



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 04:57 am GMT

PDB ID : 2WXK
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

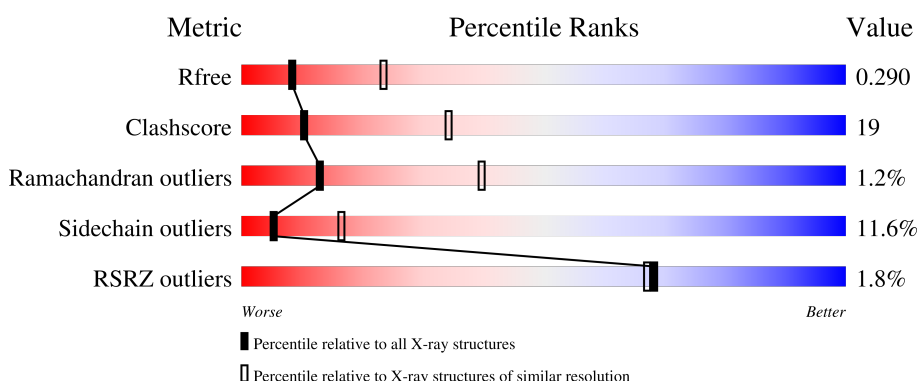
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6777 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.

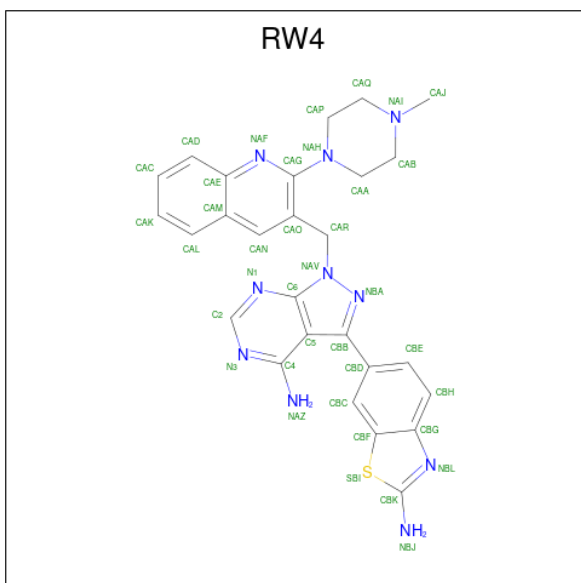
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	835	6739	4315	1144	1226	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 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 (three-letter code: RW4) (formula: C₂₇H₂₆N₁₀S).

