Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 09:24 AM UTC

PDB ID	:	3TL5 / pdb_00003tl5
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

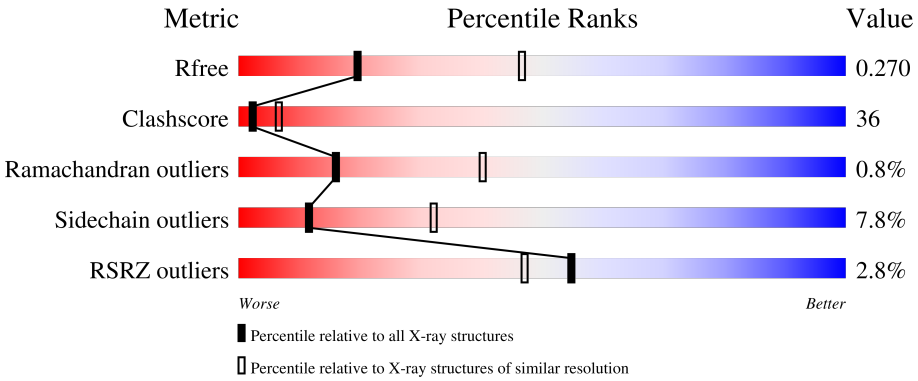
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.79 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	2% 42% 37% 8% • 13%

2 Entry composition (i)

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.

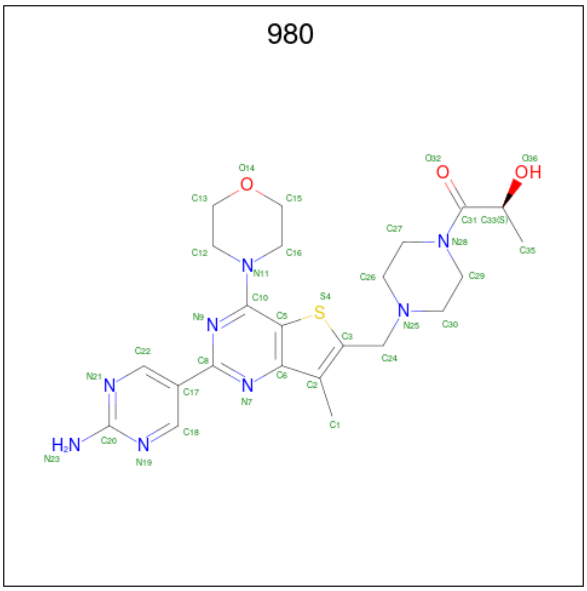
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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

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 (CCD ID: 980) (formula: $C_{23}H_{30}N_8O_3S$).



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.

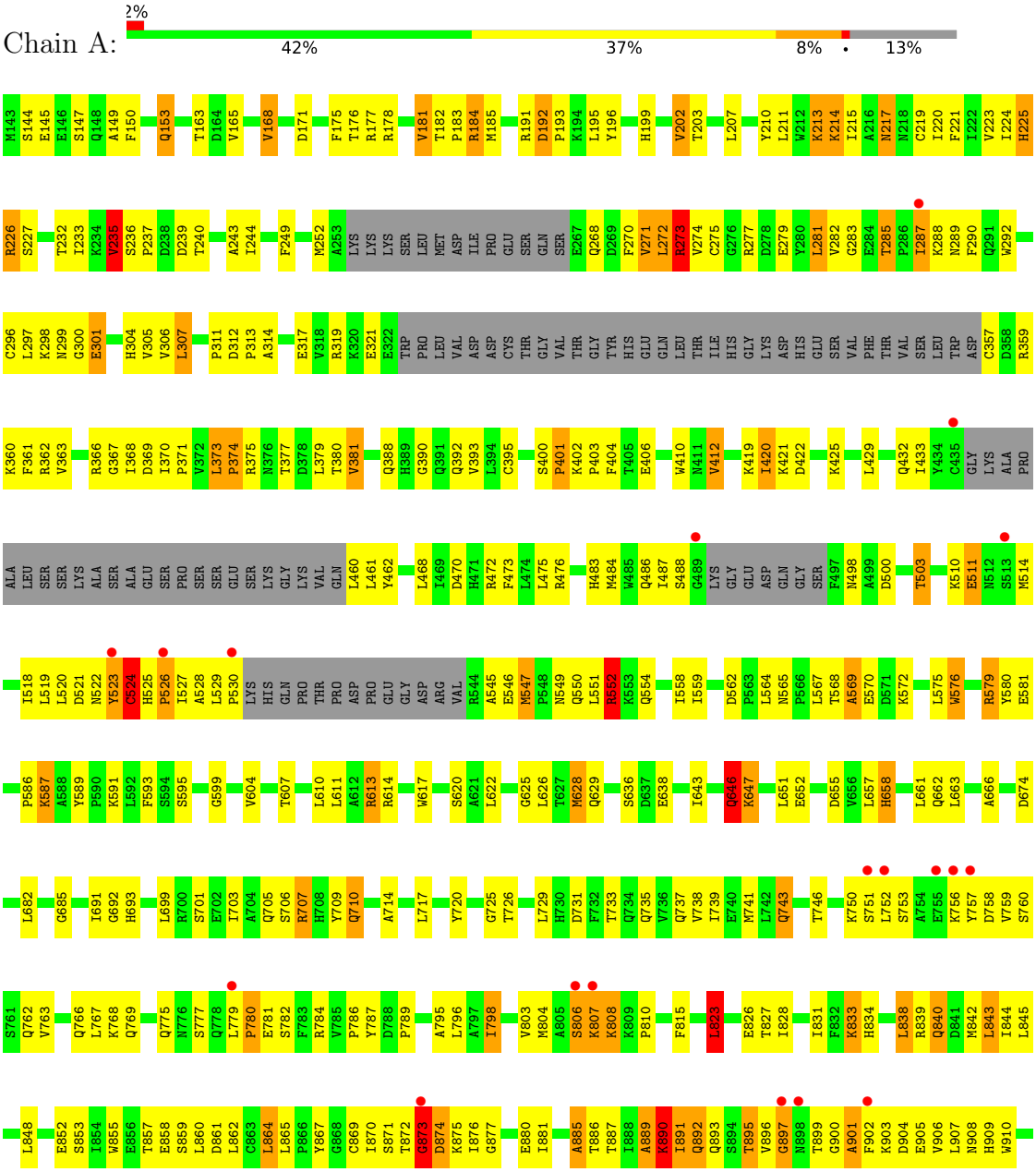
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		

