Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:57 am BST

PDB ID	:	4ANX
Title	:	Complexes of PI3Kgamma with isoform selective inhibitors.
Authors	:	Foster, P.G.; Lougheed, J.C.
Deposited on	:	2012-03-22
Resolution	:	2.73 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

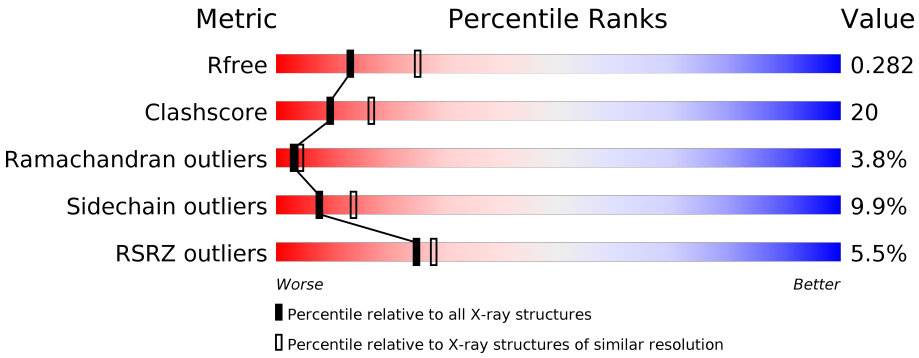
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	5% 51% 28% 5% • 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6828 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.

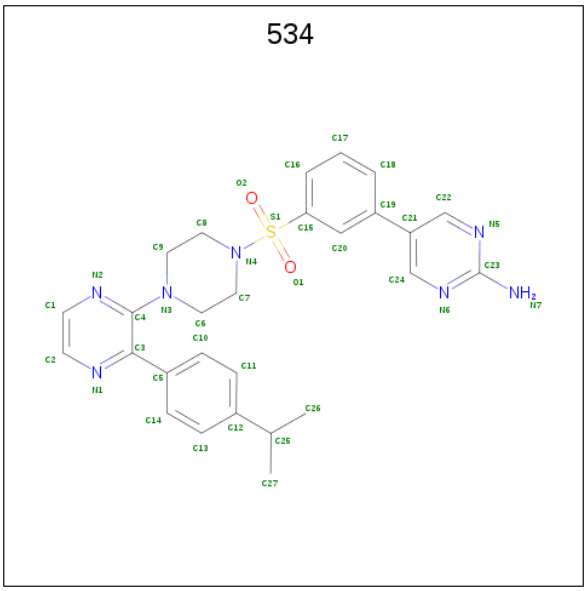
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

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 5-{3-[(4-{3-[4-(1-methylethyl)phenyl]pyrazin-2-yl}piperazin-1-yl)sulfonyl]phenyl}pyrimidin-2-amine (three-letter code: 534) (formula: $C_{27}H_{29}N_7O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	27	7	2	1		

- Molecule 3 is water.

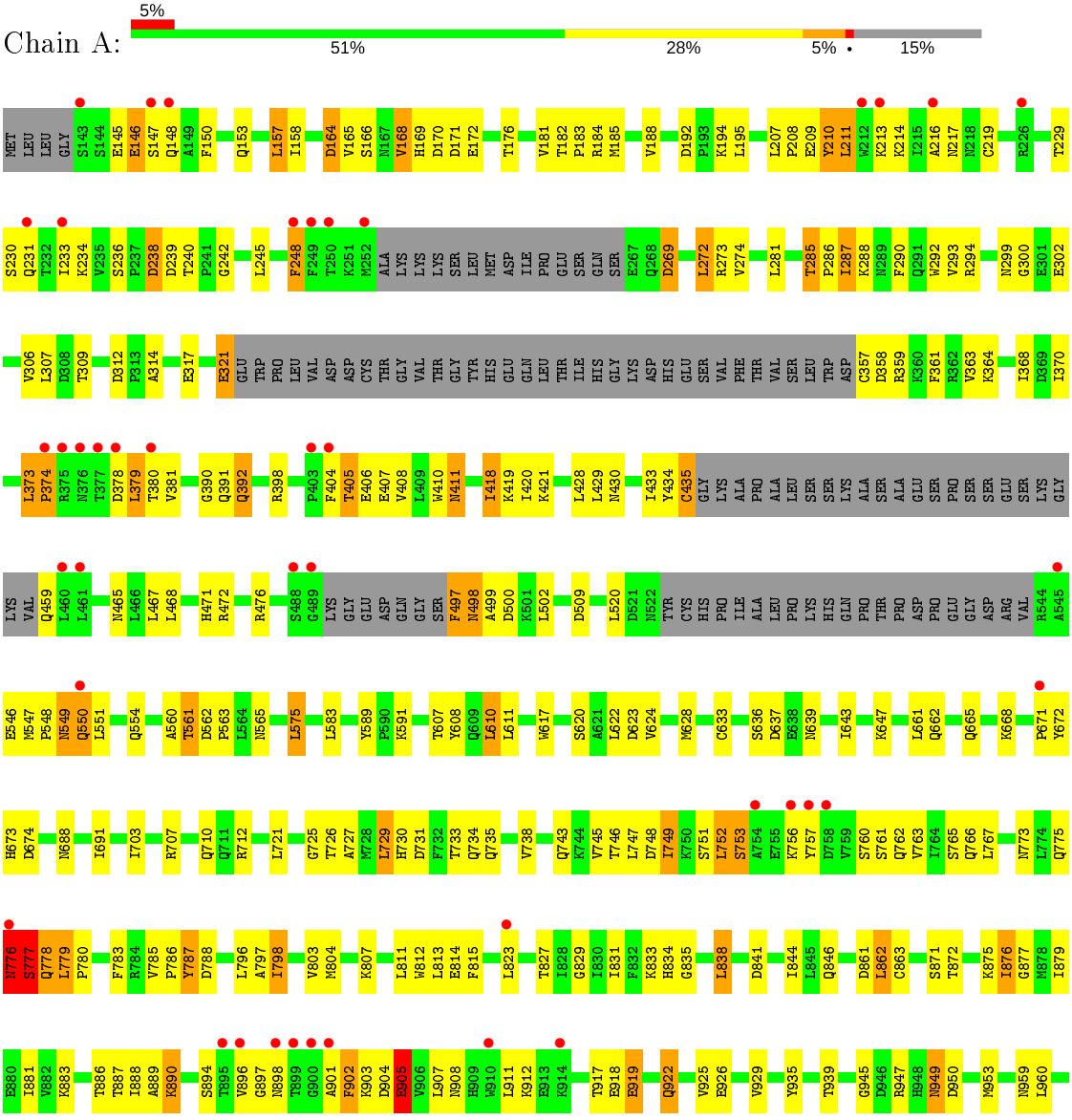
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		

