WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 07:31 pm GMT

PDB ID	:	2WXQ
Title	:	The crystal structure of the murine class IA PI 3-kinase p110delta in complex with AS15.
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	:	2.70 Å(reported)

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

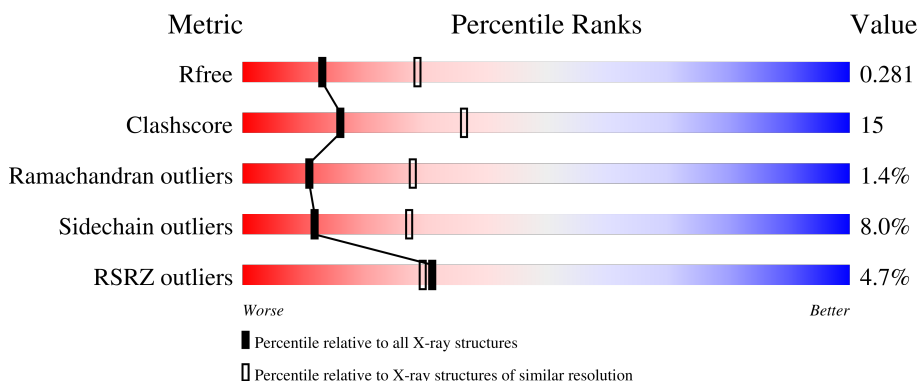|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.70 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	Percentile Ranks	Value
Rfree		0.281
Clashscore		15
Ramachandran outliers		1.4%
Sidechain outliers		8.0%
RSRZ outliers		4.7%

Worse *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	4% ... 61% ... 23% · 13%

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
2	ZZQ	A	1500	-	-	X	-

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2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6667 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	822	Total 6633	C 4254	N 1126	O 1199	S 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-{[3-(2-METHOXYPHENYL)-4-OXO-3,4,5,6,7,8-HEXAHYDROQUINAZOLIN-2-YL]SULFANYL}-N-QUINOXALIN-6-YLACETAMIDE (three-letter code: ZZQ) (formula: $C_{25}H_{23}N_5O_3S$).
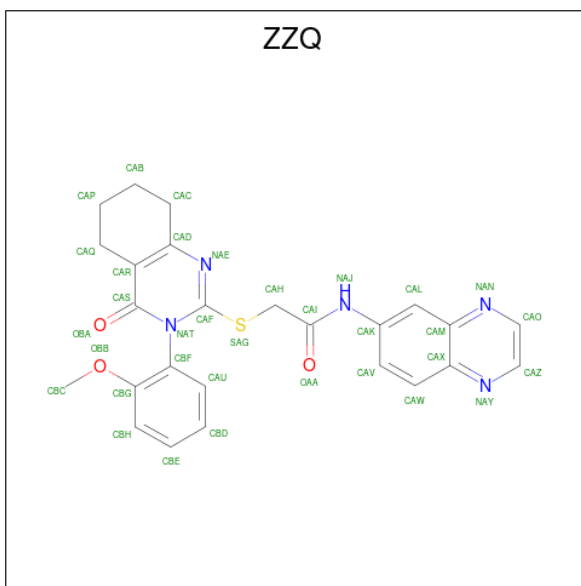

