



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:25 PM UTC

PDB ID : 6AAY / pdb_00006aay
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

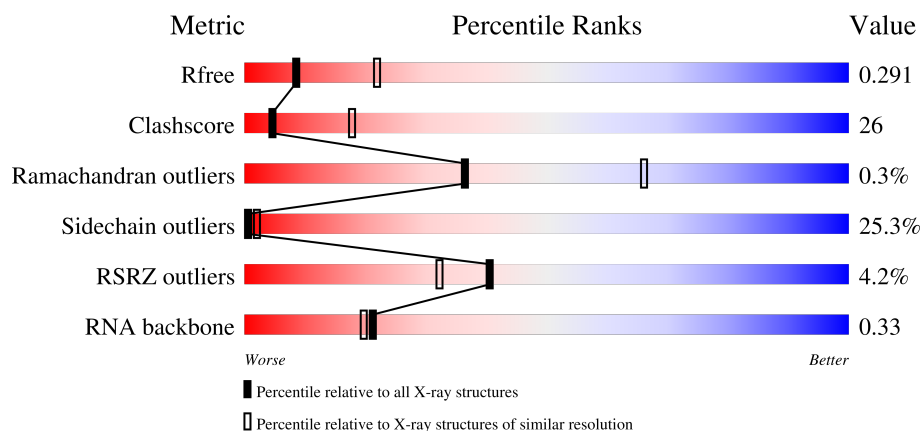
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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% 49% 35% 13% • •
2	B	59	5% 37% 32% 19% 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			

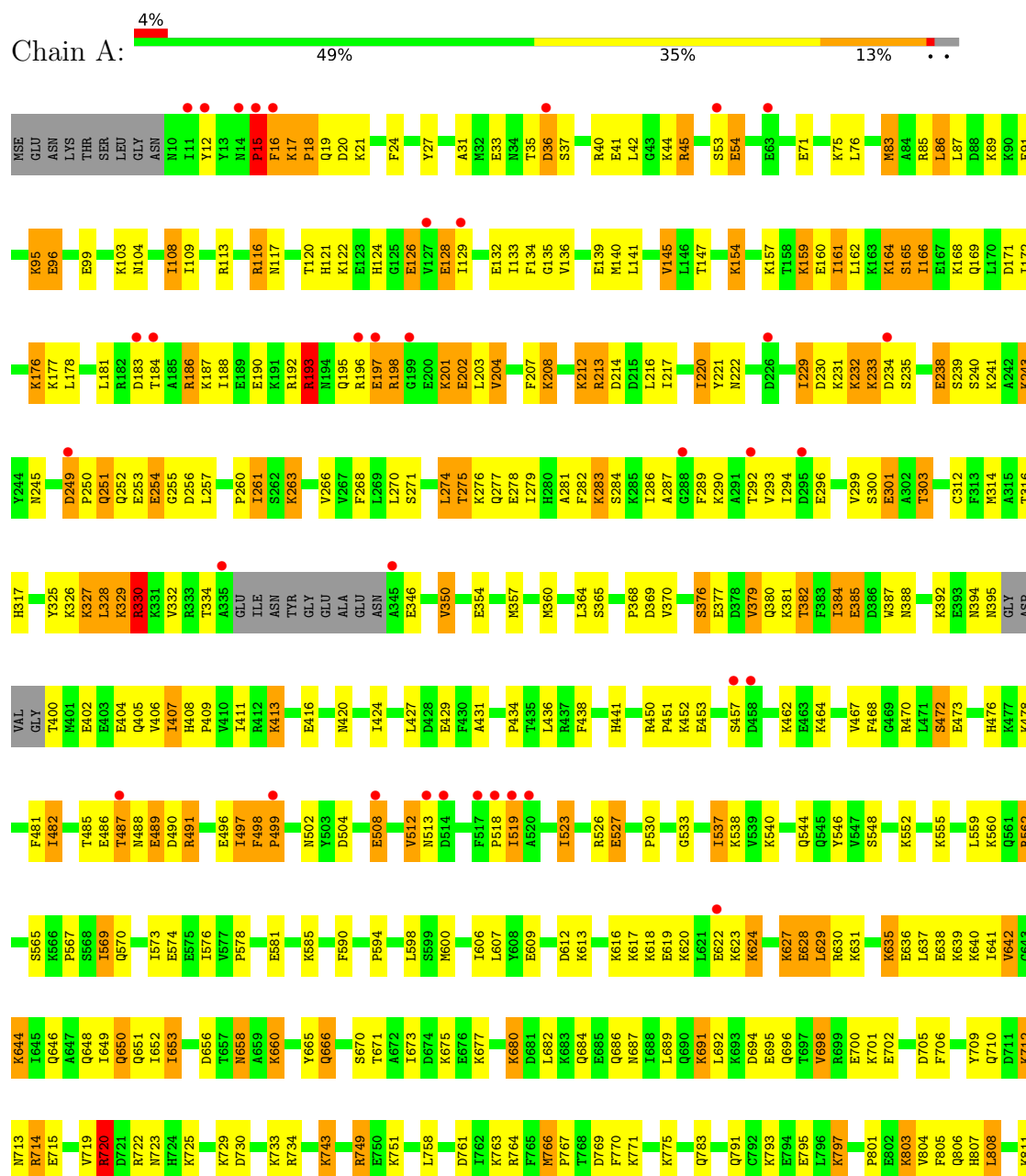
- Molecule 3 is water.

