



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:52 PM 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 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/ValidationPDFNotes.html>

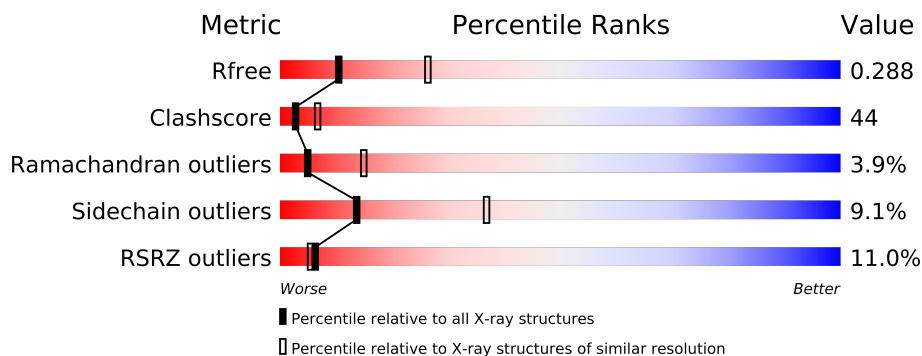
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

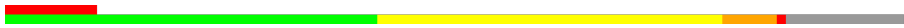
The reported resolution of this entry is 2.80 Å.

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	966	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6938 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

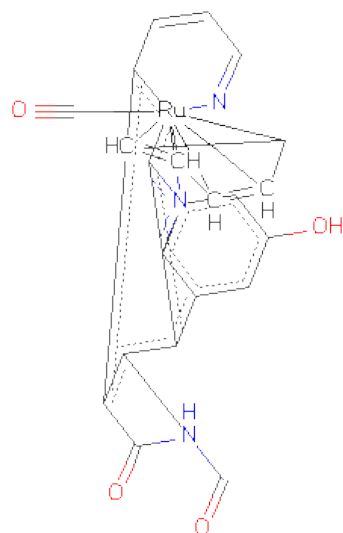
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6801	4369	1159	1238	35			

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		

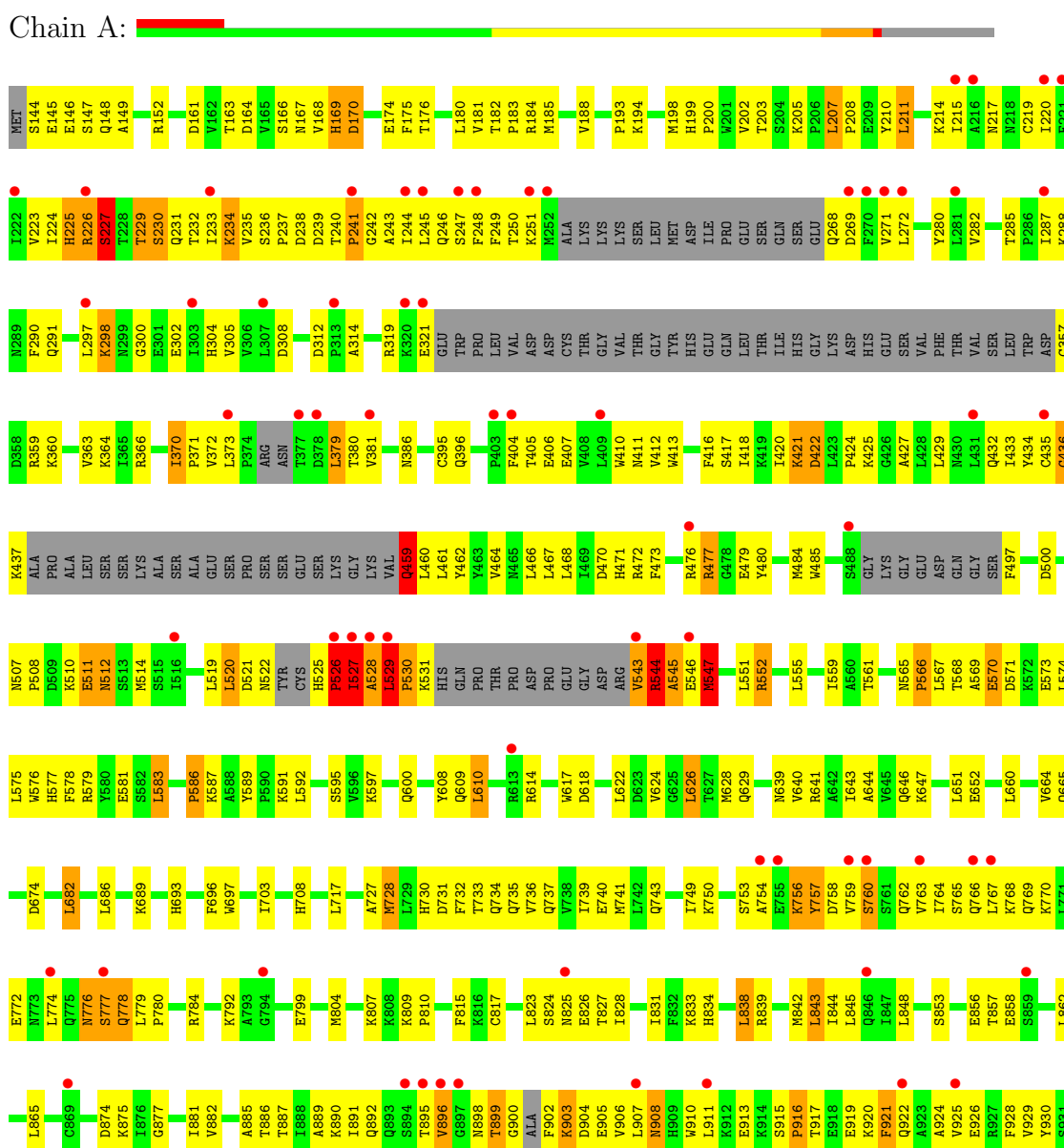
- Molecule 3 is water.

