



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:28 PM UTC

PDB ID : 8Y07 / pdb_00008y07
Title : Crystal structure of LbCas12a in complex with crRNA and 13nt target DNA
Authors : Lin, X.; Chen, J.; Liu, L.
Deposited on : 2024-01-22
Resolution : 2.85 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

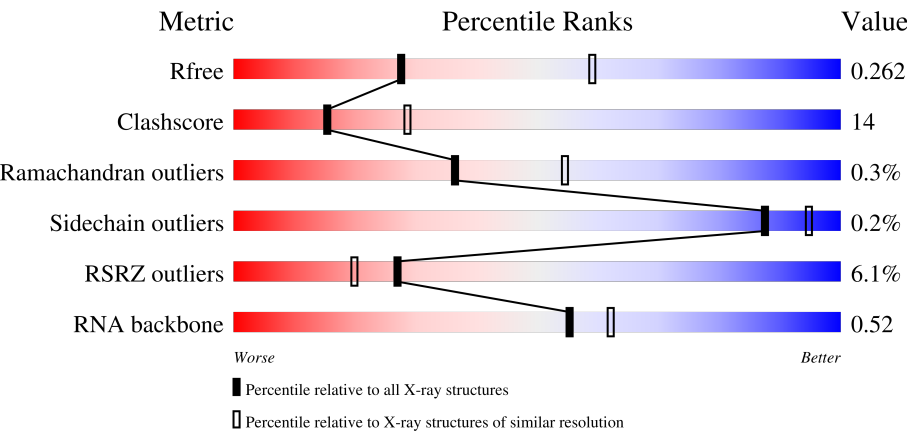
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)
RNA backbone	3983	1009 (3.06-2.66)

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	4% 73% 25% ..
1	E	1228	8% 69% 29% ..
2	B	40	48% 28% 8% 18%
2	F	40	62% 18% . 18%

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Mol	Chain	Length	Quality of chain
3	C	22	
3	G	22	
4	D	11	
4	H	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	LI	A	1301	-	-	-	X
5	LI	E	1301	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22604 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	E	1214	Total	C	N	O	S	0	0	0
			9902	6371	1618	1884	29			
1	A	1214	Total	C	N	O	S	0	0	0
			9949	6402	1626	1892	29			

- Molecule 2 is a RNA chain called RNA (33-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	33	Total	C	N	O	P	0	0	0
			696	314	123	227	32			
2	B	33	Total	C	N	O	P	0	0	0
			696	314	123	227	32			

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*TP*TP*AP*CP*TP*GP*GP*AP*TP*GP*CP*GP*TP*AP*AP*AP*GP*GP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	22	Total	C	N	O	P	0	0	0
			457	217	86	132	22			
3	C	22	Total	C	N	O	P	0	0	0
			457	217	86	132	22			

- 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	H	11	Total	C	N	O	P	0	0	0
			217	107	31	69	10			
4	D	11	Total	C	N	O	P	0	0	0
			217	107	31	69	10			

- Molecule 5 is LITHIUM ION (CCD ID: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total 1	Li 1	0	0
5	F	1	Total 1	Li 1	0	0
5	A	1	Total 1	Li 1	0	0
5	B	1	Total 1	Li 1	0	0

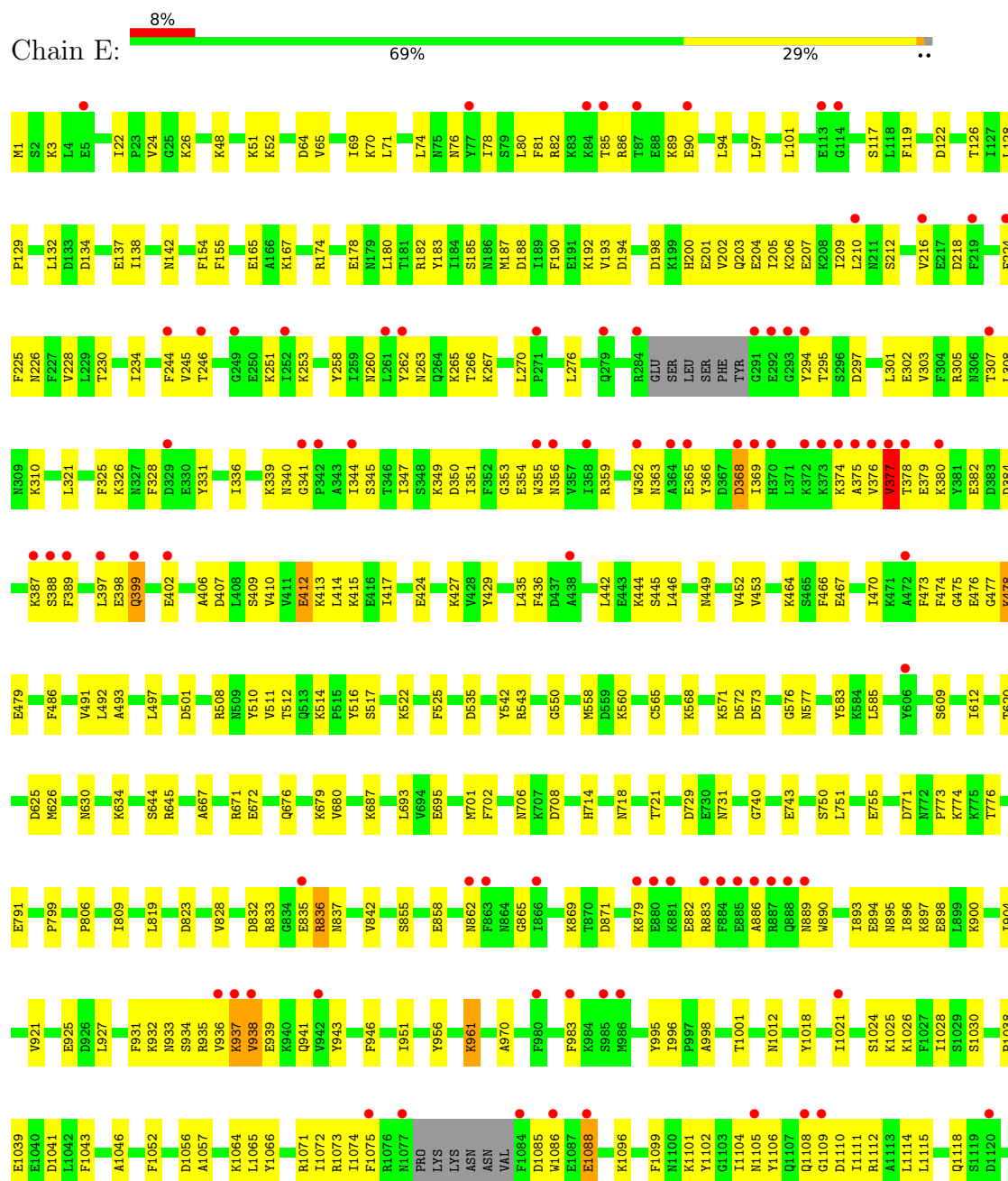
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	4	Total 4	O 4	0	0
6	A	5	Total 5	O 5	0	0

3 Residue-property plots

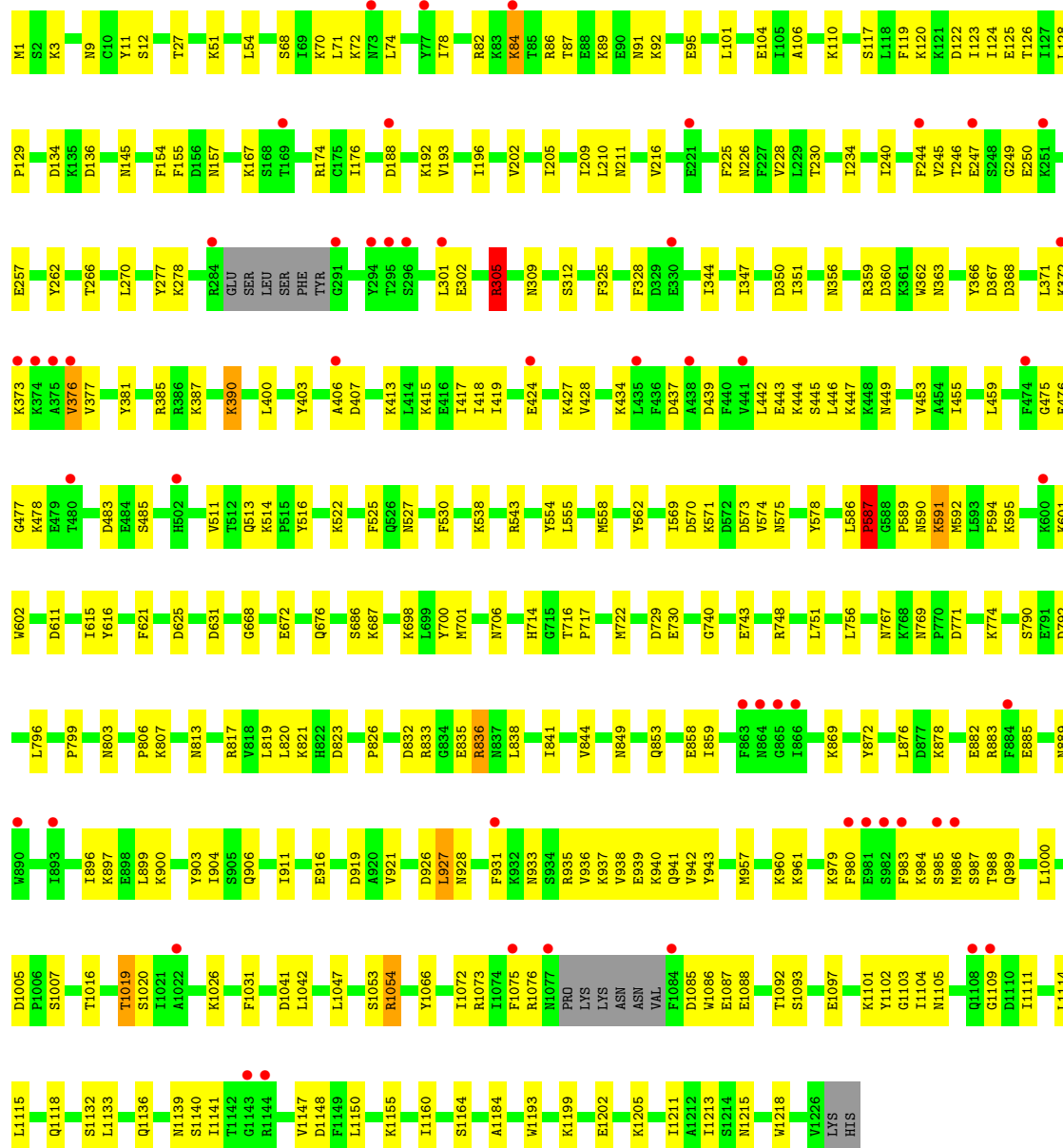
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 (33-MER)



