



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:45 AM EDT

PDB ID : 8Y0A / pdb_00008y0a
Title : Crystal structure of LbCas12a in complex with crRNA and 18nt target DNA
Authors : Lin, X.; Chen, J.; Liu, L.
Deposited on : 2024-01-22
Resolution : 3.51 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
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

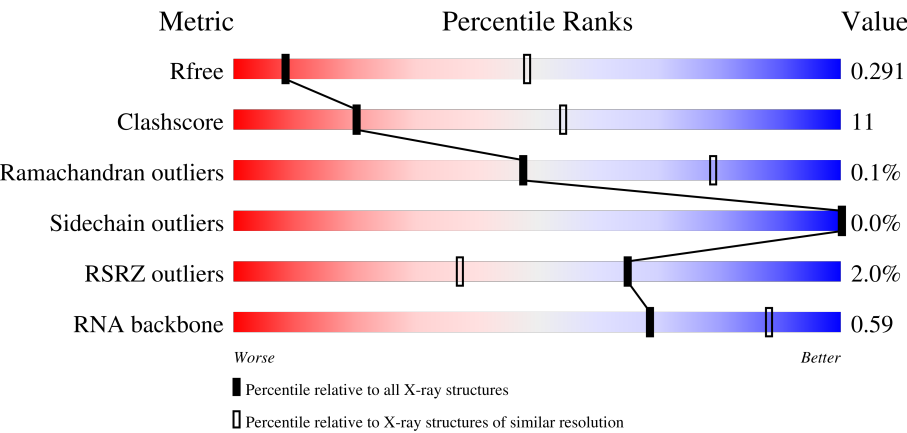
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)
RNA backbone	3983	1018 (4.00-3.04)

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	1228	2% 75% 25%
1	E	1228	2% 73% 27%
2	B	40	42% 52% 5%
2	F	40	45% 48% 5%

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Mol	Chain	Length	Quality of chain
3	C	27	 4% 56% 44%
3	G	27	 52% 48%
4	D	11	 9% 64% 36%
4	H	11	 45% 55%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23102 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 LbCas12a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1223	Total	C	N	O	S	0	0	0
			9964	6412	1623	1900	29			
1	E	1223	Total	C	N	O	S	0	0	0
			9958	6409	1626	1894	29			

- Molecule 2 is a RNA chain called RNA (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	38	Total	C	N	O	P	0	0	0
			805	362	144	262	37			
2	F	38	Total	C	N	O	P	0	0	0
			805	362	144	262	37			

- Molecule 3 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	27	Total	C	N	O	P	0	0	0
			558	264	105	162	27			
3	G	27	Total	C	N	O	P	0	0	0
			558	264	105	162	27			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			217	107	31	69	10			
4	H	11	Total	C	N	O	P	0	0	0
			217	107	31	69	10			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	E	2	Total	Mg	0	0
			2	2		

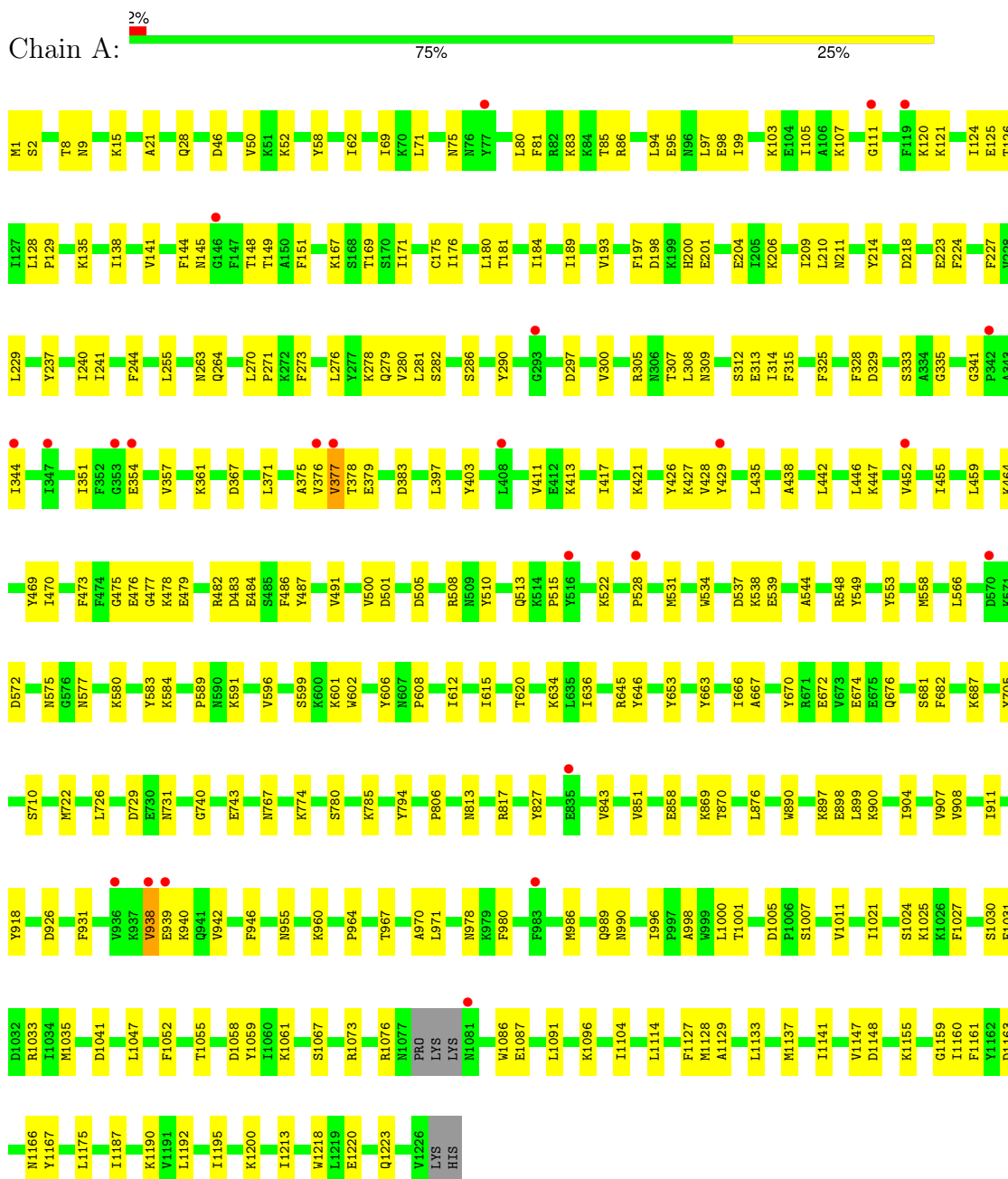
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	E	6	Total	O	0	0
			6	6		