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 34	C 25	N 5	O 3	S 1	0	0

3   Residue-property plots ⓘ

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
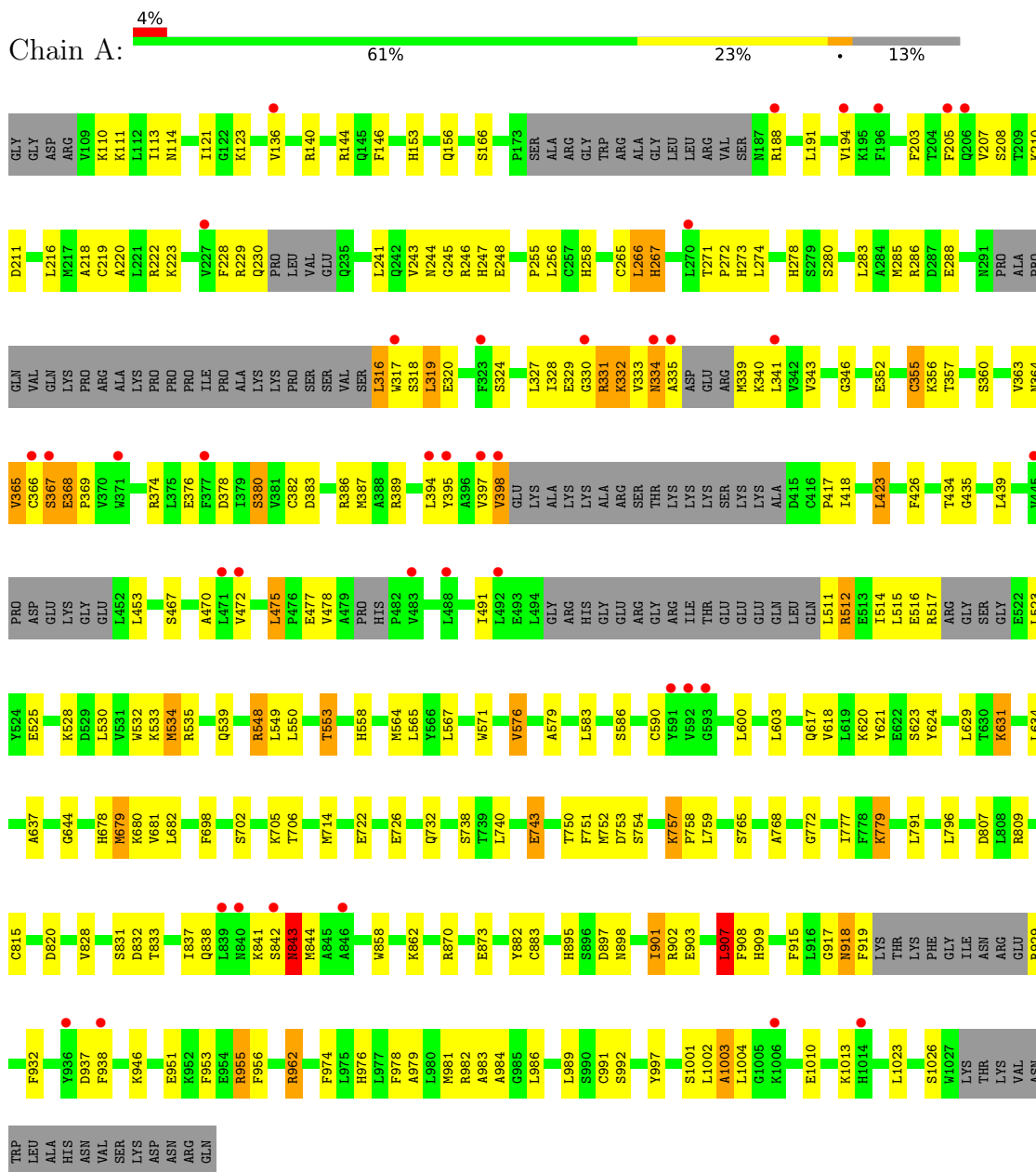
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.13Å 63.86Å 116.63Å 90.00° 102.62° 90.00°	Depositor
Resolution (Å)	65.94 – 2.70 65.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (65.94-2.70) 99.5 (65.97-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.225 , 0.286 0.225 , 0.281	Depositor DCC
R_{free} test set	896 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å²)	54.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6667	wwPDB-VP
Average B, all atoms (Å²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ 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: ZZQ

