



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 02:19 am GMT

PDB ID : 6I1L  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

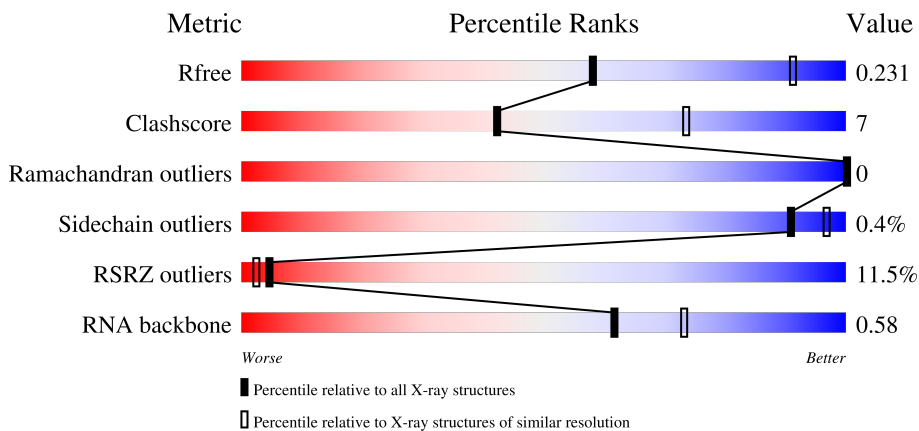
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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))
$R_{free}$	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)
RNA backbone	3102	1088 (3.26-2.70)

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  $\geq 3$ , 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	
1	D	1301	
2	B	40	
2	E	40	

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Mol	Chain	Length	Quality of chain
3	C	20	
3	F	20	

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	CIT	A	1406	-	-	-	X
5	CIT	E	103	-	-	-	X
6	K	D	1411	-	-	-	X
6	K	E	105	-	-	-	X

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
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
			Total	C	N	O	P			
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			

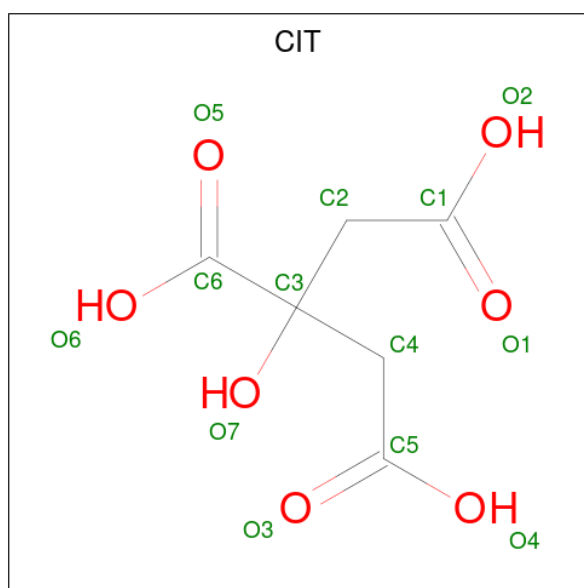
- Molecule 3 is a DNA chain called ssDNA target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
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 (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0
5	A	1	Total C O 13 6 7	0	0
5	A	1	Total C O 13 6 7	0	0
5	B	1	Total C O 13 6 7	0	0
5	B	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 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 (three-letter code: 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		