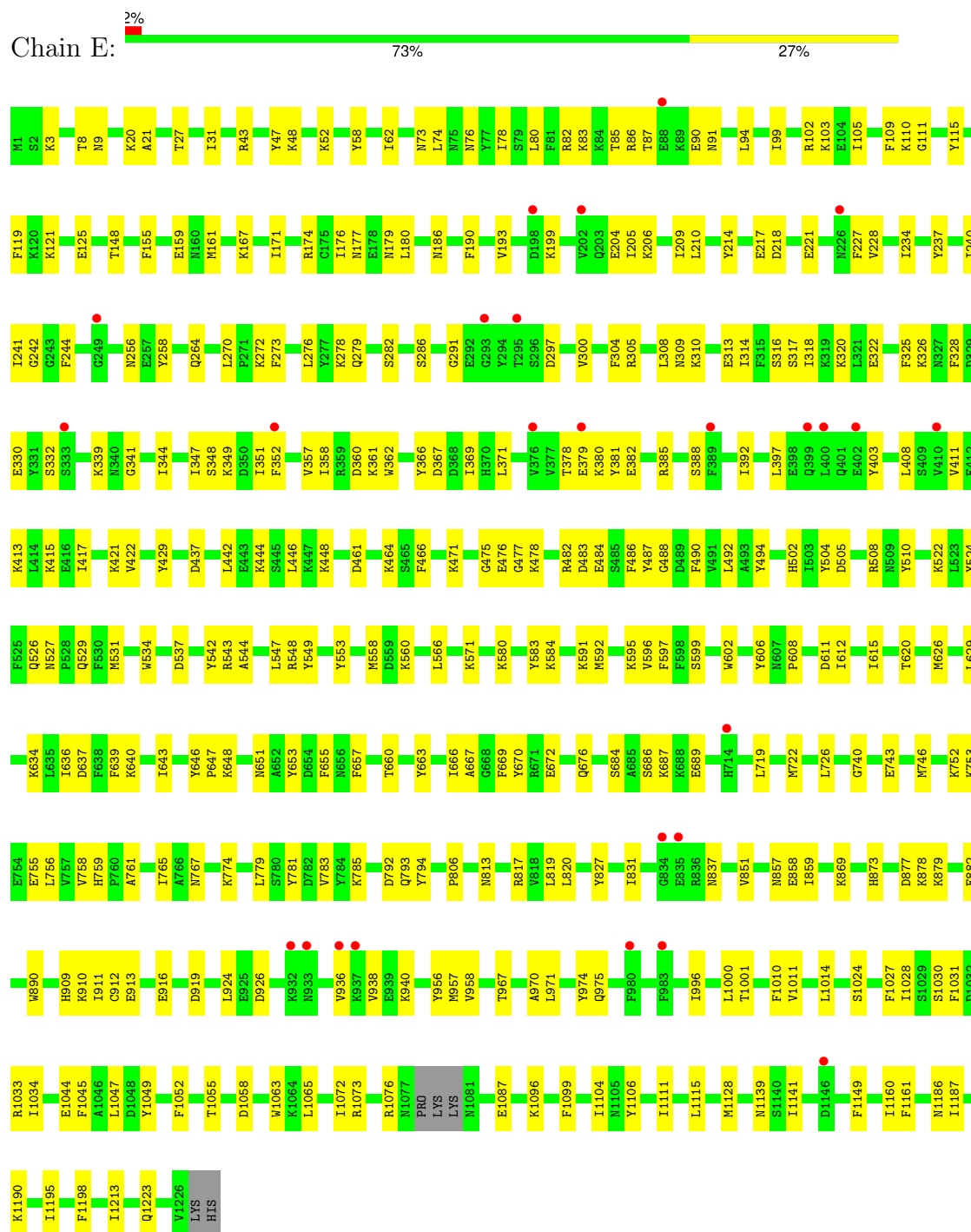
3 Residue-property plots

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: LbCas12a



- Molecule 1: LbCas12a



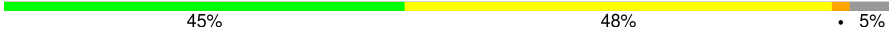
- Molecule 2: RNA (38-MER)

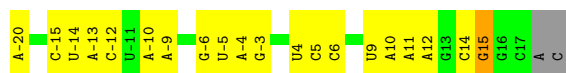
Chain B:

42% 52% 5%



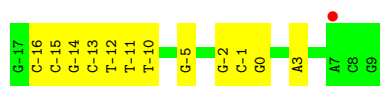
- Molecule 2: RNA (38-MER)

Chain F:  45% 48% 5%



- Molecule 3: DNA (27-MER)

Chain C:  4% 56% 44%



- Molecule 3: DNA (27-MER)

Chain G:  52% 48%



- Molecule 4: DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3')

Chain D:  9% 64% 36%



- Molecule 4: DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3')

Chain H:  45% 55%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.78Å 142.67Å 209.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.87 – 3.51 25.87 – 3.51	Depositor EDS
% Data completeness (in resolution range)	96.2 (25.87-3.51) 96.1 (25.87-3.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.238 , 0.294 0.237 , 0.291	Depositor DCC
R_{free} test set	2220 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23102	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6372e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.18	0/10174	0.41	0/13698
1	E	0.19	0/10168	0.43	1/13690 (0.0%)
2	B	0.15	0/900	0.31	0/1400
2	F	0.15	0/900	0.32	0/1400
3	C	0.22	0/626	0.38	0/965
3	G	0.21	0/626	0.38	0/965
4	D	0.24	0/240	0.52	0/368
4	H	0.25	0/240	0.52	0/368
All	All	0.19	0/23874	0.41	1/32854 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	180	LEU	CB-CG-CD2	-6.06	92.51	110.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	938	VAL	Peptide

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	9964	0	9743	232	0
1	E	9958	0	9742	233	0
2	B	805	0	410	17	0
2	F	805	0	410	20	0
3	C	558	0	304	15	0
3	G	558	0	304	15	0
4	D	217	0	129	5	0
4	H	217	0	129	6	0
5	A	2	0	0	0	0
5	E	2	0	0	0	0
6	A	8	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	6	0	0	1	0
All	All	23102	0	21171	498	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 11.

