



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:15 am BST

PDB ID : 3TL5
Title : Discovery of GDC-0980: a Potent, Selective, and Orally Available Class I Phosphatidylinositol 3-Kinase (PI3K)/Mammalian Target of Rapamycin (mTOR) Kinase Inhibitor for the Treatment of Cancer
Authors : Murray, J.M.; Wiesmann, C.
Deposited on : 2011-08-29
Resolution : 2.79 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

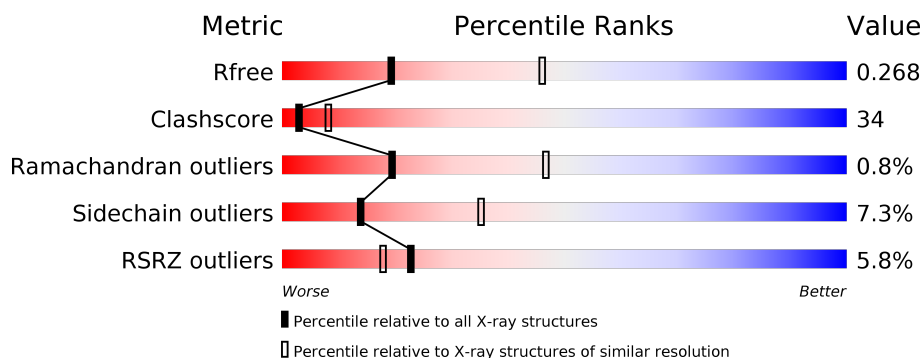
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	<div> <div>5%</div> <div>45%</div> <div>38%</div> <div>5%</div> <div>13%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6868 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.

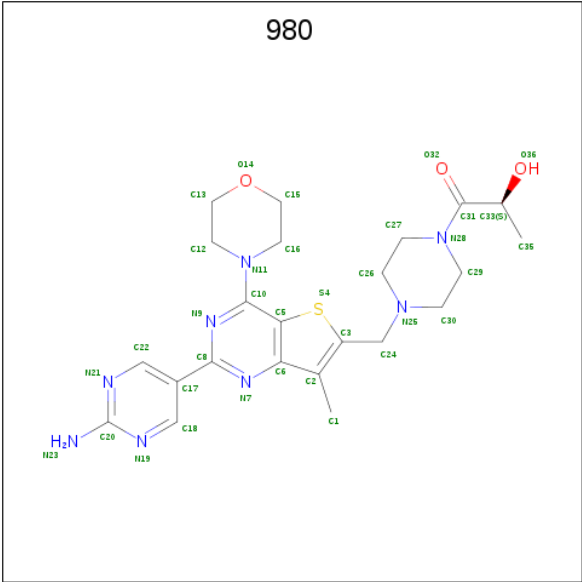
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	845	Total	C	N	O	S	0	0	0
			6820	4376	1162	1246	36			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	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

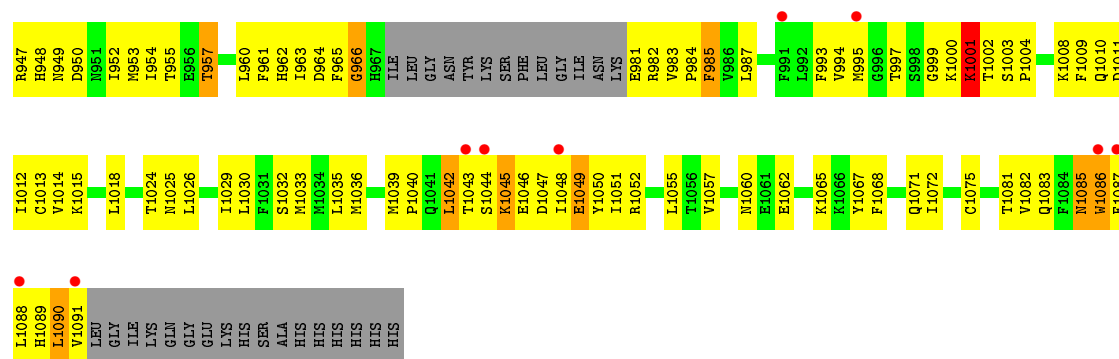
- Molecule 2 is (2S)-1-(4-{[2-(2-aminopyrimidin-5-yl)-7-methyl-4-(morpholin-4-yl)thieno[3,2-d]pyrimidin-6-yl]methyl}piperazin-1-yl)-2-hydroxypropan-1-one (three-letter code: 980) (formula: C₂₃H₃₀N₈O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	23	8	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.87Å 67.01Å 105.81Å 90.00° 96.77° 90.00°	Depositor
Resolution (Å)	61.67 – 2.79 61.67 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.1 (61.67-2.79) 93.4 (61.67-2.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.199 , 0.267 0.211 , 0.268	Depositor DCC
R_{free} test set	1236 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6868	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 980

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	1/6968 (0.0%)	0.98	10/9434 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	PRO	CA-C	5.29	1.63	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	897	GLY	N-CA-C	9.37	136.53	113.10
1	A	873	GLY	N-CA-C	8.49	134.32	113.10
1	A	874	ASP	N-CA-C	-7.01	92.07	111.00
1	A	375	ARG	N-CA-C	-6.83	92.55	111.00
1	A	544	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	579	ARG	CB-CA-C	-5.79	98.82	110.40
1	A	379	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	890	LYS	CB-CA-C	-5.33	99.74	110.40
1	A	1001	LYS	CB-CA-C	-5.21	99.99	110.40
1	A	658	HIS	N-CA-CB	-5.17	101.30	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	ARG	Sidechain
1	A	780	PRO	Peptide
1	A	873	GLY	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6820	0	6825	471	0
2	A	35	0	30	3	0
3	A	13	0	0	2	0
All	All	6868	0	6855	471	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 34.

