Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 02:51 PM JST

PDB ID	:	7CR6
Title	:	Synechocystis Cas1-Cas2/prespacer binary complex
Authors	:	Yu, Y.; Chen, Q.
Deposited on	:	2020-08-12
Resolution	:	3.72 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:

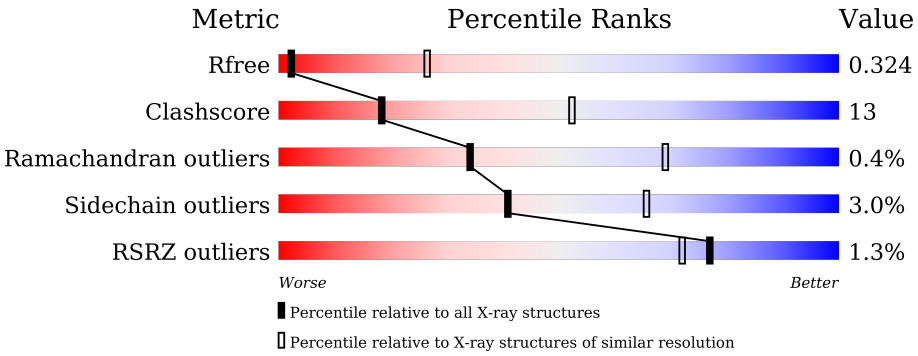
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.72 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	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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 <=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	336	2% 74% 21%
1	B	336	66% 29%
1	C	336	66% 29%
1	D	336	69% 23% 7%
2	E	105	2% 66% 21% 12%
2	F	105	67% 21% 12%

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Mol	Chain	Length	Quality of chain
3	G	36	3% 8% 64% 28%
4	H	36	19% 50% 31%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24088 atoms, of which 11235 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 Cas1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	322	Total	C	H	N	O	S	0	0	0
			5072	1661	2484	462	460	5			
1	B	323	Total	C	H	N	O	S	0	0	0
			5038	1663	2445	461	464	5			
1	C	325	Total	C	H	N	O	S	0	0	0
			4966	1674	2354	466	466	6			
1	D	313	Total	C	H	N	O	S	0	0	0
			4970	1622	2445	451	447	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP Q6ZEI2
A	-9	ALA	-	expression tag	UNP Q6ZEI2
A	-8	SER	-	expression tag	UNP Q6ZEI2
A	-7	GLY	-	expression tag	UNP Q6ZEI2
A	-6	SER	-	expression tag	UNP Q6ZEI2
A	-5	GLY	-	expression tag	UNP Q6ZEI2
A	-4	THR	-	expression tag	UNP Q6ZEI2
A	-3	GLY	-	expression tag	UNP Q6ZEI2
A	-2	SER	-	expression tag	UNP Q6ZEI2
A	-1	GLY	-	expression tag	UNP Q6ZEI2
A	0	SER	-	expression tag	UNP Q6ZEI2
B	-10	GLY	-	expression tag	UNP Q6ZEI2
B	-9	ALA	-	expression tag	UNP Q6ZEI2
B	-8	SER	-	expression tag	UNP Q6ZEI2
B	-7	GLY	-	expression tag	UNP Q6ZEI2
B	-6	SER	-	expression tag	UNP Q6ZEI2
B	-5	GLY	-	expression tag	UNP Q6ZEI2
B	-4	THR	-	expression tag	UNP Q6ZEI2
B	-3	GLY	-	expression tag	UNP Q6ZEI2
B	-2	SER	-	expression tag	UNP Q6ZEI2
B	-1	GLY	-	expression tag	UNP Q6ZEI2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP Q6ZEI2
C	-10	GLY	-	expression tag	UNP Q6ZEI2
C	-9	ALA	-	expression tag	UNP Q6ZEI2
C	-8	SER	-	expression tag	UNP Q6ZEI2
C	-7	GLY	-	expression tag	UNP Q6ZEI2
C	-6	SER	-	expression tag	UNP Q6ZEI2
C	-5	GLY	-	expression tag	UNP Q6ZEI2
C	-4	THR	-	expression tag	UNP Q6ZEI2
C	-3	GLY	-	expression tag	UNP Q6ZEI2
C	-2	SER	-	expression tag	UNP Q6ZEI2
C	-1	GLY	-	expression tag	UNP Q6ZEI2
C	0	SER	-	expression tag	UNP Q6ZEI2
D	-10	GLY	-	expression tag	UNP Q6ZEI2
D	-9	ALA	-	expression tag	UNP Q6ZEI2
D	-8	SER	-	expression tag	UNP Q6ZEI2
D	-7	GLY	-	expression tag	UNP Q6ZEI2
D	-6	SER	-	expression tag	UNP Q6ZEI2
D	-5	GLY	-	expression tag	UNP Q6ZEI2
D	-4	THR	-	expression tag	UNP Q6ZEI2
D	-3	GLY	-	expression tag	UNP Q6ZEI2
D	-2	SER	-	expression tag	UNP Q6ZEI2
D	-1	GLY	-	expression tag	UNP Q6ZEI2
D	0	SER	-	expression tag	UNP Q6ZEI2

- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	92	Total	C	H	N	O	S	0	0	0
			1494	485	748	123	135	3			
2	F	92	Total	C	H	N	O	S	0	0	0
			1505	485	759	123	135	3			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	GLY	-	expression tag	UNP Q6ZEI1
E	-9	ALA	-	expression tag	UNP Q6ZEI1
E	-8	SER	-	expression tag	UNP Q6ZEI1
E	-7	GLY	-	expression tag	UNP Q6ZEI1
E	-6	SER	-	expression tag	UNP Q6ZEI1
E	-5	GLY	-	expression tag	UNP Q6ZEI1
E	-4	THR	-	expression tag	UNP Q6ZEI1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP Q6ZEI1
E	-2	SER	-	expression tag	UNP Q6ZEI1
E	-1	GLY	-	expression tag	UNP Q6ZEI1
E	0	SER	-	expression tag	UNP Q6ZEI1
F	-10	GLY	-	expression tag	UNP Q6ZEI1
F	-9	ALA	-	expression tag	UNP Q6ZEI1
F	-8	SER	-	expression tag	UNP Q6ZEI1
F	-7	GLY	-	expression tag	UNP Q6ZEI1
F	-6	SER	-	expression tag	UNP Q6ZEI1
F	-5	GLY	-	expression tag	UNP Q6ZEI1
F	-4	THR	-	expression tag	UNP Q6ZEI1
F	-3	GLY	-	expression tag	UNP Q6ZEI1
F	-2	SER	-	expression tag	UNP Q6ZEI1
F	-1	GLY	-	expression tag	UNP Q6ZEI1
F	0	SER	-	expression tag	UNP Q6ZEI1

- Molecule 3 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	26	Total	C	N	O	P	0	0	0
			526	252	81	167	26			

- Molecule 4 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	25	Total	C	N	O	P	0	0	0
			516	243	102	146	25			

- Molecule 5 is water.

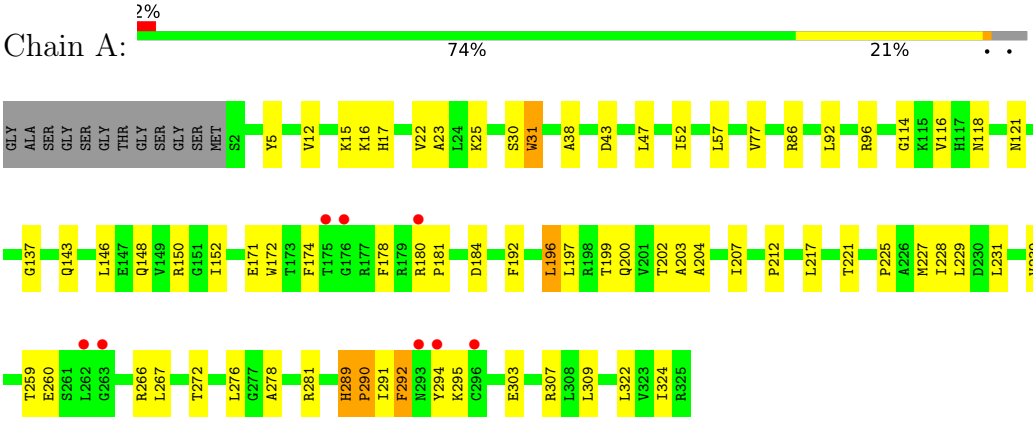
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		

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.

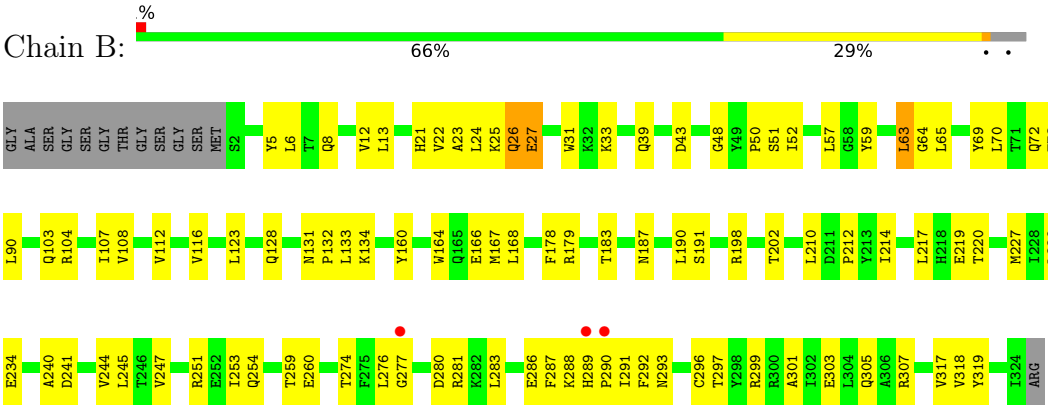
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain A:



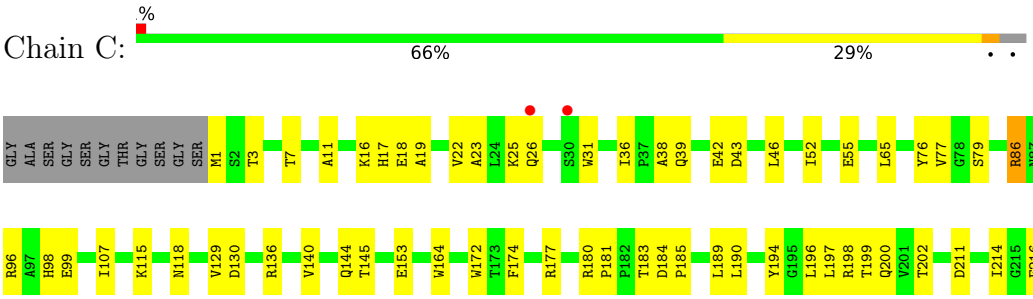
• Molecule 1: CRISPR-associated endonuclease Cas1