All (498) 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:1033:ARG:NH2	1:A:1035:MET:SD	2.47	0.87
1:E:522:LYS:HE3	1:E:743:GLU:HG2	1.62	0.81
1:A:539:GLU:OE2	1:A:580:LYS:NZ	2.13	0.80
1:E:442:LEU:HD11	1:E:446:LEU:HD13	1.63	0.80
1:E:612:ILE:HD11	1:E:634:LYS:HG2	1.63	0.79
1:A:328:PHE:HE2	1:A:397:LEU:HD11	1.46	0.79
1:E:367:ASP:OD1	1:E:381:TYR:OH	2.02	0.77
1:A:211:ASN:O	1:A:211:ASN:ND2	2.18	0.76
1:A:376:VAL:HG13	1:A:377:VAL:HG22	1.68	0.76
1:A:479:GLU:OE2	1:A:482:ARG:NH1	2.18	0.75
1:E:653:TYR:HB2	1:E:655:PHE:CE1	2.21	0.74
1:E:596:VAL:HG11	1:E:646:TYR:HE1	1.51	0.74
1:E:537:ASP:OD2	1:E:584:LYS:NZ	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:ARG:O	1:E:309:ASN:ND2	2.19	0.74
1:A:305:ARG:O	1:A:309:ASN:ND2	2.18	0.74
1:A:897:LYS:NZ	1:A:898:GLU:OE2	2.21	0.73
1:E:1058:ASP:OD1	1:E:1223:GLN:NE2	2.16	0.73
1:E:48:LYS:O	1:E:48:LYS:HD3	1.89	0.72
1:E:1073:ARG:HH22	1:E:1076:ARG:NH2	1.88	0.72
1:E:297:ASP:OD2	1:E:446:LEU:HB2	1.89	0.71
1:A:314:ILE:HD13	1:A:500:VAL:HG12	1.72	0.71
1:A:596:VAL:HG11	1:A:646:TYR:HE1	1.57	0.70
1:E:1001:THR:O	1:E:1186:ASN:ND2	2.21	0.69
1:A:612:ILE:HD11	1:A:634:LYS:HG2	1.74	0.69
1:E:595:LYS:NZ	3:G:3:DA:N3	2.39	0.69
1:E:325:PHE:HA	1:E:328:PHE:CD1	2.28	0.69
1:E:636:ILE:HD13	1:E:663:TYR:HD2	1.57	0.68
1:A:537:ASP:OD2	1:A:584:LYS:NZ	2.24	0.68
1:A:176:ILE:HA	1:A:180:LEU:HD23	1.74	0.68
1:A:279:GLN:HG3	1:A:282:SER:HB3	1.75	0.68
1:A:1155:LYS:HB3	1:A:1159:GLY:HA2	1.74	0.68
1:A:1058:ASP:OD1	1:A:1223:GLN:NE2	2.24	0.67
1:A:636:ILE:HD13	1:A:663:TYR:HD2	1.59	0.67
1:E:653:TYR:HB2	1:E:655:PHE:HE1	1.60	0.67
1:E:647:PRO:O	1:E:651:ASN:ND2	2.27	0.67
1:E:1000:LEU:HD13	1:E:1011:VAL:HG11	1.77	0.67
1:A:176:ILE:O	1:A:180:LEU:HB2	1.94	0.67
1:A:209:ILE:HG12	1:A:244:PHE:HE1	1.61	0.66
1:E:595:LYS:O	1:E:599:SER:OG	2.13	0.66
1:A:1129:ALA:O	1:A:1133:LEU:HD12	1.95	0.66
1:A:729:ASP:OD1	1:A:731:ASN:ND2	2.29	0.66
1:A:167:LYS:NZ	3:C:-2:DG:OP1	2.22	0.66
1:A:575:ASN:O	1:A:577:ASN:ND2	2.29	0.66
1:E:464:LYS:NZ	2:F:14:C:OP1	2.29	0.66
1:A:200:HIS:O	1:A:204:GLU:N	2.25	0.66
1:A:80:LEU:O	1:A:86:ARG:NH1	2.29	0.65
1:A:83:LYS:HG3	1:A:85:THR:H	1.61	0.65
1:A:538:LYS:NZ	3:C:3:DA:N7	2.44	0.65
1:A:1190:LYS:HE3	1:A:1213:ILE:HG21	1.78	0.65
1:A:876:LEU:HD23	1:A:899:LEU:HG	1.79	0.64
1:E:640:LYS:NZ	1:E:660:THR:OG1	2.20	0.64
1:A:69:ILE:HD11	1:A:105:ILE:HG12	1.80	0.64
1:E:938:VAL:HG23	1:E:940:LYS:H	1.62	0.64
1:E:996:ILE:HD11	1:E:1187:ILE:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:HG23	1:A:271:PRO:HG2	1.81	0.63
1:A:81:PHE:HZ	1:A:181:THR:HG23	1.64	0.62
2:F:11:A:H2'	2:F:12:A:C8	2.34	0.62
1:A:28:GLN:HE22	1:A:794:TYR:HE1	1.46	0.62
1:E:606:TYR:O	1:E:608:PRO:HD3	1.99	0.62
1:A:964:PRO:HB3	1:A:970:ALA:HB3	1.80	0.62
1:A:297:ASP:OD1	1:A:510:TYR:OH	2.18	0.62
1:A:464:LYS:NZ	1:A:501:ASP:OD2	2.32	0.62
1:E:87:THR:O	1:E:91:ASN:ND2	2.26	0.62
1:A:464:LYS:NZ	2:B:14:C:OP1	2.33	0.62
1:E:526:GLN:HB3	1:E:560:LYS:HD2	1.83	0.61
1:E:352:PHE:CD1	1:E:408:LEU:HD23	2.36	0.61
1:A:596:VAL:O	1:A:599:SER:OG	2.19	0.60
1:E:310:LYS:HE3	1:E:429:TYR:CG	2.36	0.60
1:A:996:ILE:HD11	1:A:1187:ILE:HG23	1.82	0.60
1:E:80:LEU:HB3	1:E:94:LEU:HD13	1.83	0.60
1:E:80:LEU:O	1:E:86:ARG:NH1	2.34	0.60
1:A:483:ASP:O	1:A:486:PHE:N	2.34	0.60
1:A:80:LEU:HB3	1:A:94:LEU:HD13	1.83	0.59
1:E:726:LEU:HD13	1:E:971:LEU:HG	1.83	0.59
1:E:279:GLN:HG3	1:E:282:SER:HB2	1.84	0.59
1:E:367:ASP:O	1:E:371:LEU:N	2.35	0.59
1:A:305:ARG:HH21	1:A:438:ALA:HA	1.68	0.59
1:E:936:VAL:HG21	2:F:9:U:H5''	1.85	0.59
1:E:218:ASP:HA	1:E:221:GLU:HG3	1.83	0.59
1:A:904:ILE:HD11	1:A:942:VAL:HG22	1.84	0.58
1:E:325:PHE:HA	1:E:328:PHE:HD1	1.68	0.58
1:E:548:ARG:HD3	1:E:553:TYR:CE2	2.39	0.58
1:E:640:LYS:HE2	1:E:657:PHE:HD1	1.66	0.58
2:F:15:G:H1	3:G:-15:DC:H42	1.50	0.58
1:E:21:ALA:HB3	1:E:794:TYR:HB2	1.85	0.58
1:A:361:LYS:NZ	1:A:403:TYR:O	2.37	0.58
1:A:964:PRO:HA	1:A:970:ALA:H	1.68	0.58
1:A:171:ILE:HG12	1:A:280:VAL:HB	1.84	0.58
1:E:326:LYS:HA	1:E:415:LYS:HG3	1.84	0.58
1:E:655:PHE:HD2	1:E:657:PHE:CZ	2.22	0.58
1:E:206:LYS:HA	1:E:210:LEU:HB2	1.86	0.57
1:A:375:ALA:O	1:A:376:VAL:HG12	2.04	0.57
1:A:722:MET:HE1	1:A:960:LYS:HA	1.86	0.57
1:E:305:ARG:NH2	1:E:437:ASP:O	2.37	0.57
1:A:286:SER:OG	3:C:-12:DT:OP1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:ILE:HD12	1:A:1147:VAL:HG21	1.85	0.57
1:E:322:GLU:CD	1:E:422:VAL:HG21	2.30	0.57
1:A:148:THR:OG1	4:D:-4:DT:OP1	2.21	0.57
1:A:376:VAL:O	1:A:377:VAL:HG13	2.04	0.57