All (471) 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:760:SER:HB2	1:A:763:VAL:HG23	1.22	1.14
1:A:756:LYS:CD	1:A:758:ASP:HB2	1.78	1.11
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.28	1.11
1:A:527:ILE:CG2	1:A:528:ALA:H	1.61	1.11
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.33	1.08
1:A:223:VAL:HG12	1:A:225:HIS:CE1	1.90	1.05
1:A:486:GLN:HG2	1:A:487:ILE:H	1.20	1.05
1:A:217:ASN:HD22	1:A:219:CYS:HB3	1.19	1.05
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.36	1.04
1:A:743:GLN:HE21	1:A:876:ILE:HG12	1.22	1.02
1:A:1043:THR:CG2	1:A:1046:GLU:H	1.74	1.01
1:A:527:ILE:HG22	1:A:528:ALA:N	1.72	1.00
1:A:893:GLN:HG3	1:A:897:GLY:CA	1.91	0.99
1:A:274:VAL:HG23	1:A:277:ARG:HB2	1.44	0.99
1:A:1060:ASN:HD21	1:A:1062:GLU:HB2	1.24	0.99
1:A:274:VAL:CG2	1:A:277:ARG:HB2	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LYS:HD2	1:A:758:ASP:CB	1.91	0.99
1:A:235:VAL:HG11	1:A:244:ILE:HD11	1.42	0.99
1:A:874:ASP:H	1:A:876:ILE:HG22	1.25	0.98
1:A:893:GLN:HG3	1:A:897:GLY:HA3	0.99	0.97
1:A:893:GLN:CG	1:A:897:GLY:HA3	1.93	0.97
1:A:527:ILE:CG2	1:A:528:ALA:N	2.25	0.95
1:A:756:LYS:HD2	1:A:758:ASP:HB2	0.96	0.95
1:A:210:TYR:O	1:A:213:LYS:HD3	1.67	0.94
1:A:223:VAL:CG1	1:A:225:HIS:CE1	2.51	0.94
1:A:527:ILE:HG22	1:A:528:ALA:H	1.29	0.93
1:A:1090:LEU:O	1:A:1091:VAL:HG23	1.71	0.90
1:A:779:LEU:HD12	1:A:780:PRO:HD2	1.54	0.90
1:A:760:SER:HB2	1:A:763:VAL:CG2	2.02	0.89
1:A:743:GLN:NE2	1:A:876:ILE:HG12	1.87	0.89
1:A:997:THR:HG23	1:A:1001:LYS:HB3	1.52	0.89
1:A:756:LYS:HB2	1:A:758:ASP:N	1.89	0.88
1:A:564:LEU:HD11	1:A:1048:ILE:CG2	2.04	0.88
1:A:1060:ASN:ND2	1:A:1062:GLU:HB2	1.91	0.85
1:A:1090:LEU:HD12	1:A:1090:LEU:O	1.76	0.84
1:A:225:HIS:HE2	1:A:304:HIS:HD2	1.27	0.83
1:A:272:LEU:HB3	1:A:305:VAL:CG1	2.09	0.83
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.58	0.83
1:A:527:ILE:HG23	1:A:528:ALA:H	1.43	0.82
1:A:1043:THR:HG21	1:A:1046:GLU:H	1.41	0.82
1:A:163:THR:HG22	1:A:177:ARG:HH12	1.43	0.82
1:A:1043:THR:HG22	1:A:1046:GLU:H	1.43	0.82
1:A:873:GLY:HA3	1:A:876:ILE:CG2	2.10	0.81
1:A:706:SER:O	1:A:710:GLN:HB3	1.79	0.81
1:A:857:THR:OG1	1:A:858:GLU:OE1	1.98	0.80
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.16	0.80
1:A:1042:LEU:H	1:A:1042:LEU:HD13	1.47	0.79
1:A:737:GLN:O	1:A:741:MET:HG3	1.83	0.79
1:A:775:GLN:HE21	1:A:798:ILE:HD11	1.47	0.78
1:A:643:ILE:O	1:A:646:GLN:HB3	1.84	0.78
1:A:903:LYS:O	1:A:906:VAL:HG22	1.84	0.78
1:A:576:TRP:O	1:A:579:ARG:HD3	1.84	0.78
1:A:905:GLU:HG2	1:A:993:PHE:CZ	2.19	0.77
1:A:1035:LEU:HD12	1:A:1048:ILE:CD1	2.12	0.77
1:A:486:GLN:HG2	1:A:487:ILE:N	1.99	0.77
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.65	0.77
1:A:810:PRO:HB3	1:A:833:LYS:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:VAL:HB	1:A:225:HIS:HE1	1.50	0.75
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.14	0.75
1:A:874:ASP:N	1:A:876:ILE:HG22	2.02	0.75
1:A:1008:LYS:O	1:A:1012:ILE:HG13	1.86	0.75
1:A:902:PHE:CZ	1:A:1083:GLN:HB3	2.22	0.75
1:A:925:VAL:O	1:A:929:VAL:HG23	1.86	0.75
1:A:273:ARG:H	1:A:305:VAL:HG13	1.52	0.74
1:A:470:ASP:HB3	1:A:476:ARG:HH21	1.51	0.74
1:A:1043:THR:CG2	1:A:1046:GLU:N	2.51	0.74
1:A:210:TYR:CE1	1:A:211:LEU:HG	2.23	0.74
1:A:1087:PHE:HD1	1:A:1090:LEU:HD23	1.52	0.74
1:A:182:THR:HB	1:A:183:PRO:HD3	1.69	0.73
1:A:838:LEU:HD23	1:A:877:GLY:CA	2.18	0.73
1:A:483:HIS:CE1	1:A:510:LYS:HG2	2.23	0.72
1:A:1010:GLN:HG2	1:A:1072:ILE:HD12	1.72	0.72
1:A:760:SER:CB	1:A:763:VAL:HG23	2.12	0.72
1:A:1091:VAL:O	1:A:1091:VAL:HG12	1.88	0.71
1:A:275:CYS:HB2	1:A:823:LEU:HD22	1.71	0.71
1:A:273:ARG:O	1:A:305:VAL:HA	1.90	0.71
1:A:905:GLU:HG2	1:A:993:PHE:CE2	2.25	0.71
1:A:1090:LEU:O	1:A:1091:VAL:CG2	2.37	0.71
1:A:568:THR:HG22	1:A:569:ALA:N	2.06	0.71
1:A:524:CYS:O	1:A:526:PRO:HD3	1.91	0.70
1:A:223:VAL:CB	1:A:225:HIS:HE1	2.04	0.70
1:A:756:LYS:N	1:A:757:TYR:HA	2.07	0.70
1:A:652:GLU:HG2	3:A:2:HOH:O	1.90	0.70
1:A:150:PHE:CE2	1:A:319:ARG:HD3	2.26	0.70
1:A:207:LEU:HD11	1:A:288:LYS:HB2	1.73	0.70
1:A:285:THR:HG22	1:A:289:ASN:HB2	1.72	0.69
1:A:1086:TRP:O	1:A:1087:PHE:HB3	1.91	0.69
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.73	0.69
1:A:1067:TYR:O	1:A:1071:GLN:HG2	1.93	0.69
1:A:892:GLN:OE1	1:A:906:VAL:HG21	1.94	0.68
1:A:1043:THR:HG22	1:A:1046:GLU:N	2.09	0.67
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.08	0.67
1:A:756:LYS:H	1:A:757:TYR:HA	1.57	0.67
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.58	0.67
1:A:892:GLN:O	1:A:903:LYS:HE3	1.95	0.67
1:A:1010:GLN:HG2	1:A:1072:ILE:CD1	2.25	0.67
1:A:274:VAL:O	1:A:274:VAL:HG23	1.95	0.67
1:A:1043:THR:HB	1:A:1047:ASP:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:OD1	1:A:472:ARG:NH2	2.22	0.66
1:A:225:HIS:N	1:A:225:HIS:ND1	2.44	0.66
1:A:217:ASN:HD22	1:A:219:CYS:CB	2.05	0.66
1:A:181:VAL:HG22	1:A:184:ARG:NH2	2.11	0.66
1:A:1025:ASN:O	1:A:1029:ILE:HG22	1.96	0.66
1:A:1081:THR:O	1:A:1085:ASN:ND2	2.29	0.66
1:A:366:ARG:NH1	1:A:519:LEU:HB2	2.10	0.66
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.60	0.65
1:A:981:GLU:O	1:A:982:ARG:HD3	1.97	0.65
1:A:1087:PHE:CD1	1:A:1090:LEU:HD23	2.31	0.65
1:A:699:LEU:O	1:A:703:ILE:HG13	1.97	0.65
1:A:810:PRO:CB	1:A:833:LYS:HB2	2.26	0.65
1:A:768:LYS:HE3	1:A:798:ILE:O	1.97	0.65
1:A:900:GLY:O	1:A:901:ALA:HB3	1.96	0.64
1:A:317:GLU:O	1:A:726:THR:HG23	1.98	0.64
1:A:936:CYS:HG	1:A:985:PHE:HD1	1.45	0.64
1:A:296:CYS:HB3	1:A:301:GLU:O	1.98	0.64
1:A:775:GLN:OE1	1:A:795:ALA:HB1	1.98	0.64
1:A:486:GLN:CG	1:A:487:ILE:H	2.03	0.63