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	0.59	0/6776	0.70	3/9142 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	423	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	907	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	603	LEU	CA-CB-CG	5.12	127.09	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	6633	0	6615	191	0
2	A	34	0	22	11	0
All	All	6667	0	6637	193	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 (193) 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:367:SER:HB3	1:A:368:GLU:HB3	1.34	1.08
1:A:549:LEU:HG	1:A:564:MET:HE1	1.16	1.08
1:A:548:ARG:HH11	1:A:548:ARG:HG3	1.04	1.08
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.19	1.04
1:A:205:PHE:HE1	1:A:223:LYS:HG3	1.21	1.02
1:A:752:MET:HB3	2:A:1500:ZZQ:CBC	1.90	0.99
1:A:549:LEU:HG	1:A:564:MET:CE	1.92	0.99
1:A:752:MET:HB3	2:A:1500:ZZQ:HBC3	1.43	0.99
1:A:828:VAL:H	2:A:1500:ZZQ:HAZ	1.27	0.98
1:A:367:SER:HB3	1:A:368:GLU:CB	1.98	0.94
1:A:548:ARG:HG3	1:A:548:ARG:NH1	1.83	0.91
1:A:267:HIS:HE1	1:A:870:ARG:NH2	1.70	0.90
1:A:205:PHE:CE1	1:A:223:LYS:HG3	2.09	0.84
1:A:534:MET:HA	1:A:534:MET:HE2	1.62	0.81
1:A:828:VAL:H	2:A:1500:ZZQ:CAZ	1.92	0.81
1:A:828:VAL:N	2:A:1500:ZZQ:HAZ	1.97	0.80
1:A:434:THR:HG21	1:A:477:GLU:HA	1.63	0.80
1:A:534:MET:HA	1:A:534:MET:CE	2.12	0.79
1:A:962:ARG:HH11	1:A:962:ARG:CG	1.94	0.79
1:A:962:ARG:HG2	1:A:962:ARG:NH1	1.96	0.78
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.66	0.77
1:A:838:GLN:NE2	1:A:937:ASP:OD2	2.18	0.77
1:A:110:LYS:HE3	1:A:114:ASN:HD21	1.50	0.76
1:A:698:PHE:HZ	1:A:714:MET:HG2	1.50	0.76
1:A:334:ASN:HD22	1:A:335:ALA:H	1.34	0.75
1:A:553:THR:HG21	1:A:564:MET:HE3	1.66	0.75
1:A:367:SER:HB3	1:A:368:GLU:CA	2.17	0.74
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.68	0.73
1:A:267:HIS:CE1	1:A:870:ARG:NH2	2.56	0.73
1:A:901:ILE:HD12	1:A:901:ILE:H	1.53	0.71
1:A:752:MET:HB3	2:A:1500:ZZQ:HBC1	1.73	0.71
1:A:271:THR:O	1:A:273:HIS:HD2	1.75	0.69
1:A:758:PRO:HB3	1:A:779:LYS:HG2	1.74	0.69
1:A:267:HIS:CE1	1:A:870:ARG:HH21	2.10	0.69
1:A:549:LEU:CG	1:A:564:MET:HE1	2.10	0.69
1:A:367:SER:CB	1:A:368:GLU:HB3	2.19	0.68
1:A:283:LEU:HD22	1:A:286:ARG:HH21	1.58	0.67
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.93	0.67
1:A:247:HIS:HB2	1:A:738:SER:HA	1.77	0.66
1:A:278:HIS:CD2	1:A:280:SER:H	2.13	0.66
1:A:435:GLY:HA2	1:A:475:LEU:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:ARG:NH2	1:A:991:CYS:HA	2.11	0.66
1:A:367:SER:CB	1:A:368:GLU:C	2.64	0.65
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.33	0.63
1:A:553:THR:CG2	1:A:564:MET:HE3	2.28	0.63
1:A:681:VAL:CG1	1:A:732:GLN:NE2	2.62	0.62
1:A:617:GLN:HE22	1:A:620:LYS:NZ	1.95	0.62
1:A:387:MET:CE	1:A:590:CYS:SG	2.88	0.62
1:A:698:PHE:CZ	1:A:714:MET:HG2	2.35	0.61
1:A:618:VAL:HG12	1:A:629:LEU:CD2	2.31	0.61
1:A:435:GLY:O	1:A:475:LEU:N	2.30	0.61
1:A:367:SER:HB2	1:A:368:GLU:C	2.21	0.61
1:A:367:SER:CB	1:A:368:GLU:CA	2.80	0.60
1:A:832:ASP:O	1:A:901:ILE:HD12	2.01	0.60
1:A:873:GLU:HA	1:A:873:GLU:OE1	2.00	0.60
1:A:617:GLN:HE22	1:A:620:LYS:HZ2	1.49	0.60
1:A:267:HIS:HE1	1:A:870:ARG:HH21	1.42	0.59
1:A:681:VAL:HG11	1:A:732:GLN:NE2	2.17	0.59
1:A:395:TYR:HB3	1:A:417:PRO:HA	1.84	0.59
1:A:548:ARG:HH11	1:A:548:ARG:CG	1.95	0.59
1:A:837:ILE:CD1	1:A:901:ILE:HD11	2.32	0.58
1:A:367:SER:HB3	1:A:368:GLU:C	2.23	0.58
1:A:917:GLY:HA3	1:A:997:TYR:CE1	2.38	0.58
1:A:539:GLN:HG3	1:A:571:TRP:CE3	2.39	0.58
1:A:328:ILE:HG22	1:A:329:GLU:HG2	1.87	0.57
1:A:334:ASN:ND2	1:A:335:ALA:H	2.00	0.57
1:A:278:HIS:HD2	1:A:280:SER:H	1.52	0.57
1:A:330:GLY:O	1:A:368:GLU:HA	2.05	0.57
1:A:387:MET:HE3	1:A:590:CYS:SG	2.45	0.57
1:A:153:HIS:O	1:A:156:GLN:HG2	2.05	0.57
1:A:229:ARG:O	1:A:230:GLN:HB3	2.04	0.57
1:A:363:VAL:HG12	1:A:364:ASN:N	2.20	0.57
1:A:981:MET:HB3	1:A:989:LEU:HD21	1.87	0.56
1:A:535:ARG:HG3	1:A:567:LEU:HD11	1.87	0.56
1:A:841:LYS:HB3	1:A:844:MET:HE3	1.87	0.55
1:A:842:SER:O	1:A:843:ASN:CB	2.54	0.55
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.89	0.55
1:A:833:THR:O	1:A:837:ILE:HG13	2.06	0.55
1:A:283:LEU:HD22	1:A:286:ARG:NH2	2.20	0.55
1:A:579:ALA:HB1	1:A:600:LEU:HG	1.89	0.54
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.40	0.54
1:A:426:PHE:O	1:A:624:TYR:OH	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:PHE:O	1:A:956:PHE:HB3	2.08	0.54
1:A:617:GLN:O	1:A:620:LYS:HB2	2.07	0.53
1:A:330:GLY:C	1:A:331:ARG:HG2	2.29	0.53
1:A:807:ASP:OD1	1:A:807:ASP:C	2.47	0.53
1:A:146:PHE:CZ	1:A:631:LYS:HD2	2.43	0.53
1:A:316:LEU:HD12	1:A:318:SER:H	1.72	0.53
1:A:681:VAL:HG13	1:A:732:GLN:NE2	2.24	0.52
1:A:981:MET:CB	1:A:989:LEU:HD21	2.39	0.52
1:A:842:SER:O	1:A:843:ASN:HB2	2.09	0.52
1:A:216:LEU:HD22	1:A:241:LEU:HD11	1.91	0.52
1:A:984:ALA:HB3	1:A:986:LEU:HD13	1.90	0.52