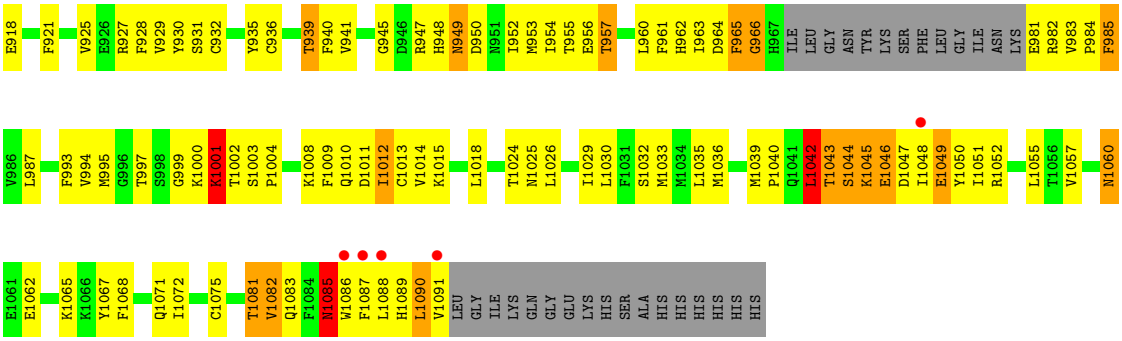
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

Chain A:




E918 F921 V925 E926 R927 F928 V929 Y930 S931 C932 Y935 C936 T939 F940 V941 G945 D946 R947 H948 N949 D950 N951 I952 M953 I954 T955 E956 T957 L960 F961 H962 I963 D964 F965 G966 H967 ILE LEU GLY ASN TYR LYS SER PHE LEU GLY ILE ASN LYS E981 R982 V983 P984 F985
V986 L987 F993 V994 M995 G996 T997 S998 G999 K1000 K1001 T1002 S1003 P1004 K1008 F1009 Q1010 D1011 I1012 C1013 V1014 K1015 L1018 T1024 N1025 L1026 I1029 L1030 F1031 S1032 M1033 M1034 L1035 M1036 M1039 P1040 Q1041 L1042 T1043 S1044 K1045 E1046 D1047 I1048 E1049 Y1050 I1051 R1052 L1055 T1056 V1057 N1060
E1061 E1062 K1065 K1066 Y1067 F1068 Q1071 I1072 C1075 T1081 V1082 Q1083 F1084 N1085 W1086 F1087 L1088 H1089 L1090 V1091 LEU GLY ILE LYS GLN GLY GLU LYS HIS SER ALA HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.03 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.199 , 0.267 0.213 , 0.270	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)	0.30 , 70.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[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: 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	0.79	3/6968 (0.0%)	1.39	92/9434 (1.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	PRO	CA-C	8.74	1.63	1.52
1	A	828	ILE	CA-CB	-5.40	1.47	1.53
1	A	168	VAL	CA-CB	5.20	1.61	1.55