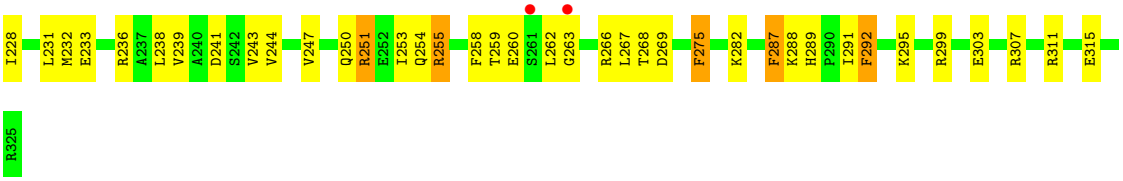
Chain B:



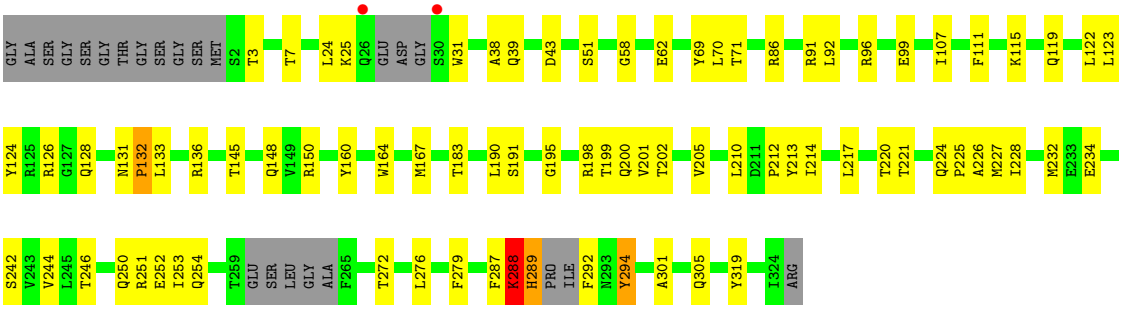
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain C:



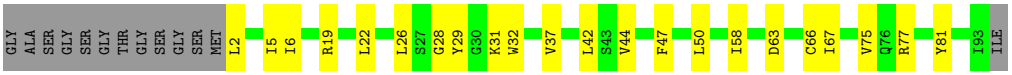


• Molecule 1: CRISPR-associated endonuclease Cas1

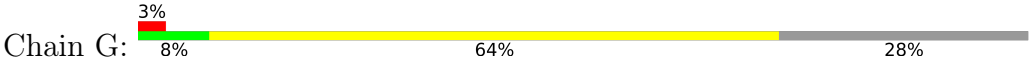


• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

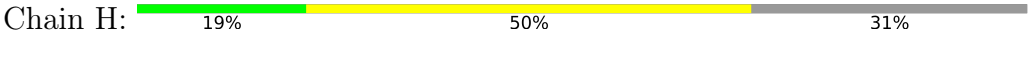
• Molecule 2: CRISPR-associated endoribonuclease Cas2 1

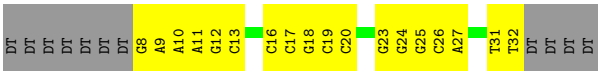


• Molecule 3: DNA (36-MER)



• Molecule 4: DNA (36-MER)





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	125.56Å 215.16Å 191.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.81 – 3.72 33.81 – 3.72	Depositor EDS
% Data completeness (in resolution range)	91.9 (33.81-3.72) 92.0 (33.81-3.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 3.76Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.276 , 0.324 0.276 , 0.324	Depositor DCC
R_{free} test set	1058 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 23.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.022 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.035 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	24088	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.25	0/2646	0.49	0/3577
1	B	0.26	0/2652	0.49	0/3589
1	C	0.25	0/2671	0.49	0/3613
1	D	0.25	0/2580	0.47	0/3486
2	E	0.25	0/761	0.46	0/1028
2	F	0.25	0/761	0.51	0/1028
3	G	0.47	0/584	0.97	0/899
4	H	0.49	0/580	0.80	0/893
All	All	0.28	0/13235	0.54	0/18113

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	288	LYS	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2588	2484	2621	48	0
1	B	2593	2445	2618	82	1
1	C	2612	2354	2643	82	1
1	D	2525	2445	2554	70	0
2	E	746	748	767	25	0
2	F	746	759	767	14	0
3	G	526	0	298	29	0
4	H	516	0	279	17	0
5	A	1	0	0	0	0
All	All	12853	11235	12547	337	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 13.

