GLN
1	A	193	ASN
1	A	278	HIS
1	A	289	GLN
1	A	291	ASN
1	A	431	GLN
1	A	617	GLN

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Mol	Chain	Res	Type
1	A	685	GLN
1	A	795	GLN
1	A	898	ASN
1	A	918	ASN
1	A	926	ASN
1	A	976	HIS
1	A	1014	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RW4	A	1500	-	44,44,44	2.41	16 (36%)	63,65,65	3.34	22 (34%)

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	RW4	A	1500	-	-	3/12/22/22	0/7/7/7

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	RW4	CBD-CBB	-7.64	1.38	1.49
2	A	1500	RW4	NAV-NBA	-5.75	1.25	1.36
2	A	1500	RW4	CAG-NAF	4.97	1.37	1.31
2	A	1500	RW4	CAA-NAH	3.82	1.53	1.46
2	A	1500	RW4	CAQ-NAI	3.75	1.55	1.46
2	A	1500	RW4	CBK-NBL	3.57	1.35	1.31
2	A	1500	RW4	CBB-NBA	2.99	1.36	1.33
2	A	1500	RW4	C5-C4	-2.94	1.39	1.42
2	A	1500	RW4	CAB-NAI	2.85	1.53	1.46
2	A	1500	RW4	CAK-CAC	2.84	1.44	1.38
2	A	1500	RW4	CAR-NAV	2.67	1.49	1.46
2	A	1500	RW4	CAK-CAL	2.65	1.42	1.36
2	A	1500	RW4	C5-CBB	-2.65	1.37	1.44
2	A	1500	RW4	CAJ-NAI	2.64	1.53	1.46
2	A	1500	RW4	CAC-CAD	2.36	1.41	1.36
2	A	1500	RW4	CAP-NAH	2.35	1.50	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	RW4	CBF-SBI-CBK	10.02	93.63	88.89
2	A	1500	RW4	CAO-CAR-NAV	-9.24	103.41	112.80
2	A	1500	RW4	SBI-CBK-NBL	-9.19	110.02	115.72
2	A	1500	RW4	C5-C6-N1	-7.31	119.22	126.97
2	A	1500	RW4	CAP-NAH-CAA	6.97	127.25	111.57
2	A	1500	RW4	CBG-NBL-CBK	6.74	114.57	110.57
2	A	1500	RW4	C5-CBB-CBD	-5.47	124.79	131.28
2	A	1500	RW4	CBD-CBB-NBA	5.36	125.89	118.91
2	A	1500	RW4	N1-C6-NAV	5.32	133.65	125.34
2	A	1500	RW4	C4-C5-C6	5.19	119.62	115.74
2	A	1500	RW4	CAR-NAV-NBA	4.06	123.13	119.98
2	A	1500	RW4	CAR-NAV-C6	-3.80	125.40	127.81
2	A	1500	RW4	N3-C2-N1	-3.62	123.11	128.58
2	A	1500	RW4	CAA-CAB-NAI	-3.54	105.16	110.86
2	A	1500	RW4	SBI-CBK-NBJ	3.45	123.88	120.13
2	A	1500	RW4	C2-N1-C6	3.22	119.69	111.83
2	A	1500	RW4	CAD-CAE-CAM	3.08	122.12	119.04
2	A	1500	RW4	C4-C5-CBB	-2.65	136.39	139.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	RW4	NBJ-CBK-NBL	2.50	126.10	124.13
2	A	1500	RW4	CBB-NBA-NAV	2.23	108.11	106.02
2	A	1500	RW4	NAF-CAG-NAH	-2.22	115.81	117.62
2	A	1500	RW4	CAR-CAO-CAN	-2.07	116.83	122.06

There are no chirality outliers.

