Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 11:36 AM EDT

PDB ID	:	3CSF
Title	:	Crystal structure of PI3K p110gamma catalytical domain in complex with organoruthenium inhibitor DW2
Authors	:	Xie, P.; Marmorstein, R.
Deposited on	:	2008-04-09
Resolution	:	2.80 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:

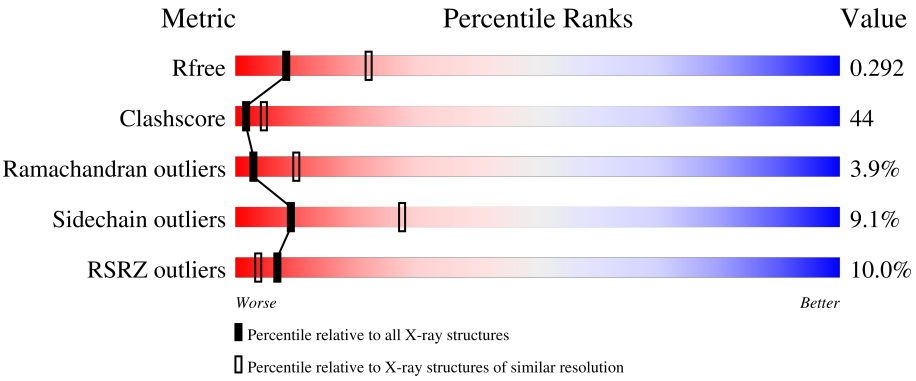
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	9%, 41%, 38%, 6%, 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6938 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.

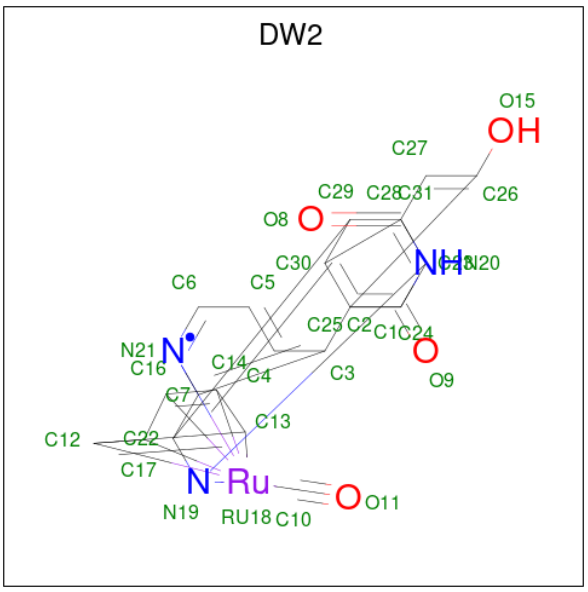
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	839	6801	4369	1159	1238	35	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 RU-PYRIDOCARBAZOLE-2 (three-letter code: DW2) (formula: $C_{23}H_{13}N_3O_4Ru$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Ru	0	0
			31	23	3	4	1		

- Molecule 3 is water.

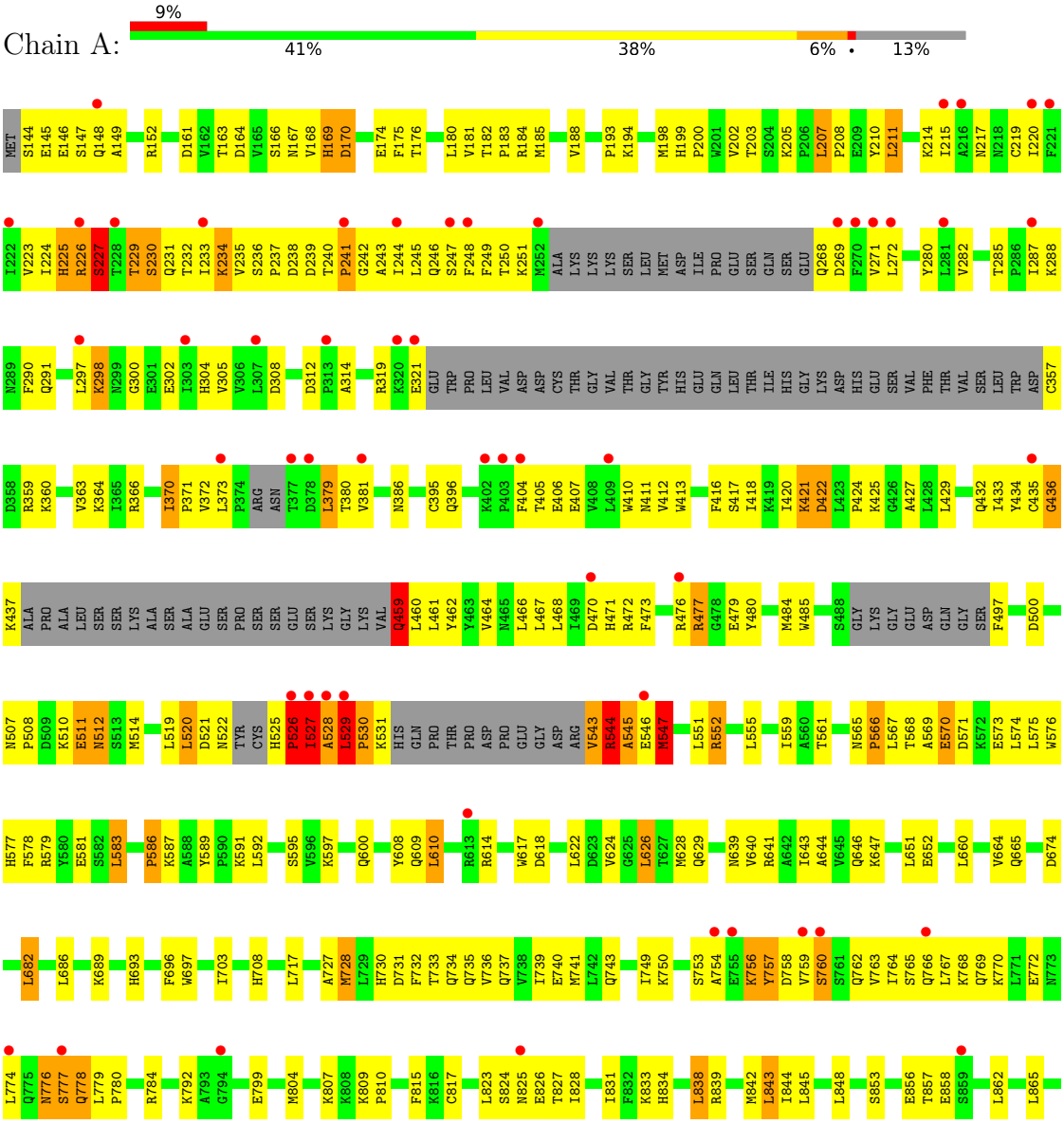
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		

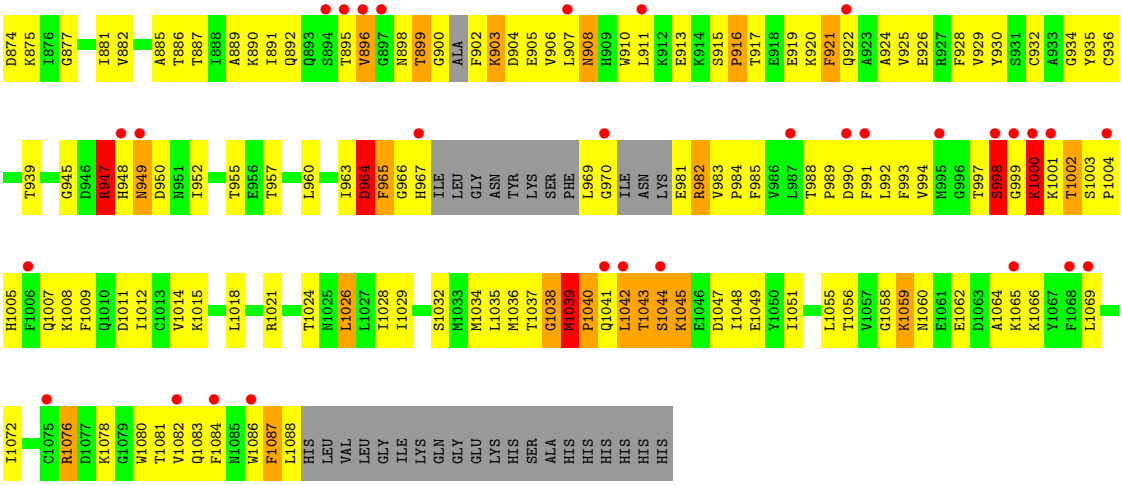
3 Residue-property plots (i)

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:




