Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 03:55 am BST

PDB ID	:	4ANW
Title	:	Complexes of PI3Kgamma with isoform selective inhibitors.
Authors	:	Foster, P.G.; Lougheed, J.C.
Deposited on	:	2012-03-22
Resolution	:	2.31 Å(reported)

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

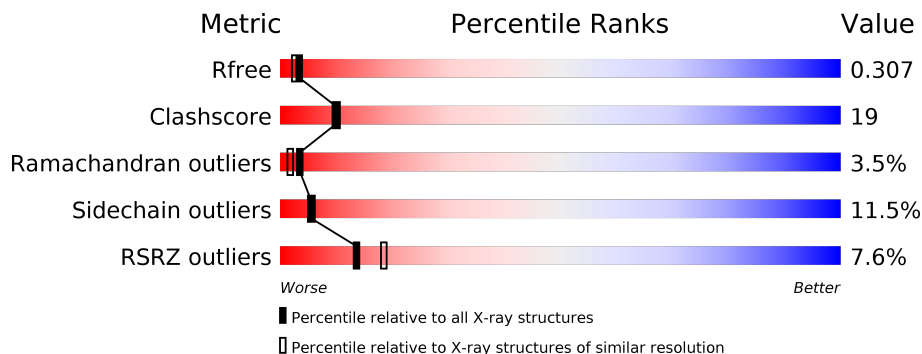|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.31 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		0.307
Clashscore		19
Ramachandran outliers		3.5%
Sidechain outliers		11.5%
RSRZ outliers		7.6%

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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	980	6% / 49% / 29% / 6% · / 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6888 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	833	6757	4334	1153	1235	35	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	expression tag	UNP P48736
A	140	LEU	-	expression tag	UNP P48736
A	141	LEU	-	expression tag	UNP P48736
A	142	GLY	-	expression tag	UNP P48736
A	143	SER	-	expression tag	UNP P48736
A	1103	GLU	-	expression tag	UNP P48736
A	1104	PHE	-	expression tag	UNP P48736
A	1105	GLY	-	expression tag	UNP P48736
A	1106	LEU	-	expression tag	UNP P48736
A	1107	VAL	-	expression tag	UNP P48736
A	1108	PRO	-	expression tag	UNP P48736
A	1109	ARG	-	expression tag	UNP P48736
A	1110	GLY	-	expression tag	UNP P48736
A	1111	SER	-	expression tag	UNP P48736
A	1112	GLY	-	expression tag	UNP P48736
A	1113	HIS	-	expression tag	UNP P48736
A	1114	HIS	-	expression tag	UNP P48736
A	1115	HIS	-	expression tag	UNP P48736
A	1116	HIS	-	expression tag	UNP P48736
A	1117	HIS	-	expression tag	UNP P48736
A	1118	HIS	-	expression tag	UNP P48736

