Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:27 am BST

PDB ID	:	6AAY
Title	:	the Cas13b binary complex
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Deposited on	:	2018-07-19
Resolution	:	2.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

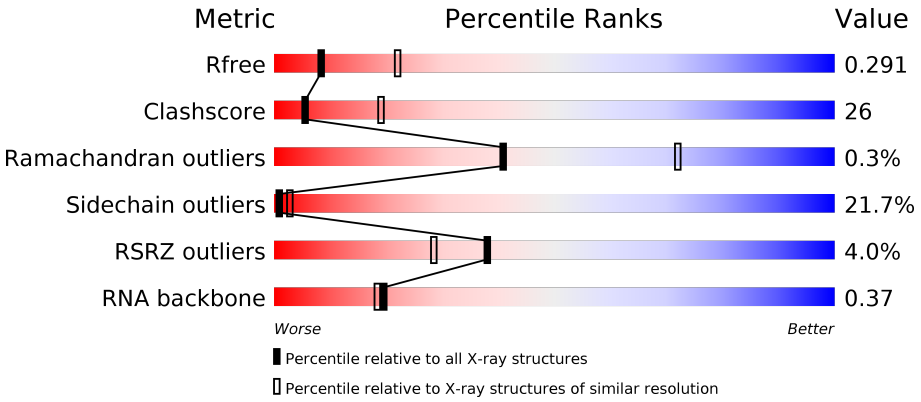
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	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)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1232	4% 51% 35% 11%
2	B	59	3% 34% 32% 20% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11262 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 Bergeyella zoohelcum Cas13b (R1177A) mutant.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1199	Total	C	N	O	S	Se	0	0	0
			10107	6494	1706	1888	7	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP K1LVU1
A	1177	ALA	ARG	engineered mutation	UNP K1LVU1
A	1225	LEU	-	expression tag	UNP K1LVU1
A	1226	GLU	-	expression tag	UNP K1LVU1
A	1227	HIS	-	expression tag	UNP K1LVU1
A	1228	HIS	-	expression tag	UNP K1LVU1
A	1229	HIS	-	expression tag	UNP K1LVU1
A	1230	HIS	-	expression tag	UNP K1LVU1
A	1231	HIS	-	expression tag	UNP K1LVU1
A	1232	HIS	-	expression tag	UNP K1LVU1

- Molecule 2 is a RNA chain called RNA (52-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	52	Total	C	N	O	P	0	0	0
			1118	501	210	355	52			

- Molecule 3 is water.

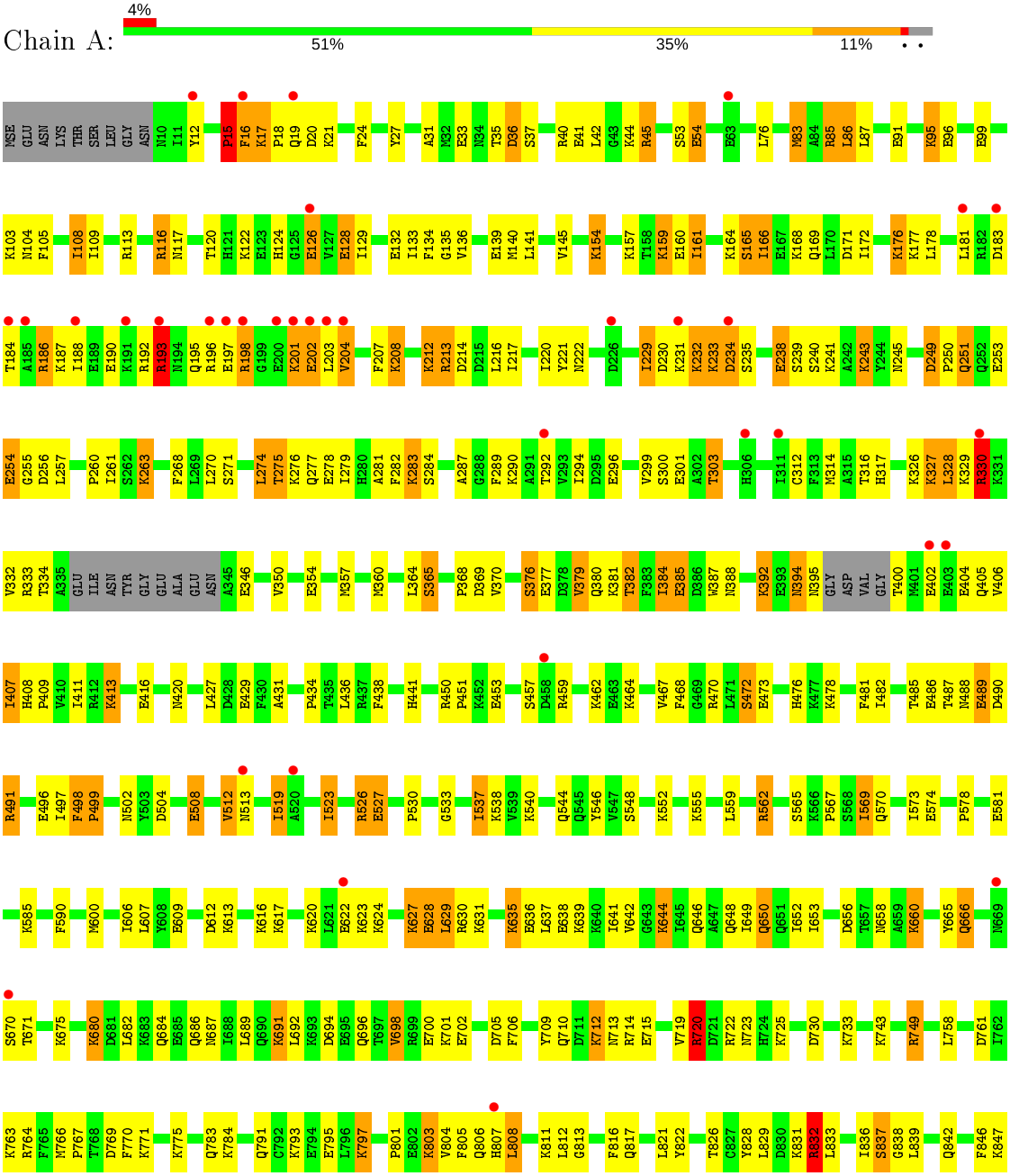
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	1	Total	O	0	0
			1	1		

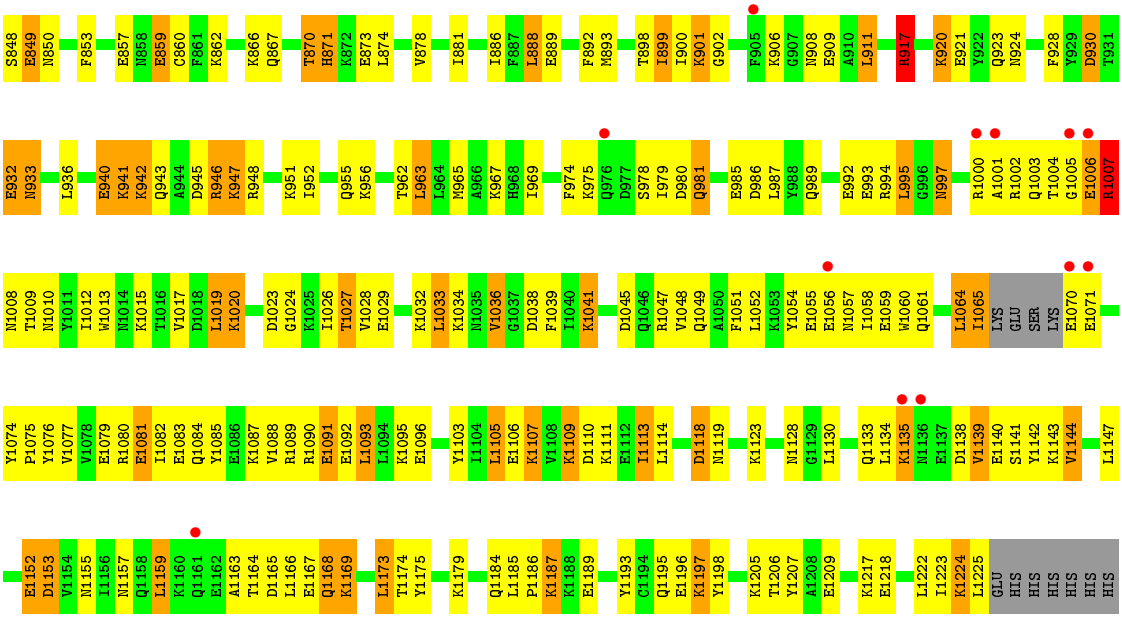
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Bergeyella zoohelcum Cas13b (R1177A) mutant

