



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:04 AM UTC

PDB ID : 6I1L / pdb_00006i1l
Title : Crystal structure of FnCas12a in complex with a crRNA guide and ssDNA target
Authors : Jinek, M.; Swarts, D.C.
Deposited on : 2018-10-29
Resolution : 2.98 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

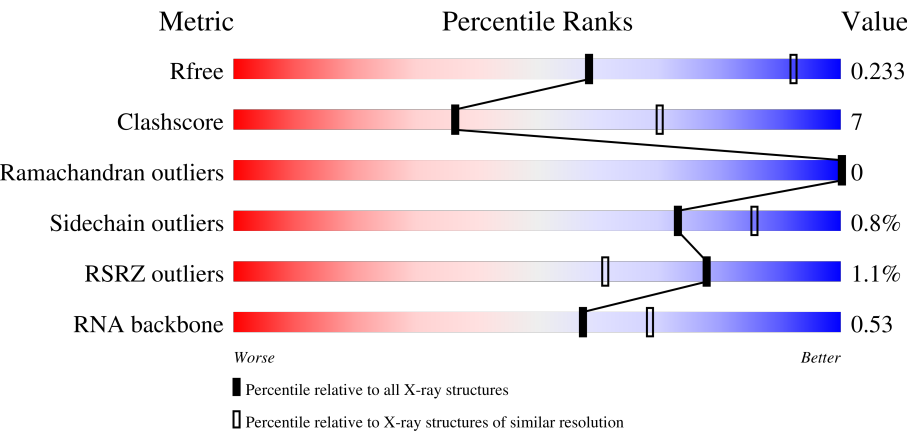
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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.



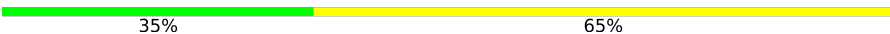
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)
RNA backbone	3983	1013 (3.18-2.78)

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	1301	0.2% 82% 16% 2%
1	D	1301	2% 79% 17% 2%
2	B	40	38% 52% 10%
2	E	40	32% 55% 12%

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Mol	Chain	Length	Quality of chain
3	C	20	 35%65%
3	F	20	 35%65%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23637 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 CRISPR-associated endonuclease Cas12a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1277	Total	C	N	O	S	0	0	0
			10551	6784	1743	2003	21			
1	D	1254	Total	C	N	O	S	0	0	0
			10351	6662	1702	1966	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ASN	-	expression tag	UNP A0Q7Q2
A	1	ALA	-	expression tag	UNP A0Q7Q2
A	1006	GLN	GLU	engineered mutation	UNP A0Q7Q2
D	0	ASN	-	expression tag	UNP A0Q7Q2
D	1	ALA	-	expression tag	UNP A0Q7Q2
D	1006	GLN	GLU	engineered mutation	UNP A0Q7Q2

- Molecule 2 is a RNA chain called crRNA (40-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	P	0	0	0
			843	380	144	280	39			
2	E	40	Total	C	N	O	P	0	0	0
			827	371	141	276	39			

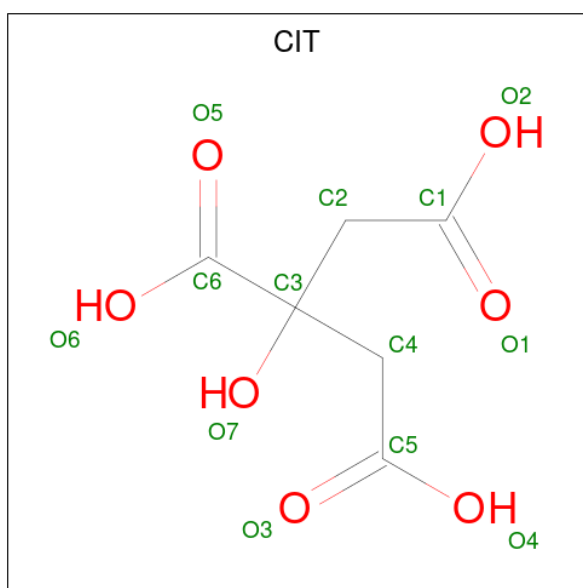
- Molecule 3 is a DNA chain called ssDNA target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	20	Total	C	N	O	P	0	0	0
			403	197	67	120	19			
3	F	20	Total	C	N	O	P	0	0	0
			403	197	67	120	19			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total 4 Mg 4	0	0
4	B	1	Total 1 Mg 1	0	0
4	D	3	Total 3 Mg 3	0	0
4	E	1	Total 1 Mg 1	0	0

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total 13 C 6 O 7	0	0
5	A	1	Total 13 C 6 O 7	0	0
5	A	1	Total 13 C 6 O 7	0	0
5	B	1	Total 13 C 6 O 7	0	0
5	B	1	Total 13 C 6 O 7	0	0
5	D	1	Total 13 C 6 O 7	0	0
5	D	1	Total 13 C 6 O 7	0	0
5	D	1	Total 13 C 6 O 7	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			13	6	7		
5	E	1	Total	C	O	0	0
			13	6	7		
5	E	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	K	0	0
			5	5		
6	B	1	Total	K	0	0
			1	1		
6	D	5	Total	K	0	0
			5	5		
6	E	1	Total	K	0	0
			1	1		

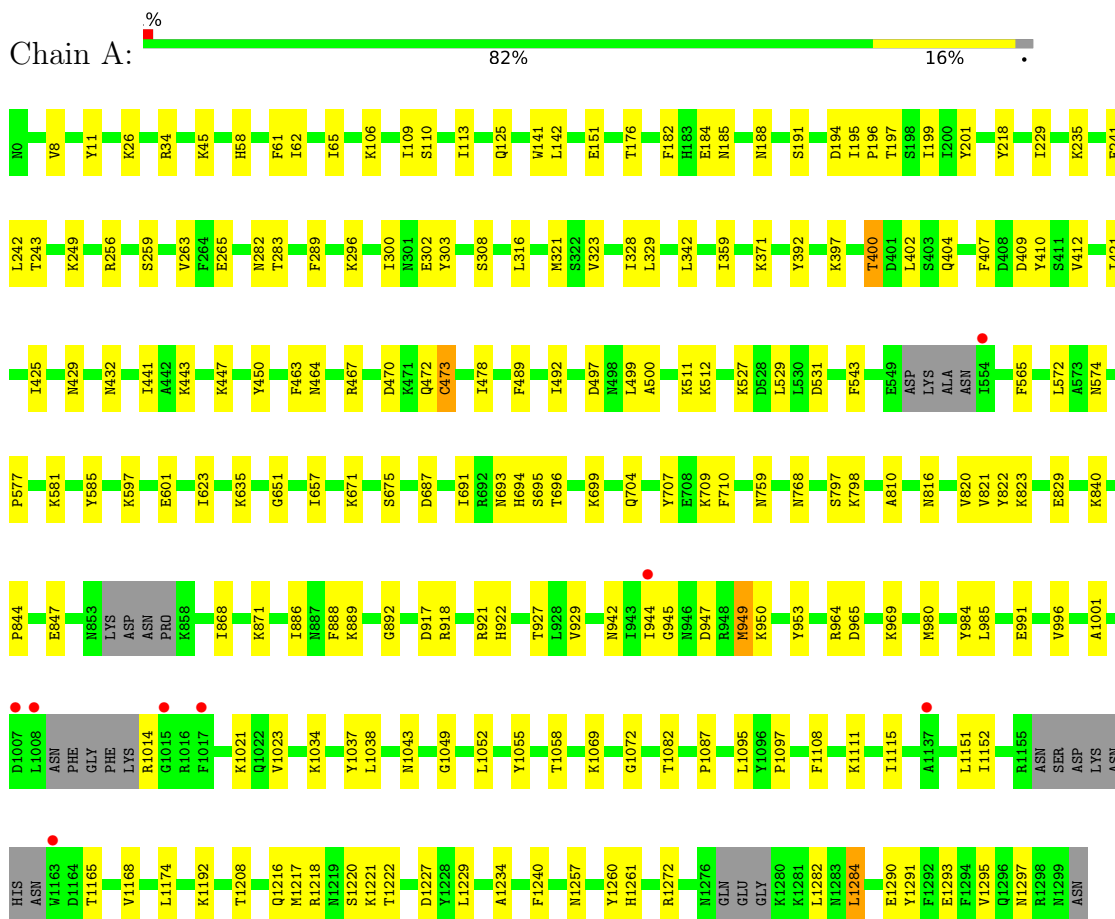
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	45	Total	O	0	0
			45	45		
7	B	10	Total	O	0	0
			10	10		
7	C	3	Total	O	0	0
			3	3		
7	D	26	Total	O	0	0
			26	26		
7	E	11	Total	O	0	0
			11	11		