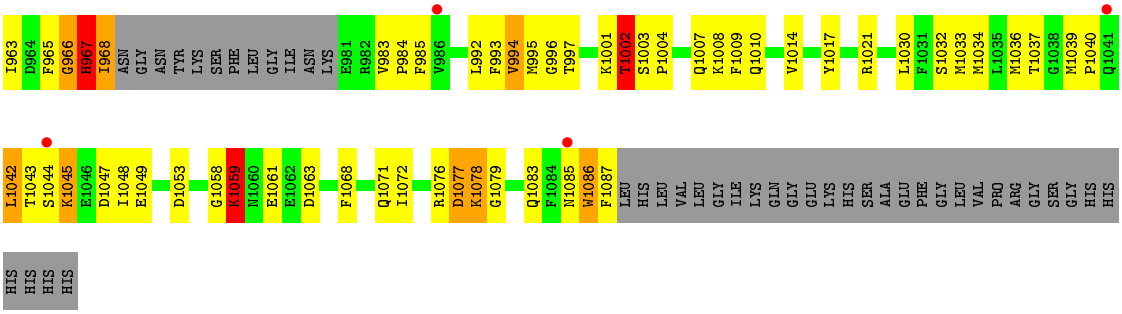
3 Residue-property plots (i)

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

Chain A:




I963 D964 F965 G966 H967 I968 ASN GLY ASN TYR LYS SER PHE LEU GLY ILE ASN LYS E981 R982 V983 P984 F985 V986 L992 F993 V994 M995 G996 T997 K1001 T1002 S1003 P1004 Q1007 K1008 F1009 Q1010 V1014 Y1017 R1021 L1030 F1031 S1032 M1033 M1034 L1035 M1036 T1037 G1038 M1039 P1040 Q1041
L1042 T1043 S1044 K1045 E1046 D1047 I1048 E1049 D1053 G1058 K1059 N1060 E1061 E1062 D1063 F1068 Q1071 I1072 R1076 D1077 K1078 G1079 Q1083 F1084 N1085 W1086 F1087 LEU HIS LEU VAL LEU GLY ILE LYS GLN GLY GLU LYS HIS SER ALA GLU PHE GLY LEU VAL PRO ARG GLY SER GLY 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	143.42Å 68.53Å 106.26Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	32.60 – 2.73 32.60 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.60-2.73) 99.5 (32.60-2.73)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.282 0.226 , 0.282	Depositor DCC
R_{free} test set	1375 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	70.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6828	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 534

