Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:56 am BST

PDB ID	:	5OQ4
Title	:	PQR309 - a Potent, Brain-Penetrant, Orally Bioavailable, pan-Class I PI3K/mTOR Inhibitor as Clinical Candidate in Oncology
Authors	:	Williams, R.L.; Zhang, X.
Deposited on	:	2017-08-10
Resolution	:	2.70 Å(reported)

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

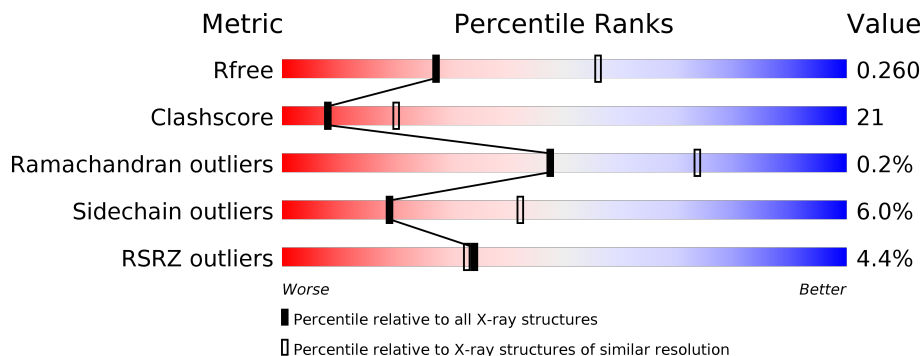|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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		0.260
Clashscore		21
Ramachandran outliers		0.2%
Sidechain outliers		6.0%
RSRZ outliers		4.4%

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 on 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	966	4% ... 54% ... 28% ... • ... 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6851 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.
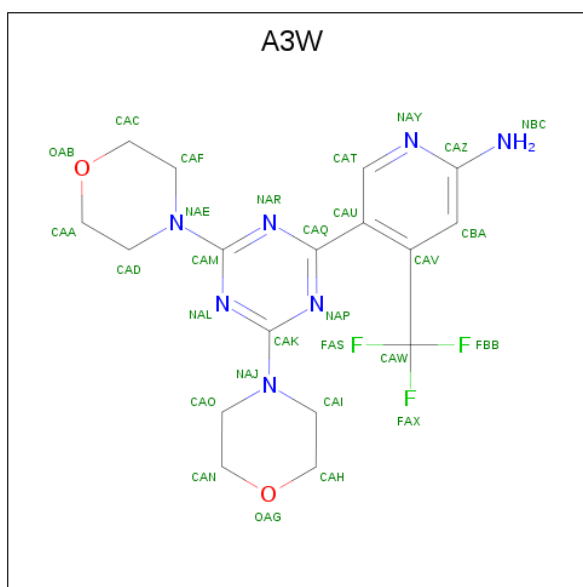
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	834	6776	4353	1158	1231	34	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	UNP P48736
A	459	ARG	GLN	conflict	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is 5-(4,6-dimorpholin-4-yl-1,3,5-triazin-2-yl)-4-(trifluoromethyl)pyridin-2-amine (three-letter code: A3W) (formula: $C_{17}H_{20}F_3N_7O_2$) (labeled as "Ligand of Interest" by author).

A3W

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			29	17	3	7	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total 36	O 36	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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 gamma isoform

D1047 I1048 E1049 R1052 D1053 A1054 L1055 T1056 N1060 E1061 E1062 D1063 Y1067 F1068 L1069 E1073 V1074 C1075 R1076 T1081 N1085 W1086 F1087 L1088 H1089 L1090 V1091 LEU GLY ILE LYS GLN GLY GLU LYS HIS SER ALA HIS HIS HIS HIS HIS HIS

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.49Å 67.36Å 103.61Å 90.00° 96.94° 90.00°	Depositor
Resolution (Å)	61.00 – 2.70 60.57 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (61.00-2.70) 97.0 (60.57-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.01 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.196 , 0.264 0.200 , 0.260	Depositor DCC
R_{free} test set	1292 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 79.4	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6851	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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: A3W, SO4

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	1.00	5/6922 (0.1%)	1.04	29/9358 (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	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	573	GLU	CD-OE2	8.50	1.34	1.25
1	A	967[A]	HIS	N-CA	-7.18	1.31	1.46
1	A	967[B]	HIS	N-CA	-7.18	1.31	1.46
1	A	867	TYR	CE1-CZ	-6.49	1.30	1.38
1	A	852	GLU	CD-OE2	5.46	1.31	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	967[A]	HIS	CA-C-O	-9.19	100.81	120.10
1	A	967[B]	HIS	CA-C-O	-9.19	100.81	120.10
1	A	579	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A	967[A]	HIS	CA-C-N	8.60	136.13	117.20
1	A	967[B]	HIS	CA-C-N	8.60	136.13	117.20
1	A	397	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	579	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	964	ASP	CB-CG-OD2	-7.69	111.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	966	GLY	CA-C-N	6.68	131.90	117.20
1	A	679	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	500	ASP	CB-CG-OD1	6.65	124.28	118.30
1	A	1052	ARG	C-N-CA	-6.62	105.16	121.70
1	A	728	MET	CG-SD-CE	6.36	110.38	100.20
1	A	842	MET	CG-SD-CE	-6.26	90.18	100.20
1	A	191	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	618	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	502	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	843	LEU	CB-CG-CD1	5.92	121.06	111.00
1	A	278	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	690	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	500	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	520	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	573	GLU	OE1-CD-OE2	5.44	129.83	123.30
1	A	947	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	964	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	690	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	177	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	170	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	841	ASP	CB-CG-OD1	-5.04	113.77	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	967[A]	HIS	Mainchain,Peptide
1	A	967[B]	HIS	Peptide

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	6776	0	6818	290	0
2	A	29	0	0	0	0
3	A	10	0	0	0	0
4	A	36	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6851	0	6818	290	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 21.