All (337) 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)
4:H:12:DG:H2"	4:H:13:DC:H5"	1.31	1.07
1:B:25:LYS:HD2	1:B:25:LYS:O	1.63	0.97
1:D:288:LYS:HD2	1:D:289:HIS:H	1.34	0.90
1:C:46:LEU:HD21	1:C:52:ILE:HD11	1.52	0.90
1:B:25:LYS:HE2	1:B:31:TRP:HE1	1.36	0.90
1:C:99:GLU:OE2	1:D:96:ARG:NH1	2.06	0.89
1:D:24:LEU:HD23	1:D:25:LYS:H	1.37	0.88
1:C:288:LYS:HE2	1:C:295:LYS:HE3	1.55	0.87
1:C:43:ASP:OD2	1:C:200:GLN:NE2	2.06	0.87
1:D:150:ARG:NH2	1:D:217:LEU:O	2.09	0.85
1:C:254:GLN:OE1	1:C:255:ARG:N	2.09	0.85
1:D:201:VAL:O	1:D:205:VAL:HG23	1.79	0.82
1:B:303:GLU:OE2	1:B:307:ARG:NH1	2.14	0.81
1:B:25:LYS:O	1:B:26:GLN:HG2	1.80	0.81
1:B:234:GLU:OE2	1:B:319:TYR:OH	1.97	0.80
1:C:253:ILE:HD12	1:C:254:GLN:H	1.46	0.80
1:C:255:ARG:HG2	1:C:255:ARG:O	1.82	0.78
1:A:143:GLN:NE2	1:A:148:GLN:OE1	2.17	0.78
1:D:212:PRO:HA	1:D:227:MET:HB3	1.64	0.78
1:D:123:LEU:HD12	1:D:132:PRO:HB3	1.66	0.76
1:C:253:ILE:HD12	1:C:254:GLN:N	2.02	0.74
1:C:288:LYS:HA	1:C:295:LYS:HA	1.70	0.73
1:A:260:GLU:N	1:A:260:GLU:OE1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:ARG:NH1	2:F:66:CYS:SG	2.62	0.73
1:C:211:ASP:OD1	1:D:91:ARG:NH1	2.22	0.73
4:H:12:DG:C2'	4:H:13:DC:H5"	2.14	0.73
1:C:115:LYS:NZ	1:C:153:GLU:OE1	2.23	0.71
1:D:288:LYS:HD2	1:D:289:HIS:N	2.06	0.70
1:B:241:ASP:O	1:B:245:LEU:HD13	1.90	0.70
1:C:262:LEU:HD13	1:C:262:LEU:O	1.91	0.70
1:B:25:LYS:O	1:B:26:GLN:CG	2.39	0.70
1:B:43:ASP:OD2	1:B:307:ARG:NH2	2.24	0.70
1:C:46:LEU:HD21	1:C:52:ILE:CD1	2.21	0.70
1:A:114:GLY:O	1:A:118:ASN:ND2	2.25	0.70
1:A:303:GLU:OE2	1:A:307:ARG:NH2	2.25	0.70
1:B:253:ILE:HG22	1:B:254:GLN:H	1.55	0.70
1:C:303:GLU:OE2	1:C:307:ARG:NH2	2.24	0.69
1:D:198:ARG:O	1:D:202:THR:OG1	2.09	0.69
3:G:9:DG:H2'	3:G:10:DT:H72	1.74	0.69
1:D:288:LYS:O	1:D:289:HIS:HB2	1.92	0.68
4:H:10:DA:H2'	4:H:11:DA:C8	2.28	0.68
1:C:190:LEU:O	1:C:194:TYR:N	2.27	0.68
1:B:212:PRO:HA	1:B:227:MET:HB3	1.75	0.67
1:C:236:ARG:O	1:C:241:ASP:HB2	1.95	0.67
1:D:24:LEU:CD2	1:D:25:LYS:H	2.07	0.67
2:E:7:TYR:OH	3:G:21:DG:OP1	2.10	0.67
1:B:51:SER:OG	4:H:9:DA:H5'	1.95	0.66
1:B:128:GLN:NE2	1:B:166:GLU:OE1	2.29	0.66
3:G:15:DC:H2"	3:G:16:DT:H71	1.78	0.66
1:D:288:LYS:HG2	1:D:294:TYR:CB	2.26	0.65
1:C:189:LEU:HD22	1:C:244:VAL:HG13	1.77	0.65
1:C:55:GLU:N	1:C:55:GLU:OE1	2.29	0.65
2:E:9:VAL:HG12	2:E:10:PRO:HD2	1.78	0.65
1:B:164:TRP:O	1:B:168:LEU:HD12	1.97	0.65
1:B:198:ARG:HB2	1:B:232:MET:HE1	1.79	0.64
1:C:260:GLU:HB2	1:C:266:ARG:NH2	2.11	0.64
2:F:29:TYR:CG	2:F:50:LEU:HD12	2.33	0.64
1:C:1:MET:HB3	1:C:42:GLU:OE1	1.98	0.64
1:A:22:VAL:HG11	2:E:93:ILE:CD1	2.28	0.63
1:C:197:LEU:HG	1:C:232:MET:HG3	1.81	0.63
1:C:190:LEU:CD2	1:C:244:VAL:HG21	2.29	0.62
1:C:287:PHE:CE1	1:C:289:HIS:HA	2.34	0.62
2:E:88:LYS:H	2:E:88:LYS:HD3	1.64	0.62
1:B:259:THR:HG22	1:B:260:GLU:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:12:DC:H2"	3:G:13:DC:O5'	2.00	0.62