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	0.67	2/6901 (0.0%)	0.79	5/9334 (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	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	HIS	C-N	-5.82	1.20	1.34
1	A	435	CYS	CB-SG	-5.02	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	575	LEU	CA-CB-CG	6.71	130.72	115.30
1	A	210	TYR	N-CA-C	6.59	128.80	111.00
1	A	967	HIS	O-C-N	-6.08	112.97	122.70
1	A	777	SER	CB-CA-C	5.51	120.58	110.10
1	A	1077	ASP	C-N-CA	5.43	135.28	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	GLU	Peptide
1	A	210	TYR	Peptide
1	A	777	SER	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	266	0
2	A	37	0	29	4	0
3	A	34	0	0	4	0
All	All	6828	0	6818	266	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (266) 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:967:HIS:H	1:A:968:ILE:HA	1.07	1.11
1:A:775:GLN:HE22	1:A:798:ILE:HD11	1.21	1.02
1:A:827:THR:HG22	1:A:883:LYS:NZ	1.81	0.95
1:A:561:THR:HG22	1:A:591:LYS:NZ	1.81	0.95
1:A:967:HIS:N	1:A:968:ILE:HA	1.73	0.94
1:A:827:THR:HG22	1:A:883:LYS:HZ2	1.38	0.89
1:A:967:HIS:H	1:A:968:ILE:CA	1.86	0.89
1:A:925:VAL:O	1:A:929:VAL:HG23	1.73	0.88
1:A:966:GLY:HA3	1:A:967:HIS:HB2	1.54	0.87
1:A:430:ASN:HD22	1:A:465:ASN:HD21	1.23	0.86
1:A:145:GLU:HA	1:A:146:GLU:O	1.75	0.86
1:A:777:SER:HB3	1:A:778:GLN:CB	2.06	0.85
1:A:907:LEU:HD23	1:A:994:VAL:HG21	1.58	0.83
1:A:233:ILE:HG22	1:A:234:LYS:O	1.81	0.81
1:A:903:LYS:HG2	1:A:905:GLU:OE2	1.82	0.80
1:A:1077:ASP:N	1:A:1078:LYS:HB2	1.98	0.79
1:A:620:SER:O	1:A:647:LYS:NZ	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:GLU:OE1	1:A:827:THR:HG21	1.84	0.77
1:A:775:GLN:N	1:A:776:ASN:HB2	1.99	0.77
1:A:497:PHE:O	1:A:1042:LEU:HD11	1.83	0.77
1:A:777:SER:CB	1:A:778:GLN:HB2	2.15	0.77
1:A:430:ASN:HD22	1:A:465:ASN:ND2	1.82	0.77
1:A:926:GLU:OE2	1:A:1008:LYS:NZ	2.18	0.76
1:A:777:SER:HB3	1:A:778:GLN:HB3	1.67	0.76
1:A:811:LEU:HB3	1:A:813:LEU:HD21	1.68	0.75
1:A:168:VAL:HG13	1:A:170:ASP:H	1.52	0.75
1:A:165:VAL:HG12	1:A:165:VAL:O	1.87	0.75
1:A:907:LEU:O	1:A:911:LEU:HD23	1.87	0.75
1:A:146:GLU:O	1:A:148:GLN:N	2.20	0.74
1:A:245:LEU:HD21	1:A:272:LEU:HD22	1.70	0.74
1:A:775:GLN:CA	1:A:776:ASN:HB2	2.18	0.73
1:A:182:THR:HB	1:A:183:PRO:HD3	1.72	0.72
1:A:236:SER:OG	1:A:239:ASP:OD1	2.08	0.71
1:A:748:ASP:O	1:A:752:LEU:HD13	1.88	0.71
1:A:777:SER:HB3	1:A:778:GLN:HB2	1.70	0.71
1:A:207:LEU:HD21	1:A:211:LEU:HB3	1.73	0.70
1:A:966:GLY:CA	1:A:967:HIS:HB2	2.22	0.70
1:A:761:SER:O	1:A:765:SER:N	2.26	0.69
1:A:907:LEU:O	1:A:911:LEU:CD2	2.40	0.69
1:A:953:MET:O	1:A:960:LEU:HD12	1.93	0.69
1:A:673:HIS:HD2	1:A:712:ARG:HE	1.39	0.68
1:A:583:LEU:HD22	1:A:589:TYR:OH	1.92	0.68
1:A:662:GLN:OE1	1:A:1030:LEU:HD22	1.93	0.68
1:A:185:MET:HE1	1:A:321:GLU:HG3	1.75	0.68
1:A:405:THR:HG23	1:A:408:VAL:HG22	1.76	0.68
1:A:561:THR:HG22	1:A:591:LYS:CE	2.23	0.68
1:A:947:ARG:NH2	1:A:963:ILE:O	2.26	0.68
1:A:561:THR:HG22	1:A:591:LYS:HZ1	1.58	0.67
1:A:731:ASP:O	1:A:735:GLN:HG3	1.95	0.67
1:A:498:ASN:C	1:A:498:ASN:OD1	2.32	0.67
1:A:997:THR:HG23	1:A:1002:THR:N	2.08	0.67
1:A:834:HIS:CA	1:A:876:ILE:HD12	2.24	0.67
1:A:240:THR:HG22	1:A:242:GLY:N	2.10	0.67
1:A:775:GLN:NE2	1:A:798:ILE:HD11	2.04	0.67
1:A:1077:ASP:HB2	1:A:1078:LYS:HG2	1.78	0.66
1:A:561:THR:HG23	1:A:565:ASN:HB3	1.78	0.65
1:A:1048:ILE:HD12	1:A:1048:ILE:H	1.62	0.65
1:A:185:MET:CE	1:A:321:GLU:HG3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:CD2	1:A:272:LEU:HD22	2.26	0.64
1:A:673:HIS:CD2	1:A:712:ARG:HE	2.15	0.64
1:A:379:LEU:HD13	1:A:380:THR:HG22	1.80	0.64
1:A:725:GLY:O	1:A:729:LEU:HD22	1.98	0.63
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.78	0.63
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.28	0.63
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.80	0.63
1:A:775:GLN:H	1:A:776:ASN:HB2	1.64	0.63
1:A:1068:PHE:O	1:A:1071:GLN:HB2	1.99	0.62
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.39	0.62
1:A:287:ILE:HG22	1:A:293:VAL:HG21	1.81	0.62
1:A:834:HIS:N	1:A:876:ILE:HD12	2.15	0.62
1:A:171:ASP:OD2	1:A:472:ARG:NH2	2.32	0.61
1:A:966:GLY:HA3	1:A:967:HIS:CB	2.26	0.61
1:A:812:TRP:C	1:A:813:LEU:HD23	2.20	0.61
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.47	0.61
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.36	0.61
1:A:476:ARG:O	1:A:520:LEU:HD23	2.02	0.60