All (290) 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:948:HIS:HB3	1:A:969:LEU:HD21	1.28	1.07
1:A:620:SER:O	1:A:647:LYS:NZ	1.91	1.02
1:A:953:MET:O	1:A:960:LEU:HD12	1.60	1.00
1:A:997:THR:OG1	1:A:1003:SER:OG	1.86	0.93
1:A:583:LEU:HD13	1:A:610:LEU:HD22	1.51	0.93
1:A:583:LEU:HD21	1:A:613:ARG:O	1.68	0.93
1:A:212:TRP:O	1:A:215:ILE:O	1.87	0.92
1:A:220:ILE:N	1:A:235:VAL:O	2.02	0.91
1:A:576:TRP:O	1:A:579:ARG:HG2	1.71	0.88
1:A:1042:LEU:HG	1:A:1047:ASP:OD2	1.73	0.88
1:A:498:ASN:ND2	1:A:1040:PRO:O	2.07	0.88
1:A:1060:ASN:OD1	1:A:1063:ASP:OD2	1.92	0.87
1:A:470:ASP:OD1	1:A:474:LEU:HG	1.75	0.87
1:A:948:HIS:ND1	1:A:950:ASP:OD1	2.08	0.87
1:A:765:SER:O	1:A:769:GLN:HG3	1.73	0.86
1:A:220:ILE:O	1:A:235:VAL:N	2.08	0.85
1:A:997:THR:CG2	1:A:1001:LYS:O	2.24	0.85
1:A:477:ARG:NH1	1:A:521:ASP:OD1	2.09	0.85
1:A:964:ASP:OD2	1:A:968:ILE:HG21	1.79	0.82
1:A:760:SER:O	1:A:763:VAL:HG12	1.79	0.82
1:A:948:HIS:HB3	1:A:969:LEU:CD2	2.11	0.80
1:A:948:HIS:HD1	1:A:950:ASP:CG	1.84	0.80
1:A:611:LEU:O	1:A:614:ARG:HB2	1.82	0.79
1:A:743:GLN:CD	1:A:876:ILE:HD13	2.03	0.79
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.11	0.79
1:A:743:GLN:NE2	1:A:876:ILE:HG21	1.98	0.78
1:A:221:PHE:CE2	1:A:234:LYS:HB3	2.18	0.78
1:A:997:THR:HG23	1:A:1001:LYS:O	1.84	0.77
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.67	0.76
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.67	0.76
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.67	0.76
1:A:278:ASP:OD1	1:A:280:TYR:CE1	2.39	0.76
1:A:470:ASP:CG	1:A:474:LEU:HG	2.06	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:TYR:O	1:A:939:THR:HB	1.85	0.76
1:A:622:LEU:HD21	1:A:651:LEU:HD21	1.70	0.74
1:A:210:TYR:OH	1:A:856:GLU:HG3	1.87	0.73
1:A:360:LYS:HD3	1:A:416:PHE:O	1.89	0.73
1:A:221:PHE:CD2	1:A:234:LYS:HB3	2.24	0.73
1:A:226:ARG:HB2	1:A:229:THR:OG1	1.88	0.73
1:A:997:THR:HG21	1:A:1001:LYS:O	1.88	0.73
1:A:410:TRP:HB3	1:A:412:VAL:HG23	1.69	0.72
1:A:701:SER:O	1:A:705:GLN:HG2	1.89	0.72
1:A:568:THR:HG22	1:A:570:GLU:H	1.55	0.72
1:A:272:LEU:CD2	1:A:305:VAL:HG11	2.21	0.71
1:A:701:SER:OG	1:A:871:SER:OG	2.08	0.71
1:A:226:ARG:O	1:A:229:THR:OG1	2.07	0.70
1:A:964:ASP:OD2	1:A:968:ILE:CG2	2.39	0.70
1:A:743:GLN:CG	1:A:876:ILE:HD13	2.20	0.70
1:A:219:CYS:SG	4:A:1336:HOH:O	2.49	0.70
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.74	0.69
1:A:743:GLN:HE22	1:A:876:ILE:HG21	1.55	0.69
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.58	0.68
1:A:386:ASN:OD1	1:A:396:GLN:HG3	1.92	0.68
1:A:735:GLN:O	1:A:739:ILE:HG23	1.93	0.68
1:A:743:GLN:HG3	1:A:876:ILE:HD13	1.76	0.67
1:A:518:ILE:HD12	1:A:520:LEU:HD22	1.75	0.67
1:A:737:GLN:O	1:A:741:MET:HG3	1.96	0.66
1:A:948:HIS:HB2	1:A:969:LEU:HD11	1.77	0.65
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.25	0.65
1:A:1081:THR:O	1:A:1085:ASN:OD1	2.14	0.65
1:A:278:ASP:OD1	1:A:280:TYR:HE1	1.78	0.65
1:A:738:VAL:HG12	1:A:742:LEU:HD12	1.77	0.65
1:A:196:TYR:OH	1:A:724:CYS:O	2.06	0.64
1:A:395:CYS:HB2	1:A:418:ILE:CD1	2.27	0.64
1:A:221:PHE:CE2	1:A:234:LYS:CB	2.80	0.64
1:A:367:GLY:HA3	1:A:409:LEU:HD23	1.79	0.64
1:A:912:LYS:HA	1:A:921:PHE:CD1	2.33	0.64
1:A:172:GLU:O	1:A:176:THR:OG1	2.14	0.63
1:A:814:GLU:HG2	1:A:827:THR:OG1	1.98	0.63
1:A:887:THR:HG21	1:A:950:ASP:HA	1.80	0.63
1:A:750:LYS:NZ	1:A:808:LYS:HD2	2.14	0.63
1:A:272:LEU:HD22	1:A:305:VAL:HG11	1.80	0.63
1:A:750:LYS:HZ1	1:A:808:LYS:HD2	1.64	0.62