1:A:550:GLN:O	1:A:554:GLN:HG3	1.97	0.63
1:A:890:LYS:HA	1:A:893:GLN:HB3	1.79	0.63
1:A:1043:THR:HG22	1:A:1045:LYS:H	1.63	0.63
1:A:213:LYS:HG2	1:A:214:LYS:N	2.11	0.63
1:A:1086:TRP:CE3	1:A:1087:PHE:N	2.67	0.63
1:A:225:HIS:NE2	1:A:304:HIS:HD2	1.97	0.63
1:A:547:MET:CE	1:A:551:LEU:HB3	2.29	0.63
1:A:1043:THR:HG21	1:A:1046:GLU:CB	2.28	0.63
1:A:948:HIS:CD2	1:A:950:ASP:HB2	2.34	0.63
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.80	0.62
1:A:873:GLY:H	1:A:876:ILE:HG23	1.64	0.62
1:A:1085:ASN:O	1:A:1088:LEU:HG	2.00	0.62
1:A:271:VAL:HG23	1:A:282:VAL:HG12	1.81	0.62
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.81	0.62
1:A:890:LYS:HA	1:A:893:GLN:CB	2.30	0.62
1:A:240:THR:HG23	1:A:243:ALA:H	1.64	0.62
1:A:368:ILE:O	1:A:368:ILE:HG13	2.00	0.62
1:A:983:VAL:HG13	1:A:985:PHE:O	2.00	0.62
1:A:1032:SER:HA	1:A:1048:ILE:HD12	1.82	0.61
1:A:949:ASN:N	1:A:1083:GLN:HE22	1.98	0.61
1:A:202:VAL:HG12	1:A:203:THR:N	2.15	0.61
1:A:287:ILE:HD12	1:A:288:LYS:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:THR:HG22	1:A:569:ALA:H	1.64	0.61
1:A:500:ASP:O	1:A:503:THR:HG22	2.01	0.61
1:A:304:HIS:CB	1:A:823:LEU:HD21	2.30	0.61
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.49	0.61
1:A:614:ARG:NH1	1:A:643:ILE:HG22	2.15	0.61
1:A:756:LYS:HD3	1:A:758:ASP:OD2	2.01	0.61
1:A:905:GLU:HG2	1:A:993:PHE:CE1	2.35	0.61
1:A:217:ASN:OD1	1:A:217:ASN:N	2.33	0.60
1:A:273:ARG:N	1:A:305:VAL:HG13	2.16	0.60
1:A:175:PHE:HD1	1:A:178:ARG:NH2	1.99	0.60
1:A:833:LYS:HG3	1:A:834:HIS:N	2.15	0.60
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.83	0.60
1:A:806:SER:O	1:A:807:LYS:CB	2.49	0.60
1:A:564:LEU:HD21	1:A:1048:ILE:HG21	1.82	0.60
1:A:853:SER:O	1:A:857:THR:HG23	2.01	0.60
1:A:743:GLN:HG2	1:A:876:ILE:CD1	2.32	0.59
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.33	0.59
1:A:1011:ASP:O	1:A:1015:LYS:HD3	2.02	0.59
1:A:217:ASN:ND2	1:A:219:CYS:HB3	2.04	0.59
1:A:1024:THR:HG23	1:A:1055:LEU:HD12	1.84	0.59
1:A:815:PHE:O	1:A:827:THR:HB	2.02	0.59
1:A:225:HIS:O	1:A:306:VAL:HG23	2.03	0.59
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.02	0.58
1:A:705:GLN:NE2	1:A:839:ARG:HD3	2.18	0.58
1:A:798:ILE:HD12	1:A:798:ILE:N	2.18	0.58
1:A:796:LEU:HG	1:A:815:PHE:CE2	2.37	0.58
1:A:235:VAL:HG12	1:A:239:ASP:OD2	2.04	0.58
1:A:743:GLN:NE2	1:A:872:THR:OG1	2.35	0.58
1:A:873:GLY:CA	1:A:876:ILE:CG2	2.81	0.58
1:A:1024:THR:HG23	1:A:1055:LEU:CD1	2.34	0.58
1:A:895:THR:OG1	1:A:903:LYS:NZ	2.36	0.58
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.03	0.58
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.85	0.58
1:A:1049:GLU:O	1:A:1050:TYR:C	2.43	0.58
1:A:271:VAL:CG2	1:A:282:VAL:HG12	2.33	0.58
1:A:775:GLN:NE2	1:A:796:LEU:HB2	2.19	0.58
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.04	0.58
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.03	0.57
1:A:756:LYS:CD	1:A:758:ASP:CB	2.65	0.57
1:A:1001:LYS:HG2	1:A:1002:THR:H	1.68	0.57
1:A:1091:VAL:O	1:A:1091:VAL:CG1	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HG22	1:A:235:VAL:HG22	1.87	0.57
1:A:273:ARG:NH1	1:A:273:ARG:HG2	2.19	0.57
1:A:547:MET:HE2	1:A:552:ARG:N	2.20	0.57
1:A:1043:THR:HG21	1:A:1046:GLU:N	2.16	0.57
1:A:217:ASN:ND2	1:A:219:CYS:O	2.38	0.57
1:A:885:ALA:HA	1:A:954:ILE:O	2.05	0.57
1:A:810:PRO:HB3	1:A:833:LYS:CB	2.34	0.57
1:A:285:THR:CG2	1:A:289:ASN:HB2	2.35	0.57
1:A:550:GLN:OE1	1:A:550:GLN:HA	2.05	0.57
1:A:572:LYS:HA	1:A:575:LEU:HD12	1.87	0.57
1:A:249:PHE:CE1	1:A:268:GLN:OE1	2.58	0.56
1:A:733:THR:HG22	1:A:737:GLN:NE2	2.19	0.56
1:A:840:GLN:O	1:A:844:ILE:HG12	2.05	0.56
1:A:743:GLN:HG2	1:A:876:ILE:HD13	1.87	0.56
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.87	0.56
1:A:202:VAL:CG1	1:A:203:THR:N	2.68	0.56
1:A:271:VAL:HG21	1:A:282:VAL:HG11	1.86	0.56
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.86	0.56
1:A:655:ASP:O	1:A:658:HIS:HB2	2.05	0.56
1:A:311:PRO:O	1:A:313:PRO:HD3	2.04	0.56
1:A:287:ILE:HD12	1:A:288:LYS:H	1.71	0.56
1:A:1001:LYS:CG	1:A:1002:THR:H	2.18	0.56
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.35	0.56
1:A:901:ALA:O	1:A:902:PHE:CG	2.58	0.56
1:A:272:LEU:CB	1:A:305:VAL:HG11	2.23	0.56
1:A:739:ILE:O	1:A:743:GLN:HB2	2.06	0.56
1:A:948:HIS:ND1	1:A:949:ASN:N	2.54	0.56
1:A:1090:LEU:HD12	1:A:1090:LEU:C	2.27	0.56
1:A:373:LEU:N	1:A:374:PRO:CD	2.69	0.56
1:A:498:ASN:ND2	1:A:1036:MET:O	2.38	0.55
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.86	0.55
1:A:554:GLN:O	1:A:558:ILE:HG13	2.06	0.55
1:A:586:PRO:HA	1:A:589:TYR:CE1	2.41	0.55
1:A:987:LEU:HB3	1:A:1075:CYS:HB3	1.89	0.55
1:A:804:MET:HE1	1:A:831:ILE:HG12	1.88	0.55
1:A:271:VAL:HG22	1:A:272:LEU:N	2.22	0.55
1:A:567:LEU:HD21	1:A:591:LYS:HD2	1.88	0.55
1:A:163:THR:HG22	1:A:177:ARG:NH1	2.20	0.54
1:A:784:ARG:HH11	1:A:784:ARG:HG2	1.71	0.54
1:A:1042:LEU:N	1:A:1042:LEU:HD13	2.18	0.54
1:A:997:THR:CG2	1:A:1001:LYS:HB3	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ILE:O	1:A:235:VAL:N	2.37	0.54
1:A:874:ASP:O	1:A:875:LYS:C	2.46	0.54
1:A:1090:LEU:C	1:A:1091:VAL:HG23	2.28	0.54
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.73	0.54
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.42	0.54
1:A:701:SER:O	1:A:705:GLN:HG2	2.07	0.54
1:A:223:VAL:CG1	1:A:225:HIS:HE1	2.08	0.54
1:A:787:TYR:CE1	1:A:880:GLU:HB2	2.43	0.54
1:A:272:LEU:CD2	1:A:305:VAL:HG11	2.38	0.54
1:A:568:THR:HG22	1:A:570:GLU:H	1.73	0.53
1:A:271:VAL:HG21	1:A:282:VAL:CG1	2.39	0.53
1:A:410:TRP:HB3	1:A:412:VAL:HG12	1.90	0.53
1:A:575:LEU:HD13	1:A:595:SER:OG	2.09	0.53