1:A:827:THR:CG2	1:A:883:LYS:NZ	2.62	0.60
1:A:671:PRO:HD2	3:A:2024:HOH:O	2.00	0.60
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.84	0.60
1:A:287:ILE:H	1:A:287:ILE:HD12	1.67	0.60
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.84	0.59
1:A:950:ASP:HB2	2:A:2088:534:C2	2.32	0.59
1:A:862:LEU:CD2	1:A:862:LEU:N	2.65	0.59
1:A:887:THR:HG22	1:A:890:LYS:H	1.68	0.59
1:A:207:LEU:HD23	1:A:208:PRO:N	2.17	0.58
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.04	0.58
1:A:560:ALA:HB3	3:A:2013:HOH:O	2.03	0.58
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.03	0.58
1:A:1032:SER:O	1:A:1036:MET:HG3	2.04	0.57
1:A:963:ILE:HB	2:A:2088:534:C17	2.35	0.57
1:A:172:GLU:HG3	1:A:471:HIS:CD2	2.39	0.57
1:A:207:LEU:CD2	1:A:211:LEU:HB3	2.34	0.57
1:A:608:TYR:OH	1:A:637:ASP:OD1	2.23	0.57
1:A:827:THR:HG22	1:A:883:LYS:HZ1	1.66	0.57
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.35	0.57
1:A:150:PHE:O	1:A:153:GLN:N	2.39	0.56
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.06	0.56
1:A:1003:SER:OG	1:A:1004:PRO:HD2	2.05	0.56
1:A:831:ILE:HB	1:A:879:ILE:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:THR:HG22	1:A:591:LYS:HE2	1.88	0.55
1:A:668:LYS:O	3:A:2023:HOH:O	2.18	0.55
1:A:661:LEU:O	1:A:665:GLN:HG2	2.07	0.55
1:A:207:LEU:HD23	1:A:207:LEU:C	2.27	0.55
1:A:381:VAL:HG12	1:A:435:CYS:SG	2.47	0.55
1:A:1072:ILE:O	1:A:1076:ARG:HG3	2.07	0.55
1:A:707:ARG:HH11	1:A:710:GLN:HE22	1.55	0.55
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.42	0.54
1:A:887:THR:CG2	1:A:889:ALA:HB3	2.37	0.54
1:A:1033:MET:O	1:A:1037:THR:HG23	2.07	0.54
1:A:583:LEU:CD2	1:A:589:TYR:OH	2.54	0.54
1:A:165:VAL:O	1:A:165:VAL:CG1	2.55	0.54
1:A:804:MET:CE	2:A:2088:534:H261	2.38	0.54
1:A:498:ASN:OD1	1:A:500:ASP:N	2.39	0.54
1:A:168:VAL:HG13	1:A:170:ASP:N	2.20	0.54
1:A:363:VAL:HG23	1:A:520:LEU:HD12	1.89	0.54
1:A:561:THR:CG2	1:A:591:LYS:HE2	2.37	0.53
1:A:967:HIS:N	1:A:968:ILE:CA	2.55	0.53
1:A:617:TRP:CE2	1:A:643:ILE:HD12	2.44	0.53
1:A:357:CYS:SG	1:A:359:ARG:NE	2.82	0.53
1:A:181:VAL:O	1:A:185:MET:HG3	2.09	0.53
1:A:996:GLY:O	1:A:1003:SER:HB2	2.09	0.53
1:A:1048:ILE:N	1:A:1048:ILE:HD12	2.24	0.52
1:A:622:LEU:HD12	1:A:623:ASP:H	1.72	0.52
1:A:949:ASN:HD22	1:A:949:ASN:C	2.12	0.52
1:A:547:MET:HE2	1:A:551:LEU:HB3	1.92	0.52
1:A:548:PRO:O	1:A:549:ASN:C	2.48	0.52
1:A:158:ILE:HG23	1:A:703:ILE:HD13	1.91	0.52
1:A:434:TYR:HA	1:A:459:GLN:O	2.10	0.52
1:A:992:LEU:O	1:A:995:MET:HB2	2.09	0.52
1:A:428:LEU:CD2	1:A:467:LEU:HD12	2.40	0.52
1:A:688:ASN:HB3	1:A:691:ILE:HD12	1.93	0.51
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.92	0.51
1:A:379:LEU:HD13	1:A:380:THR:H	1.75	0.51
1:A:726:THR:O	1:A:727:ALA:C	2.47	0.51
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.91	0.51
1:A:1043:THR:O	1:A:1045:LYS:N	2.43	0.51
1:A:777:SER:OG	1:A:778:GLN:HB2	2.11	0.51
1:A:827:THR:CG2	1:A:883:LYS:HZ1	2.22	0.51
1:A:391:GLN:NE2	1:A:633:CYS:SG	2.84	0.51
1:A:285:THR:HB	1:A:290:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:GLN:CB	1:A:776:ASN:HB2	2.41	0.51
1:A:561:THR:HG22	1:A:591:LYS:HZ3	1.69	0.51
1:A:919:GLU:HA	1:A:922:GLN:HB2	1.93	0.50
1:A:1009:PHE:HE2	1:A:1072:ILE:HD13	1.76	0.50
1:A:302:GLU:HG3	3:A:2008:HOH:O	2.11	0.50
1:A:184:ARG:O	1:A:188:VAL:HG23	2.11	0.50
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.47	0.50
1:A:786:PRO:O	1:A:787:TYR:CG	2.65	0.50
1:A:901:ALA:HB1	1:A:902:PHE:HA	1.92	0.50
1:A:1049:GLU:O	1:A:1053:ASP:OD2	2.30	0.49
1:A:1058:GLY:O	1:A:1059:LYS:O	2.29	0.49
1:A:269:ASP:O	1:A:309:THR:HG22	2.11	0.49
1:A:390:GLY:C	1:A:392:GLN:H	2.16	0.49
1:A:887:THR:HG21	1:A:889:ALA:HB3	1.95	0.49
1:A:829:GLY:HA3	1:A:881:ILE:HD12	1.95	0.49
1:A:726:THR:HA	1:A:729:LEU:HD23	1.94	0.49
1:A:993:PHE:O	1:A:994:VAL:CB	2.61	0.49
1:A:993:PHE:O	1:A:994:VAL:HG23	2.13	0.48
1:A:760:SER:OG	1:A:763:VAL:HG23	2.13	0.48
1:A:993:PHE:O	1:A:994:VAL:HB	2.13	0.48
1:A:245:LEU:HD11	1:A:272:LEU:HD13	1.94	0.48
1:A:317:GLU:O	1:A:726:THR:HG23	2.14	0.48
1:A:904:ASP:O	1:A:905:GLU:O	2.30	0.48
1:A:1077:ASP:CA	1:A:1078:LYS:HB2	2.43	0.48
1:A:370:ILE:O	1:A:370:ILE:HG23	2.12	0.48
1:A:779:LEU:HD13	1:A:780:PRO:HD2	1.96	0.48
1:A:835:GLY:O	1:A:875:LYS:HD3	2.14	0.48
1:A:207:LEU:HD23	1:A:208:PRO:CD	2.44	0.48
1:A:498:ASN:OD1	1:A:499:ALA:N	2.47	0.48
1:A:373:LEU:HD22	1:A:404:PHE:CE2	2.49	0.48
1:A:887:THR:HG22	1:A:889:ALA:N	2.29	0.48