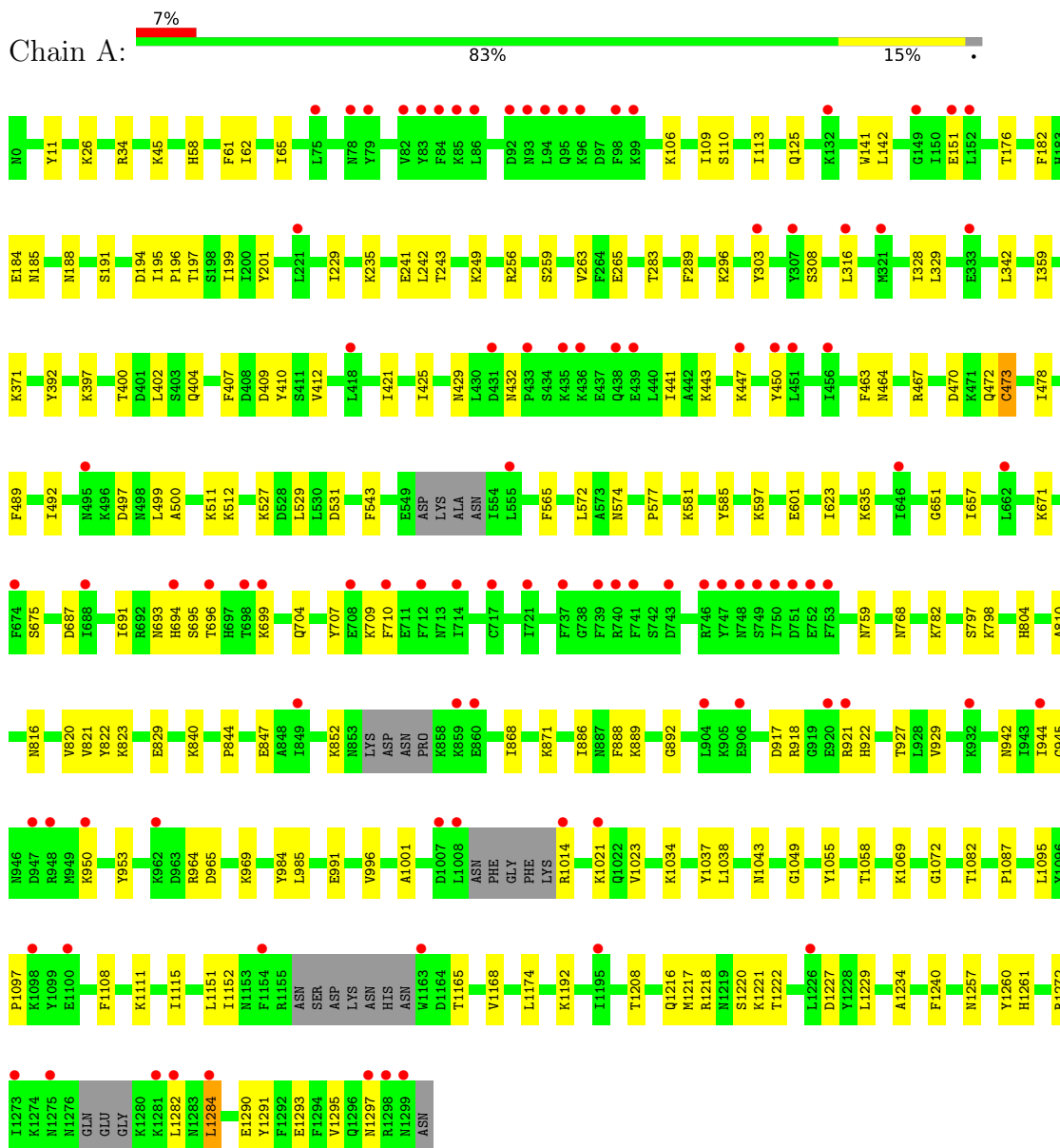
- Molecule 7 is water.