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 3 is 3-AMINO-6-{4-CHLORO-3-[(2,3-DIFLUOROPHENYL)SULFAMOYL]PH ENYL}-N-METHYLPYRAZINE-2-CARBOXAMIDE (three-letter code: O92) (formula: $C_{18}H_{14}ClF_2N_5O_3S$).
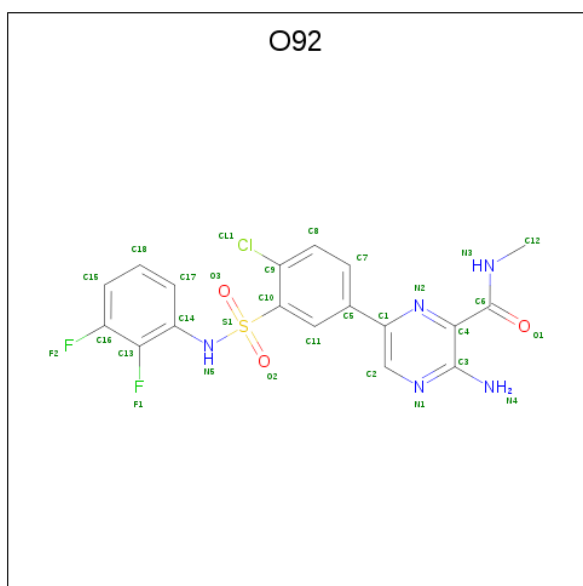
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	1
			60	36	2	4	10	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total 66	O 66	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
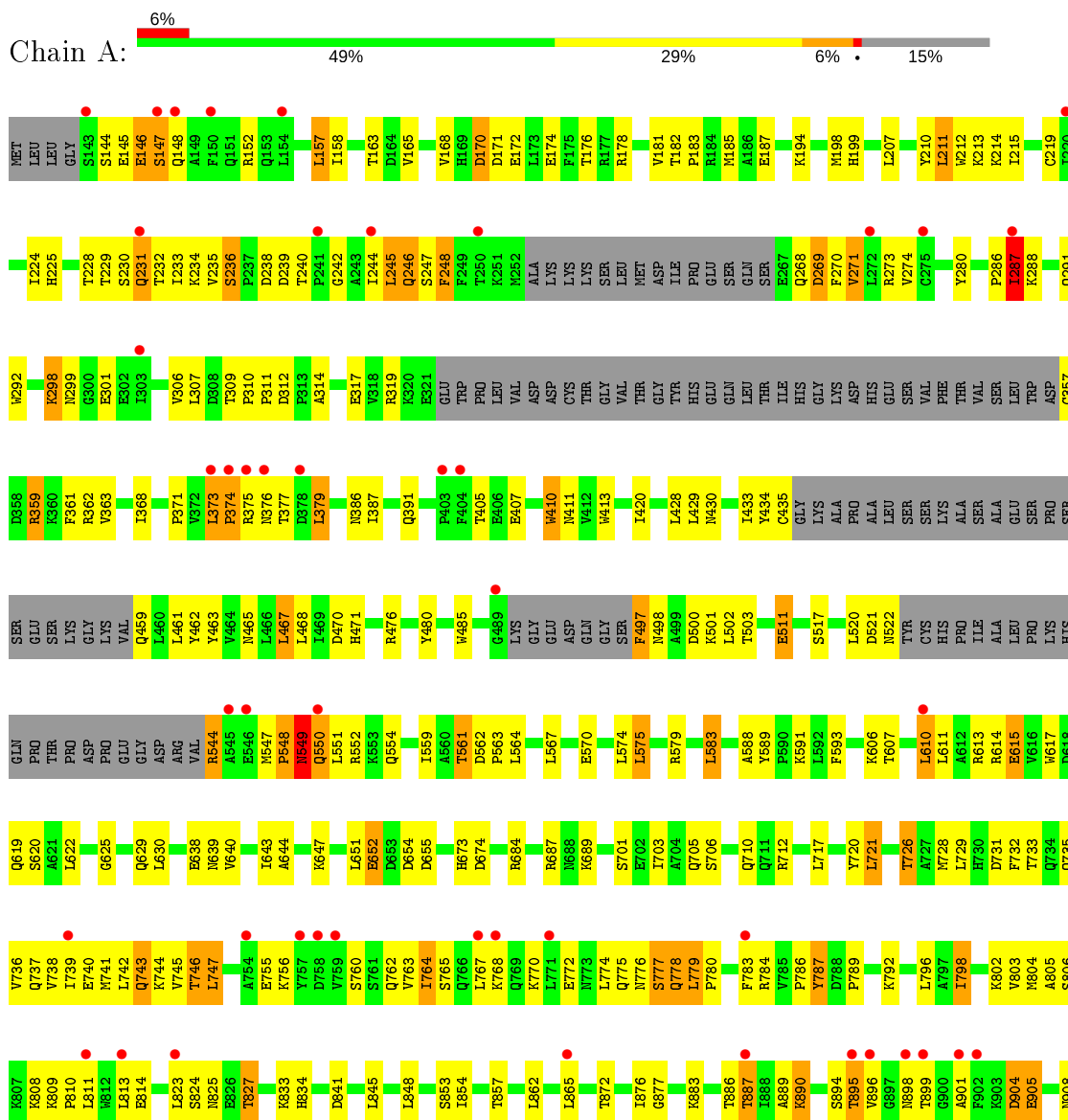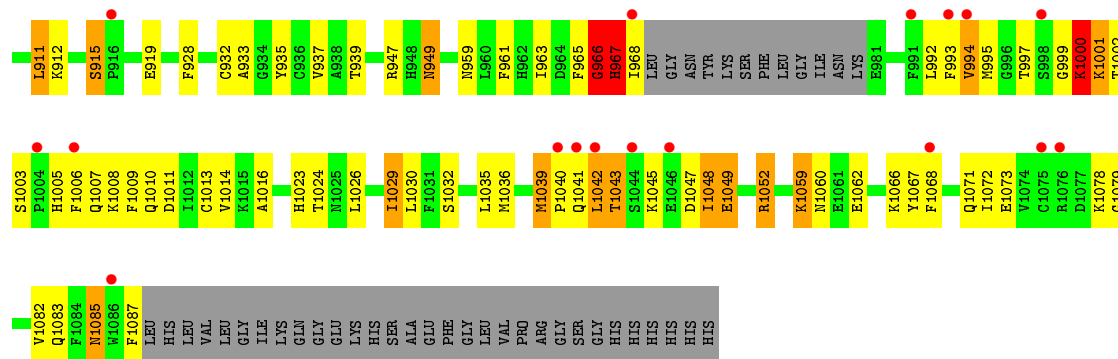
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.42Å 68.53Å 106.26Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	71.43 – 2.31 71.41 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.2 (71.43-2.31) 98.3 (71.41-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.296 0.246 , 0.307	Depositor DCC
R_{free} test set	2248 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.9	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	6888	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: O92, 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	0.89	2/6901 (0.0%)	0.92	11/9334 (0.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	570	GLU	CB-CG	5.87	1.63	1.52
1	A	480	TYR	CG-CD2	-5.18	1.32	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	A	684	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	575	LEU	CA-CB-CG	6.77	130.88	115.30
1	A	170	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	966	GLY	N-CA-C	5.98	128.04	113.10
1	A	470	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	967	HIS	O-C-N	-5.42	114.04	122.70
1	A	319	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	848	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	967	HIS	C-N-CA	-5.18	108.76	121.70
1	A	552	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1039	MET	Peptide
1	A	410	TRP	Peptide
1	A	965	PHE	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	6757	0	6789	262	0
2	A	5	0	0	0	0
3	A	60	0	28	4	0
4	A	66	0	0	1	0
All	All	6888	0	6817	262	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 (262) 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:777:SER:CB	1:A:778:GLN:HB2	1.59	1.31
1:A:967:HIS:H	1:A:968:ILE:HA	0.99	1.15
1:A:777:SER:HB3	1:A:778:GLN:CB	1.76	1.14
1:A:966:GLY:HA3	1:A:967:HIS:HB2	1.31	1.08
1:A:967:HIS:N	1:A:968:ILE:HA	1.61	1.02
1:A:210:TYR:O	1:A:211:LEU:HB2	1.62	0.97
1:A:947:ARG:NH2	1:A:963:ILE:O	1.98	0.95
1:A:775:GLN:HB3	1:A:776:ASN:HB2	1.47	0.95
1:A:428:LEU:HD23	1:A:467:LEU:HD12	1.47	0.95
1:A:673:HIS:HD2	1:A:712:ARG:HE	1.12	0.93
1:A:777:SER:HB3	1:A:778:GLN:HB2	0.90	0.89
1:A:430:ASN:HD22	1:A:465:ASN:ND2	1.72	0.86
1:A:652:GLU:OE2	1:A:654:ASP:HB3	1.76	0.86
1:A:298:LYS:NZ	1:A:299:ASN:HD21	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.64	0.80
1:A:145:GLU:HA	1:A:146:GLU:O	1.82	0.79
1:A:219:CYS:SG	1:A:234:LYS:HG3	2.23	0.79
1:A:966:GLY:CA	1:A:967:HIS:HB2	2.12	0.78
1:A:551:LEU:O	1:A:554:GLN:HB2	1.85	0.77
1:A:428:LEU:CD2	1:A:467:LEU:HD12	2.15	0.76
1:A:772:GLU:O	1:A:776:ASN:HB3	1.84	0.76
1:A:497:PHE:O	1:A:1042:LEU:CD1	2.34	0.76
1:A:435:CYS:SG	1:A:461:LEU:HD11	2.27	0.74
1:A:207:LEU:HD21	1:A:211:LEU:HB3	1.69	0.74
1:A:967:HIS:H	1:A:968:ILE:CA	1.92	0.73
1:A:928:PHE:O	1:A:932:CYS:HB2	1.88	0.73
1:A:219:CYS:SG	1:A:234:LYS:CG	2.77	0.73
1:A:405:THR:HG23	1:A:407:GLU:O	1.88	0.73
1:A:814:GLU:OE1	1:A:827:THR:HG21	1.89	0.73
1:A:430:ASN:HD22	1:A:465:ASN:HD21	1.32	0.72
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.37	0.72
1:A:212:TRP:HA	1:A:215:ILE:HD12	1.72	0.71
1:A:172:GLU:HG3	1:A:471:HIS:CD2	2.25	0.70