1:A:208:SER:OG	1:A:210:LYS:HG2	2.09	0.51
1:A:211:ASP:O	1:A:256:LEU:HG	2.10	0.51
1:A:681:VAL:HG11	1:A:732:GLN:HE22	1.74	0.51
1:A:191:LEU:O	1:A:272:PRO:HD2	2.11	0.51
1:A:981:MET:HB3	1:A:989:LEU:CD2	2.40	0.51
1:A:228:PHE:O	1:A:229:ARG:HB2	2.11	0.51
1:A:110:LYS:HZ3	1:A:144:ARG:HH12	1.59	0.51
1:A:324:SER:HB3	1:A:376:GLU:HG3	1.93	0.51
1:A:395:TYR:HA	1:A:418:ILE:HD12	1.92	0.51
1:A:245:GLY:HA3	1:A:768:ALA:CB	2.39	0.50
1:A:343:VAL:H	1:A:360:SER:HB2	1.76	0.50
1:A:753:ASP:N	2:A:1500:ZZQ:HBC3	2.26	0.49
1:A:617:GLN:NE2	1:A:620:LYS:HZ2	2.11	0.49
1:A:828:VAL:CG1	1:A:902:ARG:HD3	2.43	0.49
1:A:255:PRO:HG2	1:A:258:HIS:CD2	2.48	0.49
1:A:550:LEU:HA	1:A:553:THR:CG2	2.43	0.49
1:A:976:HIS:O	1:A:979:ALA:HB3	2.11	0.49
1:A:837:ILE:HD12	1:A:901:ILE:HD11	1.95	0.49
1:A:1002:LEU:O	1:A:1003:ALA:C	2.50	0.48
1:A:532:TRP:CZ3	1:A:553:THR:HB	2.49	0.48
1:A:918:ASN:HD22	1:A:918:ASN:HA	1.54	0.48
1:A:1023:LEU:O	1:A:1026:SER:HB3	2.14	0.48
1:A:1010:GLU:O	1:A:1013:LYS:HB3	2.13	0.47
2:A:1500:ZZQ:HAV	2:A:1500:ZZQ:HAH1	1.96	0.47
1:A:512:ARG:O	1:A:516:GLU:HB2	2.14	0.47
1:A:702:SER:O	1:A:706:THR:HG22	2.14	0.47
1:A:332:LYS:HE3	1:A:333:VAL:N	2.29	0.47
1:A:320:GLU:O	1:A:380:SER:HB2	2.14	0.47
1:A:962:ARG:CG	1:A:962:ARG:NH1	2.63	0.47
1:A:553:THR:HG21	1:A:564:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:ALA:HB3	1:A:772:GLY:HA3	1.97	0.47
1:A:951:GLU:O	1:A:955:ARG:HG3	2.15	0.47
1:A:113:ILE:HG23	1:A:679:MET:CE	2.45	0.47
1:A:548:ARG:NH1	1:A:548:ARG:CG	2.64	0.46
2:A:1500:ZZQ:CBG	2:A:1500:ZZQ:SAG	3.03	0.46
1:A:387:MET:HE2	1:A:590:CYS:SG	2.54	0.46
1:A:368:GLU:O	1:A:368:GLU:HG3	2.15	0.46
1:A:907:LEU:HD23	1:A:908:PHE:N	2.31	0.46
1:A:366:CYS:O	1:A:367:SER:HB2	2.15	0.46
1:A:765:SER:HB3	1:A:768:ALA:HB3	1.97	0.46
1:A:363:VAL:CG1	1:A:364:ASN:N	2.78	0.45
1:A:974:PHE:O	1:A:978:PHE:HD1	2.00	0.45
1:A:383:ASP:HA	1:A:558:HIS:HB3	1.98	0.45
1:A:218:ALA:O	1:A:222:ARG:HG3	2.16	0.45
1:A:984:ALA:CB	1:A:986:LEU:HD13	2.46	0.45
1:A:434:THR:CG2	1:A:477:GLU:HA	2.40	0.45
1:A:327:LEU:CD2	1:A:360:SER:OG	2.64	0.44
1:A:753:ASP:H	2:A:1500:ZZQ:HBC3	1.82	0.44
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.98	0.44
1:A:791:LEU:HD13	1:A:815:CYS:HB2	2.00	0.44
1:A:938:PHE:CD1	1:A:938:PHE:N	2.84	0.44
1:A:247:HIS:CD2	1:A:740:LEU:HD21	2.52	0.44
1:A:955:ARG:HE	1:A:955:ARG:HB3	1.55	0.44
1:A:862:LYS:HG3	1:A:903:GLU:HG2	1.99	0.44
1:A:895:HIS:ND1	1:A:897:ASP:HB2	2.33	0.44
1:A:341:LEU:HG	1:A:365:VAL:HG22	2.00	0.43
1:A:841:LYS:HE2	1:A:844:MET:HE3	1.98	0.43
1:A:439:LEU:O	1:A:470:ALA:HA	2.18	0.43
1:A:512:ARG:O	1:A:515:LEU:HG	2.18	0.43
1:A:386:ARG:HG3	1:A:386:ARG:NH1	2.34	0.43
1:A:397:VAL:HG22	1:A:398:VAL:H	1.83	0.43
1:A:285:MET:O	1:A:288:GLU:HG2	2.19	0.43
1:A:329:GLU:HB2	1:A:369:PRO:O	2.18	0.43
1:A:491:ILE:HG21	1:A:565:LEU:HD23	2.00	0.43
1:A:759:LEU:O	1:A:777:ILE:HA	2.19	0.43
1:A:882:TYR:HB3	1:A:909:HIS:CD2	2.54	0.43
1:A:244:ASN:ND2	1:A:273:HIS:HB3	2.34	0.43
1:A:525:GLU:O	1:A:528:LYS:HB2	2.18	0.43
1:A:194:VAL:HG21	1:A:216:LEU:HD21	2.01	0.42
1:A:265:CYS:O	1:A:267:HIS:N	2.51	0.42
1:A:332:LYS:NZ	1:A:341:LEU:HD21	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLY:HA3	1:A:357:THR:HG22	2.01	0.42
1:A:752:MET:CB	2:A:1500:ZZQ:HBC3	2.32	0.42
1:A:844:MET:SD	1:A:844:MET:N	2.92	0.42
1:A:750:THR:OG1	1:A:751:PHE:N	2.52	0.42
1:A:809:ARG:HH11	1:A:809:ARG:HD2	1.70	0.42
1:A:380:SER:OG	1:A:382:CYS:SG	2.75	0.42
1:A:617:GLN:NE2	1:A:984:ALA:HA	2.35	0.42
1:A:907:LEU:HD23	1:A:907:LEU:C	2.40	0.42
1:A:553:THR:HG21	1:A:564:MET:CE	2.42	0.42
1:A:121:ILE:HG13	1:A:123:LYS:H	1.85	0.41
1:A:319:LEU:O	1:A:382:CYS:HB3	2.19	0.41
1:A:831:SER:HB3	1:A:902:ARG:HG2	2.01	0.41
1:A:394:LEU:HD23	1:A:418:ILE:HB	2.01	0.41
1:A:743:GLU:H	1:A:743:GLU:HG2	1.69	0.41
1:A:355:CYS:HB2	1:A:378:ASP:HB3	2.03	0.41
1:A:984:ALA:HB1	1:A:986:LEU:CD1	2.51	0.41
1:A:681:VAL:HG13	1:A:732:GLN:HE21	1.85	0.41
1:A:929:ARG:HH22	1:A:1001:SER:HA	1.85	0.41
1:A:113:ILE:HG23	1:A:679:MET:HE1	2.03	0.41
1:A:754:SER:O	1:A:757:LYS:HE3	2.21	0.41
1:A:832:ASP:O	1:A:901:ILE:CD1	2.69	0.41
1:A:389:ARG:NH2	1:A:623:SER:OG	2.54	0.40
1:A:883:CYS:HB3	1:A:932:PHE:CZ	2.56	0.40
1:A:219:CYS:O	1:A:220:ALA:C	2.59	0.40
1:A:678:HIS:O	1:A:682:LEU:HG	2.22	0.40
1:A:837:ILE:HD13	1:A:858:TRP:CE2	2.56	0.40
1:A:136:VAL:O	1:A:140:ARG:HG3	2.21	0.40
1:A:618:VAL:HG12	1:A:629:LEU:HD22	2.03	0.40
1:A:243:VAL:HA	1:A:274:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	800/940 (85%)	741 (93%)	48 (6%)	11 (1%)	11	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	LEU
1	A	367	SER
1	A	843	ASN
1	A	820	ASP
1	A	368	GLU
1	A	355	CYS
1	A	586	SER
1	A	1003	ALA
1	A	365	VAL
1	A	478	VAL
1	A	576	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	728/827 (88%)	670 (92%)	58 (8%)	12	27