D874 K875 I876 G877 I881 V882 A885 T886 T887 I888 A889 K890 I891 Q892 Q893 S894 T895 V896 G897 N898 T899 G900 ALA F902 K903 D904 E905 V906 L907 N908 H909 W910 L911 K912 E913 K914 S915 P916 T917 E918 E919 K920 F921 Q922 A923 A924 V925 E926 R927 F928 V929 Y930 S931 C932 A933 G934 Y935 C936
T939 G945 D946 R947 H948 N949 D950 N951 I952 T955 E956 T957 L960 I963 D964 F965 G966 H967 ILE LEU GLY ASN TYR LYS SER PHE L969 G970 ILE ASN LYS E981 R982 V983 P984 F985 V986 L987 T988 P989 D990 F991 L992 F993 V994 M995 G996 T997 S998 G999 K1000 K1001 T1002 S1003 P1004
H1005 F1006 Q1007 K1008 F1009 Q1010 D1011 I1012 C1013 V1014 K1015 L1018 R1021 T1024 N1025 L1026 L1027 I1028 I1029 S1032 M1033 M1034 L1035 M1036 T1037 G1038 M1039 P1040 Q1041 L1042 T1043 S1044 K1045 E1046 D1047 I1048 E1049 Y1050 I1051 L1055 T1056 V1057 G1058 K1059 N1060 E1061 E1062 D1063 A1064 K1065 K1066 Y1067 F1068 L1069
I1072 C1075 R1076 D1077 K1078 G1079 W1080 T1081 V1082 Q1083 F1084 N1085 W1086 F1087 L1088 HIS LEU VAL 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	143.63Å 68.08Å 106.27Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 40.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (50.00-2.80) 93.0 (40.91-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.287 0.257 , 0.292	Depositor DCC
R_{free} test set	2457 reflections (9.90%)	wwPDB-VP
Wilson B-factor (Å^2)	69.9	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 73.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6938	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% 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: DW2

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	0.58	3/6944 (0.0%)	0.86	22/9387 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	756	LYS	CB-CG	-10.78	1.23	1.52
1	A	756	LYS	CA-CB	-8.46	1.35	1.53
1	A	530	PRO	N-CD	-6.62	1.38	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	756	LYS	CA-CB-CG	16.95	150.68	113.40
1	A	529	LEU	C-N-CD	-15.84	85.74	120.60
1	A	459	GLN	O-C-N	-10.55	105.82	122.70
1	A	528	ALA	N-CA-C	9.73	137.26	111.00
1	A	756	LYS	N-CA-CB	9.10	126.98	110.60
1	A	459	GLN	C-N-CA	8.55	143.07	121.70
1	A	526	PRO	O-C-N	7.01	133.91	122.70
1	A	459	GLN	CA-C-N	6.92	132.42	117.20
1	A	896	VAL	CB-CA-C	-6.68	98.71	111.40
1	A	526	PRO	CA-C-N	-6.28	103.39	117.20
1	A	269	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	998	SER	O-C-N	6.10	133.57	123.20
1	A	756	LYS	N-CA-C	-6.05	94.66	111.00
1	A	756	LYS	CB-CG-CD	5.95	127.07	111.60
1	A	1004	PRO	O-C-N	5.79	131.96	122.70
1	A	527	ILE	N-CA-C	5.67	126.30	111.00
1	A	547	MET	N-CA-C	-5.66	95.72	111.00
1	A	998	SER	CA-C-N	-5.66	104.88	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	ILE	C-N-CA	-5.50	107.95	121.70
1	A	964	ASP	N-CA-C	5.23	125.11	111.00
1	A	1043	THR	N-CA-C	-5.22	96.91	111.00
1	A	947	ARG	N-CA-C	5.21	125.06	111.00

There are no chirality outliers.

There are no planarity outliers.

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	6801	0	6849	596	0
2	A	31	0	12	3	0
3	A	106	0	0	15	0
All	All	6938	0	6861	596	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 44.