1:A:569:ALA:O	1:A:573:GLU:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:GLN:NE2	1:A:876:ILE:HD13	2.14	0.62
1:A:614:ARG:NH1	1:A:646:GLN:NE2	2.47	0.62
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.30	0.62
1:A:410:TRP:HB3	1:A:412:VAL:CG2	2.31	0.61
1:A:579:ARG:HG2	1:A:579:ARG:HH11	1.65	0.61
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.16	0.61
1:A:896:VAL:HG12	1:A:897:GLY:H	1.65	0.61
1:A:899:THR:HB	1:A:1087:PHE:CE1	2.36	0.61
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.82	0.61
1:A:214:LYS:HD3	1:A:297:LEU:O	2.00	0.60
1:A:887:THR:HG22	1:A:889:ALA:H	1.66	0.60
1:A:964:ASP:CG	1:A:968:ILE:HG23	2.22	0.60
1:A:387:ILE:HD12	1:A:418:ILE:HD12	1.82	0.60
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.67	0.60
1:A:576:TRP:O	1:A:579:ARG:NH1	2.31	0.60
1:A:640:VAL:O	1:A:643:ILE:HG12	2.01	0.60
1:A:221:PHE:CD2	1:A:234:LYS:CB	2.84	0.60
1:A:1085:ASN:N	1:A:1085:ASN:OD1	2.32	0.59
1:A:806:SER:O	1:A:808:LYS:O	2.19	0.59
1:A:555:LEU:HD11	1:A:575:LEU:HD12	1.84	0.59
1:A:1087:PHE:CE1	1:A:1091:VAL:HG21	2.38	0.59
1:A:804:MET:HB2	1:A:810:PRO:HG2	1.85	0.58
1:A:736:VAL:O	1:A:740:GLU:HB2	2.03	0.58
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.02	0.58
1:A:273:ARG:NH2	1:A:819:ASP:OD2	2.37	0.58
1:A:498:ASN:HD22	1:A:1041:GLN:HA	1.67	0.58
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.04	0.58
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.39	0.57
1:A:202:VAL:HG12	1:A:203:THR:N	2.19	0.57
1:A:765:SER:O	1:A:769:GLN:CG	2.51	0.57
1:A:1035:LEU:HD12	1:A:1048:ILE:CD1	2.34	0.57
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.85	0.57
1:A:562:ASP:OD1	1:A:1052:ARG:CZ	2.53	0.57
1:A:272:LEU:HD23	1:A:305:VAL:CG1	2.35	0.57
1:A:948:HIS:CB	1:A:969:LEU:HD11	2.34	0.57
1:A:1052:ARG:O	1:A:1053:ASP:C	2.36	0.57
1:A:215:ILE:HG13	1:A:215:ILE:O	2.03	0.57
1:A:165:VAL:O	1:A:165:VAL:HG12	2.05	0.57
1:A:395:CYS:SG	1:A:418:ILE:HG13	2.45	0.57
1:A:291:GLN:NE2	1:A:291:GLN:HA	2.19	0.56
1:A:757:TYR:CD1	1:A:757:TYR:O	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:THR:HB	1:A:1087:PHE:HE1	1.71	0.55
1:A:425:LYS:HE3	1:A:473:PHE:CZ	2.41	0.55
1:A:317:GLU:O	1:A:726:THR:HG23	2.06	0.55
1:A:564:LEU:HD11	1:A:1048:ILE:CG2	2.36	0.55
1:A:236:SER:N	1:A:239:ASP:OD2	2.34	0.55
1:A:1087:PHE:O	1:A:1091:VAL:HG23	2.06	0.55
1:A:614:ARG:HH11	1:A:646:GLN:NE2	2.05	0.55
1:A:205:LYS:NZ	1:A:652:GLU:OE1	2.40	0.55
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.88	0.55
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.88	0.54
1:A:223:VAL:C	1:A:224:ILE:HD12	2.28	0.54
1:A:564:LEU:CD1	1:A:1048:ILE:HG22	2.36	0.54
1:A:474:LEU:HD12	1:A:474:LEU:O	2.07	0.54
1:A:224:ILE:HD12	1:A:224:ILE:N	2.23	0.54
1:A:617:TRP:O	1:A:647:LYS:HE2	2.07	0.54
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.88	0.53
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.07	0.53
1:A:896:VAL:HG12	1:A:897:GLY:N	2.22	0.53
1:A:964:ASP:OD1	1:A:968:ILE:HG23	2.09	0.53
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.91	0.52
1:A:819:ASP:OD2	1:A:821:THR:OG1	2.25	0.52
1:A:948:HIS:CB	1:A:969:LEU:HD21	2.20	0.52
1:A:239:ASP:HB3	1:A:244:ILE:CG2	2.39	0.52
1:A:992:LEU:HD23	1:A:995:MET:HE3	1.91	0.52
1:A:769:GLN:O	1:A:772:GLU:HB2	2.09	0.52
1:A:996:GLY:O	1:A:1003:SER:OG	2.28	0.52
1:A:779:LEU:HD12	1:A:780:PRO:N	2.25	0.51
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.93	0.51