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		

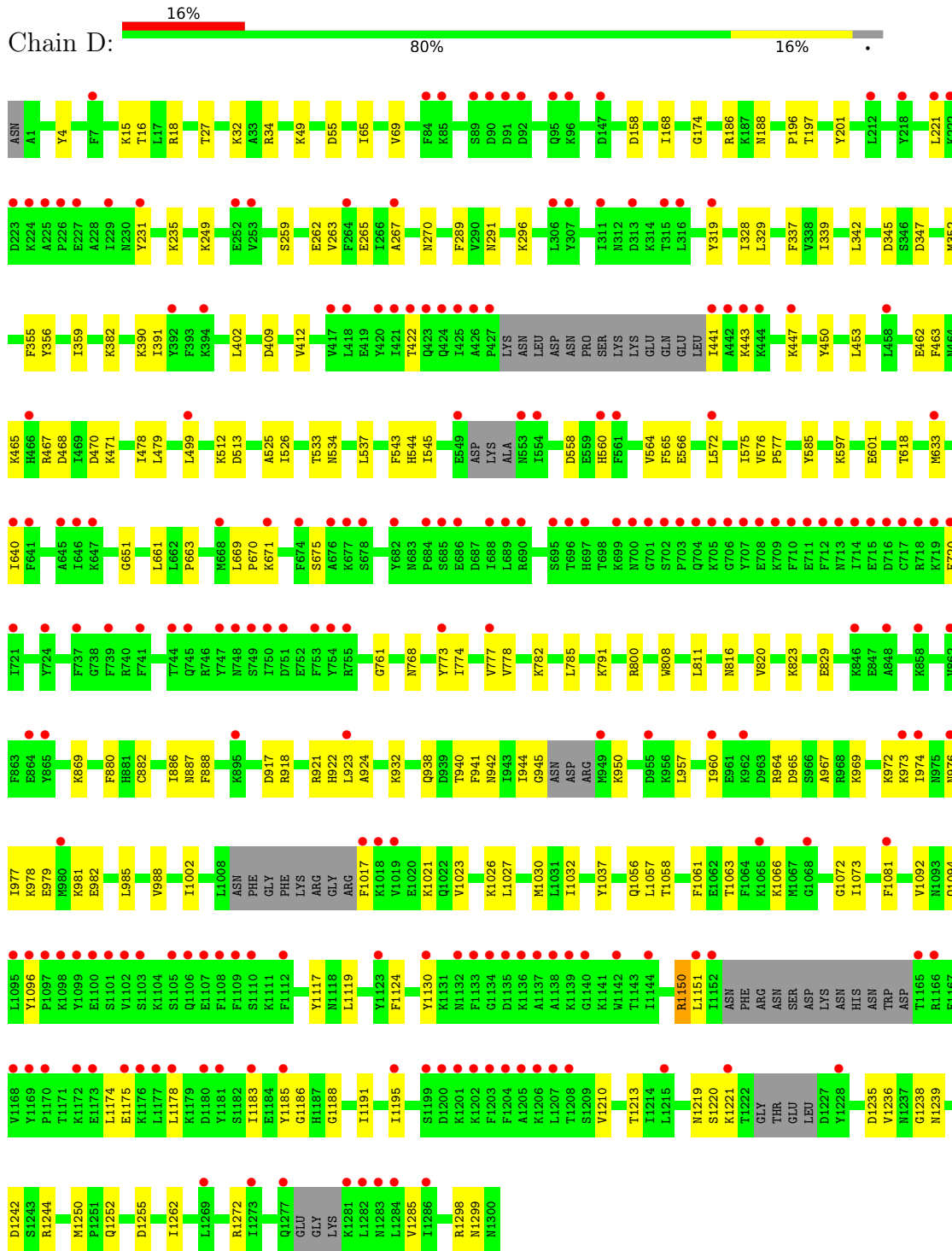
### 3 Residue-property plots [i](#)

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



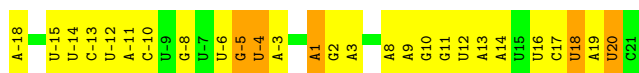
• Molecule 2: crRNA (40-MER)



• Molecule 2: crRNA (40-MER)

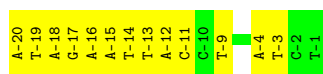


Chain E:  32% 55% 12%



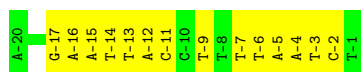
- Molecule 3: ssDNA target strand

Chain C:  35% 65%



- Molecule 3: ssDNA target strand

Chain F:  30% 70%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 97.2 (49.14-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.96Å)	Xtrriage
Refinement program	PHENIX (1.14_3211: ???)	Depositor
R, $R_{free}$	0.204 , 0.231 0.204 , 0.231	Depositor DCC
$R_{free}$ test set	8753 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23637	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CIT, MG, K

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	0.32	0/10758	0.45	0/14440
1	D	0.30	0/10553	0.44	0/14165
2	B	0.45	0/942	0.90	0/1464
2	E	0.37	0/924	0.84	0/1437
3	C	0.74	0/450	1.01	0/692
3	F	0.69	0/450	1.00	0/692
All	All	0.34	0/24077	0.53	0/32890