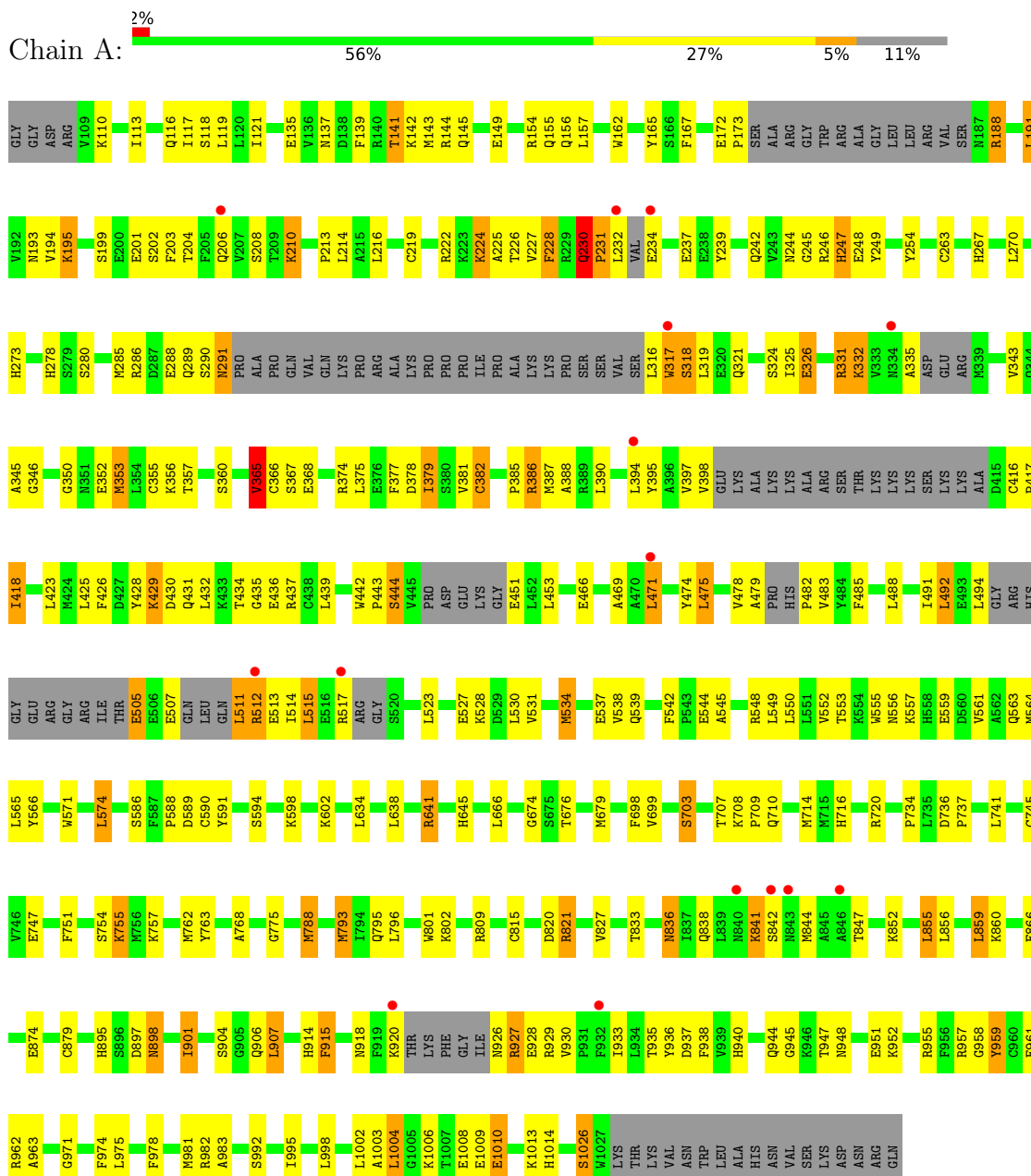


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
2	A	1	38	27	10	1	0	0

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 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 68.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.36-2.90) 100.0 (68.38-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.213 , 0.287 0.214 , 0.290	Depositor DCC
R_{free} test set	733 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6777	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.75	5/6882 (0.1%)	0.82	0/9281

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	745	CYS	CB-SG	-8.00	1.68	1.82
1	A	866	GLU	CD-OE1	6.65	1.32	1.25
1	A	879	CYS	CB-SG	-6.16	1.71	1.82
1	A	505	GLU	CD-OE2	5.66	1.31	1.25
1	A	326	GLU	CD-OE1	5.32	1.31	1.25

There are no bond angle outliers.

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	247	0
2	A	38	0	26	6	0
All	All	6777	0	6730	253	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 19.