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	806	SER	N-CA-C	12.03	124.39	111.28
1	A	375	ARG	N-CA-C	-11.36	92.55	108.23
1	A	874	ASP	N-CA-C	-9.91	92.07	108.32
1	A	897	GLY	N-CA-C	9.85	136.53	113.18
1	A	826	GLU	N-CA-C	8.92	123.17	110.23
1	A	873	GLY	N-CA-C	8.92	134.32	113.18
1	A	889	ALA	N-CA-C	-8.62	99.14	110.43
1	A	1044	SER	N-CA-C	-8.54	101.11	112.72
1	A	202	VAL	N-CA-CB	-8.19	102.90	112.32
1	A	1085	ASN	N-CA-C	8.05	120.06	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	226	ARG	N-CA-C	-7.50	103.86	113.16
1	A	235	VAL	N-CA-C	7.48	119.26	108.48
1	A	214	LYS	N-CA-C	-7.48	103.90	112.87
1	A	552	ARG	N-CA-C	-7.17	103.47	111.71
1	A	165	VAL	N-CA-C	7.16	119.02	112.29
1	A	511	GLU	N-CA-C	7.07	119.07	111.36
1	A	956	GLU	N-CA-C	-7.04	104.66	113.18
1	A	895	THR	N-CA-C	7.01	120.31	111.69
1	A	746	THR	CB-CA-C	-6.97	99.21	110.79
1	A	521	ASP	N-CA-C	6.95	120.38	108.02
1	A	546	GLU	N-CA-C	-6.83	99.17	110.17
1	A	524	CYS	N-CA-C	6.79	119.55	108.08
1	A	400	SER	CA-C-N	-6.75	113.34	120.03
1	A	400	SER	C-N-CA	-6.75	113.34	120.03
1	A	767	LEU	N-CA-C	-6.70	103.98	111.28
1	A	743	GLN	N-CA-C	-6.65	103.51	111.69
1	A	147	SER	N-CA-C	-6.55	104.18	111.71
1	A	1081	THR	CB-CA-C	-6.54	99.93	110.79
1	A	1046	GLU	N-CA-C	6.53	118.48	111.36
1	A	524	CYS	CB-CA-C	-6.49	109.11	116.63
1	A	949	ASN	N-CA-C	-6.41	104.34	111.71
1	A	569	ALA	N-CA-C	-6.40	104.39	111.36
1	A	184	ARG	CB-CA-C	-6.39	100.75	110.92
1	A	401	PRO	CB-CA-C	6.35	119.27	110.95
1	A	547	MET	CA-C-N	-6.32	113.16	119.92
1	A	547	MET	C-N-CA	-6.32	113.16	119.92
1	A	885	ALA	N-CA-C	-6.21	99.78	109.72
1	A	1043	THR	N-CA-C	-6.20	98.42	108.41
1	A	576	TRP	N-CA-C	6.14	117.84	111.03
1	A	777	SER	N-CA-C	6.12	117.75	111.14
1	A	658	HIS	N-CA-CB	-6.00	101.30	110.01
1	A	710	GLN	N-CA-C	5.97	118.57	111.71
1	A	153	GLN	N-CA-C	-5.92	104.74	111.14
1	A	1042	LEU	N-CA-C	5.88	118.42	109.95
1	A	1082	VAL	N-CA-C	5.88	116.06	110.42
1	A	579	ARG	CB-CA-C	-5.83	98.82	110.42
1	A	909	HIS	N-CA-CB	5.83	118.78	110.16
1	A	1012	ILE	CB-CA-C	-5.81	104.41	112.02
1	A	549	ASN	CB-CA-C	5.81	120.00	110.88
1	A	891	ILE	N-CA-C	-5.81	104.85	113.39
1	A	762	GLN	CB-CA-C	-5.75	101.24	110.79
1	A	559	ILE	CB-CA-C	-5.75	103.25	112.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	503	THR	N-CA-C	5.75	118.66	110.10
1	A	283	GLY	CA-C-O	-5.67	118.04	122.52
1	A	864	LEU	CA-C-N	-5.66	117.10	122.37
1	A	864	LEU	C-N-CA	-5.66	117.10	122.37
1	A	420	ILE	N-CA-C	5.63	117.04	110.62
1	A	412	VAL	N-CA-C	5.63	116.05	108.17
1	A	927	ARG	N-CA-C	5.62	117.41	111.28
1	A	870	ILE	N-CA-C	5.57	115.89	107.75
1	A	562	ASP	CA-C-N	5.51	125.61	119.32
1	A	562	ASP	C-N-CA	5.51	125.61	119.32
1	A	707	ARG	N-CA-C	-5.46	105.35	112.23
1	A	149	ALA	N-CA-C	-5.40	105.55	111.82
1	A	892	GLN	N-CA-C	-5.40	105.42	112.23
1	A	890	LYS	CB-CA-C	-5.37	99.74	110.42
1	A	646	GLN	CB-CA-C	-5.35	102.26	110.81
1	A	823	LEU	N-CA-C	5.33	117.09	111.28
1	A	565	ASN	CA-C-N	5.26	125.16	119.85
1	A	565	ASN	C-N-CA	5.26	125.16	119.85
1	A	271	VAL	N-CA-C	5.25	117.17	108.99
1	A	1001	LYS	CB-CA-C	-5.24	99.99	110.42
1	A	362	ARG	N-CA-C	5.24	117.22	108.99
1	A	965	PHE	N-CA-C	5.20	119.61	113.16
1	A	523	TYR	N-CA-C	5.18	117.88	107.41
1	A	803	VAL	CA-C-N	5.15	129.71	122.09
1	A	803	VAL	C-N-CA	5.15	129.71	122.09
1	A	192	ASP	CA-C-N	5.14	124.45	118.85
1	A	192	ASP	C-N-CA	5.14	124.45	118.85
1	A	545	ALA	CA-C-N	-5.12	113.94	122.64
1	A	545	ALA	C-N-CA	-5.12	113.94	122.64
1	A	283	GLY	CA-C-N	-5.08	114.94	122.41
1	A	283	GLY	C-N-CA	-5.08	114.94	122.41
1	A	285	THR	CA-C-N	5.08	125.32	119.83
1	A	285	THR	C-N-CA	5.08	125.32	119.83
1	A	377	THR	N-CA-C	5.08	116.58	108.41
1	A	1060	ASN	N-CA-C	-5.07	102.28	110.14
1	A	522	ASN	CB-CA-C	-5.05	101.86	112.82
1	A	840	GLN	N-CA-C	-5.04	105.87	111.36
1	A	709	TYR	N-CA-C	5.04	119.52	113.17
1	A	381	VAL	N-CA-C	5.03	115.21	107.77
1	A	808	LYS	N-CA-C	-5.01	107.02	114.64

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 (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	6820	0	6825	491	0
2	A	35	0	30	3	0
3	A	13	0	0	2	0
All	All	6868	0	6855	491	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 36.