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	10551	0	10545	118	0
1	D	10351	0	10342	141	0
2	B	843	0	426	16	0
2	E	827	0	414	21	0
3	C	403	0	231	12	0
3	F	403	0	231	17	0
4	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	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	314	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 (314) 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: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
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:D:537:LEU:HB2	1:D:575:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:106:LYS:NZ	1:A:194:ASP:OD1	2.27	0.64
1:D:49:LYS:NZ	1:D:158:ASP:O	2.30	0.63
1:D:981:LYS:HD2	1:D:1023:VAL:HG22	1.81	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: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
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:D:973:LYS:NZ	3:F:-9:DT:OP1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1235:ASP:OD1	1:D:1239:ASN:N	2.37	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:A:965:ASP:OD2	1:A:969:LYS:NZ	2.27	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:A:651:GLY:O	1:A:768:ASN:HB3	2.06	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
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
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:C2'	3:F:-5:DA:H5''	2.40	0.51
3:F:-6:DT:H2'	3:F:-5:DA:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:982:GLU:HG2	1:D:1030:MET:HE1	1.92	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
2:B:-10:C:O2'	2:B:-8:G:N7	2.38	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
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: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:499:LEU:HD21	1:D:525:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:MET:CE	1:D:526:ILE:HG23	2.48	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:1151:LEU:O	1:A:1216:GLN:NE2	2.45	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:1026:LYS:HZ3	3:F:-7:DT:P	2.42	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
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:329:LEU:HD23	1:A:329:LEU:HA	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:782:LYS:HZ3	5:A:1405:CIT:H22	1.86	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
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:342:LEU:HG	1:A:581:LYS:HB3	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	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 [i](#)

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%)	1156 (99%)	7 (1%)	86	94
1	D	1142/1184 (96%)	1139 (100%)	3 (0%)	92	97
All	All	2305/2368 (97%)	2295 (100%)	10 (0%)	91	97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	GLU
1	A	473	CYS
1	A	694	HIS
1	A	804	HIS
1	A	852	LYS
1	A	1014	ARG
1	A	1284	LEU
1	D	720	PHE
1	D	1130	TYR
1	D	1150	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	538	HIS

### 5.3.3 RNA [i](#)

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

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Mol	Chain	Res	Type
2	E	-10	C
2	E	-8	G
2	E	-6	U
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 monosaccharides 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	E	104	-	12,12,12	1.03	0	17,17,17	1.61	2 (11%)
5	CIT	E	102	-	12,12,12	1.01	0	17,17,17	1.70	3 (17%)
5	CIT	E	103	-	12,12,12	0.99	0	17,17,17	1.69	4 (23%)
5	CIT	B	103	-	12,12,12	1.00	0	17,17,17	1.57	2 (11%)
5	CIT	D	1406	-	12,12,12	0.99	0	17,17,17	1.75	1 (5%)
5	CIT	A	1407	-	12,12,12	0.95	0	17,17,17	1.73	2 (11%)
5	CIT	B	102	6	12,12,12	0.97	0	17,17,17	1.96	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CIT	A	1406	-	12,12,12	0.98	0	17,17,17	1.57	2 (11%)
5	CIT	A	1405	-	12,12,12	1.03	0	17,17,17	1.77	4 (23%)
5	CIT	D	1405	6	12,12,12	1.09	0	17,17,17	1.53	3 (17%)
5	CIT	D	1404	-	12,12,12	1.01	0	17,17,17	1.71	4 (23%)

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	E	104	-	-	4/16/16/16	-
5	CIT	E	102	-	-	9/16/16/16	-
5	CIT	E	103	-	-	11/16/16/16	-
5	CIT	B	103	-	-	4/16/16/16	-
5	CIT	D	1406	-	-	4/16/16/16	-
5	CIT	A	1407	-	-	6/16/16/16	-
5	CIT	B	102	6	-	8/16/16/16	-
5	CIT	A	1406	-	-	3/16/16/16	-
5	CIT	A	1405	-	-	11/16/16/16	-
5	CIT	D	1405	6	-	5/16/16/16	-
5	CIT	D	1404	-	-	0/16/16/16	-