1:A:645:ARG:HH21	1:A:645:ARG:HG3	1.69	0.57
1:A:767:ASN:ND2	1:A:774:LYS:O	2.30	0.57
1:A:375:ALA:HB1	1:A:378:THR:OG1	2.04	0.57
1:A:486:PHE:HD2	1:A:487:TYR:HD2	1.52	0.57
1:E:48:LYS:HD2	1:E:52:LYS:HD3	1.85	0.57
1:E:362:TRP:CD1	1:E:403:TYR:HH	2.23	0.57
1:A:813:ASN:OD1	1:A:978:ASN:ND2	2.35	0.57
1:E:328:PHE:HE2	1:E:397:LEU:HD11	1.70	0.57
1:A:308:LEU:O	1:A:429:TYR:OH	2.09	0.56
1:A:1073:ARG:HH12	1:A:1076:ARG:NH2	2.03	0.56
1:E:471:LYS:HD2	1:E:494:TYR:OH	2.05	0.56
1:A:1055:THR:O	1:A:1061:LYS:NZ	2.38	0.56
1:A:531:MET:HG3	1:A:544:ALA:HB3	1.87	0.56
1:A:572:ASP:OD1	1:A:575:ASN:N	2.28	0.56
1:E:286:SER:OG	3:G:-12:DT:OP1	2.16	0.56
1:A:75:ASN:ND2	1:A:223:GLU:OE2	2.31	0.56
1:E:328:PHE:HB3	1:E:411:VAL:HG23	1.88	0.56
1:A:1192:LEU:HD23	1:A:1195:ILE:HD12	1.86	0.56
1:A:482:ARG:O	1:A:484:GLU:N	2.38	0.56
1:A:596:VAL:HG11	1:A:646:TYR:CE1	2.38	0.56
1:E:592:MET:HA	1:E:595:LYS:HG2	1.88	0.56
1:A:442:LEU:HD21	1:A:452:VAL:HG21	1.88	0.56
1:A:667:ALA:HB2	4:D:1:DT:H2'	1.88	0.56
1:A:672:GLU:O	1:A:676:GLN:HG3	2.06	0.56
1:E:205:ILE:HG23	1:E:209:ILE:HD12	1.87	0.56
1:E:486:PHE:HD2	1:E:487:TYR:CD2	2.24	0.56
1:E:110:LYS:HG2	1:E:115:TYR:CD2	2.41	0.55
1:E:486:PHE:HD2	1:E:487:TYR:HD2	1.52	0.55
1:A:1027:PHE:O	1:A:1030:SER:OG	2.23	0.55
1:E:328:PHE:CE2	1:E:397:LEU:HD11	2.41	0.55
1:A:558:MET:HE3	1:A:566:LEU:HD12	1.87	0.55
1:E:378:THR:H	1:E:381:TYR:HB3	1.71	0.55
1:A:522:LYS:HE3	1:A:743:GLU:HG2	1.89	0.55
1:E:1024:SER:O	1:E:1028:ILE:HD12	2.07	0.55
1:E:300:VAL:HG21	1:E:510:TYR:CD2	2.42	0.55
1:E:379:GLU:OE1	1:E:379:GLU:N	2.40	0.54
3:C:-2:DG:H2'	3:C:-1:DC:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:767:ASN:ND2	1:E:774:LYS:O	2.31	0.54
1:E:1072:ILE:HD13	1:E:1141:ILE:HD11	1.87	0.54
1:E:1033:ARG:NH2	1:E:1044:GLU:OE2	2.40	0.54
1:A:94:LEU:HA	1:A:97:LEU:HD12	1.90	0.54
1:A:341:GLY:H	1:A:344:ILE:HG12	1.71	0.54
1:E:956:TYR:OH	1:E:970:ALA:O	2.18	0.54
2:F:-4:A:H2'	2:F:-3:G:C8	2.43	0.54
1:A:447:LYS:HB3	1:A:515:PRO:HG3	1.90	0.54
1:E:21:ALA:HB3	1:E:794:TYR:CB	2.36	0.54
1:E:264:GLN:NE2	3:G:-16:DC:O2	2.39	0.54
1:A:606:TYR:O	1:A:608:PRO:HD3	2.08	0.54
1:E:522:LYS:HD3	1:E:524:TYR:CZ	2.43	0.54
1:E:637:ASP:OD1	1:E:660:THR:HG21	2.07	0.54
1:E:597:PHE:HE1	1:E:646:TYR:HD1	1.54	0.54
1:A:325:PHE:HA	1:A:328:PHE:HD1	1.73	0.53
1:A:300:VAL:HG21	1:A:510:TYR:CD2	2.43	0.53
1:A:128:LEU:HD23	1:A:141:VAL:HG21	1.90	0.53
1:A:144:PHE:CD2	1:A:151:PHE:HE1	2.26	0.53
1:E:332:SER:N	1:E:483:ASP:OD1	2.30	0.53
1:A:726:LEU:HB3	1:A:971:LEU:HD21	1.91	0.53
1:E:3:LYS:HB2	1:E:919:ASP:OD2	2.08	0.53
1:E:193:VAL:HG13	1:E:270:LEU:HD13	1.91	0.53
1:E:508:ARG:HB2	1:E:890:TRP:CZ2	2.44	0.53
1:A:1:MET:HE3	1:A:2:SER:HA	1.90	0.53
1:E:531:MET:HG3	1:E:544:ALA:HB3	1.90	0.53
1:E:534:TRP:O	1:E:583:TYR:HB3	2.09	0.53
1:A:591:LYS:HB2	4:D:-1:DA:H1'	1.91	0.53
1:A:1021:ILE:O	1:A:1025:LYS:HG3	2.09	0.53
1:A:325:PHE:HE1	1:A:473:PHE:HE2	1.56	0.53
1:E:1073:ARG:HH22	1:E:1076:ARG:HH22	1.56	0.53
3:C:-12:DT:H2'	3:C:-11:DT:C6	2.43	0.53
2:F:4:U:H2'	2:F:5:C:C6	2.44	0.53
1:A:305:ARG:NH2	1:A:438:ALA:HA	2.24	0.52
1:E:242:GLY:HA2	3:G:-14:DG:H4'	1.90	0.52
1:E:740:GLY:O	3:G:0:DG:H2''	2.09	0.52
1:A:210:LEU:HD21	1:A:240:ILE:HD11	1.91	0.52
1:E:380:LYS:HE3	1:E:380:LYS:HA	1.91	0.52
1:E:957:MET:HE2	1:E:974:TYR:HD2	1.73	0.52
1:A:1076:ARG:H	1:A:1076:ARG:HE	1.58	0.52
1:E:909:HIS:CD2	2:F:-3:G:H4'	2.45	0.52
1:E:487:TYR:HA	1:E:490:PHE:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:LEU:HD13	1:A:1011:VAL:HG11	1.92	0.52
1:E:73:ASN:O	1:E:73:ASN:ND2	2.43	0.52
1:E:1027:PHE:CE1	1:E:1031:PHE:HE1	2.27	0.51
1:A:904:ILE:HD12	1:A:946:PHE:HA	1.92	0.51
1:E:330:GLU:N	1:E:330:GLU:OE1	2.43	0.51
1:A:417:ILE:O	1:A:421:LYS:HG3	2.11	0.51
1:A:121:LYS:H	4:D:-3:DT:P	2.34	0.51
1:A:740:GLY:O	3:C:0:DG:H2''	2.11	0.51
1:A:328:PHE:CE2	1:A:397:LEU:HD11	2.35	0.51
1:A:1213:ILE:HG12	1:A:1218:TRP:HB2	1.93	0.51
1:E:596:VAL:HG11	1:E:646:TYR:CE1	2.39	0.51
1:A:325:PHE:O	1:A:328:PHE:HB2	2.11	0.51
1:A:813:ASN:O	1:A:817:ARG:HG3	2.10	0.51
1:E:571:LYS:HG3	1:E:684:SER:HB2	1.93	0.51
1:A:75:ASN:HD21	1:A:223:GLU:CD	2.17	0.50
1:E:74:LEU:O	1:E:78:ILE:HG13	2.11	0.50
1:A:206:LYS:HA	1:A:210:LEU:HB2	1.92	0.50
2:B:9:U:H2'	2:B:10:A:H8	1.76	0.50
1:E:1045:PHE:HB2	1:E:1065:LEU:HB2	1.92	0.50
1:A:129:PRO:HA	1:A:138:ILE:HD11	1.93	0.50
1:E:667:ALA:HB2	4:H:1:DT:H2''	1.94	0.50
1:E:179:ASN:HD21	1:E:234:ILE:HD11	1.77	0.50
1:E:304:PHE:O	1:E:308:LEU:HB2	2.11	0.50