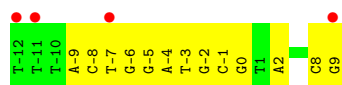
- Molecule 2: RNA (33-MER)

Chain B: 



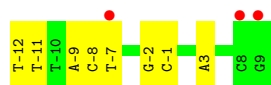
- Molecule 3: DNA (5'-D(P*TP*TP*TP*AP*CP*TP*GP*GP*AP*TP*GP*CP*GP*TP*AP*AP*AP*GP*GP*AP*CP*G)-3')

Chain G: 



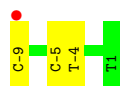
- Molecule 3: DNA (5'-D(P*TP*TP*TP*AP*CP*TP*GP*GP*AP*TP*GP*CP*GP*TP*AP*AP*AP*GP*GP*AP*CP*G)-3')

Chain C: 



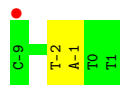
- Molecule 4: DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3')

Chain H: 



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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.66Å 142.67Å 202.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 2.85 49.05 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.05-2.85) 98.2 (49.05-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.209 , 0.264 0.208 , 0.262	Depositor DCC
R_{free} test set	4044 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22604	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% 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

5.1 Standard geometry

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

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	0.54	6/10158 (0.1%)	0.81	29/13664 (0.2%)
1	E	0.48	3/10108 (0.0%)	0.77	10/13601 (0.1%)
2	B	0.43	0/778	0.68	0/1209
2	F	0.43	0/778	0.68	0/1209
3	C	0.48	0/513	0.75	0/791
3	G	0.44	0/513	0.68	0/791
4	D	0.64	0/240	0.79	0/368
4	H	0.59	0/240	0.72	0/368
All	All	0.50	9/23328 (0.0%)	0.78	39/32001 (0.1%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	LYS	CG-CD	16.52	2.02	1.52
1	A	84	LYS	CE-NZ	9.51	1.77	1.49
1	A	84	LYS	CB-CG	9.40	1.80	1.52
1	A	1104	ILE	C-N	7.46	1.44	1.33
1	E	937	LYS	CB-CG	6.96	1.73	1.52
1	A	84	LYS	CA-CB	6.89	1.64	1.53
1	E	377	VAL	CB-CG1	-6.32	1.31	1.52
1	E	937	LYS	CE-NZ	5.96	1.67	1.49
1	A	589	PRO	N-CD	5.17	1.54	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LYS	CA-CB-CG	10.42	134.94	114.10
1	A	84	LYS	CG-CD-CE	10.09	134.50	111.30
1	A	1104	ILE	CA-C-N	-9.29	109.51	123.07
1	A	1104	ILE	C-N-CA	-9.29	109.51	123.07
1	A	305	ARG	CD-NE-CZ	8.61	136.46	124.40
1	E	399	GLN	CA-CB-CG	-8.59	96.93	114.10
1	A	424	GLU	CA-CB-CG	7.90	129.90	114.10
1	A	1054	ARG	CG-CD-NE	-6.92	96.78	112.00
1	A	192	LYS	CD-CE-NZ	-6.79	90.16	111.90
1	A	84	LYS	CD-CE-NZ	6.74	133.47	111.90
1	E	938	VAL	CA-C-N	-6.71	110.31	121.92
1	E	938	VAL	C-N-CA	-6.71	110.31	121.92
1	A	1103	GLY	CA-C-N	6.63	134.44	122.43
1	A	1103	GLY	C-N-CA	6.63	134.44	122.43
1	A	84	LYS	CB-CG-CD	6.54	126.34	111.30
1	E	89	LYS	CB-CG-CD	6.29	125.77	111.30
1	A	167	LYS	CB-CG-CD	6.26	125.70	111.30
1	E	412	GLU	CB-CG-CD	-6.07	102.28	112.60
1	E	1088	GLU	N-CA-C	5.99	118.17	108.41
1	A	1054	ARG	N-CA-CB	-5.96	102.67	113.10
1	A	390	LYS	CA-CB-CG	5.75	125.59	114.10
1	A	257	GLU	CA-CB-CG	5.69	125.49	114.10
1	E	377	VAL	CG1-CB-CG2	-5.69	98.28	110.80
1	A	587	PRO	CA-N-CD	-5.61	104.15	112.00
1	A	167	LYS	CA-CB-CG	-5.61	102.89	114.10
1	E	791	GLU	CA-CB-CG	5.52	125.14	114.10
1	A	167	LYS	CD-CE-NZ	5.49	129.47	111.90
1	A	1105	ASN	N-CA-CB	5.46	119.27	110.65
1	A	84	LYS	N-CA-CB	5.43	118.08	109.82
1	A	192	LYS	CB-CA-C	-5.38	100.69	109.56
1	A	1103	GLY	N-CA-C	5.29	123.22	115.08
1	A	591	LYS	N-CA-C	5.25	117.08	111.36
1	E	478	LYS	CB-CG-CD	-5.21	99.32	111.30
1	A	586	LEU	CA-C-N	-5.15	113.40	119.84
1	A	586	LEU	C-N-CA	-5.15	113.40	119.84
1	E	356	ASN	CB-CA-C	5.13	119.29	111.02
1	A	1105	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	927	LEU	CA-CB-CG	-5.08	98.51	116.30
1	A	305	ARG	NE-CZ-NH2	-5.05	114.66	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	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	9949	0	9786	248	1
1	E	9902	0	9719	318	1
2	B	696	0	355	13	0
2	F	696	0	355	4	0
3	C	457	0	249	9	0
3	G	457	0	249	19	0
4	D	217	0	129	2	0
4	H	217	0	129	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	5	0	0	0	0
6	E	4	0	0	0	0
All	All	22604	0	20971	584	1

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 14.