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	102	CIT	O6-C6-C3	5.37	122.38	113.05
5	D	1406	CIT	O6-C6-C3	4.94	121.63	113.05
5	A	1407	CIT	O6-C6-C3	4.89	121.55	113.05
5	E	103	CIT	O6-C6-C3	4.73	121.26	113.05
5	E	102	CIT	O6-C6-C3	4.67	121.15	113.05
5	A	1406	CIT	O6-C6-C3	4.54	120.93	113.05
5	A	1405	CIT	O6-C6-C3	4.49	120.84	113.05
5	D	1404	CIT	O6-C6-C3	4.47	120.82	113.05
5	B	103	CIT	O6-C6-C3	4.25	120.43	113.05
5	E	104	CIT	O6-C6-C3	4.13	120.22	113.05
5	D	1405	CIT	O6-C6-C3	3.70	119.48	113.05
5	A	1405	CIT	O2-C1-C2	2.59	122.65	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	102	CIT	O2-C1-C2	2.52	122.45	114.35
5	B	102	CIT	O4-C5-C4	2.42	122.13	114.35
5	E	103	CIT	O4-C5-C4	2.40	122.05	114.35
5	A	1405	CIT	O2-C1-O1	-2.35	117.45	123.30
5	E	104	CIT	C3-C4-C5	-2.32	108.19	113.81
5	D	1404	CIT	O2-C1-C2	2.30	121.75	114.35
5	E	102	CIT	O2-C1-C2	2.28	121.66	114.35
5	B	102	CIT	O2-C1-O1	-2.25	117.68	123.30
5	E	103	CIT	O4-C5-O3	-2.25	117.69	123.30
5	B	102	CIT	O5-C6-C3	-2.21	119.12	122.25
5	B	102	CIT	O4-C5-O3	-2.17	117.90	123.30
5	D	1404	CIT	C3-C4-C5	-2.14	108.64	113.81
5	A	1406	CIT	O5-C6-C3	-2.11	119.27	122.25
5	A	1407	CIT	O4-C5-C4	2.10	121.08	114.35
5	E	103	CIT	O2-C1-O1	-2.08	118.11	123.30
5	B	103	CIT	O2-C1-O1	-2.04	118.20	123.30
5	D	1404	CIT	O2-C1-O1	-2.04	118.21	123.30
5	A	1405	CIT	O4-C5-O3	-2.04	118.22	123.30
5	D	1405	CIT	O4-C5-C4	2.03	120.88	114.35
5	E	102	CIT	O2-C1-O1	-2.02	118.25	123.30
5	D	1405	CIT	O2-C1-C2	2.01	120.80	114.35

There are no chirality outliers.

All (65) 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	C2-C3-C4-C5
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-C4
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