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.95	0.48
1:A:192:ASP:CG	1:A:195:LEU:HD23	2.34	0.47
1:A:997:THR:HG23	1:A:1002:THR:H	1.78	0.47
1:A:164:ASP:OD1	1:A:166:SER:OG	2.27	0.47
1:A:639:ASN:O	1:A:643:ILE:HG23	2.13	0.47
1:A:743:GLN:O	1:A:746:THR:HG22	2.14	0.47
1:A:171:ASP:HB3	1:A:471:HIS:CE1	2.50	0.47
1:A:467:LEU:HD23	1:A:672:TYR:CE1	2.49	0.47
1:A:1059:LYS:HG3	1:A:1063:ASP:HB2	1.96	0.47
1:A:607:THR:O	1:A:610:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:LEU:CD2	1:A:803:VAL:HG23	2.45	0.47
1:A:861:ASP:C	1:A:862:LEU:HD22	2.36	0.47
1:A:734:GLN:HE21	1:A:780:PRO:HB2	1.79	0.46
1:A:497:PHE:HB2	1:A:1042:LEU:HD21	1.96	0.46
1:A:405:THR:HG23	1:A:407:GLU:O	2.15	0.46
1:A:813:LEU:HD23	1:A:813:LEU:N	2.30	0.46
1:A:168:VAL:HG13	1:A:169:HIS:N	2.30	0.46
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.98	0.46
1:A:745:VAL:O	1:A:749:ILE:HD13	2.16	0.46
1:A:361:PHE:HB2	1:A:420:ILE:HD12	1.98	0.45
1:A:796:LEU:HD13	1:A:815:PHE:CE2	2.50	0.45
1:A:192:ASP:OD1	1:A:192:ASP:C	2.55	0.45
1:A:373:LEU:O	1:A:374:PRO:C	2.55	0.45
1:A:738:VAL:HG21	1:A:783:PHE:CG	2.50	0.45
1:A:418:ILE:HG13	1:A:419:LYS:N	2.32	0.45
1:A:703:ILE:HG22	1:A:703:ILE:O	2.17	0.45
1:A:738:VAL:HG21	1:A:783:PHE:CB	2.47	0.44
1:A:804:MET:HE3	2:A:2088:534:H261	1.99	0.44
1:A:239:ASP:HB2	1:A:287:ILE:HD11	2.00	0.44
1:A:145:GLU:CA	1:A:146:GLU:O	2.58	0.44
1:A:738:VAL:HG21	1:A:783:PHE:HB3	2.00	0.43
1:A:214:LYS:HE3	1:A:300:GLY:HA2	2.00	0.43
1:A:471:HIS:H	1:A:471:HIS:CD2	2.35	0.43
1:A:779:LEU:HD13	1:A:780:PRO:N	2.33	0.43
1:A:192:ASP:OD2	1:A:195:LEU:HD23	2.18	0.43
1:A:207:LEU:CD2	1:A:208:PRO:O	2.66	0.43
1:A:411:ASN:O	1:A:411:ASN:CG	2.57	0.43
1:A:561:THR:HG23	1:A:562:ASP:O	2.18	0.43
1:A:834:HIS:HA	1:A:876:ILE:HD12	1.98	0.43
1:A:617:TRP:O	1:A:620:SER:OG	2.26	0.43
1:A:550:GLN:O	1:A:554:GLN:HG3	2.18	0.43
1:A:823:LEU:O	1:A:823:LEU:HG	2.18	0.43
1:A:207:LEU:HD23	1:A:208:PRO:O	2.19	0.43
1:A:797:ALA:O	1:A:798:ILE:C	2.57	0.43
1:A:357:CYS:SG	1:A:359:ARG:HG2	2.60	0.42
1:A:1085:ASN:C	1:A:1087:PHE:H	2.23	0.42
1:A:611:LEU:HD22	1:A:643:ILE:HG21	2.01	0.42
1:A:497:PHE:CD1	1:A:497:PHE:N	2.87	0.42
1:A:207:LEU:HD23	1:A:208:PRO:HD2	2.02	0.42
1:A:380:THR:O	1:A:381:VAL:HG13	2.20	0.42
1:A:862:LEU:HD22	1:A:862:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:LEU:HD13	1:A:780:PRO:CD	2.50	0.42
1:A:935:TYR:O	1:A:939:THR:HG23	2.19	0.42
1:A:1043:THR:OG1	1:A:1047:ASP:N	2.40	0.42
1:A:624:VAL:CG1	1:A:628:MET:HE1	2.49	0.42
1:A:785:VAL:HG12	1:A:786:PRO:O	2.19	0.42
1:A:777:SER:CB	1:A:778:GLN:CB	2.78	0.42
1:A:896:VAL:O	1:A:896:VAL:HG12	2.20	0.42
1:A:727:ALA:O	1:A:730:HIS:HB3	2.19	0.42
1:A:1071:GLN:HA	1:A:1071:GLN:NE2	2.35	0.42
1:A:238:ASP:HA	1:A:286:PRO:HB3	2.02	0.42
1:A:468:LEU:HA	1:A:468:LEU:HD23	1.90	0.42
1:A:1002:THR:OG1	1:A:1003:SER:N	2.53	0.41
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.85	0.41
1:A:273:ARG:HB3	1:A:306:VAL:HG13	2.03	0.41
1:A:561:THR:CG2	1:A:591:LYS:HZ1	2.30	0.41
1:A:611:LEU:CD2	1:A:643:ILE:HG21	2.50	0.41
1:A:373:LEU:HD11	1:A:406:GLU:N	2.36	0.41
1:A:373:LEU:HD22	1:A:404:PHE:CZ	2.55	0.41
1:A:939:THR:HB	1:A:945:GLY:HA2	2.01	0.41
1:A:306:VAL:HG22	1:A:307:LEU:N	2.35	0.41
1:A:743:GLN:HA	1:A:746:THR:HG22	2.01	0.41
1:A:786:PRO:C	1:A:788:ASP:H	2.24	0.41
1:A:757:TYR:HE1	1:A:807:LYS:HA	1.86	0.41
1:A:168:VAL:CG1	1:A:169:HIS:N	2.84	0.41
1:A:844:ILE:CD1	1:A:1034:MET:SD	3.08	0.41
1:A:787:TYR:C	1:A:787:TYR:CD1	2.95	0.41
1:A:834:HIS:HB2	1:A:876:ILE:CD1	2.50	0.41
1:A:216:ALA:HB3	1:A:219:CYS:HB3	2.03	0.41
1:A:245:LEU:O	1:A:248:PHE:HB3	2.21	0.41
1:A:364:LYS:HD3	1:A:411:ASN:HD21	1.86	0.41
1:A:561:THR:CG2	1:A:591:LYS:CE	2.94	0.41
1:A:509:ASP:C	1:A:509:ASP:OD1	2.59	0.40
1:A:551:LEU:HA	1:A:551:LEU:HD23	1.83	0.40
1:A:751:SER:C	1:A:753:SER:H	2.24	0.40
1:A:182:THR:HB	1:A:183:PRO:CD	2.48	0.40
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.87	0.40
1:A:379:LEU:CD1	1:A:380:THR:H	2.34	0.40
1:A:562:ASP:HB2	1:A:563:PRO:CD	2.51	0.40
1:A:623:ASP:OD1	1:A:623:ASP:C	2.58	0.40
1:A:157:LEU:HD11	1:A:733:THR:HA	2.02	0.40
1:A:833:LYS:O	1:A:876:ILE:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LEU:CD2	1:A:589:TYR:CZ	3.04	0.40
1:A:1078:LYS:HA	1:A:1078:LYS:HD3	1.98	0.40
1:A:290:PHE:O	1:A:294:ARG:HG3	2.21	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%)	703 (86%)	85 (10%)	31 (4%)	3 4