All (596) 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:988:THR:CG2	1:A:989:PRO:HD2	1.46	1.46
1:A:379:LEU:HG	1:A:435:CYS:SG	1.81	1.20
1:A:988:THR:CG2	1:A:989:PRO:CD	2.21	1.16
1:A:370:ILE:HG21	1:A:373:LEU:HG	1.26	1.14
1:A:988:THR:HG23	1:A:989:PRO:CD	1.79	1.11
1:A:511:GLU:HG2	1:A:512:ASN:HD22	0.96	1.10
1:A:988:THR:HG22	1:A:989:PRO:HD2	1.33	1.08
1:A:896:VAL:HG13	1:A:903:LYS:HE2	1.33	1.08
1:A:899:THR:HG22	1:A:900:GLY:H	1.13	1.08
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.30	1.08
1:A:900:GLY:HA3	1:A:902:PHE:N	1.69	1.07
1:A:982:ARG:HH11	1:A:982:ARG:HG3	1.21	1.04
1:A:988:THR:HG23	1:A:989:PRO:HD2	1.07	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:GLU:HG2	1:A:512:ASN:ND2	1.75	1.01
1:A:181:VAL:HG13	1:A:185:MET:CE	1.89	1.00
1:A:181:VAL:HG13	1:A:185:MET:HE3	1.39	1.00
1:A:473:PHE:O	1:A:526:PRO:HB3	1.61	1.00
1:A:1000:LYS:HA	1:A:1076:ARG:NH2	1.79	0.98
1:A:1076:ARG:HG3	1:A:1076:ARG:HH11	1.22	0.98
1:A:1043:THR:CG2	1:A:1047:ASP:H	1.75	0.97
1:A:1000:LYS:HD3	1:A:1000:LYS:N	1.79	0.96
1:A:568:THR:HG22	1:A:570:GLU:H	1.30	0.96
1:A:1036:MET:HG2	1:A:1042:LEU:CD1	1.95	0.96
1:A:1014:VAL:HG11	1:A:1065:LYS:HE3	1.49	0.94
1:A:900:GLY:CA	1:A:902:PHE:N	2.30	0.94
1:A:997:THR:HG22	1:A:998:SER:H	1.31	0.94
1:A:370:ILE:HD13	1:A:371:PRO:HD2	1.49	0.94
1:A:988:THR:HG22	1:A:989:PRO:CD	1.93	0.93
1:A:231:GLN:HG3	1:A:232:THR:H	1.32	0.93
1:A:234:LYS:O	1:A:234:LYS:HD3	1.69	0.91
1:A:370:ILE:HG21	1:A:373:LEU:CG	1.98	0.91
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.51	0.91
1:A:916:PRO:HG2	1:A:917:THR:H	1.35	0.91
1:A:1039:MET:O	1:A:1041:GLN:N	2.04	0.90
1:A:370:ILE:CG2	1:A:373:LEU:HG	2.02	0.89
1:A:1038:GLY:C	1:A:1040:PRO:HD3	1.92	0.89
1:A:246:GLN:O	1:A:250:THR:HG22	1.73	0.87
1:A:210:TYR:CD1	1:A:211:LEU:HD23	2.09	0.87
1:A:887:THR:HG22	1:A:889:ALA:H	1.39	0.86
1:A:1002:THR:CG2	1:A:1007:GLN:HE21	1.87	0.86
1:A:760:SER:O	1:A:763:VAL:HG12	1.76	0.85
1:A:379:LEU:HD21	1:A:404:PHE:HD2	1.38	0.85
1:A:410:TRP:HB3	1:A:412:VAL:HG12	1.56	0.85
1:A:1036:MET:HG2	1:A:1042:LEU:HD12	1.58	0.85
1:A:900:GLY:C	1:A:902:PHE:N	2.30	0.85
1:A:899:THR:HG22	1:A:900:GLY:N	1.92	0.84
1:A:922:GLN:O	1:A:926:GLU:HG2	1.76	0.84
1:A:1011:ASP:OD2	1:A:1015:LYS:HE3	1.78	0.84
1:A:477:ARG:HD2	1:A:522:ASN:H	1.40	0.84
1:A:964:ASP:O	1:A:966:GLY:N	2.11	0.84
1:A:1060:ASN:HD21	1:A:1062:GLU:HB2	1.42	0.83
1:A:1002:THR:HG21	1:A:1007:GLN:HE21	1.41	0.83
1:A:895:THR:HB	1:A:903:LYS:HE3	1.60	0.83
1:A:433:ILE:HD12	1:A:484:MET:HE1	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:LYS:O	1:A:772:GLU:HG2	1.79	0.82
1:A:896:VAL:CG1	1:A:903:LYS:HE2	2.09	0.82
1:A:960:LEU:HD11	1:A:991:PHE:HE2	1.43	0.82
1:A:741:MET:HE1	1:A:778:GLN:HB3	1.60	0.82
1:A:1043:THR:HG22	1:A:1047:ASP:CG	2.00	0.82
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.62	0.82
1:A:1078:LYS:HD3	3:A:1132:HOH:O	1.80	0.81
1:A:373:LEU:HD13	1:A:404:PHE:HZ	1.46	0.81
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.62	0.81
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.61	0.81
1:A:207:LEU:HD23	1:A:208:PRO:HD2	1.63	0.81
1:A:629:GLN:HG2	1:A:1029:ILE:HD13	1.63	0.81
1:A:997:THR:O	1:A:998:SER:HB3	1.80	0.80
1:A:917:THR:HB	1:A:919:GLU:OE1	1.80	0.80
1:A:185:MET:HE2	1:A:321:GLU:CD	2.02	0.80
1:A:217:ASN:HD22	1:A:219:CYS:HB2	1.47	0.79
1:A:900:GLY:O	1:A:902:PHE:CG	2.35	0.79
1:A:148:GLN:O	1:A:152:ARG:HG3	1.81	0.79
1:A:895:THR:C	1:A:903:LYS:HZ1	1.87	0.78
1:A:543:VAL:C	1:A:544:ARG:HD3	2.02	0.78
1:A:1021:ARG:HE	1:A:1056:THR:CG2	1.97	0.78
1:A:380:THR:HG22	1:A:437:LYS:O	1.83	0.78
1:A:900:GLY:O	1:A:902:PHE:CD1	2.36	0.78
1:A:757:TYR:H	1:A:757:TYR:HD2	1.29	0.77
1:A:224:ILE:HD13	1:A:233:ILE:HD13	1.65	0.77
1:A:760:SER:OG	1:A:762:GLN:HB3	1.83	0.77
1:A:1034:MET:HG3	1:A:1039:MET:HE3	1.66	0.77
1:A:227:SER:HB2	3:A:1144:HOH:O	1.83	0.77
1:A:526:PRO:O	1:A:527:ILE:HG23	1.83	0.77
1:A:373:LEU:HD13	1:A:404:PHE:CZ	2.19	0.77
1:A:484:MET:HE1	1:A:514:MET:HG2	1.68	0.76
1:A:1042:LEU:HD22	1:A:1042:LEU:C	2.06	0.76
1:A:304:HIS:HB2	1:A:823:LEU:HD11	1.66	0.76
1:A:1043:THR:HG23	1:A:1043:THR:O	1.83	0.76
1:A:583:LEU:HD23	1:A:610:LEU:HD22	1.68	0.76
1:A:370:ILE:HD13	1:A:371:PRO:CD	2.16	0.76
1:A:1042:LEU:C	1:A:1042:LEU:CD2	2.53	0.76
1:A:379:LEU:HD21	1:A:404:PHE:CD2	2.21	0.75
1:A:462:TYR:HB2	1:A:484:MET:HE3	1.67	0.75
1:A:547:MET:HB3	1:A:552:ARG:NH1	2.01	0.75
1:A:982:ARG:HH11	1:A:982:ARG:CG	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1058:GLY:O	1:A:1059:LYS:O	2.05	0.74
1:A:217:ASN:ND2	1:A:219:CYS:HB2	2.02	0.73
1:A:380:THR:HG22	1:A:437:LYS:C	2.09	0.73
1:A:462:TYR:CB	1:A:484:MET:HE3	2.18	0.73
1:A:1065:LYS:O	1:A:1069:LEU:HD23	1.88	0.73
1:A:1076:ARG:HG3	1:A:1076:ARG:NH1	1.99	0.73
1:A:997:THR:HG22	1:A:998:SER:N	2.04	0.72
1:A:1034:MET:HG3	1:A:1039:MET:CE	2.19	0.72
1:A:1078:LYS:HG2	1:A:1082:VAL:HG23	1.71	0.72
1:A:226:ARG:HG2	1:A:226:ARG:HH11	1.53	0.72
1:A:529:LEU:HG	1:A:529:LEU:O	1.89	0.72
1:A:181:VAL:HG13	1:A:185:MET:HE1	1.72	0.72
1:A:988:THR:HG22	1:A:989:PRO:N	2.04	0.72
1:A:526:PRO:C	1:A:527:ILE:HG12	2.10	0.72
1:A:223:VAL:HG12	1:A:225:HIS:CE1	2.25	0.71
1:A:1078:LYS:CE	1:A:1081:THR:HB	2.19	0.71
1:A:792:LYS:HD2	3:A:1209:HOH:O	1.90	0.71
1:A:899:THR:CG2	1:A:900:GLY:H	1.98	0.71
1:A:312:ASP:OD2	1:A:314:ALA:HB3	1.90	0.70
1:A:1078:LYS:HZ1	1:A:1081:THR:HG22	1.56	0.70
1:A:215:ILE:HD11	1:A:297:LEU:HD11	1.71	0.70
1:A:887:THR:HG21	1:A:950:ASP:HA	1.74	0.70
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.56	0.70
1:A:379:LEU:N	1:A:379:LEU:HD22	2.06	0.70
1:A:739:ILE:O	1:A:743:GLN:HG3	1.91	0.70
1:A:921:PHE:HA	1:A:924:ALA:HB3	1.72	0.69
1:A:210:TYR:CD1	1:A:211:LEU:CD2	2.76	0.69
1:A:576:TRP:CZ3	1:A:579:ARG:HD2	2.27	0.69
1:A:547:MET:HB3	1:A:552:ARG:HH12	1.55	0.69
1:A:843:LEU:HD23	1:A:1039:MET:HE1	1.73	0.69
1:A:1014:VAL:HG11	1:A:1065:LYS:CE	2.23	0.69
1:A:1009:PHE:HE2	1:A:1072:ILE:HD12	1.58	0.68
1:A:1078:LYS:HZ1	1:A:1081:THR:CG2	2.07	0.68
1:A:583:LEU:HD23	1:A:610:LEU:CD2	2.24	0.68
1:A:921:PHE:O	1:A:925:VAL:HG23	1.92	0.68
1:A:1036:MET:HG2	1:A:1042:LEU:HD11	1.73	0.68
1:A:180:LEU:O	1:A:183:PRO:HD2	1.93	0.68
1:A:185:MET:HE2	1:A:321:GLU:OE1	1.94	0.68
1:A:640:VAL:O	1:A:643:ILE:HG12	1.94	0.68
1:A:198:MET:HE2	1:A:282:VAL:CG2	2.24	0.67
1:A:420:ILE:HD13	1:A:522:ASN:HB3	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:ARG:HG2	1:A:1055:LEU:CD2	2.24	0.67
1:A:1014:VAL:CG2	1:A:1069:LEU:HD21	2.24	0.67
1:A:660:LEU:O	1:A:664:VAL:HG23	1.94	0.67
1:A:762:GLN:O	1:A:766:GLN:HG2	1.94	0.67
1:A:583:LEU:CD2	1:A:610:LEU:HD22	2.24	0.67
1:A:211:LEU:HD12	1:A:297:LEU:HD23	1.76	0.67
1:A:1028:ILE:HD12	1:A:1051:ILE:HG23	1.75	0.67
1:A:1043:THR:HG22	1:A:1047:ASP:OD2	1.95	0.67
1:A:960:LEU:CD1	1:A:991:PHE:HE2	2.08	0.66
1:A:235:VAL:HG11	1:A:244:ILE:HD13	1.77	0.66
1:A:180:LEU:C	1:A:183:PRO:HD2	2.15	0.66