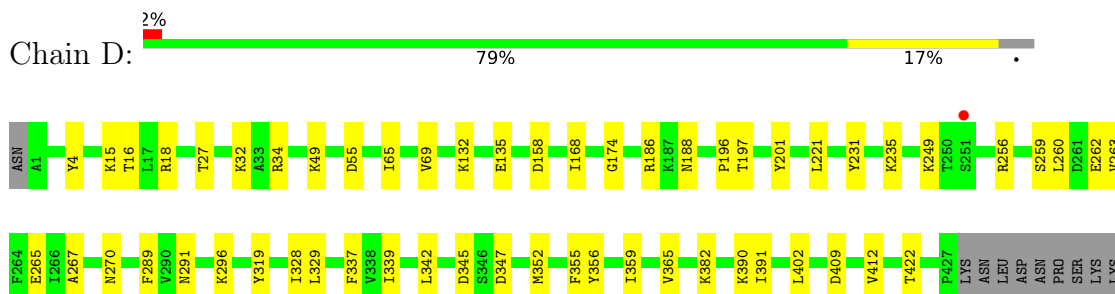
3 Residue-property plots

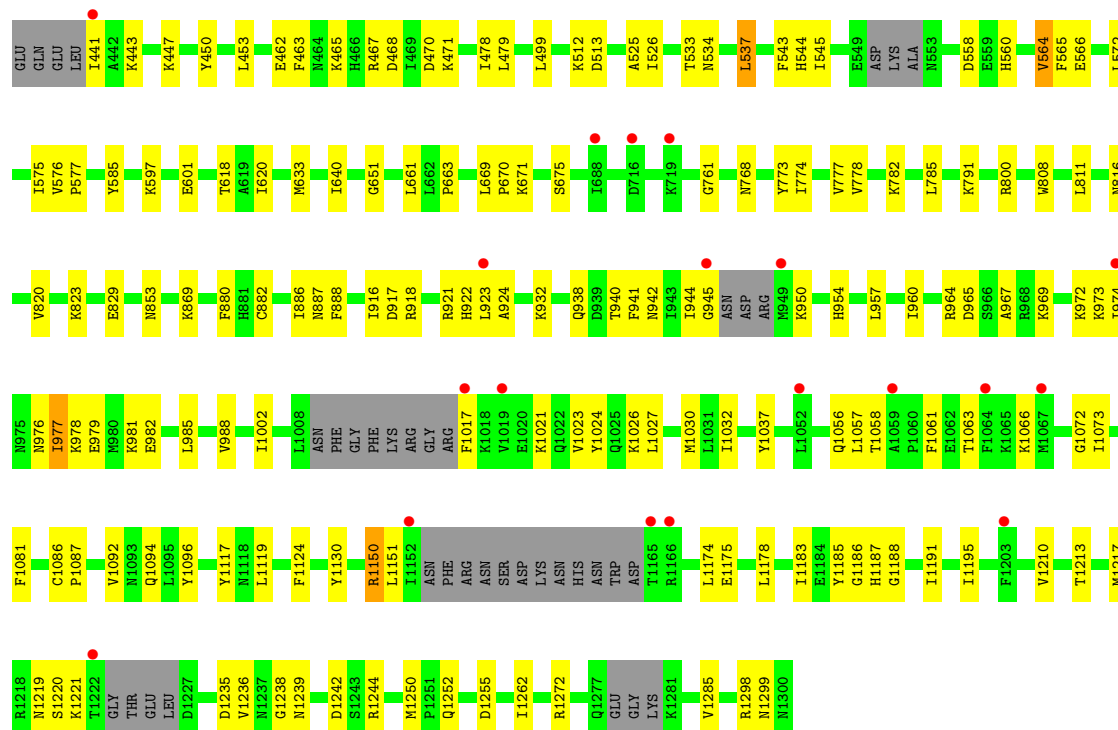
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CRISPR-associated endonuclease Cas12a



• Molecule 1: CRISPR-associated endonuclease Cas12a

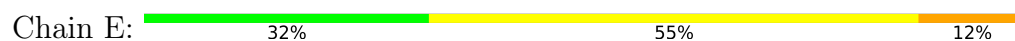




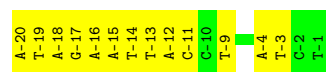
• Molecule 2: crRNA (40-MER)



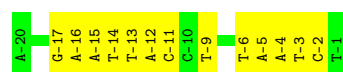
• Molecule 2: crRNA (40-MER)



• Molecule 3: ssDNA target strand



• Molecule 3: ssDNA target strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.80Å 188.58Å 284.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 2.98 49.14 – 2.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.14-2.98) 97.1 (49.14-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.14_3211: ???)	Depositor
R, R_{free}	0.204 , 0.231 0.207 , 0.233	Depositor DCC
R_{free} test set	8753 reflections (8.32%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23637	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, K, 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	0.22	0/10758	0.40	1/14440 (0.0%)
1	D	0.21	0/10553	0.39	1/14165 (0.0%)
2	B	0.25	0/942	0.45	0/1464
2	E	0.22	0/924	0.41	0/1437
3	C	0.33	0/450	0.46	0/692
3	F	0.27	0/450	0.47	0/692
All	All	0.22	0/24077	0.40	2/32890 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	LYS	CB-CA-C	-8.01	107.34	116.63
1	A	947	ASP	CB-CA-C	-6.11	109.54	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10551	0	10545	124	0
1	D	10351	0	10342	150	0
2	B	843	0	426	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	827	0	414	21	0
3	C	403	0	231	12	0
3	F	403	0	231	16	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	D	3	0	0	0	0
4	E	1	0	0	0	0
5	A	39	0	15	2	0
5	B	26	0	10	1	0
5	D	39	0	15	3	0
5	E	39	0	15	1	0
6	A	5	0	0	0	0
6	B	1	0	0	0	0
6	D	5	0	0	0	0
6	E	1	0	0	0	0
7	A	45	0	0	2	0
7	B	10	0	0	0	0
7	C	3	0	0	0	0
7	D	26	0	0	1	0
7	E	11	0	0	0	0
All	All	23637	0	22244	329	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 7.