All (584) 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:84:LYS:CB	1:A:84:LYS:CG	1.80	1.54
1:A:84:LYS:CE	1:A:84:LYS:NZ	1.77	1.47
1:A:84:LYS:CG	1:A:84:LYS:CD	2.02	1.36
1:A:82:ARG:NH1	1:A:188:ASP:OD1	1.67	1.27
1:E:837:ASN:OD1	1:E:855:SER:OG	1.59	1.18
1:E:935:ARG:O	1:E:938:VAL:HG12	1.50	1.11
1:E:883:ARG:HH12	1:E:896:ILE:HB	1.17	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:835:GLU:HG2	1:E:939:GLU:OE2	1.60	1.00
1:A:1075:PHE:HD1	1:A:1085:ASP:HA	1.30	0.96
1:A:538:LYS:NZ	3:C:3:DA:N7	2.15	0.93
1:E:625:ASP:OD1	1:E:626:MET:HG2	1.70	0.92
1:E:571:LYS:HD2	1:E:577:ASN:HD21	1.34	0.92
1:E:365:GLU:O	1:E:368:ASP:CG	2.14	0.91
1:A:836:ARG:H	1:A:836:ARG:HD2	1.34	0.90
1:E:202:VAL:HG13	1:E:216:VAL:HG21	1.57	0.85
1:E:525:PHE:O	1:E:543:ARG:NH2	2.12	0.82
1:E:571:LYS:HE2	1:E:573:ASP:HB3	1.59	0.82
1:A:525:PHE:O	1:A:543:ARG:NH2	2.12	0.82
1:E:883:ARG:HD3	1:E:894:GLU:O	1.79	0.82
1:E:453:VAL:HG11	1:E:511:VAL:HG11	1.61	0.81
1:E:1046:ALA:HB1	1:E:1064:LYS:NZ	1.94	0.81
1:E:80:LEU:HG	1:E:90:GLU:HG2	1.63	0.81
1:E:833:ARG:HH21	1:E:927:LEU:HG	1.45	0.81
1:E:571:LYS:HE2	1:E:573:ASP:CB	2.12	0.80
1:E:522:LYS:HE3	1:E:743:GLU:HG2	1.63	0.80
1:E:573:ASP:O	1:E:577:ASN:ND2	2.16	0.79
1:E:706:ASN:HD21	1:E:721:THR:HG22	1.47	0.79
1:E:571:LYS:CE	1:E:573:ASP:H	1.95	0.79
1:A:722:MET:HE1	1:A:960:LYS:HB3	1.65	0.79
1:A:611:ASP:O	1:A:615:ILE:HD13	1.83	0.78
1:E:836:ARG:CD	1:E:836:ARG:H	1.95	0.78
1:A:82:ARG:NH1	1:A:188:ASP:CG	2.41	0.78
1:E:354:GLU:HG2	1:E:355:TRP:H	1.49	0.78
1:E:1046:ALA:HB1	1:E:1064:LYS:HZ2	1.46	0.78
1:E:245:VAL:HG22	1:E:251:LYS:HE2	1.67	0.76
1:E:718:ASN:HB2	1:E:721:THR:HG23	1.65	0.76
1:A:514:LYS:H	1:A:514:LYS:HD3	1.51	0.76
1:A:836:ARG:H	1:A:836:ARG:CD	1.94	0.76
1:A:359:ARG:O	1:A:363:ASN:ND2	2.18	0.76
1:E:71:LEU:HB2	1:E:74:LEU:HD21	1.68	0.75
1:A:376:VAL:O	1:A:377:VAL:HG13	1.86	0.75
1:E:80:LEU:HD23	1:E:94:LEU:HB2	1.68	0.75
1:E:571:LYS:HD3	1:E:573:ASP:H	1.52	0.75
1:E:26:LYS:HE3	1:E:695:GLU:HA	1.68	0.74
1:E:883:ARG:NH1	1:E:896:ILE:HB	1.99	0.74
1:A:838:LEU:HD11	1:A:876:LEU:HD12	1.67	0.74
1:A:1075:PHE:CD1	1:A:1085:ASP:HA	2.21	0.74
1:E:836:ARG:H	1:E:836:ARG:HD2	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:VAL:O	1:E:307:THR:HG22	1.87	0.73
1:A:756:LEU:HD11	1:A:790:SER:HB3	1.70	0.72
1:A:1053:SER:O	1:A:1054:ARG:HB2	1.89	0.72
1:A:174:ARG:NH2	1:A:278:LYS:O	2.21	0.72
1:E:202:VAL:HG13	1:E:216:VAL:CG2	2.19	0.72
1:E:350:ASP:HB3	1:E:417:ILE:HD13	1.71	0.71
1:E:835:GLU:HA	1:E:939:GLU:OE2	1.90	0.71
1:A:443:GLU:OE1	1:A:449:ASN:ND2	2.22	0.71
1:E:1021:ILE:HD12	1:E:1021:ILE:H	1.55	0.71
1:E:571:LYS:CD	1:E:573:ASP:H	2.04	0.70
1:A:774:LYS:NZ	2:B:-10:A:OP2	2.19	0.70
1:A:1016:THR:OG1	1:A:1132:SER:OG	2.08	0.70
1:A:3:LYS:HG2	1:A:819:LEU:HB3	1.72	0.70
1:A:832:ASP:HB2	1:A:1184:ALA:HB2	1.73	0.69
1:A:350:ASP:HB3	1:A:417:ILE:HD13	1.74	0.69
1:E:378:THR:HG21	1:E:380:LYS:HZ3	1.58	0.69
1:E:464:LYS:NZ	1:E:501:ASP:OD2	2.17	0.69
1:A:87:THR:OG1	1:A:89:LYS:HB3	1.93	0.69
1:E:571:LYS:HD2	1:E:577:ASN:ND2	2.07	0.68
1:E:983:PHE:CZ	3:G:-5:DG:H5''	2.28	0.68
1:A:1016:THR:HG1	1:A:1132:SER:HG	1.37	0.68
1:E:512:THR:O	1:E:893:ILE:HG13	1.93	0.68
1:E:365:GLU:O	1:E:368:ASP:OD1	2.11	0.68
1:A:356:ASN:ND2	1:A:360:ASP:OD1	2.27	0.68
1:E:625:ASP:OD1	1:E:626:MET:N	2.27	0.68
1:E:424:GLU:HA	1:E:427:LYS:HG2	1.75	0.68
1:E:200:HIS:O	1:E:204:GLU:N	2.27	0.67
1:A:885:GLU:O	1:A:889:ASN:ND2	2.28	0.67
1:E:297:ASP:OD1	1:E:510:TYR:OH	2.09	0.67
1:A:372:LYS:H	1:A:372:LYS:HD3	1.58	0.67
1:A:1075:PHE:HB2	1:A:1085:ASP:O	1.95	0.67
3:G:9:DG:H22	4:H:-9:DC:H42	1.41	0.67
1:E:543:ARG:HA	1:E:558:MET:HE2	1.75	0.67
1:E:996:ILE:HD11	1:E:1187:ILE:HG23	1.75	0.67
1:A:885:GLU:HG3	1:A:889:ASN:ND2	2.09	0.67
1:E:201:GLU:HB3	1:E:258:TYR:CE2	2.30	0.67
1:E:326:LYS:HG2	1:E:415:LYS:HE3	1.76	0.67
1:E:833:ARG:NH2	1:E:927:LEU:HG	2.11	0.66
1:A:302:GLU:HA	1:A:305:ARG:NH1	2.11	0.66
1:E:167:LYS:HB3	3:G:-3:DT:H5'	1.76	0.66
1:E:983:PHE:CE2	3:G:-5:DG:H5''	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LYS:CE	1:E:695:GLU:HA	2.25	0.65
1:E:174:ARG:NE	1:E:178:GLU:OE2	2.28	0.65
1:A:595:LYS:NZ	4:D:-2:DT:O2	2.30	0.65
1:E:129:PRO:HB3	1:E:138:ILE:HG23	1.76	0.65
1:E:225:PHE:O	1:E:228:VAL:HG12	1.97	0.65
1:E:1071:ARG:O	1:E:1088:GLU:HG2	1.97	0.65
1:A:442:LEU:HD11	1:A:446:LEU:HD13	1.79	0.65
1:E:205:ILE:HG23	1:E:209:ILE:HD12	1.78	0.65
1:A:444:LYS:HD2	1:A:449:ASN:HA	1.79	0.65
1:E:351:ILE:HG21	1:E:410:VAL:HG13	1.79	0.65
1:E:375:ALA:O	1:E:377:VAL:N	2.29	0.65
1:A:1109:GLY:O	1:A:1111:ILE:HG23	1.96	0.64
1:E:1140:SER:OG	1:E:1148:ASP:HA	1.98	0.64
1:E:70:LYS:HA	1:E:226:ASN:OD1	1.98	0.64
1:A:1111:ILE:HD12	1:A:1115:LEU:HD21	1.80	0.64
1:E:1141:ILE:HB	1:E:1144:ARG:CB	2.28	0.64
1:E:865:GLY:HA2	1:A:730:GLU:H	1.61	0.63
1:E:1086:TRP:CD1	1:E:1141:ILE:HG21	2.33	0.63
1:A:301:LEU:C	1:A:305:ARG:NH1	2.56	0.63
1:A:983:PHE:HB3	1:A:984:LYS:HA	1.79	0.63
1:E:307:THR:HG23	1:E:308:LEU:HD23	1.81	0.63
1:E:209:ILE:HG22	1:E:210:LEU:HD23	1.80	0.63
1:A:413:LYS:O	1:A:417:ILE:HG13	1.98	0.63
1:E:983:PHE:CZ	3:G:-5:DG:OP1	2.52	0.63
1:A:209:ILE:HG12	1:A:244:PHE:CE1	2.34	0.63
1:E:65:VAL:O	1:E:69:ILE:HG12	1.99	0.62
1:E:180:LEU:HG	1:E:225:PHE:CZ	2.35	0.62