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.76	0.66
1:A:1034:MET:O	1:A:1039:MET:HE2	1.96	0.66
1:A:957:THR:HG22	1:A:957:THR:O	1.95	0.65
1:A:241:PRO:HD3	1:A:285:THR:O	1.95	0.65
1:A:1078:LYS:NZ	1:A:1081:THR:CG2	2.60	0.65
1:A:287:ILE:HD12	1:A:288:LYS:N	2.12	0.65
1:A:198:MET:HE2	1:A:282:VAL:HG21	1.78	0.64
1:A:185:MET:CE	1:A:321:GLU:CD	2.65	0.64
1:A:1021:ARG:HG2	1:A:1055:LEU:HD23	1.79	0.64
1:A:357:CYS:O	1:A:421:LYS:HB2	1.98	0.64
1:A:526:PRO:O	1:A:527:ILE:HG12	1.97	0.64
1:A:235:VAL:HG12	1:A:236:SER:N	2.12	0.64
1:A:215:ILE:HD11	1:A:297:LEU:CD1	2.27	0.64
1:A:926:GLU:OE1	1:A:1005:HIS:HE1	1.81	0.64
1:A:1038:GLY:C	1:A:1040:PRO:CD	2.65	0.64
1:A:579:ARG:HG2	1:A:610:LEU:HD11	1.79	0.64
1:A:233:ILE:H	1:A:233:ILE:HD12	1.62	0.63
1:A:1043:THR:HG21	1:A:1047:ASP:H	1.60	0.63
1:A:169:HIS:HD2	1:A:170:ASP:HB3	1.61	0.63
1:A:998:SER:O	1:A:1001:LYS:HG3	1.97	0.63
1:A:766:GLN:O	1:A:770:LYS:HG3	1.98	0.63
1:A:807:LYS:HG2	3:A:1177:HOH:O	1.97	0.63
1:A:928:PHE:CZ	1:A:991:PHE:HD2	2.17	0.63
1:A:1056:THR:HG23	1:A:1056:THR:O	1.98	0.63
1:A:464:VAL:HB	1:A:484:MET:HG2	1.81	0.63
1:A:964:ASP:O	1:A:965:PHE:C	2.36	0.63
1:A:210:TYR:HD1	1:A:211:LEU:CD2	2.10	0.62
1:A:757:TYR:N	1:A:757:TYR:CD2	2.64	0.62
1:A:1000:LYS:N	1:A:1000:LYS:CD	2.58	0.62
1:A:198:MET:HE3	1:A:280:TYR:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:THR:O	1:A:1045:LYS:N	2.31	0.62
1:A:928:PHE:HZ	1:A:991:PHE:HD2	1.47	0.62
1:A:149:ALA:O	1:A:152:ARG:HB2	1.99	0.62
1:A:239:ASP:HB3	1:A:244:ILE:HD11	1.79	0.62
1:A:1009:PHE:CE2	1:A:1072:ILE:HD12	2.35	0.62
1:A:1043:THR:C	1:A:1045:LYS:H	2.03	0.62
1:A:251:LYS:O	1:A:251:LYS:HD3	1.99	0.62
1:A:890:LYS:HZ2	2:A:1:DW2:H131	1.64	0.62
1:A:916:PRO:HG2	1:A:917:THR:N	2.13	0.62
1:A:239:ASP:CB	1:A:244:ILE:HD11	2.30	0.62
1:A:246:GLN:NE2	1:A:246:GLN:HA	2.14	0.62
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.64	0.61
1:A:202:VAL:HG12	1:A:203:THR:N	2.15	0.61
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.35	0.61
1:A:569:ALA:O	1:A:573:GLU:HG3	2.00	0.61
1:A:997:THR:HG23	1:A:1002:THR:N	2.15	0.61
1:A:576:TRP:CH2	1:A:579:ARG:HD2	2.36	0.61
1:A:887:THR:CG2	1:A:950:ASP:HA	2.31	0.61
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.16	0.61
1:A:843:LEU:HD23	1:A:1039:MET:CE	2.31	0.61
1:A:497:PHE:N	1:A:1044:SER:HG	1.99	0.61
1:A:989:PRO:HG2	1:A:1080:TRP:CD1	2.35	0.61
1:A:890:LYS:NZ	2:A:1:DW2:H131	2.15	0.61
1:A:168:VAL:HG13	1:A:170:ASP:H	1.64	0.60
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.82	0.60
1:A:202:VAL:HG11	1:A:285:THR:HG21	1.84	0.60
1:A:916:PRO:CG	1:A:917:THR:H	2.13	0.60
1:A:1078:LYS:HE3	1:A:1082:VAL:N	2.16	0.60
1:A:373:LEU:CD1	1:A:404:PHE:CZ	2.84	0.60
1:A:824:SER:OG	1:A:826:GLU:HG3	2.01	0.60
1:A:198:MET:HE1	1:A:282:VAL:CG1	2.32	0.60
1:A:473:PHE:HB3	1:A:526:PRO:CB	2.32	0.59
1:A:484:MET:CE	1:A:514:MET:HG2	2.32	0.59
1:A:462:TYR:CB	1:A:484:MET:CE	2.80	0.59
1:A:1078:LYS:HE3	1:A:1082:VAL:HG23	1.85	0.59
1:A:223:VAL:HG12	1:A:225:HIS:HE1	1.66	0.59
1:A:233:ILE:HD12	1:A:233:ILE:N	2.18	0.59
1:A:753:SER:HB3	1:A:809:LYS:HG3	1.84	0.59
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.83	0.59
1:A:547:MET:CB	1:A:552:ARG:HH12	2.14	0.59
1:A:1018:LEU:HD23	1:A:1021:ARG:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:ARG:HD3	1:A:544:ARG:N	2.18	0.59
1:A:1043:THR:CG2	1:A:1043:THR:O	2.50	0.59
1:A:380:THR:CG2	1:A:437:LYS:O	2.51	0.58
1:A:543:VAL:O	1:A:544:ARG:HB2	2.03	0.58
1:A:960:LEU:HD11	1:A:991:PHE:CE2	2.31	0.58
1:A:1002:THR:HG22	1:A:1007:GLN:HE21	1.66	0.58
1:A:472:ARG:O	1:A:473:PHE:HB2	2.02	0.58
1:A:891:ILE:HD12	1:A:910:TRP:CD1	2.37	0.58
1:A:181:VAL:CG1	1:A:185:MET:HE3	2.24	0.58
1:A:568:THR:HG22	1:A:570:GLU:N	2.11	0.58
1:A:198:MET:HE3	1:A:280:TYR:CG	2.39	0.58
1:A:886:THR:HG22	1:A:887:THR:N	2.19	0.58
1:A:1002:THR:HG22	1:A:1003:SER:H	1.68	0.58
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.33	0.58
1:A:903:LYS:HD2	1:A:906:VAL:HG22	1.84	0.58
1:A:930:TYR:HE1	1:A:1008:LYS:HE2	1.69	0.58
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.03	0.58
1:A:1028:ILE:CD1	1:A:1051:ILE:HG23	2.33	0.58
1:A:169:HIS:HE1	3:A:1128:HOH:O	1.87	0.58
1:A:198:MET:HE1	1:A:282:VAL:HG11	1.85	0.58
1:A:982:ARG:HG3	1:A:982:ARG:NH1	2.01	0.58
1:A:895:THR:HG22	1:A:903:LYS:NZ	2.18	0.58
1:A:1043:THR:HG23	1:A:1047:ASP:H	1.66	0.58
1:A:982:ARG:CG	1:A:982:ARG:NH1	2.63	0.57
1:A:215:ILE:HD11	1:A:297:LEU:HD21	1.84	0.57
1:A:839:ARG:HA	1:A:842:MET:HE2	1.85	0.57
1:A:1078:LYS:CE	1:A:1082:VAL:HG23	2.35	0.57
1:A:733:THR:O	1:A:737:GLN:HG3	2.03	0.57
1:A:896:VAL:N	1:A:903:LYS:HZ1	2.02	0.57
1:A:1042:LEU:CD2	1:A:1043:THR:C	2.73	0.57
1:A:207:LEU:CD2	1:A:208:PRO:HD2	2.32	0.57
1:A:231:GLN:HG3	1:A:232:THR:N	2.11	0.57
1:A:753:SER:OG	1:A:763:VAL:HG21	2.05	0.57
1:A:1018:LEU:HD21	1:A:1064:ALA:HB3	1.86	0.57
1:A:1000:LYS:HD3	1:A:1000:LYS:H	1.70	0.56
1:A:988:THR:HG21	1:A:1080:TRP:CE3	2.39	0.56
1:A:1026:LEU:O	1:A:1029:ILE:HG22	2.05	0.56
1:A:1078:LYS:CD	1:A:1081:THR:HB	2.35	0.56
1:A:930:TYR:CE1	1:A:1008:LYS:HE2	2.40	0.56
1:A:1024:THR:O	1:A:1028:ILE:HG12	2.05	0.56
1:A:145:GLU:HA	1:A:148:GLN:CD	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.33	0.56
1:A:433:ILE:CD1	1:A:484:MET:HE1	2.31	0.56
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.20	0.56
1:A:421:LYS:HZ2	1:A:527:ILE:HD11	1.71	0.56
1:A:831:ILE:HG13	1:A:881:ILE:HG12	1.87	0.56
1:A:181:VAL:CG1	1:A:185:MET:CE	2.75	0.56
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.35	0.56
1:A:512:ASN:ND2	1:A:512:ASN:N	2.54	0.56
1:A:379:LEU:CG	1:A:435:CYS:SG	2.74	0.56
1:A:736:VAL:O	1:A:740:GLU:HB2	2.05	0.56
1:A:210:TYR:CE1	1:A:211:LEU:HD23	2.40	0.55
1:A:211:LEU:HD11	1:A:298:LYS:HB2	1.88	0.55
1:A:776:ASN:O	1:A:778:GLN:N	2.39	0.55
1:A:874:ASP:OD1	1:A:875:LYS:HG2	2.07	0.55
1:A:1045:LYS:O	1:A:1049:GLU:HG3	2.06	0.55
1:A:579:ARG:HG2	1:A:610:LEU:CD1	2.37	0.55
1:A:215:ILE:HD11	1:A:297:LEU:CD2	2.37	0.55
1:A:890:LYS:HG3	2:A:1:DW2:O11	2.06	0.55
1:A:963:ILE:O	1:A:965:PHE:N	2.38	0.55
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.37	0.55
1:A:1036:MET:CG	1:A:1042:LEU:CD1	2.80	0.55
1:A:1038:GLY:O	1:A:1040:PRO:CD	2.55	0.55
1:A:435:CYS:HB3	1:A:461:LEU:CD1	2.37	0.55
1:A:1008:LYS:O	1:A:1012:ILE:HG12	2.07	0.55
1:A:379:LEU:HD23	1:A:379:LEU:C	2.28	0.55
1:A:765:SER:O	1:A:769:GLN:HG3	2.07	0.55
1:A:224:ILE:N	1:A:224:ILE:HD12	2.22	0.54
1:A:211:LEU:CD1	1:A:297:LEU:HD23	2.36	0.54
1:A:576:TRP:O	1:A:579:ARG:HD3	2.07	0.54
1:A:737:GLN:O	1:A:741:MET:HG3	2.06	0.54
1:A:896:VAL:N	1:A:903:LYS:CE	2.70	0.54
1:A:1060:ASN:ND2	1:A:1062:GLU:HB2	2.17	0.54
1:A:462:TYR:HB3	1:A:484:MET:CE	2.37	0.54
1:A:1043:THR:HG22	1:A:1047:ASP:CB	2.36	0.54
1:A:1078:LYS:CE	1:A:1082:VAL:CG2	2.85	0.54
1:A:223:VAL:CG1	1:A:225:HIS:HE1	2.20	0.54
1:A:544:ARG:O	1:A:545:ALA:CB	2.55	0.54
1:A:764:ILE:O	1:A:768:LYS:HG3	2.08	0.54