All (3) torsion outliers are listed below:

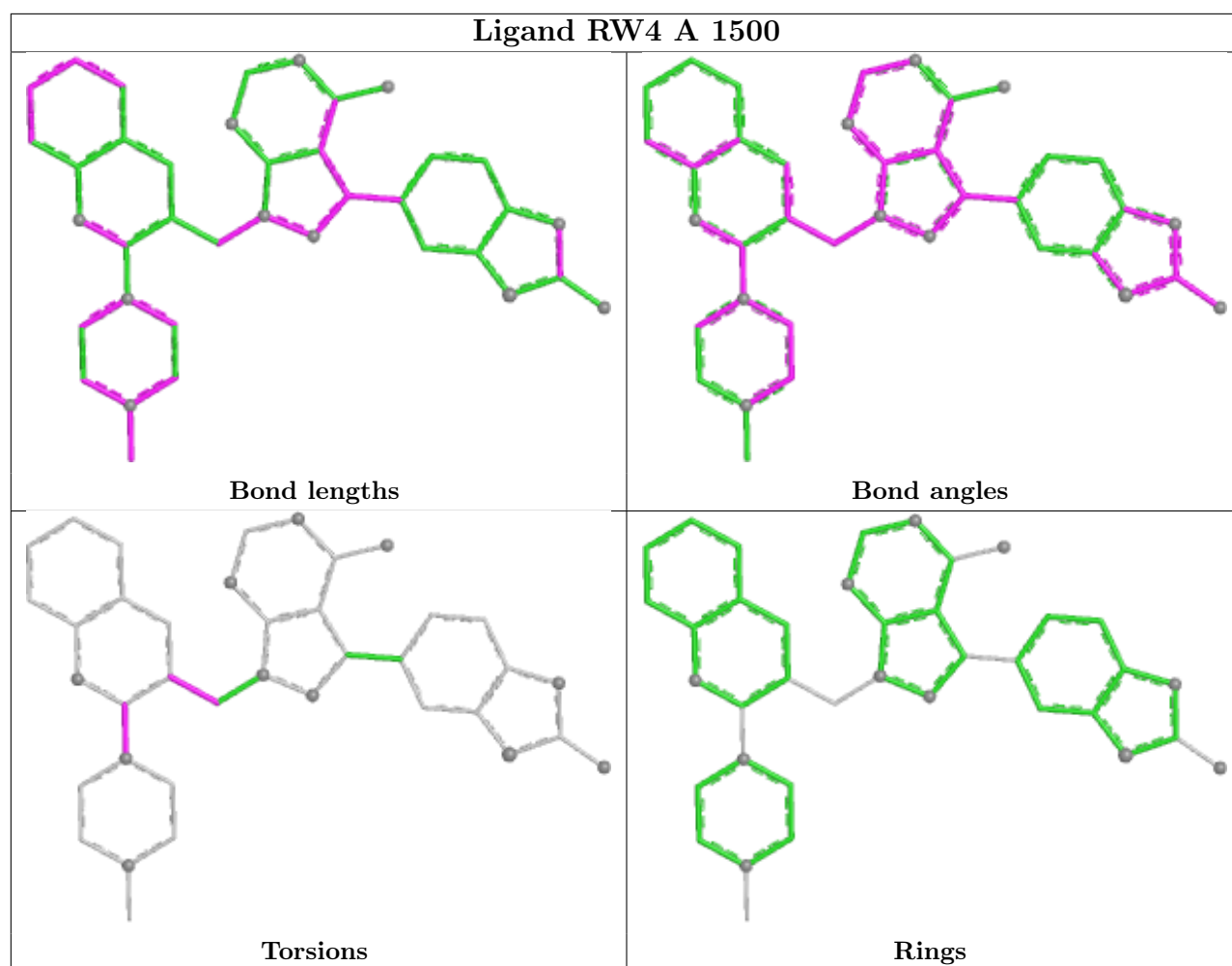
Mol	Chain	Res	Type	Atoms
2	A	1500	RW4	NAF-CAG-NAH-CAA
2	A	1500	RW4	CAO-CAG-NAH-CAA
2	A	1500	RW4	CAG-CAO-CAR-NAV

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	RW4	6	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 [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	835/940 (88%)	0.10	16 (1%) 66 58	7, 22, 38, 58	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	842	SER	4.9
1	A	335	ALA	4.2
1	A	846	ALA	4.0
1	A	1027	TRP	3.2
1	A	445	VAL	3.0
1	A	173	PRO	2.9
1	A	317	TRP	2.9
1	A	232	LEU	2.7
1	A	843	ASN	2.6
1	A	507	GLU	2.3
1	A	187	ASN	2.3
1	A	932	PHE	2.3
1	A	289	GLN	2.3
1	A	840	ASN	2.2
1	A	479	ALA	2.1
1	A	511	LEU	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](#)