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	166	SER
1	A	188	ARG
1	A	203	PHE
1	A	207	VAL
1	A	266	LEU
1	A	267	HIS
1	A	316	LEU
1	A	317	TRP
1	A	319	LEU

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Mol	Chain	Res	Type
1	A	331	ARG
1	A	332	LYS
1	A	334	ASN
1	A	339	MET
1	A	340	LYS
1	A	352	GLU
1	A	356	LYS
1	A	374	ARG
1	A	380	SER
1	A	398	VAL
1	A	423	LEU
1	A	453	LEU
1	A	467	SER
1	A	475	LEU
1	A	511	LEU
1	A	512	ARG
1	A	514	ILE
1	A	517	ARG
1	A	523	LEU
1	A	530	LEU
1	A	533	LYS
1	A	534	MET
1	A	548	ARG
1	A	553	THR
1	A	576	VAL
1	A	631	LYS
1	A	634	LEU
1	A	679	MET
1	A	680	LYS
1	A	705	LYS
1	A	722	GLU
1	A	726	GLU
1	A	743	GLU
1	A	757	LYS
1	A	779	LYS
1	A	796	LEU
1	A	843	ASN
1	A	898	ASN
1	A	901	ILE
1	A	907	LEU
1	A	915	PHE
1	A	918	ASN