1:A:271:VAL:HG13	1:A:310:PRO:HG3	1.74	0.70
1:A:497:PHE:O	1:A:1042:LEU:HD13	1.91	0.69
1:A:146:GLU:O	1:A:148:GLN:N	2.25	0.69
1:A:689:LYS:HG2	1:A:728:MET:SD	2.32	0.69
1:A:476:ARG:O	1:A:520:LEU:HD23	1.93	0.69
1:A:997:THR:OG1	1:A:1003:SER:HB2	1.92	0.68
1:A:774:LEU:O	1:A:778:GLN:HB3	1.93	0.68
1:A:298:LYS:HZ1	1:A:299:ASN:HD21	1.39	0.68
1:A:615:GLU:O	1:A:619:GLN:HG3	1.94	0.67
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.74	0.67
1:A:701:SER:O	1:A:705:GLN:HG2	1.95	0.67
1:A:168:VAL:CG1	1:A:170:ASP:O	2.43	0.67
1:A:363:VAL:HG23	1:A:520:LEU:HD12	1.77	0.67
1:A:743:GLN:O	1:A:747:LEU:HD22	1.94	0.67
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.77	0.66
1:A:673:HIS:CD2	1:A:712:ARG:HE	2.04	0.66
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.76	0.66
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.77	0.65
1:A:244:ILE:HD11	1:A:287:ILE:HG12	1.78	0.65
1:A:762:GLN:HA	1:A:765:SER:HB3	1.79	0.65
1:A:770:LYS:O	1:A:774:LEU:HB2	1.96	0.65
1:A:579:ARG:HD2	1:A:610:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:THR:HG22	1:A:890:LYS:H	1.63	0.64
1:A:738:VAL:HG12	1:A:742:LEU:HD12	1.79	0.64
1:A:968:ILE:O	1:A:968:ILE:HG12	1.98	0.62
1:A:224:ILE:HG22	1:A:225:HIS:N	2.15	0.62
1:A:240:THR:HG22	1:A:242:GLY:H	1.64	0.62
1:A:834:HIS:HB2	1:A:876:ILE:CD1	2.30	0.61
1:A:933:ALA:O	1:A:937:VAL:HG23	2.00	0.61
1:A:174:GLU:O	1:A:178:ARG:HG3	1.99	0.61
1:A:361:PHE:HA	1:A:420:ILE:CD1	2.30	0.61
1:A:561:THR:CG2	1:A:591:LYS:HE2	2.31	0.61
1:A:804:MET:HB2	1:A:810:PRO:HD2	1.82	0.61
1:A:993:PHE:O	1:A:994:VAL:HG23	2.01	0.61
1:A:833:LYS:NZ	3:A:1189[B]:O92:O3	2.23	0.60
1:A:471:HIS:H	1:A:471:HIS:CD2	2.17	0.60
1:A:617:TRP:O	1:A:620:SER:OG	2.15	0.60
1:A:497:PHE:O	1:A:1042:LEU:HD11	2.01	0.60
1:A:767:LEU:HD22	1:A:803:VAL:CG2	2.31	0.60
1:A:777:SER:CB	1:A:778:GLN:CB	2.55	0.60
1:A:357:CYS:SG	1:A:359:ARG:HG2	2.42	0.60
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.84	0.59
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.36	0.59
1:A:1003:SER:O	1:A:1007:GLN:HB2	2.00	0.59
1:A:887:THR:HG23	1:A:889:ALA:H	1.66	0.59
1:A:210:TYR:O	1:A:211:LEU:CB	2.43	0.59
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.01	0.59
1:A:706:SER:O	1:A:710:GLN:HB3	2.02	0.59
1:A:967:HIS:N	1:A:968:ILE:CA	2.53	0.59
1:A:1060:ASN:OD1	1:A:1062:GLU:HB2	2.02	0.58
1:A:434:TYR:HA	1:A:459:GLN:O	2.04	0.58
1:A:165:VAL:O	1:A:165:VAL:HG12	2.04	0.57
1:A:298:LYS:NZ	1:A:299:ASN:ND2	2.51	0.57
1:A:548:PRO:O	1:A:549:ASN:C	2.43	0.57
1:A:911:LEU:O	1:A:915:SER:OG	2.22	0.57
1:A:232:THR:CG2	1:A:233:ILE:N	2.67	0.57
1:A:230:SER:O	1:A:231:GLN:HB2	2.05	0.57
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.39	0.56
1:A:742:LEU:HD22	1:A:813:LEU:HD11	1.87	0.56
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.05	0.56
1:A:168:VAL:HG13	1:A:170:ASP:H	1.70	0.56
1:A:182:THR:HB	1:A:183:PRO:CD	2.36	0.56
1:A:1002:THR:HG22	1:A:1003:SER:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:PRO:HG2	1:A:511:GLU:O	2.06	0.55
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.89	0.55
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.88	0.55
1:A:498:ASN:HD22	1:A:1041:GLN:HE22	1.54	0.55
1:A:775:GLN:NE2	1:A:798:ILE:HD11	2.21	0.55
1:A:547:MET:O	1:A:548:PRO:C	2.42	0.55
1:A:298:LYS:HZ3	1:A:299:ASN:HD21	1.51	0.54
1:A:833:LYS:NZ	3:A:1189[A]:O92:O3	2.28	0.54
1:A:236:SER:O	1:A:287:ILE:HD11	2.07	0.54
1:A:273:ARG:HG3	1:A:280:TYR:CE2	2.43	0.54
1:A:742:LEU:O	1:A:746:THR:HG22	2.06	0.54
1:A:1032:SER:O	1:A:1036:MET:HG3	2.08	0.54
1:A:428:LEU:CD2	1:A:467:LEU:CD1	2.86	0.54
1:A:583:LEU:HD12	1:A:613:ARG:HD3	1.88	0.54
1:A:738:VAL:CG1	1:A:742:LEU:HD12	2.38	0.54