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

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

- Molecule 1: *Bergeyella zoohelcum* Cas13b (R1177A) mutant





4 Data and refinement statistics

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 65.02 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.02-2.79) 99.9 (65.02-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.97	3/10294 (0.0%)	1.32	22/13778 (0.2%)
2	B	0.73	2/1253 (0.2%)	0.92	2/1949 (0.1%)
All	All	0.95	5/11547 (0.0%)	1.28	24/15727 (0.2%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	22	A	O3'-P	-5.89	1.52	1.61
2	B	23	G	O3'-P	-5.74	1.52	1.61
1	A	766	MSE	CA-C	-5.23	1.47	1.53
1	A	594	PRO	C-O	-5.11	1.18	1.23
1	A	518	PRO	C-O	-5.03	1.17	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	PRO	N-CA-CB	-12.91	89.69	103.25
1	A	499	PRO	CA-N-CD	-11.64	95.70	112.00
1	A	499	PRO	CB-CA-C	8.06	124.86	111.56
1	A	498	PHE	CB-CA-C	7.99	125.91	110.17
1	A	658	ASN	N-CA-C	-7.41	104.24	113.28
1	A	15	PRO	N-CD-CG	-7.01	92.68	103.20
1	A	695	GLU	CB-CA-C	-6.33	100.94	110.88
1	A	16	PHE	CA-CB-CG	6.31	120.11	113.80
1	A	16	PHE	CB-CA-C	6.24	122.83	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	PHE	CA-C-N	6.10	127.47	119.84
1	A	498	PHE	C-N-CA	6.10	127.47	119.84
1	A	893	MSE	N-CA-C	6.02	117.92	111.36
1	A	18	PRO	N-CA-C	-5.97	100.17	112.47
1	A	325	TYR	CB-CA-C	5.88	119.70	109.65
1	A	121	HIS	CA-C-N	5.82	128.08	120.28
1	A	121	HIS	C-N-CA	5.82	128.08	120.28
1	A	498	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	1064	LEU	CA-C-N	5.62	131.82	121.70
1	A	1064	LEU	C-N-CA	5.62	131.82	121.70
2	B	3	A	C3'-C2'-O2'	5.58	119.07	110.70
1	A	1008	ASN	CA-C-N	5.30	129.87	122.08
1	A	1008	ASN	C-N-CA	5.30	129.87	122.08
1	A	487	THR	O-C-N	5.29	127.53	122.03
2	B	17	A	C3'-C2'-O2'	5.03	118.25	110.70

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

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Mol	Chain	Res	Type	Group
1	A	946	ARG	Sidechain