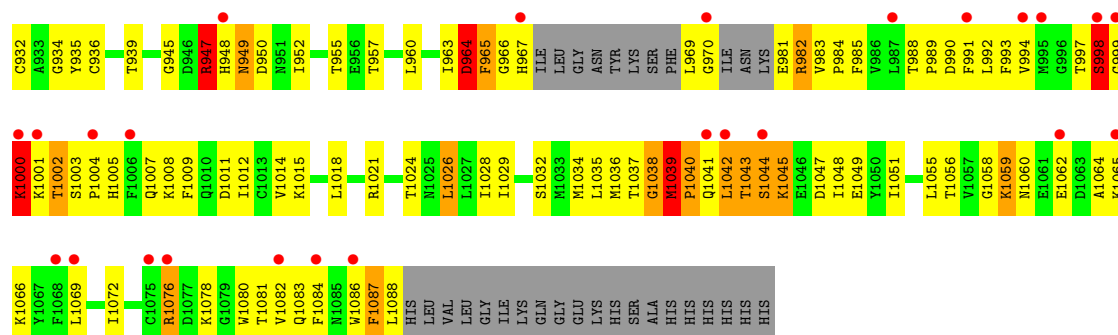
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		

3 Residue-property plots

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-bisphosphate3-kinase catalytic subunit gamma isoform





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.287 0.261 , 0.288	Depositor DCC
R_{free} test set	2348 reflections (10.97%)	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 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 44.

All (596) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:A:768:LYS:O	1:A:772:GLU:HG2	1.79	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

5.3.1 Protein backbone ⓘ

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%)	5 15

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
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

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Mol	Chain	Res	Type
1	A	242	GLY
1	A	436	GLY
1	A	1039	MET

5.3.2 Protein sidechains ⓘ

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%)	14	37

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains 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	1.79	5 (19%)	22,90,90	2.04	6 (27%)