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.43	0.53
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.09	0.53
1:A:246:GLN:C	1:A:248:PHE:H	2.12	0.53
1:A:625:GLY:O	1:A:629:GLN:HG3	2.08	0.53
1:A:798:ILE:HD12	1:A:798:ILE:H	1.73	0.53
1:A:362:ARG:H	1:A:522:ASN:HD21	1.57	0.53
1:A:1041:GLN:HA	1:A:1041:GLN:NE2	2.23	0.53
1:A:145:GLU:CA	1:A:146:GLU:O	2.56	0.52
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.91	0.52
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.44	0.52
1:A:561:THR:HG22	1:A:591:LYS:HE2	1.90	0.52
1:A:735:GLN:O	1:A:739:ILE:CD1	2.58	0.52
1:A:291:GLN:NE2	1:A:654:ASP:OD1	2.41	0.52
1:A:168:VAL:CG1	1:A:170:ASP:H	2.23	0.52
1:A:224:ILE:HG22	1:A:225:HIS:H	1.75	0.51
1:A:317:GLU:O	1:A:726:THR:HG23	2.10	0.51
1:A:786:PRO:O	1:A:787:TYR:CG	2.64	0.51
1:A:853:SER:O	1:A:857:THR:HG23	2.10	0.51
1:A:992:LEU:O	1:A:995:MET:HB2	2.11	0.51
1:A:168:VAL:HG11	1:A:170:ASP:O	2.10	0.51
1:A:373:LEU:O	1:A:374:PRO:C	2.49	0.51
1:A:834:HIS:CA	1:A:876:ILE:HD12	2.40	0.51
1:A:1049:GLU:O	1:A:1049:GLU:HG3	2.10	0.50
1:A:740:GLU:O	1:A:744:LYS:HG3	2.11	0.50
1:A:163:THR:O	1:A:165:VAL:HG23	2.11	0.50
1:A:639:ASN:O	1:A:643:ILE:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:HIS:CB	1:A:876:ILE:HD12	2.41	0.50
1:A:775:GLN:HE22	1:A:798:ILE:HD11	1.76	0.49
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.94	0.49
1:A:559:ILE:O	1:A:559:ILE:CG2	2.60	0.49
1:A:760:SER:OG	1:A:763:VAL:HG23	2.12	0.49
1:A:181:VAL:O	1:A:185:MET:HG3	2.13	0.49
1:A:904:ASP:OD1	1:A:904:ASP:N	2.46	0.49
1:A:1073:GLU:HA	1:A:1073:GLU:OE1	2.12	0.48
1:A:187:GLU:OE2	1:A:687:ARG:HB2	2.13	0.48
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.96	0.48
1:A:567:LEU:HD21	1:A:591:LYS:HD3	1.95	0.48
1:A:224:ILE:CG2	1:A:225:HIS:N	2.77	0.48
1:A:739:ILE:O	1:A:743:GLN:HB2	2.13	0.48
1:A:824:SER:OG	1:A:825:ASN:N	2.46	0.48
1:A:219:CYS:SG	1:A:234:LYS:HG2	2.51	0.48
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.12	0.48
1:A:269:ASP:OD1	1:A:269:ASP:N	2.47	0.48
1:A:583:LEU:HD22	1:A:589:TYR:CZ	2.48	0.48
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.14	0.48
1:A:1002:THR:CG2	1:A:1003:SER:N	2.77	0.47
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.79	0.47
1:A:717:LEU:HG	1:A:721:LEU:HD22	1.96	0.47
1:A:746:THR:HB	1:A:811:LEU:HG	1.96	0.47
1:A:270:PHE:HB3	1:A:307:LEU:HD11	1.96	0.47
1:A:198:MET:O	1:A:199:HIS:C	2.53	0.47
1:A:548:PRO:O	1:A:550:GLN:N	2.47	0.47
1:A:224:ILE:CG2	1:A:225:HIS:H	2.28	0.47
1:A:212:TRP:C	1:A:214:LYS:H	2.17	0.47
1:A:391:GLN:HE21	1:A:391:GLN:HB3	1.57	0.47
1:A:775:GLN:CB	1:A:776:ASN:HB2	2.31	0.47
1:A:606:LYS:O	1:A:610:LEU:HD23	2.14	0.47
1:A:273:ARG:HB3	1:A:306:VAL:HG12	1.98	0.46
1:A:207:LEU:HD12	1:A:288:LYS:HB2	1.97	0.46
1:A:207:LEU:HD23	1:A:207:LEU:C	2.35	0.46
1:A:246:GLN:O	1:A:248:PHE:N	2.40	0.46
1:A:430:ASN:ND2	1:A:465:ASN:HD21	2.06	0.46
1:A:784:ARG:HD3	1:A:789:PRO:O	2.16	0.46
1:A:1009:PHE:CE1	1:A:1072:ILE:HD13	2.51	0.46
1:A:246:GLN:C	1:A:248:PHE:N	2.69	0.46
1:A:361:PHE:CD1	1:A:387:ILE:HD11	2.51	0.46
1:A:865:LEU:HD12	1:A:961:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:GLY:O	1:A:1000:LYS:HB2	2.16	0.46
1:A:375:ARG:HG3	1:A:376:ASN:H	1.80	0.46
1:A:742:LEU:HD22	1:A:813:LEU:CD1	2.45	0.45
1:A:232:THR:HG22	1:A:233:ILE:N	2.31	0.45
1:A:640:VAL:O	1:A:643:ILE:HG12	2.17	0.45
1:A:735:GLN:O	1:A:739:ILE:HD13	2.16	0.45
1:A:171:ASP:HB3	1:A:471:HIS:HE1	1.82	0.45
1:A:182:THR:HB	1:A:183:PRO:HD3	1.98	0.45
1:A:629:GLN:HG2	1:A:1029:ILE:HG12	1.99	0.45
1:A:862:LEU:HD21	1:A:1016:ALA:HB2	1.99	0.45
1:A:413:TRP:HH2	1:A:521:ASP:HB2	1.82	0.45
1:A:559:ILE:O	1:A:559:ILE:HG22	2.17	0.45