All (253) 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: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:234:GLU:OE2	1:A:239:TYR:OH	1.97	0.81
1:A:549:LEU:HG	1:A:564:MET:CE	2.10	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:549:LEU:HG	1:A:564:MET:HE3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:365:VAL:O	1:A:365:VAL:CG1	2.38	0.71
1:A:928:GLU:HG3	1:A:929:ARG:N	2.07	0.70
1:A:345:ALA:O	1:A:357:THR:HB	1.92	0.70
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: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: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: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
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:332:LYS:HE3	1:A:332:LYS:C	2.21	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:332:LYS:HB2	1:A:332:LYS:HZ2	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:C	1:A:515:LEU:HD13	2.22	0.60
1:A:762:MET:CE	1:A:827:VAL:HG11	2.32	0.60
1:A:901:ILE:N	1:A:901:ILE:CD1	2.65	0.59
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: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:550:LEU:C	1:A:553:THR:HG22	2.24	0.56
1:A:397:VAL:HG22	1:A:398:VAL:N	2.21	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:842:SER:O	1:A:844:MET:CE	2.54	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:335:ALA:C	1:A:365:VAL:HG11	2.28	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: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: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:507:GLU:C	1:A:511:LEU:N	2.61	0.54
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:549:LEU:HG	1:A:564:MET:HE1	1.88	0.53
1:A:904:SER:OG	1:A:906:GLN:NE2	2.40	0.52
1:A:895:HIS:N	1:A:898:ASN:HD21	2.07	0.52
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.91	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:820:ASP:O	1:A:821:ARG:C	2.47	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: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:762:MET:HE1	1:A:827:VAL:HG11	1.93	0.50
1:A:116:GLN:HE21	1:A:679:MET:CE	2.25	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:191:LEU:HD22	1:A:204:THR:CG2	2.42	0.49
1:A:378:ASP:CG	1:A:378:ASP:O	2.49	0.49
1:A:809:ARG:HG3	1:A:874:GLU:OE2	2.11	0.49
1:A:907:LEU:HD23	1:A:907:LEU:C	2.33	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: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:754:SER:O	1:A:755:LYS:HB2	2.12	0.49
1:A:898:ASN:C	1:A:898:ASN:HD22	2.15	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:317:TRP:CD1	1:A:317:TRP:C	2.87	0.48
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: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: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:842:SER:O	1:A:844:MET:HE3	2.13	0.47
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:116:GLN:HE21	1:A:679:MET:HE1	1.79	0.47
1:A:793:MET:HE2	1:A:978:PHE:CE1	2.50	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:762:MET:CE	1:A:775:GLY:HA3	2.46	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: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:379:ILE:CD1	1:A:379:ILE:N	2.79	0.45
1:A:842:SER:O	1:A:844:MET:HE2	2.16	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:394:LEU:HD23	1:A:418:ILE:CD1	2.39	0.45
1:A:553:THR:HB	1:A:564:MET:HE2	1.98	0.45
1:A:135:GLU:HG3	1:A:428:TYR:CD1	2.52	0.45
1:A:418:ILE:C	1:A:444:SER:HB2	2.37	0.45
1:A:1002:LEU:O	1:A:1003:ALA:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:841:LYS:HZ2	1:A:844:MET:CE	2.31	0.44
1:A:914:HIS:NE2	1:A:920:LYS:HB3	2.32	0.44
1:A:793:MET:HE3	1:A:978:PHE:CE1	2.53	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:958:GLY:O	1:A:959:TYR:C	2.54	0.44
1:A:982:ARG:CD	1:A:995:ILE:HD11	2.40	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:793:MET:HE3	1:A:978:PHE:CD1	2.54	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:708:LYS:O	1:A:709:PRO:C	2.56	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:142:LYS:HG2	1:A:143:MET:CE	2.49	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:981:MET:C	1:A:983:ALA:N	2.73	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:512:ARG:NH2	1:A:542:PHE:CD2	2.85	0.41
1:A:434:THR:C	1:A:437:ARG:HH12	2.24	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: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: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:355:CYS:HG	1:A:379:ILE:HD12	1.75	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%)	13 40

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	740/827 (90%)	654 (88%)	86 (12%)	5 16

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ILE
1	A	118	SER
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	228	PHE
1	A	230	GLN
1	A	247	HIS
1	A	263	CYS
1	A	267	HIS

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Mol	Chain	Res	Type
1	A	291	ASN
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	356	LYS
1	A	365	VAL
1	A	368	GLU
1	A	374	ARG
1	A	379	ILE
1	A	382	CYS
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	475	LEU
1	A	483	VAL
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	534	MET
1	A	548	ARG
1	A	574	LEU
1	A	586	SER
1	A	594	SER
1	A	598	LYS
1	A	634	LEU
1	A	641	ARG
1	A	703	SER
1	A	710	GLN
1	A	736	ASP

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Mol	Chain	Res	Type
1	A	757	LYS
1	A	788	MET
1	A	793	MET
1	A	795	GLN
1	A	821	ARG
1	A	836	ASN
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	907	LEU
1	A	915	PHE
1	A	926	ASN
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	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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	155	GLN
1	A	170	GLN
1	A	193	ASN
1	A	278	HIS
1	A	291	ASN
1	A	431	GLN
1	A	617	GLN
1	A	721	GLN
1	A	898	ASN
1	A	906	GLN

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Mol	Chain	Res	Type
1	A	918	ASN
1	A	926	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	RW4	A	1500	-	36,44,44	1.87	10 (27%)	41,65,65	2.22	12 (29%)