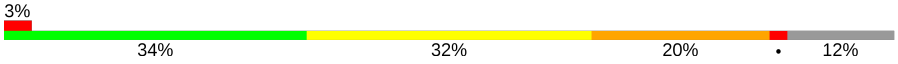
Chain A:

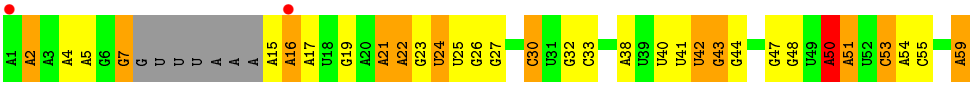




- Molecule 2: RNA (52-MER)

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	196.74Å 196.74Å 96.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.02 – 2.79 64.93 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.02-2.79) 99.9 (64.93-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.221 , 0.276 0.232 , 0.291	Depositor DCC
R_{free} test set	2390 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	72.3	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11262	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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

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	0.66	0/10294	0.77	6/13778 (0.0%)
2	B	0.84	7/1253 (0.6%)	0.81	0/1949
All	All	0.68	7/11547 (0.1%)	0.77	6/15727 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	23

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	22	A	O3'-P	-7.36	1.52	1.61
2	B	23	G	O3'-P	-7.17	1.52	1.61
2	B	47	G	O3'-P	-6.09	1.53	1.61
2	B	24	U	O3'-P	-5.94	1.54	1.61
2	B	25	U	O3'-P	-5.80	1.54	1.61
2	B	50	A	O3'-P	-5.55	1.54	1.61
2	B	48	G	O3'-P	-5.12	1.55	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	PRO	N-CA-CB	-11.34	89.69	103.30
1	A	499	PRO	CA-N-CD	-11.29	95.70	111.50
1	A	498	PHE	CB-CA-C	7.75	125.91	110.40
1	A	15	PRO	N-CD-CG	-7.01	92.68	103.20
1	A	16	PHE	CB-CA-C	6.22	122.83	110.40
1	A	499	PRO	CB-CA-C	5.14	124.86	112.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1002	ARG	Sidechain
1	A	1007	ARG	Sidechain
1	A	1047	ARG	Sidechain
1	A	1089	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	193	ARG	Sidechain
1	A	196	ARG	Sidechain
1	A	198	ARG	Sidechain
1	A	330	ARG	Sidechain
1	A	45	ARG	Sidechain
1	A	491	ARG	Sidechain
1	A	498	PHE	Mainchain
1	A	526	ARG	Sidechain
1	A	562	ARG	Sidechain
1	A	714	ARG	Sidechain
1	A	720	ARG	Sidechain
1	A	722	ARG	Sidechain
1	A	749	ARG	Sidechain
1	A	764	ARG	Sidechain
1	A	832	ARG	Sidechain
1	A	85	ARG	Sidechain
1	A	917	ARG	Sidechain
1	A	946	ARG	Sidechain

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	10107	0	10188	556	0
2	B	1118	0	562	36	0
3	A	36	0	0	0	0
3	B	1	0	0	0	0
All	All	11262	0	10750	567	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 26.