1:A:157:LEU:HD11	1:A:733:THR:HA	1.99	0.45
1:A:562:ASP:HB2	1:A:563:PRO:HD2	1.99	0.44
1:A:741:MET:O	1:A:745:VAL:HG23	2.18	0.44
1:A:997:THR:HG23	1:A:1001:LYS:HB2	1.98	0.44
1:A:500:ASP:O	1:A:503:THR:HG22	2.16	0.44
1:A:551:LEU:HD22	1:A:574:LEU:HD11	1.98	0.44
1:A:245:LEU:O	1:A:248:PHE:HB3	2.17	0.44
1:A:1036:MET:HG2	1:A:1042:LEU:HD21	2.00	0.44
1:A:775:GLN:NE2	1:A:796:LEU:HB2	2.33	0.44
1:A:777:SER:OG	1:A:778:GLN:HB2	2.12	0.44
1:A:198:MET:SD	1:A:271:VAL:HG11	2.58	0.44
1:A:777:SER:CA	1:A:778:GLN:HB2	2.39	0.44
1:A:732:PHE:O	1:A:736:VAL:HG23	2.16	0.44
1:A:497:PHE:CD1	1:A:497:PHE:N	2.85	0.43
1:A:550:GLN:HB3	1:A:550:GLN:HE21	1.68	0.43
1:A:548:PRO:CG	1:A:551:LEU:HD12	2.42	0.43
1:A:239:ASP:O	1:A:287:ILE:HG13	2.18	0.43
1:A:735:GLN:O	1:A:739:ILE:HD12	2.18	0.43
1:A:548:PRO:O	1:A:551:LEU:N	2.51	0.43
1:A:559:ILE:HG12	1:A:588:ALA:HB2	2.00	0.43
1:A:772:GLU:C	1:A:774:LEU:H	2.20	0.43
1:A:809:LYS:N	1:A:810:PRO:HD3	2.34	0.43
1:A:993:PHE:O	1:A:994:VAL:CB	2.66	0.43
1:A:386:ASN:HB2	1:A:430:ASN:HB3	1.99	0.43
1:A:804:MET:O	1:A:806:SER:N	2.50	0.43
1:A:720:TYR:OH	4:A:2007:HOH:O	2.20	0.43
1:A:1082:VAL:HA	1:A:1085:ASN:HB2	2.00	0.43
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.19	0.43
1:A:935:TYR:O	1:A:939:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:MET:O	1:A:549:ASN:N	2.52	0.42
1:A:158:ILE:HG23	1:A:703:ILE:HD13	2.01	0.42
1:A:1043:THR:HB	1:A:1047:ASP:H	1.84	0.42
1:A:1009:PHE:HE1	1:A:1072:ILE:HD13	1.85	0.42
1:A:361:PHE:CA	1:A:420:ILE:CD1	2.97	0.42
1:A:738:VAL:HG21	1:A:783:PHE:CD1	2.54	0.42
1:A:804:MET:CE	3:A:1189[A]:O92:C17	2.97	0.42
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.55	0.42
1:A:411:ASN:O	1:A:411:ASN:CG	2.58	0.42
1:A:630:LEU:HB2	1:A:644:ALA:HB2	2.02	0.42
1:A:298:LYS:HZ3	1:A:299:ASN:ND2	2.16	0.41
1:A:804:MET:HB3	3:A:1189[A]:O92:H18	2.01	0.41
1:A:775:GLN:H	1:A:776:ASN:HB3	1.84	0.41
1:A:1042:LEU:HD23	1:A:1048:ILE:HD11	2.01	0.41
1:A:210:TYR:CD2	1:A:211:LEU:HD13	2.55	0.41
1:A:467:LEU:HB2	1:A:476:ARG:HH21	1.85	0.41
1:A:768:LYS:HG2	1:A:798:ILE:CG2	2.51	0.41
1:A:562:ASP:OD2	1:A:1052:ARG:HD2	2.21	0.41
1:A:741:MET:HE1	1:A:780:PRO:HD3	2.02	0.41
1:A:144:SER:OG	1:A:146:GLU:HB3	2.20	0.41
1:A:270:PHE:HB3	1:A:307:LEU:CD1	2.51	0.41
1:A:310:PRO:HA	1:A:311:PRO:HD2	1.93	0.41
1:A:779:LEU:HD13	1:A:780:PRO:HD2	2.02	0.41
1:A:911:LEU:HD12	1:A:911:LEU:HA	2.00	0.41
1:A:1008:LYS:O	1:A:1011:ASP:HB3	2.20	0.41
1:A:361:PHE:CA	1:A:420:ILE:HD12	2.51	0.41
1:A:607:THR:HA	1:A:610:LEU:CD2	2.51	0.41
1:A:1003:SER:HB3	1:A:1006:PHE:H	1.85	0.41
1:A:544:ARG:CZ	1:A:544:ARG:HA	2.51	0.41
1:A:995:MET:O	1:A:1005:HIS:HB2	2.21	0.41
1:A:1043:THR:HG22	1:A:1045:LYS:H	1.87	0.40
1:A:1059:LYS:HA	1:A:1059:LYS:HD3	1.77	0.40
1:A:731:ASP:O	1:A:735:GLN:HG3	2.21	0.40
1:A:317:GLU:O	1:A:726:THR:CG2	2.69	0.40
1:A:233:ILE:CD1	1:A:248:PHE:HB2	2.51	0.40
1:A:286:PRO:O	1:A:287:ILE:C	2.58	0.40
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.57	0.40
1:A:827:THR:HG22	1:A:883:LYS:NZ	2.35	0.40
1:A:176:THR:HG23	1:A:674:ASP:HB2	2.02	0.40
1:A:359:ARG:HG3	1:A:420:ILE:HD13	2.02	0.40
1:A:462:TYR:HA	1:A:485:TRP:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:ILE:HG13	1:A:764:ILE:H	1.67	0.40
1:A:775:GLN:HB3	1:A:776:ASN:CB	2.33	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	819/980 (84%)	720 (88%)	70 (8%)	29 (4%)	3 2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	147	SER
1	A	211	LEU
1	A	374	PRO
1	A	778	GLN
1	A	805	ALA
1	A	967	HIS
1	A	994	VAL
1	A	1000	LYS
1	A	1040	PRO
1	A	213	LYS
1	A	247	SER
1	A	777	SER
1	A	798	ILE
1	A	896	VAL
1	A	901	ALA
1	A	966	GLY
1	A	1079	GLY
1	A	231	GLN