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Mol	Chain	Res	Type
1	A	919	PHE
1	A	946	LYS
1	A	955	ARG
1	A	962	ARG
1	A	992	SER
1	A	1004	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	156	GLN
1	A	206	GLN
1	A	267	HIS
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	334	ASN
1	A	344	GLN
1	A	539	GLN
1	A	610	GLN
1	A	617	GLN
1	A	780	ASN
1	A	851	ASN
1	A	898	ASN
1	A	914	HIS
1	A	918	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	ZZQ	A	1500	-	38,38,38	1.70	7 (18%)	45,53,53	2.59	21 (46%)

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	ZZQ	A	1500	-	-	4/15/22/22	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ZZQ	CAK-NAJ	-4.79	1.31	1.41
2	A	1500	ZZQ	CAC-CAD	3.77	1.56	1.50
2	A	1500	ZZQ	CAL-CAM	-3.68	1.36	1.41
2	A	1500	ZZQ	CAH-SAG	3.56	1.86	1.80
2	A	1500	ZZQ	CAW-CAV	2.74	1.42	1.36
2	A	1500	ZZQ	CAI-NAJ	-2.61	1.29	1.35
2	A	1500	ZZQ	CAR-CAD	2.49	1.42	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ZZQ	CAK-NAJ-CAI	7.27	140.22	127.50
2	A	1500	ZZQ	CBC-OBB-CBG	-5.99	108.49	117.53
2	A	1500	ZZQ	CAM-CAX-NAY	-5.61	115.64	121.00
2	A	1500	ZZQ	CAL-CAK-NAJ	-4.37	108.58	123.13
2	A	1500	ZZQ	CAH-CAI-NAJ	4.06	119.97	114.41
2	A	1500	ZZQ	CAZ-CAO-NAN	-3.53	117.07	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1500	ZZQ	CAI-CAH-SAG	-3.49	97.52	111.42
2	A	1500	ZZQ	OBA-CAS-CAR	-3.22	118.94	125.08
2	A	1500	ZZQ	CBF-NAT-CAF	-3.13	114.80	119.77
2	A	1500	ZZQ	NAT-CAF-NAE	-3.03	121.36	124.58
2	A	1500	ZZQ	CAR-CAD-NAE	-2.96	119.38	123.68
2	A	1500	ZZQ	CAZ-NAY-CAX	2.91	121.44	116.93
2	A	1500	ZZQ	CAV-CAK-NAJ	2.91	130.18	120.40
2	A	1500	ZZQ	CAW-CAX-NAY	2.85	123.19	118.52
2	A	1500	ZZQ	OAA-CAI-NAJ	-2.81	118.49	123.63
2	A	1500	ZZQ	CAW-CAV-CAK	-2.65	116.12	120.93
2	A	1500	ZZQ	CBG-CBF-NAT	2.51	121.62	119.17
2	A	1500	ZZQ	CAK-CAL-CAM	2.46	123.20	120.50
2	A	1500	ZZQ	CAX-CAM-NAN	2.45	123.33	121.00
2	A	1500	ZZQ	CAO-NAN-CAM	2.32	120.52	116.93
2	A	1500	ZZQ	CAL-CAM-CAX	-2.03	117.31	119.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
2	A	1500	ZZQ	CAH-CAI-NAJ-CAK
2	A	1500	ZZQ	OAA-CAI-NAJ-CAK
2	A	1500	ZZQ	CBF-CBG-OBB-CBC
2	A	1500	ZZQ	CBH-CBG-OBB-CBC