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

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

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	104	CIT	1	0
5	B	103	CIT	1	0
5	D	1406	CIT	1	0
5	A	1406	CIT	1	0
5	A	1405	CIT	2	0
5	D	1405	CIT	1	0
5	D	1404	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1277/1301 (98%)	0.57	96 (7%) 14 7	43, 72, 120, 206	0
1	D	1254/1301 (96%)	0.91	209 (16%) 1 1	52, 90, 166, 207	0
2	B	40/40 (100%)	0.40	0 100 100	48, 56, 96, 192	0
2	E	40/40 (100%)	-0.02	0 100 100	59, 69, 96, 129	0
3	C	20/20 (100%)	-0.05	0 100 100	50, 57, 75, 76	0
3	F	20/20 (100%)	-0.31	0 100 100	63, 74, 97, 99	0
All	All	2651/2722 (97%)	0.71	305 (11%) 4 2	43, 80, 147, 207	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1166	ARG	10.1
1	A	1163	TRP	10.0
1	D	748	ASN	8.6
1	D	1099	TYR	8.6
1	D	1201	LYS	8.3
1	D	750	ILE	8.2
1	D	1204	PHE	8.1
1	D	1200	ASP	7.4
1	D	1203	PHE	7.4
1	D	1205	ALA	7.1
1	D	674	PHE	7.1
1	A	948	ARG	6.9
1	D	716	ASP	6.8
1	D	1101	SER	6.7
1	D	700	ASN	6.6
1	D	1137	ALA	6.6
1	D	749	SER	6.6
1	D	686	GLU	6.4
1	D	1282	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
1	D	1109	PHE	6.1
1	D	1202	LYS	6.1
1	D	745	GLN	6.0
1	D	1138	ALA	6.0
1	D	668	MET	5.8
1	D	227	GLU	5.7
1	D	720	PHE	5.6
1	D	1199	SER	5.6
1	D	1176	LYS	5.5
1	D	1100	GLU	5.5
1	D	1133	PHE	5.4
1	D	1102	VAL	5.3
1	D	712	PHE	5.2
1	D	226	PRO	5.2
1	D	1169	TYR	5.0
1	D	1108	PHE	4.9
1	D	697	HIS	4.9
1	D	92	ASP	4.8
1	D	754	TYR	4.7
1	D	447	LYS	4.7
1	A	151	GLU	4.6
1	D	1165	THR	4.6
1	D	425	ILE	4.6
1	D	1106	GLN	4.6
1	A	96	LYS	4.5
1	D	724	TYR	4.5
1	D	444	LYS	4.5
1	A	947	ASP	4.5
1	D	747	TYR	4.5
1	D	315	THR	4.5
1	D	696	THR	4.5
1	A	85	LYS	4.5
1	D	1281	LYS	4.4
1	A	708	GLU	4.4
1	D	737	PHE	4.3
1	D	751	ASP	4.3
1	A	149	GLY	4.3
1	D	1134	GLY	4.3
1	D	690	ARG	4.3
1	D	441	ILE	4.3
1	D	1152	ILE	4.2
1	D	1283	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	1207	LEU	4.2
1	D	974	ILE	4.2
1	A	95	GLN	4.1
1	A	1282	LEU	4.1
1	D	699	LYS	4.1
1	D	677	LYS	4.1
1	D	307	TYR	4.0
1	D	443	LYS	3.9
1	D	701	GLY	3.9
1	D	1130	TYR	3.9
1	D	427	PRO	3.9
1	A	86	LEU	3.9
1	D	744	THR	3.9
1	D	1206	LYS	3.9
1	D	1136	LYS	3.9
1	D	1135	ASP	3.8
1	D	704	GLN	3.8
1	A	860	GLU	3.8
1	D	682	TYR	3.8
1	D	955	ASP	3.7
1	D	1208	THR	3.7
1	D	89	SER	3.7
1	D	418	LEU	3.7
1	D	424	GLN	3.7
1	D	688	ILE	3.7
1	D	1132	ASN	3.7
1	A	94	LEU	3.7
1	D	229	ILE	3.6
1	D	421	ILE	3.6
1	D	1181	TYR	3.6
1	D	1269	LEU	3.6
1	D	707	TYR	3.6
1	D	676	ALA	3.6
1	A	447	LYS	3.5
1	A	436	LYS	3.5
1	D	715	GLU	3.5
1	D	711	GLU	3.4
1	D	1018	LYS	3.4
1	D	311	ILE	3.4
1	D	1151	LEU	3.4