1:E:351:ILE:O	1:E:413:LYS:HG2	2.12	0.50
1:E:756:LEU:O	1:E:758:VAL:HG23	2.11	0.50
1:A:351:ILE:HG23	1:A:413:LYS:HB3	1.94	0.50
2:F:9:U:H2'	2:F:10:A:H8	1.77	0.50
1:A:328:PHE:HD2	1:A:411:VAL:HG23	1.77	0.50
1:A:780:SER:O	1:A:780:SER:OG	2.25	0.50
1:E:310:LYS:HE3	1:E:429:TYR:CD1	2.47	0.50
1:E:464:LYS:HZ1	2:F:14:C:P	2.34	0.50
1:A:81:PHE:CZ	1:A:181:THR:HG23	2.46	0.49
1:A:379:GLU:O	1:A:383:ASP:HB2	2.12	0.49
1:A:986:MET:HE1	1:A:990:ASN:HD22	1.77	0.49
1:A:264:GLN:NE2	3:C:-16:DC:O2	2.41	0.49
1:A:1041:ASP:OD1	1:A:1096:LYS:NZ	2.33	0.49
1:E:115:TYR:CE1	1:E:119:PHE:HE2	2.29	0.49
1:E:837:ASN:HA	1:E:857:ASN:HD21	1.77	0.49
1:E:318:ILE:HG23	1:E:466:PHE:CE2	2.47	0.49
1:A:584:LYS:HB3	1:A:653:TYR:HE1	1.78	0.49
1:E:9:ASN:OD1	1:E:806:PRO:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:813:ASN:O	1:E:817:ARG:HG3	2.13	0.49
1:A:105:ILE:HD11	1:A:176:ILE:HD11	1.93	0.49
1:E:209:ILE:HG12	1:E:244:PHE:HE1	1.78	0.49
1:A:218:ASP:HB3	1:A:224:PHE:CE1	2.48	0.49
1:A:729:ASP:CG	1:A:731:ASN:HD22	2.21	0.48
1:A:907:VAL:O	1:A:911:ILE:HD12	2.13	0.48
1:E:109:PHE:O	1:E:111:GLY:HA3	2.13	0.48
1:A:367:ASP:O	1:A:371:LEU:N	2.46	0.48
1:A:1104:ILE:HG23	1:A:1114:LEU:HG	1.95	0.48
1:E:785:LYS:HB2	2:F:-20:A:H5''	1.96	0.48
1:E:78:ILE:HG22	1:E:82:ARG:HD2	1.96	0.48
1:E:909:HIS:O	1:E:913:GLU:HG3	2.13	0.48
1:A:813:ASN:ND2	1:A:989:GLN:HG2	2.29	0.48
2:B:7:A:H2'	2:B:8:G:C8	2.48	0.48
1:E:83:LYS:HG3	1:E:85:THR:H	1.77	0.48
1:E:291:GLY:HA3	1:E:502:HIS:NE2	2.29	0.48
1:A:9:ASN:OD1	1:A:806:PRO:HA	2.12	0.48
1:E:461:ASP:OD1	1:E:504:TYR:OH	2.16	0.48
1:A:785:LYS:HD2	2:B:-20:A:H5''	1.95	0.48
1:A:998:ALA:O	1:A:1001:THR:OG1	2.26	0.48
1:E:73:ASN:HB2	1:E:76:ASN:HB2	1.94	0.48
1:E:102:ARG:HD3	1:E:177:ASN:OD1	2.13	0.48
1:E:325:PHE:HA	1:E:328:PHE:CE1	2.48	0.48
1:E:1031:PHE:CE2	1:E:1045:PHE:HB3	2.49	0.48
1:A:1:MET:HG3	1:A:2:SER:N	2.28	0.48
1:A:193:VAL:HG13	1:A:270:LEU:HD13	1.95	0.48
1:A:354:GLU:HB3	1:A:357:VAL:HG23	1.95	0.48
1:E:626:MET:H	1:E:626:MET:HG2	1.48	0.48
1:A:615:ILE:HG23	1:A:620:THR:OG1	2.13	0.48
1:A:307:THR:O	1:A:312:SER:OG	2.27	0.47
1:E:161:MET:O	1:E:171:ILE:HG13	2.13	0.47
1:A:938:VAL:HB	1:A:940:LYS:H	1.79	0.47
1:E:446:LEU:HD23	1:E:510:TYR:HE2	1.79	0.47
1:A:1031:PHE:CE2	1:A:1047:LEU:HD23	2.49	0.47
1:A:1167:TYR:CE2	1:A:1175:LEU:HB2	2.49	0.47
1:E:527:ASN:OD1	1:E:529:GLN:N	2.47	0.47
1:E:1073:ARG:NH2	1:E:1087:GLU:OE1	2.46	0.47
2:F:9:U:H2'	2:F:10:A:C8	2.49	0.47
2:B:7:A:H2'	2:B:8:G:H8	1.78	0.47
1:E:87:THR:OG1	1:E:90:GLU:HG3	2.14	0.47
1:E:558:MET:HE3	1:E:566:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:OD1	1:A:200:HIS:N	2.37	0.47
1:A:477:GLY:HA2	1:A:478:LYS:HB3	1.96	0.47
1:A:843:VAL:HG11	1:A:918:TYR:CD2	2.50	0.47
2:B:9:U:H2'	2:B:10:A:C8	2.50	0.47
1:E:121:LYS:H	4:H:-3:DT:P	2.37	0.47
1:A:278:LYS:NZ	2:B:6:C:OP1	2.42	0.47
1:A:645:ARG:HG3	1:A:645:ARG:NH2	2.29	0.47
2:B:11:A:H2'	2:B:12:A:C8	2.49	0.47
1:E:62:ILE:HD13	1:E:171:ILE:HD11	1.97	0.47
1:E:752:LYS:HB2	1:E:755:GLU:HG3	1.97	0.47
1:E:476:GLU:OE1	1:E:478:LYS:HE2	2.15	0.47
1:E:611:ASP:O	1:E:615:ILE:HG12	2.15	0.47
1:E:1099:PHE:O	1:E:1104:ILE:N	2.41	0.47
1:A:209:ILE:HG12	1:A:244:PHE:CE1	2.44	0.46
2:B:-5:U:H2'	2:B:-4:A:H8	1.80	0.46
1:E:148:THR:OG1	4:H:-4:DT:OP1	2.19	0.46
1:E:316:SER:O	1:E:320:LYS:HG3	2.15	0.46
1:A:125:GLU:HG2	1:A:145:ASN:OD1	2.15	0.46
1:E:174:ARG:NH2	1:E:278:LYS:O	2.44	0.46
1:E:827:TYR:HE2	1:E:851:VAL:HG21	1.80	0.46
1:A:69:ILE:CD1	1:A:105:ILE:HG12	2.45	0.46
1:E:640:LYS:HE2	1:E:657:PHE:CD1	2.47	0.46
1:E:779:LEU:HD13	1:E:781:TYR:CZ	2.50	0.46
1:A:926:ASP:HB2	1:A:996:ILE:C	2.40	0.46
2:B:5:C:H42	3:C:-5:DG:H1	1.63	0.46
1:E:3:LYS:HE3	1:E:919:ASP:OD2	2.16	0.46
1:E:20:LYS:HG3	1:E:793:GLN:HG3	1.96	0.46
1:E:347:ILE:O	1:E:351:ILE:HG12	2.16	0.46
1:E:352:PHE:HD1	1:E:408:LEU:HD23	1.80	0.46
1:E:719:LEU:HD11	1:E:958:VAL:HG11	1.97	0.46
2:F:-5:U:H2'	2:F:-4:A:C8	2.51	0.46
1:A:290:TYR:HE1	3:C:-12:DT:H1'	1.79	0.46
1:A:297:ASP:OD2	1:A:446:LEU:HB2	2.15	0.46
1:E:228:VAL:HG21	1:E:276:LEU:HD12	1.97	0.46
1:E:580:LYS:HB3	1:E:580:LYS:HE2	1.62	0.46
1:E:1111:ILE:HG22	1:E:1115:LEU:HG	1.97	0.46
1:A:52:LYS:HA	1:A:52:LYS:HD2	1.70	0.46
1:A:308:LEU:HD12	1:A:459:LEU:CD2	2.46	0.46
1:E:817:ARG:HD3	1:E:1198:PHE:CE1	2.49	0.46
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.73	0.46
1:A:1073:ARG:NH2	1:A:1087:GLU:OE1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HD11	1:A:446:LEU:HD13	1.98	0.46
1:A:477:GLY:HA3	1:A:479:GLU:OE2	2.15	0.46