1:A:997:THR:HG23	1:A:1002:THR:H	1.70	0.54
1:A:462:TYR:HB3	1:A:484:MET:HE3	1.90	0.54
1:A:892:GLN:O	1:A:896:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.08	0.53
1:A:1084:PHE:O	1:A:1087:PHE:CE1	2.61	0.53
1:A:436:GLY:O	1:A:437:LYS:HG3	2.08	0.53
1:A:583:LEU:CD2	1:A:610:LEU:HD13	2.38	0.53
1:A:220:ILE:HD11	1:A:237:PRO:HG3	1.89	0.53
1:A:249:PHE:CE1	1:A:268:GLN:HA	2.44	0.53
1:A:526:PRO:O	1:A:527:ILE:CG1	2.56	0.53
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.90	0.53
1:A:1032:SER:HB3	1:A:1048:ILE:HG23	1.90	0.53
1:A:1078:LYS:CG	1:A:1082:VAL:HG23	2.37	0.53
1:A:226:ARG:HH11	1:A:226:ARG:CG	2.20	0.53
1:A:467:LEU:O	1:A:476:ARG:HD2	2.09	0.53
1:A:215:ILE:HD12	1:A:215:ILE:N	2.22	0.53
1:A:592:LEU:O	1:A:595:SER:HB2	2.08	0.53
1:A:947:ARG:NH2	1:A:963:ILE:O	2.41	0.53
1:A:1036:MET:CG	1:A:1042:LEU:HD12	2.35	0.53
1:A:381:VAL:HG13	1:A:404:PHE:HB2	1.91	0.53
1:A:144:SER:O	1:A:147:SER:HB3	2.09	0.53
1:A:366:ARG:HH21	1:A:519:LEU:HD22	1.74	0.53
1:A:1062:GLU:O	1:A:1066:LYS:HG3	2.09	0.52
1:A:366:ARG:NH2	1:A:519:LEU:HD22	2.24	0.52
1:A:589:TYR:CD1	1:A:589:TYR:N	2.75	0.52
1:A:395:CYS:SG	1:A:418:ILE:HG13	2.50	0.52
1:A:886:THR:HG22	1:A:887:THR:H	1.73	0.52
1:A:1078:LYS:HE3	1:A:1082:VAL:CG2	2.40	0.52
1:A:168:VAL:CG1	1:A:169:HIS:N	2.73	0.52
1:A:555:LEU:O	1:A:559:ILE:HG12	2.09	0.52
1:A:229:THR:HB	3:A:1113:HOH:O	2.10	0.52
1:A:433:ILE:HD12	1:A:484:MET:CE	2.37	0.52
1:A:693:HIS:O	1:A:696:PHE:HB3	2.09	0.52
1:A:379:LEU:CD2	1:A:404:PHE:HD2	2.19	0.51
1:A:476:ARG:HG3	1:A:480:TYR:OH	2.10	0.51
1:A:484:MET:HE1	1:A:514:MET:CG	2.37	0.51
1:A:561:THR:OG1	1:A:591:LYS:HE2	2.10	0.51
1:A:198:MET:CE	1:A:280:TYR:HB3	2.39	0.51
1:A:244:ILE:HA	1:A:247:SER:OG	2.10	0.51
1:A:905:GLU:HG3	1:A:993:PHE:CE2	2.44	0.51
1:A:568:THR:HB	1:A:571:ASP:OD2	2.10	0.51
1:A:828:ILE:N	1:A:828:ILE:HD12	2.26	0.51
1:A:915:SER:CB	1:A:921:PHE:HB2	2.40	0.51
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LYS:HD3	1:A:297:LEU:HD12	1.93	0.51
1:A:479:GLU:OE1	1:A:479:GLU:HA	2.11	0.51
1:A:566:PRO:O	1:A:567:LEU:HG	2.10	0.51
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.92	0.51
1:A:997:THR:CG2	1:A:1001:LYS:HB2	2.40	0.51
1:A:291:GLN:NE2	1:A:291:GLN:HA	2.25	0.51
1:A:928:PHE:HZ	1:A:991:PHE:CD2	2.26	0.51
1:A:161:ASP:O	1:A:164:ASP:HB3	2.11	0.51
1:A:1078:LYS:HE2	1:A:1082:VAL:HG22	1.92	0.51
1:A:198:MET:HE1	1:A:271:VAL:HG21	1.92	0.51
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.40	0.51
1:A:215:ILE:CD1	1:A:297:LEU:HD21	2.41	0.50
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.76	0.50
1:A:526:PRO:O	1:A:527:ILE:CG2	2.57	0.50
1:A:997:THR:HG23	1:A:1001:LYS:HB2	1.94	0.50
1:A:1014:VAL:HG11	1:A:1065:LYS:CD	2.42	0.50
1:A:1014:VAL:CG2	1:A:1065:LYS:HG3	2.41	0.50
1:A:166:SER:O	1:A:510:LYS:HE3	2.11	0.50
1:A:997:THR:CG2	1:A:1002:THR:N	2.74	0.50
1:A:839:ARG:HA	1:A:842:MET:CE	2.41	0.50
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.92	0.50
1:A:586:PRO:HA	1:A:589:TYR:CE1	2.46	0.50
1:A:689:LYS:HA	1:A:728:MET:HE1	1.92	0.50
1:A:470:ASP:CB	1:A:476:ARG:NH2	2.75	0.50
1:A:198:MET:CE	1:A:282:VAL:HG11	2.41	0.50
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.10	0.50
1:A:777:SER:O	1:A:778:GLN:HG3	2.12	0.50
1:A:1014:VAL:HG21	1:A:1069:LEU:HD21	1.94	0.50
1:A:185:MET:CE	1:A:321:GLU:OE2	2.60	0.50
1:A:202:VAL:CG1	1:A:203:THR:N	2.74	0.50
1:A:526:PRO:CG	1:A:527:ILE:N	2.69	0.50
1:A:233:ILE:H	1:A:233:ILE:CD1	2.25	0.49
1:A:939:THR:OG1	1:A:945:GLY:HA2	2.12	0.49
1:A:379:LEU:C	1:A:379:LEU:CD2	2.80	0.49
1:A:896:VAL:N	1:A:903:LYS:NZ	2.60	0.49
1:A:360:LYS:HE2	1:A:417:SER:HA	1.94	0.49
1:A:697:TRP:CH2	1:A:739:ILE:HD13	2.48	0.49
1:A:753:SER:O	1:A:754:ALA:HB3	2.12	0.49
1:A:1038:GLY:O	1:A:1040:PRO:HD3	2.11	0.49
1:A:287:ILE:HA	1:A:290:PHE:CD1	2.48	0.49
1:A:948:HIS:O	1:A:950:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:ARG:NE	1:A:1056:THR:CG2	2.72	0.49
1:A:810:PRO:HB3	1:A:833:LYS:HB2	1.93	0.49
1:A:896:VAL:HA	1:A:903:LYS:NZ	2.27	0.49
1:A:935:TYR:O	1:A:939:THR:HG22	2.11	0.49
1:A:413:TRP:HD1	3:A:1187:HOH:O	1.96	0.49
1:A:760:SER:HG	1:A:763:VAL:H	1.57	0.49
1:A:1042:LEU:HD23	1:A:1043:THR:N	2.28	0.49
1:A:1078:LYS:HD2	1:A:1081:THR:HB	1.93	0.49
1:A:434:TYR:HD1	1:A:459:GLN:C	2.15	0.49
1:A:911:LEU:HD11	1:A:924:ALA:HB1	1.93	0.49
1:A:370:ILE:HG21	1:A:373:LEU:CD1	2.40	0.48
1:A:425:LYS:HD2	1:A:473:PHE:CE2	2.48	0.48
1:A:547:MET:HE2	1:A:552:ARG:N	2.28	0.48
1:A:379:LEU:HD22	1:A:379:LEU:H	1.74	0.48
1:A:614:ARG:HD2	1:A:618:ASP:OD1	2.14	0.48
1:A:920:LYS:O	1:A:921:PHE:CB	2.60	0.48
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.96	0.48
1:A:473:PHE:HB3	1:A:526:PRO:HB3	1.95	0.48
1:A:895:THR:HG22	1:A:903:LYS:HZ2	1.79	0.48
1:A:1042:LEU:CD2	1:A:1043:THR:N	2.77	0.48
1:A:421:LYS:HZ1	1:A:527:ILE:HD13	1.79	0.48
1:A:1021:ARG:HE	1:A:1056:THR:HG23	1.77	0.48
1:A:1043:THR:C	1:A:1045:LYS:N	2.67	0.48
1:A:589:TYR:HD1	1:A:589:TYR:H	1.61	0.48
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.44	0.48
1:A:589:TYR:N	1:A:589:TYR:HD1	2.11	0.48
1:A:1038:GLY:O	1:A:1040:PRO:HD2	2.14	0.47
1:A:211:LEU:O	1:A:297:LEU:HD21	2.14	0.47
1:A:235:VAL:CG1	1:A:236:SER:N	2.77	0.47
1:A:241:PRO:O	1:A:243:ALA:N	2.48	0.47
1:A:381:VAL:HG12	1:A:435:CYS:HB2	1.96	0.47
1:A:885:ALA:HA	1:A:955:THR:HA	1.96	0.47
1:A:998:SER:O	1:A:1001:LYS:CG	2.62	0.47
1:A:1078:LYS:HE2	1:A:1082:VAL:CG2	2.44	0.47
1:A:319:ARG:HD3	3:A:1199:HOH:O	2.13	0.47
1:A:268:GLN:O	1:A:268:GLN:HG3	2.15	0.47
1:A:753:SER:CB	1:A:809:LYS:HG3	2.43	0.47
1:A:1000:LYS:CA	1:A:1076:ARG:NH2	2.64	0.47
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.62	0.47
1:A:804:MET:CE	1:A:810:PRO:HG2	2.45	0.47
1:A:948:HIS:CE1	1:A:1086:TRP:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:SER:HB3	1:A:1048:ILE:CG2	2.45	0.47
1:A:181:VAL:CG1	1:A:185:MET:HE1	2.43	0.47
1:A:462:TYR:HB2	1:A:484:MET:CE	2.41	0.47
1:A:597:LYS:HD2	1:A:600:GLN:OE1	2.14	0.47
1:A:831:ILE:HG13	1:A:881:ILE:CG1	2.45	0.47
1:A:1060:ASN:ND2	1:A:1062:GLU:H	2.12	0.47
1:A:899:THR:CG2	1:A:900:GLY:N	2.65	0.47
1:A:948:HIS:ND1	1:A:1086:TRP:HB3	2.29	0.47
1:A:1042:LEU:HD22	1:A:1043:THR:C	2.35	0.47
1:A:925:VAL:O	1:A:929:VAL:HG23	2.15	0.47
1:A:815:PHE:O	1:A:827:THR:HB	2.14	0.46
1:A:175:PHE:CG	1:A:471:HIS:CD2	3.03	0.46
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.44	0.46
1:A:907:LEU:HD23	1:A:994:VAL:HG21	1.98	0.46
1:A:198:MET:CE	1:A:280:TYR:CB	2.92	0.46
1:A:207:LEU:HD22	1:A:211:LEU:HB2	1.97	0.46
1:A:1051:ILE:O	1:A:1055:LEU:HB2	2.15	0.46
1:A:245:LEU:HD21	1:A:272:LEU:HG	1.98	0.46
1:A:370:ILE:HG13	1:A:373:LEU:HD21	1.97	0.46
1:A:363:VAL:O	1:A:363:VAL:HG13	2.14	0.46
1:A:420:ILE:CD1	1:A:522:ASN:HB3	2.43	0.46
1:A:988:THR:HG21	1:A:1080:TRP:CZ3	2.51	0.46
1:A:198:MET:CE	1:A:282:VAL:CG1	2.94	0.46
1:A:511:GLU:HB3	3:A:1145:HOH:O	2.15	0.46
1:A:565:ASN:O	1:A:566:PRO:O	2.33	0.46