All (329) 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:D:940:THR:HG22	1:D:942:ASN:H	1.39	0.87
1:D:922:HIS:HA	1:D:942:ASN:HD21	1.41	0.85
1:D:15:LYS:HG3	2:E:1:A:H5"	1.59	0.84
1:A:1293:GLU:O	1:A:1297:ASN:HB2	1.80	0.81
1:D:1191:ILE:HG22	1:D:1195:ILE:HG13	1.61	0.81
1:A:1165:THR:HG21	1:A:1221:LYS:HA	1.60	0.80
1:A:400:THR:HG23	1:A:410:TYR:HB2	1.64	0.79
1:A:400:THR:HG21	3:C:-20:DA:H62	1.50	0.75
1:D:352:MET:HE1	1:D:526:ILE:HG23	1.67	0.74
1:A:443:LYS:HA	1:A:447:LYS:HB3	1.70	0.72
1:D:249:LYS:HD2	1:D:265:GLU:HG2	1.70	0.72
1:D:55:ASP:OD1	1:D:186:ARG:NH1	2.23	0.72
1:D:921:ARG:NH2	1:D:1221:LYS:O	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:LYS:HA	1:D:447:LYS:HB3	1.73	0.71
1:A:191:SER:HB3	1:A:195:ILE:HD11	1.72	0.71
1:D:923:LEU:HD21	1:D:1023:VAL:HG11	1.74	0.70
1:A:1108:PHE:HA	1:A:1111:LYS:HE3	1.75	0.68
1:A:106:LYS:NZ	1:A:194:ASP:OD1	2.27	0.68
1:D:537:LEU:HB2	1:D:575:ILE:HD11	1.76	0.67
1:D:985:LEU:HA	1:D:988:VAL:HG12	1.76	0.67
1:A:125:GLN:HG3	1:A:176:THR:HG21	1.76	0.66
1:D:945:GLY:HA3	1:D:950:LYS:HA	1.79	0.65
3:C:-17:DG:H2'	3:C:-16:DA:C8	2.32	0.65
1:D:27:THR:HG21	1:D:785:LEU:H	1.62	0.65
1:D:887:ASN:ND2	1:D:1056:GLN:OE1	2.30	0.65
1:A:11:TYR:HB2	1:A:892:GLY:HA2	1.79	0.64
1:D:1002:ILE:HA	1:D:1073:ILE:HG22	1.79	0.64
1:A:65:ILE:HD13	1:A:113:ILE:HG22	1.79	0.64
1:D:981:LYS:HD2	1:D:1023:VAL:HG22	1.81	0.63
1:D:982:GLU:HA	1:D:1030:MET:HE1	1.80	0.63
1:A:1038:LEU:HB3	1:A:1055:TYR:HB2	1.81	0.62
3:F:-6:DT:H2''	3:F:-5:DA:H5''	1.82	0.61
1:D:391:ILE:HG22	1:D:453:LEU:HD13	1.81	0.61
1:D:534:ASN:HA	1:D:575:ILE:HD12	1.81	0.60
2:B:-3:A:H8	2:B:-3:A:H5''	1.66	0.60
1:D:973:LYS:NZ	3:F:-9:DT:OP1	2.28	0.60
1:A:953:TYR:HD1	1:A:980:MET:HE1	1.68	0.59
1:A:922:HIS:HA	1:A:942:ASN:HD21	1.67	0.59
1:D:342:LEU:HD22	1:D:347:ASP:HB3	1.84	0.59
5:A:1406:CIT:O3	5:A:1406:CIT:O7	2.21	0.59
1:D:964:ARG:HA	1:D:974:ILE:HD13	1.85	0.59
1:A:497:ASP:O	1:A:500:ALA:HB3	2.03	0.59
1:A:693:ASN:HB3	1:A:707:TYR:CD1	2.38	0.59
1:D:18:ARG:NH2	5:D:1405:CIT:O6	2.36	0.59
1:A:463:PHE:CE2	1:A:467:ARG:HD2	2.38	0.58
2:E:10:G:H2'	2:E:11:G:H8	1.67	0.58
1:A:404:GLN:HG2	1:A:410:TYR:HB3	1.85	0.58
1:D:1174:LEU:HG	1:D:1210:VAL:HG11	1.84	0.58
1:A:235:LYS:HD3	1:A:242:LEU:HD13	1.85	0.58
1:A:400:THR:HG21	3:C:-20:DA:N6	2.17	0.58
1:A:687:ASP:O	1:A:691:ILE:HG12	2.04	0.58
1:A:964:ARG:NH2	3:C:-9:DT:O3'	2.36	0.58
1:A:1069:LYS:HB2	1:A:1284:LEU:HD13	1.85	0.57
1:A:696:THR:HG22	1:A:710:PHE:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:PHE:CZ	1:D:575:ILE:HG23	2.39	0.57
1:A:409:ASP:HB3	1:A:412:VAL:HG23	1.86	0.57
3:F:-5:DA:H2''	3:F:-4:DA:H8	1.70	0.57
1:A:823:LYS:HD2	1:A:888:PHE:CE1	2.41	0.56
3:C:-12:DA:H2'	3:C:-11:DC:C6	2.39	0.56
1:D:328:ILE:HG22	1:D:329:LEU:HD13	1.85	0.56
1:D:1235:ASP:OD1	1:D:1239:ASN:N	2.37	0.56
2:B:-10:C:O2'	2:B:-8:G:N7	2.38	0.56
1:D:640:ILE:HG21	1:D:777:VAL:HG11	1.86	0.56
1:A:821:VAL:HG23	1:A:822:TYR:CD2	2.40	0.56
1:A:425:ILE:HD12	1:A:441:ILE:HD13	1.88	0.56
1:D:390:LYS:HB3	1:D:558:ASP:N	2.20	0.56
1:D:462:GLU:HA	1:D:465:LYS:HE3	1.88	0.55
1:A:1058:THR:HA	1:A:1072:GLY:HA3	1.89	0.55
1:D:49:LYS:NZ	1:D:158:ASP:O	2.30	0.55
1:A:651:GLY:O	1:A:768:ASN:HB3	2.06	0.55
1:A:965:ASP:OD2	1:A:969:LYS:NZ	2.27	0.55
1:D:976:ASN:HB3	1:D:979:GLU:HB2	1.88	0.55
3:F:-17:DG:H2'	3:F:-16:DA:C8	2.41	0.54
1:D:974:ILE:HD12	1:D:977:ILE:HD11	1.89	0.54
1:D:791:LYS:N	2:E:-15:U:OP1	2.40	0.54
1:D:259:SER:HB3	1:D:262:GLU:HG3	1.90	0.54
3:C:-15:DA:H3'	3:C:-14:DT:H71	1.90	0.53
1:D:1117:TYR:HD1	1:D:1124:PHE:CE1	2.26	0.53
1:A:61:PHE:CZ	1:A:65:ILE:HD11	2.43	0.53
1:D:1017:PHE:N	1:D:1021:LYS:HD2	2.23	0.53
5:E:104:CIT:O4	5:E:104:CIT:O7	2.26	0.53
2:B:16:U:H2'	2:B:17:C:C6	2.44	0.53
1:D:938:GLN:NE2	1:D:1250:MET:O	2.42	0.53
3:F:-12:DA:H2'	3:F:-11:DC:C6	2.44	0.53
1:D:174:GLY:HA2	5:D:1406:CIT:H22	1.90	0.52
1:A:300:ILE:HG21	1:A:321:MET:HE3	1.91	0.52