1:A:274:VAL:HG21	1:A:277:ARG:HB2	1.84	0.53
1:A:921:PHE:O	1:A:925:VAL:HG23	2.08	0.53
1:A:804:MET:CG	2:A:1:980:H29	2.38	0.53
1:A:735:GLN:O	1:A:739:ILE:HG12	2.09	0.53
1:A:935:TYR:O	1:A:939:THR:HB	2.08	0.53
1:A:487:ILE:HG22	1:A:488:SER:N	2.24	0.53
1:A:625:GLY:O	1:A:629:GLN:HG3	2.08	0.53
1:A:984:PRO:HB2	1:A:985:PHE:CD2	2.44	0.53
1:A:632:ASP:HB3	1:A:1033:MET:HE2	1.91	0.53
1:A:210:TYR:CD1	1:A:211:LEU:HG	2.44	0.53
1:A:223:VAL:O	1:A:225:HIS:CE1	2.62	0.53
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.44	0.53
1:A:268:GLN:HA	1:A:268:GLN:OE1	2.09	0.53
1:A:955:THR:OG1	1:A:957:THR:HG22	2.09	0.53
1:A:750:LYS:HG3	1:A:808:LYS:O	2.09	0.53
1:A:370:ILE:O	1:A:370:ILE:HG23	2.08	0.52
1:A:576:TRP:CE2	1:A:579:ARG:HD2	2.44	0.52
1:A:892:GLN:HA	1:A:892:GLN:OE1	2.09	0.52
1:A:271:VAL:CG2	1:A:282:VAL:CG1	2.86	0.52
1:A:547:MET:HE3	1:A:551:LEU:HB3	1.91	0.52
1:A:784:ARG:HG2	1:A:784:ARG:NH1	2.24	0.52
1:A:470:ASP:CB	1:A:476:ARG:NH2	2.72	0.52
1:A:775:GLN:HE22	1:A:796:LEU:HB2	1.74	0.52
1:A:947:ARG:NH2	1:A:964:ASP:O	2.42	0.52
1:A:887:THR:HG22	1:A:889:ALA:H	1.75	0.52
1:A:547:MET:CE	1:A:551:LEU:CB	2.88	0.52
1:A:1085:ASN:H	1:A:1085:ASN:HD22	1.57	0.52
1:A:145:GLU:OE2	1:A:145:GLU:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:LEU:HD23	1:A:476:ARG:N	2.25	0.52
1:A:1086:TRP:HZ3	1:A:1090:LEU:HD22	1.73	0.52
1:A:604:VAL:O	1:A:607:THR:HB	2.10	0.51
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.91	0.51
1:A:199:HIS:CD2	1:A:199:HIS:O	2.63	0.51
1:A:575:LEU:CD1	1:A:595:SER:OG	2.58	0.51
1:A:685:GLY:HA2	1:A:691:ILE:HG22	1.93	0.51
1:A:1043:THR:HG21	1:A:1046:GLU:HB3	1.92	0.51
1:A:965:PHE:O	1:A:966:GLY:C	2.49	0.51
1:A:899:THR:OG1	1:A:900:GLY:N	2.43	0.51
1:A:1043:THR:C	1:A:1045:LYS:H	2.15	0.50
1:A:221:PHE:HA	1:A:233:ILE:O	2.11	0.50
1:A:225:HIS:HE2	1:A:304:HIS:CD2	2.17	0.50
1:A:529:LEU:HB3	1:A:530:PRO:HD2	1.93	0.50
1:A:214:LYS:NZ	1:A:297:LEU:HA	2.27	0.50
1:A:357:CYS:SG	1:A:359:ARG:HB3	2.51	0.50
1:A:766:GLN:HA	1:A:769:GLN:HB2	1.93	0.50
1:A:983:VAL:HB	1:A:1082:VAL:HG21	1.92	0.50
1:A:249:PHE:CD1	1:A:268:GLN:NE2	2.79	0.50
1:A:1003:SER:HB2	1:A:1004:PRO:CD	2.42	0.50
1:A:226:ARG:O	1:A:227:SER:CB	2.59	0.50
1:A:373:LEU:N	1:A:374:PRO:HD3	2.27	0.50
1:A:483:HIS:NE2	1:A:510:LYS:HG2	2.26	0.50
1:A:798:ILE:HD12	1:A:798:ILE:H	1.76	0.50
1:A:366:ARG:NH1	1:A:519:LEU:CB	2.73	0.50
1:A:873:GLY:N	1:A:876:ILE:HG23	2.26	0.50
1:A:984:PRO:HG2	1:A:1075:CYS:SG	2.52	0.49
1:A:845:LEU:CD1	1:A:869:CYS:HB3	2.42	0.49
1:A:889:ALA:O	1:A:890:LYS:CB	2.59	0.49
1:A:905:GLU:HG2	1:A:993:PHE:CD2	2.48	0.49
1:A:932:CYS:HA	1:A:960:LEU:HD23	1.94	0.49
1:A:184:ARG:NE	1:A:321:GLU:OE2	2.38	0.49
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.95	0.49
1:A:425:LYS:HD2	1:A:473:PHE:CE2	2.48	0.49
1:A:952:ILE:CG2	1:A:960:LEU:HD11	2.42	0.49
1:A:941:VAL:O	1:A:1051:ILE:HG13	2.13	0.49
1:A:646:GLN:HG2	1:A:647:LYS:N	2.27	0.49
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.95	0.49
1:A:1086:TRP:HE3	1:A:1087:PHE:N	2.10	0.48
1:A:839:ARG:HA	1:A:842:MET:HE2	1.95	0.48
1:A:890:LYS:HG2	1:A:893:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASP:HB3	1:A:599:GLY:O	2.14	0.48
1:A:366:ARG:HH12	1:A:519:LEU:HD22	1.76	0.48
1:A:784:ARG:NH1	1:A:789:PRO:O	2.46	0.48
1:A:873:GLY:HA3	1:A:876:ILE:HG23	1.91	0.48
1:A:567:LEU:HD22	1:A:575:LEU:HD11	1.93	0.48
1:A:312:ASP:OD2	1:A:314:ALA:CB	2.61	0.48
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.43	0.48
1:A:360:LYS:HA	1:A:419:LYS:HA	1.94	0.48
1:A:380:THR:OG1	1:A:401:PRO:HB2	2.13	0.48
1:A:523:TYR:CD2	1:A:524:CYS:HB2	2.49	0.48
1:A:298:LYS:HD2	1:A:299:ASN:OD1	2.14	0.48
1:A:433:ILE:O	1:A:460:LEU:HD12	2.13	0.48
1:A:589:TYR:O	1:A:593:PHE:CD1	2.67	0.48
1:A:842:MET:CE	1:A:871:SER:HB3	2.43	0.48
1:A:891:ILE:HD13	1:A:910:TRP:CD2	2.49	0.48
1:A:1086:TRP:O	1:A:1087:PHE:CB	2.60	0.47
1:A:779:LEU:HD12	1:A:780:PRO:CD	2.35	0.47
1:A:210:TYR:HD2	1:A:859:SER:O	1.97	0.47
1:A:395:CYS:HG	1:A:417:SER:HG	1.54	0.47
1:A:887:THR:O	1:A:889:ALA:O	2.32	0.47
1:A:367:GLY:HA2	1:A:410:TRP:HE3	1.79	0.47
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.14	0.47
1:A:999:GLY:O	1:A:1000:LYS:C	2.53	0.47
1:A:232:THR:HG22	1:A:233:ILE:N	2.28	0.47
1:A:576:TRP:CD2	1:A:579:ARG:HD2	2.49	0.47
1:A:274:VAL:CG2	1:A:279:GLU:HB3	2.45	0.47
1:A:150:PHE:HB2	1:A:319:ARG:NH1	2.30	0.47
1:A:620:SER:O	1:A:647:LYS:NZ	2.47	0.47
1:A:804:MET:HG3	2:A:1:980:H29	1.97	0.47
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.44	0.47
1:A:780:PRO:O	1:A:782:SER:N	2.48	0.47
1:A:725:GLY:O	1:A:729:LEU:HG	2.15	0.47
1:A:855:TRP:HB3	1:A:860:LEU:HB2	1.96	0.47
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.95	0.47
1:A:1052:ARG:HG3	1:A:1057:VAL:HG21	1.96	0.47
1:A:552:ARG:HD2	1:A:552:ARG:HH11	1.57	0.47
1:A:1085:ASN:HA	1:A:1088:LEU:CD1	2.44	0.46
1:A:731:ASP:OD2	1:A:784:ARG:NE	2.47	0.46
1:A:461:LEU:HB3	1:A:462:TYR:CD2	2.51	0.46
1:A:524:CYS:HB3	1:A:525:HIS:H	1.45	0.46
1:A:705:GLN:HE21	1:A:839:ARG:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ASP:CB	1:A:476:ARG:HH21	2.26	0.46
1:A:756:LYS:N	1:A:757:TYR:CA	2.75	0.46
1:A:743:GLN:CG	1:A:876:ILE:CD1	2.93	0.46
1:A:1001:LYS:CG	1:A:1002:THR:N	2.78	0.46
1:A:214:LYS:CE	1:A:300:GLY:HA2	2.45	0.46
1:A:214:LYS:HE3	1:A:300:GLY:HA2	1.98	0.46
1:A:957:THR:O	1:A:957:THR:HG23	2.16	0.46
1:A:1049:GLU:O	1:A:1052:ARG:N	2.43	0.46
1:A:175:PHE:HD1	1:A:178:ARG:HH22	1.62	0.46
1:A:373:LEU:O	1:A:374:PRO:C	2.52	0.46
1:A:568:THR:CG2	1:A:569:ALA:N	2.74	0.46
1:A:873:GLY:CA	1:A:876:ILE:HG23	2.46	0.46