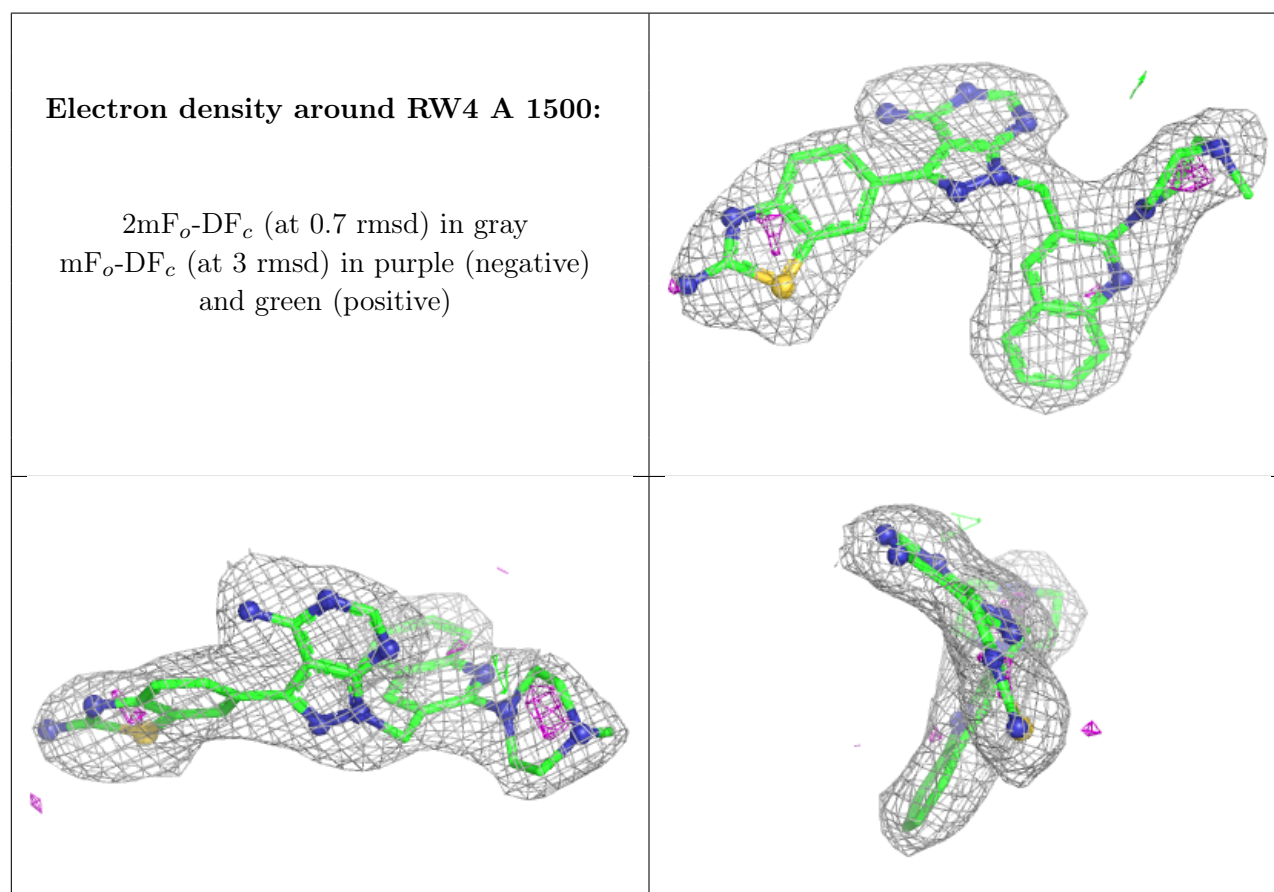
There are no oligosaccharides in this entry.

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
2	RW4	A	1500	38/38	0.95	0.08	26,29,32,34	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 [i](#)

There are no such residues in this entry.