5:A:1405:CIT:O4	5:A:1405:CIT:O7	2.27	0.52
2:B:-18:A:O5'	5:B:103:CIT:H41	2.09	0.52
1:D:27:THR:CG2	1:D:785:LEU:H	2.22	0.52
2:E:10:G:H2'	2:E:11:G:C8	2.43	0.52
2:E:16:U:H2'	2:E:17:C:C6	2.45	0.52
1:A:1097:PRO:HB2	1:A:1208:THR:HG23	1.90	0.52
1:A:109:ILE:O	1:A:113:ILE:HG23	2.10	0.52
1:A:512:LYS:HA	1:A:585:TYR:OH	2.10	0.52
1:D:470:ASP:N	1:D:470:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:A:H1'	2:E:2:G:C8	2.44	0.51
1:A:759:ASN:HB3	1:A:889:LYS:HG2	1.93	0.51
1:A:810:ALA:O	1:A:816:ASN:ND2	2.43	0.51
1:D:922:HIS:HA	1:D:942:ASN:ND2	2.19	0.51
1:D:1063:THR:HG23	1:D:1066:LYS:H	1.76	0.51
1:D:1057:LEU:HB3	1:D:1073:ILE:CD1	2.40	0.51
1:D:409:ASP:HB3	1:D:412:VAL:HG23	1.93	0.51
3:F:-6:DT:H2'	3:F:-5:DA:H8	1.76	0.51
3:F:-6:DT:C2'	3:F:-5:DA:H5''	2.40	0.51
1:A:243:THR:HA	1:A:256:ARG:O	2.11	0.51
1:D:1032:ILE:HG21	1:D:1061:PHE:HB2	1.92	0.51
1:D:1151:LEU:N	1:D:1219:ASN:OD1	2.40	0.50
1:D:661:LEU:HA	1:D:761:GLY:O	2.10	0.50
2:B:20:U:H5'	2:B:21:C:OP1	2.11	0.50
1:D:1124:PHE:CE2	1:D:1174:LEU:HB3	2.46	0.50
1:A:1095:LEU:O	1:A:1097:PRO:HD3	2.11	0.50
1:D:921:ARG:NH2	1:D:1220:SER:HB2	2.26	0.50
1:D:669:LEU:HB2	1:D:670:PRO:HD3	1.93	0.50
1:D:957:LEU:O	1:D:960:ILE:HG22	2.12	0.50
1:A:397:LYS:NZ	3:C:-19:DT:O4	2.44	0.50
1:A:26:LYS:NZ	7:A:1505:HOH:O	2.45	0.49
1:A:821:VAL:HG23	1:A:822:TYR:HD2	1.76	0.49
1:A:1218:ARG:NH1	1:A:1227:ASP:OD2	2.45	0.49
2:B:-3:A:H5''	2:B:-3:A:C8	2.46	0.49
1:D:267:ALA:O	1:D:270:ASN:ND2	2.46	0.49
1:A:985:LEU:HD11	1:A:1023:VAL:HG12	1.94	0.49
1:A:1272:ARG:NH2	1:A:1290:GLU:OE1	2.45	0.49
1:D:468:ASP:HB2	1:D:471:LYS:HE3	1.94	0.49
1:A:1234:ALA:HB2	1:A:1240:PHE:CZ	2.47	0.49
1:D:221:LEU:HB2	1:D:319:TYR:HD1	1.78	0.49
1:A:289:PHE:CE2	1:A:296:LYS:HD2	2.47	0.49
1:A:464:ASN:HB3	1:A:472:GLN:NE2	2.28	0.49
1:D:1272:ARG:NH1	1:D:1285:VAL:O	2.39	0.48
1:A:953:TYR:CD1	1:A:984:TYR:HB2	2.48	0.48
1:D:924:ALA:HB3	1:D:941:PHE:HB2	1.94	0.48
2:E:13:A:H2'	2:E:14:A:C8	2.48	0.48
3:C:-15:DA:H5''	3:C:-15:DA:H8	1.78	0.48
1:D:231:TYR:O	1:D:235:LYS:HG2	2.13	0.48
1:A:407:PHE:CD1	1:A:473:CYS:HB3	2.48	0.48
1:D:259:SER:O	1:D:263:VAL:HG13	2.13	0.48
1:A:597:LYS:HE2	1:A:829:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:PHE:CE2	1:D:467:ARG:HD2	2.49	0.48
1:D:560:HIS:O	1:D:564:VAL:HG23	2.13	0.48
1:A:218:TYR:HB2	1:A:321:MET:HE1	1.96	0.48
1:D:345:ASP:OD2	1:D:513:ASP:N	2.36	0.48
1:D:382:LYS:HA	1:D:479:LEU:HD13	1.95	0.48
1:D:618:THR:HG22	1:D:633:MET:H	1.77	0.48
1:D:661:LEU:HG	1:D:663:PRO:HD3	1.95	0.48
1:D:1026:LYS:HG2	1:D:1030:MET:HE3	1.96	0.48
1:D:499:LEU:HD21	1:D:525:ALA:HB1	1.95	0.48
1:D:800:ARG:NH2	7:D:1502:HOH:O	2.47	0.48
1:A:996:VAL:HA	1:A:1001:ALA:HB3	1.95	0.47
1:D:359:ILE:HD12	1:D:572:LEU:HD23	1.96	0.47
1:D:4:TYR:CZ	1:D:1073:ILE:HD13	2.49	0.47
1:D:256:ARG:HH12	1:D:262:GLU:CD	2.19	0.47
1:D:823:LYS:HD2	1:D:888:PHE:CE1	2.49	0.47
1:A:945:GLY:HA3	1:A:950:LYS:HA	1.95	0.47
2:E:-12:U:H2'	2:E:-11:A:C8	2.48	0.47
1:A:58:HIS:O	1:A:62:ILE:HG13	2.15	0.47
1:A:1023:VAL:HG12	1:A:1023:VAL:O	2.15	0.47
1:D:671:LYS:O	1:D:675:SER:HB3	2.14	0.47
1:D:945:GLY:HA3	1:D:950:LYS:HG2	1.97	0.47
1:D:964:ARG:CZ	1:D:977:ILE:HD12	2.45	0.47
2:B:-14:U:H2'	2:B:-13:C:C6	2.50	0.47
1:D:390:LYS:HB3	1:D:558:ASP:H	1.79	0.47
1:D:463:PHE:CZ	1:D:467:ARG:HD2	2.49	0.47
1:A:470:ASP:OD2	1:A:470:ASP:N	2.47	0.47
3:F:-13:DT:H2'	3:F:-12:DA:C8	2.50	0.47
1:A:199:ILE:HG22	1:A:328:ILE:HB	1.95	0.47
1:A:623:ILE:HG13	1:A:657:ILE:HD11	1.97	0.47
1:A:695:SER:O	1:A:709:LYS:HE3	2.14	0.47
1:A:574:ASN:O	1:A:577:PRO:HD2	2.15	0.47
1:D:967:ALA:HB1	1:D:972:LYS:HG2	1.97	0.47
1:D:932:LYS:O	1:D:1298:ARG:NH2	2.46	0.46
1:A:229:ILE:HG22	1:A:303:TYR:HB2	1.97	0.46
1:A:543:PHE:HB2	1:A:565:PHE:CZ	2.50	0.46
1:A:844:PRO:HG2	1:A:847:GLU:OE1	2.15	0.46
1:D:921:ARG:HH22	1:D:1220:SER:HB2	1.79	0.46
1:A:110:SER:O	1:A:113:ILE:HG12	2.15	0.46
1:A:182:PHE:O	1:A:185:ASN:HB2	2.15	0.46
1:D:188:ASN:HB3	1:D:197:THR:OG1	2.15	0.46