1	A	79	TYR	3.4
1	D	713	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	1177	LEU	3.4
1	D	1105	SER	3.4
1	D	895	LYS	3.4
1	A	1098	LYS	3.3
1	D	1195	ILE	3.3
1	D	1065	LYS	3.3
1	A	747	TYR	3.3
1	D	755	ARG	3.3
1	D	646	ILE	3.3
1	D	1168	VAL	3.3
1	A	859	LYS	3.3
1	D	253	VAL	3.2
1	D	1098	LYS	3.2
1	A	717	CYS	3.2
1	D	91	ASP	3.2
1	A	98	PHE	3.2
1	D	739	PHE	3.2
1	D	702	SER	3.2
1	D	1068	GLY	3.2
1	A	741	PHE	3.2
1	D	1103	SER	3.2
1	D	90	ASP	3.2
1	D	316	LEU	3.2
1	D	466	HIS	3.2
1	A	439	GLU	3.1
1	D	572	LEU	3.1
1	A	450	TYR	3.1
1	D	1170	PRO	3.1
1	A	950	LYS	3.1
1	A	1275	ASN	3.1
1	D	423	GLN	3.1
1	A	82	VAL	3.0
1	D	1107	GLU	3.0
1	A	84	PHE	3.0
1	D	1284	LEU	3.0
1	A	920	GLU	3.0
1	A	1281	LYS	3.0
1	D	222	LYS	3.0
1	D	420	TYR	3.0
1	A	1226	LEU	3.0
1	D	313	ASP	3.0
1	A	1021	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	303	TYR	2.9
1	A	92	ASP	2.9
1	A	749	SER	2.9
1	D	231	TYR	2.9
1	D	714	ILE	2.9
1	A	321	MET	2.9
1	D	1173	GLU	2.9
1	D	717	CYS	2.9
1	A	93	ASN	2.9
1	D	976	ASN	2.9
1	D	1221	LYS	2.9
1	D	1139	LYS	2.9
1	D	1142	TRP	2.8
1	D	96	LYS	2.8
1	D	225	ALA	2.8
1	D	721	ILE	2.8
1	D	923	LEU	2.8
1	D	705	LYS	2.8
1	D	641	PHE	2.8
1	D	1183	ILE	2.8
1	A	1008	LEU	2.8
1	A	99	LYS	2.8
1	A	1298	ARG	2.7
1	A	904	LEU	2.7
1	D	252	GLU	2.7
1	D	85	LYS	2.7
1	D	1185	TYR	2.7
1	D	1228	TYR	2.7
1	A	932	LYS	2.7
1	D	773	TYR	2.7
1	D	1178	LEU	2.7
1	D	84	PHE	2.7
1	D	865	TYR	2.7
1	D	949	MET	2.6
1	A	721	ILE	2.6
1	D	306	LEU	2.6
1	D	685	SER	2.6
1	D	422	THR	2.6
1	D	1112	PHE	2.6
1	A	1284	LEU	2.6
1	D	695	SER	2.6
1	D	224	LYS	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	78	ASN	2.6
1	D	442	ALA	2.6
1	D	1095	LEU	2.6
1	A	495	ASN	2.6
1	A	221	LEU	2.6
1	A	906	GLU	2.6
1	D	1180	ASP	2.6
1	D	741	PHE	2.6
1	A	737	PHE	2.5
1	D	7	PHE	2.5
1	D	1215	LEU	2.5
1	A	748	ASN	2.5
1	D	95	GLN	2.5
1	D	554	ILE	2.5
1	D	499	LEU	2.5
1	D	678	SER	2.5
1	D	703	PRO	2.5
1	D	1175	GLU	2.5
1	A	1014	ARG	2.5
1	D	223	ASP	2.5
1	A	435	LYS	2.5
1	D	319	TYR	2.5
1	D	458	LEU	2.5
1	D	553	ASN	2.5
1	A	83	TYR	2.4
1	A	674	PHE	2.4
1	D	1019	VAL	2.4
1	D	1110	SER	2.4
1	A	451	LEU	2.4
1	A	714	ILE	2.4
1	A	944	ILE	2.4
1	A	307	TYR	2.4
1	A	712	PHE	2.4
1	D	1273	ILE	2.4
1	A	333	GLU	2.3
1	D	1017	PHE	2.3
1	D	264	PHE	2.3
1	A	746	ARG	2.3
1	D	862	VAL	2.3
1	A	751	ASP	2.3
1	D	267	ALA	2.3
1	D	426	ALA	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	549	GLU	2.3
1	D	753	PHE	2.3
1	D	417	VAL	2.3
1	D	1097	PRO	2.3
1	A	456	ILE	2.3
1	D	1277	GLN	2.3
1	D	1123	TYR	2.3
1	D	710	PHE	2.3
1	D	973	LYS	2.3
1	D	1172	LYS	2.3
1	A	316	LEU	2.3
1	A	418	LEU	2.3
1	A	740	ARG	2.3
1	D	645	ALA	2.3