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	A	211	LEU
1	A	217	ASN
1	A	778	GLN
1	A	905	GLU
1	A	966	GLY
1	A	967	HIS
1	A	994	VAL
1	A	1045	LYS
1	A	1059	LYS
1	A	1078	LYS
1	A	248	PHE
1	A	374	PRO
1	A	378	ASP
1	A	549	ASN
1	A	752	LEU
1	A	776	ASN
1	A	898	ASN

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Mol	Chain	Res	Type
1	A	1040	PRO
1	A	1079	GLY
1	A	231	GLN
1	A	894	SER
1	A	1002	THR
1	A	1044	SER
1	A	146	GLU
1	A	897	GLY
1	A	1086	TRP
1	A	798	ILE
1	A	918	GLU
1	A	213	LYS
1	A	373	LEU

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%)	675 (90%)	74 (10%)	8 14

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	LEU
1	A	164	ASP
1	A	168	VAL
1	A	194	LYS
1	A	229	THR
1	A	230	SER
1	A	238	ASP
1	A	269	ASP
1	A	272	LEU
1	A	281	LEU
1	A	285	THR
1	A	287	ILE
1	A	288	LYS

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Mol	Chain	Res	Type
1	A	299	ASN
1	A	321	GLU
1	A	358	ASP
1	A	379	LEU
1	A	392	GLN
1	A	398	ARG
1	A	405	THR
1	A	410	TRP
1	A	411	ASN
1	A	418	ILE
1	A	421	LYS
1	A	497	PHE
1	A	498	ASN
1	A	502	LEU
1	A	546	GLU
1	A	550	GLN
1	A	561	THR
1	A	575	LEU
1	A	610	LEU
1	A	636	SER
1	A	721	LEU
1	A	729	LEU
1	A	747	LEU
1	A	749	ILE
1	A	753	SER
1	A	756	LYS
1	A	762	GLN
1	A	766	GLN
1	A	773	ASN
1	A	776	ASN
1	A	779	LEU
1	A	787	TYR
1	A	838	LEU
1	A	841	ASP
1	A	846	GLN
1	A	862	LEU
1	A	863	CYS
1	A	871	SER
1	A	876	ILE
1	A	886	THR
1	A	888	ILE
1	A	890	LYS

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Mol	Chain	Res	Type
1	A	902	PHE
1	A	905	GLU
1	A	908	ASN
1	A	912	LYS
1	A	917	THR
1	A	919	GLU
1	A	922	GLN
1	A	949	ASN
1	A	959	ASN
1	A	968	ILE
1	A	985	PHE
1	A	1001	LYS
1	A	1002	THR
1	A	1007	GLN
1	A	1039	MET
1	A	1042	LEU
1	A	1059	LYS
1	A	1061	GLU
1	A	1086	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	304	HIS
1	A	391	GLN
1	A	411	ASN
1	A	465	ASN
1	A	471	HIS
1	A	512	ASN
1	A	565	ASN
1	A	634	ASN
1	A	646	GLN
1	A	658	HIS
1	A	673	HIS
1	A	710	GLN
1	A	734	GLN
1	A	766	GLN
1	A	775	GLN
1	A	776	ASN
1	A	840	GLN
1	A	893	GLN

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Mol	Chain	Res	Type
1	A	908	ASN
1	A	949	ASN
1	A	951	ASN
1	A	1071	GLN
1	A	1083	GLN

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 carbohydrates 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	534	A	2088	-	41,41,41	2.35	8 (19%)	56,59,59	2.22	18 (32%)