1:A:391:GLN:NE2	1:A:633:CYS:SG	2.84	0.51
1:A:586:PRO:HA	1:A:589:TYR:CE1	2.46	0.51
1:A:948:HIS:ND1	1:A:950:ASP:CG	2.61	0.51
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.46	0.51
1:A:768:LYS:O	1:A:772:GLU:HG2	2.10	0.51
1:A:273:ARG:NH2	1:A:821:THR:OG1	2.42	0.51
1:A:272:LEU:CD2	1:A:305:VAL:CG1	2.89	0.51
1:A:568:THR:HG22	1:A:570:GLU:N	2.22	0.51
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.59	0.51
1:A:232:THR:O	1:A:232:THR:HG22	2.10	0.50
1:A:804:MET:CE	1:A:810:PRO:HG2	2.41	0.50
1:A:826:GLU:O	1:A:826:GLU:HG3	2.11	0.50
1:A:969:LEU:HD12	1:A:969:LEU:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.58	0.50
1:A:845:LEU:HD13	1:A:867:TYR:O	2.12	0.50
1:A:364:LYS:HA	1:A:412:VAL:O	2.11	0.50
1:A:871:SER:OG	1:A:871:SER:O	2.27	0.50
1:A:1024:THR:HG23	1:A:1055:LEU:HD13	1.94	0.50
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.94	0.50
1:A:208:PRO:HB3	1:A:210:TYR:CE2	2.46	0.50
1:A:360:LYS:NZ	4:A:1305:HOH:O	2.44	0.50
1:A:787:TYR:HB3	1:A:870:ILE:HD12	1.94	0.50
1:A:235:VAL:HB	1:A:239:ASP:OD2	2.12	0.49
1:A:964:ASP:CG	1:A:968:ILE:CG2	2.80	0.49
1:A:219:CYS:HA	1:A:235:VAL:O	2.11	0.49
1:A:277:ARG:HD2	1:A:292:TRP:CH2	2.47	0.49
1:A:808:LYS:HB2	1:A:833:LYS:NZ	2.28	0.49
1:A:220:ILE:HD12	1:A:287:ILE:CD1	2.42	0.49
1:A:518:ILE:CD1	1:A:520:LEU:HD22	2.41	0.49
1:A:158:ILE:HG12	1:A:717:LEU:HD23	1.95	0.49
1:A:995:MET:O	1:A:1005:HIS:HB2	2.12	0.49
1:A:272:LEU:HD23	1:A:305:VAL:HG12	1.95	0.49
1:A:395:CYS:SG	1:A:418:ILE:HD11	2.53	0.49
1:A:804:MET:CE	1:A:810:PRO:CG	2.90	0.49
1:A:224:ILE:HA	1:A:305:VAL:O	2.13	0.49
1:A:948:HIS:HB2	1:A:969:LEU:CD1	2.43	0.49
1:A:952:ILE:HG22	1:A:960:LEU:HD11	1.95	0.49
1:A:220:ILE:HG22	1:A:221:PHE:N	2.28	0.48
1:A:236:SER:HB3	1:A:239:ASP:OD1	2.13	0.48
1:A:583:LEU:CD2	1:A:613:ARG:O	2.50	0.48
1:A:748:ASP:O	1:A:751:SER:HB2	2.13	0.48
1:A:1044:SER:O	1:A:1048:ILE:HG12	2.13	0.48
1:A:1062:GLU:OE1	1:A:1062:GLU:HA	2.12	0.48
1:A:787:TYR:HA	1:A:870:ILE:HD11	1.95	0.48
1:A:997:THR:HG21	1:A:1076:ARG:HH12	1.79	0.48
1:A:240:THR:O	1:A:244:ILE:HG12	2.14	0.48
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.48	0.48
1:A:947:ARG:NH2	1:A:963:ILE:O	2.46	0.48
1:A:689:LYS:HD3	1:A:728:MET:SD	2.54	0.48
1:A:787:TYR:CE1	1:A:880:GLU:HB2	2.49	0.48
1:A:225:HIS:O	1:A:226:ARG:HG3	2.13	0.47
1:A:743:GLN:HG3	1:A:876:ILE:CD1	2.42	0.47
1:A:435:CYS:SG	1:A:461:LEU:HD11	2.54	0.47
1:A:555:LEU:HD11	1:A:575:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:HG22	1:A:177:ARG:HH12	1.80	0.47
1:A:547:MET:O	1:A:552:ARG:NH1	2.48	0.47
1:A:202:VAL:CG1	1:A:203:THR:N	2.78	0.47
1:A:233:ILE:N	1:A:233:ILE:HD12	2.30	0.47
1:A:1043:THR:O	1:A:1044:SER:C	2.53	0.47
1:A:581:GLU:HA	1:A:581:GLU:OE1	2.15	0.47
1:A:833:LYS:O	1:A:876:ILE:HG13	2.15	0.47
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.44	0.47
1:A:214:LYS:CD	1:A:297:LEU:O	2.62	0.47
1:A:180:LEU:O	1:A:183:PRO:HG2	2.14	0.46
1:A:466:LEU:HD21	1:A:476:ARG:HD3	1.97	0.46
1:A:887:THR:CG2	1:A:950:ASP:HA	2.46	0.46
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.50	0.46
1:A:804:MET:HE2	1:A:810:PRO:HG2	1.96	0.46
1:A:497:PHE:CD1	1:A:497:PHE:N	2.83	0.46
1:A:952:ILE:CG2	1:A:960:LEU:HD11	2.46	0.46
1:A:945:GLY:HA3	1:A:984:PRO:O	2.15	0.46
1:A:961:PHE:N	1:A:961:PHE:CD1	2.84	0.46
1:A:667:VAL:O	1:A:712:ARG:NH1	2.49	0.45
1:A:787:TYR:HB3	1:A:870:ILE:CD1	2.47	0.45
1:A:697:TRP:CZ3	1:A:872:THR:HG22	2.51	0.45