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	0/0/11/11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	DW2	C3-C2	4.91	1.47	1.41
2	A	1	DW2	C5-C4	3.32	1.44	1.36
2	A	1	DW2	C6-N21	3.00	1.37	1.34
2	A	1	DW2	C7-N21	2.41	1.40	1.36
2	A	1	DW2	C6-C5	2.31	1.44	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	DW2	C6-N21-C7	4.25	119.95	117.18
2	A	1	DW2	C4-C3-C7	-4.06	114.69	117.90
2	A	1	DW2	C4-C3-C2	3.82	129.94	123.38
2	A	1	DW2	C29-C28-C23	3.67	108.58	105.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	DW2	C2-C3-C7	-2.56	115.38	119.26
2	A	1	DW2	C5-C6-N21	-2.17	119.70	122.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	839/966 (86%)	0.67	92 (10%) 6 5	20, 90, 141, 163	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	LEU	6.7
1	A	377	THR	5.8
1	A	248	PHE	5.6
1	A	1044	SER	5.5
1	A	529	LEU	5.2
1	A	1086	TRP	5.2
1	A	307	LEU	5.1
1	A	895	THR	5.0
1	A	215	ILE	4.7
1	A	270	PHE	4.6
1	A	244	ILE	4.5
1	A	221	PHE	4.3
1	A	241	PRO	4.1
1	A	911	LEU	4.1
1	A	233	ILE	4.0
1	A	907	LEU	3.9
1	A	759	VAL	3.8
1	A	222	ILE	3.7
1	A	825	ASN	3.7
1	A	303	ILE	3.7
1	A	403	PRO	3.7
1	A	526	PRO	3.6
1	A	220	ILE	3.6
1	A	281	LEU	3.6
1	A	998	SER	3.5
1	A	948	HIS	3.5
1	A	546	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	252	MET	3.5
1	A	320	LYS	3.4
1	A	1082	VAL	3.4
1	A	1075	CYS	3.4
1	A	272	LEU	3.4
1	A	528	ALA	3.3
1	A	378	ASP	3.3
1	A	613	ARG	3.2
1	A	1068	PHE	3.2
1	A	970	GLY	3.2
1	A	755	GLU	3.1
1	A	435	CYS	3.1
1	A	271	VAL	3.1
1	A	897	GLY	3.0
1	A	216	ALA	3.0
1	A	1041	GLN	3.0
1	A	1065	LYS	3.0
1	A	527	ILE	2.9
1	A	269	ASP	2.9
1	A	754	ALA	2.8
1	A	894	SER	2.8
1	A	1004	PRO	2.8
1	A	967	HIS	2.8
1	A	1084	PHE	2.8
1	A	995	MET	2.8
1	A	991	PHE	2.8
1	A	794	GLY	2.8
1	A	1042	LEU	2.8
1	A	404	PHE	2.7
1	A	226	ARG	2.7
1	A	543	VAL	2.6
1	A	999	GLY	2.6
1	A	922	GLN	2.6
1	A	859	SER	2.6
1	A	1006	PHE	2.6
1	A	476	ARG	2.5
1	A	247	SER	2.5
1	A	1069	LEU	2.5
1	A	287	ILE	2.5
1	A	896	VAL	2.5
1	A	409	LEU	2.5
1	A	987	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1001	LYS	2.4
1	A	488	SER	2.3
1	A	760	SER	2.3
1	A	774	LEU	2.3
1	A	763	VAL	2.3
1	A	245	LEU	2.2
1	A	1000	LYS	2.2
1	A	766	GLN	2.2
1	A	516	ILE	2.2
1	A	381	VAL	2.2
1	A	777	SER	2.2
1	A	846	GLN	2.2
1	A	297	LEU	2.1
1	A	251	LYS	2.1
1	A	869	CYS	2.1
1	A	1062	GLU	2.1
1	A	321	GLU	2.1
1	A	994	VAL	2.1
1	A	313	PRO	2.0
1	A	1076	ARG	2.0
1	A	767	LEU	2.0
1	A	925	VAL	2.0
1	A	431	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	DW2	A	1	31/31	0.26	0.94	158,161,191,191	0

6.5 Other polymers ⓘ

There are no such residues in this entry.