1:E:313:GLU:O	1:E:317:SER:N	2.45	0.46
1:E:859:ILE:HG23	1:E:910:LYS:HE2	1.97	0.46
1:A:198:ASP:HB3	1:A:201:GLU:HG3	1.98	0.46
1:E:121:LYS:HD2	1:E:125:GLU:OE2	2.16	0.46
1:E:190:PHE:CZ	1:E:217:GLU:HG3	2.52	0.46
1:E:444:LYS:HG2	1:E:448:LYS:HB3	1.97	0.46
1:A:858:GLU:OE2	1:A:869:LYS:HD3	2.16	0.45
1:A:1058:ASP:O	1:A:1061:LYS:HE2	2.16	0.45
1:A:241:ILE:HG23	1:A:273:PHE:HB2	1.98	0.45
2:B:-5:U:H2'	2:B:-4:A:C8	2.50	0.45
3:C:-15:DC:H2'	3:C:-14:DG:C8	2.51	0.45
1:E:672:GLU:O	1:E:676:GLN:HG3	2.17	0.45
3:G:-15:DC:H2'	3:G:-14:DG:H8	1.80	0.45
1:E:548:ARG:HD3	1:E:553:TYR:CZ	2.51	0.45
1:E:722:MET:HE2	1:E:970:ALA:HB2	1.99	0.45
3:C:-14:DG:H2'	3:C:-13:DC:H6	1.81	0.45
1:E:1024:SER:HB3	1:E:1128:MET:HE3	1.99	0.45
3:G:-15:DC:H2'	3:G:-14:DG:C8	2.52	0.45
3:C:-15:DC:H2'	3:C:-14:DG:H8	1.81	0.45
1:A:46:ASP:O	1:A:50:VAL:HG23	2.16	0.45
1:A:58:TYR:O	1:A:62:ILE:HG13	2.16	0.45
3:G:1:DT:H3	4:H:-1:DA:H61	1.65	0.45
1:A:95:GLU:O	1:A:98:GLU:HG2	2.17	0.45
1:E:615:ILE:HG23	1:E:620:THR:OG1	2.17	0.45
1:A:180:LEU:O	1:A:184:ILE:HG13	2.16	0.45
1:A:939:GLU:O	1:A:942:VAL:HG12	2.17	0.45
1:E:366:TYR:O	1:E:369:ILE:HG13	2.16	0.45
1:A:325:PHE:CE1	1:A:473:PHE:HE2	2.35	0.44
1:A:548:ARG:HD3	1:A:553:TYR:CZ	2.51	0.44
1:A:1073:ARG:HH22	1:A:1076:ARG:NH2	2.14	0.44
1:E:666:ILE:HG13	1:E:670:TYR:CE2	2.51	0.44
1:A:469:TYR:HD2	1:A:470:ILE:HD12	1.82	0.44
1:A:1005:ASP:OD1	1:A:1007:SER:N	2.51	0.44
1:E:155:PHE:O	1:E:159:GLU:HG3	2.17	0.44
1:E:186:ASN:ND2	1:E:237:TYR:OH	2.35	0.44
1:E:204:GLU:OE1	1:E:258:TYR:OH	2.34	0.44
1:E:543:ARG:HG2	1:E:558:MET:HB2	1.99	0.44
1:E:820:LEU:HD13	1:E:1195:ILE:HG12	1.98	0.44
1:A:135:LYS:O	1:A:138:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:THR:HG21	2:B:-13:A:H4'	1.98	0.44
1:A:876:LEU:CD2	1:A:899:LEU:HG	2.45	0.44
1:A:931:PHE:HD1	1:A:931:PHE:O	2.00	0.44
1:E:52:LYS:HA	1:E:52:LYS:HD2	1.82	0.44
1:E:105:ILE:HD11	1:E:176:ILE:HD11	2.00	0.44
1:E:655:PHE:HD2	1:E:657:PHE:CE2	2.35	0.44
1:E:210:LEU:HD21	1:E:240:ILE:HD11	1.98	0.44
1:E:1000:LEU:HD23	1:E:1000:LEU:HA	1.78	0.44
1:A:71:LEU:HD21	1:A:229:LEU:HD11	1.99	0.44
1:A:333:SER:O	1:A:397:LEU:HB2	2.17	0.44
1:A:169:THR:HG22	2:B:5:C:H1'	2.00	0.44
1:E:1030:SER:HB2	1:E:1052:PHE:CZ	2.53	0.44
1:A:197:PHE:CE2	1:A:255:LEU:HD22	2.53	0.44
3:C:-11:DT:H2'	3:C:-10:DT:C6	2.52	0.44
1:E:397:LEU:HD23	1:E:397:LEU:HA	1.82	0.44
1:E:926:ASP:N	1:E:996:ILE:O	2.40	0.44
1:E:1049:TYR:O	1:E:1055:THR:OG1	2.27	0.43
2:F:15:G:H1	3:G:-15:DC:N4	2.14	0.43
1:A:315:PHE:HE2	1:A:426:TYR:CZ	2.36	0.43
1:E:314:ILE:HD12	1:E:314:ILE:H	1.83	0.43
1:A:1052:PHE:HB2	1:A:1055:THR:HG21	2.00	0.43
1:A:21:ALA:O	1:A:794:TYR:HB2	2.18	0.43
1:A:124:ILE:HD12	1:A:148:THR:HG22	2.00	0.43
1:A:263:ASN:ND2	1:A:270:LEU:H	2.15	0.43
1:E:8:THR:HG21	1:E:967:THR:HG23	1.99	0.43
1:E:967:THR:HG22	1:E:974:TYR:HE1	1.82	0.43
1:A:900:LYS:O	1:A:904:ILE:HG12	2.18	0.43
1:E:349:LYS:HB3	1:E:349:LYS:HE2	1.86	0.43
1:E:505:ASP:OD1	1:E:508:ARG:NH2	2.49	0.43
1:A:149:THR:OG1	1:A:528:PRO:HB2	2.18	0.43
1:A:534:TRP:O	1:A:583:TYR:HB3	2.18	0.43
1:E:547:LEU:HD23	1:E:580:LYS:HA	2.00	0.43
1:E:1014:LEU:HD11	1:E:1047:LEU:HD21	2.00	0.43
2:F:-4:A:H2'	2:F:-3:G:H8	1.80	0.43
1:A:505:ASP:OD1	2:B:13:G:O2'	2.20	0.43
1:A:589:PRO:HG2	1:A:674:GLU:HB2	2.00	0.43
1:A:601:LYS:HG2	1:A:602:TRP:CD1	2.54	0.43
1:E:348:SER:HB2	1:E:358:ILE:HG13	2.00	0.43
1:A:21:ALA:HB3	1:A:794:TYR:HB3	2.00	0.43
1:A:475:GLY:C	1:A:476:GLU:HG3	2.44	0.43
1:A:1160:ILE:HD12	1:A:1161:PHE:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:475:GLY:C	1:E:476:GLU:HG3	2.43	0.43
1:A:427:LYS:HZ1	1:A:428:VAL:N	2.16	0.43
1:A:681:SER:OG	1:A:682:PHE:N	2.51	0.43
1:E:726:LEU:HD22	1:E:971:LEU:HD11	2.01	0.43
1:A:126:THR:C	1:A:129:PRO:HD2	2.43	0.42
1:A:175:CYS:O	1:A:180:LEU:HD23	2.19	0.42
1:E:477:GLY:HA2	1:E:478:LYS:C	2.43	0.42
1:E:549:TYR:CE1	1:E:687:LYS:HD2	2.54	0.42
1:A:99:ILE:HG22	1:A:103:LYS:HE3	2.01	0.42
1:E:27:THR:O	1:E:31:ILE:HG13	2.19	0.42
1:E:214:TYR:CE1	1:E:227:PHE:HE1	2.38	0.42
1:E:584:LYS:HD2	1:E:584:LYS:HA	1.83	0.42
1:E:1139:ASN:HB2	1:E:1149:PHE:CE1	2.54	0.42
1:A:120:LYS:HB3	4:D:-3:DT:OP1	2.20	0.42
1:A:584:LYS:HD2	1:A:584:LYS:HA	1.77	0.42
1:A:785:LYS:HB2	2:B:-20:A:H5''	2.01	0.42
1:A:1086:TRP:CE2	1:A:1141:ILE:HD13	2.55	0.42
1:E:602:TRP:NE1	3:G:4:DA:OP1	2.49	0.42
2:F:-14:U:H2'	2:F:-13:A:O4'	2.20	0.42
1:A:121:LYS:HD2	1:A:125:GLU:OE2	2.20	0.42
1:A:1076:ARG:HE	1:A:1076:ARG:N	2.16	0.42