1:E:1104:ILE:HG23	1:E:1114:LEU:HD13	1.81	0.62
1:E:1111:ILE:HD12	1:E:1115:LEU:HD21	1.81	0.62
1:A:475:GLY:O	1:A:476:GLU:HG3	1.99	0.61
1:E:359:ARG:HD2	1:E:359:ARG:O	2.00	0.61
1:A:86:ARG:HB3	1:A:91:ASN:OD1	2.00	0.61
1:E:134:ASP:O	1:E:138:ILE:HG13	1.99	0.61
1:E:363:ASN:HA	1:E:366:TYR:HB3	1.83	0.61
1:E:117:SER:HB3	1:E:122:ASP:HB2	1.82	0.61
1:E:477:GLY:HA2	1:E:478:LYS:HB2	1.83	0.61
1:A:68:SER:O	1:A:68:SER:OG	2.17	0.61
1:E:858:GLU:HG2	1:E:871:ASP:HA	1.83	0.60
1:E:1072:ILE:HG12	1:E:1088:GLU:HG3	1.83	0.60
1:E:1150:LEU:HD23	1:E:1162:TYR:HE2	1.66	0.60
1:E:64:ASP:OD1	1:E:65:VAL:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:O	1:A:234:ILE:HG13	2.01	0.60
1:A:587:PRO:O	1:A:592:MET:HG3	2.01	0.60
1:A:1140:SER:OG	1:A:1148:ASP:HA	2.01	0.60
1:E:889:ASN:O	1:E:890:TRP:HB2	2.00	0.60
3:C:-9:DA:C2'	3:C:-8:DC:H5''	2.31	0.60
1:E:1109:GLY:O	1:E:1111:ILE:HG23	2.02	0.60
1:E:165:GLU:HB2	1:E:167:LYS:HE3	1.82	0.60
1:A:305:ARG:HH11	1:A:305:ARG:HB2	1.66	0.60
1:A:371:LEU:HD13	1:A:381:TYR:CZ	2.36	0.60
1:E:326:LYS:HA	1:E:415:LYS:HD2	1.83	0.60
1:E:1163:ASP:OD1	1:E:1165:ARG:NH1	2.35	0.60
1:A:483:ASP:OD2	1:A:485:SER:HB3	2.02	0.60
1:A:937:LYS:O	1:A:941:GLN:HG2	2.03	0.59
1:A:1202:GLU:HB2	1:A:1205:LYS:HE3	1.83	0.59
1:E:81:PHE:O	1:E:86:ARG:NH2	2.36	0.59
3:G:9:DG:H22	4:H:-9:DC:N4	2.01	0.59
1:A:428:VAL:HG11	1:A:459:LEU:HA	1.85	0.58
1:E:1057:ALA:HA	1:E:1216:LYS:HG2	1.84	0.58
1:E:253:LYS:HB2	1:E:258:TYR:CE1	2.38	0.58
1:A:368:ASP:N	1:A:368:ASP:OD1	2.36	0.58
1:E:206:LYS:HD2	1:E:212:SER:HA	1.86	0.58
1:E:78:ILE:O	1:E:82:ARG:HB2	2.04	0.57
1:E:336:ILE:CD1	1:E:486:PHE:CD2	2.88	0.57
1:A:722:MET:HE1	1:A:960:LYS:CB	2.34	0.57
1:E:961:LYS:O	1:A:961:LYS:HB3	2.03	0.57
1:E:1041:ASP:OD1	1:E:1096:LYS:NZ	2.36	0.57
1:E:3:LYS:HG2	1:E:819:LEU:HB3	1.86	0.57
2:F:-15:C:H2'	2:F:-14:U:C6	2.40	0.57
1:E:378:THR:HG21	1:E:380:LYS:NZ	2.19	0.57
1:E:399:GLN:O	1:E:399:GLN:HG3	1.94	0.57
1:A:193:VAL:HG12	1:A:270:LEU:HD13	1.86	0.57
1:A:927:LEU:HD12	1:A:943:TYR:CD2	2.40	0.57
1:E:1043:PHE:HE1	1:E:1106:TYR:HB2	1.70	0.57
1:E:51:LYS:HD2	1:E:154:PHE:CD1	2.40	0.57
1:E:475:GLY:O	1:E:476:GLU:HG3	2.05	0.57
1:A:363:ASN:OD1	1:A:385:ARG:HD3	2.04	0.56
1:A:933:ASN:HB3	1:A:936:VAL:HG23	1.86	0.56
1:E:983:PHE:HZ	3:G:-5:DG:OP1	1.86	0.56
1:A:82:ARG:HH11	1:A:188:ASP:CG	2.12	0.56
1:E:571:LYS:HD3	1:E:573:ASP:N	2.20	0.56
1:E:706:ASN:ND2	1:E:721:THR:HG22	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:GLU:HG2	1:E:355:TRP:N	2.20	0.56
3:G:9:DG:N2	4:H:-9:DC:H42	2.03	0.56
2:B:-10:A:H5'	2:B:-8:G:N1	2.21	0.56
1:E:571:LYS:HD2	1:E:573:ASP:O	2.05	0.56
1:E:571:LYS:CD	1:E:577:ASN:HD21	2.14	0.56
1:E:806:PRO:O	1:E:809:ILE:HD11	2.06	0.56
1:A:387:LYS:O	1:A:390:LYS:HB2	2.05	0.56
1:E:245:VAL:CG2	1:E:251:LYS:HE2	2.36	0.56
1:E:679:LYS:HG3	1:E:680:VAL:N	2.20	0.56
1:E:835:GLU:HA	1:E:939:GLU:CD	2.30	0.56
1:E:302:GLU:HG2	1:E:305:ARG:HH12	1.70	0.55
1:E:359:ARG:HD2	1:E:359:ARG:C	2.31	0.55
1:E:837:ASN:OD1	1:E:855:SER:CB	2.53	0.55
1:A:1101:LYS:HG2	1:A:1102:TYR:CE1	2.41	0.55
1:A:748:ARG:HA	1:A:792:ASP:OD1	2.06	0.55
1:E:477:GLY:HA3	1:E:479:GLU:OE1	2.06	0.55
1:A:838:LEU:CD1	1:A:876:LEU:HD12	2.37	0.55
1:E:571:LYS:HD3	1:E:572:ASP:N	2.21	0.55
2:F:-10:A:H5'	2:F:-8:G:N1	2.21	0.55
1:A:119:PHE:HB3	1:A:155:PHE:HB3	1.88	0.55
1:A:1141:ILE:HG13	1:A:1147:VAL:HG21	1.89	0.55
1:A:928:ASN:HB2	1:A:940:LYS:HZ3	1.72	0.55
2:B:8:G:H1	3:C:-8:DC:H42	1.54	0.55
1:E:310:LYS:HG3	1:E:429:TYR:CZ	2.42	0.55
1:A:301:LEU:O	1:A:305:ARG:HB2	2.06	0.55
1:E:80:LEU:O	1:E:86:ARG:NE	2.40	0.55
1:E:230:THR:O	1:E:234:ILE:HG13	2.07	0.55
1:E:203:GLN:HA	1:E:206:LYS:HB3	1.89	0.54
1:E:560:LYS:NZ	4:H:-5:DC:OP1	2.35	0.54
1:A:245:VAL:HG22	1:A:246:THR:O	2.07	0.54
1:E:1046:ALA:HA	1:E:1064:LYS:HD3	1.89	0.54
1:E:209:ILE:HG12	1:E:244:PHE:CE1	2.42	0.54
1:E:359:ARG:HD2	1:E:363:ASN:HD21	1.73	0.54
1:E:714:HIS:CD2	1:A:714:HIS:HD2	2.26	0.54
1:A:70:LYS:HA	1:A:226:ASN:OD1	2.07	0.54
1:A:885:GLU:HG3	1:A:889:ASN:HD21	1.71	0.54
1:A:751:LEU:HD13	1:A:756:LEU:HD21	1.88	0.54
1:A:841:ILE:HD11	1:A:911:ILE:HD11	1.88	0.54
1:A:301:LEU:O	1:A:305:ARG:NH1	2.39	0.54
1:E:328:PHE:CE2	1:E:397:LEU:HD11	2.43	0.54
1:E:1072:ILE:HD13	1:E:1141:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1150:LEU:HD23	1:E:1162:TYR:CE2	2.42	0.54
1:E:571:LYS:CD	1:E:573:ASP:O	2.56	0.54
1:E:1074:ILE:HD13	1:E:1086:TRP:HB3	1.90	0.54
1:E:183:TYR:O	1:E:187:MET:HG3	2.08	0.53
1:A:833:ARG:HD3	1:A:927:LEU:CD1	2.38	0.53
1:A:126:THR:C	1:A:129:PRO:HD2	2.34	0.53
1:E:345:SER:OG	1:E:355:TRP:HB3	2.09	0.53
1:A:988:THR:HB	1:A:1211:ILE:HD11	1.89	0.53
1:A:1202:GLU:HB2	1:A:1205:LYS:CE	2.39	0.53
1:E:925:GLU:HB2	1:E:1187:ILE:HD13	1.89	0.53
1:A:1075:PHE:HD1	1:A:1085:ASP:CA	2.14	0.53
1:E:193:VAL:HG23	1:E:270:LEU:HD13	1.91	0.53
1:A:302:GLU:CA	1:A:305:ARG:NH1	2.72	0.52
1:E:514:LYS:HZ1	1:E:895:ASN:HB2	1.72	0.52
3:C:-9:DA:H2''	3:C:-8:DC:O4'	2.09	0.52
1:E:644:SER:O	1:E:645:ARG:HB2	2.08	0.52
1:E:1075:PHE:HB2	1:E:1085:ASP:O	2.10	0.52
1:A:92:LYS:HA	1:A:95:GLU:HB3	1.91	0.52
1:E:80:LEU:CG	1:E:90:GLU:HG2	2.37	0.52
1:A:11:TYR:CD1	1:A:979:LYS:HG2	2.44	0.52
1:A:302:GLU:N	1:A:305:ARG:HH12	2.08	0.52