All (491) 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:274:VAL:CG2	1:A:277:ARG:HB2	1.91	0.99
1:A:756:LYS:HD2	1:A:758:ASP:CB	1.91	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:ASN:HD21	1:A:1062:GLU:HB2	1.24	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: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:527:ILE:CG2	1:A:528:ALA:N	2.25	0.86
1:A:1060:ASN:ND2	1:A:1062:GLU:HB2	1.91	0.85
1:A:1090:LEU:O	1:A:1090:LEU:HD12	1.76	0.84
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:163:THR:HG22	1:A:177:ARG:HH12	1.43	0.82
1:A:1043:THR:HG21	1:A:1046:GLU:H	1.41	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:HD13	1:A:1042:LEU:H	1.47	0.79
1:A:737:GLN:O	1:A:741:MET:HG3	1.83	0.79
1:A:225:HIS:N	1:A:225:HIS:HD1	1.81	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:486:GLN:HG2	1:A:487:ILE:N	1.99	0.77
1:A:1035:LEU:HD12	1:A:1048:ILE:CD1	2.12	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

Continued on next page...

Continued from previous page...

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: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:1008:LYS:O	1:A:1012:ILE:HG13	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:210:TYR:CE1	1:A:211:LEU:HG	2.23	0.74
1:A:1043:THR:CG2	1:A:1046:GLU:N	2.51	0.74
1:A:1087:PHE:HD1	1:A:1090:LEU:HD23	1.52	0.74
1:A:628:MET:HE3	1:A:1030:LEU:HD21	1.70	0.73
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:275:CYS:HB2	1:A:823:LEU:HD22	1.71	0.71
1:A:1091:VAL:HG12	1:A:1091:VAL:O	1.88	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:842:MET:HE2	1:A:871:SER:HB3	1.71	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:176:THR:HG23	1:A:674:ASP:HB2	1.73	0.69
1:A:1086:TRP:O	1:A:1087:PHE:HB3	1.91	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:892:GLN:O	1:A:903:LYS:HE3	1.95	0.67
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.58	0.67
1:A:274:VAL:HG23	1:A:274:VAL:O	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:GLN:HG2	1:A:1072:ILE:CD1	2.25	0.67
1:A:224:ILE:C	1:A:225:HIS:HD1	2.03	0.67
1:A:171:ASP:OD1	1:A:472:ARG:NH2	2.22	0.66
1:A:1043:THR:HB	1:A:1047:ASP:H	1.59	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:366:ARG:NH1	1:A:519:LEU:HB2	2.10	0.66
1:A:1081:THR:O	1:A:1085:ASN:ND2	2.29	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:699:LEU:O	1:A:703:ILE:HG13	1.97	0.65
1:A:1087:PHE:CD1	1:A:1090:LEU:HD23	2.31	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:1029:ILE:HD11	1:A:1033:MET:HE3	1.79	0.64
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: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:213:LYS:HG2	1:A:214:LYS:N	2.11	0.63
1:A:1043:THR:HG22	1:A:1045:LYS:H	1.63	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:1086:TRP:CE3	1:A:1087:PHE:N	2.67	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:1049:GLU:O	1:A:1050:TYR:C	2.43	0.62
1:A:271:VAL:HG23	1:A:282:VAL:HG12	1.81	0.62
1:A:1085:ASN:O	1:A:1088:LEU:HG	2.00	0.62
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.81	0.62
1:A:737:GLN:HB3	1:A:741:MET:HE3	1.82	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:MET:HE1	1:A:1009:PHE:CD1	2.34	0.61
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:287:ILE:HD12	1:A:288:LYS:N	2.15	0.61
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:202:VAL:HG12	1:A:203:THR:N	2.15	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:1090:LEU:HD12	1:A:1090:LEU:C	2.27	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:217:ASN:ND2	1:A:219:CYS:HB3	2.04	0.59
1:A:1011:ASP:O	1:A:1015:LYS:HD3	2.02	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:874:ASP:O	1:A:875:LYS:C	2.46	0.59
1:A:1090:LEU:C	1:A:1091:VAL:HG23	2.28	0.59
1:A:225:HIS:O	1:A:306:VAL:HG23	2.03	0.59
1:A:705:GLN:NE2	1:A:839:ARG:HD3	2.18	0.58
1:A:796:LEU:HG	1:A:815:PHE:CE2	2.37	0.58
1:A:798:ILE:N	1:A:798:ILE:HD12	2.18	0.58
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.02	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:895:THR:OG1	1:A:903:LYS:NZ	2.36	0.58
1:A:1024:THR:HG23	1:A:1055:LEU:CD1	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:233:ILE:HG22	1:A:235:VAL:HG22	1.87	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
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: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:1043:THR:HG21	1:A:1046:GLU:N	2.16	0.57
1:A:810:PRO:HB3	1:A:833:LYS:CB	2.34	0.57
1:A:145:GLU:OE2	1:A:145:GLU:C	2.48	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:202:VAL:CG1	1:A:203:THR:N	2.68	0.56
1:A:225:HIS:N	1:A:225:HIS:ND1	2.44	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: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: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:901:ALA:O	1:A:902:PHE:CG	2.58	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: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:965:PHE:O	1:A:966:GLY:C	2.49	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:THR:C	1:A:1045:LYS:H	2.15	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: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:HD13	1:A:1042:LEU:N	2.18	0.54
1:A:220:ILE:O	1:A:235:VAL:N	2.37	0.54
1:A:997:THR:CG2	1:A:1001:LYS:HB3	2.31	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:735:GLN:O	1:A:739:ILE:HG12	2.09	0.53
1:A:804:MET:CG	2:A:1:980:H29	2.38	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: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: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:HG23	1:A:370:ILE:O	2.08	0.52
1:A:576:TRP:CE2	1:A:579:ARG:HD2	2.44	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:804:MET:HE1	1:A:831:ILE:HD13	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:475:LEU:HD23	1:A:476:ARG:N	2.25	0.52
1:A:999:GLY:O	1:A:1000:LYS:C	2.53	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:892:GLN:OE1	1:A:892:GLN:HA	2.09	0.51
