Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:57 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

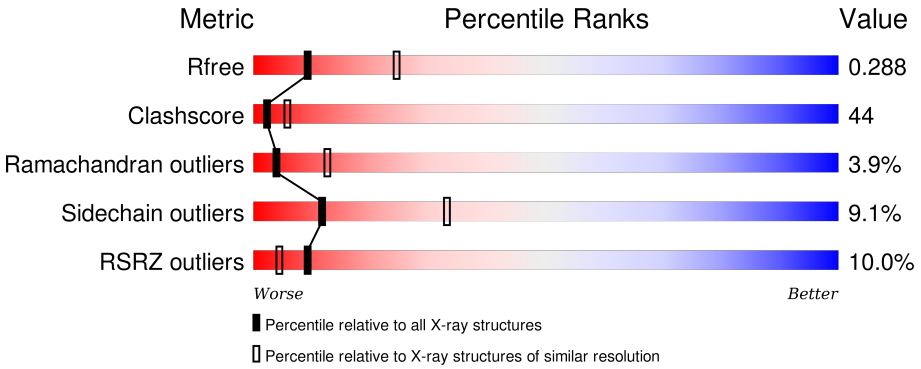
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

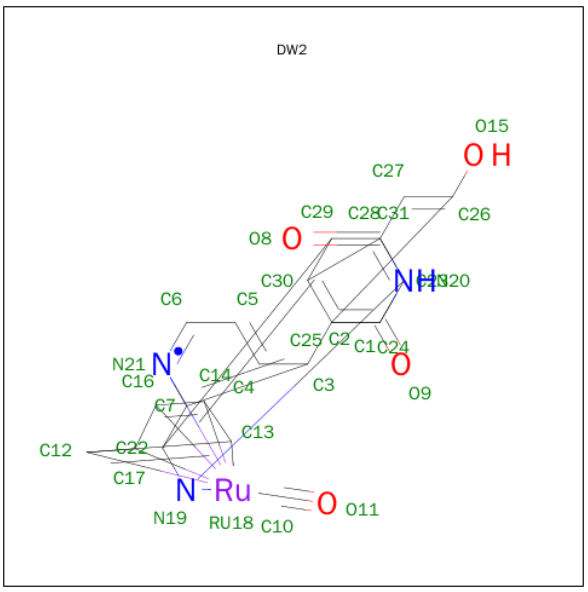
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

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.

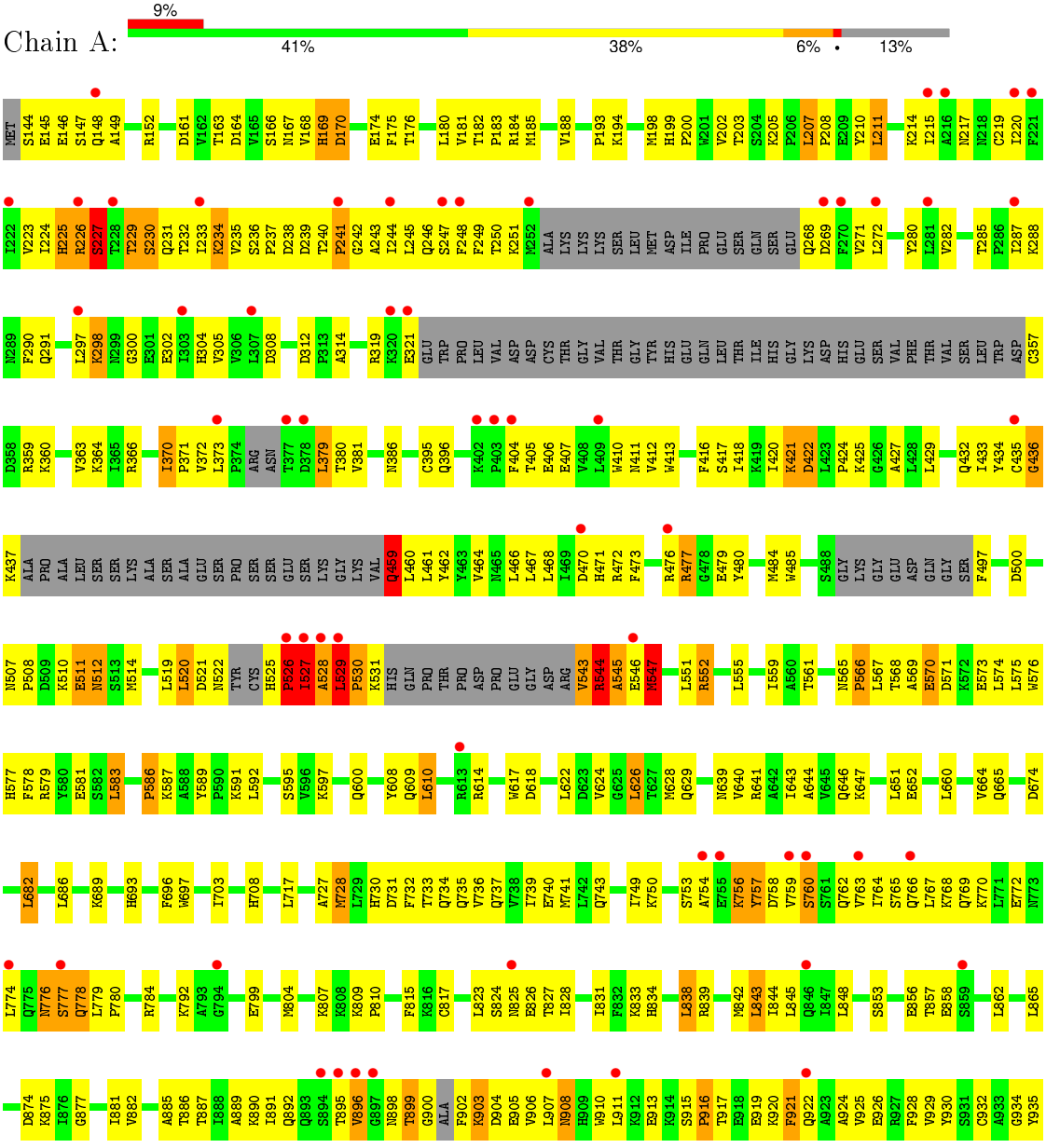
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		