1:A:952:ILE:HG22	1:A:960:LEU:HD11	1.97	0.46
1:A:225:HIS:O	1:A:306:VAL:HA	2.16	0.46
1:A:661:LEU:HD21	1:A:843:LEU:HD13	1.97	0.46
1:A:840:GLN:OE1	1:A:966:GLY:O	2.34	0.46
1:A:366:ARG:HH12	1:A:519:LEU:CD2	2.29	0.46
1:A:953:MET:O	1:A:960:LEU:HD12	2.16	0.46
1:A:468:LEU:HA	1:A:468:LEU:HD23	1.68	0.46
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.46	0.46
1:A:731:ASP:HB3	1:A:735:GLN:HE21	1.81	0.46
1:A:693:HIS:HE2	1:A:786:PRO:HA	1.81	0.46
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.16	0.45
1:A:274:VAL:O	1:A:274:VAL:CG2	2.61	0.45
1:A:287:ILE:HA	1:A:290:PHE:CD1	2.51	0.45
1:A:628:MET:CE	1:A:1030:LEU:HD21	2.47	0.45
1:A:780:PRO:O	1:A:781:GLU:C	2.55	0.45
1:A:865:LEU:HD23	1:A:961:PHE:CD2	2.51	0.45
1:A:845:LEU:HD12	1:A:869:CYS:HB3	1.98	0.45
1:A:371:PRO:HG2	1:A:511:GLU:O	2.17	0.45
1:A:756:LYS:HB2	1:A:758:ASP:H	1.79	0.45
1:A:901:ALA:O	1:A:902:PHE:CD2	2.70	0.45
1:A:983:VAL:CG1	1:A:985:PHE:O	2.63	0.45
1:A:587:LYS:HB3	1:A:587:LYS:HE2	1.80	0.45
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.75	0.45
1:A:647:LYS:HA	1:A:647:LYS:HD2	1.78	0.44
1:A:1043:THR:HG22	1:A:1045:LYS:N	2.31	0.44
1:A:220:ILE:N	1:A:235:VAL:O	2.39	0.44
1:A:249:PHE:CE1	1:A:268:GLN:CD	2.90	0.44
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.16	0.44
1:A:887:THR:HG22	1:A:889:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PHE:O	1:A:153:GLN:HB3	2.18	0.44
1:A:750:LYS:HE3	1:A:808:LYS:HA	2.00	0.44
1:A:472:ARG:O	1:A:473:PHE:HB2	2.17	0.44
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.18	0.44
1:A:304:HIS:HB2	1:A:823:LEU:HD21	1.98	0.44
1:A:935:TYR:HB3	1:A:962:HIS:CD2	2.53	0.44
1:A:240:THR:CG2	1:A:243:ALA:H	2.31	0.44
1:A:270:PHE:HB3	1:A:307:LEU:HD11	1.99	0.44
1:A:1001:LYS:HG2	1:A:1002:THR:N	2.33	0.44
1:A:652:GLU:N	3:A:2:HOH:O	2.33	0.43
1:A:842:MET:HG2	1:A:869:CYS:O	2.19	0.43
1:A:487:ILE:CG2	1:A:488:SER:N	2.81	0.43
1:A:738:VAL:HG23	1:A:780:PRO:HG3	2.00	0.43
1:A:1030:LEU:HA	1:A:1030:LEU:HD23	1.63	0.43
1:A:995:MET:CE	1:A:1009:PHE:CD1	3.01	0.43
1:A:199:HIS:HD2	1:A:199:HIS:O	2.00	0.43
1:A:657:LEU:HA	1:A:657:LEU:HD23	1.90	0.43
1:A:887:THR:O	1:A:891:ILE:HG13	2.18	0.43
1:A:184:ARG:HB2	1:A:184:ARG:NH1	2.34	0.43
1:A:867:TYR:OH	1:A:963:ILE:HA	2.19	0.43
1:A:366:ARG:HH12	1:A:519:LEU:CB	2.31	0.43
1:A:550:GLN:OE1	1:A:550:GLN:CA	2.67	0.43
1:A:881:ILE:HG23	2:A:1:980:H13	2.00	0.43
1:A:191:ARG:HD2	1:A:196:TYR:CG	2.54	0.43
1:A:236:SER:HA	1:A:237:PRO:HD3	1.91	0.43
1:A:274:VAL:CG1	1:A:292:TRP:CD1	3.01	0.43
1:A:281:LEU:C	1:A:282:VAL:HG13	2.38	0.43
1:A:576:TRP:O	1:A:579:ARG:CD	2.61	0.43
1:A:756:LYS:HB2	1:A:758:ASP:CB	2.48	0.43
1:A:810:PRO:HB3	1:A:833:LYS:HA	2.01	0.43
1:A:862:LEU:N	1:A:862:LEU:HD22	2.34	0.43
1:A:945:GLY:O	1:A:985:PHE:HA	2.19	0.43
1:A:900:GLY:O	1:A:901:ALA:CB	2.61	0.42
1:A:939:THR:CG2	1:A:940:PHE:N	2.81	0.42
1:A:568:THR:CG2	1:A:569:ALA:H	2.29	0.42
1:A:865:LEU:HD12	1:A:865:LEU:HA	1.87	0.42
1:A:930:TYR:CD2	1:A:1012:ILE:HD13	2.54	0.42
1:A:145:GLU:OE2	1:A:145:GLU:O	2.36	0.42
1:A:184:ARG:HB2	1:A:184:ARG:HH11	1.84	0.42
1:A:486:GLN:O	1:A:487:ILE:HD13	2.20	0.42
1:A:580:TYR:HE2	1:A:613:ARG:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:TYR:CD2	1:A:593:PHE:HE1	2.37	0.42
1:A:271:VAL:CG2	1:A:272:LEU:N	2.81	0.42
1:A:1085:ASN:HA	1:A:1088:LEU:HD11	2.02	0.42
1:A:402:LYS:HB3	1:A:403:PRO:CD	2.49	0.42
1:A:823:LEU:HA	1:A:823:LEU:HD12	1.86	0.42
1:A:661:LEU:CD2	1:A:843:LEU:HD13	2.49	0.42
1:A:731:ASP:O	1:A:735:GLN:HG3	2.20	0.42
1:A:273:ARG:NH1	1:A:277:ARG:O	2.51	0.42
1:A:622:LEU:HD21	1:A:651:LEU:HG	2.02	0.42
1:A:1087:PHE:HA	1:A:1090:LEU:HB2	2.00	0.42
1:A:1086:TRP:CZ3	1:A:1090:LEU:HD22	2.54	0.42
1:A:663:LEU:O	1:A:666:ALA:HB3	2.20	0.42
1:A:905:GLU:HG2	1:A:993:PHE:CD1	2.54	0.41
1:A:240:THR:HG22	1:A:243:ALA:HB2	2.02	0.41
1:A:862:LEU:O	1:A:931:SER:HA	2.20	0.41
1:A:904:ASP:O	1:A:905:GLU:HB2	2.20	0.41
1:A:889:ALA:HB2	1:A:949:ASN:HB3	2.02	0.41
1:A:518:ILE:HD12	1:A:520:LEU:HD13	2.02	0.41
1:A:862:LEU:CD2	1:A:862:LEU:N	2.83	0.41
1:A:388:GLN:HG2	1:A:393:VAL:HG22	2.03	0.41
1:A:150:PHE:CD2	1:A:319:ARG:HD3	2.56	0.41
1:A:192:ASP:HA	1:A:193:PRO:HD3	1.91	0.41
1:A:390:GLY:C	1:A:392:GLN:H	2.24	0.41
1:A:484:MET:SD	1:A:514:MET:HG2	2.61	0.41
1:A:703:ILE:CD1	1:A:714:ALA:HA	2.51	0.41
1:A:223:VAL:HB	1:A:225:HIS:CE1	2.41	0.41
1:A:674:ASP:C	1:A:674:ASP:OD1	2.58	0.41
1:A:1014:VAL:HG11	1:A:1065:LYS:CG	2.45	0.41
1:A:432:GLN:HB3	1:A:460:LEU:HD13	2.03	0.40
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.56	0.40
1:A:861:ASP:C	1:A:862:LEU:HD22	2.42	0.40
1:A:743:GLN:CG	1:A:876:ILE:HD11	2.51	0.40
1:A:890:LYS:HA	1:A:893:GLN:HB2	2.02	0.40
1:A:939:THR:HG23	1:A:945:GLY:CA	2.51	0.40
1:A:369:ASP:OD1	1:A:406:GLU:O	2.39	0.40
1:A:611:LEU:HA	1:A:611:LEU:HD23	1.85	0.40
1:A:628:MET:HE3	1:A:1030:LEU:HD21	2.02	0.40
1:A:1060:ASN:ND2	1:A:1062:GLU:CB	2.75	0.40
1:A:274:VAL:HG12	1:A:292:TRP:CD1	2.57	0.40
1:A:379:LEU:O	1:A:404:PHE:HB2	2.22	0.40
1:A:484:MET:SD	1:A:514:MET:CG	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LYS:CB	1:A:758:ASP:CG	2.89	0.40
1:A:886:THR:HG22	1:A:887:THR:N	2.36	0.40
1:A:729:LEU:HA	1:A:729:LEU:HD23	1.92	0.40
1:A:885:ALA:HA	1:A:955:THR:HA	2.04	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	831/966 (86%)	786 (95%)	38 (5%)	7 (1%)	19	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	807	LYS
1	A	966	GLY
1	A	1001	LYS
1	A	374	PRO
1	A	526	PRO
1	A	901	ALA
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	753/864 (87%)	698 (93%)	55 (7%)	14	35