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.16	0.46
1:A:214:LYS:HZ2	1:A:300:GLY:HA2	1.80	0.46
1:A:784:ARG:HH11	1:A:784:ARG:HG2	1.81	0.46
1:A:947:ARG:HB3	1:A:948:HIS:H	1.48	0.46
1:A:211:LEU:HB3	1:A:297:LEU:HD23	1.97	0.45
1:A:366:ARG:NH2	1:A:519:LEU:HB2	2.31	0.45
1:A:528:ALA:HB1	1:A:529:LEU:H	1.49	0.45
1:A:817:CYS:HB2	1:A:828:ILE:HD11	1.98	0.45
1:A:220:ILE:CD1	1:A:237:PRO:HG3	2.46	0.45
1:A:169:HIS:C	1:A:169:HIS:CD2	2.88	0.45
1:A:198:MET:HE2	1:A:282:VAL:HG22	1.99	0.45
1:A:163:THR:HB	3:A:1204:HOH:O	2.17	0.45
1:A:193:PRO:HA	3:A:1115:HOH:O	2.17	0.45
1:A:304:HIS:CB	1:A:823:LEU:HD11	2.42	0.45
1:A:981:GLU:CD	1:A:1078:LYS:HZ3	2.19	0.45
1:A:988:THR:HG23	1:A:989:PRO:HD3	1.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:PRO:HG2	1:A:511:GLU:O	2.16	0.45
1:A:1018:LEU:HD21	1:A:1064:ALA:CB	2.46	0.45
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.80	0.45
1:A:184:ARG:O	1:A:188:VAL:HG23	2.17	0.45
1:A:435:CYS:SG	1:A:436:GLY:N	2.90	0.45
1:A:373:LEU:HD12	1:A:404:PHE:CE1	2.52	0.45
1:A:1076:ARG:NH1	1:A:1076:ARG:CG	2.73	0.45
1:A:774:LEU:C	1:A:776:ASN:H	2.20	0.44
1:A:774:LEU:C	1:A:776:ASN:N	2.70	0.44
1:A:779:LEU:HD23	1:A:780:PRO:O	2.16	0.44
1:A:862:LEU:CD2	1:A:862:LEU:N	2.80	0.44
1:A:967:HIS:NE2	1:A:970:GLY:HA2	2.32	0.44
1:A:1036:MET:CG	1:A:1042:LEU:HD11	2.43	0.44
1:A:215:ILE:CD1	1:A:297:LEU:HD11	2.43	0.44
1:A:731:ASP:O	1:A:735:GLN:HG3	2.16	0.44
1:A:739:ILE:HG13	1:A:740:GLU:N	2.31	0.44
1:A:992:LEU:HD11	1:A:1076:ARG:CD	2.48	0.44
1:A:641:ARG:O	1:A:644:ALA:HB3	2.17	0.44
1:A:732:PHE:O	1:A:736:VAL:HG23	2.18	0.44
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.99	0.44
1:A:960:LEU:CD1	1:A:991:PHE:CE2	2.96	0.44
1:A:552:ARG:HH11	1:A:552:ARG:HB2	1.82	0.44
1:A:421:LYS:NZ	1:A:527:ILE:CD1	2.80	0.44
1:A:1001:LYS:H	1:A:1076:ARG:HH22	1.64	0.44
1:A:182:THR:HB	1:A:183:PRO:HD3	1.98	0.44
1:A:235:VAL:HG12	1:A:236:SER:H	1.82	0.44
1:A:370:ILE:HD13	1:A:371:PRO:N	2.31	0.44
1:A:421:LYS:NZ	1:A:527:ILE:HD11	2.32	0.44
1:A:477:ARG:HD2	1:A:522:ASN:N	2.20	0.44
1:A:526:PRO:HG2	1:A:527:ILE:N	2.32	0.44
1:A:862:LEU:N	1:A:862:LEU:HD22	2.32	0.44
1:A:999:GLY:C	1:A:1000:LYS:HD3	2.36	0.44
1:A:1086:TRP:O	1:A:1087:PHE:CD2	2.71	0.44
1:A:198:MET:HE1	1:A:282:VAL:HG13	2.00	0.44
1:A:436:GLY:O	1:A:437:LYS:CB	2.66	0.44
1:A:853:SER:O	1:A:857:THR:HG23	2.17	0.44
1:A:957:THR:O	1:A:957:THR:CG2	2.65	0.44
1:A:175:PHE:CG	1:A:471:HIS:HD2	2.36	0.43
1:A:916:PRO:CG	1:A:917:THR:N	2.75	0.43
1:A:145:GLU:HA	1:A:148:GLN:NE2	2.33	0.43
1:A:226:ARG:O	1:A:227:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PRO:C	1:A:243:ALA:H	2.21	0.43
1:A:363:VAL:HG23	1:A:520:LEU:HD13	2.01	0.43
1:A:424:PRO:HG2	1:A:427:ALA:HB2	2.00	0.43
1:A:576:TRP:CE3	1:A:579:ARG:HD2	2.52	0.43
1:A:915:SER:HB3	1:A:921:PHE:HB2	1.99	0.43
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.54	0.43
1:A:882:VAL:HA	3:A:1120:HOH:O	2.18	0.43
1:A:410:TRP:HB3	1:A:412:VAL:CG1	2.39	0.43
1:A:531:LYS:HD3	1:A:609:GLN:HG2	2.01	0.43
1:A:194:LYS:HE3	3:A:1168:HOH:O	2.17	0.43
1:A:386:ASN:OD1	1:A:396:GLN:HG3	2.19	0.43
1:A:484:MET:CE	1:A:514:MET:CG	2.94	0.43
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.86	0.43
1:A:149:ALA:HA	1:A:152:ARG:HD2	2.01	0.43
1:A:168:VAL:HG13	1:A:169:HIS:N	2.34	0.43
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.49	0.43
1:A:682:LEU:HD22	1:A:686:LEU:CD1	2.49	0.43
1:A:1078:LYS:NZ	1:A:1081:THR:HB	2.34	0.43
1:A:577:HIS:CD2	3:A:1159:HOH:O	2.71	0.43
1:A:665:GLN:OE1	1:A:1037:THR:HB	2.18	0.43
1:A:727:ALA:O	1:A:730:HIS:HB3	2.19	0.43
1:A:1001:LYS:H	1:A:1076:ARG:NH2	2.16	0.43
1:A:246:GLN:C	1:A:248:PHE:H	2.20	0.43
1:A:308:ASP:N	1:A:308:ASP:OD1	2.52	0.43
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.49	0.43
1:A:435:CYS:HB3	1:A:461:LEU:HD11	1.99	0.43
1:A:904:ASP:O	1:A:990:ASP:HA	2.19	0.43
1:A:587:LYS:HA	1:A:626:LEU:HD11	2.01	0.42
1:A:862:LEU:HB3	1:A:934:GLY:HA3	2.00	0.42
1:A:184:ARG:NH2	1:A:321:GLU:OE1	2.52	0.42
1:A:824:SER:OG	1:A:825:ASN:N	2.52	0.42
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.60	0.42
1:A:856:GLU:C	1:A:858:GLU:H	2.21	0.42
1:A:932:CYS:O	1:A:936:CYS:SG	2.74	0.42
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	2.01	0.42
1:A:236:SER:HA	1:A:237:PRO:HD3	1.85	0.42
1:A:583:LEU:HD12	1:A:589:TYR:OH	2.18	0.42
1:A:885:ALA:HB2	1:A:955:THR:HG22	2.01	0.42
1:A:405:THR:O	1:A:407:GLU:N	2.53	0.42
1:A:521:ASP:OD1	1:A:521:ASP:C	2.57	0.42
1:A:983:VAL:HB	1:A:1082:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:LYS:HE3	1:A:1081:THR:HB	1.97	0.42
1:A:485:TRP:CH2	1:A:508:PRO:HD3	2.54	0.42
1:A:766:GLN:OE1	1:A:766:GLN:HA	2.19	0.42
1:A:908:ASN:HB2	1:A:993:PHE:HD2	1.84	0.42
1:A:1078:LYS:HZ2	1:A:1081:THR:HG21	1.85	0.42
1:A:900:GLY:C	1:A:902:PHE:HB2	2.40	0.42
1:A:1000:LYS:HA	1:A:1076:ARG:CZ	2.46	0.42
1:A:241:PRO:C	1:A:243:ALA:N	2.71	0.42
1:A:359:ARG:HA	1:A:359:ARG:HD3	1.83	0.42
1:A:512:ASN:HD22	1:A:512:ASN:N	2.17	0.42
1:A:608:TYR:N	1:A:608:TYR:CD2	2.87	0.42
1:A:734:GLN:OE1	1:A:780:PRO:HB3	2.20	0.42
1:A:935:TYR:O	1:A:939:THR:CG2	2.67	0.42
1:A:1002:THR:HG21	1:A:1007:GLN:NE2	2.22	0.42
1:A:1069:LEU:HD13	1:A:1069:LEU:HA	1.84	0.42
1:A:205:LYS:NZ	1:A:652:GLU:OE1	2.53	0.42
1:A:167:ASN:O	1:A:167:ASN:CG	2.58	0.41
1:A:547:MET:HG2	1:A:578:PHE:CD2	2.55	0.41
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.91	0.41
1:A:291:GLN:NE2	1:A:291:GLN:CA	2.84	0.41
1:A:1039:MET:N	1:A:1040:PRO:CD	2.82	0.41
1:A:199:HIS:O	1:A:200:PRO:C	2.59	0.41
1:A:964:ASP:C	1:A:966:GLY:N	2.74	0.41
1:A:364:LYS:CE	1:A:411:ASN:OD1	2.68	0.41
1:A:436:GLY:O	1:A:437:LYS:CG	2.69	0.41
1:A:226:ARG:CG	1:A:226:ARG:NH1	2.80	0.41
1:A:370:ILE:HD12	1:A:372:VAL:O	2.21	0.41
1:A:552:ARG:NH2	1:A:581:GLU:CD	2.74	0.41
1:A:875:LYS:HB3	1:A:875:LYS:HE3	1.74	0.41
1:A:896:VAL:HA	1:A:903:LYS:HZ3	1.85	0.41
1:A:900:GLY:O	1:A:902:PHE:CB	2.68	0.41
1:A:214:LYS:HD3	1:A:297:LEU:CD1	2.51	0.41
1:A:922:GLN:O	1:A:926:GLU:CG	2.59	0.41
1:A:985:PHE:CE1	1:A:1072:ILE:HD13	2.55	0.41
1:A:246:GLN:NE2	1:A:246:GLN:CA	2.81	0.41
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.56	0.41
1:A:624:VAL:O	1:A:628:MET:HG2	2.20	0.41
1:A:834:HIS:HA	1:A:875:LYS:O	2.21	0.41
1:A:224:ILE:O	1:A:230:SER:HA	2.21	0.40
1:A:248:PHE:O	1:A:249:PHE:C	2.60	0.40
1:A:887:THR:HB	1:A:890:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:MET:N	1:A:1040:PRO:HD3	2.33	0.40
1:A:319:ARG:CD	3:A:1199:HOH:O	2.67	0.40
1:A:526:PRO:HB2	1:A:527:ILE:H	1.19	0.40
1:A:435:CYS:HB3	1:A:461:LEU:HG	2.03	0.40
1:A:484:MET:HB2	1:A:484:MET:HE2	1.65	0.40
1:A:543:VAL:O	1:A:544:ARG:CB	2.70	0.40
1:A:703:ILE:O	1:A:703:ILE:HG22	2.21	0.40
1:A:547:MET:HE1	1:A:551:LEU:C	2.42	0.40
1:A:512:ASN:ND2	1:A:512:ASN:H	2.18	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	817/966 (85%)	721 (88%)	64 (8%)	32 (4%)	3 10