1:A:268:GLN:OE1	1:A:268:GLN:HA	2.09	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:373:LEU:O	1:A:374:PRO:C	2.52	0.51
1:A:221:PHE:HA	1:A:233:ILE:O	2.11	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:780:PRO:O	1:A:781:GLU:C	2.55	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:1003:SER:HB2	1:A:1004:PRO:CD	2.42	0.50
1:A:798:ILE:HD12	1:A:798:ILE:H	1.76	0.50
1:A:249:PHE:CE1	1:A:268:GLN:CD	2.90	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:899:THR:OG1	1:A:900:GLY:N	2.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:890:LYS:HG2	1:A:893:GLN:OE1	2.13	0.48
1:A:1086:TRP:HE3	1:A:1087:PHE:N	2.10	0.48
1:A:366:ARG:HH12	1:A:519:LEU:HD22	1.76	0.48
1:A:422:ASP:HB3	1:A:599:GLY:O	2.14	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:891:ILE:HD13	1:A:910:TRP:CD2	2.49	0.48
1:A:210:TYR:HD2	1:A:859:SER:O	1.97	0.47
1:A:779:LEU:HD12	1:A:780:PRO:CD	2.35	0.47
1:A:1086:TRP:O	1:A:1087:PHE:CB	2.60	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:842:MET:CE	1:A:871:SER:HB3	2.43	0.47
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.14	0.47
1:A:281:LEU:C	1:A:282:VAL:HG13	2.38	0.47
1:A:150:PHE:HB2	1:A:319:ARG:NH1	2.30	0.47
1:A:232:THR:HG22	1:A:233:ILE:N	2.28	0.47
1:A:274:VAL:CG2	1:A:279:GLU:HB3	2.45	0.47
1:A:576:TRP:CD2	1:A:579:ARG:HD2	2.49	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:552:ARG:HH11	1:A:552:ARG:HD2	1.57	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ASP:OD2	1:A:784:ARG:NE	2.47	0.46
1:A:1085:ASN:HA	1:A:1088:LEU:CD1	2.44	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
1:A:470:ASP:CB	1:A:476:ARG:HH21	2.26	0.46
1:A:743:GLN:CG	1:A:876:ILE:CD1	2.93	0.46
1:A:756:LYS:N	1:A:757:TYR:CA	2.75	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:1001:LYS:CG	1:A:1002:THR:N	2.78	0.46
1:A:175:PHE:HD1	1:A:178:ARG:HH22	1.62	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:1049:GLU:O	1:A:1052:ARG:N	2.43	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:390:GLY:C	1:A:392:GLN:H	2.24	0.46
1:A:953:MET:O	1:A:960:LEU:HD12	2.16	0.46
1:A:468:LEU:HD23	1:A:468:LEU:HA	1.68	0.46
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.46	0.46
1:A:693:HIS:HE2	1:A:786:PRO:HA	1.81	0.46
1:A:731:ASP:HB3	1:A:735:GLN:HE21	1.81	0.46
1:A:274:VAL:CG2	1:A:274:VAL:O	2.61	0.45
1:A:674:ASP:C	1:A:674:ASP:OD1	2.58	0.45
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.16	0.45
1:A:287:ILE:HA	1:A:290:PHE:CD1	2.51	0.45
1:A:756:LYS:HB2	1:A:757:TYR:C	2.41	0.45
1:A:845:LEU:HD12	1:A:869:CYS:HB3	1.98	0.45
1:A:865:LEU:HD23	1:A:961:PHE:CD2	2.51	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:861:ASP:C	1:A:862:LEU:HD22	2.42	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:756:LYS:CB	1:A:758:ASP:CG	2.89	0.45
1:A:587:LYS:HE2	1:A:587:LYS:HB3	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:MET:HE1	1:A:831:ILE:CD1	2.47	0.45
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.75	0.45
1:A:281:LEU:C	1:A:282:VAL:CG1	2.90	0.45
1:A:647:LYS:HA	1:A:647:LYS:HD2	1.78	0.44
1:A:220:ILE:N	1:A:235:VAL:O	2.39	0.44
1:A:1043:THR:HG22	1:A:1045:LYS:N	2.31	0.44
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.16	0.44
1:A:733:THR:C	1:A:737:GLN:HE21	2.25	0.44
1:A:887:THR:HG22	1:A:889:ALA:N	2.32	0.44
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: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:1048:ILE:O	1:A:1051:ILE:HG22	2.18	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:1049:GLU:CD	1:A:1052:ARG:CZ	2.91	0.43
1:A:199:HIS:O	1:A:199:HIS:HD2	2.00	0.43
1:A:657:LEU:HD23	1:A:657:LEU:HA	1.90	0.43
1:A:865:LEU:H	1:A:935:TYR:HH	1.61	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:842:MET:HE2	1:A:871:SER:CB	2.46	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:213:LYS:C	1:A:215:ILE:N	2.74	0.43
1:A:274:VAL:CG1	1:A:292:TRP:CD1	3.01	0.43
1:A:514:MET:HE2	1:A:514:MET:HB2	1.70	0.43
1:A:552:ARG:HH21	1:A:581:GLU:CD	2.27	0.43
1:A:576:TRP:O	1:A:579:ARG:CD	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:A:862:LEU:N	2.34	0.43
1:A:945:GLY:O	1:A:985:PHE:HA	2.19	0.43
1:A:981:GLU:C	1:A:982:ARG:HD3	2.43	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:370:ILE:HD12	1:A:514:MET:HE2	2.01	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
1:A:589:TYR:CD2	1:A:593:PHE:HE1	2.37	0.42
1:A:928:PHE:CD2	1:A:928:PHE:C	2.96	0.42
1:A:271:VAL:CG2	1:A:272:LEU:N	2.81	0.42
1:A:402:LYS:HB3	1:A:403:PRO:CD	2.49	0.42
1:A:823:LEU:HD12	1:A:823:LEU:HA	1.86	0.42
1:A:1085:ASN:HA	1:A:1088:LEU:HD11	2.02	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:663:LEU:O	1:A:666:ALA:HB3	2.20	0.42
1:A:995:MET:CE	1:A:1009:PHE:CD1	3.01	0.42
1:A:1086:TRP:CZ3	1:A:1090:LEU:HD22	2.54	0.42
1:A:1087:PHE:HA	1:A:1090:LEU:HB2	2.00	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:889:ALA:HB2	1:A:949:ASN:HB3	2.02	0.41
1:A:904:ASP:O	1:A:905:GLU:HB2	2.20	0.41
1:A:948:HIS:O	1:A:949:ASN:C	2.62	0.41
1:A:518:ILE:HD12	1:A:520:LEU:HD13	2.02	0.41
1:A:628:MET:CE	1:A:1030:LEU:HD21	2.47	0.41
1:A:862:LEU:N	1:A:862:LEU:CD2	2.83	0.41
1:A:902:PHE:C	1:A:903:LYS:HG2	2.40	0.41
1:A:388:GLN:HG2	1:A:393:VAL:HG22	2.03	0.41
1:A:865:LEU:N	1:A:935:TYR:HH	2.17	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PHE:CD2	1:A:319:ARG:HD3	2.56	0.41
1:A:756:LYS:HB3	1:A:758:ASP:CG	2.45	0.41
1:A:1085:ASN:O	1:A:1086:TRP:C	2.64	0.41
1:A:192:ASP:HA	1:A:193:PRO:HD3	1.91	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: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: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:214:LYS:HZ2	1:A:297:LEU:HA	1.86	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:936:CYS:SG	1:A:985:PHE:HD1	2.44	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
1:A:886:THR:HG22	1:A:887:THR:N	2.36	0.40
1:A:1060:ASN:ND2	1:A:1062:GLU:CB	2.75	0.40
1:A:729:LEU:HD23	1:A:729:LEU:HA	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%)	16 40