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	10107	0	10188	561	0
2	B	1118	0	562	33	0
3	A	36	0	0	0	0
3	B	1	0	0	0	0
All	All	11262	0	10750	571	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 (571) 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:HE2	1:A:232:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:420:ASN:CG	1:A:600:MSE:HE2	1.82	1.04
1:A:41:GLU:OE1	1:A:328:LEU:HG	1.58	1.01
1:A:1175:TYR:HE1	1:A:1186:PRO:HB3	1.24	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: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:HH11	1:A:832:ARG:HG2	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:188:ILE:HD12	1:A:207:PHE:CB	1.98	0.92
1:A:1070:GLU:OE2	1:A:1074:TYR:HB2	1.70	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
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:N	1:A:405:GLN:OE1	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:HE21	1:A:666:GLN:HA	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:O	1:A:233:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:609:GLU:HG3	1:A:893:MSE:CE	2.12	0.79
1:A:696:GLN:HG2	1:A:826:THR:CG2	2.11	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
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:497:ILE:HD12	1:A:497:ILE:N	2.01	0.75
1:A:1061:GLN:CG	1:A:1074:TYR:CD2	2.70	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:O	1:A:650:GLN:NE2	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:462:LYS:HD3	1:A:496:GLU:OE1	1.86	0.75
1:A:1130:LEU:HD21	1:A:1222:LEU:HB3	1.66	0.75
1:A:1038:ASP:O	1:A:1041:LYS:HG2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD23	1:A:436:LEU:C	2.13	0.74
1:A:997:ASN:HD22	1:A:997:ASN:N	1.86	0.73
1:A:1159:LEU:C	1:A:1159:LEU:HD22	2.13	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:981:GLN:CD	1:A:981:GLN:H	1.96	0.72
1:A:17:LYS:HD2	1:A:17:LYS:N	2.03	0.72
1:A:270:LEU:O	1:A:274:LEU:HB2	1.89	0.72
1:A:1019:LEU:HD12	1:A:1019:LEU:O	1.89	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:624:LYS:CG	1:A:628:GLU:HG2	2.17	0.71
1:A:1144:VAL:HG23	1:A:1163:ALA:HB2	1.72	0.71
1:A:15:PRO:CA	1:A:24:PHE:CZ	2.61	0.70
1:A:128:GLU:OE1	1:A:260:PRO:HG3	1.90	0.70
1:A:202:GLU:C	1:A:203:LEU:HD23	2.16	0.70
1:A:369:ASP:OD1	1:A:413:LYS:CE	2.40	0.70
1:A:232:LYS:HA	1:A:232:LYS:CE	2.16	0.69
1:A:1028:VAL:HG11	1:A:1039:PHE:CE2	2.27	0.69
1:A:277:GLN:CG	1:A:402:GLU:HG3	2.23	0.69
1:A:350:VAL:O	1:A:354:GLU:HG3	1.92	0.69
1:A:15:PRO:CD	1:A:21:LYS:HZ3	2.06	0.69
1:A:942:LYS:HG2	1:A:942:LYS:O	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:201:LYS:C	1:A:202:GLU:OE2	2.36	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: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:940:GLU:H	1:A:940:GLU:CD	2.01	0.67
1:A:666:GLN:HE21	1:A:666:GLN:CA	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:GLN:HA	1:A:666:GLN:NE2	2.05	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:N	1:A:995:LEU:HD23	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:HE2	1:A:232:LYS:CA	2.22	0.66
1:A:497:ILE:H	1:A:497:ILE:CD1	2.06	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:979:ILE:HD13	1:A:1015:LYS:HD3	1.73	0.66
1:A:249:ASP:OD1	1:A:249:ASP:N	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:190:GLU:OE2	1:A:193:ARG:HD2	1.98	0.64
1:A:1081:GLU:HG3	1:A:1206:THR:CG2	2.18	0.64
1:A:696:GLN:CG	1:A:826:THR:HG22	2.24	0.64
1:A:317:HIS:CD2	1:A:406:VAL:HG11	2.33	0.64
1:A:1168:GLN:CG	1:A:1193:TYR:OH	2.46	0.64
1:A:192:ARG:NH1	1:A:204:VAL:O	2.24	0.63
1:A:660:LYS:CD	1:A:660:LYS:H	2.09	0.63
1:A:867:GLN:NE2	2:B:27:G:OP2	2.31	0.63
1:A:20:ASP:C	1:A:21:LYS:HD3	2.24	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: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:HD12	1:A:963:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1142:TYR:CE1	1:A:1167:GLU:HB2	2.35	0.61