1:D:25:LYS:O	1:D:31:TRP:HB2	1.99	0.61
1:C:196:LEU:O	1:C:199:THR:HG22	1.99	0.61
3:G:25:DC:H2'	3:G:26:DT:C7	2.30	0.60
1:B:73:PHE:HB2	3:G:30:DT:H2'	1.82	0.60
1:D:288:LYS:HG3	1:D:292:PHE:O	2.02	0.60
1:B:190:LEU:HD12	1:B:244:VAL:HG21	1.83	0.60
2:E:2:LEU:N	2:E:70:LEU:O	2.34	0.60
1:A:25:LYS:HG2	1:A:30:SER:HB2	1.84	0.59
1:B:288:LYS:HE3	1:B:292:PHE:HB3	1.85	0.59
2:E:88:LYS:HD3	2:E:88:LYS:N	2.17	0.59
1:A:180:ARG:HG3	1:A:181:PRO:HD3	1.85	0.59
1:D:287:PHE:O	1:D:288:LYS:HB2	2.00	0.59
2:E:11:ALA:HB2	3:G:19:DC:H6	1.68	0.59
3:G:18:DG:N2	4:H:20:DC:O2	2.37	0.58
1:C:17:HIS:CE1	3:G:10:DT:H3'	2.39	0.58
1:D:160:TYR:O	1:D:164:TRP:NE1	2.38	0.57
1:B:214:ILE:O	1:B:227:MET:HE2	2.05	0.57
1:A:77:VAL:O	1:B:83:SER:N	2.37	0.56
1:B:108:VAL:HG22	1:B:217:LEU:HB2	1.87	0.56
1:A:197:LEU:HD13	1:A:239:VAL:HG21	1.88	0.56
1:B:8:GLN:HE22	1:B:25:LYS:HG2	1.71	0.56
2:E:51:GLN:OE1	2:F:81:TYR:OH	2.23	0.56
1:A:43:ASP:OD2	1:A:200:GLN:NE2	2.38	0.56
1:A:121:ASN:ND2	1:A:324:ILE:O	2.35	0.55
1:B:25:LYS:CE	1:B:31:TRP:HE1	2.14	0.55
1:A:12:VAL:HG12	1:A:23:ALA:HB3	1.87	0.55
1:D:183:THR:O	1:D:183:THR:HG22	2.06	0.55
1:B:191:SER:O	3:G:32:DT:H73	2.07	0.55
1:B:164:TRP:O	1:B:167:MET:N	2.37	0.54
2:E:34:GLN:NE2	2:E:83:THR:HG21	2.22	0.54
1:B:69:TYR:C	1:B:70:LEU:HD12	2.27	0.54
1:D:224:GLN:O	1:D:226:ALA:N	2.40	0.54
3:G:25:DC:H2'	3:G:26:DT:H71	1.90	0.54
1:C:288:LYS:CE	1:C:295:LYS:HE3	2.34	0.53
1:D:288:LYS:CB	1:D:294:TYR:H	2.20	0.53
1:A:196:LEU:O	1:A:199:THR:HG22	2.08	0.53
1:C:266:ARG:HG3	1:C:267:LEU:O	2.09	0.53
1:C:250:GLN:N	1:C:250:GLN:OE1	2.42	0.53
1:C:259:THR:OG1	1:C:263:GLY:O	2.18	0.53
1:C:38:ALA:O	1:C:65:LEU:HD11	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:GLU:HA	1:C:260:GLU:OE1	2.08	0.53
1:C:287:PHE:HE1	1:C:289:HIS:HA	1.74	0.52
1:C:214:ILE:O	1:C:227:MET:HG2	2.10	0.52
1:C:221:THR:HG22	1:C:221:THR:O	2.09	0.52
4:H:16:DC:H2"	4:H:17:DC:O5'	2.09	0.52
1:C:190:LEU:HD22	1:C:244:VAL:HG21	1.92	0.52
1:D:220:THR:O	1:D:221:THR:HG23	2.08	0.52
1:D:253:ILE:HG22	1:D:254:GLN:H	1.74	0.52
4:H:18:DG:H2"	4:H:19:DC:O5'	2.09	0.52
1:A:244:VAL:HA	1:A:247:VAL:HG22	1.89	0.52
1:B:6:LEU:HD12	1:B:13:LEU:HD11	1.91	0.52
1:C:76:TYR:OH	1:C:79:SER:OG	2.12	0.52
1:D:234:GLU:OE2	1:D:319:TYR:OH	2.28	0.52
4:H:24:DG:H2"	4:H:25:DG:O5'	2.10	0.52
1:A:192:PHE:CE2	1:A:196:LEU:HD21	2.45	0.52
4:H:17:DC:H2"	4:H:18:DG:C8	2.44	0.52
1:B:178:PHE:N	1:B:187:ASN:OD1	2.39	0.52
1:C:136:ARG:O	1:C:140:VAL:HG23	2.09	0.52
1:C:288:LYS:HE2	1:C:295:LYS:CE	2.32	0.51
1:A:272:THR:O	1:A:276:LEU:HG	2.11	0.51
1:B:296:CYS:SG	1:B:297:THR:N	2.82	0.51
2:F:5:ILE:HD13	2:F:26:LEU:HD21	1.92	0.51
1:A:5:TYR:CG	1:A:276:LEU:HD13	2.45	0.51
1:A:203:ALA:O	1:A:207:ILE:HG13	2.11	0.51
2:F:50:LEU:HD23	2:F:50:LEU:C	2.31	0.51
1:B:291:ILE:O	1:B:291:ILE:HG22	2.10	0.51
1:D:7:THR:O	1:D:7:THR:HG22	2.11	0.51
3:G:13:DC:C2'	3:G:14:DC:H5'	2.41	0.50