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	ZZQ	11	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 then 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.

Ligand ZZQ A 1500

Bond lengths

Bond angles

Torsions

Rings
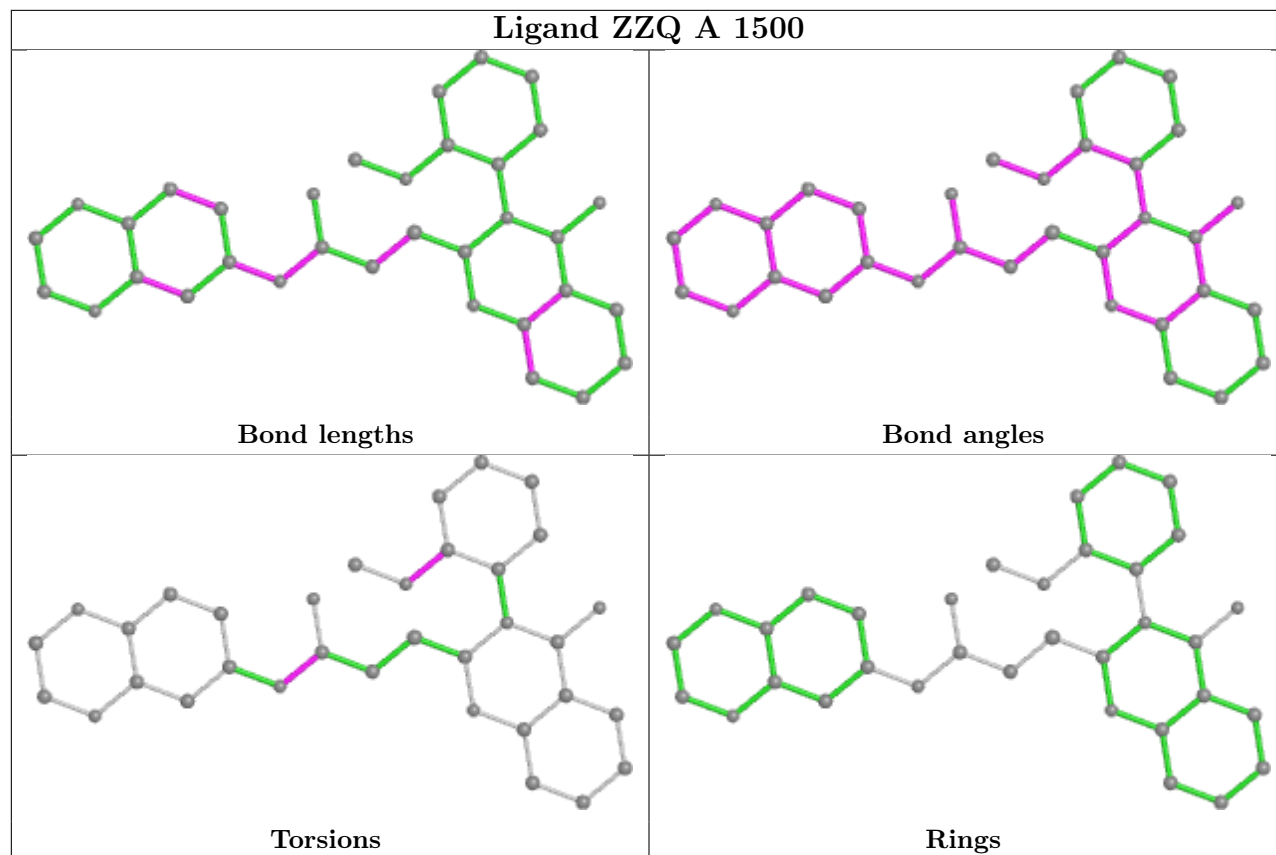
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	822/940 (87%)	0.24	39 (4%)	31	30	22, 39, 56, 75	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	846	ALA	4.8
1	A	341	LEU	4.7
1	A	330	GLY	3.6
1	A	591	TYR	3.5
1	A	323	PHE	3.5
1	A	205	PHE	3.2
1	A	196	PHE	3.2
1	A	377	PHE	3.2
1	A	842	SER	3.1
1	A	593	GLY	2.9
1	A	317	TRP	2.8
1	A	840	ASN	2.8
1	A	367	SER	2.8
1	A	1014	HIS	2.7
1	A	270	LEU	2.7
1	A	483	VAL	2.6
1	A	471	LEU	2.6
1	A	206	GLN	2.5
1	A	397	VAL	2.5
1	A	445	VAL	2.5
1	A	1006	LYS	2.5
1	A	136	VAL	2.4
1	A	472	VAL	2.4
1	A	334	ASN	2.4
1	A	492	LEU	2.4
1	A	395	TYR	2.4
1	A	227	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	592	VAL	2.3
1	A	839	LEU	2.3
1	A	936	TYR	2.3
1	A	188	ARG	2.3
1	A	366	CYS	2.3
1	A	194	VAL	2.3
1	A	394	LEU	2.2
1	A	488	LEU	2.2
1	A	335	ALA	2.1
1	A	371	TRP	2.1
1	A	938	PHE	2.0
1	A	398	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