1:A:519:ILE:O	1:A:519:ILE:HG22	2.01	0.61
1:A:997:ASN:HD22	1:A:997:ASN:H	1.47	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:1061:GLN:HG2	1:A:1074:TYR:CD2	2.34	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:1001:ALA:HB2	1:A:1007:ARG:CB	2.31	0.61
1:A:947:LYS:CD	1:A:951:LYS:HE2	2.30	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:1187:LYS:NZ	1:A:1189:GLU:OE1	2.23	0.61
1:A:979:ILE:CD1	1:A:1015:LYS:HD2	2.25	0.61
1:A:394:ASN:HB3	1:A:1032:LYS:NZ	2.07	0.60
1:A:19:GLN:O	1:A:19:GLN:HG2	2.01	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:947:LYS:HE3	1:A:951:LYS:HE3	1.69	0.60
1:A:1135:LYS:HE2	1:A:1222:LEU:O	2.01	0.60
1:A:326:LYS:O	1:A:327:LYS:HB2	2.02	0.60
1:A:981:GLN:OE1	1:A:981:GLN:N	2.33	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: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:832:ARG:HG2	1:A:832:ARG:NH1	1.99	0.59
1:A:1009:THR:OG1	1:A:1009:THR:O	2.13	0.59
1:A:1110:ASP:O	1:A:1133:GLN:NE2	2.31	0.59
2:B:4:A:C5	2:B:5:A:C2	2.91	0.59
1:A:684:GLN:OE1	1:A:684:GLN:HA	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:962:THR:HA	1:A:965:MSE:HE3	1.85	0.58
1:A:330:ARG:HD2	2:B:16:A:N3	2.19	0.58
1:A:523:ILE:HG23	1:A:692:LEU:HD21	1.86	0.58
1:A:202:GLU:O	1:A:203:LEU:HD23	2.02	0.58
1:A:87:LEU:HD22	1:A:104:ASN:HB2	1.86	0.57
1:A:660:LYS:N	1:A:660:LYS:HD3	2.19	0.57
1:A:848:SER:HB2	1:A:849:GLU:OE2	2.04	0.57
1:A:300:SER:O	1:A:303:THR:OG1	2.22	0.57
1:A:1007:ARG:CZ	1:A:1009:THR:HB	2.35	0.57
1:A:1070:GLU:OE2	1:A:1074:TYR:CB	2.50	0.57
1:A:1075:PRO:HB2	1:A:1076:TYR:CE1	2.39	0.57
1:A:1076:TYR:CD1	1:A:1076:TYR:N	2.72	0.57
1:A:527:GLU:N	1:A:527:GLU:OE2	2.37	0.57
1:A:650:GLN:HE21	1:A:650:GLN:C	2.13	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
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:1163:ALA:HB1	1:A:1167:GLU:CD	2.30	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:197:GLU:OE2	1:A:197:GLU:HA	2.04	0.55
1:A:370:VAL:HG21	1:A:951:LYS:HB2	1.88	0.55
1:A:1054:TYR:HD2	1:A:1207:TYR:CE2	2.24	0.55
1:A:135:GLY:O	1:A:139:GLU:HG2	2.07	0.55
1:A:192:ARG:HD2	1:A:204:VAL:O	2.06	0.55
1:A:1045:ASP:O	1:A:1049:GLN:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:LYS:O	1:A:482:ILE:HG12	2.06	0.55
1:A:1074:TYR:O	1:A:1080:ARG:NH1	2.40	0.55
1:A:1046:GLN:H	1:A:1046:GLN:CD	2.14	0.54
1:A:609:GLU:O	1:A:613:LYS:HG3	2.08	0.54
1:A:906:LYS:HZ2	2:B:40:U:H2'	1.71	0.54
2:B:50:A:C8	2:B:50:A:H5''	2.43	0.54
1:A:574:GLU:CG	1:A:578:PRO:HA	2.36	0.54
1:A:395:ASN:C	1:A:1032:LYS:HE2	2.31	0.54
1:A:901:LYS:HD3	1:A:902:GLY:H	1.72	0.54
1:A:906:LYS:NZ	2:B:40:U:O2	2.40	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: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:866:LYS:O	1:A:870:THR:HG22	2.08	0.53
1:A:1123:LYS:HG3	1:A:1174:THR:HG21	1.89	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:986:ASP:CG	1:A:1010:ASN:HB3	2.34	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:O	1:A:233:LYS:HD2	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
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:848:SER:C	1:A:849:GLU:OE2	2.53	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:4:A:N7	2:B:5:A:C2	2.78	0.52
2:B:15:A:H2'	2:B:16:A:H2'	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:357:MSE:O	1:A:357:MSE:HG2	2.10	0.51
1:A:400:THR:HG23	1:A:400:THR:O	2.10	0.51
1:A:901:LYS:H	1:A:901:LYS:HD2	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: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:1064:LEU:HG	1:A:1077:VAL:HG11	1.91	0.51
1:A:828:TYR:OH	1:A:832:ARG:HD2	2.10	0.51
1:A:1070:GLU:OE2	1:A:1074:TYR:N	2.43	0.51
1:A:253:GLU:C	1:A:255:GLY:H	2.19	0.51
1:A:803:LYS:HD2	1:A:806:GLN:OE1	2.10	0.51