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	ILE
1	A	530	PRO
1	A	545	ALA
1	A	566	PRO
1	A	756	LYS
1	A	758	ASP
1	A	777	SER
1	A	916	PRO
1	A	949	ASN
1	A	964	ASP
1	A	965	PHE
1	A	998	SER

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Mol	Chain	Res	Type
1	A	1040	PRO
1	A	1059	LYS
1	A	227	SER
1	A	230	SER
1	A	921	PHE
1	A	526	PRO
1	A	899	THR
1	A	1044	SER
1	A	406	GLU
1	A	422	ASP
1	A	778	GLN
1	A	1000	LYS
1	A	1045	LYS
1	A	759	VAL
1	A	1038	GLY
1	A	544	ARG
1	A	241	PRO
1	A	242	GLY
1	A	436	GLY
1	A	1039	MET

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	755/864 (87%)	686 (91%)	69 (9%)	9 27

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	169	HIS
1	A	170	ASP
1	A	174	GLU
1	A	207	LEU
1	A	211	LEU

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Mol	Chain	Res	Type
1	A	225	HIS
1	A	226	ARG
1	A	227	SER
1	A	229	THR
1	A	234	LYS
1	A	238	ASP
1	A	298	LYS
1	A	370	ILE
1	A	379	LEU
1	A	421	LYS
1	A	422	ASP
1	A	459	GLN
1	A	477	ARG
1	A	511	GLU
1	A	512	ASN
1	A	520	LEU
1	A	525	HIS
1	A	527	ILE
1	A	529	LEU
1	A	543	VAL
1	A	544	ARG
1	A	546	GLU
1	A	547	MET
1	A	552	ARG
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	583	LEU
1	A	586	PRO
1	A	610	LEU
1	A	626	LEU
1	A	647	LYS
1	A	682	LEU
1	A	717	LEU
1	A	728	MET
1	A	749	ILE
1	A	757	TYR
1	A	760	SER
1	A	767	LEU
1	A	776	ASN
1	A	799	GLU
1	A	838	LEU

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Mol	Chain	Res	Type
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	898	ASN
1	A	903	LYS
1	A	908	ASN
1	A	913	GLU
1	A	947	ARG
1	A	952	ILE
1	A	969	LEU
1	A	982	ARG
1	A	998	SER
1	A	1000	LYS
1	A	1002	THR
1	A	1026	LEU
1	A	1039	MET
1	A	1042	LEU
1	A	1076	ARG
1	A	1087	PHE
1	A	1088	LEU

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

Mol	Chain	Res	Type
1	A	169	HIS
1	A	217	ASN
1	A	225	HIS
1	A	246	GLN
1	A	291	GLN
1	A	295	HIS
1	A	299	ASN
1	A	304	HIS
1	A	391	GLN
1	A	459	GLN
1	A	512	ASN
1	A	549	ASN
1	A	565	ASN
1	A	646	GLN
1	A	743	GLN
1	A	773	ASN
1	A	834	HIS

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Mol	Chain	Res	Type
1	A	908	ASN
1	A	951	ASN
1	A	959	ASN
1	A	1005	HIS
1	A	1007	GLN
1	A	1060	ASN
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 monosaccharides 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	DW2	A	1	-	15,41,41	2.35	5 (33%)	8,90,90	2.59	3 (37%)

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	DW2	A	1	-	-	-	0/12/11/11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	DW2	C6-N21	5.41	1.37	1.29
2	A	1	DW2	C23-N19	3.89	1.40	1.36
2	A	1	DW2	C26-C27	3.38	1.44	1.37
2	A	1	DW2	C7-C3	3.11	1.44	1.39
2	A	1	DW2	C25-C26	2.78	1.43	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	DW2	C30-C29-C28	5.24	140.60	132.71
2	A	1	DW2	C25-C26-C27	-3.46	119.37	123.04
2	A	1	DW2	C2-C30-C29	-2.67	120.96	124.02

There are no chirality outliers.

There are no torsion outliers.