All (567) 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:947:LYS:HE3	1:A:951:LYS:CE	1.52	1.39
1:A:15:PRO:HA	1:A:24:PHE:CZ	1.70	1.26
1:A:1144:VAL:CG2	1:A:1163:ALA:HB2	1.65	1.25
1:A:979:ILE:CD1	1:A:1015:LYS:HD3	1.64	1.25
1:A:1084:GLN:O	1:A:1088:VAL:HG23	1.37	1.23
1:A:947:LYS:CE	1:A:951:LYS:HE2	1.72	1.17
1:A:250:PRO:HG2	1:A:263:LYS:HG2	1.18	1.16
1:A:330:ARG:HG3	2:B:16:A:C2	1.83	1.14
1:A:979:ILE:CD1	1:A:1015:LYS:CD	2.26	1.14
1:A:188:ILE:HD12	1:A:207:PHE:HB2	1.14	1.13
1:A:624:LYS:HG3	1:A:628:GLU:HG2	1.29	1.13
1:A:979:ILE:HD11	1:A:1015:LYS:CD	1.80	1.09
1:A:188:ILE:CD1	1:A:207:PHE:HB2	1.82	1.08
1:A:979:ILE:HD11	1:A:1015:LYS:HD3	1.12	1.07
1:A:232:LYS:HA	1:A:232:LYS:HE2	1.36	1.07
1:A:1081:GLU:HG3	1:A:1206:THR:HG23	1.28	1.06
1:A:1144:VAL:HG11	1:A:1159:LEU:HA	1.34	1.06
1:A:15:PRO:HA	1:A:24:PHE:HZ	0.92	1.05
1:A:45:ARG:NH1	1:A:329:LYS:HD2	1.71	1.05
1:A:1169:LYS:HD3	1:A:1218:GLU:OE1	1.57	1.04
1:A:1175:TYR:HE1	1:A:1186:PRO:HB3	1.24	1.01
1:A:41:GLU:OE1	1:A:328:LEU:HG	1.58	1.01
1:A:987:LEU:HD23	1:A:1012:ILE:HG21	1.39	1.00
1:A:394:ASN:HB3	1:A:1032:LYS:HZ1	1.23	1.00
1:A:696:GLN:HG2	1:A:826:THR:HG22	1.43	0.99
1:A:420:ASN:CG	1:A:600:MSE:HE2	1.82	0.99
1:A:360:MSE:CE	1:A:969:ILE:HD12	1.92	0.99
1:A:1144:VAL:HG21	1:A:1163:ALA:CB	1.93	0.98
1:A:1144:VAL:HG21	1:A:1163:ALA:HB2	0.98	0.97
1:A:832:ARG:HG2	1:A:832:ARG:HH11	1.27	0.96
1:A:427:LEU:O	1:A:431:ALA:HB3	1.65	0.96
1:A:250:PRO:CG	1:A:263:LYS:HG2	1.95	0.96
1:A:497:ILE:H	1:A:497:ILE:HD12	1.30	0.96
1:A:379:VAL:O	1:A:382:THR:HG23	1.66	0.95
1:A:141:LEU:O	1:A:145:VAL:HG13	1.67	0.94
1:A:15:PRO:CA	1:A:24:PHE:HZ	1.80	0.93
1:A:1070:GLU:OE2	1:A:1074:TYR:HB2	1.70	0.92
1:A:188:ILE:HD12	1:A:207:PHE:CB	1.98	0.92
1:A:775:LYS:HD2	2:B:59:A:O2'	1.70	0.91
1:A:987:LEU:CD2	1:A:1012:ILE:HG21	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLN:HG3	1:A:402:GLU:HG3	1.54	0.89
1:A:1144:VAL:HG11	1:A:1159:LEU:CA	2.02	0.89
1:A:184:THR:CG2	1:A:207:PHE:CE2	2.55	0.89
1:A:1033:LEU:O	1:A:1036:VAL:CG1	2.20	0.88
1:A:420:ASN:OD1	1:A:600:MSE:HE2	1.73	0.88
1:A:405:GLN:OE1	1:A:405:GLN:N	2.07	0.88
1:A:947:LYS:HE3	1:A:951:LYS:HE2	0.88	0.87
1:A:1033:LEU:O	1:A:1036:VAL:HG13	1.74	0.87
1:A:184:THR:HG23	1:A:207:PHE:CD2	2.09	0.87
1:A:793:LYS:HE2	1:A:816:PHE:O	1.74	0.87
1:A:666:GLN:HA	1:A:666:GLN:HE21	1.40	0.86
1:A:849:GLU:OE2	1:A:849:GLU:N	2.07	0.86
1:A:987:LEU:HD23	1:A:1012:ILE:CG2	2.06	0.86
1:A:451:PRO:HB3	1:A:457:SER:O	1.76	0.85
1:A:233:LYS:NZ	1:A:233:LYS:O	2.08	0.85
1:A:1175:TYR:CE1	1:A:1186:PRO:HB3	2.10	0.85
1:A:181:LEU:O	1:A:184:THR:HG22	1.78	0.84
1:A:250:PRO:HG2	1:A:263:LYS:CG	2.04	0.83
1:A:161:ILE:HD12	1:A:161:ILE:O	1.78	0.83
1:A:874:LEU:O	1:A:878:VAL:HG23	1.79	0.82
1:A:1084:GLN:O	1:A:1088:VAL:CG2	2.26	0.81
1:A:208:LYS:H	1:A:208:LYS:HD3	1.45	0.81
1:A:360:MSE:CE	1:A:969:ILE:CD1	2.59	0.81
1:A:1001:ALA:CB	1:A:1007:ARG:HB3	2.10	0.81
1:A:1081:GLU:CG	1:A:1206:THR:HG23	2.09	0.81
1:A:1060:TRP:HZ3	1:A:1081:GLU:OE2	1.64	0.80
1:A:1152:GLU:OE2	1:A:1187:LYS:HE3	1.81	0.80
1:A:665:TYR:CE2	1:A:871:HIS:HB2	2.15	0.80
1:A:671:THR:HA	1:A:871:HIS:CE1	2.17	0.80
1:A:1001:ALA:HB2	1:A:1007:ARG:HB3	1.63	0.80
1:A:1168:GLN:HG2	1:A:1193:TYR:OH	1.82	0.80
1:A:184:THR:HG21	1:A:207:PHE:CE2	2.16	0.80
1:A:427:LEU:O	1:A:431:ALA:CB	2.30	0.80
1:A:696:GLN:HG2	1:A:826:THR:CG2	2.11	0.79
1:A:609:GLU:HG3	1:A:893:MSE:CE	2.12	0.79
1:A:649:ILE:O	1:A:653:ILE:HG13	1.81	0.79
1:A:917:ARG:O	1:A:921:GLU:HG3	1.83	0.79
1:A:1142:TYR:HB3	1:A:1167:GLU:OE2	1.81	0.79
1:A:1175:TYR:OH	1:A:1187:LYS:HG2	1.82	0.79
1:A:208:LYS:HD3	1:A:208:LYS:N	1.97	0.78
1:A:1061:GLN:HG3	1:A:1074:TYR:CD2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.13	0.78
1:A:1061:GLN:HG2	1:A:1074:TYR:CE2	2.19	0.78
1:A:1205:LYS:HD2	1:A:1209:GLU:OE1	1.84	0.78
1:A:574:GLU:HG2	1:A:578:PRO:HA	1.65	0.78
1:A:1138:ASP:OD2	1:A:1166:LEU:HD23	1.84	0.77
1:A:947:LYS:CE	1:A:951:LYS:CE	2.47	0.77
1:A:395:ASN:H	1:A:1032:LYS:HZ1	1.33	0.77
1:A:254:GLU:O	1:A:254:GLU:HG2	1.83	0.77
1:A:126:GLU:O	1:A:128:GLU:HG3	1.86	0.75
1:A:1061:GLN:CG	1:A:1074:TYR:CD2	2.70	0.75
1:A:497:ILE:N	1:A:497:ILE:HD12	2.01	0.75
1:A:1060:TRP:CZ3	1:A:1081:GLU:OE2	2.40	0.75
1:A:17:LYS:HB2	1:A:257:LEU:HB2	1.67	0.75
1:A:650:GLN:NE2	1:A:650:GLN:O	2.20	0.75
1:A:906:LYS:NZ	2:B:40:U:H2'	2.02	0.75
1:A:1074:TYR:CD1	1:A:1075:PRO:HD2	2.21	0.75
1:A:1130:LEU:HD21	1:A:1222:LEU:HB3	1.66	0.75
1:A:462:LYS:HD3	1:A:496:GLU:OE1	1.86	0.75
1:A:1038:ASP:O	1:A:1041:LYS:HG2	1.86	0.74
1:A:997:ASN:HD22	1:A:997:ASN:N	1.86	0.73
1:A:1197:LYS:HG2	1:A:1198:TYR:CE1	2.24	0.73
1:A:360:MSE:HE1	1:A:969:ILE:CD1	2.17	0.73
1:A:763:LYS:HE3	2:B:24:U:OP1	1.88	0.73
1:A:462:LYS:HE3	2:B:21:A:C2	2.23	0.73
1:A:17:LYS:HD2	1:A:17:LYS:N	2.03	0.72
1:A:1019:LEU:O	1:A:1019:LEU:HD12	1.89	0.72
1:A:270:LEU:O	1:A:274:LEU:HB2	1.89	0.72
1:A:666:GLN:NE2	1:A:666:GLN:HA	2.05	0.72
1:A:275:THR:HG22	1:A:278:GLU:H	1.53	0.72
1:A:513:ASN:O	1:A:680:LYS:NZ	2.23	0.72
1:A:1175:TYR:HE1	1:A:1186:PRO:CB	2.01	0.71
1:A:420:ASN:OD1	1:A:600:MSE:CE	2.38	0.71
1:A:438:PHE:CE1	1:A:537:ILE:HD11	2.26	0.71
1:A:41:GLU:OE1	1:A:328:LEU:CG	2.38	0.71
1:A:811:LYS:HG3	1:A:813:GLY:H	1.56	0.71
1:A:1159:LEU:HD22	1:A:1159:LEU:O	1.90	0.71
1:A:1144:VAL:HG23	1:A:1163:ALA:HB2	1.72	0.71
1:A:624:LYS:CG	1:A:628:GLU:HG2	2.17	0.71
1:A:128:GLU:OE1	1:A:260:PRO:HG3	1.90	0.70
1:A:15:PRO:CA	1:A:24:PHE:CZ	2.61	0.70
1:A:369:ASP:OD1	1:A:413:LYS:CE	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:VAL:HG11	1:A:1039:PHE:CE2	2.27	0.69
1:A:232:LYS:HA	1:A:232:LYS:CE	2.16	0.69
1:A:277:GLN:CG	1:A:402:GLU:HG3	2.23	0.69
1:A:436:LEU:HD23	1:A:436:LEU:C	2.13	0.69
1:A:350:VAL:O	1:A:354:GLU:HG3	1.92	0.69
1:A:1159:LEU:HD22	1:A:1159:LEU:C	2.13	0.69
1:A:942:LYS:O	1:A:942:LYS:HG2	1.91	0.69
1:A:369:ASP:OD1	1:A:413:LYS:HE3	1.93	0.68
1:A:979:ILE:HD12	1:A:1015:LYS:CD	2.19	0.68
1:A:15:PRO:CD	1:A:21:LYS:HZ3	2.06	0.68
1:A:184:THR:HG23	1:A:207:PHE:CE2	2.23	0.68
1:A:1144:VAL:CG2	1:A:1163:ALA:CB	2.60	0.68
1:A:1169:LYS:HB3	1:A:1218:GLU:OE1	1.94	0.68
1:A:981:GLN:H	1:A:981:GLN:CD	1.96	0.68
1:A:828:TYR:CZ	1:A:832:ARG:HD2	2.28	0.68
1:A:377:GLU:HG3	1:A:381:LYS:HZ3	1.59	0.67
1:A:666:GLN:CA	1:A:666:GLN:HE21	2.03	0.67
1:A:234:ASP:OD2	2:B:7:G:N7	2.27	0.67
1:A:83:MSE:O	1:A:86:LEU:HB2	1.95	0.67