1:A:605:ALA:O	1:A:609:GLN:HG3	2.16	0.45
1:A:158:ILE:HG23	1:A:717:LEU:HD23	1.98	0.45
1:A:526:PRO:O	1:A:527:ILE:HB	2.17	0.45
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.47	0.45
1:A:743:GLN:CD	1:A:876:ILE:HG21	2.37	0.45
1:A:430:ASN:ND2	1:A:465:ASN:OD1	2.33	0.45
1:A:614:ARG:NH1	1:A:646:GLN:HE21	2.13	0.44
1:A:1056:THR:HG21	1:A:1067:TYR:CD2	2.52	0.44
1:A:182:THR:N	1:A:183:PRO:HD2	2.32	0.44
1:A:547:MET:HE1	1:A:552:ARG:HA	1.98	0.44
1:A:618:ASP:OD1	1:A:646:GLN:OE1	2.35	0.44
1:A:724:CYS:HB2	1:A:728:MET:HG3	1.99	0.44
1:A:775:GLN:HA	1:A:779:LEU:HD23	1.98	0.44
1:A:226:ARG:O	1:A:227:SER:OG	2.31	0.44
1:A:643:ILE:O	1:A:646:GLN:HB3	2.17	0.44
1:A:507:ASN:OD1	1:A:508:PRO:HD2	2.17	0.44
1:A:1049:GLU:OE2	1:A:1052:ARG:NH1	2.51	0.43
1:A:272:LEU:HB3	1:A:305:VAL:CG1	2.49	0.43
1:A:614:ARG:NH1	1:A:643:ILE:HG22	2.33	0.43
1:A:987:LEU:HB3	1:A:1075:CYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:LEU:HD12	1:A:1048:ILE:HD12	2.01	0.42
1:A:751:SER:C	1:A:752:LEU:HD23	2.39	0.42
1:A:834:HIS:C	1:A:834:HIS:CD2	2.92	0.42
1:A:913:GLU:HG3	1:A:914:LYS:N	2.34	0.42
1:A:824:SER:OG	1:A:825:ASN:N	2.53	0.42
1:A:379:LEU:HD23	1:A:435:CYS:SG	2.58	0.42
1:A:988:THR:HB	1:A:989:PRO:CD	2.49	0.42
1:A:467:LEU:O	1:A:476:ARG:HD2	2.19	0.42
1:A:889:ALA:HB2	1:A:949:ASN:HB3	2.01	0.42
1:A:198:MET:O	1:A:199:HIS:CG	2.73	0.42
1:A:617:TRP:O	1:A:647:LYS:CE	2.68	0.42
1:A:498:ASN:C	1:A:498:ASN:OD1	2.58	0.42
1:A:745:VAL:O	1:A:749:ILE:HD13	2.19	0.42
1:A:970:GLY:HA3	1:A:1086:TRP:CH2	2.55	0.42
1:A:240:THR:HG22	1:A:242:GLY:H	1.84	0.42
1:A:395:CYS:SG	1:A:418:ILE:CD1	3.08	0.42
1:A:667:VAL:HG12	1:A:667:VAL:O	2.19	0.42
1:A:948:HIS:CG	1:A:949:ASN:N	2.88	0.42
1:A:602:GLU:O	1:A:606:LYS:HG3	2.19	0.42
1:A:804:MET:HE3	1:A:810:PRO:CG	2.49	0.42
1:A:170:ASP:OD2	1:A:476:ARG:NH2	2.53	0.41
1:A:834:HIS:HA	1:A:875:LYS:O	2.19	0.41
1:A:226:ARG:C	1:A:227:SER:OG	2.57	0.41
1:A:763:VAL:HG13	1:A:764:ILE:N	2.35	0.41
1:A:271:VAL:CG2	1:A:282:VAL:HG12	2.50	0.41
1:A:558:ILE:HD11	1:A:571:ASP:OD1	2.20	0.41
1:A:287:ILE:HA	1:A:290:PHE:HD2	1.86	0.41
1:A:614:ARG:HG2	1:A:617:TRP:HB3	2.01	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.21	0.41
1:A:929:VAL:HG22	1:A:995:MET:HG2	2.02	0.41
1:A:239:ASP:HB3	1:A:244:ILE:HG23	2.03	0.41
1:A:241:PRO:HA	1:A:244:ILE:HD11	2.03	0.41
1:A:372:VAL:HG12	1:A:373:LEU:N	2.35	0.41
1:A:474:LEU:HD12	1:A:474:LEU:C	2.42	0.41
1:A:834:HIS:HB2	1:A:876:ILE:HD12	2.02	0.41
1:A:1035:LEU:HD13	1:A:1042:LEU:HD23	2.02	0.41
1:A:1069:LEU:O	1:A:1073:GLU:HG2	2.21	0.41
1:A:611:LEU:HD23	1:A:611:LEU:HA	1.84	0.41
1:A:686:LEU:HD23	1:A:686:LEU:HA	1.87	0.41
1:A:804:MET:HE2	1:A:810:PRO:CG	2.50	0.40
1:A:992:LEU:HA	1:A:995:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PHE:HE2	1:A:234:LYS:HB3	1.77	0.40
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.94	0.40
1:A:608:TYR:CD1	1:A:608:TYR:N	2.90	0.40
1:A:809:LYS:HD2	1:A:809:LYS:HA	1.86	0.40
1:A:933:ALA:O	1:A:937:VAL:HG23	2.22	0.40
1:A:435:CYS:O	1:A:435:CYS:SG	2.79	0.40
1:A:425:LYS:HE3	1:A:473:PHE:CE2	2.57	0.40
1:A:622:LEU:HD21	1:A:651:LEU:HD23	1.98	0.40
1:A:518:ILE:CD1	1:A:520:LEU:CD2	3.00	0.40
1:A:808:LYS:O	1:A:809:LYS:HD2	2.21	0.40
1:A:865:LEU:HD12	1:A:865:LEU:HA	1.92	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	813/966 (84%)	787 (97%)	23 (3%)	3 (0%)	34 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1044	SER
1	A	967[A]	HIS
1	A	967[B]	HIS