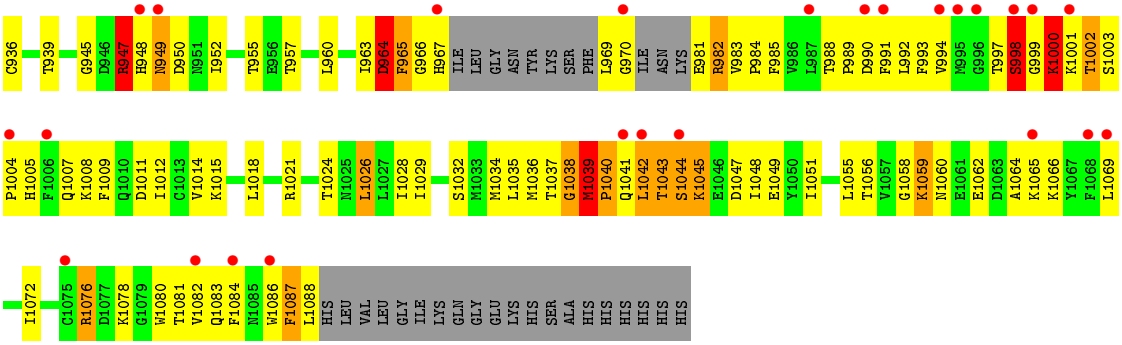
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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:




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 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 0.260 , 0.288	Depositor DCC
R_{free} test set	2457 reflections (11.50%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 24815 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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