1:A:609:GLU:HG3	1:A:893:MSE:HE3	1.75	0.67
1:A:691:LYS:NZ	1:A:694:ASP:OD2	2.27	0.66
1:A:995:LEU:HD23	1:A:995:LEU:N	2.09	0.66
1:A:470:ARG:HB3	1:A:473:GLU:HG3	1.75	0.66
1:A:761:ASP:OD2	1:A:832:ARG:NE	2.29	0.66
1:A:232:LYS:CA	1:A:232:LYS:HE2	2.22	0.66
1:A:497:ILE:H	1:A:497:ILE:CD1	2.06	0.66
1:A:979:ILE:HD13	1:A:1015:LYS:HD3	1.73	0.66
1:A:141:LEU:O	1:A:145:VAL:CG1	2.42	0.66
1:A:395:ASN:H	1:A:1032:LYS:NZ	1.94	0.66
1:A:202:GLU:C	1:A:203:LEU:HD23	2.16	0.65
1:A:249:ASP:N	1:A:249:ASP:OD1	2.21	0.65
1:A:453:GLU:O	1:A:453:GLU:HG2	1.97	0.65
1:A:839:LEU:HD21	1:A:859:GLU:HG2	1.78	0.65
1:A:141:LEU:O	1:A:141:LEU:HD12	1.97	0.65
1:A:275:THR:O	1:A:279:ILE:HG22	1.97	0.65
1:A:644:LYS:HG3	1:A:892:PHE:HB2	1.79	0.65
1:A:523:ILE:O	1:A:523:ILE:HG13	1.95	0.64
1:A:1054:TYR:HD2	1:A:1207:TYR:CD2	2.16	0.64
1:A:965:MSE:O	1:A:969:ILE:HG13	1.97	0.64
1:A:1000:ARG:NH2	1:A:1007:ARG:HE	1.95	0.64
1:A:1081:GLU:HG3	1:A:1206:THR:CG2	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLU:OE2	1:A:193:ARG:HD2	1.98	0.64
1:A:201:LYS:C	1:A:202:GLU:OE2	2.36	0.64
1:A:696:GLN:CG	1:A:826:THR:HG22	2.24	0.64
1:A:1168:GLN:CG	1:A:1193:TYR:OH	2.46	0.64
1:A:317:HIS:CD2	1:A:406:VAL:HG11	2.33	0.64
1:A:192:ARG:NH1	1:A:204:VAL:O	2.24	0.63
1:A:660:LYS:H	1:A:660:LYS:CD	2.09	0.63
1:A:867:GLN:NE2	2:B:27:G:OP2	2.31	0.63
1:A:376:SER:OG	1:A:379:VAL:HG23	1.98	0.63
1:A:508:GLU:HB3	1:A:530:PRO:HG2	1.80	0.63
1:A:1153:ASP:OD1	1:A:1153:ASP:N	2.31	0.63
1:A:250:PRO:HG3	1:A:263:LYS:HE3	1.81	0.63
1:A:940:GLU:H	1:A:940:GLU:CD	2.01	0.63
1:A:330:ARG:HG3	2:B:16:A:N3	2.14	0.62
1:A:434:PRO:HG2	1:A:638:GLU:OE2	2.00	0.62
1:A:963:LEU:O	1:A:963:LEU:HD12	1.98	0.62
1:A:1007:ARG:NE	1:A:1009:THR:HB	2.14	0.62
1:A:360:MSE:HE2	1:A:969:ILE:HD12	1.79	0.62
1:A:1142:TYR:CE1	1:A:1167:GLU:HB2	2.35	0.61
1:A:519:ILE:HG22	1:A:519:ILE:O	2.01	0.61
1:A:997:ASN:HD22	1:A:997:ASN:H	1.47	0.61
1:A:1061:GLN:HG2	1:A:1074:TYR:CD2	2.34	0.61
1:A:388:ASN:O	1:A:392:LYS:HD2	2.00	0.61
1:A:438:PHE:CD1	1:A:537:ILE:HD11	2.36	0.61
1:A:1001:ALA:HB2	1:A:1007:ARG:CB	2.31	0.61
1:A:462:LYS:CD	1:A:496:GLU:OE1	2.48	0.61
1:A:698:VAL:O	1:A:702:GLU:HG3	2.00	0.61
1:A:947:LYS:CD	1:A:951:LYS:HE2	2.30	0.61
1:A:1187:LYS:NZ	1:A:1189:GLU:OE1	2.23	0.61
1:A:15:PRO:HA	1:A:24:PHE:CE1	2.33	0.61
1:A:544:GLN:HA	1:A:544:GLN:NE2	2.15	0.61
1:A:979:ILE:CD1	1:A:1015:LYS:HD2	2.25	0.61
1:A:19:GLN:HG2	1:A:19:GLN:O	2.01	0.60
1:A:394:ASN:HB3	1:A:1032:LYS:NZ	2.07	0.60
1:A:395:ASN:N	1:A:1032:LYS:HZ1	1.99	0.60
1:A:686:GLN:OE1	1:A:837:SER:HB2	2.02	0.60
1:A:1135:LYS:HE2	1:A:1222:LEU:O	2.01	0.60
1:A:947:LYS:HE3	1:A:951:LYS:HE3	1.69	0.60
1:A:1000:ARG:NH2	1:A:1007:ARG:NE	2.50	0.60
1:A:1033:LEU:O	1:A:1036:VAL:HG12	2.00	0.60
1:A:326:LYS:O	1:A:327:LYS:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:GLN:N	1:A:981:GLN:OE1	2.33	0.60
1:A:1038:ASP:O	1:A:1041:LYS:CD	2.50	0.60
1:A:793:LYS:O	1:A:797:LYS:HD3	2.02	0.60
1:A:979:ILE:HD11	1:A:1015:LYS:HD2	1.79	0.60
1:A:1001:ALA:HB1	1:A:1007:ARG:HB3	1.84	0.59
1:A:1009:THR:O	1:A:1009:THR:OG1	2.13	0.59
1:A:1110:ASP:O	1:A:1133:GLN:NE2	2.31	0.59
1:A:832:ARG:NH1	1:A:832:ARG:HG2	1.99	0.59
2:B:4:A:C5	2:B:5:A:C2	2.91	0.59
1:A:684:GLN:HA	1:A:684:GLN:OE1	2.02	0.59
1:A:15:PRO:CD	1:A:21:LYS:NZ	2.66	0.59
1:A:376:SER:OG	1:A:379:VAL:CG2	2.50	0.59
1:A:696:GLN:CG	1:A:826:THR:CG2	2.81	0.59
1:A:1055:GLU:HG3	1:A:1207:TYR:OH	2.03	0.59
1:A:232:LYS:O	1:A:232:LYS:HD3	2.02	0.58
1:A:20:ASP:C	1:A:21:LYS:HD3	2.24	0.58
1:A:920:LYS:HE3	2:B:42:U:OP1	2.03	0.58
1:A:243:LYS:O	1:A:245:ASN:ND2	2.35	0.58
1:A:360:MSE:HE1	1:A:969:ILE:HD11	1.84	0.58
1:A:801:PRO:HD2	1:A:804:VAL:CG2	2.34	0.58
1:A:613:LYS:NZ	1:A:636:GLU:OE2	2.35	0.58
1:A:775:LYS:HD2	2:B:59:A:HO2'	1.66	0.58
1:A:962:THR:HA	1:A:965:MSE:HE3	1.85	0.58
1:A:523:ILE:HG23	1:A:692:LEU:HD21	1.86	0.58
1:A:330:ARG:HD2	2:B:16:A:N3	2.19	0.58
1:A:202:GLU:O	1:A:203:LEU:HD23	2.02	0.58
1:A:660:LYS:HD3	1:A:660:LYS:N	2.19	0.57
1:A:87:LEU:HD22	1:A:104:ASN:HB2	1.86	0.57
1:A:848:SER:HB2	1:A:849:GLU:OE2	2.04	0.57
1:A:1007:ARG:CZ	1:A:1009:THR:HB	2.35	0.57
1:A:300:SER:O	1:A:303:THR:OG1	2.22	0.57
1:A:1070:GLU:OE2	1:A:1074:TYR:CB	2.50	0.57
1:A:1076:TYR:CD1	1:A:1076:TYR:N	2.72	0.57
1:A:1075:PRO:HB2	1:A:1076:TYR:CE1	2.39	0.57
1:A:527:GLU:OE2	1:A:527:GLU:N	2.37	0.57
1:A:154:LYS:HD3	1:A:221:TYR:HB3	1.87	0.57
1:A:1039:PHE:HD1	1:A:1039:PHE:H	1.53	0.57
1:A:377:GLU:CG	1:A:381:LYS:NZ	2.68	0.56
1:A:377:GLU:CG	1:A:381:LYS:HZ3	2.17	0.56
1:A:31:ALA:O	1:A:35:THR:HG23	2.05	0.56
1:A:979:ILE:CD1	1:A:1015:LYS:CE	2.82	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:PHE:N	1:A:1039:PHE:CD1	2.73	0.56
1:A:253:GLU:O	1:A:253:GLU:HG3	2.06	0.56
1:A:33:GLU:OE1	1:A:33:GLU:HA	2.06	0.56
1:A:1038:ASP:O	1:A:1041:LYS:CG	2.53	0.56
1:A:1224:LYS:O	1:A:1224:LYS:HE3	2.05	0.56
1:A:801:PRO:HD2	1:A:804:VAL:HG21	1.88	0.56
1:A:1054:TYR:HD2	1:A:1207:TYR:CE2	2.24	0.55
1:A:197:GLU:HA	1:A:197:GLU:OE2	2.04	0.55
1:A:370:VAL:HG21	1:A:951:LYS:HB2	1.88	0.55
1:A:135:GLY:O	1:A:139:GLU:HG2	2.07	0.55
1:A:1045:ASP:O	1:A:1049:GLN:HG3	2.06	0.55
1:A:192:ARG:HD2	1:A:204:VAL:O	2.06	0.55
1:A:116:ARG:O	1:A:120:THR:HG23	2.06	0.55
1:A:281:ALA:O	1:A:284:SER:OG	2.20	0.55
1:A:930:ASP:OD2	1:A:932:GLU:HB2	2.06	0.55
1:A:1142:TYR:CD1	1:A:1167:GLU:HB2	2.41	0.55
1:A:161:ILE:O	1:A:165:SER:OG	2.22	0.55
1:A:940:GLU:N	1:A:940:GLU:OE1	2.40	0.55
1:A:1074:TYR:O	1:A:1080:ARG:NH1	2.40	0.55
1:A:478:LYS:O	1:A:482:ILE:HG12	2.06	0.55
1:A:609:GLU:O	1:A:613:LYS:HG3	2.08	0.54
2:B:50:A:H5”	2:B:50:A:C8	2.43	0.54
1:A:574:GLU:CG	1:A:578:PRO:HA	2.36	0.54
1:A:901:LYS:HD3	1:A:902:GLY:H	1.72	0.54
1:A:974:PHE:CE1	1:A:1017:VAL:HG21	2.42	0.54
1:A:979:ILE:O	1:A:979:ILE:HG23	2.07	0.54
1:A:906:LYS:NZ	2:B:40:U:O2	2.40	0.54
1:A:1004:THR:HG23	1:A:1005:GLY:N	2.23	0.54
1:A:15:PRO:HG2	1:A:16:PHE:HD1	1.73	0.54
1:A:1123:LYS:HG3	1:A:1174:THR:HG21	1.89	0.53
1:A:866:LYS:O	1:A:870:THR:HG22	2.08	0.53
1:A:15:PRO:HD2	1:A:15:PRO:O	2.07	0.53
1:A:420:ASN:CB	1:A:600:MSE:HE2	2.38	0.53
1:A:612:ASP:OD2	1:A:616:LYS:HE2	2.09	0.53
1:A:1020:LYS:HA	1:A:1026:ILE:O	2.08	0.53
1:A:232:LYS:O	1:A:232:LYS:NZ	2.39	0.53
1:A:171:ASP:OD2	1:A:213:ARG:NH2	2.42	0.53
1:A:233:LYS:HD2	1:A:233:LYS:O	2.08	0.53
1:A:671:THR:HA	1:A:871:HIS:HE1	1.70	0.53
1:A:909:GLU:O	1:A:917:ARG:HD2	2.08	0.53