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	752/864 (87%)	706 (94%)	46 (6%)	18	41

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	A	241	PRO
1	A	250	THR
1	A	271	VAL
1	A	288	LYS
1	A	298	LYS
1	A	435	CYS
1	A	470	ASP
1	A	476	ARG
1	A	488	SER
1	A	497	PHE
1	A	498	ASN
1	A	513	SER
1	A	518	ILE
1	A	520	LEU
1	A	562	ASP
1	A	574	LEU
1	A	575	LEU
1	A	579	ARG
1	A	601	GLN
1	A	610	LEU
1	A	646	GLN
1	A	658	HIS
1	A	734	GLN
1	A	739	ILE
1	A	740	GLU
1	A	755	GLU
1	A	799	GLU
1	A	809	LYS
1	A	819	ASP
1	A	821	THR
1	A	823	LEU
1	A	832	PHE
1	A	862	LEU
1	A	888	ILE

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Mol	Chain	Res	Type
1	A	905	GLU
1	A	907	LEU
1	A	912	LYS
1	A	939	THR
1	A	967[A]	HIS
1	A	967[B]	HIS
1	A	1003	SER
1	A	1015	LYS
1	A	1029	ILE
1	A	1085	ASN
1	A	1087	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	225	HIS
1	A	291	GLN
1	A	304	HIS
1	A	391	GLN
1	A	646	GLN
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	769	GLN
1	A	834	HIS
1	A	840	GLN
1	A	959	ASN
1	A	1089	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	#$|Z| > 2$
3	SO4	A	1203	-	4,4,4	0.39	0	6,6,6	0.25	0
2	A3W	A	1201	-	32,32,32	2.08	9 (28%)	43,46,46	2.32	12 (27%)
3	SO4	A	1202	-	4,4,4	0.29	0	6,6,6	0.21	0