1:A:359:ARG:HG2	1:A:363:ASN:HD21	1.74	0.52
1:A:876:LEU:HD23	1:A:899:LEU:HD23	1.92	0.52
1:E:203:GLN:HA	1:E:206:LYS:CB	2.40	0.52
1:E:740:GLY:O	3:G:0:DG:H2''	2.10	0.52
1:E:882:GLU:O	1:E:886:ALA:HB3	2.09	0.52
1:E:442:LEU:HD11	1:E:446:LEU:HD13	1.92	0.51
1:A:591:LYS:HD2	4:D:-1:DA:C2	2.46	0.51
1:A:1202:GLU:HB2	1:A:1205:LYS:NZ	2.24	0.51
1:E:209:ILE:HG12	1:E:244:PHE:CD1	2.45	0.51
1:A:543:ARG:HG2	1:A:558:MET:HB2	1.92	0.51
1:E:776:THR:OG1	1:A:573:ASP:OD1	2.28	0.51
1:A:1019:THR:OG1	1:A:1020:SER:N	2.43	0.51
1:E:879:LYS:HA	1:E:882:GLU:HB2	1.91	0.51
1:A:51:LYS:HG2	1:A:154:PHE:CE1	2.46	0.51
2:B:9:U:H2'	2:B:10:A:C8	2.44	0.51
3:G:8:DC:H2''	3:G:9:DG:C4	2.46	0.51
1:A:226:ASN:H	1:A:226:ASN:HD22	1.57	0.51
1:E:1073:ARG:O	1:E:1086:TRP:HB2	2.11	0.51
1:A:309:ASN:O	1:A:312:SER:HB3	2.10	0.51
1:A:823:ASP:O	1:A:826:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:LEU:H	1:A:1164:SER:HB3	1.75	0.51
1:E:307:THR:HG23	1:E:308:LEU:CD2	2.41	0.51
4:H:-5:DC:C6	4:H:-4:DT:H72	2.46	0.51
1:E:833:ARG:HB2	1:E:943:TYR:CD1	2.46	0.50
1:A:477:GLY:HA2	1:A:478:LYS:C	2.36	0.50
1:E:351:ILE:HA	1:E:413:LYS:HG2	1.93	0.50
1:E:368:ASP:OD1	1:E:369:ILE:N	2.43	0.50
1:E:85:THR:O	1:E:85:THR:OG1	2.25	0.50
1:E:937:LYS:O	1:E:938:VAL:C	2.54	0.50
1:A:205:ILE:HG23	1:A:209:ILE:HD12	1.94	0.50
1:E:326:LYS:CG	1:E:415:LYS:HE3	2.42	0.50
1:E:1146:ASP:OD1	1:E:1146:ASP:N	2.44	0.50
1:E:226:ASN:N	1:E:226:ASN:HD22	2.07	0.50
1:E:1038:PRO:HD2	1:E:1039:GLU:OE2	2.12	0.50
1:A:1042:LEU:HD23	1:A:1066:TYR:CD2	2.46	0.50
1:E:362:TRP:CZ3	1:E:389:PHE:HB2	2.47	0.50
1:E:398:GLU:O	1:E:402:GLU:HG3	2.12	0.50
1:E:630:ASN:O	1:E:634:LYS:HG3	2.11	0.50
1:A:1111:ILE:O	1:A:1115:LEU:HG	2.11	0.50
1:E:336:ILE:CD1	1:E:486:PHE:CG	2.95	0.50
1:E:882:GLU:O	1:E:886:ALA:N	2.38	0.50
1:A:51:LYS:HG2	1:A:154:PHE:CZ	2.47	0.50
1:E:996:ILE:HD11	1:E:1187:ILE:O	2.11	0.50
1:A:1076:ARG:HG3	1:A:1076:ARG:HH11	1.76	0.50
1:E:516:TYR:HB3	1:E:751:LEU:HD11	1.94	0.49
1:E:126:THR:C	1:E:129:PRO:HD2	2.36	0.49
1:E:198:ASP:HB3	1:E:201:GLU:CD	2.37	0.49
1:E:773:PRO:O	1:A:574:VAL:HG23	2.12	0.49
1:A:935:ARG:O	1:A:939:GLU:HG3	2.12	0.49
1:E:550:GLY:HA2	2:B:-10:A:N3	2.27	0.49
1:A:562:TYR:CE2	1:A:698:LYS:HE2	2.48	0.49
1:A:1213:ILE:HG12	1:A:1218:TRP:HB2	1.95	0.49
1:E:1111:ILE:O	1:E:1115:LEU:HG	2.13	0.49
2:F:-15:C:H2'	2:F:-14:U:H6	1.76	0.49
1:A:415:LYS:O	1:A:419:ILE:HG12	2.13	0.49
1:A:1031:PHE:CE2	1:A:1047:LEU:HB3	2.48	0.49
1:E:833:ARG:NH2	1:E:927:LEU:HA	2.28	0.49
1:E:76:ASN:O	1:E:80:LEU:HD13	2.12	0.49
1:A:418:ILE:HG22	1:A:419:ILE:HD13	1.94	0.49
1:E:1:MET:O	1:A:1:MET:HE3	2.13	0.49
1:E:466:PHE:O	1:E:470:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ILE:O	1:A:351:ILE:HG13	2.12	0.49
1:A:916:GLU:OE2	1:A:957:MET:HE3	2.13	0.49
1:E:180:LEU:HG	1:E:225:PHE:CE2	2.47	0.48
1:E:1104:ILE:HD11	1:E:1118:GLN:CG	2.43	0.48
1:A:106:ALA:O	1:A:110:LYS:HG3	2.13	0.48
1:A:444:LYS:HG2	1:A:445:SER:N	2.28	0.48
1:E:444:LYS:HG2	1:E:755:GLU:HG2	1.95	0.48
1:A:202:VAL:HG13	1:A:216:VAL:HB	1.94	0.48
1:A:928:ASN:HB2	1:A:940:LYS:NZ	2.27	0.48
1:A:833:ARG:HD3	1:A:927:LEU:HD11	1.94	0.48
1:E:467:GLU:HA	1:E:497:LEU:HD21	1.95	0.48
1:E:474:PHE:HE2	1:E:491:VAL:HG22	1.78	0.48
1:A:210:LEU:HD21	1:A:240:ILE:HD11	1.95	0.48
1:E:305:ARG:HG3	1:E:305:ARG:HH11	1.79	0.48
1:E:336:ILE:HD11	1:E:486:PHE:CG	2.48	0.48
1:A:813:ASN:O	1:A:817:ARG:HG3	2.14	0.48
1:E:1001:THR:O	1:E:1186:ASN:ND2	2.43	0.48
2:B:9:U:H2'	2:B:10:A:H8	1.79	0.48
1:E:1110:ASP:OD1	1:E:1112:ARG:HD3	2.14	0.48
1:A:740:GLY:O	1:A:799:PRO:HG2	2.14	0.48
1:E:409:SER:OG	1:E:412:GLU:HB2	2.14	0.48
1:A:625:ASP:OD2	1:A:625:ASP:N	2.47	0.48
1:E:349:LYS:HG3	1:E:353:GLY:C	2.39	0.48
1:E:1172:ASN:OD1	1:E:1172:ASN:N	2.46	0.48
1:E:26:LYS:HE2	1:E:26:LYS:H	1.79	0.48
1:E:862:ASN:OD1	1:E:862:ASN:N	2.43	0.48
1:A:587:PRO:HD2	1:A:592:MET:HG3	1.95	0.48
3:C:-9:DA:H2''	3:C:-8:DC:H5''	1.96	0.48
1:E:310:LYS:HE3	1:E:429:TYR:CD2	2.49	0.47
1:E:1018:TYR:CD1	1:E:1125:SER:HA	2.49	0.47
1:A:522:LYS:HE3	1:A:743:GLU:HG2	1.96	0.47
1:A:1066:TYR:CZ	1:A:1155:LYS:HE3	2.49	0.47
1:E:937:LYS:HB3	1:E:941:GLN:CB	2.43	0.47
1:E:1024:SER:O	1:E:1028:ILE:HG13	2.14	0.47
1:A:174:ARG:HA	1:A:174:ARG:HD3	1.68	0.47
1:E:1175:LEU:HD23	1:E:1175:LEU:HA	1.75	0.47
1:A:262:TYR:CZ	1:A:266:THR:HG21	2.49	0.47
1:A:833:ARG:CD	1:A:927:LEU:HD11	2.43	0.47
1:A:807:LYS:HA	1:A:807:LYS:HD3	1.76	0.47
1:A:1073:ARG:HB2	1:A:1133:LEU:HD21	1.95	0.47
1:E:203:GLN:O	1:E:206:LYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:O	1:A:78:ILE:HG13	2.14	0.47
1:E:933:ASN:HA	1:E:934:SER:HA	1.56	0.47
1:E:1196:GLY:O	1:E:1200:LYS:HG3	2.15	0.47
1:E:132:LEU:HD13	1:E:137:GLU:HB3	1.97	0.47
1:E:262:TYR:CZ	1:E:266:THR:HG21	2.49	0.47
1:E:996:ILE:HD11	1:E:1187:ILE:CG2	2.42	0.47
1:A:522:LYS:HE3	1:A:743:GLU:OE2	2.15	0.47
1:A:570:ASP:OD1	1:A:571:LYS:N	2.47	0.47
1:A:1041:ASP:O	1:A:1092:THR:HG21	2.14	0.47
1:E:932:LYS:O	1:E:936:VAL:HG12	2.14	0.47
1:E:983:PHE:CZ	3:G:-5:DG:C5'	2.98	0.47
1:A:11:TYR:CE1	1:A:979:LYS:HG2	2.49	0.47
1:A:101:LEU:HB3	1:A:176:ILE:HG12	1.97	0.47
1:A:616:TYR:HA	1:A:621:PHE:HE2	1.79	0.47
1:E:774:LYS:HE2	1:A:575:ASN:HA	1.97	0.47
1:E:1151:ILE:HA	1:E:1162:TYR:O	2.15	0.47