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:HG3	1:A:982:ARG:HH11	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:473:PHE:O	1:A:526:PRO:HB3	1.61	1.00
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: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:N	1:A:1000:LYS:HD3	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:1002:THR:CG2	1:A:1007:GLN:HE21	1.87	0.86
1:A:887:THR:HG22	1:A:889:ALA:H	1.39	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:964:ASP:O	1:A:966:GLY:N	2.11	0.84
1:A:477:ARG:HD2	1:A:522:ASN:H	1.40	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:896:VAL:CG1	1:A:903:LYS:HE2	2.09	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:433:ILE:HD12	1:A:484:MET:HE1	1.61	0.82
1:A:960:LEU:HD11	1:A:991:PHE:HE2	1.43	0.82
1:A:1043:THR:HG22	1:A:1047:ASP:CG	2.00	0.82
1:A:741:MET:HE1	1:A:778:GLN:HB3	1.60	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:1034:MET:HG3	1:A:1039:MET:HE3	1.66	0.77
1:A:760:SER:OG	1:A:762:GLN:HB3	1.83	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:1043:THR:O	1:A:1043:THR:HG23	1.83	0.76
1:A:304:HIS:HB2	1:A:823:LEU:HD11	1.66	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:CD2	1:A:1042:LEU:C	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:CG	1:A:982:ARG:HH11	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: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:217:ASN:ND2	1:A:219:CYS:HB2	2.02	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:HH11	1:A:226:ARG:HG2	1.53	0.72
1:A:529:LEU:O	1:A:529:LEU:HG	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:1078:LYS:CE	1:A:1081:THR:HB	2.19	0.71
1:A:223:VAL:HG12	1:A:225:HIS:CE1	2.25	0.71
1:A:899:THR:CG2	1:A:900:GLY:H	1.98	0.71
1:A:792:LYS:HD2	3:A:1209:HOH:O	1.90	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:HD22	1:A:379:LEU:N	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:1036:MET:HG2	1:A:1042:LEU:HD11	1.73	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: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:420:ILE:HD13	1:A:522:ASN:HB3	1.74	0.67
1:A:198:MET:HE2	1:A:282:VAL:CG2	2.24	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:762:GLN:O	1:A:766:GLN:HG2	1.94	0.67
1:A:660:LEU:O	1:A:664:VAL:HG23	1.94	0.67
1:A:583:LEU:CD2	1:A:610:LEU:HD22	2.24	0.67
1:A:1043:THR:HG22	1:A:1047:ASP:OD2	1.95	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: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:1038:GLY:C	1:A:1040:PRO:CD	2.65	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:579:ARG:HG2	1:A:610:LEU:HD11	1.79	0.64
1:A:1043:THR:HG21	1:A:1047:ASP:H	1.60	0.63
1:A:233:ILE:HD12	1:A:233:ILE:H	1.62	0.63
1:A:998:SER:O	1:A:1001:LYS:HG3	1.97	0.63
1:A:169:HIS:HD2	1:A:170:ASP:HB3	1.61	0.63
1:A:766:GLN:O	1:A:770:LYS:HG3	1.98	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:807:LYS:HG2	3:A:1177:HOH:O	1.97	0.63
1:A:964:ASP:O	1:A:965:PHE:C	2.36	0.63
1:A:464:VAL:HB	1:A:484:MET:HG2	1.81	0.63
1:A:1000:LYS:N	1:A:1000:LYS:CD	2.58	0.62
1:A:210:TYR:HD1	1:A:211:LEU:CD2	2.10	0.62
1:A:757:TYR:CD2	1:A:757:TYR:N	2.64	0.62
1:A:1043:THR:O	1:A:1045:LYS:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:MET:HE3	1:A:280:TYR:CB	2.29	0.62
1:A:928:PHE:HZ	1:A:991:PHE:HD2	1.47	0.62
1:A:239:ASP:HB3	1:A:244:ILE:HD11	1.79	0.62
1:A:149:ALA:O	1:A:152:ARG:HB2	1.99	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:HD3	1:A:251:LYS:O	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:246:GLN:NE2	1:A:246:GLN:HA	2.14	0.62