1:B:59:TYR:O	1:B:63:LEU:HD23	2.10	0.50
1:C:259:THR:O	1:C:260:GLU:HG2	2.10	0.50
1:C:289:HIS:CE1	1:C:291:ILE:HD12	2.47	0.50
1:D:69:TYR:O	1:D:70:LEU:HD12	2.10	0.50
1:C:94:GLN:HE21	1:C:227:MET:HG3	1.75	0.50
1:D:225:PRO:HB2	1:D:228:ILE:HD12	1.91	0.50
2:E:92:ILE:O	2:E:93:ILE:HG23	2.11	0.50
1:B:22:VAL:HG12	1:B:24:LEU:HD12	1.93	0.50
1:C:19:ALA:HB2	2:F:28:GLY:CA	2.42	0.50
1:B:6:LEU:CD1	1:B:13:LEU:HD11	2.41	0.50
1:A:259:THR:O	1:A:259:THR:HG22	2.11	0.50
1:D:51:SER:OG	3:G:8:DT:OP1	2.25	0.50
1:B:5:TYR:OH	1:B:303:GLU:OE1	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD11	1:B:210:LEU:HD23	1.94	0.50
1:D:133:LEU:HD23	1:D:136:ARG:HG3	1.94	0.50
3:G:19:DC:H2"	3:G:20:DG:O5'	2.11	0.50
2:E:9:VAL:HG12	2:E:10:PRO:CD	2.42	0.49
1:A:289:HIS:CD2	1:A:290:PRO:HD2	2.47	0.49
1:B:22:VAL:CG1	1:B:24:LEU:HD12	2.42	0.49
1:A:150:ARG:NH2	1:A:217:LEU:O	2.45	0.49
1:A:116:VAL:HG21	1:A:137:GLY:HA2	1.94	0.49
1:B:103:GLN:O	1:B:107:ILE:HD12	2.12	0.49
1:C:7:THR:HG22	1:C:7:THR:O	2.13	0.49
1:B:39:GLN:O	1:B:39:GLN:NE2	2.46	0.49
1:C:95:PHE:HA	1:C:98:HIS:HB3	1.95	0.49
1:A:52:ILE:HG21	1:A:57:LEU:HD13	1.95	0.49
1:B:198:ARG:CB	1:B:232:MET:HE1	2.43	0.49
1:C:289:HIS:HE1	1:C:291:ILE:HD12	1.77	0.49
1:D:128:GLN:OE1	1:D:167:MET:HB2	2.13	0.49
1:B:52:ILE:HD13	1:B:57:LEU:HD11	1.95	0.49
1:D:253:ILE:HG22	1:D:254:GLN:N	2.27	0.48
1:C:94:GLN:NE2	1:C:227:MET:HG3	2.28	0.48
1:C:43:ASP:OD1	1:C:43:ASP:N	2.43	0.48
1:A:92:LEU:O	1:A:96:ARG:HG3	2.13	0.48
1:D:115:LYS:NZ	1:D:119:GLN:OE1	2.45	0.48
1:B:220:THR:HG23	1:B:220:THR:O	2.13	0.48
1:C:311:ARG:O	1:C:315:GLU:N	2.37	0.48
1:D:221:THR:O	1:D:224:GLN:N	2.45	0.48
2:F:2:LEU:HD13	2:F:75:VAL:HG11	1.95	0.48
3:G:11:DG:H2"	3:G:12:DC:C6	2.49	0.48
1:B:317:VAL:HG12	1:B:318:VAL:N	2.29	0.48
1:D:69:TYR:C	1:D:70:LEU:HD12	2.34	0.48
1:A:212:PRO:HA	1:A:227:MET:HB3	1.95	0.48
1:A:289:HIS:CD2	1:A:322:LEU:HD11	2.48	0.48
1:B:259:THR:HG22	1:B:260:GLU:N	2.26	0.48
1:C:1:MET:O	1:C:1:MET:HG3	2.12	0.48
1:B:164:TRP:CZ3	1:B:245:LEU:HD11	2.49	0.48
1:B:198:ARG:O	1:B:202:THR:OG1	2.20	0.48
1:B:240:ALA:O	1:B:244:VAL:HG23	2.13	0.48
2:F:44:VAL:O	2:F:47:PHE:N	2.46	0.47
3:G:11:DG:H4'	3:G:11:DG:OP1	2.14	0.47
1:D:107:ILE:HG22	1:D:111:PHE:HE2	1.79	0.47
1:A:22:VAL:HG11	2:E:93:ILE:HD11	1.96	0.47
1:A:289:HIS:O	1:A:291:ILE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PHE:HB2	1:A:295:LYS:HD3	1.96	0.47
1:D:272:THR:O	1:D:276:LEU:HD13	2.14	0.47
1:D:288:LYS:HG2	1:D:294:TYR:HB2	1.96	0.47
2:E:9:VAL:O	2:E:19:ARG:NH2	2.48	0.47
3:G:7:DT:O4'	3:G:8:DT:H73	2.14	0.47
1:B:183:THR:HG22	1:B:183:THR:O	2.15	0.47
2:F:5:ILE:HD13	2:F:26:LEU:CD2	2.44	0.47
1:A:92:LEU:HD11	1:B:214:ILE:HD12	1.97	0.46
3:G:9:DG:H2'	3:G:10:DT:C7	2.43	0.46
4:H:23:DG:H2"	4:H:24:DG:O5'	2.14	0.46
1:A:92:LEU:CD1	1:B:214:ILE:HD12	2.45	0.46
2:E:59:LYS:N	2:E:63:ASP:OD2	2.43	0.46