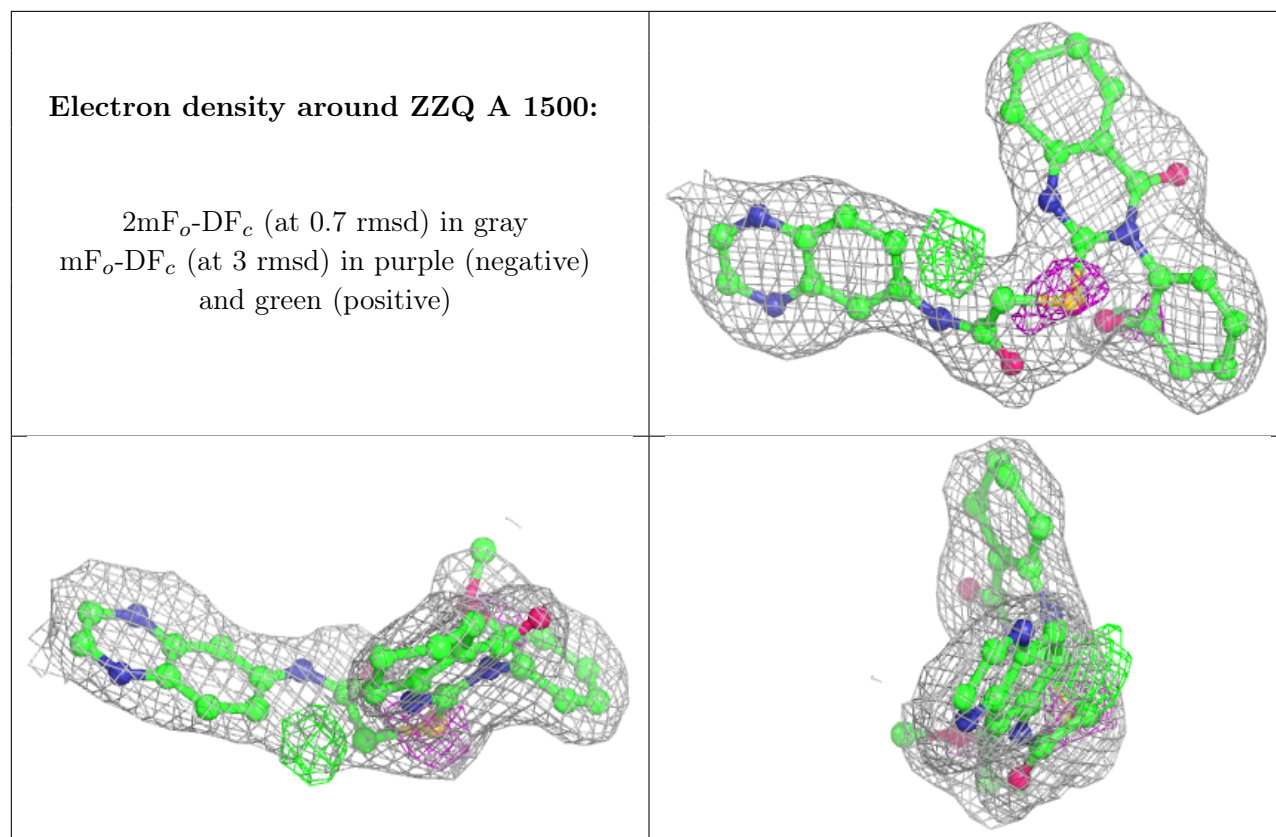There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
2	ZZQ	A	1500	34/34	0.95	0.17	33,37,46,50	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.

Electron density around ZZQ A 1500:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.