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	168	VAL
1	A	185	MET
1	A	213	LYS
1	A	217	ASN
1	A	225	HIS
1	A	226	ARG
1	A	235	VAL
1	A	252	MET
1	A	272	LEU
1	A	273	ARG
1	A	281	LEU
1	A	301	GLU
1	A	307	LEU
1	A	376	ASN
1	A	395	CYS
1	A	404	PHE
1	A	523	TYR
1	A	524	CYS
1	A	552	ARG
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	636	SER
1	A	638	GLU
1	A	646	GLN
1	A	647	LYS
1	A	662	GLN
1	A	682	LEU
1	A	717	LEU
1	A	751	SER
1	A	752	LEU
1	A	753	SER
1	A	759	VAL
1	A	823	LEU
1	A	824	SER
1	A	833	LYS
1	A	838	LEU

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Mol	Chain	Res	Type
1	A	841	ASP
1	A	843	LEU
1	A	878	MET
1	A	896	VAL
1	A	907	LEU
1	A	939	THR
1	A	957	THR
1	A	985	PHE
1	A	1026	LEU
1	A	1042	LEU
1	A	1044	SER
1	A	1045	LYS
1	A	1049	GLU
1	A	1085	ASN
1	A	1086	TRP
1	A	1089	HIS
1	A	1090	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
1	A	217	ASN
1	A	304	HIS
1	A	432	GLN
1	A	646	GLN
1	A	705	GLN
1	A	737	GLN
1	A	743	GLN
1	A	908	ASN
1	A	962	HIS
1	A	1060	ASN
1	A	1083	GLN
1	A	1085	ASN