1:E:571:LYS:HE2	1:E:573:ASP:H	1.75	0.46
1:E:1099:PHE:CD2	1:E:1106:TYR:HB3	2.50	0.46
1:E:48:LYS:O	1:E:52:LYS:HG3	2.16	0.46
1:E:344:ILE:HD12	1:E:347:ILE:HB	1.97	0.46
1:E:1101:LYS:HZ3	1:E:1102:TYR:HE1	1.63	0.46
1:A:54:LEU:HD23	1:A:128:LEU:HD22	1.96	0.46
1:E:265:LYS:HD2	1:E:265:LYS:HA	1.68	0.46
1:A:878:LYS:O	1:A:882:GLU:HG3	2.16	0.46
1:E:349:LYS:HE2	1:E:355:TRP:CE2	2.49	0.46
1:E:1131:MET:HE3	1:E:1131:MET:HB3	1.75	0.46
1:A:876:LEU:HD23	1:A:876:LEU:HA	1.72	0.46
1:E:203:GLN:O	1:E:207:GLU:HG2	2.16	0.46
1:E:302:GLU:HG2	1:E:305:ARG:NH1	2.31	0.46
1:E:900:LYS:O	1:E:904:ILE:HG12	2.15	0.46
1:E:543:ARG:HG2	1:E:558:MET:HB2	1.96	0.46
1:E:1193:TRP:CD2	1:E:1213:ILE:HD12	2.50	0.46
1:A:301:LEU:C	1:A:305:ARG:HH12	2.23	0.46
1:E:190:PHE:O	1:E:194:ASP:HB2	2.16	0.46
1:A:120:LYS:O	1:A:123:ILE:HG22	2.16	0.46
1:E:832:ASP:HB2	1:E:1184:ALA:HB2	1.97	0.45
1:A:12:SER:HB3	1:A:803:ASN:O	2.15	0.45
1:E:302:GLU:OE1	1:E:305:ARG:NH2	2.50	0.45
1:E:336:ILE:HB	1:E:397:LEU:HG	1.97	0.45
1:E:576:GLY:O	1:E:687:LYS:HB3	2.16	0.45
1:E:1065:LEU:HD13	1:E:1135:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLU:CA	1:A:305:ARG:HH12	2.29	0.45
1:A:439:ASP:OD1	1:A:439:ASP:N	2.49	0.45
1:A:590:ASN:O	1:A:594:PRO:CD	2.65	0.45
3:C:-12:DT:H2'	3:C:-11:DT:C6	2.51	0.45
1:E:305:ARG:HD2	1:E:436:PHE:HA	1.98	0.45
1:E:406:ALA:HA	1:E:407:ASP:HA	1.63	0.45
1:E:1021:ILE:H	1:E:1021:ILE:CD1	2.24	0.45
1:A:362:TRP:CH2	1:A:366:TYR:HD1	2.33	0.45
1:A:400:LEU:O	1:A:403:TYR:HB2	2.15	0.45
1:E:477:GLY:HA2	1:E:478:LYS:CB	2.44	0.45
1:A:516:TYR:HB3	1:A:751:LEU:HD11	1.99	0.45
1:E:672:GLU:O	1:E:676:GLN:HG3	2.16	0.45
1:E:1096:LYS:HG2	1:E:1106:TYR:CZ	2.52	0.45
1:A:767:ASN:ND2	2:B:-11:U:H3'	2.31	0.45
1:E:542:TYR:OH	3:G:2:DA:OP2	2.32	0.45
1:E:492:LEU:HD23	1:E:492:LEU:HA	1.83	0.45
1:A:1133:LEU:HA	1:A:1136:GLN:HG2	1.99	0.45
1:E:842:VAL:HG23	1:E:1184:ALA:HB3	1.97	0.45
2:B:-15:C:H2'	2:B:-14:U:C6	2.52	0.45
1:E:897:LYS:HZ3	1:E:900:LYS:HZ3	1.64	0.45
1:A:601:LYS:HD3	1:A:602:TRP:NE1	2.31	0.45
1:A:858:GLU:OE1	1:A:869:LYS:HD2	2.17	0.45
1:E:384:ASP:O	1:E:388:SER:N	2.42	0.44
1:E:1025:LYS:HE2	1:E:1124:TYR:OH	2.18	0.44
1:E:1030:SER:HB2	1:E:1052:PHE:CZ	2.53	0.44
1:A:668:GLY:O	1:A:672:GLU:HG3	2.18	0.44
1:A:706:ASN:HB2	2:B:-17:U:OP1	2.17	0.44
1:A:1136:GLN:O	1:A:1136:GLN:HG3	2.18	0.44
1:A:1136:GLN:HG3	1:A:1139:ASN:HD21	1.81	0.44
1:A:1031:PHE:CD2	1:A:1047:LEU:HB3	2.53	0.44
1:E:336:ILE:HD13	1:E:486:PHE:CD2	2.52	0.44
1:E:359:ARG:HD2	1:E:363:ASN:ND2	2.32	0.44
1:E:771:ASP:OD2	1:E:869:LYS:NZ	2.50	0.44
1:A:246:THR:HG22	1:A:250:GLU:H	1.82	0.44
1:A:325:PHE:CG	1:A:418:ILE:HG21	2.52	0.44
1:A:616:TYR:HA	1:A:621:PHE:CE2	2.53	0.44
1:A:926:ASP:O	1:A:927:LEU:HD23	2.17	0.44
1:E:568:LYS:HD3	1:E:568:LYS:HA	1.85	0.44
1:E:931:PHE:CB	1:E:936:VAL:HB	2.47	0.44
3:G:-9:DA:H2'	3:G:-8:DC:C6	2.53	0.44
1:A:277:TYR:HE1	2:B:8:G:OP1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:SER:OG	1:A:988:THR:N	2.51	0.44
1:A:1114:LEU:HD12	1:A:1114:LEU:HA	1.76	0.44
3:C:-9:DA:C3'	3:C:-8:DC:H5''	2.48	0.44
1:A:72:LYS:HE2	1:A:104:GLU:CD	2.42	0.44
1:A:72:LYS:HE2	1:A:104:GLU:OE1	2.18	0.44
1:E:71:LEU:CB	1:E:74:LEU:HD21	2.44	0.44
1:E:138:ILE:HG22	1:E:142:ASN:ND2	2.33	0.44
1:E:182:ARG:HA	1:E:185:SER:HB3	1.99	0.44
1:E:1026:LYS:O	1:E:1030:SER:OG	2.30	0.44
1:E:24:VAL:HG21	1:E:701:MET:HE2	2.00	0.44
1:E:445:SER:N	1:E:755:GLU:OE1	2.50	0.44
1:E:708:ASP:OD2	1:E:721:THR:HG21	2.18	0.44
3:G:-2:DG:H2'	3:G:-1:DC:C6	2.52	0.44
1:A:883:ARG:NH2	1:A:896:ILE:HG21	2.33	0.44
1:A:71:LEU:HB2	1:A:74:LEU:HB2	2.00	0.44
1:A:193:VAL:O	1:A:196:ILE:HG12	2.18	0.44
1:A:1136:GLN:OE1	1:A:1139:ASN:ND2	2.50	0.44
1:A:373:LYS:HA	1:A:373:LYS:HD3	1.86	0.43
1:A:527:ASN:HB3	1:A:530:PHE:HB2	2.00	0.43
1:E:667:ALA:O	1:E:671:ARG:HG3	2.18	0.43
1:E:983:PHE:CE1	3:G:-5:DG:H5'	2.53	0.43
1:E:1066:TYR:CZ	1:E:1155:LYS:HE3	2.52	0.43
1:A:27:THR:HG23	1:A:700:TYR:HB3	2.00	0.43
1:A:128:LEU:HD12	1:A:128:LEU:HA	1.81	0.43
1:A:134:ASP:OD2	1:A:136:ASP:N	2.50	0.43
1:E:1101:LYS:HG2	1:E:1102:TYR:CE1	2.54	0.43
1:A:427:LYS:HA	1:A:427:LYS:HD3	1.81	0.43
1:E:260:ASN:HA	1:E:263:ASN:HB2	2.00	0.43
1:E:1018:TYR:CD2	1:E:1018:TYR:C	2.96	0.43
1:A:1072:ILE:HD13	1:A:1088:GLU:HG3	2.00	0.43
1:A:1075:PHE:N	1:A:1085:ASP:O	2.51	0.43
1:E:267:LYS:HA	1:E:267:LYS:HD3	1.89	0.43
1:A:569:ILE:HG22	1:A:686:SER:H	1.84	0.43
1:A:900:LYS:O	1:A:904:ILE:HG12	2.18	0.43
1:A:1086:TRP:H	1:A:1086:TRP:CD1	2.35	0.43
1:E:245:VAL:HG12	1:E:246:THR:O	2.18	0.43
1:E:321:LEU:HG	1:E:493:ALA:HB1	2.01	0.43
1:E:409:SER:HG	1:E:412:GLU:HB2	1.84	0.43
1:E:897:LYS:NZ	1:E:900:LYS:NZ	2.65	0.43
1:A:615:ILE:HD11	1:A:631:ASP:OD2	2.18	0.43
1:A:813:ASN:ND2	1:A:989:GLN:HG3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:TRP:CD2	1:A:1213:ILE:HD12	2.53	0.43
1:E:379:GLU:OE1	1:E:382:GLU:HB3	2.19	0.43
1:E:729:ASP:OD2	1:E:731:ASN:HB2	2.19	0.43
1:A:897:LYS:HE3	3:C:-7:DT:H3'	2.00	0.43
1:E:609:SER:HB2	1:E:612:ILE:HG12	2.00	0.43
1:A:117:SER:HB3	1:A:122:ASP:HB2	2.01	0.43
1:E:128:LEU:HB3	1:E:129:PRO:HD3	1.99	0.43
1:E:620:THR:HA	1:E:626:MET:O	2.19	0.43
1:E:951:ILE:HD11	1:E:995:TYR:OH	2.18	0.43
3:G:-4:DA:H2''	3:G:-3:DT:O5'	2.19	0.43
1:A:12:SER:O	1:A:979:LYS:HE2	2.19	0.43