3:F:-13:DT:H2'	3:F:-12:DA:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LEU:HD21	1:A:478:ILE:HG23	1.98	0.46
1:A:871:LYS:HE2	2:B:-16:U:OP1	2.15	0.46
1:A:1021:LYS:O	1:A:1023:VAL:HG23	2.16	0.46
2:E:12:U:H2'	2:E:13:A:C8	2.51	0.46
1:D:544:HIS:ND1	1:D:566:GLU:OE1	2.40	0.46
1:D:978:LYS:O	1:D:982:GLU:HG3	2.16	0.46
3:F:-6:DT:H2'	3:F:-5:DA:C8	2.51	0.46
1:A:241:GLU:HG2	1:A:283:THR:HB	1.96	0.46
1:A:371:LYS:HD3	1:A:489:PHE:HB2	1.97	0.46
1:A:693:ASN:HA	1:A:704:GLN:HB2	1.98	0.46
1:A:1152:ILE:HD12	1:A:1168:VAL:HG21	1.98	0.46
1:D:65:ILE:O	1:D:69:VAL:HG23	2.16	0.46
1:D:512:LYS:HA	1:D:585:TYR:OH	2.16	0.46
1:D:880:PHE:CE2	1:D:882:CYS:HB2	2.51	0.46
1:A:917:ASP:OD1	1:A:918:ARG:N	2.46	0.45
3:C:-4:DA:H3'	3:C:-3:DT:H71	1.98	0.45
1:D:917:ASP:HB2	1:D:1262:ILE:HD12	1.97	0.45
1:D:1087:PRO:HB2	1:D:1250:MET:HE3	1.98	0.45
3:F:-14:DT:H2'	3:F:-13:DT:C6	2.51	0.45
1:D:402:LEU:HD21	1:D:478:ILE:HG23	1.99	0.45
1:D:1117:TYR:CE2	1:D:1119:LEU:HD23	2.51	0.45
3:F:-4:DA:H3'	3:F:-3:DT:H71	1.98	0.45
1:A:1291:TYR:O	1:A:1295:VAL:HG12	2.17	0.45
2:B:13:A:H2'	2:B:14:A:C8	2.51	0.45
1:D:543:PHE:HB2	1:D:565:PHE:CZ	2.51	0.45
1:D:640:ILE:HD11	1:D:782:LYS:HB3	1.99	0.45
2:E:13:A:H2'	2:E:14:A:H8	1.82	0.45
1:A:944:ILE:HD11	1:A:991:GLU:HG3	1.99	0.45
1:D:965:ASP:O	1:D:969:LYS:HD3	2.17	0.45
1:A:259:SER:O	1:A:263:VAL:HG13	2.16	0.45
2:E:8:A:H2'	2:E:9:A:C8	2.52	0.45
1:D:34:ARG:NH1	1:D:601:GLU:OE2	2.49	0.45
1:A:597:LYS:NZ	7:A:1503:HOH:O	2.39	0.45
1:A:840:LYS:O	1:A:868:ILE:HG23	2.16	0.45
1:D:620:ILE:HD11	1:D:633:MET:HE2	1.98	0.45
1:D:1185:TYR:HB3	1:D:1191:ILE:HD11	1.99	0.45
2:B:-13:C:H2'	2:B:-12:U:C6	2.52	0.44
1:A:1272:ARG:HB3	1:A:1282:LEU:HD11	1.99	0.44
1:D:1236:VAL:HG21	1:D:1299:ASN:HD21	1.83	0.44
1:D:537:LEU:CB	1:D:575:ILE:HD11	2.45	0.44
1:A:196:PRO:HA	1:A:201:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1175:GLU:HG2	1:D:1185:TYR:CE1	2.52	0.44
1:D:1242:ASP:OD2	1:D:1244:ARG:HG3	2.18	0.44
1:A:886:ILE:HG21	1:A:1037:TYR:CZ	2.53	0.44
1:A:949:MET:HE3	1:A:949:MET:HB2	1.78	0.44
1:D:922:HIS:HB3	1:D:940:THR:HG23	2.00	0.44
1:A:184:GLU:HG2	3:C:-3:DT:H2''	1.99	0.44
2:B:-5:G:C2	2:B:-4:U:C5	3.06	0.44
2:E:-5:G:H2'	2:E:-4:U:H5'	2.00	0.44
1:D:1026:LYS:CG	1:D:1030:MET:HE3	2.48	0.44
1:A:699:LYS:O	1:A:699:LYS:HD3	2.17	0.43
1:D:356:TYR:CE2	1:D:533:THR:HG21	2.53	0.43
2:E:17:C:H2'	2:E:18:U:O4'	2.18	0.43
1:A:359:ILE:HD12	1:A:572:LEU:HD23	2.01	0.43
1:D:196:PRO:HA	1:D:201:TYR:CD2	2.52	0.43
1:D:886:ILE:HG21	1:D:1037:TYR:CZ	2.53	0.43
2:B:2:G:H2'	2:B:3:A:C8	2.53	0.43
1:A:1174:LEU:HD12	1:A:1174:LEU:HA	1.86	0.43
3:C:-18:DA:H2'	3:C:-17:DG:H8	1.83	0.43
1:D:808:TRP:O	1:D:811:LEU:HB2	2.18	0.43
1:D:869:LYS:HB2	2:E:-18:A:H5''	1.99	0.43
1:A:34:ARG:NH1	1:A:601:GLU:OE1	2.50	0.43
1:A:289:PHE:CE1	1:A:296:LYS:HB2	2.52	0.43
1:A:953:TYR:CD1	1:A:980:MET:HE1	2.52	0.43
1:A:1151:LEU:O	1:A:1216:GLN:NE2	2.45	0.43
1:D:982:GLU:HG2	1:D:1030:MET:HE1	2.00	0.43
1:D:572:LEU:O	1:D:575:ILE:HG12	2.19	0.43
1:D:974:ILE:CD1	1:D:977:ILE:HD11	2.48	0.43
1:D:289:PHE:CE1	1:D:296:LYS:HB2	2.54	0.43
1:D:545:ILE:HG12	1:D:566:GLU:OE2	2.19	0.43
1:A:511:LYS:HA	1:A:511:LYS:HD3	1.73	0.42
1:D:15:LYS:HE3	1:D:15:LYS:HB2	1.84	0.42
1:D:651:GLY:O	1:D:768:ASN:HB3	2.20	0.42
1:D:1081:PHE:CD1	1:D:1092:VAL:HG11	2.54	0.42
1:D:576:VAL:HB	1:D:577:PRO:HD3	2.01	0.42
1:D:774:ILE:O	1:D:778:VAL:HG12	2.19	0.42
1:D:941:PHE:HD1	1:D:944:ILE:HD11	1.85	0.42
1:D:979:GLU:N	1:D:979:GLU:OE2	2.53	0.42
1:D:1117:TYR:HB3	1:D:1188:GLY:HA2	2.00	0.42
1:A:671:LYS:O	1:A:675:SER:HB3	2.19	0.42
1:A:820:VAL:H	1:A:889:LYS:NZ	2.18	0.42
1:D:782:LYS:NZ	5:D:1404:CIT:O4	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:941:PHE:CD1	1:D:988:VAL:HG23	2.54	0.42
1:A:429:ASN:HB3	1:A:432:ASN:O	2.19	0.42
1:A:499:LEU:CD1	1:A:529:LEU:HD22	2.50	0.42
1:A:927:THR:HG21	1:A:1260:TYR:HA	2.00	0.42
1:D:773:TYR:O	1:D:777:VAL:HG23	2.20	0.42