1:A:160:GLU:OE2	1:A:164:LYS:HE3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:VAL:HG21	1:A:951:LYS:CB	2.39	0.53
1:A:995:LEU:N	1:A:995:LEU:CD2	2.72	0.53
1:A:775:LYS:CD	2:B:59:A:O2'	2.52	0.52
1:A:27:TYR:CD2	1:A:282:PHE:HD1	2.28	0.52
1:A:429:GLU:OE1	1:A:472:SER:OG	2.24	0.52
1:A:660:LYS:CD	1:A:660:LYS:N	2.72	0.52
1:A:682:LEU:HD11	1:A:860:CYS:SG	2.49	0.52
1:A:462:LYS:CE	2:B:21:A:C2	2.92	0.52
1:A:533:GLY:O	1:A:600:MSE:CG	2.58	0.52
1:A:906:LYS:HZ2	2:B:40:U:H2'	1.73	0.52
1:A:232:LYS:CE	1:A:232:LYS:CA	2.85	0.52
1:A:630:ARG:HG2	1:A:630:ARG:HH11	1.75	0.52
2:B:15:A:H2'	2:B:16:A:H2'	1.91	0.52
2:B:4:A:N7	2:B:5:A:C2	2.78	0.52
1:A:95:LYS:O	1:A:99:GLU:HG3	2.09	0.51
1:A:346:GLU:OE1	1:A:476:HIS:HD2	1.94	0.51
1:A:650:GLN:NE2	1:A:650:GLN:CA	2.73	0.51
1:A:1163:ALA:HB1	1:A:1167:GLU:CD	2.30	0.51
1:A:357:MSE:O	1:A:357:MSE:HG2	2.10	0.51
1:A:400:THR:O	1:A:400:THR:HG23	2.10	0.51
1:A:901:LYS:HD2	1:A:901:LYS:H	1.75	0.51
1:A:192:ARG:HG2	1:A:204:VAL:HG23	1.92	0.51
1:A:212:LYS:HE2	1:A:214:ASP:OD1	2.11	0.51
1:A:948:ARG:O	1:A:952:ILE:HG12	2.10	0.51
1:A:1064:LEU:HG	1:A:1077:VAL:HG11	1.91	0.51
1:A:438:PHE:CD1	1:A:537:ILE:CD1	2.94	0.51
1:A:481:PHE:O	1:A:485:THR:HG23	2.11	0.51
1:A:652:ILE:HD13	1:A:881:ILE:HG21	1.93	0.51
1:A:1070:GLU:OE2	1:A:1074:TYR:N	2.43	0.51
1:A:828:TYR:OH	1:A:832:ARG:HD2	2.10	0.51
1:A:803:LYS:HD2	1:A:806:GLN:OE1	2.10	0.51
1:A:1175:TYR:OH	1:A:1187:LYS:CG	2.57	0.51
1:A:86:LEU:HB3	1:A:140:MSE:HG2	1.93	0.51
1:A:1061:GLN:HG3	1:A:1074:TYR:HD2	1.71	0.50
1:A:113:ARG:O	1:A:117:ASN:ND2	2.42	0.50
1:A:533:GLY:O	1:A:600:MSE:N	2.37	0.50
1:A:36:ASP:O	1:A:40:ARG:HG3	2.11	0.50
1:A:665:TYR:CZ	1:A:871:HIS:HB2	2.46	0.50
1:A:166:ILE:HG23	1:A:166:ILE:O	2.11	0.50
1:A:222:ASN:ND2	2:B:5:A:OP2	2.44	0.50
1:A:908:ASN:O	1:A:911:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:GLU:HA	1:A:1206:THR:HG21	1.94	0.50
1:A:268:PHE:O	1:A:271:SER:HB3	2.11	0.50
1:A:544:GLN:CA	1:A:544:GLN:NE2	2.75	0.50
1:A:464:LYS:NZ	1:A:504:ASP:OD1	2.44	0.50
1:A:948:ARG:O	1:A:952:ILE:CG1	2.60	0.50
1:A:767:PRO:HG2	1:A:770:PHE:HB3	1.94	0.50
1:A:395:ASN:C	1:A:1032:LYS:HE2	2.31	0.49
1:A:652:ILE:HD11	2:B:30:C:H41	1.76	0.49
1:A:166:ILE:HG12	1:A:169:GLN:NE2	2.28	0.49
1:A:606:ILE:HG13	1:A:893:MSE:HG3	1.94	0.49
1:A:1113:ILE:HG22	1:A:1128:ASN:HB3	1.94	0.49
1:A:1004:THR:HG23	1:A:1006:GLU:N	2.27	0.49
1:A:395:ASN:N	1:A:1032:LYS:NZ	2.59	0.49
1:A:997:ASN:N	1:A:997:ASN:ND2	2.59	0.49
1:A:1000:ARG:HH21	1:A:1007:ARG:NE	2.10	0.49
1:A:1107:LYS:O	1:A:1134:LEU:HD11	2.13	0.49
1:A:1061:GLN:CG	1:A:1074:TYR:CE2	2.90	0.49
1:A:238:GLU:HA	1:A:241:LYS:HD2	1.95	0.49
1:A:650:GLN:HA	1:A:650:GLN:NE2	2.26	0.49
1:A:986:ASP:CG	1:A:1010:ASN:HB3	2.34	0.49
1:A:1058:ILE:HD13	1:A:1076:TYR:CE2	2.48	0.49
1:A:485:THR:O	1:A:485:THR:OG1	2.21	0.49
1:A:427:LEU:HA	1:A:431:ALA:HB2	1.95	0.48
1:A:1075:PRO:HG2	1:A:1076:TYR:CD1	2.48	0.48
1:A:1109:LYS:HA	1:A:1109:LYS:HD3	1.55	0.48
1:A:487:THR:OG1	1:A:488:ASN:N	2.46	0.48
1:A:979:ILE:HD12	1:A:1015:LYS:CE	2.43	0.48
1:A:1139:VAL:CG1	1:A:1141:SER:HB2	2.42	0.48
1:A:87:LEU:CD2	1:A:104:ASN:HB2	2.43	0.48
1:A:376:SER:O	1:A:380:GLN:HG3	2.13	0.48
1:A:489:GLU:H	1:A:489:GLU:HG2	1.34	0.48
1:A:985:GLU:O	1:A:985:GLU:HG2	2.14	0.48
1:A:263:LYS:HE2	1:A:287:ALA:O	2.13	0.48
1:A:296:GLU:O	1:A:296:GLU:HG3	2.14	0.48
1:A:650:GLN:HE21	1:A:650:GLN:C	2.13	0.48
1:A:963:LEU:O	1:A:967:LYS:HG3	2.14	0.48
1:A:1001:ALA:CB	1:A:1007:ARG:CB	2.87	0.48
1:A:1195:GLN:HA	1:A:1195:GLN:OE1	2.14	0.48
1:A:691:LYS:HD3	1:A:691:LYS:HA	1.61	0.48
1:A:846:PHE:N	1:A:846:PHE:CD1	2.80	0.48
1:A:104:ASN:O	1:A:108:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:GLN:OE1	1:A:889:GLU:HG3	2.14	0.48
1:A:624:LYS:HG3	1:A:628:GLU:CG	2.22	0.47
1:A:689:LEU:HD11	1:A:832:ARG:NH2	2.29	0.47
1:A:87:LEU:CD2	1:A:104:ASN:CB	2.93	0.47
1:A:1048:VAL:O	1:A:1052:LEU:HG	2.14	0.47
1:A:1105:LEU:HD23	1:A:1105:LEU:HA	1.70	0.47
2:B:54:A:C6	2:B:55:C:C4	3.02	0.47
1:A:1007:ARG:NH1	1:A:1009:THR:HA	2.29	0.47
1:A:1019:LEU:HD11	1:A:1028:VAL:HB	1.95	0.47
1:A:160:GLU:HB3	1:A:384:ILE:HD11	1.97	0.47
1:A:644:LYS:O	1:A:644:LYS:HD2	2.14	0.47
1:A:848:SER:C	1:A:849:GLU:OE2	2.53	0.47
1:A:533:GLY:O	1:A:600:MSE:CB	2.63	0.47
1:A:17:LYS:H	1:A:17:LYS:HD2	1.77	0.47
1:A:134:PHE:HE1	1:A:261:ILE:HG13	1.78	0.47
1:A:360:MSE:HE2	1:A:969:ILE:CD1	2.40	0.47
1:A:365:SER:HG	1:A:1013:TRP:HZ2	1.61	0.47
1:A:145:VAL:HG22	1:A:229:ILE:HD11	1.97	0.47
1:A:256:ASP:HB3	1:A:257:LEU:H	1.53	0.47
1:A:533:GLY:O	1:A:600:MSE:HG2	2.15	0.47
1:A:468:PHE:HB2	1:A:590:PHE:HB2	1.97	0.47
1:A:838:GLY:O	1:A:842:GLN:HB2	2.15	0.47
1:A:898:THR:OG1	2:B:43:G:H2'	2.14	0.46
1:A:1061:GLN:HG2	1:A:1074:TYR:HE2	1.77	0.46
1:A:1164:THR:HB	1:A:1167:GLU:HB3	1.96	0.46
1:A:15:PRO:HD3	1:A:21:LYS:NZ	2.30	0.46
1:A:1054:TYR:CD2	1:A:1207:TYR:CD2	2.99	0.46
1:A:1020:LYS:HB3	1:A:1024:GLY:HA2	1.97	0.46
1:A:234:ASP:OD1	1:A:234:ASP:N	2.49	0.46
1:A:27:TYR:CD2	1:A:282:PHE:CD1	3.04	0.46
1:A:635:LYS:HE2	1:A:635:LYS:HB2	1.49	0.46
1:A:15:PRO:HD2	1:A:21:LYS:NZ	2.30	0.46
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.70	0.46
1:A:1168:GLN:HG2	1:A:1193:TYR:HH	1.81	0.46
1:A:665:TYR:CE2	1:A:871:HIS:CB	2.95	0.46
1:A:822:TYR:O	1:A:826:THR:HG23	2.16	0.46
1:A:1087:LYS:O	1:A:1091:GLU:HB2	2.16	0.46
1:A:128:GLU:OE1	1:A:260:PRO:CG	2.62	0.46
1:A:637:LEU:O	1:A:641:ILE:HD12	2.16	0.46
1:A:696:GLN:O	1:A:700:GLU:HG3	2.16	0.46
1:A:1093:LEU:O	1:A:1093:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:PRO:HB2	1:A:1076:TYR:CD1	2.51	0.45
1:A:1128:ASN:ND2	1:A:1147:LEU:HD21	2.31	0.45
1:A:364:LEU:HB3	1:A:987:LEU:HD13	1.98	0.45
1:A:712:LYS:HE3	1:A:715:GLU:OE1	2.16	0.45
1:A:967:LYS:HD2	1:A:980:ASP:HA	1.98	0.45
1:A:519:ILE:HD12	1:A:519:ILE:HA	1.79	0.45
1:A:569:ILE:HG12	1:A:569:ILE:H	1.65	0.45
1:A:253:GLU:C	1:A:255:GLY:H	2.19	0.45
1:A:54:GLU:HG2	1:A:54:GLU:H	1.44	0.45
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.75	0.45
1:A:627:LYS:HE2	1:A:631:LYS:HE3	1.98	0.45
1:A:761:ASP:OD2	1:A:828:TYR:OH	2.26	0.45
1:A:453:GLU:H	1:A:453:GLU:CD	2.20	0.45
1:A:648:GLN:NE2	1:A:886:ILE:CG2	2.80	0.45
1:A:930:ASP:OD1	1:A:933:ASN:OD1	2.35	0.45
1:A:979:ILE:HD12	1:A:1015:LYS:HE2	1.99	0.45
1:A:202:GLU:N	1:A:202:GLU:OE2	2.50	0.45
1:A:312:CYS:O	1:A:316:THR:HG22	2.17	0.45
1:A:888:LEU:HD12	1:A:888:LEU:HA	1.76	0.45