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Mol	Chain	Res	Type
1	A	287	ILE
1	A	898	ASN
1	A	1085	ASN
1	A	248	PHE
1	A	549	ASN
1	A	905	GLU
1	A	1001	LYS
1	A	379	LEU
1	A	895	THR
1	A	548	PRO

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	749/874 (86%)	663 (88%)	86 (12%)	5	6

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

Mol	Chain	Res	Type
1	A	147	SER
1	A	152	ARG
1	A	157	LEU
1	A	194	LYS
1	A	228	THR
1	A	229	THR
1	A	235	VAL
1	A	236	SER
1	A	238	ASP
1	A	245	LEU
1	A	246	GLN
1	A	268	GLN
1	A	269	ASP
1	A	271	VAL
1	A	287	ILE
1	A	298	LYS

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Mol	Chain	Res	Type
1	A	301	GLU
1	A	309	THR
1	A	359	ARG
1	A	373	LEU
1	A	377	THR
1	A	379	LEU
1	A	410	TRP
1	A	467	LEU
1	A	497	PHE
1	A	502	LEU
1	A	511	GLU
1	A	517	SER
1	A	544	ARG
1	A	549	ASN
1	A	550	GLN
1	A	561	THR
1	A	575	LEU
1	A	583	LEU
1	A	610	LEU
1	A	614	ARG
1	A	615	GLU
1	A	638	GLU
1	A	652	GLU
1	A	721	LEU
1	A	726	THR
1	A	729	LEU
1	A	737	GLN
1	A	743	GLN
1	A	746	THR
1	A	747	LEU
1	A	755	GLU
1	A	756	LYS
1	A	764	ILE
1	A	779	LEU
1	A	787	TYR
1	A	792	LYS
1	A	802	LYS
1	A	808	LYS
1	A	823	LEU
1	A	827	THR
1	A	841	ASP
1	A	845	LEU

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Mol	Chain	Res	Type
1	A	886	THR
1	A	887	THR
1	A	890	LYS
1	A	894	SER
1	A	895	THR
1	A	899	THR
1	A	904	ASP
1	A	905	GLU
1	A	908	ASN
1	A	911	LEU
1	A	912	LYS
1	A	915	SER
1	A	919	GLU
1	A	949	ASN
1	A	959	ASN
1	A	967	HIS
1	A	1000	LYS
1	A	1024	THR
1	A	1029	ILE
1	A	1042	LEU
1	A	1043	THR
1	A	1048	ILE
1	A	1049	GLU
1	A	1052	ARG
1	A	1059	LYS
1	A	1066	LYS
1	A	1078	LYS
1	A	1087	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	268	GLN
1	A	299	ASN
1	A	386	ASN
1	A	389	HIS
1	A	391	GLN
1	A	396	GLN
1	A	465	ASN
1	A	471	HIS
1	A	522	ASN

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Mol	Chain	Res	Type
1	A	550	GLN
1	A	554	GLN
1	A	585	HIS
1	A	629	GLN
1	A	646	GLN
1	A	673	HIS
1	A	710	GLN
1	A	743	GLN
1	A	766	GLN
1	A	775	GLN
1	A	778	GLN
1	A	893	GLN
1	A	908	ASN
1	A	922	GLN
1	A	949	ASN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN

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	O92	A	1189[A]	-	32,32,32	2.48	8 (25%)	43,47,47	2.00	8 (18%)
2	SO4	A	1188	-	4,4,4	0.33	0	6,6,6	0.75	0
3	O92	A	1189[B]	-	32,32,32	2.47	8 (25%)	43,47,47	2.11	8 (18%)

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
3	O92	A	1189[A]	-	-	7/21/21/21	0/3/3/3
3	O92	A	1189[B]	-	-	2/21/21/21	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1189[B]	O92	O2-S1	8.02	1.52	1.43
3	A	1189[A]	O92	O2-S1	7.64	1.52	1.43
3	A	1189[A]	O92	C5-C1	-5.47	1.40	1.48
3	A	1189[B]	O92	C5-C1	-5.34	1.40	1.48
3	A	1189[B]	O92	O3-S1	5.33	1.49	1.43
3	A	1189[A]	O92	O3-S1	5.14	1.49	1.43
3	A	1189[B]	O92	C10-S1	5.02	1.84	1.77
3	A	1189[A]	O92	C14-N5	-4.57	1.35	1.42
3	A	1189[A]	O92	C10-S1	4.26	1.83	1.77
3	A	1189[B]	O92	C14-N5	-4.21	1.35	1.42
3	A	1189[A]	O92	C18-C17	3.90	1.47	1.38
3	A	1189[A]	O92	C4-C6	2.94	1.55	1.50
3	A	1189[B]	O92	C4-C6	2.60	1.54	1.50
3	A	1189[A]	O92	C17-C14	2.23	1.43	1.39
3	A	1189[B]	O92	O1-C6	2.20	1.27	1.23
3	A	1189[B]	O92	C6-N3	2.11	1.36	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1189[B]	O92	O3-S1-O2	-10.45	106.70	119.55
3	A	1189[A]	O92	O3-S1-O2	-9.16	108.29	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1189[A]	O92	C15-C18-C17	-2.97	116.03	120.25
3	A	1189[B]	O92	O3-S1-N5	2.82	113.79	106.73
3	A	1189[B]	O92	O3-S1-C10	2.64	112.00	107.66
3	A	1189[A]	O92	F1-C13-C14	2.52	122.48	118.32
3	A	1189[A]	O92	C17-C14-N5	-2.42	116.05	120.88
3	A	1189[A]	O92	C2-N1-C3	2.32	121.08	118.70
3	A	1189[A]	O92	O1-C6-N3	2.32	125.98	122.47
3	A	1189[A]	O92	C4-N2-C1	2.22	121.49	118.19
3	A	1189[A]	O92	C18-C17-C14	2.21	123.20	118.62
3	A	1189[B]	O92	C2-N1-C3	2.18	120.94	118.70
3	A	1189[B]	O92	C4-C3-N4	-2.17	120.29	122.84
3	A	1189[B]	O92	C10-S1-N5	-2.07	104.86	107.27
3	A	1189[B]	O92	C18-C17-C14	2.06	122.89	118.62
3	A	1189[B]	O92	O2-S1-C10	2.04	111.03	107.66

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1189[A]	O92	C9-C10-S1-N5
3	A	1189[A]	O92	C17-C14-N5-S1
3	A	1189[A]	O92	C13-C14-N5-S1
3	A	1189[B]	O92	C9-C10-S1-N5
3	A	1189[B]	O92	C11-C10-S1-N5
3	A	1189[A]	O92	C11-C10-S1-N5
3	A	1189[A]	O92	C14-N5-S1-O3
3	A	1189[A]	O92	C14-N5-S1-O2
3	A	1189[A]	O92	C14-N5-S1-C10