1:A:86:LEU:HB3	1:A:140:MSE:HG2	1.93	0.51
1:A:1175:TYR:OH	1:A:1187:LYS:CG	2.57	0.51
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:1061:GLN:HG3	1:A:1074:TYR:HD2	1.71	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
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: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: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:453:GLU:CD	1:A:453:GLU:H	2.20	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:232:LYS:HD3	1:A:232:LYS:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:238:GLU:HA	1:A:241:LYS:HD2	1.95	0.49
1:A:650:GLN:NE2	1:A:650:GLN:HA	2.26	0.49
1:A:1061:GLN:CG	1:A:1074:TYR:CE2	2.90	0.49
1:A:161:ILE:HD12	1:A:161:ILE:C	2.35	0.49
1:A:485:THR:O	1:A:485:THR:OG1	2.21	0.49
1:A:1058:ILE:HD13	1:A:1076:TYR:CE2	2.48	0.49
1:A:427:LEU:HA	1:A:431:ALA:HB2	1.95	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: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: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:HG3	1:A:296:GLU:O	2.14	0.48
1:A:963:LEU:O	1:A:967:LYS:HG3	2.14	0.48
1:A:691:LYS:HA	1:A:691:LYS:HD3	1.61	0.48
1:A:846:PHE:N	1:A:846:PHE:CD1	2.80	0.48
1:A:1001:ALA:CB	1:A:1007:ARG:CB	2.87	0.48
1:A:104:ASN:O	1:A:108:ILE:HG13	2.14	0.48
1:A:648:GLN:OE1	1:A:889:GLU:HG3	2.14	0.48
1:A:87:LEU:CD2	1:A:104:ASN:CB	2.93	0.47
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:1083:GLU:O	1:A:1084:GLN:C	2.55	0.47
1:A:124:HIS:ND1	1:A:124:HIS:C	2.72	0.47
1:A:712:LYS:HE3	1:A:715:GLU:CD	2.39	0.47
1:A:1048:VAL:O	1:A:1052:LEU:HG	2.14	0.47
1:A:1105:LEU:HA	1:A:1105:LEU:HD23	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:160:GLU:HB3	1:A:384:ILE:HD11	1.97	0.47
1:A:527:GLU:N	1:A:527:GLU:CD	2.73	0.47
1:A:644:LYS:HD2	1:A:644:LYS:O	2.14	0.47
1:A:1019:LEU:HD11	1:A:1028:VAL:HB	1.95	0.47
1:A:17:LYS:HD2	1:A:17:LYS:H	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:377:GLU:CD	1:A:381:LYS:NZ	2.72	0.47
1:A:533:GLY:O	1:A:600:MSE:CB	2.63	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:468:PHE:HB2	1:A:590:PHE:HB2	1.97	0.47
1:A:533:GLY:O	1:A:600:MSE:HG2	2.15	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:27:TYR:CD2	1:A:282:PHE:CD1	3.04	0.46
1:A:635:LYS:HB2	1:A:635:LYS:HE2	1.49	0.46
1:A:15:PRO:HD2	1:A:21:LYS:NZ	2.30	0.46
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.70	0.46
1:A:234:ASP:N	1:A:234:ASP:OD1	2.49	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: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:1087:LYS:O	1:A:1091:GLU:HB2	2.16	0.46
1:A:15:PRO:C	1:A:24:PHE:CZ	2.94	0.45
1:A:1093:LEU:HD13	1:A:1093:LEU:O	2.16	0.45
1:A:364:LEU:HB3	1:A:987:LEU:HD13	1.98	0.45
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:1168:GLN:HG2	1:A:1193:TYR:HH	1.81	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:H	1:A:569:ILE:HG12	1.65	0.45
1:A:54:GLU:H	1:A:54:GLU:HG2	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:436:LEU:C	1:A:436:LEU:CD2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE2	1:A:202:GLU:N	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: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:1103:TYR:CE2	1:A:1223:ILE:HD13	2.52	0.44
1:A:128:GLU:C	1:A:128:GLU:CD	2.85	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:533:GLY:O	1:A:600:MSE:HB2	2.18	0.44
1:A:906:LYS:CE	2:B:40:U:H2'	2.47	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:1085:TYR:CD1	1:A:1085:TYR:C	2.94	0.44
2:B:32:G:H2'	2:B:33:C:O4'	2.18	0.44
1:A:832:ARG:NH1	1:A:832:ARG:CG	2.73	0.44
1:A:1033:LEU:HD22	1:A:1036:VAL:HG11	2.00	0.44
1:A:478:LYS:O	1:A:482:ILE:CG1	2.66	0.44
1:A:96:GLU:CD	1:A:96:GLU:H	2.25	0.44
1:A:609:GLU:HG3	1:A:893:MSE:HE2	1.97	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