1:E:414:LEU:HD13	1:E:473:PHE:HZ	1.84	0.42
1:E:897:LYS:NZ	1:E:900:LYS:HZ3	2.17	0.42
1:E:904:ILE:HD12	1:E:946:PHE:HB2	2.01	0.42
1:A:820:LEU:HD11	1:A:921:VAL:HG11	2.01	0.42
1:A:938:VAL:O	1:A:942:VAL:HG23	2.19	0.42
1:E:22:ILE:O	1:E:702:PHE:HA	2.19	0.42
1:A:1000:LEU:HD12	1:A:1215:ASN:OD1	2.19	0.42
3:G:-7:DT:C2	3:G:-6:DG:C8	3.07	0.42
1:A:9:ASN:OD1	1:A:806:PRO:HA	2.19	0.42
1:A:376:VAL:O	1:A:377:VAL:CG1	2.64	0.42
1:A:833:ARG:CD	1:A:927:LEU:CD1	2.97	0.42
1:E:192:LYS:HD2	1:E:192:LYS:HA	1.35	0.42
1:E:414:LEU:HD13	1:E:473:PHE:CZ	2.54	0.42
1:E:435:LEU:HD11	1:E:452:VAL:HG13	2.01	0.42
1:A:210:LEU:O	1:A:211:ASN:HB2	2.19	0.42
1:E:228:VAL:HG21	1:E:276:LEU:HD12	2.01	0.42
1:E:359:ARG:HE	1:E:359:ARG:HB3	1.70	0.42
1:E:740:GLY:O	1:E:799:PRO:HG2	2.19	0.42
1:E:898:GLU:HG2	2:F:-15:C:H4'	2.00	0.42
1:A:554:TYR:CG	1:A:701:MET:HE3	2.55	0.42
1:E:119:PHE:HB3	1:E:155:PHE:HB3	2.02	0.42
1:E:301:LEU:HD11	1:E:442:LEU:HG	2.02	0.42
1:A:125:GLU:HG2	1:A:145:ASN:OD1	2.20	0.42
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.74	0.42
1:E:359:ARG:O	1:E:363:ASN:ND2	2.52	0.42
1:E:585:LEU:O	3:G:2:DA:H4'	2.19	0.42
1:E:883:ARG:HH22	1:E:896:ILE:HG21	1.85	0.42
1:E:937:LYS:NZ	1:E:941:GLN:HA	2.34	0.42
1:A:1086:TRP:CE2	1:A:1141:ILE:HD13	2.55	0.42
1:A:1087:GLU:HG2	1:A:1088:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:886:ALA:O	1:E:889:ASN:HB2	2.20	0.42
1:A:246:THR:CG2	1:A:250:GLU:H	2.32	0.42
1:A:672:GLU:O	1:A:676:GLN:HG3	2.20	0.42
2:B:7:A:H2'	2:B:8:G:O4'	2.20	0.42
1:E:245:VAL:HG22	1:E:251:LYS:CE	2.44	0.42
1:E:349:LYS:HG3	1:E:354:GLU:HA	2.01	0.42
1:E:828:VAL:HG22	1:E:921:VAL:CG2	2.50	0.42
1:A:578:TYR:CE2	1:A:687:LYS:HG3	2.55	0.42
1:A:1093:SER:O	1:A:1097:GLU:HG3	2.20	0.42
1:A:54:LEU:HD11	1:A:124:ILE:HD11	2.00	0.41
1:A:154:PHE:HA	1:A:157:ASN:OD1	2.20	0.41
1:A:722:MET:CE	1:A:960:LYS:HD2	2.50	0.41
1:A:980:PHE:HZ	1:A:985:SER:HB3	1.85	0.41
1:E:26:LYS:HE2	1:E:26:LYS:HB2	1.69	0.41
1:E:218:ASP:HB3	1:E:224:PHE:CD1	2.55	0.41
1:A:406:ALA:HA	1:A:407:ASP:HA	1.67	0.41
1:A:434:LYS:HA	1:A:437:ASP:OD1	2.21	0.41
1:A:476:GLU:O	1:A:478:LYS:HB2	2.19	0.41
1:A:587:PRO:O	1:A:587:PRO:HD2	2.20	0.41
1:A:1102:TYR:HB3	1:A:1118:GLN:OE1	2.20	0.41
1:E:82:ARG:HH12	1:E:188:ASP:HA	1.86	0.41
1:E:365:GLU:O	1:E:368:ASP:OD2	2.35	0.41
1:E:937:LYS:O	1:E:941:GLN:N	2.41	0.41
1:A:1101:LYS:HG2	1:A:1102:TYR:CD1	2.54	0.41
1:E:294:TYR:CZ	1:E:303:VAL:HG11	2.55	0.41
1:E:325:PHE:O	1:E:328:PHE:HB2	2.21	0.41
1:E:1145:THR:OG1	1:E:1146:ASP:OD1	2.38	0.41
1:E:97:LEU:O	1:E:101:LEU:HB2	2.20	0.41
1:E:1012:ASN:OD1	1:E:1135:LEU:HD13	2.20	0.41
1:A:325:PHE:O	1:A:328:PHE:HB2	2.21	0.41
1:A:367:ASP:OD1	1:A:381:TYR:OH	2.21	0.41
3:C:-2:DG:H2'	3:C:-1:DC:C6	2.55	0.41
1:E:193:VAL:HG23	1:E:270:LEU:CD1	2.50	0.41
1:E:925:GLU:HG3	1:E:998:ALA:HB2	2.03	0.41
1:E:1128:MET:HE3	1:E:1128:MET:HB3	1.78	0.41
1:A:247:GLU:C	1:A:249:GLY:N	2.77	0.41
1:A:716:THR:HA	1:A:717:PRO:HD3	1.92	0.41
2:B:11:A:H2'	2:B:12:A:C8	2.56	0.41
1:E:1:MET:HE3	1:A:919:ASP:OD2	2.21	0.41
1:E:961:LYS:HB3	1:A:961:LYS:O	2.20	0.41
3:G:-8:DC:H2''	3:G:-7:DT:O5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LYS:HD2	1:A:449:ASN:CA	2.47	0.41
1:A:841:ILE:O	1:A:853:GLN:HA	2.20	0.41
1:A:1005:ASP:OD1	1:A:1007:SER:OG	2.37	0.41
1:E:339:LYS:HG2	1:E:340:ASN:N	2.35	0.41
1:E:535:ASP:HA	1:E:583:TYR:O	2.21	0.41
1:E:1105:ASN:ND2	1:E:1108:GLN:HB2	2.35	0.41
1:E:1192:LEU:HD23	1:E:1192:LEU:HA	1.78	0.41
1:A:844:VAL:HA	1:A:849:ASN:O	2.20	0.41
1:A:859:ILE:HG21	1:A:906:GLN:HB3	2.03	0.41
1:A:933:ASN:HB3	1:A:936:VAL:CG2	2.50	0.41
1:E:331:TYR:CD1	1:E:486:PHE:HB2	2.55	0.41
1:E:359:ARG:CD	1:E:363:ASN:HD21	2.32	0.41
1:E:565:CYS:SG	1:E:693:LEU:HD13	2.61	0.41
1:E:571:LYS:HE2	1:E:573:ASP:N	2.34	0.41
4:H:-9:DC:H6	4:H:-9:DC:H2'	1.75	0.41
1:A:246:THR:HG22	1:A:250:GLU:N	2.35	0.41
1:A:247:GLU:O	1:A:247:GLU:HG2	2.21	0.41
1:A:447:LYS:NZ	1:A:513:GLN:OE1	2.53	0.41
1:A:453:VAL:HG11	1:A:511:VAL:HG11	2.02	0.41
1:A:455:ILE:HD13	1:A:455:ILE:HA	1.89	0.41
1:A:555:LEU:HD22	1:A:796:LEU:HD22	2.03	0.41
1:A:767:ASN:HD21	2:B:-11:U:H3'	1.86	0.41
1:A:769:ASN:HD21	1:A:771:ASP:HB2	1.86	0.41
1:A:931:PHE:O	1:A:931:PHE:CG	2.73	0.41
1:E:3:LYS:HE2	1:E:823:ASP:OD2	2.21	0.41
1:E:341:GLY:O	1:E:344:ILE:HG22	2.21	0.41
1:E:571:LYS:CE	1:E:573:ASP:N	2.73	0.41
1:E:1202:GLU:O	1:E:1203:ASP:C	2.64	0.41
1:A:1026:LYS:HE2	1:A:1026:LYS:HB2	1.69	0.41
1:E:387:LYS:HD2	1:E:387:LYS:HA	1.69	0.40
1:E:449:ASN:O	1:E:453:VAL:HG23	2.21	0.40
1:E:956:TYR:OH	1:E:970:ALA:O	2.32	0.40
1:E:508:ARG:HG3	1:E:890:TRP:CE2	2.56	0.40
1:A:225:PHE:O	1:A:228:VAL:HG12	2.20	0.40
1:A:821:LYS:HG3	1:A:1199:LYS:HA	2.03	0.40
1:A:1075:PHE:CB	1:A:1085:ASP:O	2.67	0.40
1:E:295:THR:O	1:E:510:TYR:HE1	2.04	0.40
1:A:363:ASN:N	1:A:363:ASN:HD22	2.19	0.40
1:A:872:TYR:CD1	1:A:903:TYR:HB2	2.56	0.40
1:E:517:SER:H	1:E:750:SER:CB	2.34	0.40
1:A:344:ILE:HD12	1:A:344:ILE:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:ASP:OD1	1:A:730:GLU:N	2.54	0.40
1:A:1160:ILE:HD12	1:A:1160:ILE:HA	1.96	0.40
1:E:3:LYS:HB2	1:E:3:LYS:HE3	1.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1056:ASP:OD1	1:A:444:LYS:NZ[3_454]	2.18	0.02