1	A	696	THR	2.3
1	A	1299	ASN	2.3
1	D	647	LYS	2.3
1	A	694	HIS	2.3
1	A	921	ARG	2.3
1	D	560	HIS	2.3
1	D	640	ILE	2.3
1	D	561	PHE	2.3
1	A	1195	ILE	2.2
1	D	960	ILE	2.2
1	D	980	MET	2.2
1	A	699	LYS	2.2
1	A	743	ASP	2.2
1	D	858	LYS	2.2
1	D	1096	TYR	2.2
1	A	555	LEU	2.2
1	A	688	ILE	2.2
1	A	739	PHE	2.2
1	A	753	PHE	2.2
1	D	221	LEU	2.2
1	D	706	GLY	2.2
1	A	710	PHE	2.2
1	D	633	MET	2.2
1	A	1154	PHE	2.2
1	D	392	TYR	2.2
1	D	1140	GLY	2.2
1	D	848	ALA	2.2
1	A	962	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	662	LEU	2.2
1	A	1273	ILE	2.2
1	A	132	LYS	2.2
1	A	431	ASP	2.1
1	D	689	LEU	2.1
1	D	212	LEU	2.1
1	D	846	LYS	2.1
1	D	1286	ILE	2.1
1	A	698	THR	2.1
1	A	752	GLU	2.1
1	A	75	LEU	2.1
1	D	218	TYR	2.1
1	D	1081	PHE	2.1
1	A	750	ILE	2.1
1	D	708	GLU	2.1
1	D	864	GLU	2.1
1	D	718	ARG	2.1
1	D	1144	ILE	2.1
1	D	709	LYS	2.0
1	D	719	LYS	2.0
1	D	777	VAL	2.0
1	A	1007	ASP	2.0
1	D	147	ASP	2.0
1	D	671	LYS	2.0
1	A	433	PRO	2.0
1	A	1297	ASN	2.0
1	A	438	GLN	2.0
1	D	394	LYS	2.0
1	A	152	LEU	2.0
1	D	684	PRO	2.0
1	A	646	ILE	2.0
1	A	849	ILE	2.0
1	A	1100	GLU	2.0
1	D	962	LYS	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	MG	B	101	1/1	0.16	0.32	85,85,85,85	0
4	MG	D	1402	1/1	0.41	0.19	86,86,86,86	0
5	CIT	E	103	13/13	0.53	0.52	116,116,116,116	0
4	MG	A	1404	1/1	0.60	0.14	78,78,78,78	0
4	MG	A	1401	1/1	0.63	0.08	74,74,74,74	0
5	CIT	E	104	13/13	0.67	0.39	131,131,131,131	0
6	K	D	1411	1/1	0.68	0.51	126,126,126,126	0
5	CIT	D	1406	13/13	0.72	0.38	112,112,112,112	0
5	CIT	A	1406	13/13	0.72	0.48	96,96,96,96	0
4	MG	A	1402	1/1	0.73	0.13	70,70,70,70	0
6	K	E	105	1/1	0.76	0.41	106,106,106,106	0
4	MG	D	1401	1/1	0.77	0.08	86,86,86,86	0
4	MG	D	1403	1/1	0.77	0.23	103,103,103,103	0
6	K	A	1411	1/1	0.80	0.26	106,106,106,106	0
6	K	A	1412	1/1	0.81	0.15	102,102,102,102	0
6	K	D	1408	1/1	0.81	0.34	93,93,93,93	0
5	CIT	A	1405	13/13	0.82	0.36	95,95,95,95	0
5	CIT	E	102	13/13	0.84	0.24	98,98,98,98	0
5	CIT	D	1404	13/13	0.85	0.52	110,110,110,110	0
5	CIT	A	1407	13/13	0.86	0.22	85,85,85,85	0
6	K	D	1410	1/1	0.86	0.14	108,108,108,108	0
4	MG	A	1403	1/1	0.88	0.17	95,95,95,95	0
5	CIT	B	103	13/13	0.88	0.79	112,112,112,112	0
6	K	D	1409	1/1	0.88	0.47	109,109,109,109	0
6	K	D	1407	1/1	0.89	0.35	104,104,104,104	0
5	CIT	B	102	13/13	0.89	0.25	79,79,79,79	0
6	K	A	1408	1/1	0.89	0.25	95,95,95,95	0
6	K	A	1409	1/1	0.90	0.18	94,94,94,94	0
5	CIT	D	1405	13/13	0.91	0.19	89,89,89,89	0
4	MG	E	101	1/1	0.92	0.12	91,91,91,91	0
6	K	B	104	1/1	0.94	0.34	81,81,81,81	0
6	K	A	1410	1/1	0.96	0.30	84,84,84,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.