5.3.3 RNA ⓘ

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](#)

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	980	A	1	-	35,39,39	3.26	11 (31%)	42,56,56	2.24	14 (33%)

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	980	A	1	-	-	9/18/38/38	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	980	C24-N25	-9.98	1.28	1.47
2	A	1	980	C29-N28	-7.59	1.33	1.47
2	A	1	980	C31-N28	7.09	1.45	1.34
2	A	1	980	C27-N28	-7.04	1.34	1.47
2	A	1	980	C20-N23	4.92	1.43	1.33
2	A	1	980	C12-N11	-4.72	1.39	1.46
2	A	1	980	C16-N11	-3.79	1.40	1.46
2	A	1	980	C30-N25	-3.72	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	980	C26-N25	-3.72	1.36	1.46
2	A	1	980	C10-N11	2.60	1.44	1.37
2	A	1	980	C10-N9	2.54	1.36	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	980	N7-C8-N9	-8.88	119.13	126.11
2	A	1	980	C8-N7-C6	4.81	121.87	116.55
2	A	1	980	C17-C22-N21	-3.60	118.39	124.32
2	A	1	980	N21-C20-N19	-3.48	120.83	124.53
2	A	1	980	C22-N21-C20	2.99	121.97	116.44
2	A	1	980	O32-C31-N28	-2.82	118.36	121.67
2	A	1	980	C10-N9-C8	2.65	122.39	116.17
2	A	1	980	C17-C18-N19	-2.57	120.08	124.32
2	A	1	980	C22-C17-C18	2.38	118.37	114.66
2	A	1	980	C26-C27-N28	2.36	115.49	110.44
2	A	1	980	C29-N28-C27	2.26	116.98	112.62
2	A	1	980	N23-C20-N19	2.22	119.69	117.44
2	A	1	980	C18-N19-C20	2.11	120.35	116.44
2	A	1	980	N23-C20-N21	2.01	119.48	117.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

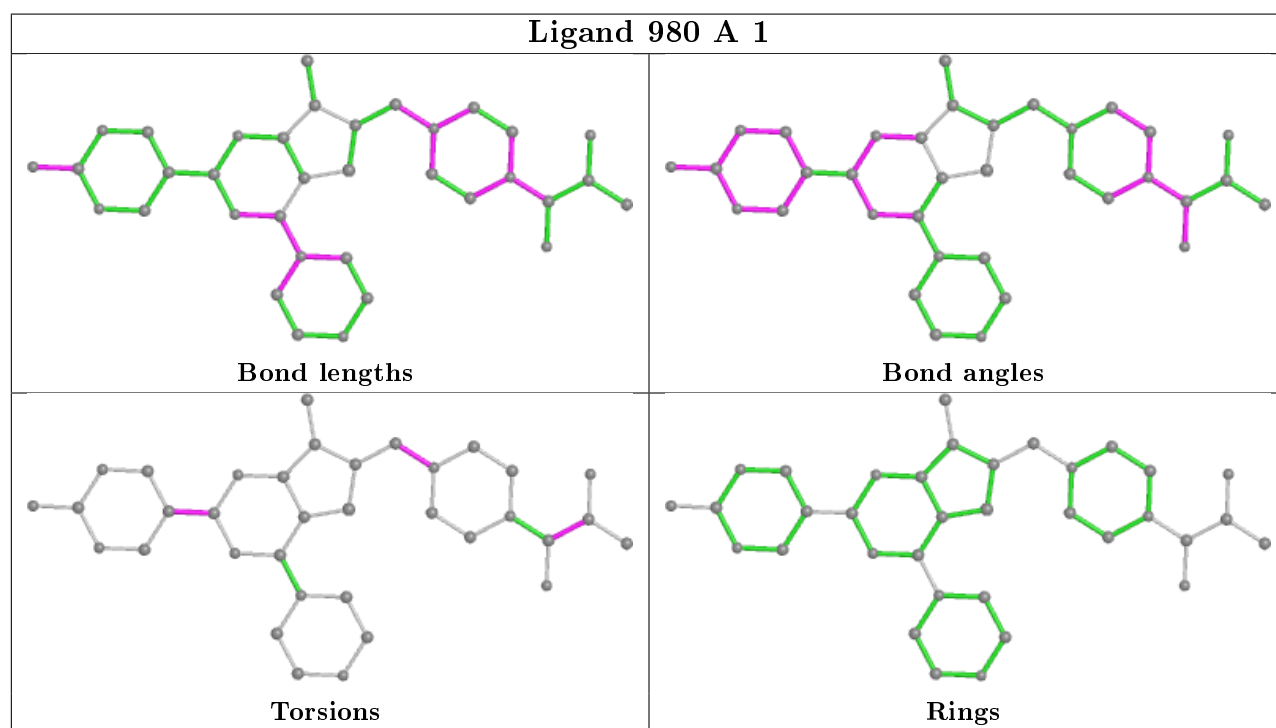
Mol	Chain	Res	Type	Atoms
2	A	1	980	N28-C31-C33-C35
2	A	1	980	O32-C31-C33-O36
2	A	1	980	C22-C17-C8-N7
2	A	1	980	C18-C17-C8-N9
2	A	1	980	C18-C17-C8-N7
2	A	1	980	C22-C17-C8-N9
2	A	1	980	C3-C24-N25-C30
2	A	1	980	N28-C31-C33-O36
2	A	1	980	O32-C31-C33-C35