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	534	A	2088	-	-	16/28/38/38	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2088	534	C5-C3	-9.46	1.38	1.49
2	A	2088	534	O2-S1	7.03	1.51	1.43
2	A	2088	534	O1-S1	6.26	1.50	1.43
2	A	2088	534	C21-C19	-3.58	1.40	1.49
2	A	2088	534	C6-N3	2.33	1.50	1.46
2	A	2088	534	S1-N4	2.23	1.66	1.63
2	A	2088	534	C4-N3	2.13	1.43	1.37
2	A	2088	534	C9-N3	2.01	1.49	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2088	534	C15-S1-N4	-6.25	99.86	107.30
2	A	2088	534	O1-S1-N4	5.86	112.04	106.69
2	A	2088	534	O2-S1-O1	-5.40	110.77	119.52
2	A	2088	534	C6-N3-C9	4.81	122.13	111.52
2	A	2088	534	O2-S1-N4	4.56	110.85	106.69
2	A	2088	534	N6-C23-N5	-3.79	120.50	124.53
2	A	2088	534	O2-S1-C15	3.58	112.58	108.05
2	A	2088	534	C1-N2-C4	3.37	122.96	115.14
2	A	2088	534	C6-C7-N4	-2.91	106.69	108.91
2	A	2088	534	C2-N1-C3	2.80	122.30	116.81
2	A	2088	534	C7-N4-S1	-2.72	112.10	117.05
2	A	2088	534	C2-C1-N2	-2.68	118.32	122.17
2	A	2088	534	C21-C24-N6	-2.50	120.19	124.32
2	A	2088	534	C24-N6-C23	2.44	120.96	116.44
2	A	2088	534	N7-C23-N5	2.41	119.88	117.44
2	A	2088	534	N7-C23-N6	2.14	119.61	117.44
2	A	2088	534	C21-C22-N5	-2.12	120.82	124.32
2	A	2088	534	C22-N5-C23	2.02	120.17	116.44

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2088	534	C3-C4-N3-C6
2	A	2088	534	C8-N4-S1-O2

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Mol	Chain	Res	Type	Atoms
2	A	2088	534	C8-N4-S1-C15
2	A	2088	534	C7-N4-S1-O1
2	A	2088	534	C8-N4-S1-O1
2	A	2088	534	N2-C4-N3-C6
2	A	2088	534	C7-N4-S1-O2
2	A	2088	534	C7-N4-S1-C15
2	A	2088	534	N1-C3-C5-C14
2	A	2088	534	N1-C3-C5-C10
2	A	2088	534	C20-C19-C21-C24
2	A	2088	534	C18-C19-C21-C22
2	A	2088	534	C4-C3-C5-C14
2	A	2088	534	C4-C3-C5-C10
2	A	2088	534	C20-C19-C21-C22
2	A	2088	534	C18-C19-C21-C24

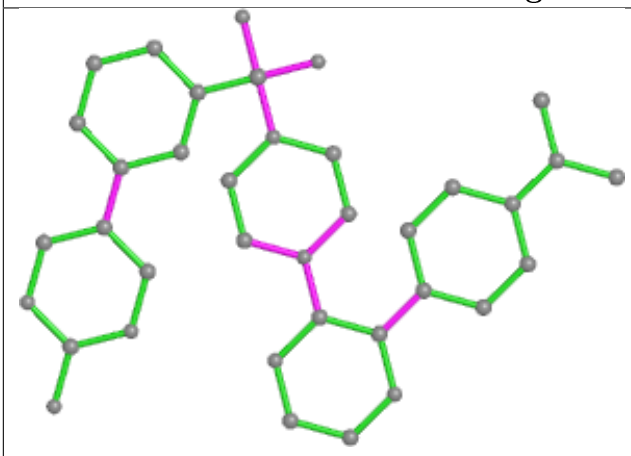
There are no ring outliers.

1 monomer is involved in 4 short contacts:

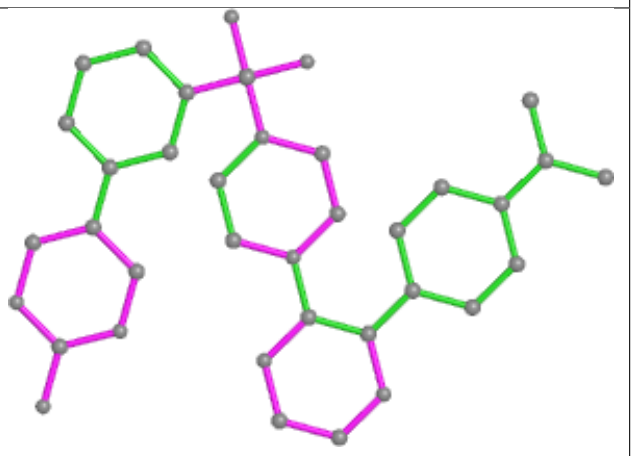
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2088	534	4	0

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.