1:A:45:LYS:NZ	1:D:32:LYS:O	2.45	0.42
2:B:-2:G:H2'	2:B:-1:A:O4'	2.19	0.42
2:E:-14:U:H2'	2:E:-13:C:C6	2.54	0.42
2:E:-5:G:C2'	2:E:-4:U:H5'	2.49	0.42
3:F:-15:DA:H2'	3:F:-14:DT:C6	2.54	0.42
1:A:296:LYS:NZ	1:A:302:GLU:OE1	2.48	0.42
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.86	0.42
1:D:916:ILE:O	1:D:1024:TYR:OH	2.36	0.42
3:F:-17:DG:H2'	3:F:-16:DA:H8	1.84	0.42
1:A:693:ASN:HB3	1:A:707:TYR:HD1	1.84	0.42
1:D:291:ASN:HB3	1:D:337:PHE:CD1	2.54	0.42
1:D:1119:LEU:HD21	1:D:1186:GLY:O	2.20	0.42
1:D:1150:ARG:HG2	1:D:1213:THR:O	2.20	0.42
2:E:-14:U:H2'	2:E:-13:C:H6	1.85	0.42
1:D:1057:LEU:O	1:D:1073:ILE:HG13	2.20	0.41
1:A:527:LYS:HE3	1:A:969:LYS:O	2.20	0.41
1:A:921:ARG:NH1	1:A:1222:THR:HA	2.35	0.41
1:A:1034:LYS:HD3	2:B:0:U:P	2.60	0.41
1:A:1115:ILE:HD12	1:A:1192:LYS:HG3	2.02	0.41
1:A:1220:SER:HB3	1:A:1227:ASP:HA	2.02	0.41
1:A:635:LYS:HA	1:A:635:LYS:HD2	1.80	0.41
1:A:1043:ASN:HD22	1:A:1049:GLY:HA3	1.85	0.41
2:B:12:U:H2'	2:B:13:A:C8	2.55	0.41
1:D:1124:PHE:CZ	1:D:1178:LEU:HD12	2.56	0.41
1:A:249:LYS:HD2	1:A:265:GLU:HG2	2.02	0.41
3:C:-14:DT:H2'	3:C:-13:DT:C6	2.56	0.41
1:D:16:THR:HG21	2:E:2:G:H1'	2.02	0.41
1:D:422:THR:HG22	1:D:441:ILE:HD13	2.01	0.41
1:D:450:TYR:OH	1:D:545:ILE:HA	2.21	0.41
1:D:942:ASN:CG	1:D:954:HIS:HB2	2.45	0.41
3:F:-3:DT:H2'	3:F:-2:DC:C6	2.55	0.41
1:D:597:LYS:NZ	1:D:829:GLU:HG2	2.35	0.41
1:D:922:HIS:ND1	1:D:1255:ASP:OD2	2.52	0.41
1:A:188:ASN:HB3	1:A:197:THR:OG1	2.20	0.41
1:A:282:ASN:CG	1:A:323:VAL:HG13	2.46	0.41
1:A:342:LEU:HG	1:A:581:LYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1086:CYS:N	1:D:1217:MET:HE1	2.35	0.41
1:A:141:TRP:CE3	1:A:142:LEU:HD12	2.56	0.41
1:A:308:SER:HA	1:A:316:LEU:HD12	2.03	0.41
1:A:392:TYR:HB3	1:A:450:TYR:HB3	2.02	0.41
1:A:1217:MET:O	1:A:1229:LEU:HA	2.21	0.41
1:D:918:ARG:HH11	1:D:1021:LYS:HG2	1.85	0.41
1:D:964:ARG:HA	1:D:974:ILE:CD1	2.51	0.41
1:D:1058:THR:HA	1:D:1072:GLY:HA3	2.03	0.41
1:D:1183:ILE:HG21	1:D:1191:ILE:HG23	2.02	0.41
1:D:816:ASN:O	1:D:820:VAL:HA	2.21	0.41
1:D:1119:LEU:HD11	1:D:1187:HIS:C	2.46	0.41
1:A:927:THR:HG22	1:A:929:VAL:HG23	2.03	0.40
1:D:1094:GLN:HA	1:D:1096:TYR:CE2	2.56	0.40
2:E:-4:U:H2'	2:E:-3:A:C8	2.56	0.40
3:F:-5:DA:H2''	3:F:-4:DA:C8	2.55	0.40
2:B:2:G:H2'	2:B:3:A:H8	1.86	0.40
1:D:49:LYS:HB3	1:D:168:ILE:HD13	2.02	0.40
1:D:1235:ASP:OD1	1:D:1238:GLY:N	2.53	0.40
2:E:2:G:H2'	2:E:3:A:C8	2.56	0.40
1:A:421:ILE:HG22	1:A:441:ILE:HD13	2.03	0.40
1:A:1087:PRO:HG3	1:A:1257:ASN:OD1	2.21	0.40
1:A:492:ILE:HG23	1:A:529:LEU:HD11	2.03	0.40
1:A:1082:THR:O	1:A:1261:HIS:HB2	2.22	0.40
1:D:985:LEU:HD22	1:D:1027:LEU:HB2	2.02	0.40
1:A:527:LYS:NZ	1:A:531:ASP:OD1	2.54	0.40
1:A:797:SER:OG	1:A:798:LYS:N	2.54	0.40
1:D:337:PHE:CE2	1:D:339:ILE:HD13	2.56	0.40
1:D:938:GLN:NE2	1:D:1252:GLN:HG2	2.37	0.40
2:E:19:A:H2'	2:E:20:U:C6	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	1265/1301 (97%)	1217 (96%)	48 (4%)	0	100	100
1	D	1238/1301 (95%)	1213 (98%)	25 (2%)	0	100	100
All	All	2503/2602 (96%)	2430 (97%)	73 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1163/1184 (98%)	1154 (99%)	9 (1%)	73	86
1	D	1142/1184 (96%)	1133 (99%)	9 (1%)	73	86
All	All	2305/2368 (97%)	2287 (99%)	18 (1%)	73	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	151	GLU
1	A	400	THR
1	A	473	CYS
1	A	694	HIS
1	A	949	MET
1	A	1014	ARG
1	A	1052	LEU
1	A	1284	LEU
1	D	135	GLU
1	D	260	LEU
1	D	365	VAL
1	D	537	LEU
1	D	564	VAL
1	D	853	ASN
1	D	977	ILE
1	D	1130	TYR
1	D	1150	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	507	GLN
1	A	509	GLN
1	A	532	GLN
1	A	637	ASN
1	A	748	ASN
1	A	787	GLN
1	D	9	ASN
1	D	30	ASN
1	D	52	GLN
1	D	121	ASN
1	D	404	GLN
1	D	538	HIS
1	D	599	ASN
1	D	780	GLN
1	D	887	ASN
1	D	987	GLN
1	D	1299	ASN
1	D	1300	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	39/40 (97%)	7 (17%)	0
2	E	38/40 (95%)	8 (21%)	0
All	All	77/80 (96%)	15 (19%)	0