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:86:LEU:HD23	1:A:86:LEU:N	2.33	0.44
1:A:190:GLU:HA	1:A:193:ARG:HB3	2.00	0.44
1:A:1038:ASP:O	1:A:1041:LYS:HD3	2.18	0.44
1:A:706:PHE:CZ	1:A:743:LYS:HD3	2.52	0.44
1:A:1134:LEU:HB3	1:A:1135:LYS:H	1.39	0.44
1:A:159:LYS:HE2	1:A:159:LYS:HB3	1.49	0.43
1:A:249:ASP:CB	1:A:250:PRO:HD3	2.47	0.43
1:A:364:LEU:HB3	1:A:987:LEU:CD1	2.48	0.43
1:A:364:LEU:CB	1:A:987:LEU:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:652:ILE:CD1	2:B:30:C:H41	2.32	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:330:ARG:HH21	2:B:17:A:H5''	1.83	0.43
1:A:1185:LEU:HD23	1:A:1185:LEU:HA	1.85	0.43
1:A:650:GLN:NE2	1:A:650:GLN:C	2.76	0.43
1:A:1123:LYS:NZ	1:A:1147:LEU:O	2.39	0.43
1:A:408:HIS:O	1:A:408:HIS:CG	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:1195:GLN:OE1	1:A:1195:GLN:HA	2.14	0.43
1:A:546:TYR:N	1:A:546:TYR:CD1	2.85	0.43
1:A:1058:ILE:CD1	1:A:1076:TYR:CE2	3.02	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:83:MSE:SE	1:A:87:LEU:HD12	2.68	0.43
1:A:377:GLU:O	1:A:381:LYS:HG3	2.19	0.43
1:A:544:GLN:CA	1:A:544:GLN:HE21	2.31	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:HE3	1:A:600:MSE:HB3	1.67	0.42
1:A:41:GLU:O	1:A:45:ARG:HG3	2.19	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:299:VAL:O	1:A:299:VAL:HG13	2.19	0.42
1:A:901:LYS:H	1:A:901:LYS:CD	2.31	0.42
1:A:941:LYS:HA	1:A:941:LYS:HD3	1.61	0.42
1:A:986:ASP:OD2	1:A:1010:ASN:HB3	2.19	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:1159:LEU:C	1:A:1159:LEU:CD2	2.85	0.42
1:A:1165:ASP:O	1:A:1169:LYS:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1175:TYR:HH	1:A:1187:LYS:HG2	1.82	0.42
1:A:96:GLU:CD	1:A:96:GLU:N	2.77	0.42
1:A:195:GLN:HB3	1:A:203:LEU:HD22	2.00	0.42
1:A:1179:LYS:HD2	1:A:1186:PRO:HA	2.01	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:660:LYS:HE2	2:B:30:C:O2	2.20	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:1003:GLN:OE1	1:A:1003:GLN:N	2.52	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:1027:THR:CG2	1:A:1059:GLU:OE2	2.68	0.42
1:A:251:GLN:HE21	1:A:251:GLN:HB2	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:720:ARG:CD	1:A:720:ARG:H	2.33	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:O	1:A:807:HIS:CG	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
1:A:906:LYS:HE3	2:B:41:U:OP1	2.20	0.41
1:A:18:PRO:O	1:A:20:ASP:N	2.47	0.41
1:A:208:LYS:O	1:A:208:LYS:HG2	2.21	0.41
1:A:801:PRO:HD2	1:A:804:VAL:HG23	2.03	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
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:15:PRO:O	1:A:18:PRO:HD3	2.20	0.41
1:A:166:ILE:O	1:A:166:ILE:CG2	2.68	0.41
1:A:176:LYS:HE3	1:A:301:GLU:O	2.21	0.41
1:A:533:GLY:C	1:A:600:MSE:CG	2.94	0.41
1:A:730:ASP:N	1:A:730:ASP:OD1	2.51	0.41
1:A:1128:ASN:O	1:A:1133:GLN:HG3	2.20	0.41
1:A:451:PRO:CB	1:A:457:SER:O	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:LYS:HD2	1:A:712:LYS:HA	1.77	0.41
1:A:758:LEU:HD23	1:A:758:LEU:HA	1.88	0.41
1:A:1057:ASN:HD22	1:A:1057:ASN:HA	1.73	0.41
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.80	0.41
1:A:675:LYS:HG2	1:A:853:PHE:CE2	2.56	0.41
1:A:1147:LEU:HD12	1:A:1147:LEU:HA	1.76	0.41
1:A:719:VAL:HG12	1:A:725:LYS:HB2	2.03	0.41
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:HA	1:A:682:LEU:HD23	1.88	0.40
1:A:1173:LEU:HD22	1:A:1173:LEU:HA	1.93	0.40
1:A:671:THR:HA	1:A:871:HIS:ND1	2.35	0.40
1:A:831:LYS:HA	1:A:831:LYS:HD2	1.77	0.40
1:A:963:LEU:HD12	1:A:963:LEU:C	2.45	0.40
1:A:1060:TRP:CE3	1:A:1076:TYR:HB3	2.55	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:O	1:A:979:ILE:CG2	2.70	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	1191/1232 (97%)	1140 (96%)	48 (4%)	3 (0%)	36 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	PRO