1:A:933:ASN:OD1	1:A:933:ASN:N	2.49	0.45
1:A:1083:GLU:O	1:A:1084:GLN:C	2.55	0.44
1:A:1103:TYR:CE2	1:A:1223:ILE:HD13	2.52	0.44
1:A:233:LYS:HD2	1:A:233:LYS:HA	1.67	0.44
1:A:250:PRO:CG	1:A:263:LYS:HE3	2.46	0.44
1:A:274:LEU:HG	1:A:278:GLU:HB3	2.00	0.44
1:A:803:LYS:HD2	1:A:803:LYS:HA	1.73	0.44
1:A:899:ILE:HG12	2:B:44:G:O4'	2.17	0.44
1:A:385:GLU:OE1	1:A:994:ARG:NH1	2.32	0.44
1:A:656:ASP:OD1	1:A:658:ASN:HB2	2.17	0.44
1:A:828:TYR:CE1	1:A:832:ARG:HD2	2.52	0.44
1:A:1048:VAL:HG23	1:A:1082:ILE:HD11	1.97	0.44
1:A:1065:ILE:HD13	1:A:1065:ILE:HA	1.73	0.44
1:A:533:GLY:O	1:A:600:MSE:HB2	2.18	0.44
2:B:32:G:H2'	2:B:33:C:O4'	2.18	0.44
1:A:906:LYS:CE	2:B:40:U:H2'	2.47	0.44
1:A:1033:LEU:HD22	1:A:1036:VAL:HG11	2.00	0.44
1:A:832:ARG:NH1	1:A:832:ARG:CG	2.73	0.44
1:A:478:LYS:O	1:A:482:ILE:CG1	2.66	0.44
1:A:730:ASP:OD1	1:A:730:ASP:N	2.51	0.44
1:A:1075:PRO:HG2	1:A:1076:TYR:CE1	2.53	0.44
1:A:1163:ALA:HB1	1:A:1167:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:GLU:HG3	1:A:893:MSE:HE2	1.97	0.44
1:A:184:THR:O	1:A:188:ILE:HG13	2.17	0.44
1:A:629:LEU:HD23	1:A:629:LEU:HA	1.66	0.44
1:A:1038:ASP:O	1:A:1041:LYS:HD3	2.18	0.44
1:A:190:GLU:HA	1:A:193:ARG:HB3	2.00	0.44
1:A:86:LEU:N	1:A:86:LEU:HD23	2.33	0.44
1:A:1134:LEU:HB3	1:A:1135:LYS:H	1.39	0.44
1:A:706:PHE:CZ	1:A:743:LYS:HD3	2.52	0.44
1:A:159:LYS:HB3	1:A:159:LYS:HE2	1.49	0.43
1:A:249:ASP:CB	1:A:250:PRO:HD3	2.47	0.43
1:A:364:LEU:CB	1:A:987:LEU:HD13	2.48	0.43
1:A:364:LEU:HB3	1:A:987:LEU:CD1	2.48	0.43
2:B:51:A:O2'	2:B:53:C:OP2	2.30	0.43
1:A:467:VAL:HG12	1:A:573:ILE:HD13	2.00	0.43
1:A:652:ILE:HG22	1:A:878:VAL:HG13	2.01	0.43
1:A:805:PHE:HA	1:A:808:LEU:HD22	2.01	0.43
1:A:979:ILE:HD12	1:A:1015:LYS:HD2	1.97	0.43
1:A:652:ILE:CD1	2:B:30:C:H41	2.32	0.43
1:A:1185:LEU:HA	1:A:1185:LEU:HD23	1.85	0.43
1:A:330:ARG:HH21	2:B:17:A:H5"	1.83	0.43
1:A:232:LYS:C	1:A:232:LYS:HD3	2.38	0.43
1:A:408:HIS:CG	1:A:408:HIS:O	2.71	0.43
1:A:642:VAL:O	1:A:646:GLN:HG3	2.19	0.43
1:A:1144:VAL:HG11	1:A:1159:LEU:N	2.33	0.43
1:A:1058:ILE:CD1	1:A:1076:TYR:CE2	3.02	0.43
1:A:546:TYR:CD1	1:A:546:TYR:N	2.85	0.43
2:B:26:G:H2'	2:B:27:G:C8	2.53	0.43
2:B:50:A:H5"	2:B:50:A:H8	1.83	0.43
1:A:377:GLU:O	1:A:381:LYS:HG3	2.19	0.43
1:A:544:GLN:HE21	1:A:544:GLN:CA	2.31	0.43
1:A:712:LYS:HE3	1:A:715:GLU:CD	2.39	0.43
1:A:83:MSE:SE	1:A:87:LEU:HD12	2.68	0.43
1:A:124:HIS:C	1:A:124:HIS:ND1	2.72	0.43
1:A:213:ARG:O	1:A:217:ILE:HG12	2.19	0.43
1:A:523:ILE:HG23	1:A:692:LEU:CD2	2.49	0.43
1:A:128:GLU:HG2	1:A:260:PRO:HD3	2.01	0.42
1:A:216:LEU:O	1:A:220:ILE:HD12	2.18	0.42
1:A:763:LYS:O	1:A:771:LYS:HE3	2.19	0.42
2:B:38:A:C2	2:B:44:G:C6	3.08	0.42
1:A:512:VAL:HG23	1:A:512:VAL:O	2.19	0.42
1:A:600:MSE:HB3	1:A:600:MSE:HE3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:HZ1	2:B:2:A:H2	1.66	0.42
1:A:116:ARG:HD3	1:A:120:THR:HG21	2.01	0.42
1:A:388:ASN:O	1:A:392:LYS:CD	2.65	0.42
1:A:411:ILE:HG22	1:A:413:LYS:HB3	2.00	0.42
1:A:41:GLU:O	1:A:45:ARG:HG3	2.19	0.42
1:A:527:GLU:N	1:A:527:GLU:CD	2.73	0.42
1:A:986:ASP:OD2	1:A:1010:ASN:HB3	2.19	0.42
1:A:299:VAL:O	1:A:299:VAL:HG13	2.19	0.42
1:A:901:LYS:CD	1:A:901:LYS:H	2.31	0.42
1:A:941:LYS:HA	1:A:941:LYS:HD3	1.61	0.42
1:A:1165:ASP:O	1:A:1169:LYS:HG2	2.18	0.42
1:A:1175:TYR:HH	1:A:1187:LYS:HG2	1.82	0.42
1:A:377:GLU:CD	1:A:381:LYS:NZ	2.72	0.42
1:A:540:LYS:HE3	1:A:581:GLU:HG3	2.00	0.42
1:A:652:ILE:HD13	1:A:881:ILE:CG2	2.48	0.42
1:A:694:ASP:O	1:A:698:VAL:HG13	2.19	0.42
1:A:1179:LYS:HD2	1:A:1186:PRO:HA	2.01	0.42
1:A:195:GLN:HB3	1:A:203:LEU:HD22	2.00	0.42
1:A:1003:GLN:N	1:A:1003:GLN:OE1	2.52	0.42
1:A:136:VAL:HA	1:A:139:GLU:CG	2.50	0.42
1:A:392:LYS:NZ	1:A:404:GLU:HG2	2.34	0.42
1:A:407:ILE:HG22	1:A:409:PRO:HD3	2.01	0.42
1:A:719:VAL:CG1	1:A:725:LYS:HB2	2.50	0.42
1:A:963:LEU:HD12	1:A:967:LYS:HG3	2.02	0.42
1:A:660:LYS:HE2	2:B:30:C:O2	2.20	0.42
1:A:1027:THR:CG2	1:A:1059:GLU:OE2	2.68	0.42
1:A:370:VAL:HG13	1:A:952:ILE:HD13	2.02	0.42
1:A:441:HIS:CD2	1:A:464:LYS:HG3	2.54	0.42
1:A:701:LYS:NZ	1:A:705:ASP:OD1	2.53	0.42
1:A:836:ILE:HD13	1:A:836:ILE:HA	1.82	0.42
1:A:251:GLN:HB2	1:A:251:GLN:HE21	1.65	0.42
1:A:283:LYS:HG3	1:A:289:PHE:HB3	2.01	0.42
1:A:763:LYS:HA	1:A:766:MSE:HE3	2.01	0.42
1:A:436:LEU:CD2	1:A:436:LEU:C	2.85	0.42
1:A:720:ARG:H	1:A:720:ARG:CD	2.33	0.42
1:A:940:GLU:N	1:A:940:GLU:CD	2.72	0.42
1:A:177:LYS:HD2	1:A:177:LYS:HA	1.79	0.41
1:A:368:PRO:HB3	1:A:955:GLN:HG2	2.03	0.41
1:A:807:HIS:CG	1:A:807:HIS:O	2.73	0.41
1:A:562:ARG:NH1	1:A:567:PRO:O	2.51	0.41
1:A:901:LYS:CD	1:A:901:LYS:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:LYS:HE3	2:B:41:U:OP1	2.20	0.41
1:A:1061:GLN:CG	1:A:1074:TYR:HD2	2.28	0.41
1:A:1092:GLU:O	1:A:1096:GLU:HG3	2.20	0.41
1:A:18:PRO:O	1:A:20:ASP:N	2.47	0.41
1:A:208:LYS:HG2	1:A:208:LYS:O	2.21	0.41
1:A:801:PRO:HD2	1:A:804:VAL:HG23	2.03	0.41
2:B:53:C:O5'	2:B:53:C:H6	2.02	0.41
1:A:1007:ARG:CZ	1:A:1009:THR:CB	2.99	0.41
1:A:1087:LYS:O	1:A:1091:GLU:CB	2.69	0.41
1:A:1128:ASN:O	1:A:1133:GLN:HG3	2.20	0.41
1:A:166:ILE:CG2	1:A:166:ILE:O	2.68	0.41
1:A:15:PRO:O	1:A:18:PRO:HD3	2.20	0.41
1:A:176:LYS:HE3	1:A:301:GLU:O	2.21	0.41
1:A:1057:ASN:HD22	1:A:1057:ASN:HA	1.73	0.41
1:A:451:PRO:CB	1:A:457:SER:O	2.57	0.41
1:A:712:LYS:HA	1:A:712:LYS:HD2	1.77	0.41
1:A:758:LEU:HA	1:A:758:LEU:HD23	1.88	0.41
1:A:1085:TYR:CD1	1:A:1085:TYR:C	2.94	0.41
1:A:1147:LEU:HD12	1:A:1147:LEU:HA	1.76	0.41
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.80	0.41
1:A:15:PRO:C	1:A:24:PHE:CZ	2.94	0.41
1:A:675:LYS:HG2	1:A:853:PHE:CE2	2.56	0.41
1:A:719:VAL:HG12	1:A:725:LYS:HB2	2.03	0.41
1:A:1173:LEU:HA	1:A:1173:LEU:HD22	1.93	0.40
1:A:168:LYS:HB3	1:A:296:GLU:OE1	2.21	0.40
1:A:613:LYS:O	1:A:617:LYS:HG3	2.20	0.40
1:A:682:LEU:HD23	1:A:682:LEU:HA	1.88	0.40
1:A:1060:TRP:CE3	1:A:1076:TYR:HB3	2.55	0.40
1:A:671:THR:HA	1:A:871:HIS:ND1	2.35	0.40
1:A:831:LYS:HD2	1:A:831:LYS:HA	1.77	0.40
1:A:1133:GLN:O	1:A:1134:LEU:HD12	2.21	0.40
1:A:270:LEU:HB3	1:A:274:LEU:HD22	2.02	0.40
1:A:168:LYS:O	1:A:172:ILE:HG13	2.22	0.40
1:A:709:TYR:CE1	1:A:713:ASN:ND2	2.89	0.40
1:A:979:ILE:CG2	1:A:979:ILE:O	2.70	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	1191/1232 (97%)	1140 (96%)	48 (4%)	3 (0%)	41 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	PRO
1	A	499	PRO
1	A	1135	LYS