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	A3W	A	1201	-	-	0/18/34/34	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	A3W	CAK-NAJ	5.83	1.46	1.35
2	A	1201	A3W	CAM-NAE	4.26	1.43	1.35
2	A	1201	A3W	CAU-CAQ	4.17	1.59	1.48
2	A	1201	A3W	CAM-NAR	3.51	1.40	1.34
2	A	1201	A3W	CAK-NAP	2.69	1.39	1.34
2	A	1201	A3W	CAQ-NAP	2.35	1.39	1.34
2	A	1201	A3W	CAM-NAL	2.34	1.38	1.34
2	A	1201	A3W	CAD-CAA	2.18	1.58	1.50
2	A	1201	A3W	CAI-CAH	2.03	1.58	1.50

All (12) bond angle outliers are listed below:

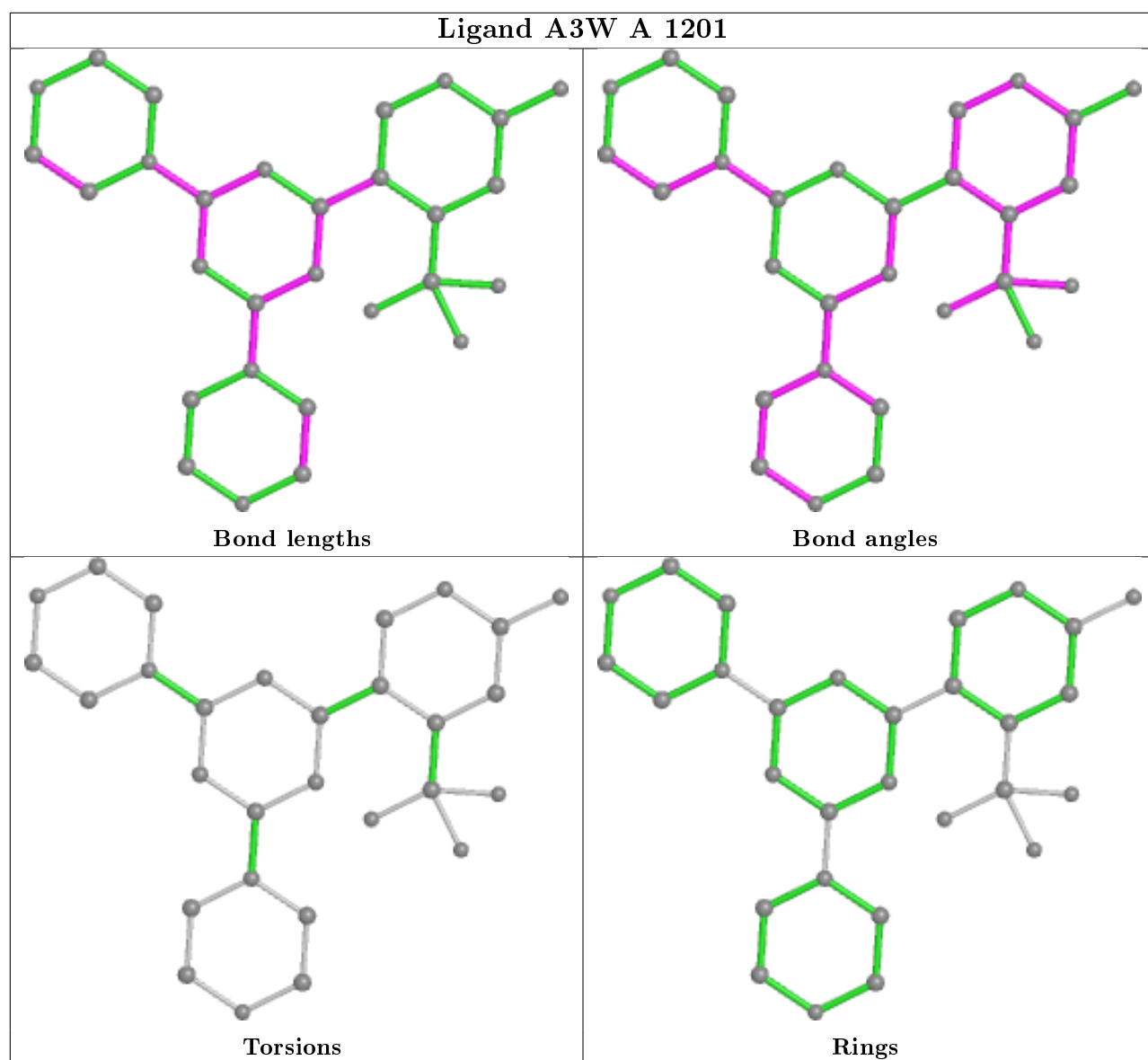| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	A3W	CBA-CAZ-NAY	-7.28	114.87	121.53
2	A	1201	A3W	CAK-NAP-CAQ	5.37	118.33	114.43
2	A	1201	A3W	CBA-CAV-CAU	4.87	125.64	119.77
2	A	1201	A3W	CAA-CAD-NAE	4.67	118.64	110.02
2	A	1201	A3W	FAS-CAW-CAV	3.71	119.16	112.70
2	A	1201	A3W	CAI-NAJ-CAK	3.26	127.09	121.69
2	A	1201	A3W	CAU-CAT-NAY	3.11	129.38	124.49
2	A	1201	A3W	NAP-CAK-NAJ	2.82	120.59	117.11
2	A	1201	A3W	OAG-CAN-CAO	-2.72	105.80	111.80
2	A	1201	A3W	CAO-NAJ-CAK	-2.60	117.38	121.69
2	A	1201	A3W	CAD-NAE-CAM	2.33	125.55	121.69
2	A	1201	A3W	FAX-CAW-CAV	-2.17	108.92	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 A3W A 1201