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%)	694 (92%)	59 (8%)	11 32

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	168	VAL
1	A	181	VAL
1	A	185	MET
1	A	213	LYS
1	A	217	ASN
1	A	225	HIS
1	A	235	VAL
1	A	252	MET
1	A	272	LEU
1	A	273	ARG
1	A	281	LEU
1	A	287	ILE
1	A	301	GLU
1	A	307	LEU
1	A	381	VAL
1	A	395	CYS
1	A	421	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	524	CYS
1	A	552	ARG
1	A	587	LYS
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	628	MET
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	707	ARG
1	A	717	LEU
1	A	751	SER
1	A	752	LEU
1	A	753	SER
1	A	759	VAL
1	A	798	ILE
1	A	823	LEU
1	A	833	LYS
1	A	838	LEU
1	A	843	LEU
1	A	848	LEU
1	A	890	LYS
1	A	896	VAL
1	A	907	LEU
1	A	918	GLU
1	A	939	THR
1	A	957	THR
1	A	985	PHE
1	A	1001	LYS
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	1089	HIS
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	199	HIS
1	A	304	HIS
1	A	432	GLN
1	A	549	ASN
1	A	634	ASN
1	A	646	GLN
1	A	705	GLN
1	A	708	HIS
1	A	737	GLN
1	A	743	GLN
1	A	834	HIS
1	A	908	ASN
1	A	962	HIS
1	A	1060	ASN
1	A	1083	GLN
1	A	1085	ASN