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	-	-	2/8/22/22	0/7/7/7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	RW4	CAG-NAF	5.02	1.37	1.31
2	A	1500	RW4	CAQ-NAI	4.19	1.55	1.46
2	A	1500	RW4	CAA-NAH	4.17	1.53	1.46
2	A	1500	RW4	CAB-NAI	3.18	1.53	1.46
2	A	1500	RW4	CAJ-NAI	2.78	1.53	1.46
2	A	1500	RW4	CAP-NAH	2.56	1.50	1.46
2	A	1500	RW4	CAK-CAL	2.47	1.42	1.36
2	A	1500	RW4	CAK-CAC	2.45	1.44	1.38
2	A	1500	RW4	CBE-CBH	2.23	1.41	1.35
2	A	1500	RW4	CAC-CAD	2.20	1.41	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	RW4	CAP-NAH-CAA	7.13	127.25	111.52
2	A	1500	RW4	CAA-CAB-NAI	-5.00	105.16	110.80
2	A	1500	RW4	CAO-CAR-NAV	-3.79	103.41	112.83
2	A	1500	RW4	CBG-CBF-SBI	-3.62	107.05	111.85
2	A	1500	RW4	N1-C2-N3	-3.57	123.11	128.68
2	A	1500	RW4	CAD-CAE-CAM	2.93	122.12	119.04
2	A	1500	RW4	CBF-CBG-NBL	2.88	114.74	108.04
2	A	1500	RW4	CBC-CBF-SBI	2.68	130.45	125.10
2	A	1500	RW4	NAF-CAG-NAH	-2.54	115.81	117.62
2	A	1500	RW4	NBJ-CBK-NBL	2.25	126.10	123.19
2	A	1500	RW4	CBC-CBD-CBE	2.16	120.84	118.15
2	A	1500	RW4	CAJ-NAI-CAB	-2.02	107.64	110.66

There are no chirality outliers.

All (2) 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

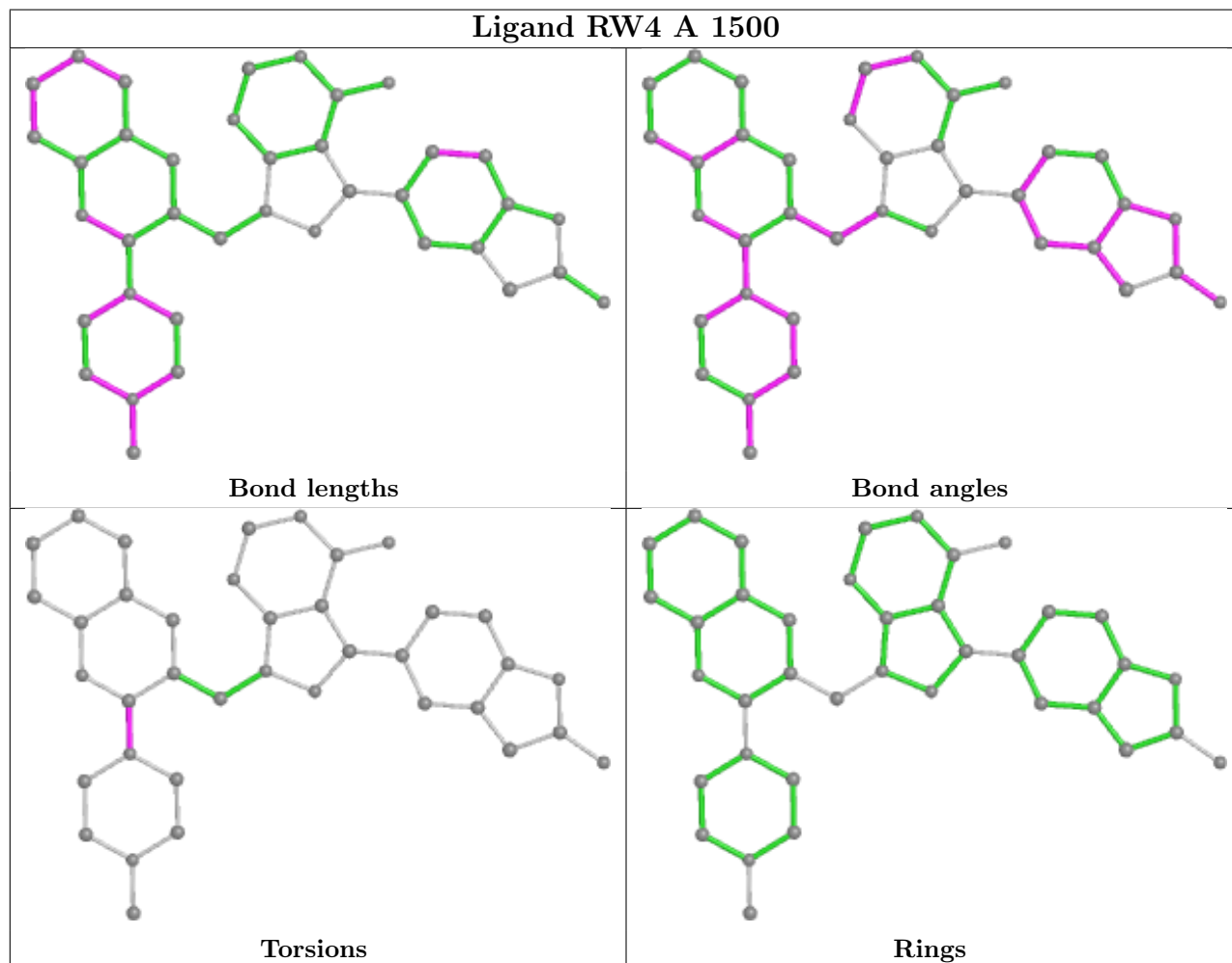
There are no ring outliers.