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-8	G
2	B	-6	U
2	B	-5	G
2	B	-4	U
2	B	1	A
2	B	18	U
2	B	21	C
2	E	-10	C
2	E	-8	G
2	E	-6	U

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Mol	Chain	Res	Type
2	E	-5	G
2	E	-4	U
2	E	1	A
2	E	18	U
2	E	20	U

There are no RNA pucker outliers to report.

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](#)

Of 32 ligands modelled in this entry, 21 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	CIT	B	103	-	12,12,12	1.05	0	17,17,17	1.47	2 (11%)
5	CIT	E	102	-	12,12,12	1.05	0	17,17,17	1.58	2 (11%)
5	CIT	B	102	6	12,12,12	1.01	0	17,17,17	1.83	5 (29%)
5	CIT	A	1405	-	12,12,12	1.07	0	17,17,17	1.65	3 (17%)
5	CIT	E	104	-	12,12,12	1.08	0	17,17,17	1.49	2 (11%)
5	CIT	D	1404	-	12,12,12	1.06	0	17,17,17	1.61	2 (11%)
5	CIT	D	1405	6	12,12,12	1.14	0	17,17,17	1.43	3 (17%)
5	CIT	E	103	-	12,12,12	1.03	0	17,17,17	1.58	4 (23%)
5	CIT	A	1406	-	12,12,12	1.03	0	17,17,17	1.44	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CIT	A	1407	-	12,12,12	1.00	0	17,17,17	1.60	3 (17%)
5	CIT	D	1406	-	12,12,12	1.04	0	17,17,17	1.63	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CIT	B	103	-	-	4/16/16/16	-
5	CIT	E	102	-	-	9/16/16/16	-
5	CIT	B	102	6	-	8/16/16/16	-
5	CIT	A	1405	-	-	10/16/16/16	-
5	CIT	E	104	-	-	3/16/16/16	-
5	CIT	D	1404	-	-	0/16/16/16	-
5	CIT	D	1405	6	-	4/16/16/16	-
5	CIT	E	103	-	-	11/16/16/16	-
5	CIT	A	1406	-	-	3/16/16/16	-
5	CIT	A	1407	-	-	6/16/16/16	-
5	CIT	D	1406	-	-	4/16/16/16	-

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	102	CIT	O6-C6-C3	4.82	122.38	113.14
5	D	1406	CIT	O6-C6-C3	4.43	121.63	113.14
5	A	1407	CIT	O6-C6-C3	4.38	121.55	113.14
5	E	103	CIT	O6-C6-C3	4.23	121.26	113.14
5	E	102	CIT	O6-C6-C3	4.18	121.15	113.14
5	A	1406	CIT	O6-C6-C3	4.06	120.93	113.14
5	A	1405	CIT	O6-C6-C3	4.02	120.84	113.14
5	D	1404	CIT	O6-C6-C3	4.00	120.82	113.14
5	B	103	CIT	O6-C6-C3	3.80	120.43	113.14
5	E	104	CIT	O6-C6-C3	3.69	120.22	113.14
5	D	1405	CIT	O6-C6-C3	3.31	119.48	113.14
5	A	1405	CIT	O2-C1-C2	2.62	122.65	114.35
5	B	102	CIT	O2-C1-C2	2.56	122.45	114.35
5	B	102	CIT	O4-C5-C4	2.46	122.13	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	103	CIT	O4-C5-C4	2.43	122.05	114.35
5	D	1404	CIT	O2-C1-C2	2.34	121.75	114.35
5	E	102	CIT	O2-C1-C2	2.31	121.66	114.35
5	A	1405	CIT	O2-C1-O1	-2.29	117.45	123.33
5	B	102	CIT	O2-C1-O1	-2.20	117.68	123.33
5	E	103	CIT	O4-C5-O3	-2.19	117.69	123.33
5	A	1407	CIT	O4-C5-C4	2.13	121.08	114.35
5	B	102	CIT	O4-C5-O3	-2.11	117.90	123.33
5	E	104	CIT	C3-C4-C5	-2.10	108.19	113.92
5	D	1405	CIT	O4-C5-C4	2.06	120.88	114.35
5	D	1405	CIT	O2-C1-C2	2.04	120.80	114.35
5	E	103	CIT	O2-C1-O1	-2.03	118.11	123.33
5	B	103	CIT	O2-C1-C2	2.02	120.75	114.35
5	A	1407	CIT	O2-C1-C2	2.01	120.72	114.35

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1405	CIT	C2-C3-C6-O5
5	A	1405	CIT	C2-C3-C6-O6
5	A	1405	CIT	O7-C3-C6-O5
5	A	1405	CIT	O7-C3-C6-O6
5	A	1406	CIT	O7-C3-C4-C5
5	A	1406	CIT	C6-C3-C4-C5
5	A	1407	CIT	C1-C2-C3-O7
5	A	1407	CIT	C1-C2-C3-C6
5	B	102	CIT	O7-C3-C6-O5
5	B	102	CIT	O7-C3-C6-O6
5	B	102	CIT	C4-C3-C6-O5
5	B	102	CIT	C4-C3-C6-O6
5	E	102	CIT	O7-C3-C6-O5
5	E	102	CIT	O7-C3-C6-O6
5	E	102	CIT	C4-C3-C6-O5
5	E	102	CIT	C4-C3-C6-O6
5	A	1406	CIT	C2-C3-C4-C5
5	A	1407	CIT	C1-C2-C3-C4
5	A	1407	CIT	O7-C3-C4-C5
5	B	103	CIT	C1-C2-C3-C4
5	A	1407	CIT	C6-C3-C4-C5
5	E	102	CIT	C6-C3-C4-C5
5	A	1405	CIT	C3-C4-C5-O4