1:A:239:ASP:CB	1:A:244:ILE:HD11	2.30	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:997:THR:HG23	1:A:1002:THR:N	2.15	0.61
1:A:569:ALA:O	1:A:573:GLU:HG3	2.00	0.61
1:A:887:THR:CG2	1:A:950:ASP:HA	2.31	0.61
1:A:576:TRP:CH2	1:A:579:ARG:HD2	2.36	0.61
1:A:843:LEU:HD23	1:A:1039:MET:CE	2.31	0.61
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.16	0.61
1:A:989:PRO:HG2	1:A:1080:TRP:CD1	2.35	0.61
1:A:497:PHE:N	1:A:1044:SER:HG	1.99	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:753:SER:HB3	1:A:809:LYS:HG3	1.84	0.59
1:A:233:ILE:N	1:A:233:ILE:HD12	2.18	0.59
1:A:223:VAL:HG12	1:A:225:HIS:HE1	1.66	0.59
1:A:1018:LEU:HD23	1:A:1021:ARG:HD3	1.85	0.59
1:A:547:MET:CB	1:A:552:ARG:HH12	2.14	0.59
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:THR:O	1:A:1043:THR:CG2	2.50	0.59
1:A:544:ARG:HD3	1:A:544:ARG:N	2.18	0.59
1:A:380:THR:CG2	1:A:437:LYS:O	2.51	0.58
1:A:1002:THR:HG22	1:A:1007:GLN:HE21	1.66	0.58
1:A:960:LEU:HD11	1:A:991:PHE:CE2	2.31	0.58
1:A:543:VAL:O	1:A:544:ARG:HB2	2.03	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:1002:THR:HG22	1:A:1003:SER:H	1.68	0.58
1:A:886:THR:HG22	1:A:887:THR:N	2.19	0.58
1:A:198:MET:HE3	1:A:280:TYR:CG	2.39	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: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:930:TYR:HE1	1:A:1008:LYS:HE2	1.69	0.58
1:A:982:ARG:HG3	1:A:982:ARG:NH1	2.01	0.58
1:A:198:MET:HE1	1:A:282:VAL:HG11	1.85	0.58
1:A:169:HIS:HE1	3:A:1128:HOH:O	1.87	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:231:GLN:HG3	1:A:232:THR:N	2.11	0.57
1:A:207:LEU:CD2	1:A:208:PRO:HD2	2.32	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:1078:LYS:CD	1:A:1081:THR:HB	2.35	0.56
1:A:1026:LEU:O	1:A:1029:ILE:HG22	2.05	0.56
1:A:1024:THR:O	1:A:1028:ILE:HG12	2.05	0.56
1:A:930:TYR:CE1	1:A:1008:LYS:HE2	2.40	0.56
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ILE:CD1	1:A:484:MET:HE1	2.31	0.56
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.33	0.56
1:A:145:GLU:HA	1:A:148:GLN:CD	2.26	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:512:ASN:N	1:A:512:ASN:ND2	2.54	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: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:1045:LYS:O	1:A:1049:GLU:HG3	2.06	0.55
1:A:211:LEU:HD11	1:A:298:LYS:HB2	1.88	0.55
1:A:210:TYR:CE1	1:A:211:LEU:HD23	2.40	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:579:ARG:HG2	1:A:610:LEU:CD1	2.37	0.55
1:A:1038:GLY:O	1:A:1040:PRO:CD	2.55	0.55
1:A:1036:MET:CG	1:A:1042:LEU:CD1	2.80	0.55
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	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: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:HD12	1:A:224:ILE:N	2.22	0.54
1:A:896:VAL:N	1:A:903:LYS:CE	2.70	0.54
1:A:211:LEU:CD1	1:A:297:LEU:HD23	2.36	0.54
1:A:1060:ASN:ND2	1:A:1062:GLU:HB2	2.17	0.54
1:A:737:GLN:O	1:A:741:MET:HG3	2.06	0.54
1:A:576:TRP:O	1:A:579:ARG:HD3	2.07	0.54
1:A:1043:THR:HG22	1:A:1047:ASP:CB	2.36	0.54
1:A:462:TYR:HB3	1:A:484:MET:CE	2.37	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:997:THR:HG23	1:A:1002:THR:H	1.70	0.54
1:A:764:ILE:O	1:A:768:LYS:HG3	2.08	0.54
1:A:892:GLN:O	1:A:896:VAL:HG22	2.08	0.54
1:A:462:TYR:HB3	1:A:484:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:PHE:O	1:A:1087:PHE:CE1	2.61	0.53