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	1104/1119 (99%)	864 (78%)	240 (22%)	1 3

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	17	LYS
1	A	36	ASP
1	A	37	SER
1	A	42	LEU
1	A	44	LYS
1	A	53	SER
1	A	54	GLU

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Mol	Chain	Res	Type
1	A	76	LEU
1	A	83	MSE
1	A	85	ARG
1	A	86	LEU
1	A	91	GLU
1	A	95	LYS
1	A	96	GLU
1	A	103	LYS
1	A	105	PHE
1	A	108	ILE
1	A	109	ILE
1	A	116	ARG
1	A	122	LYS
1	A	126	GLU
1	A	128	GLU
1	A	129	ILE
1	A	132	GLU
1	A	133	ILE
1	A	154	LYS
1	A	157	LYS
1	A	159	LYS
1	A	161	ILE
1	A	165	SER
1	A	166	ILE
1	A	176	LYS
1	A	183	ASP
1	A	186	ARG
1	A	187	LYS
1	A	193	ARG
1	A	198	ARG
1	A	201	LYS
1	A	202	GLU
1	A	204	VAL
1	A	208	LYS
1	A	212	LYS
1	A	213	ARG
1	A	229	ILE
1	A	230	ASP
1	A	231	LYS
1	A	232	LYS
1	A	233	LYS
1	A	234	ASP