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Mol	Chain	Res	Type	Atoms
5	E	102	CIT	O7-C3-C4-C5
5	A	1405	CIT	C3-C4-C5-O3
5	D	1406	CIT	O7-C3-C4-C5
5	E	103	CIT	O7-C3-C6-O5
5	A	1407	CIT	C2-C3-C4-C5
5	B	103	CIT	C1-C2-C3-C6
5	D	1406	CIT	C6-C3-C4-C5
5	E	102	CIT	C2-C3-C4-C5
5	D	1405	CIT	C1-C2-C3-O7
5	E	103	CIT	C2-C3-C6-O5
5	E	103	CIT	C2-C3-C6-O6
5	E	103	CIT	C4-C3-C6-O5
5	E	103	CIT	C4-C3-C6-O6
5	E	102	CIT	O2-C1-C2-C3
5	B	103	CIT	C1-C2-C3-O7
5	D	1405	CIT	C1-C2-C3-C6
5	D	1406	CIT	C2-C3-C4-C5
5	E	103	CIT	C6-C3-C4-C5
5	E	102	CIT	O1-C1-C2-C3
5	E	103	CIT	C3-C4-C5-O4
5	D	1405	CIT	C3-C4-C5-O4
5	A	1405	CIT	C4-C3-C6-O5
5	A	1405	CIT	C4-C3-C6-O6
5	E	103	CIT	C3-C4-C5-O3
5	D	1405	CIT	C3-C4-C5-O3
5	E	103	CIT	O7-C3-C4-C5
5	E	104	CIT	O7-C3-C4-C5
5	D	1406	CIT	C4-C3-C6-O6
5	B	102	CIT	C3-C4-C5-O4
5	E	103	CIT	O7-C3-C6-O6
5	B	102	CIT	O2-C1-C2-C3
5	B	102	CIT	C3-C4-C5-O3
5	E	104	CIT	C3-C4-C5-O3
5	A	1405	CIT	O1-C1-C2-C3
5	B	102	CIT	O1-C1-C2-C3
5	E	103	CIT	C2-C3-C4-C5
5	A	1405	CIT	O2-C1-C2-C3
5	E	104	CIT	C3-C4-C5-O4
5	B	103	CIT	O7-C3-C4-C5

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	103	CIT	1	0
5	A	1405	CIT	1	0
5	E	104	CIT	1	0
5	D	1404	CIT	1	0
5	D	1405	CIT	1	0
5	A	1406	CIT	1	0
5	D	1406	CIT	1	0

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	1277/1301 (98%)	-0.17	8 (0%) 85 72	43, 72, 120, 206	0
1	D	1254/1301 (96%)	0.01	20 (1%) 70 51	52, 90, 166, 207	0
2	B	40/40 (100%)	-0.86	0 100 100	48, 56, 96, 192	0
2	E	40/40 (100%)	-0.89	0 100 100	59, 69, 96, 129	0
3	C	20/20 (100%)	-0.99	0 100 100	50, 57, 75, 76	0
3	F	20/20 (100%)	-0.81	0 100 100	63, 74, 97, 99	0
All	All	2651/2722 (97%)	-0.12	28 (1%) 78 61	43, 80, 147, 207	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1008	LEU	4.3
1	D	1067	MET	4.1
1	D	945	GLY	3.4
1	D	1019	VAL	3.4
1	D	441	ILE	3.0
1	D	1166	ARG	2.9
1	A	1137	ALA	2.9
1	D	949	MET	2.8
1	D	719	LYS	2.7
1	D	1165	THR	2.7
1	D	1052	LEU	2.6
1	D	1064	PHE	2.6
1	A	1007	ASP	2.5
1	D	974	ILE	2.5
1	A	1163	TRP	2.5
1	A	554	ILE	2.4
1	D	1059	ALA	2.4
1	D	1222	THR	2.3
1	A	1015	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	923	LEU	2.3
1	D	1203	PHE	2.2
1	D	688	ILE	2.2
1	D	251	SER	2.2
1	D	716	ASP	2.2
1	A	1017	PHE	2.1
1	A	944	ILE	2.1
1	D	1017	PHE	2.0
1	D	1152	ILE	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(Å ²)	Q<0.9
5	CIT	D	1406	13/13	0.35	0.13	112,112,112,112	0
5	CIT	E	103	13/13	0.54	0.15	116,116,116,116	0
5	CIT	A	1407	13/13	0.56	0.12	85,85,85,85	0
5	CIT	E	104	13/13	0.60	0.12	131,131,131,131	0
6	K	D	1411	1/1	0.68	0.17	126,126,126,126	0
5	CIT	A	1406	13/13	0.70	0.14	96,96,96,96	0
6	K	D	1407	1/1	0.72	0.19	104,104,104,104	0
5	CIT	B	103	13/13	0.73	0.11	112,112,112,112	0
5	CIT	E	102	13/13	0.73	0.11	98,98,98,98	0
6	K	E	105	1/1	0.73	0.14	106,106,106,106	0
6	K	A	1411	1/1	0.74	0.14	106,106,106,106	0
6	K	D	1410	1/1	0.74	0.10	108,108,108,108	0
5	CIT	B	102	13/13	0.75	0.11	79,79,79,79	0
6	K	A	1408	1/1	0.82	0.12	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	B	101	1/1	0.83	0.17	85,85,85,85	0
5	CIT	D	1405	13/13	0.84	0.10	89,89,89,89	0
6	K	A	1412	1/1	0.84	0.10	102,102,102,102	0
5	CIT	D	1404	13/13	0.84	0.08	110,110,110,110	0
6	K	D	1409	1/1	0.85	0.14	109,109,109,109	0
4	MG	D	1402	1/1	0.85	0.10	86,86,86,86	0
5	CIT	A	1405	13/13	0.86	0.09	95,95,95,95	0
6	K	D	1408	1/1	0.86	0.16	93,93,93,93	0
4	MG	A	1404	1/1	0.87	0.07	78,78,78,78	0
4	MG	A	1403	1/1	0.89	0.08	95,95,95,95	0
4	MG	A	1401	1/1	0.90	0.07	74,74,74,74	0
4	MG	D	1403	1/1	0.90	0.14	103,103,103,103	0
6	K	A	1410	1/1	0.93	0.16	84,84,84,84	0
4	MG	A	1402	1/1	0.93	0.12	70,70,70,70	0
6	K	A	1409	1/1	0.93	0.13	94,94,94,94	0
4	MG	D	1401	1/1	0.94	0.06	86,86,86,86	0
6	K	B	104	1/1	0.94	0.14	81,81,81,81	0
4	MG	E	101	1/1	0.96	0.07	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.