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.08	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:1032:SER:HB3	1:A:1048:ILE:HG23	1.90	0.53
1:A:526:PRO:O	1:A:527:ILE:CG1	2.56	0.53
1:A:249:PHE:CE1	1:A:268:GLN:HA	2.44	0.53
1:A:1078:LYS:CG	1:A:1082:VAL:HG23	2.37	0.53
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.90	0.53
1:A:220:ILE:HD11	1:A:237:PRO:HG3	1.89	0.53
1:A:467:LEU:O	1:A:476:ARG:HD2	2.09	0.53
1:A:226:ARG:HH11	1:A:226:ARG:CG	2.20	0.53
1:A:1036:MET:CG	1:A:1042:LEU:HD12	2.35	0.53
1:A:215:ILE:HD12	1:A:215:ILE:N	2.22	0.53
1:A:947:ARG:NH2	1:A:963:ILE:O	2.41	0.53
1:A:592:LEU:O	1:A:595:SER:HB2	2.08	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:589:TYR:CD1	1:A:589:TYR:N	2.75	0.52
1:A:366:ARG:NH2	1:A:519:LEU:HD22	2.24	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:433:ILE:HD12	1:A:484:MET:CE	2.37	0.52
1:A:229:THR:HB	3:A:1113:HOH:O	2.10	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:244:ILE:HA	1:A:247:SER:OG	2.10	0.51
1:A:198:MET:CE	1:A:280:TYR:HB3	2.39	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: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
1:A:828:ILE:N	1:A:828:ILE:HD12	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:566:PRO:O	1:A:567:LEU:HG	2.10	0.51
1:A:479:GLU:OE1	1:A:479:GLU:HA	2.11	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:928:PHE:HZ	1:A:991:PHE:CD2	2.26	0.51
1:A:291:GLN:HA	1:A:291:GLN:NE2	2.25	0.51
1:A:1078:LYS:HE2	1:A:1082:VAL:HG22	1.92	0.51
1:A:161:ASP:O	1:A:164:ASP:HB3	2.11	0.51
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.40	0.51
1:A:198:MET:HE1	1:A:271:VAL:HG21	1.92	0.51
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:CG2	1:A:1065:LYS:HG3	2.41	0.50
1:A:1014:VAL:HG11	1:A:1065:LYS:CD	2.42	0.50
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:997:THR:CG2	1:A:1002:THR:N	2.74	0.50
1:A:166:SER:O	1:A:510:LYS:HE3	2.11	0.50
1:A:839:ARG:HA	1:A:842:MET:CE	2.41	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:176:THR:HG23	1:A:674:ASP:HB2	1.92	0.50
1:A:470:ASP:CB	1:A:476:ARG:NH2	2.75	0.50
1:A:777:SER:O	1:A:778:GLN:HG3	2.12	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:1014:VAL:HG21	1:A:1069:LEU:HD21	1.94	0.50
1:A:526:PRO:CG	1:A:527:ILE:N	2.69	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:233:ILE:CD1	1:A:233:ILE:H	2.25	0.49
1:A:939:THR:OG1	1:A:945:GLY:HA2	2.12	0.49
1:A:379:LEU:CD2	1:A:379:LEU:C	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:1038:GLY:O	1:A:1040:PRO:HD3	2.11	0.49
1:A:753:SER:O	1:A:754:ALA:HB3	2.12	0.49
1:A:697:TRP:CH2	1:A:739:ILE:HD13	2.48	0.49
1:A:948:HIS:O	1:A:950:ASP:N	2.45	0.49
1:A:287:ILE:HA	1:A:290:PHE:CD1	2.48	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: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:810:PRO:HB3	1:A:833:LYS:HB2	1.93	0.49
1:A:1042:LEU:HD23	1:A:1043:THR:N	2.28	0.49
1:A:760:SER:HG	1:A:763:VAL:H	1.57	0.49
1:A:1078:LYS:HD2	1:A:1081:THR:HB	1.93	0.49
1:A:413:TRP:HD1	3:A:1187:HOH:O	1.96	0.49
1:A:911:LEU:HD11	1:A:924:ALA:HB1	1.93	0.49
1:A:434:TYR:HD1	1:A:459:GLN:C	2.15	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:1035:LEU:HD23	1:A:1039:MET:HG3	1.96	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:895:THR:HG22	1:A:903:LYS:HZ2	1.79	0.48
1:A:473:PHE:HB3	1:A:526:PRO:HB3	1.95	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:1043:THR:C	1:A:1045:LYS:N	2.67	0.48
1:A:1021:ARG:HE	1:A:1056:THR:HG23	1.77	0.48