Bond lengths

Bond angles

Torsions

Rings

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	834/966 (86%)	0.13	37 (4%)	34	33	29, 60, 106, 143	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	GLY	6.2
1	A	269	ASP	4.8
1	A	268	GLN	4.5
1	A	755	GLU	4.1
1	A	379	LEU	3.3
1	A	1043	THR	3.3
1	A	522	ASN	3.2
1	A	249	PHE	3.0
1	A	220	ILE	2.9
1	A	151	GLN	2.9
1	A	747	LEU	2.9
1	A	270	PHE	2.9
1	A	758	ASP	2.7
1	A	287	ILE	2.7
1	A	743	GLN	2.7
1	A	146	GLU	2.7
1	A	823	LEU	2.7
1	A	221	PHE	2.7
1	A	377	THR	2.7
1	A	147	SER	2.6
1	A	527	ILE	2.6
1	A	1089	HIS	2.6
1	A	757	TYR	2.5
1	A	545	ALA	2.5
1	A	166	SER	2.4
1	A	236	SER	2.4
1	A	233	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	145	GLU	2.3
1	A	226	ARG	2.3
1	A	526	PRO	2.3
1	A	874	ASP	2.2
1	A	235	VAL	2.2
1	A	808	LYS	2.2
1	A	805	ALA	2.1
1	A	370	ILE	2.1
1	A	211	LEU	2.1
1	A	1087	PHE	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.
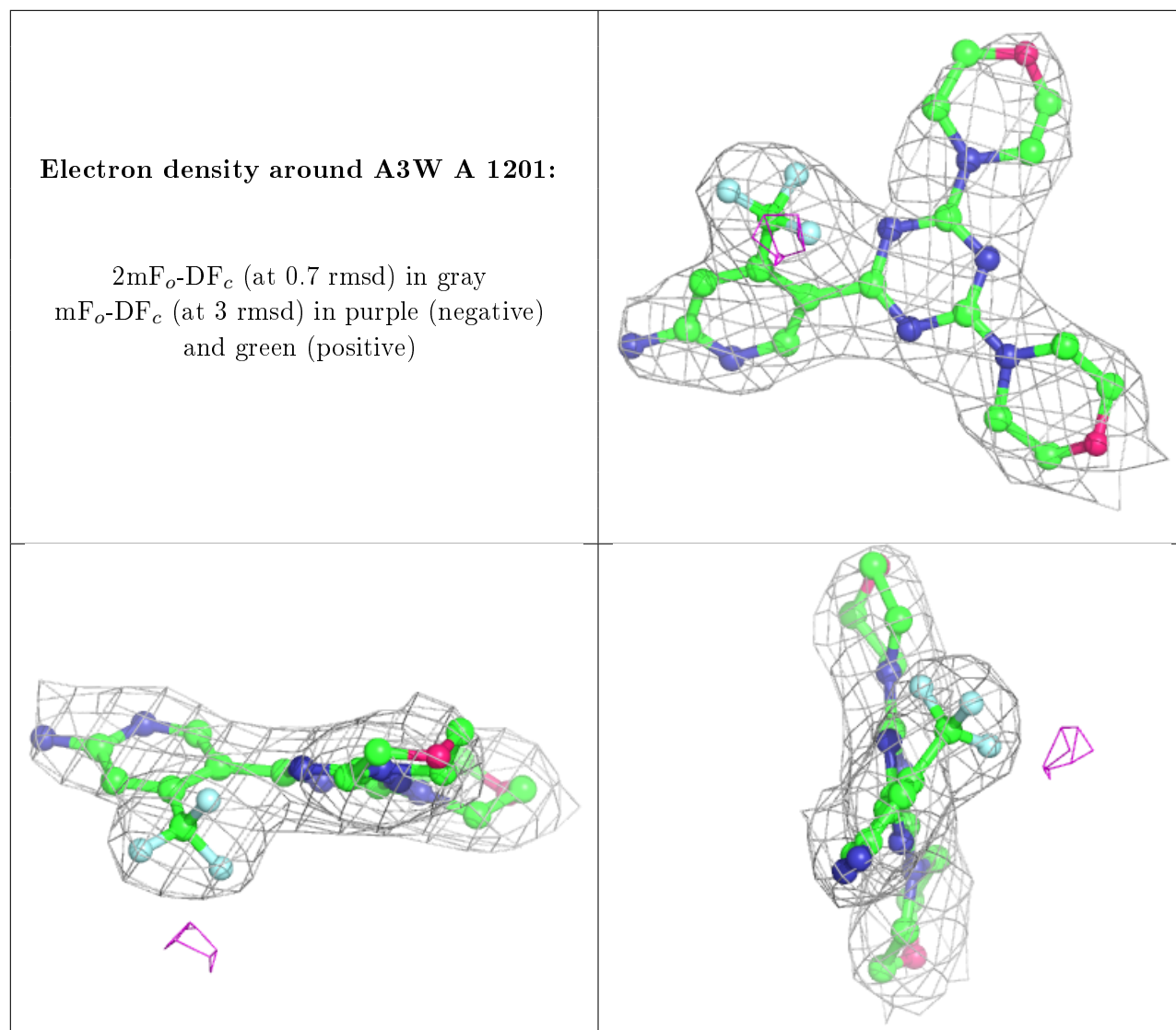
6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	SO4	A	1202	5/5	0.88	0.23	105,110,114,117	0
3	SO4	A	1203	5/5	0.91	0.13	91,93,101,107	0
2	A3W	A	1201	29/29	0.96	0.19	44,56,68,76	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 A3W A 1201:

$2mF_o$-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.