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Mol	Chain	Res	Type
1	A	235	SER
1	A	238	GLU
1	A	239	SER
1	A	240	SER
1	A	243	LYS
1	A	249	ASP
1	A	251	GLN
1	A	254	GLU
1	A	263	LYS
1	A	274	LEU
1	A	275	THR
1	A	276	LYS
1	A	283	LYS
1	A	290	LYS
1	A	292	THR
1	A	294	ILE
1	A	303	THR
1	A	314	MSE
1	A	327	LYS
1	A	328	LEU
1	A	330	ARG
1	A	332	VAL
1	A	333	ARG
1	A	334	THR
1	A	365	SER
1	A	376	SER
1	A	379	VAL
1	A	382	THR
1	A	384	ILE
1	A	385	GLU
1	A	387	TRP
1	A	392	LYS
1	A	394	ASN
1	A	407	ILE
1	A	413	LYS
1	A	416	GLU
1	A	450	ARG
1	A	459	ARG
1	A	472	SER
1	A	486	GLU
1	A	489	GLU
1	A	490	ASP

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Mol	Chain	Res	Type
1	A	491	ARG
1	A	502	ASN
1	A	508	GLU
1	A	512	VAL
1	A	519	ILE
1	A	523	ILE
1	A	526	ARG
1	A	527	GLU
1	A	537	ILE
1	A	538	LYS
1	A	548	SER
1	A	552	LYS
1	A	555	LYS
1	A	559	LEU
1	A	565	SER
1	A	569	ILE
1	A	570	GLN
1	A	585	LYS
1	A	607	LEU
1	A	620	LYS
1	A	622	GLU
1	A	623	LYS
1	A	627	LYS
1	A	628	GLU
1	A	629	LEU
1	A	635	LYS
1	A	639	LYS
1	A	644	LYS
1	A	650	GLN
1	A	660	LYS
1	A	666	GLN
1	A	670	SER
1	A	680	LYS
1	A	687	ASN
1	A	691	LYS
1	A	698	VAL
1	A	710	GLN
1	A	712	LYS
1	A	720	ARG
1	A	723	ASN
1	A	733	LYS
1	A	749	ARG

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Mol	Chain	Res	Type
1	A	769	ASP
1	A	783	GLN
1	A	784	LYS
1	A	791	GLN
1	A	795	GLU
1	A	797	LYS
1	A	803	LYS
1	A	808	LEU
1	A	812	LEU
1	A	817	GLN
1	A	821	LEU
1	A	829	LEU
1	A	832	ARG
1	A	833	LEU
1	A	837	SER
1	A	847	LYS
1	A	849	GLU
1	A	850	ASN
1	A	857	GLU
1	A	859	GLU
1	A	862	LYS
1	A	870	THR
1	A	871	HIS
1	A	873	GLU
1	A	888	LEU
1	A	899	ILE
1	A	900	ILE
1	A	901	LYS
1	A	911	LEU
1	A	917	ARG
1	A	920	LYS
1	A	923	GLN
1	A	924	ASN
1	A	928	PHE
1	A	930	ASP
1	A	932	GLU
1	A	933	ASN
1	A	936	LEU
1	A	940	GLU
1	A	941	LYS
1	A	942	LYS
1	A	943	GLN

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Mol	Chain	Res	Type
1	A	945	ASP
1	A	946	ARG
1	A	947	LYS
1	A	956	LYS
1	A	963	LEU
1	A	975	LYS
1	A	978	SER
1	A	981	GLN
1	A	989	GLN
1	A	992	GLU
1	A	993	GLU
1	A	995	LEU
1	A	997	ASN
1	A	1006	GLU
1	A	1007	ARG
1	A	1008	ASN
1	A	1019	LEU
1	A	1020	LYS
1	A	1023	ASP
1	A	1027	THR
1	A	1029	GLU
1	A	1033	LEU
1	A	1034	LYS
1	A	1036	VAL
1	A	1041	LYS
1	A	1051	PHE
1	A	1056	GLU
1	A	1064	LEU
1	A	1065	ILE
1	A	1071	GLU
1	A	1079	GLU
1	A	1081	GLU
1	A	1090	ARG
1	A	1091	GLU
1	A	1093	LEU
1	A	1095	LYS
1	A	1105	LEU
1	A	1106	GLU
1	A	1107	LYS
1	A	1109	LYS
1	A	1111	LYS
1	A	1113	ILE

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Mol	Chain	Res	Type
1	A	1114	LEU
1	A	1118	ASP
1	A	1119	ASN
1	A	1139	VAL
1	A	1140	GLU
1	A	1143	LYS
1	A	1144	VAL
1	A	1152	GLU
1	A	1153	ASP
1	A	1155	ASN
1	A	1157	ASN
1	A	1159	LEU
1	A	1168	GLN
1	A	1169	LYS
1	A	1173	LEU
1	A	1184	GLN
1	A	1187	LYS
1	A	1196	GLU
1	A	1197	LYS
1	A	1217	LYS
1	A	1224	LYS
1	A	1225	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	245	ASN
1	A	264	ASN
1	A	454	ASN
1	A	476	HIS
1	A	544	GLN
1	A	650	GLN
1	A	666	GLN
1	A	723	ASN
1	A	760	ASN
1	A	908	ASN
1	A	997	ASN
1	A	1057	ASN
1	A	1155	ASN
1	A	1168	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	50/59 (84%)	13 (26%)	3 (6%)

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	A
2	B	7	G
2	B	16	A
2	B	19	G
2	B	21	A
2	B	22	A
2	B	30	C
2	B	42	U
2	B	43	G
2	B	50	A
2	B	51	A
2	B	53	C
2	B	59	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	16	A
2	B	21	A
2	B	50	A

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

There are no ligands in this entry.

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	1187/1232 (96%)	0.44	48 (4%) 38 28	30, 68, 110, 163	0
2	B	52/59 (88%)	0.14	2 (3%) 40 30	42, 59, 139, 148	0
All	All	1239/1291 (95%)	0.43	50 (4%) 38 28	30, 68, 113, 163	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	GLU	5.7
1	A	1071	GLU	5.5
1	A	198	ARG	5.2
1	A	669	ASN	4.8
1	A	181	LEU	4.4
1	A	204	VAL	4.0
1	A	191	LYS	3.9
1	A	403	GLU	3.9
1	A	1136	ASN	3.7
1	A	234	ASP	3.5
1	A	520	ALA	3.4
1	A	670	SER	3.3
1	A	1056	GLU	3.3
1	A	12	TYR	3.2
1	A	226	ASP	3.2
1	A	197	GLU	3.1
1	A	622	GLU	3.1
1	A	1000	ARG	3.1
1	A	1005	GLY	3.0
1	A	1006	GLU	3.0
1	A	905	PHE	2.9
1	A	1161	GLN	2.8
2	B	16	A	2.8
1	A	976	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	201	LYS	2.5
1	A	16	PHE	2.5
1	A	1070	GLU	2.5
1	A	63	GLU	2.4
1	A	231	LYS	2.4
2	B	1	A	2.4
1	A	196	ARG	2.4
1	A	202	GLU	2.4
1	A	203	LEU	2.3
1	A	1135	LYS	2.2
1	A	193	ARG	2.2
1	A	185	ALA	2.2
1	A	200	GLU	2.2
1	A	513	ASN	2.2
1	A	807	HIS	2.2
1	A	311	ILE	2.2
1	A	306	HIS	2.2
1	A	184	THR	2.2
1	A	183	ASP	2.1
1	A	126	GLU	2.1
1	A	188	ILE	2.1
1	A	1001	ALA	2.1
1	A	458	ASP	2.1
1	A	292	THR	2.0
1	A	19	GLN	2.0
1	A	330	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.