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	1208/1228 (98%)	1176 (97%)	28 (2%)	4 (0%)	36	54
1	E	1208/1228 (98%)	1170 (97%)	34 (3%)	4 (0%)	36	54
All	All	2416/2456 (98%)	2346 (97%)	62 (3%)	8 (0%)	36	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	368	ASP
1	E	374	LYS
1	A	986	MET
1	A	587	PRO
1	A	1019	THR
1	E	377	VAL
1	A	376	VAL
1	E	376	VAL

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	1081/1115 (97%)	1079 (100%)	2 (0%)	87	95
1	E	1071/1115 (96%)	1069 (100%)	2 (0%)	87	95
All	All	2152/2230 (96%)	2148 (100%)	4 (0%)	87	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	836	ARG
1	E	961	LYS
1	A	835	GLU
1	A	836	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	142	ASN
1	E	203	GLN
1	E	211	ASN
1	E	311	ASN
1	E	363	ASN
1	E	399	GLN
1	E	577	ASN
1	E	607	ASN
1	E	714	HIS
1	E	909	HIS
1	E	1070	ASN
1	A	96	ASN
1	A	509	ASN
1	A	633	HIS
1	A	714	HIS
1	A	793	GLN
1	A	889	ASN
1	A	909	HIS

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Mol	Chain	Res	Type
1	A	1070	ASN
1	A	1139	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	32/40 (80%)	5 (15%)	0
2	F	32/40 (80%)	5 (15%)	0
All	All	64/80 (80%)	10 (15%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	-17	U
2	F	-10	A
2	F	-9	A
2	F	-6	G
2	F	8	G
2	B	-17	U
2	B	-10	A
2	B	-9	A
2	B	-6	G
2	B	8	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 [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	1214/1228 (98%)	0.14	52 (4%)	40	31	19, 48, 90, 148	0
1	E	1214/1228 (98%)	0.30	94 (7%)	19	14	22, 53, 105, 131	0
2	B	33/40 (82%)	-0.49	0	100	100	25, 30, 155, 178	0
2	F	33/40 (82%)	-0.53	0	100	100	25, 28, 164, 183	0
3	C	22/22 (100%)	0.61	3 (13%)	7	5	25, 63, 155, 175	0
3	G	22/22 (100%)	0.55	4 (18%)	3	3	30, 65, 178, 189	0
4	D	11/11 (100%)	0.14	1 (9%)	15	11	33, 36, 94, 110	0
4	H	11/11 (100%)	0.30	1 (9%)	15	11	39, 43, 85, 97	0
All	All	2560/2602 (98%)	0.20	155 (6%)	27	20	19, 50, 100, 189	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	883	ARG	5.4
1	E	888	GLN	5.0
1	E	1108	GLN	5.0
1	E	1077	ASN	4.7
1	E	1141	ILE	4.4
1	E	886	ALA	4.3
1	A	982	SER	4.2
1	A	1077	ASN	4.0
1	E	1075	PHE	3.9
1	E	377	VAL	3.9
1	A	866	ILE	3.9
1	E	884	PHE	3.8
1	E	374	LYS	3.7
3	C	9	DG	3.7
1	E	373	LYS	3.6
1	A	1109	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1022	ALA	3.5
4	H	-9	DC	3.4
1	E	291	GLY	3.4
1	E	1088	GLU	3.4
4	D	-9	DC	3.4
1	E	219	PHE	3.4
1	E	375	ALA	3.4
1	A	372	LYS	3.4
1	E	980	PHE	3.4
1	E	889	ASN	3.3
1	E	1109	GLY	3.3
1	E	369	ILE	3.3
1	E	885	GLU	3.3
1	A	981	GLU	3.3
1	E	1142	THR	3.3
1	E	986	MET	3.2
1	E	983	PHE	3.2
1	A	291	GLY	3.2
1	E	368	ASP	3.2
1	E	292	GLU	3.2
1	A	931	PHE	3.2
1	E	293	GLY	3.2
1	A	376	VAL	3.1
1	A	1108	GLN	3.0
1	E	389	PHE	3.0
1	E	1086	TRP	3.0
1	E	388	SER	3.0
1	A	863	PHE	3.0
1	E	113	GLU	2.9
1	E	364	ALA	2.9
1	E	863	PHE	2.9
1	A	1075	PHE	2.9
1	E	279	GLN	2.9
1	E	372	LYS	2.9
1	A	893	ILE	2.9
1	E	880	GLU	2.8
1	A	424	GLU	2.8
1	E	397	LEU	2.8
1	A	502	HIS	2.8
1	E	606	TYR	2.8
1	A	980	PHE	2.8
3	G	9	DG	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	224	PHE	2.7
1	E	378	THR	2.7
1	A	188	ASP	2.7
1	E	985	SER	2.7
1	A	330	GLU	2.7
1	E	216	VAL	2.7
1	E	365	GLU	2.7
1	A	374	LYS	2.6
1	E	887	ARG	2.6
1	E	342	PRO	2.6
1	E	246	THR	2.6
1	E	90	GLU	2.6
1	E	438	ALA	2.6
1	E	1105	ASN	2.6
1	E	271	PRO	2.5
1	E	938	VAL	2.5
1	E	84	LYS	2.5
1	E	879	LYS	2.5
1	A	373	LYS	2.5
1	A	375	ALA	2.5
1	A	296	SER	2.5
1	E	85	THR	2.5
1	A	983	PHE	2.5
1	E	362	TRP	2.5
1	E	1123	PHE	2.5
3	G	-12	DT	2.5
3	G	-7	DT	2.5
1	A	295	THR	2.5
1	A	438	ALA	2.4
1	E	356	ASN	2.4
3	C	8	DC	2.4
1	E	341	GLY	2.4
1	E	244	PHE	2.4
1	E	402	GLU	2.4
1	E	1148	ASP	2.4
1	E	472	ALA	2.4
1	A	986	MET	2.4
1	A	441	VAL	2.3
1	E	114	GLY	2.3
1	E	358	ILE	2.3
1	A	1143	GLY	2.3
1	A	244	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	884	PHE	2.3
1	A	406	ALA	2.3
1	E	252	ILE	2.3
1	E	307	THR	2.3
1	E	1021	ILE	2.3
1	E	1143	GLY	2.3
1	A	985	SER	2.3
1	E	284	ARG	2.3
1	E	294	TYR	2.3
1	E	936	VAL	2.3
1	E	1084	PHE	2.3
1	A	474	PHE	2.3
1	A	1084	PHE	2.3
1	E	835	GLU	2.3
1	A	435	LEU	2.3
1	A	284	ARG	2.3
1	A	77	TYR	2.3
1	E	380	LYS	2.2
1	E	399	GLN	2.2
1	A	1144	ARG	2.2
1	E	262	TYR	2.2
1	E	387	LYS	2.2
1	A	864	ASN	2.2
1	E	329	ASP	2.2
1	E	942	VAL	2.2
3	C	-7	DT	2.2
1	E	355	TRP	2.2
1	E	937	LYS	2.2
1	E	261	LEU	2.2
1	E	344	ILE	2.2
1	E	1145	THR	2.2
1	A	890	TRP	2.2
1	A	294	TYR	2.2
1	A	301	LEU	2.2
1	A	221	GLU	2.2
1	A	480	THR	2.1
1	A	600	LYS	2.1
1	E	862	ASN	2.1
1	A	84	LYS	2.1
1	A	251	LYS	2.1
1	E	77	TYR	2.1
1	A	247	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	210	LEU	2.1
1	E	376	VAL	2.1
1	E	1120	ASP	2.1
1	E	881	LYS	2.0
1	A	73	ASN	2.0
1	E	249	GLY	2.0
1	A	865	GLY	2.0
1	E	370	HIS	2.0
3	G	-11	DT	2.0
1	E	866	ILE	2.0
1	E	87	THR	2.0
1	A	169	THR	2.0
1	E	5	GLU	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](#)

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	LI	A	1301	1/1	0.18	0.79	12,12,12,12	0
5	LI	E	1301	1/1	0.40	0.81	16,16,16,16	0
5	LI	F	101	1/1	0.86	0.79	2,2,2,2	0
5	LI	B	101	1/1	0.92	0.81	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.