1:C:129:VAL:HG13	1:C:130:ASP:H	1.80	0.46
1:C:238:LEU:HD12	1:C:239:VAL:HG13	1.97	0.46
1:D:252:GLU:OE1	1:D:252:GLU:N	2.48	0.46
1:D:288:LYS:CD	1:D:289:HIS:H	2.16	0.46
1:C:107:ILE:HG21	1:C:216:PHE:CD2	2.50	0.46
1:C:268:THR:HG22	1:C:269:ASP:O	2.14	0.46
1:C:25:LYS:HB3	1:C:31:TRP:HA	1.97	0.46
1:A:197:LEU:HD13	1:A:239:VAL:CG2	2.45	0.46
1:D:71:THR:HG21	4:H:31:DT:OP1	2.16	0.46
1:A:231:LEU:O	1:A:231:LEU:HD23	2.16	0.46
1:B:52:ILE:HD13	1:B:57:LEU:CD1	2.46	0.46
1:D:190:LEU:O	1:D:191:SER:C	2.54	0.46
1:D:288:LYS:HG2	1:D:294:TYR:HB3	1.96	0.46
3:G:22:DT:H2"	3:G:23:DC:C6	2.50	0.46
1:C:289:HIS:CE1	1:C:291:ILE:HB	2.51	0.46
1:B:21:HIS:CE1	1:B:33:LYS:HD3	2.51	0.46
1:C:232:MET:O	1:C:232:MET:HG2	2.14	0.46
1:D:126:ARG:CB	1:D:167:MET:HE3	2.46	0.46
1:C:16:LYS:O	1:C:18:GLU:N	2.39	0.45
1:C:202:THR:HG22	1:C:202:THR:O	2.16	0.45
3:G:27:DT:H2"	3:G:28:DT:O5'	2.16	0.45
1:A:146:LEU:HD21	1:A:150:ARG:HH21	1.81	0.45
1:D:38:ALA:O	1:D:39:GLN:HG2	2.17	0.45
1:C:11:ALA:HA	1:C:23:ALA:O	2.16	0.45
2:E:11:ALA:HB2	3:G:19:DC:C6	2.51	0.45
1:D:25:LYS:HB3	1:D:31:TRP:HE3	1.81	0.45
1:B:25:LYS:O	1:B:26:GLN:CB	2.64	0.45
1:B:288:LYS:HB3	1:B:293:ASN:O	2.16	0.44
1:D:202:THR:HG23	1:D:228:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:LEU:N	1:D:276:LEU:HD12	2.32	0.44
2:E:79:ILE:O	2:F:67:ILE:N	2.49	0.44
2:F:31:LYS:HG3	2:F:32:TRP:H	1.82	0.44
1:A:38:ALA:O	2:E:28:GLY:O	2.36	0.44
1:C:289:HIS:O	1:C:292:PHE:O	2.34	0.44
1:D:228:ILE:O	1:D:232:MET:HG3	2.17	0.44
2:E:88:LYS:O	2:E:88:LYS:HG2	2.17	0.44
1:D:250:GLN:OE1	1:D:250:GLN:N	2.51	0.44
2:E:10:PRO:HA	3:G:19:DC:H5'	1.98	0.44
3:G:8:DT:H2"	3:G:9:DG:C8	2.53	0.44
1:D:3:THR:HG22	1:D:43:ASP:HB2	1.99	0.44
1:C:22:VAL:CG2	1:C:36:ILE:HD12	2.48	0.44
1:B:276:LEU:N	1:B:276:LEU:HD12	2.33	0.44
1:B:283:LEU:HB3	1:B:299:ARG:HB2	1.99	0.44
1:C:243:VAL:HG23	1:C:282:LYS:HG2	2.00	0.44
1:C:254:GLN:O	1:C:255:ARG:HB3	2.18	0.44
1:B:63:LEU:HG	1:B:65:LEU:HD13	2.00	0.44
1:A:225:PRO:O	1:A:229:LEU:HD13	2.18	0.43
1:B:112:VAL:O	1:B:116:VAL:HG12	2.18	0.43
1:B:123:LEU:HD21	1:B:160:TYR:HE1	1.83	0.43
1:D:131:ASN:N	1:D:132:PRO:CD	2.81	0.43
2:E:12:THR:HG23	2:E:15:GLY:H	1.83	0.43
1:A:204:ALA:HB1	1:A:303:GLU:HA	2.00	0.43
1:B:247:VAL:HG12	1:B:251:ARG:HD2	2.00	0.43
1:B:253:ILE:HG22	1:B:254:GLN:N	2.27	0.43
1:B:164:TRP:HB3	1:B:168:LEU:HD11	2.00	0.43
1:C:260:GLU:HB2	1:C:266:ARG:HH21	1.82	0.43
4:H:32:DT:O2	4:H:32:DT:O4'	2.36	0.43
1:B:25:LYS:C	1:B:26:GLN:HG2	2.39	0.43
1:A:31:TRP:O	1:A:31:TRP:CD1	2.72	0.43
1:B:131:ASN:N	1:B:132:PRO:CD	2.81	0.43
1:C:233:GLU:OE2	1:C:236:ARG:NH1	2.51	0.43
1:D:301:ALA:O	1:D:305:GLN:HG2	2.18	0.43
1:B:290:PRO:O	1:B:292:PHE:N	2.52	0.43
1:C:144:GLN:O	1:C:145:THR:HG23	2.18	0.43
1:D:123:LEU:HD12	1:D:132:PRO:CB	2.43	0.43
1:A:278:ALA:O	1:A:281:ARG:HB2	2.18	0.42
2:F:19:ARG:O	2:F:22:LEU:N	2.52	0.42
3:G:8:DT:OP1	3:G:8:DT:H6	2.02	0.42