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 oligosaccharides 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	-	37,39,39	3.14	12 (32%)	46,56,56	3.31	20 (43%)

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	-	-	9/20/38/38	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	980	C24-N25	-8.68	1.28	1.47
2	A	1	980	C29-N28	-7.53	1.33	1.47
2	A	1	980	C27-N28	-6.99	1.34	1.47
2	A	1	980	C31-N28	6.96	1.45	1.35
2	A	1	980	C20-N23	4.94	1.43	1.33
2	A	1	980	C12-N11	-4.34	1.39	1.46
2	A	1	980	C3-C2	4.11	1.43	1.36
2	A	1	980	C30-N25	-3.80	1.36	1.46
2	A	1	980	C26-N25	-3.79	1.36	1.46
2	A	1	980	C16-N11	-3.48	1.40	1.46
2	A	1	980	C10-N11	2.92	1.44	1.37
2	A	1	980	C3-S4	-2.70	1.72	1.74

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	980	C2-C3-S4	-12.93	106.41	113.50
2	A	1	980	C5-S4-C3	12.04	99.06	92.12
2	A	1	980	C6-N7-C8	5.07	121.87	116.19
2	A	1	980	C6-C5-S4	-4.99	106.81	112.41
2	A	1	980	C17-C22-N21	-3.70	118.39	124.28
2	A	1	980	N9-C8-N7	-3.65	119.13	125.13
2	A	1	980	N21-C20-N19	-3.63	120.83	124.54
2	A	1	980	C22-N21-C20	3.23	121.97	116.29
2	A	1	980	C10-N9-C8	2.76	122.39	115.92
2	A	1	980	O32-C31-N28	-2.72	118.36	121.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	980	C17-C18-N19	-2.64	120.08	124.28
2	A	1	980	C26-C27-N28	2.55	115.49	110.42
2	A	1	980	C17-C8-N7	2.49	121.52	117.40
2	A	1	980	C22-C17-C18	2.39	118.37	114.73
2	A	1	980	C18-N19-C20	2.30	120.35	116.29
2	A	1	980	C5-C10-N9	-2.26	119.64	122.33
2	A	1	980	N23-C20-N19	2.21	119.69	117.40
2	A	1	980	C30-C29-N28	2.14	114.67	110.42
2	A	1	980	C29-N28-C27	2.11	116.98	112.68
2	A	1	980	N23-C20-N21	2.01	119.48	117.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	980	N25-C24-C3-C2
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-N7
2	A	1	980	C18-C17-C8-N9
2	A	1	980	C22-C17-C8-N9
2	A	1	980	N28-C31-C33-O36
2	A	1	980	O32-C31-C33-C35

There are no ring outliers.

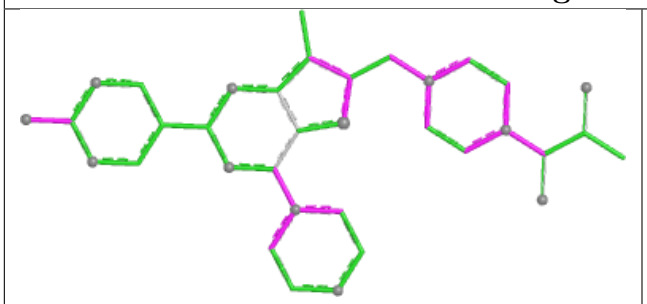
1 monomer is involved in 3 short contacts:

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

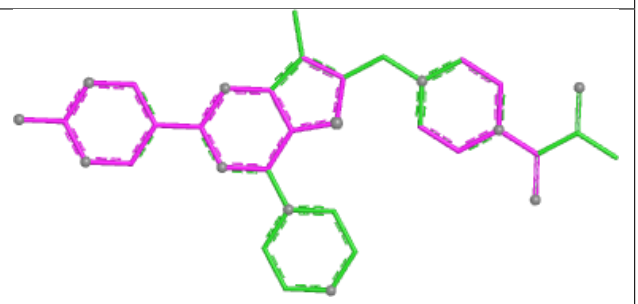
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