1:A:589:TYR:HD1	1:A:589:TYR:H	1.61	0.48
1:A:589:TYR:HD1	1:A:589:TYR:N	2.11	0.48
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.44	0.48
1:A:1038:GLY:O	1:A:1040:PRO:HD2	2.14	0.47
1:A:381:VAL:HG12	1:A:435:CYS:HB2	1.96	0.47
1:A:998:SER:O	1:A:1001:LYS:CG	2.62	0.47
1:A:211:LEU:O	1:A:297:LEU:HD21	2.14	0.47
1:A:1078:LYS:HE2	1:A:1082:VAL:CG2	2.44	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:885:ALA:HA	1:A:955:THR:HA	1.96	0.47
1:A:319:ARG:HD3	3:A:1199:HOH:O	2.13	0.47
1:A:1000:LYS:CA	1:A:1076:ARG:NH2	2.64	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:1032:SER:HB3	1:A:1048:ILE:CG2	2.45	0.47
1:A:948:HIS:CE1	1:A:1086:TRP:HB3	2.50	0.47
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:MET:CE	1:A:810:PRO:HG2	2.45	0.47
1:A:181:VAL:CG1	1:A:185:MET:HE1	2.43	0.47
1:A:1060:ASN:ND2	1:A:1062:GLU:H	2.12	0.47
1:A:462:TYR:HB2	1:A:484:MET:CE	2.41	0.47
1:A:831:ILE:HG13	1:A:881:ILE:CG1	2.45	0.47
1:A:597:LYS:HD2	1:A:600:GLN:OE1	2.14	0.47
1:A:899:THR:CG2	1:A:900:GLY:N	2.65	0.47
1:A:1042:LEU:HD22	1:A:1043:THR:C	2.35	0.47
1:A:948:HIS:ND1	1:A:1086:TRP:HB3	2.29	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:235:VAL:HG11	1:A:244:ILE:CD1	2.44	0.46
1:A:175:PHE:CG	1:A:471:HIS:CD2	3.03	0.46
1:A:907:LEU:HD23	1:A:994:VAL:HG21	1.98	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:198:MET:CE	1:A:280:TYR:CB	2.92	0.46
1:A:370:ILE:HG13	1:A:373:LEU:HD21	1.97	0.46
1:A:245:LEU:HD21	1:A:272:LEU:HG	1.98	0.46
1:A:988:THR:HG21	1:A:1080:TRP:CZ3	2.51	0.46
1:A:420:ILE:CD1	1:A:522:ASN:HB3	2.43	0.46
1:A:363:VAL:O	1:A:363:VAL:HG13	2.14	0.46
1:A:511:GLU:HB3	3:A:1145:HOH:O	2.15	0.46
1:A:198:MET:CE	1:A:282:VAL:CG1	2.94	0.46
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.16	0.46
1:A:565:ASN:O	1:A:566:PRO:O	2.33	0.46
1:A:214:LYS:HZ2	1:A:300:GLY:HA2	1.80	0.46
1:A:947:ARG:HB3	1:A:948:HIS:H	1.48	0.46
1:A:784:ARG:HH11	1:A:784:ARG:HG2	1.81	0.46
1:A:211:LEU:HB3	1:A:297:LEU:HD23	1.97	0.45
1:A:528:ALA:HB1	1:A:529:LEU:H	1.49	0.45
1:A:366:ARG:NH2	1:A:519:LEU:HB2	2.31	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:198:MET:HE2	1:A:282:VAL:HG22	1.99	0.45
1:A:169:HIS:CD2	1:A:169:HIS:C	2.88	0.45
1:A:981:GLU:CD	1:A:1078:LYS:HZ3	2.19	0.45
1:A:304:HIS:CB	1:A:823:LEU:HD11	2.42	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: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:435:CYS:SG	1:A:436:GLY:N	2.90	0.45
1:A:184:ARG:O	1:A:188:VAL:HG23	2.17	0.45
1:A:373:LEU:HD12	1:A:404:PHE:CE1	2.52	0.45
1:A:1076:ARG:CG	1:A:1076:ARG:NH1	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:1036:MET:CG	1:A:1042:LEU:HD11	2.43	0.44
1:A:967:HIS:NE2	1:A:970:GLY:HA2	2.32	0.44
1:A:862:LEU:CD2	1:A:862:LEU:N	2.80	0.44
1:A:992:LEU:HD11	1:A:1076:ARG:CD	2.48	0.44
1:A:215:ILE:CD1	1:A:297:LEU:HD11	2.43	0.44
1:A:739:ILE:HG13	1:A:740:GLU:N	2.31	0.44
1:A:731:ASP:O	1:A:735:GLN:HG3	2.16	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:732:PHE:O	1:A:736:VAL:HG23	2.18	0.44
1:A:641:ARG:O	1:A:644:ALA:HB3	2.17	0.44
1:A:552:ARG:HB2	1:A:552:ARG:HH11	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: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:526:PRO:HG2	1:A:527:ILE:N	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:477:ARG:HD2	1:A:522:ASN:N	2.20	0.44
1:A:235:VAL:HG12	1:A:236:SER:H	1.82	0.44
1:A:182:THR:HB	1:A:183:PRO:HD3	1.98	0.44
1:A:862:LEU:HD22	1:A:862:LEU:N	2.32	0.44
1:A:436:GLY:O	1:A:437:LYS:CB	2.66	0.44