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1189[A]	O92	3	0
3	A	1189[B]	O92	1	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 O92 A 1189 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand O92 A 1189 (B)

Bond lengths

Bond angles

Torsions

Rings
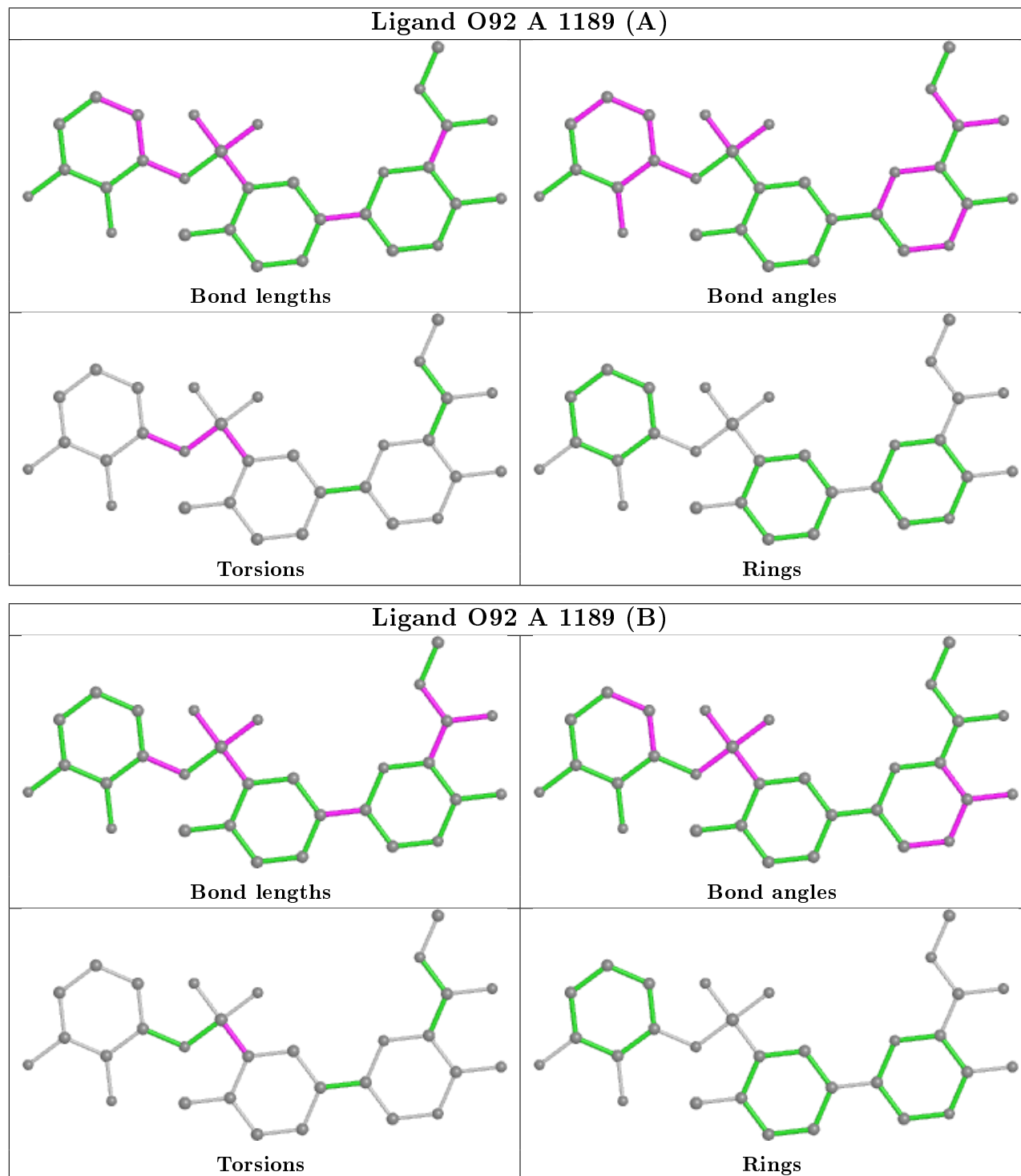
5.7 Other polymers (i)

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	833/980 (85%)	0.63	63 (7%)	13	18	36, 65, 102, 115	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	8.9
1	A	757	TYR	7.9
1	A	998	SER	5.3
1	A	1086	TRP	5.2
1	A	895	THR	4.9
1	A	373	LEU	4.4
1	A	1042	LEU	4.1
1	A	143	SER	4.1
1	A	898	ASN	4.0
1	A	916	PRO	3.9
1	A	147	SER	3.9
1	A	546	GLU	3.7
1	A	241	PRO	3.6
1	A	378	ASP	3.5
1	A	545	ALA	3.4
1	A	902	PHE	3.4
1	A	376	ASN	3.3
1	A	231	GLN	3.1
1	A	610	LEU	3.0
1	A	148	GLN	3.0
1	A	759	VAL	2.9
1	A	767	LEU	2.9
1	A	991	PHE	2.9
1	A	1004	PRO	2.9
1	A	272	LEU	2.9
1	A	1040	PRO	2.9
1	A	896	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1068	PHE	2.8
1	A	404	PHE	2.7
1	A	154	LEU	2.7
1	A	1076	ARG	2.7
1	A	1046	GLU	2.7
1	A	403	PRO	2.6
1	A	1075	CYS	2.6
1	A	1006	PHE	2.6
1	A	220	ILE	2.6
1	A	993	PHE	2.5
1	A	244	ILE	2.5
1	A	303	ILE	2.5
1	A	771	LEU	2.5
1	A	375	ARG	2.4
1	A	754	ALA	2.4
1	A	768	LYS	2.4
1	A	811	LEU	2.4
1	A	901	ALA	2.3
1	A	823	LEU	2.2
1	A	865	LEU	2.2
1	A	1041	GLN	2.2
1	A	374	PRO	2.2
1	A	813	LEU	2.2
1	A	887	THR	2.2
1	A	994	VAL	2.1
1	A	287	ILE	2.1
1	A	968	ILE	2.1
1	A	783	PHE	2.1
1	A	899	THR	2.1
1	A	489	GLY	2.1
1	A	275	CYS	2.1
1	A	150	PHE	2.1
1	A	550	GLN	2.0
1	A	250	THR	2.0
1	A	758	ASP	2.0
1	A	739	ILE	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)