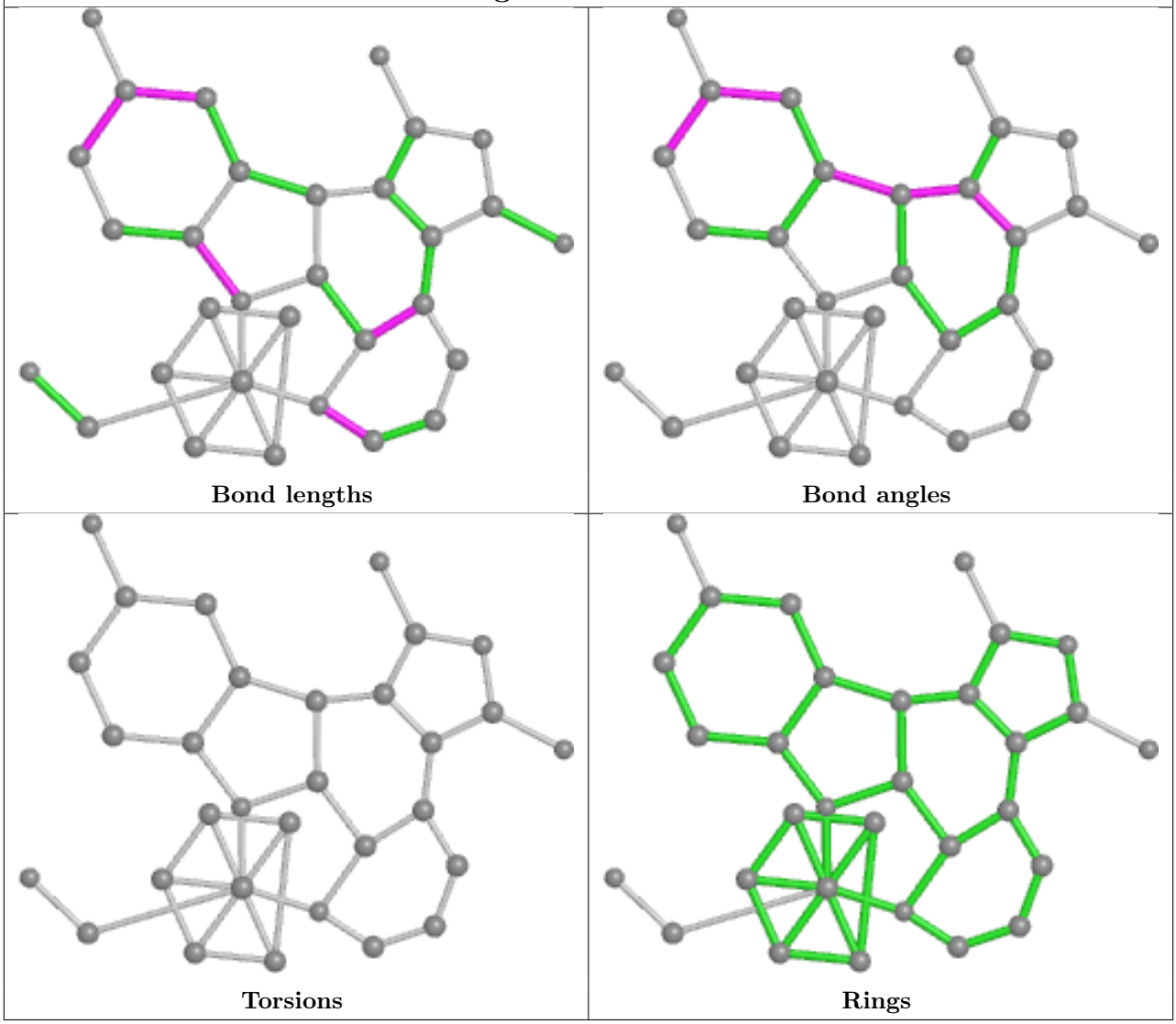
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	DW2	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 DW2 A 1



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, 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	839/966 (86%)	0.58	84 (10%) 7 4	20, 90, 141, 163	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	LEU	6.1
1	A	377	THR	5.7
1	A	529	LEU	5.6
1	A	1044	SER	5.2
1	A	248	PHE	4.7
1	A	911	LEU	4.7
1	A	1086	TRP	4.7
1	A	998	SER	4.5
1	A	307	LEU	4.5
1	A	895	THR	4.4
1	A	759	VAL	4.3
1	A	221	PHE	4.0
1	A	215	ILE	4.0
1	A	907	LEU	3.9
1	A	270	PHE	3.9
1	A	244	ILE	3.7
1	A	528	ALA	3.7
1	A	241	PRO	3.6
1	A	233	ILE	3.4
1	A	378	ASP	3.3
1	A	220	ILE	3.3
1	A	320	LYS	3.2
1	A	825	ASN	3.2
1	A	948	HIS	3.2
1	A	403	PRO	3.1
1	A	1075	CYS	3.1
1	A	435	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	995	MET	3.1
1	A	526	PRO	3.0
1	A	1082	VAL	3.0
1	A	755	GLU	3.0
1	A	252	MET	3.0
1	A	774	LEU	3.0
1	A	303	ILE	3.0
1	A	1001	LYS	2.8
1	A	1042	LEU	2.7
1	A	894	SER	2.7
1	A	269	ASP	2.7
1	A	1041	GLN	2.7
1	A	222	ILE	2.6
1	A	999	GLY	2.6
1	A	546	GLU	2.6
1	A	859	SER	2.6
1	A	216	ALA	2.6
1	A	1069	LEU	2.5
1	A	991	PHE	2.5
1	A	1006	PHE	2.5
1	A	1068	PHE	2.5
1	A	777	SER	2.5
1	A	760	SER	2.5
1	A	970	GLY	2.5
1	A	613	ARG	2.5
1	A	281	LEU	2.5
1	A	226	ARG	2.4
1	A	1004	PRO	2.4
1	A	409	LEU	2.4
1	A	754	ALA	2.4
1	A	794	GLY	2.4
1	A	287	ILE	2.4
1	A	1084	PHE	2.3
1	A	404	PHE	2.3
1	A	148	GLN	2.3
1	A	922	GLN	2.3
1	A	527	ILE	2.3
1	A	967	HIS	2.3
1	A	896	VAL	2.3
1	A	766	GLN	2.3
1	A	247	SER	2.2
1	A	321	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	313	PRO	2.2
1	A	987	LEU	2.2
1	A	228	THR	2.2
1	A	476	ARG	2.2
1	A	897	GLY	2.2
1	A	1000	LYS	2.1
1	A	297	LEU	2.1
1	A	470	ASP	2.1
1	A	272	LEU	2.1
1	A	990	ASP	2.1
1	A	381	VAL	2.1
1	A	271	VAL	2.0
1	A	402	LYS	2.0
1	A	949	ASN	2.0
1	A	1065	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

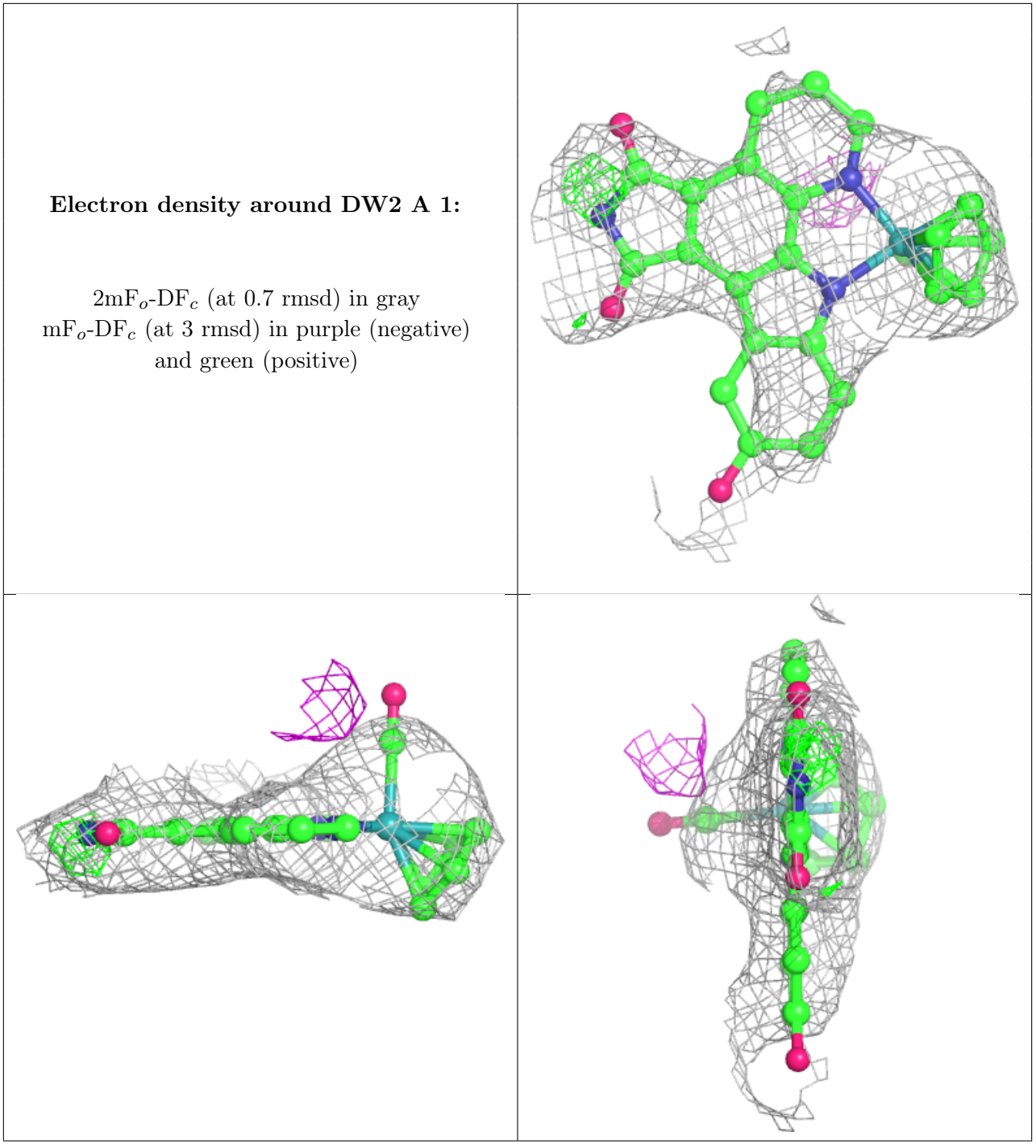
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	DW2	A	1	31/31	0.88	0.26	158,161,191,191	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 DW2 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

There are no such residues in this entry.