1:A:198:MET:HE1	1:A:282:VAL:HG13	2.00	0.44
1:A:957:THR:CG2	1:A:957:THR:O	2.65	0.44
1:A:853:SER:O	1:A:857:THR:HG23	2.17	0.44
1:A:916:PRO:CG	1:A:917:THR:N	2.75	0.43
1:A:175:PHE:CG	1:A:471:HIS:HD2	2.36	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: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: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: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:484:MET:CE	1:A:514:MET:CG	2.94	0.43
1:A:386:ASN:OD1	1:A:396:GLN:HG3	2.19	0.43
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.86	0.43
1:A:194:LYS:HE3	3:A:1168:HOH:O	2.17	0.43
1:A:149:ALA:HA	1:A:152:ARG:HD2	2.01	0.43
1:A:1078:LYS:NZ	1:A:1081:THR:HB	2.34	0.43
1:A:168:VAL:HG13	1:A:169:HIS:N	2.34	0.43
1:A:682:LEU:HD22	1:A:686:LEU:CD1	2.49	0.43
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.49	0.43
1:A:1001:LYS:H	1:A:1076:ARG:NH2	2.16	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:435:CYS:HB3	1:A:461:LEU:HD11	1.99	0.43
1:A:246:GLN:C	1:A:248:PHE:H	2.20	0.43
1:A:308:ASP:OD1	1:A:308:ASP:N	2.52	0.43
1:A:904:ASP:O	1:A:990:ASP:HA	2.19	0.43
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.49	0.43
1:A:862:LEU:HB3	1:A:934:GLY:HA3	2.00	0.42
1:A:587:LYS:HA	1:A:626:LEU:HD11	2.01	0.42
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.60	0.42
1:A:184:ARG:NH2	1:A:321:GLU:OE1	2.52	0.42
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	2.01	0.42
1:A:824:SER:OG	1:A:825:ASN:N	2.52	0.42
1:A:932:CYS:O	1:A:936:CYS:SG	2.74	0.42
1:A:856:GLU:C	1:A:858:GLU:H	2.21	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:521:ASP:C	1:A:521:ASP:OD1	2.57	0.42
1:A:405:THR:O	1:A:407:GLU:N	2.53	0.42
1:A:1078:LYS:HE3	1:A:1081:THR:HB	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:VAL:HB	1:A:1082:VAL:HG21	2.00	0.42
1:A:766:GLN:HA	1:A:766:GLN:OE1	2.19	0.42
1:A:908:ASN:HB2	1:A:993:PHE:HD2	1.84	0.42
1:A:485:TRP:CH2	1:A:508:PRO:HD3	2.54	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:512:ASN:HD22	1:A:512:ASN:N	2.17	0.42
1:A:1002:THR:HG21	1:A:1007:GLN:NE2	2.22	0.42
1:A:1069:LEU:HA	1:A:1069:LEU:HD13	1.84	0.42
1:A:241:PRO:C	1:A:243:ALA:N	2.71	0.42
1:A:935:TYR:O	1:A:939:THR:CG2	2.67	0.42
1:A:734:GLN:OE1	1:A:780:PRO:HB3	2.20	0.42
1:A:608:TYR:N	1:A:608:TYR:CD2	2.87	0.42
1:A:359:ARG:HD3	1:A:359:ARG:HA	1.83	0.42
1:A:205:LYS:NZ	1:A:652:GLU:OE1	2.53	0.42
1:A:547:MET:HG2	1:A:578:PHE:CD2	2.55	0.41
1:A:167:ASN:CG	1:A:167:ASN:O	2.58	0.41
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.91	0.41
1:A:1039:MET:N	1:A:1040:PRO:CD	2.82	0.41
1:A:291:GLN:CA	1:A:291:GLN:NE2	2.84	0.41
1:A:964:ASP:C	1:A:966:GLY:N	2.74	0.41
1:A:199:HIS:O	1:A:200:PRO:C	2.59	0.41
1:A:436:GLY:O	1:A:437:LYS:CG	2.69	0.41
1:A:364:LYS:CE	1:A:411:ASN:OD1	2.68	0.41
1:A:370:ILE:HD12	1:A:372:VAL:O	2.21	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:226:ARG:NH1	1:A:226:ARG:CG	2.80	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: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:834:HIS:HA	1:A:875:LYS:O	2.21	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:1039:MET:N	1:A:1040:PRO:HD3	2.33	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:224:ILE:O	1:A:230:SER:HA	2.21	0.40
1:A:526:PRO:HB2	1:A:527:ILE:H	1.19	0.40
1:A:319:ARG:CD	3:A:1199:HOH:O	2.67	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:H	1:A:512:ASN:ND2	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%)	4 12