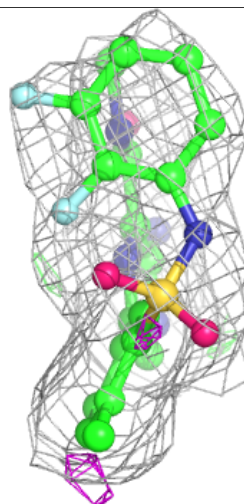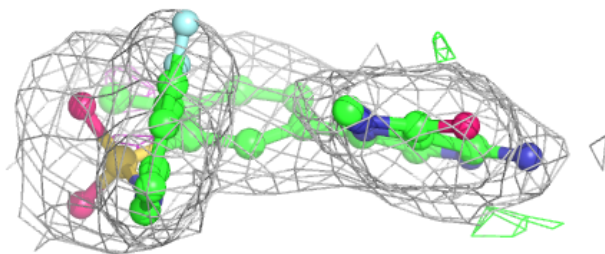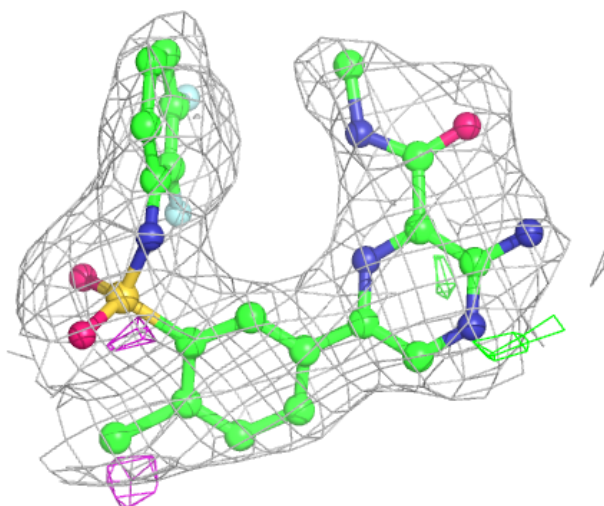There are no carbohydrates in this entry.

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.
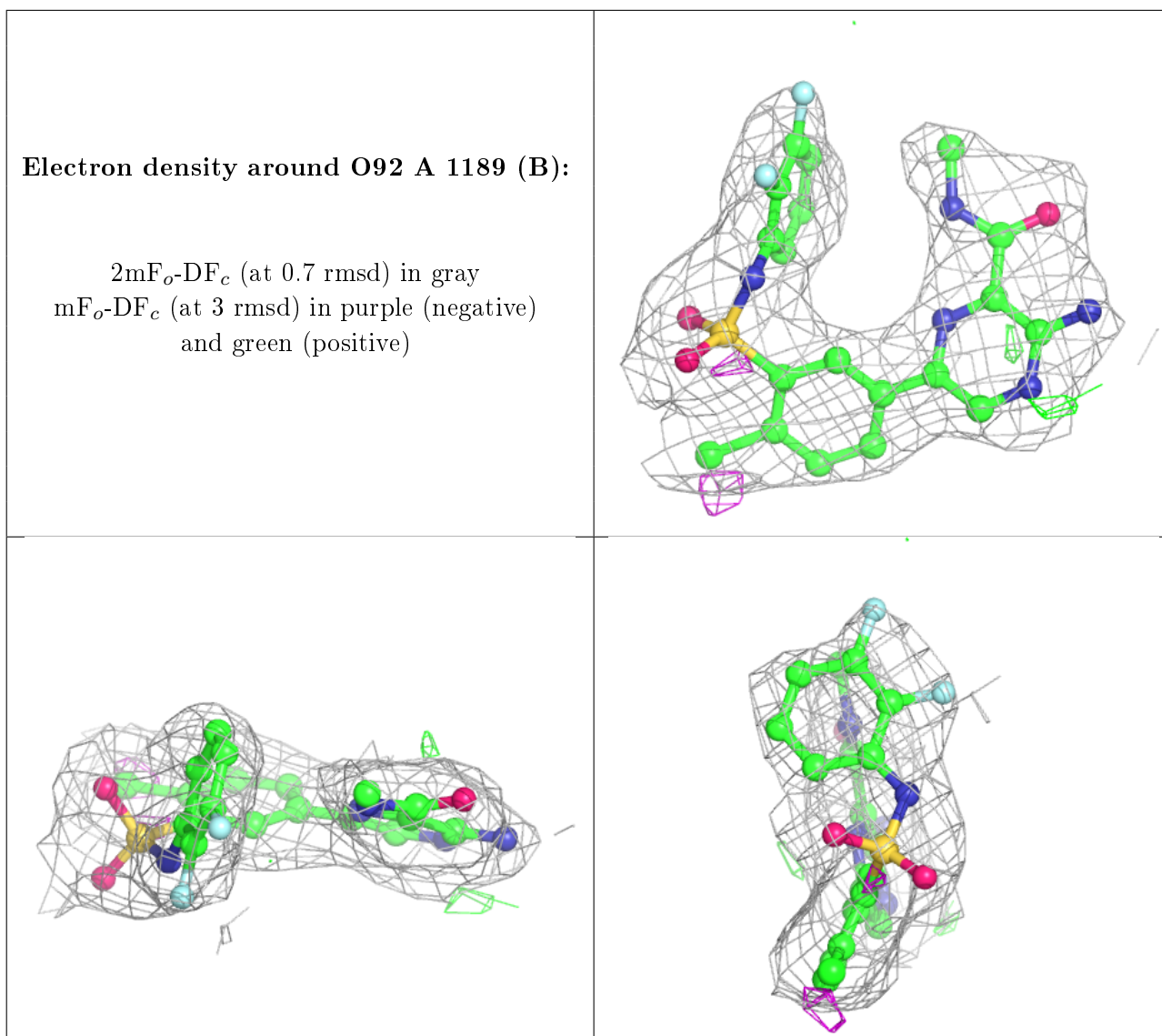
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	O92	A	1189[A]	30/30	0.94	0.15	54,59,74,75	30
2	SO4	A	1188	5/5	0.94	0.12	75,76,79,81	0
3	O92	A	1189[B]	30/30	0.94	0.15	50,57,71,71	30

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 O92 A 1189 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around O92 A 1189 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5   Other polymers ⓘ

There are no such residues in this entry.