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	980	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	845/966 (87%)	0.34	49 (5%) 23 18	35, 83, 146, 215	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	GLU	10.2
1	A	377	THR	9.3
1	A	376	ASN	8.4
1	A	1088	LEU	7.3
1	A	898	ASN	7.2
1	A	747	LEU	6.2
1	A	896	VAL	5.1
1	A	374	PRO	5.0
1	A	1044	SER	4.7
1	A	1091	VAL	4.5
1	A	897	GLY	4.3
1	A	287	ILE	4.2
1	A	1087	PHE	4.1
1	A	234	LYS	4.1
1	A	1086	TRP	3.9
1	A	378	ASP	3.9
1	A	899	THR	3.9
1	A	995	MET	3.4
1	A	526	PRO	3.4
1	A	235	VAL	3.1
1	A	253	ALA	3.0
1	A	409	LEU	3.0
1	A	752	LEU	2.9
1	A	489	GLY	2.9
1	A	902	PHE	2.8
1	A	1048	ILE	2.7
1	A	375	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	544	ARG	2.7
1	A	779	LEU	2.6
1	A	207	LEU	2.6
1	A	751	SER	2.6
1	A	321	GLU	2.6
1	A	755	GLU	2.6
1	A	750	LYS	2.5
1	A	756	LYS	2.5
1	A	403	PRO	2.5
1	A	217	ASN	2.4
1	A	528	ALA	2.4
1	A	513	SER	2.3
1	A	529	LEU	2.2
1	A	1043	THR	2.2
1	A	523	TYR	2.2
1	A	222	ILE	2.2
1	A	143	MET	2.2
1	A	832	PHE	2.2
1	A	359	ARG	2.1
1	A	991	PHE	2.1
1	A	813	LEU	2.0
1	A	363	VAL	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](#)

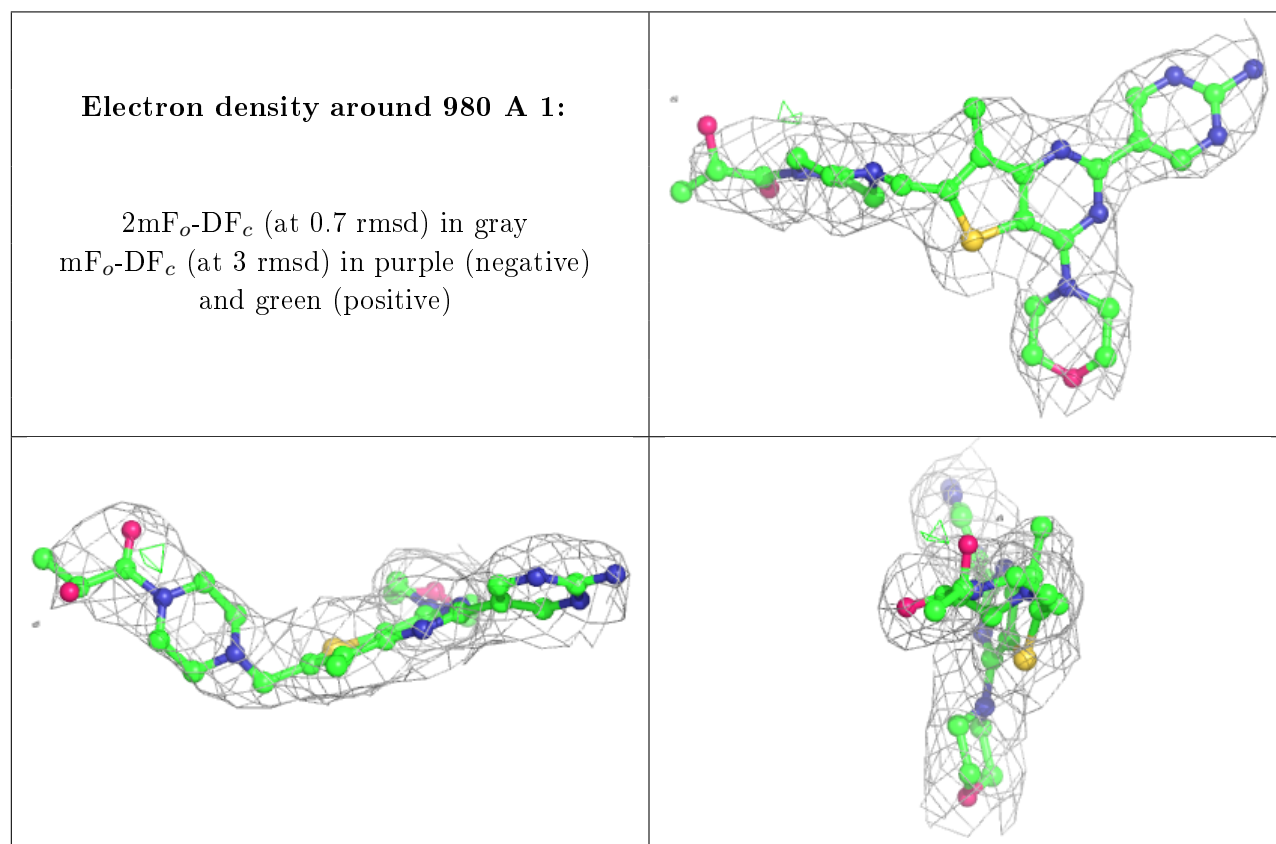
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
2	980	A	1	35/35	0.94	0.17	62,84,106,122	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.