1:E:482:ARG:O	1:E:484:GLU:N	2.51	0.42
1:A:898:GLU:HG2	2:B:-15:C:H4'	2.00	0.42
1:E:591:LYS:HB2	4:H:-1:DA:H1'	2.01	0.42
1:E:1160:ILE:HD12	1:E:1161:PHE:H	1.84	0.42
1:A:281:LEU:HD12	1:A:281:LEU:HA	1.91	0.42
1:A:549:TYR:CE1	1:A:687:LYS:HD2	2.54	0.42
1:A:955:ASN:HD21	1:A:980:PHE:H	1.67	0.42
1:A:1059:TYR:HB2	1:A:1220:GLU:HA	2.02	0.42
3:C:-14:DG:H2'	3:C:-13:DC:C6	2.54	0.42
1:A:666:ILE:HG13	1:A:670:TYR:CE2	2.54	0.42
1:E:361:LYS:HD3	1:E:361:LYS:HA	1.88	0.42
1:A:1059:TYR:HB3	1:A:1223:GLN:OE1	2.20	0.42
1:A:1067:SER:HB2	1:A:1091:LEU:HB3	2.02	0.42
1:E:256:ASN:CG	1:E:272:LYS:HB2	2.45	0.42
1:E:629:LEU:HD23	1:E:629:LEU:HA	1.89	0.42
1:E:1010:PHE:CZ	1:E:1065:LEU:HD11	2.55	0.42
1:A:211:ASN:HD22	1:A:211:ASN:C	2.25	0.42
1:E:388:SER:O	1:E:392:ILE:HG12	2.20	0.42
3:G:-14:DG:H2'	3:G:-13:DC:H6	1.85	0.42
1:E:831:ILE:HD13	1:E:911:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:831:ILE:HD12	1:E:924:LEU:HD21	2.01	0.42
1:E:873:HIS:O	1:E:877:ASP:HB2	2.20	0.42
1:A:371:LEU:HD11	1:A:376:VAL:C	2.44	0.41
1:E:464:LYS:NZ	2:F:14:C:P	2.93	0.41
1:E:746:MET:HE1	1:E:792:ASP:HB3	2.02	0.41
1:A:341:GLY:O	1:A:344:ILE:HG12	2.20	0.41
1:A:1059:TYR:CD1	1:A:1220:GLU:HG3	2.55	0.41
1:E:382:GLU:HG2	1:E:385:ARG:CZ	2.50	0.41
1:E:542:TYR:OH	3:G:2:DA:OP2	2.28	0.41
3:G:-4:DA:H2''	3:G:-3:DT:H5''	2.01	0.41
2:F:5:C:H2'	2:F:6:C:O4'	2.21	0.41
1:A:95:GLU:O	1:A:99:ILE:HG13	2.20	0.41
1:A:107:LYS:O	1:A:111:GLY:N	2.49	0.41
1:A:214:TYR:CZ	1:A:227:PHE:HE1	2.38	0.41
1:A:486:PHE:HD2	1:A:487:TYR:CD2	2.36	0.41
1:A:487:TYR:O	1:A:491:VAL:HG23	2.19	0.41
1:A:827:TYR:HE2	1:A:851:VAL:HG21	1.86	0.41
1:E:488:GLY:O	1:E:492:LEU:HG	2.21	0.41
1:E:686:SER:HB3	1:E:689:GLU:HB2	2.01	0.41
2:F:-15:C:H2'	2:F:-14:U:H6	1.85	0.41
1:A:237:TYR:CE1	1:A:276:LEU:HG	2.56	0.41
1:A:612:ILE:CD1	1:A:634:LYS:HG2	2.47	0.41
1:E:584:LYS:HB3	1:E:653:TYR:CE1	2.56	0.41
1:A:214:TYR:CE1	1:A:227:PHE:HE1	2.38	0.41
1:E:341:GLY:H	1:E:344:ILE:HG12	1.85	0.41
1:E:1058:ASP:OD2	1:E:1063:TRP:NE1	2.40	0.41
1:E:1190:LYS:HE3	1:E:1213:ILE:HG21	2.03	0.41
1:A:15:LYS:HB3	2:B:0:C:H5'	2.02	0.41
1:A:218:ASP:HB3	1:A:224:PHE:CD1	2.55	0.41
1:A:508:ARG:HB2	1:A:890:TRP:CZ2	2.55	0.41
1:E:759:HIS:CE1	1:E:765:ILE:HG23	2.56	0.41
1:E:759:HIS:HB2	1:E:783:VAL:HB	2.03	0.41
1:A:290:TYR:CE1	3:C:-12:DT:H1'	2.55	0.41
1:A:435:LEU:HD23	1:A:455:ILE:HG21	2.03	0.41
1:A:705:TYR:OH	1:A:710:SER:HB2	2.21	0.41
1:A:904:ILE:HG22	1:A:908:VAL:HG23	2.02	0.41
1:A:1127:PHE:HD2	1:A:1128:MET:HE2	1.86	0.41
1:A:1200:LYS:O	1:E:753:LYS:HD3	2.21	0.41
1:E:58:TYR:O	1:E:62:ILE:HG13	2.20	0.41
1:E:99:ILE:HG22	1:E:103:LYS:HE3	2.03	0.41
1:E:639:PHE:O	1:E:643:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:785:LYS:HD2	2:F:-20:A:H5''	2.01	0.41
1:E:878:LYS:O	1:E:882:GLU:HG3	2.21	0.41
1:A:313:GLU:H	1:A:313:GLU:HG2	1.67	0.41
1:A:325:PHE:HA	1:A:328:PHE:CD1	2.55	0.41
1:A:548:ARG:HD3	1:A:553:TYR:CE2	2.55	0.41
1:A:1024:SER:HB3	1:A:1128:MET:HE3	2.02	0.41
1:E:199:LYS:HB2	1:E:199:LYS:HE3	1.88	0.41
1:E:726:LEU:HB3	1:E:971:LEU:HD21	2.03	0.41
1:A:335:GLY:HA3	1:A:483:ASP:HB2	2.03	0.40
1:E:417:ILE:O	1:E:421:LYS:HG3	2.20	0.40
1:E:648:LYS:HB2	1:E:648:LYS:HE3	1.81	0.40
1:E:657:PHE:CE1	1:E:669:PHE:HE1	2.40	0.40
1:E:3:LYS:HG2	1:E:819:LEU:HB3	2.03	0.40
1:E:167:LYS:NZ	3:G:-2:DG:OP1	2.45	0.40
1:E:339:LYS:O	1:E:344:ILE:HD11	2.21	0.40
1:E:380:LYS:HA	1:E:380:LYS:CE	2.50	0.40
1:E:879:LYS:HB2	6:E:1403:HOH:O	2.21	0.40
1:A:477:GLY:HA3	1:A:479:GLU:HG3	2.02	0.40
1:A:1141:ILE:HB	1:A:1147:VAL:HG21	2.03	0.40
1:E:190:PHE:HZ	1:E:217:GLU:HG3	1.85	0.40
1:E:241:ILE:HG23	1:E:273:PHE:HB2	2.04	0.40
1:E:1028:ILE:HG23	1:E:1034:ILE:HD12	2.03	0.40
4:H:-6:DC:H2''	4:H:-5:DC:C6	2.56	0.40
1:A:1005:ASP:HB2	1:A:1137:MET:HE1	2.02	0.40
1:E:357:VAL:HA	1:E:360:ASP:HB2	2.03	0.40
1:E:912:CYS:O	1:E:916:GLU:HG3	2.21	0.40
1:E:956:TYR:HD1	1:E:975:GLN:HE21	1.69	0.40
2:F:-15:C:H2'	2:F:-14:U:C6	2.57	0.40
1:A:8:THR:HG21	1:A:967:THR:HG23	2.04	0.40
1:A:447:LYS:HG3	1:A:513:GLN:O	2.22	0.40
1:A:1163:ASP:HB3	1:A:1166:ASN:OD1	2.21	0.40
1:E:43:ARG:O	1:E:47:TYR:N	2.49	0.40
1:E:858:GLU:CD	1:E:869:LYS:HD3	2.46	0.40
1:E:1096:LYS:HG2	1:E:1106:TYR:CE2	2.57	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	1219/1228 (99%)	1182 (97%)	35 (3%)	2 (0%)	43	74
1	E	1219/1228 (99%)	1185 (97%)	33 (3%)	1 (0%)	48	79
All	All	2438/2456 (99%)	2367 (97%)	68 (3%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	VAL
1	A	1148	ASP
1	E	761	ALA