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%)	-0.06	15 (1%) 68 67	7, 22, 38, 58	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	LEU	4.7
1	A	920	LYS	4.1
1	A	842	SER	3.7
1	A	846	ALA	3.3
1	A	843	ASN	3.1
1	A	317	TRP	3.0
1	A	394	LEU	2.7
1	A	932	PHE	2.7
1	A	334	ASN	2.5
1	A	517	ARG	2.3
1	A	471	LEU	2.3
1	A	206	GLN	2.1
1	A	840	ASN	2.1
1	A	512	ARG	2.1
1	A	234	GLU	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](#)

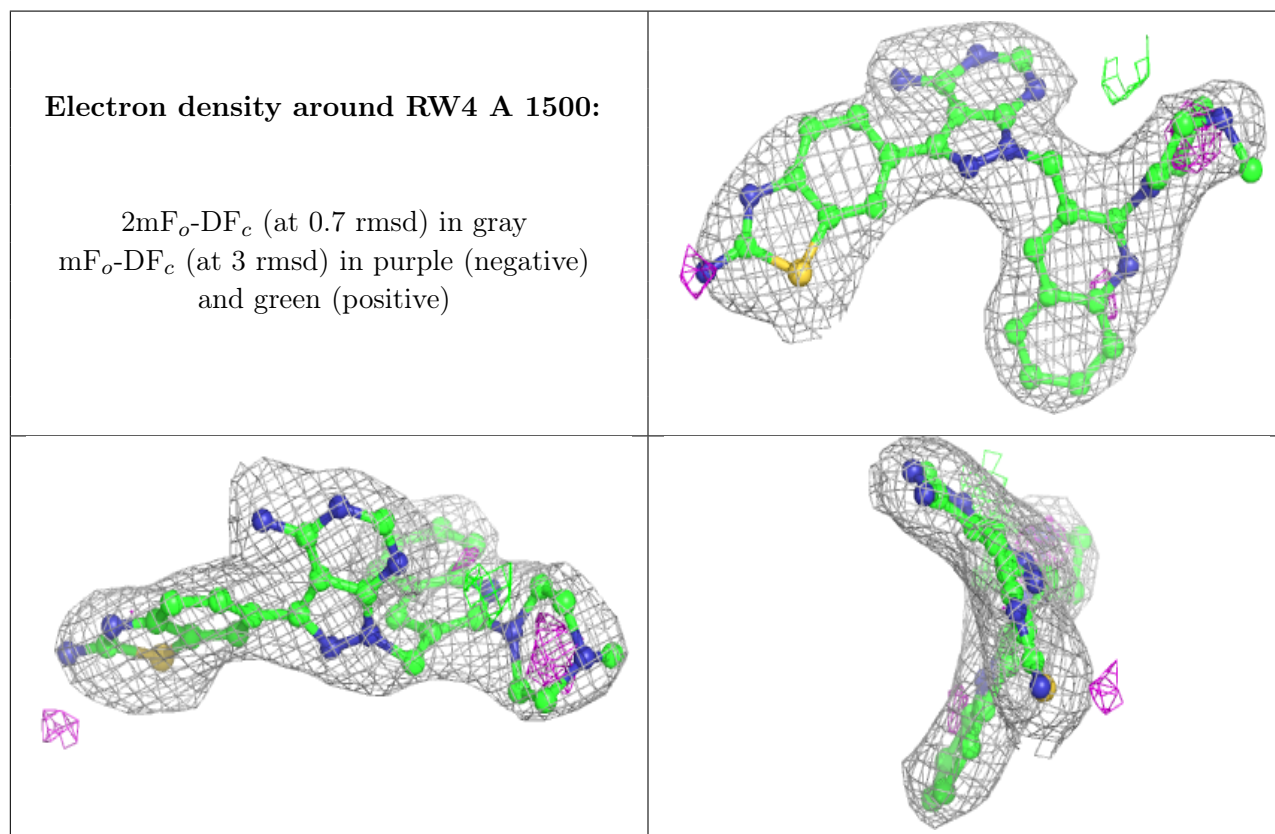
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
2	RW4	A	1500	38/38	0.97	0.22	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.