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Mol	Chain	Res	Type
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%)	825 (75%)	279 (25%)	0 2

All (279) 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
1	A	71	GLU
1	A	75	LYS
1	A	76	LEU
1	A	83	MSE
1	A	86	LEU
1	A	89	LYS
1	A	91	GLU
1	A	95	LYS
1	A	96	GLU
1	A	103	LYS
1	A	108	ILE
1	A	109	ILE
1	A	116	ARG
1	A	122	LYS
1	A	126	GLU
1	A	128	GLU

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Mol	Chain	Res	Type
1	A	129	ILE
1	A	132	GLU
1	A	133	ILE
1	A	145	VAL
1	A	147	THR
1	A	154	LYS
1	A	157	LYS
1	A	159	LYS
1	A	161	ILE
1	A	162	LEU
1	A	164	LYS
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	197	GLU
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	220	ILE
1	A	229	ILE
1	A	230	ASP
1	A	231	LYS
1	A	232	LYS
1	A	233	LYS
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	252	GLN
1	A	254	GLU
1	A	261	ILE

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Mol	Chain	Res	Type
1	A	263	LYS
1	A	266	VAL
1	A	274	LEU
1	A	275	THR
1	A	276	LYS
1	A	283	LYS
1	A	286	ILE
1	A	290	LYS
1	A	292	THR
1	A	293	VAL
1	A	294	ILE
1	A	301	GLU
1	A	303	THR
1	A	314	MSE
1	A	327	LYS
1	A	328	LEU
1	A	329	LYS
1	A	330	ARG
1	A	332	VAL
1	A	334	THR
1	A	350	VAL
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	407	ILE
1	A	413	LYS
1	A	416	GLU
1	A	424	ILE
1	A	450	ARG
1	A	452	LYS
1	A	472	SER
1	A	482	ILE
1	A	486	GLU
1	A	489	GLU
1	A	490	ASP
1	A	491	ARG
1	A	497	ILE
1	A	502	ASN

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Mol	Chain	Res	Type
1	A	508	GLU
1	A	512	VAL
1	A	519	ILE
1	A	523	ILE
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	560	LYS
1	A	565	SER
1	A	569	ILE
1	A	570	GLN
1	A	576	ILE
1	A	585	LYS
1	A	598	LEU
1	A	607	LEU
1	A	618	LYS
1	A	619	GLU
1	A	620	LYS
1	A	622	GLU
1	A	623	LYS
1	A	624	LYS
1	A	627	LYS
1	A	628	GLU
1	A	629	LEU
1	A	635	LYS
1	A	639	LYS
1	A	640	LYS
1	A	642	VAL
1	A	644	LYS
1	A	650	GLN
1	A	651	GLN
1	A	653	ILE
1	A	660	LYS
1	A	666	GLN
1	A	670	SER
1	A	673	ILE
1	A	677	LYS
1	A	680	LYS

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Mol	Chain	Res	Type
1	A	687	ASN
1	A	691	LYS
1	A	698	VAL
1	A	710	GLN
1	A	712	LYS
1	A	714	ARG
1	A	720	ARG
1	A	723	ASN
1	A	729	LYS
1	A	733	LYS
1	A	734	ARG
1	A	743	LYS
1	A	749	ARG
1	A	751	LYS
1	A	769	ASP
1	A	783	GLN
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	855	LYS
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	877	ARG
1	A	888	LEU
1	A	899	ILE
1	A	900	ILE