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	1076/1115 (96%)	1075 (100%)	1 (0%)	88	87
1	E	1074/1115 (96%)	1074 (100%)	0	100	100
All	All	2150/2230 (96%)	2149 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	73	ASN
1	A	142	ASN
1	A	211	ASN
1	A	226	ASN
1	A	340	ASN
1	A	613	GLN
1	A	633	HIS
1	A	731	ASN
1	A	793	GLN
1	A	862	ASN
1	A	1197	GLN
1	E	179	ASN
1	E	567	GLN
1	E	582	ASN
1	E	656	ASN
1	E	793	GLN
1	E	909	HIS
1	E	1136	GLN
1	E	1197	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	37/40 (92%)	5 (13%)	0
2	F	37/40 (92%)	5 (13%)	0
All	All	74/80 (92%)	10 (13%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-12	C
2	B	-10	A
2	B	-9	A
2	B	-6	G
2	B	15	G
2	F	-12	C
2	F	-10	A
2	F	-9	A
2	F	-6	G
2	F	15	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1223/1228 (99%)	0.36	24 (1%) 65 37	14, 53, 97, 136	0
1	E	1223/1228 (99%)	0.36	26 (2%) 63 36	19, 52, 97, 141	0
2	B	38/40 (95%)	0.35	0 100 100	21, 34, 82, 100	0
2	F	38/40 (95%)	0.55	0 100 100	20, 31, 77, 98	0
3	C	27/27 (100%)	0.77	1 (3%) 45 25	33, 49, 110, 139	0
3	G	27/27 (100%)	0.68	0 100 100	35, 50, 112, 129	0
4	D	11/11 (100%)	1.02	1 (9%) 15 9	51, 57, 120, 126	0
4	H	11/11 (100%)	0.68	0 100 100	49, 52, 102, 121	0
All	All	2598/2612 (99%)	0.38	52 (2%) 65 37	14, 52, 98, 141	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	937	LYS	4.8
1	A	939	GLU	4.2
1	E	333	SER	4.1
1	E	933	ASN	3.9
1	A	528	PRO	3.8
1	A	376	VAL	3.6
1	A	938	VAL	3.6
1	E	226	ASN	3.5
3	C	7	DA	3.1
1	A	377	VAL	3.1
1	A	835	GLU	3.1
1	A	119	PHE	2.9
1	E	400	LEU	2.9
1	A	1081	ASN	2.8
4	D	-9	DC	2.8
1	A	293	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	249	GLY	2.8
1	A	429	TYR	2.7
1	E	980	PHE	2.7
1	E	936	VAL	2.6
1	A	983	PHE	2.6
1	E	88	GLU	2.5
1	E	983	PHE	2.5
1	E	714	HIS	2.5
1	E	399	GLN	2.4
1	A	111	GLY	2.4
1	E	835	GLU	2.4
1	A	146	GLY	2.3
1	A	353	GLY	2.3
1	E	295	THR	2.3
1	A	344	ILE	2.3
1	A	77	TYR	2.3
1	E	376	VAL	2.3
1	E	402	GLU	2.2
1	E	1146	ASP	2.2
1	A	347	ILE	2.2
1	A	936	VAL	2.2
1	A	570	ASP	2.2
1	E	202	VAL	2.2
1	A	408	LEU	2.2
1	E	352	PHE	2.1
1	A	342	PRO	2.1
1	E	932	LYS	2.1
1	E	379	GLU	2.1
1	E	834	GLY	2.1
1	E	293	GLY	2.0
1	E	389	PHE	2.0
1	A	516	TYR	2.0
1	E	198	ASP	2.0
1	A	452	VAL	2.0
1	E	410	VAL	2.0
1	A	354	GLU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	E	1301	1/1	0.87	0.23	2,2,2,2	0
5	MG	A	1302	1/1	0.94	0.29	4,4,4,4	0
5	MG	A	1301	1/1	0.97	0.23	17,17,17,17	0
5	MG	E	1302	1/1	0.98	0.15	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.