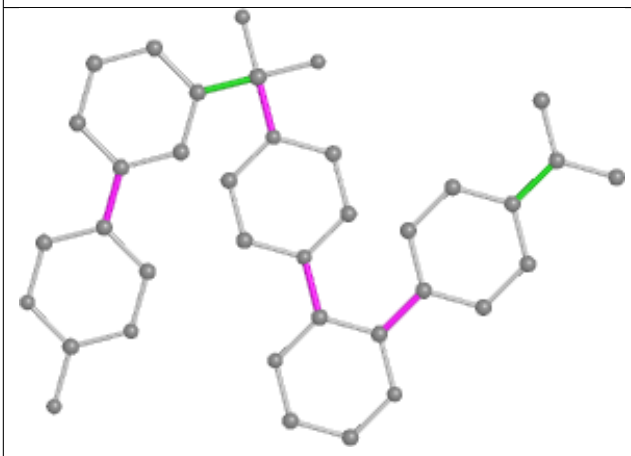
Ligand 534 A 2088



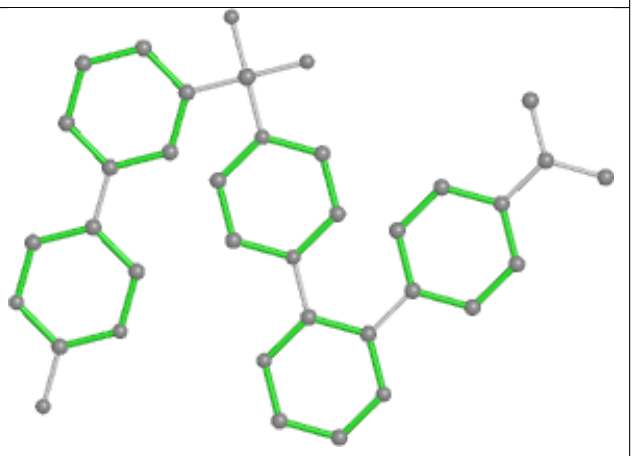
Bond lengths



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, 95^{th} 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%)	0.25	46 (5%)	25	28	39, 70, 106, 120	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	6.0
1	A	375	ARG	5.9
1	A	376	ASN	5.7
1	A	896	VAL	5.5
1	A	900	GLY	5.4
1	A	895	THR	4.7
1	A	252	MET	4.7
1	A	1044	SER	4.6
1	A	143	SER	4.3
1	A	901	ALA	4.3
1	A	404	PHE	3.8
1	A	212	TRP	3.4
1	A	754	ALA	3.4
1	A	823	LEU	3.4
1	A	147	SER	3.1
1	A	377	THR	3.0
1	A	374	PRO	2.8
1	A	233	ILE	2.8
1	A	250	THR	2.8
1	A	226	ARG	2.8
1	A	489	GLY	2.8
1	A	899	THR	2.7
1	A	758	ASP	2.7
1	A	757	TYR	2.6
1	A	910	TRP	2.5
1	A	148	GLN	2.5
1	A	671	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	545	ALA	2.4
1	A	756	LYS	2.4
1	A	248	PHE	2.3
1	A	249	PHE	2.3
1	A	550	GLN	2.3
1	A	231	GLN	2.2
1	A	898	ASN	2.2
1	A	488	SER	2.2
1	A	380	THR	2.2
1	A	403	PRO	2.1
1	A	914	LYS	2.1
1	A	213	LYS	2.1
1	A	986	VAL	2.1
1	A	216	ALA	2.1
1	A	461	LEU	2.1
1	A	776	ASN	2.1
1	A	1041	GLN	2.0
1	A	1085	ASN	2.0
1	A	460	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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.

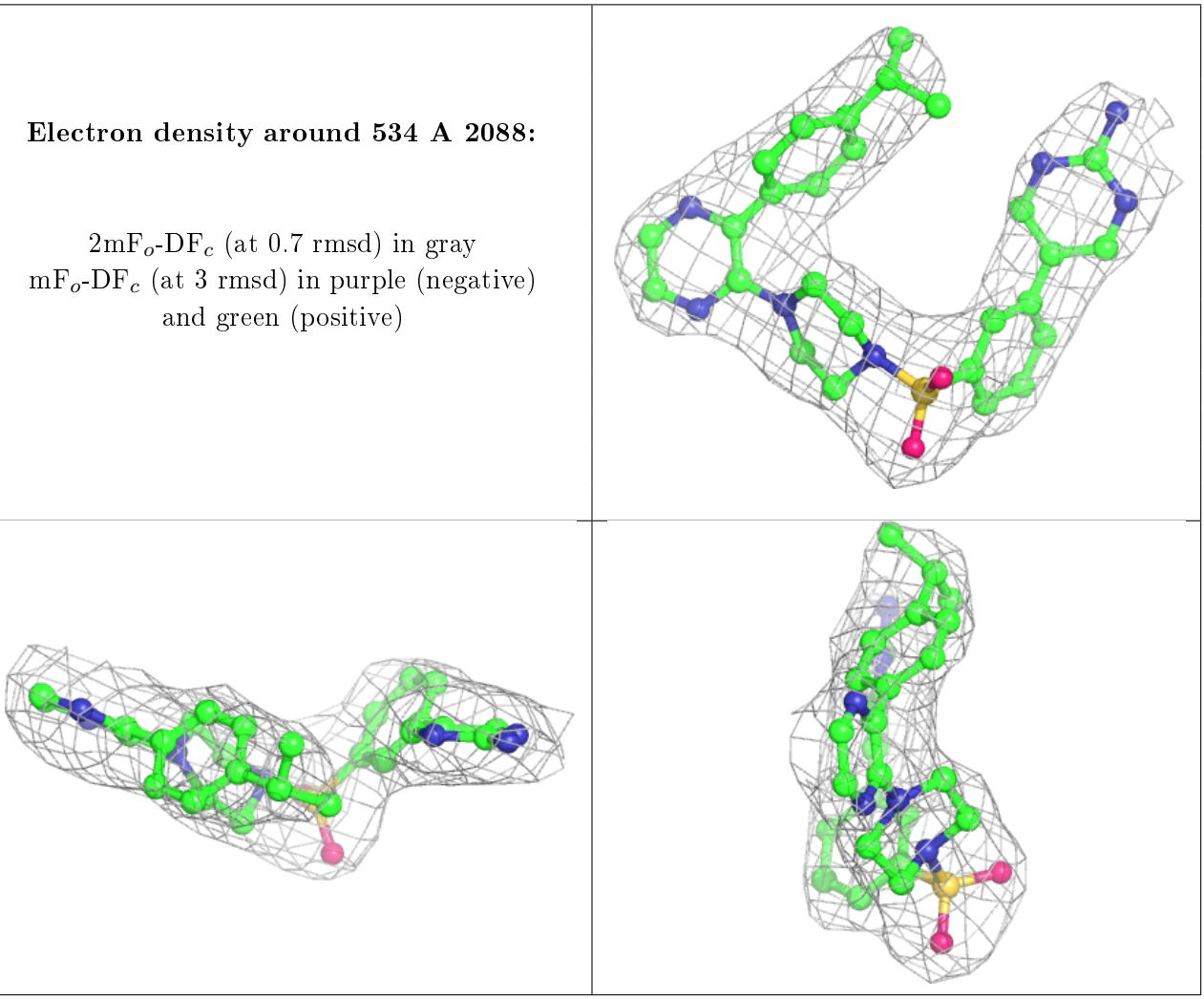
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	534	A	2088	37/37	0.97	0.14	61,66,70,71	0

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 534 A 2088:

$2mF_o$-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.