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%)	12 33

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

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

Mol	Chain	Res	Type
1	A	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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DW2	A	1	-	26,41,41	3.41	17 (65%)	25,90,90	3.23	12 (48%)

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	-	-	0/0/135/135	0/6/11/11

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	DW2	O8-C31	-6.90	1.20	1.33
2	A	1	DW2	C27-C28	-6.85	1.43	1.53
2	A	1	DW2	C29-C28	-5.02	1.41	1.51
2	A	1	DW2	C28-C23	-4.56	1.40	1.54
2	A	1	DW2	C30-C31	-4.46	1.40	1.45
2	A	1	DW2	C24-C23	-4.36	1.42	1.52
2	A	1	DW2	C27-C26	-4.02	1.44	1.51
2	A	1	DW2	C24-C25	-3.52	1.43	1.52
2	A	1	DW2	C25-C26	-3.02	1.43	1.51
2	A	1	DW2	O15-C26	-2.32	1.36	1.43
2	A	1	DW2	C23-N19	-2.05	1.40	1.47
2	A	1	DW2	C6-C5	2.40	1.44	1.38
2	A	1	DW2	C7-N21	2.41	1.40	1.36
2	A	1	DW2	C6-N21	2.80	1.37	1.34
2	A	1	DW2	C5-C4	3.31	1.44	1.36
2	A	1	DW2	C2-C30	3.96	1.45	1.38
2	A	1	DW2	C31-N20	4.61	1.36	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	DW2	C30-C2-C1	-2.39	105.78	107.98
2	A	1	DW2	C25-C24-C23	2.87	118.92	111.16
2	A	1	DW2	C6-N21-C7	3.12	119.95	117.34
2	A	1	DW2	C27-C28-C29	3.81	132.25	115.52
2	A	1	DW2	C1-N20-C31	3.91	108.90	103.62
2	A	1	DW2	C4-C3-C2	4.12	129.94	123.46
2	A	1	DW2	O15-C26-C27	4.20	118.22	109.86
2	A	1	DW2	O15-C26-C25	4.37	122.41	110.05
2	A	1	DW2	C24-C25-C26	4.54	120.00	111.59
2	A	1	DW2	C30-C29-C28	5.55	140.60	131.87
2	A	1	DW2	O9-C1-C2	6.46	129.41	122.68
2	A	1	DW2	C27-C26-C25	6.94	119.37	110.52

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

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	839/966 (86%)	0.61	84 (10%) 9 4	20, 90, 141, 163	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	THR	6.7
1	A	529	LEU	6.4
1	A	373	LEU	6.1
1	A	1044	SER	5.2
1	A	998	SER	4.9
1	A	1086	TRP	4.8
1	A	248	PHE	4.8
1	A	911	LEU	4.6
1	A	307	LEU	4.4
1	A	895	THR	4.4
1	A	759	VAL	4.4
1	A	270	PHE	4.2
1	A	215	ILE	4.0
1	A	907	LEU	4.0
1	A	221	PHE	4.0
1	A	233	ILE	3.8
1	A	244	ILE	3.7
1	A	241	PRO	3.6
1	A	528	ALA	3.6
1	A	995	MET	3.4
1	A	526	PRO	3.3
1	A	948	HIS	3.3
1	A	435	CYS	3.2
1	A	825	ASN	3.2
1	A	378	ASP	3.2
1	A	220	ILE	3.2
1	A	754	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1075	CYS	3.1
1	A	252	MET	3.1
1	A	755	GLU	3.1
1	A	269	ASP	3.0
1	A	320	LYS	2.9
1	A	859	SER	2.9
1	A	303	ILE	2.9
1	A	1082	VAL	2.9
1	A	403	PRO	2.8
1	A	894	SER	2.8
1	A	1068	PHE	2.8
1	A	774	LEU	2.7
1	A	546	GLU	2.7
1	A	1041	GLN	2.7
1	A	222	ILE	2.7
1	A	281	LEU	2.7
1	A	987	LEU	2.7
1	A	148	GLN	2.6
1	A	1004	PRO	2.6
1	A	970	GLY	2.6
1	A	226	ARG	2.6
1	A	1006	PHE	2.6
1	A	777	SER	2.6
1	A	1042	LEU	2.5
1	A	1001	LYS	2.5
1	A	991	PHE	2.5
1	A	613	ARG	2.5
1	A	321	GLU	2.5
1	A	228	THR	2.5
1	A	999	GLY	2.5
1	A	922	GLN	2.5
1	A	766	GLN	2.4
1	A	216	ALA	2.4
1	A	896	VAL	2.4
1	A	409	LEU	2.4
1	A	1069	LEU	2.4
1	A	527	ILE	2.4
1	A	794	GLY	2.4
1	A	897	GLY	2.4
1	A	760	SER	2.3
1	A	967	HIS	2.3
1	A	404	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	476	ARG	2.2
1	A	1065	LYS	2.2
1	A	763	VAL	2.2
1	A	470	ASP	2.2
1	A	1084	PHE	2.2
1	A	287	ILE	2.2
1	A	247	SER	2.2
1	A	272	LEU	2.2
1	A	990	ASP	2.1
1	A	996	GLY	2.1
1	A	297	LEU	2.1
1	A	402	LYS	2.1
1	A	846	GLN	2.0
1	A	994	VAL	2.0
1	A	949	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	DW2	A	1	31/31	0.88	0.26	0.97	158,161,191,191	0

6.5 Other polymers

There are no such residues in this entry.