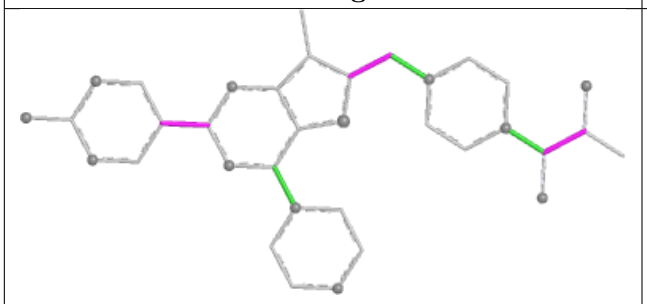
Ligand 980 A 1



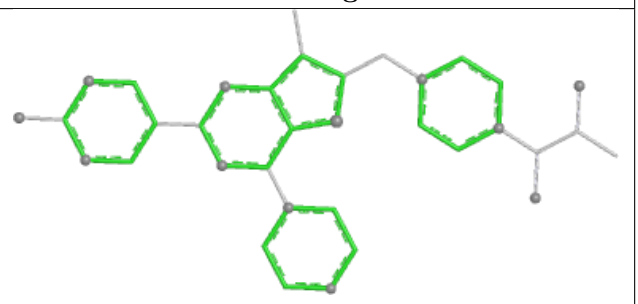
Bond lengths



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	845/966 (87%)	0.06	24 (2%) 55 47	35, 83, 146, 215	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	752	LEU	4.7
1	A	755	GLU	4.7
1	A	1088	LEU	3.1
1	A	807	LYS	3.0
1	A	513	SER	2.9
1	A	756	LYS	2.8
1	A	757	TYR	2.7
1	A	1086	TRP	2.7
1	A	779	LEU	2.5
1	A	1048	ILE	2.4
1	A	530	PRO	2.4
1	A	806	SER	2.3
1	A	1091	VAL	2.3
1	A	873	GLY	2.3
1	A	523	TYR	2.2
1	A	435	CYS	2.2
1	A	526	PRO	2.1
1	A	898	ASN	2.1
1	A	897	GLY	2.1
1	A	902	PHE	2.1
1	A	1087	PHE	2.1
1	A	287	ILE	2.1
1	A	489	GLY	2.1
1	A	751	SER	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 oligosaccharides in this entry.

6.4 Ligands (i)

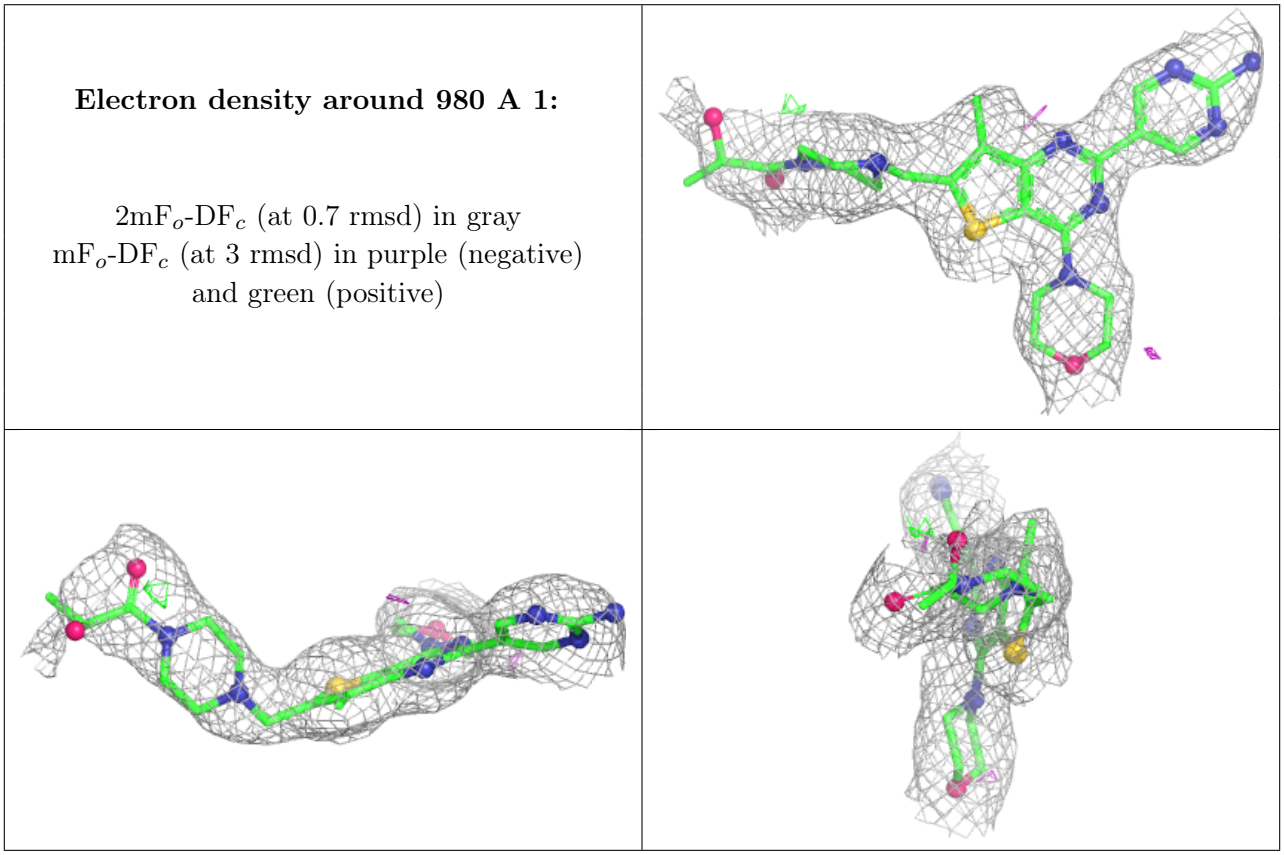
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	980	A	1	35/35	0.92	0.11	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.

Electron density around 980 A 1:

$2mF_o$-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 (i)

There are no such residues in this entry.