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Mol	Chain	Res	Type
1	A	901	LYS
1	A	911	LEU
1	A	917	ARG
1	A	920	LYS
1	A	923	GLN
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
1	A	945	ASP
1	A	946	ARG
1	A	947	LYS
1	A	952	ILE
1	A	956	LYS
1	A	963	LEU
1	A	975	LYS
1	A	978	SER
1	A	979	ILE
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	1003	GLN
1	A	1006	GLU
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	1051	PHE
1	A	1056	GLU
1	A	1058	ILE

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Mol	Chain	Res	Type
1	A	1064	LEU
1	A	1065	ILE
1	A	1071	GLU
1	A	1079	GLU
1	A	1081	GLU
1	A	1086	GLU
1	A	1088	VAL
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
1	A	1114	LEU
1	A	1115	LYS
1	A	1118	ASP
1	A	1119	ASN
1	A	1134	LEU
1	A	1139	VAL
1	A	1140	GLU
1	A	1143	LYS
1	A	1144	VAL
1	A	1147	LEU
1	A	1152	GLU
1	A	1153	ASP
1	A	1155	ASN
1	A	1157	ASN
1	A	1159	LEU
1	A	1161	GLN
1	A	1169	LYS
1	A	1173	LEU
1	A	1184	GLN
1	A	1187	LYS
1	A	1188	LYS
1	A	1196	GLU
1	A	1197	LYS
1	A	1200	LYS
1	A	1205	LYS

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Mol	Chain	Res	Type
1	A	1217	LYS
1	A	1224	LYS
1	A	1225	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	245	ASN
1	A	251	GLN
1	A	264	ASN
1	A	306	HIS
1	A	408	HIS
1	A	441	HIS
1	A	454	ASN
1	A	476	HIS
1	A	544	GLN
1	A	666	GLN
1	A	717	ASN
1	A	723	ASN
1	A	760	ASN
1	A	778	GLN
1	A	908	ASN
1	A	997	ASN
1	A	1049	GLN
1	A	1057	ASN
1	A	1128	ASN
1	A	1155	ASN
1	A	1184	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

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Mol	Chain	Res	Type
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1187/1232 (96%)	0.40	49 (4%) 41 33	30, 68, 110, 163	0
2	B	52/59 (88%)	-0.30	3 (5%) 29 22	42, 59, 139, 148	0
All	All	1239/1291 (95%)	0.37	52 (4%) 40 32	30, 68, 113, 163	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	TYR	4.4
1	A	517	PHE	4.2
1	A	16	PHE	4.1
1	A	513	ASN	3.9
1	A	499	PRO	3.9
1	A	519	ILE	3.9
1	A	1135	LYS	3.8
1	A	1225	LEU	3.8
1	A	1065	ILE	3.7
1	A	1081	GLU	3.2
1	A	197	GLU	3.1
1	A	127	VAL	3.1
1	A	11	ILE	3.0
1	A	345	ALA	3.0
1	A	518	PRO	2.9
1	A	458	ASP	2.9
1	A	15	PRO	2.8
1	A	226	ASP	2.8
1	A	1224	LYS	2.7
1	A	292	THR	2.6
1	A	63	GLU	2.6
1	A	335	ALA	2.6
1	A	814	GLY	2.5
1	A	1139	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	53	SER	2.5
1	A	865	LYS	2.5
1	A	514	ASP	2.5
1	A	508	GLU	2.5
1	A	1206	THR	2.4
1	A	14	ASN	2.4
2	B	21	A	2.4
1	A	199	GLY	2.4
1	A	1039	PHE	2.4
1	A	183	ASP	2.4
2	B	20	A	2.3
1	A	295	ASP	2.3
1	A	288	GLY	2.3
1	A	234	ASP	2.3
1	A	520	ALA	2.2
1	A	487	THR	2.2
1	A	129	ILE	2.2
1	A	622	GLU	2.1
1	A	184	THR	2.1
1	A	249	ASP	2.1
1	A	1092	GLU	2.1
1	A	1000	ARG	2.1
1	A	457	SER	2.1
2	B	16	A	2.1
1	A	846	PHE	2.1
1	A	36	ASP	2.0
1	A	196	ARG	2.0
1	A	903	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.