4:H:25:DG:H2"	4:H:26:DC:C6	2.54	0.42
4:H:27:DA:H8	4:H:27:DA:O5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ARG:HA	1:B:232:MET:HE2	2.01	0.42
2:E:10:PRO:O	2:E:19:ARG:NH2	2.52	0.42
1:B:104:ARG:NH2	1:B:219:GLU:OE2	2.51	0.42
1:B:160:TYR:O	1:B:164:TRP:CD1	2.72	0.42
1:B:274:THR:O	1:B:277:GLY:N	2.49	0.42
1:C:77:VAL:HG11	1:D:62:GLU:HG2	2.01	0.42
1:C:88:GLY:O	1:D:214:ILE:HD11	2.20	0.42
1:D:145:THR:HG22	1:D:148:GLN:OE1	2.20	0.42
1:D:160:TYR:O	1:D:164:TRP:CD1	2.73	0.42
1:D:190:LEU:HD12	1:D:244:VAL:HG21	2.01	0.42
1:B:25:LYS:O	1:B:25:LYS:CD	2.50	0.42
1:B:280:ASP:OD1	1:B:281:ARG:N	2.53	0.42
2:E:50:LEU:O	2:E:50:LEU:HD23	2.18	0.42
1:B:12:VAL:HG23	1:B:23:ALA:HB3	2.02	0.42
1:D:199:THR:OG1	1:D:200:GLN:OE1	2.36	0.42
3:G:21:DG:H1	4:H:16:DC:H42	1.67	0.42
1:C:198:ARG:HG2	1:C:228:ILE:CG2	2.50	0.42
1:D:122:LEU:HD22	1:D:160:TYR:OH	2.20	0.42
3:G:25:DC:H2'	3:G:26:DT:C5	2.54	0.42
1:C:189:LEU:HG	1:C:275:PHE:HE1	1.85	0.42
2:E:88:LYS:N	2:E:89:PRO:HD3	2.35	0.42
1:B:297:THR:O	1:B:301:ALA:N	2.47	0.42
1:D:195:GLY:O	1:D:198:ARG:HB3	2.20	0.42
1:D:205:VAL:HG13	1:D:210:LEU:HB2	2.02	0.42
2:F:6:ILE:HG22	2:F:37:VAL:HG22	2.01	0.42
2:F:58:ILE:HG23	2:F:63:ASP:OD2	2.19	0.42
1:A:22:VAL:HG11	2:E:93:ILE:HD12	2.00	0.41
1:D:58:GLY:O	1:D:62:GLU:HG3	2.20	0.41
1:D:92:LEU:O	1:D:96:ARG:HG3	2.20	0.41
1:C:96:ARG:NE	1:D:99:GLU:OE2	2.53	0.41
1:D:242:SER:O	1:D:246:THR:OG1	2.21	0.41
1:B:301:ALA:O	1:B:305:GLN:HG2	2.20	0.41
1:C:238:LEU:HD12	1:C:239:VAL:CG1	2.50	0.41
1:D:221:THR:O	1:D:224:GLN:HB2	2.20	0.41
3:G:13:DC:H2"	3:G:14:DC:H5'	2.02	0.41
1:B:48:GLY:C	1:B:50:PRO:HD3	2.40	0.41
1:B:289:HIS:HB2	1:B:290:PRO:CD	2.51	0.41
1:A:47:LEU:HD11	1:A:276:LEU:HD11	2.03	0.41
1:B:72:GLN:HB3	3:G:30:DT:H1'	2.03	0.41
1:B:286:GLU:OE2	1:B:288:LYS:HA	2.20	0.41
1:A:5:TYR:CB	1:A:276:LEU:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:HG3	1:A:17:HIS:H	1.86	0.41
1:A:202:THR:OG1	1:A:228:ILE:HD13	2.20	0.41
1:A:221:THR:O	1:A:221:THR:HG22	2.20	0.41
1:C:181:PRO:O	1:C:183:THR:N	2.54	0.41
1:D:200:GLN:OE1	1:D:200:GLN:N	2.47	0.41
1:D:288:LYS:HB2	1:D:294:TYR:O	2.21	0.41
1:B:26:GLN:HB3	1:B:27:GLU:H	1.58	0.41
1:C:231:LEU:HD23	1:C:231:LEU:O	2.20	0.41
1:A:148:GLN:O	1:A:152:ILE:HG12	2.21	0.41
1:C:3:THR:OG1	1:C:299:ARG:NH2	2.54	0.41
1:C:180:ARG:HB3	1:C:181:PRO:HD2	2.03	0.41
1:C:184:ASP:OD2	1:C:185:PRO:N	2.53	0.41
1:D:150:ARG:HH21	1:D:217:LEU:HD12	1.86	0.41
4:H:8:DG:H4'	4:H:8:DG:OP2	2.21	0.41
1:C:86:ARG:HG3	1:D:213:TYR:CE1	2.56	0.41
4:H:18:DG:OP2	4:H:18:DG:H8	2.04	0.41
1:B:64:GLY:O	1:B:65:LEU:HD12	2.20	0.40
1:B:167:MET:CE	1:B:245:LEU:HD21	2.51	0.40
1:C:247:VAL:O	1:C:251:ARG:O	2.39	0.40
3:G:28:DT:H2'	3:G:29:DC:O4'	2.21	0.40
1:A:227:MET:CE	1:A:309:LEU:HD21	2.52	0.40
1:B:229:LEU:O	1:B:233:GLU:HG2	2.21	0.40
1:A:266:ARG:NE	1:A:267:LEU:O	2.41	0.40
1:C:184:ASP:OD2	1:C:184:ASP:C	2.59	0.40
1:B:133:LEU:HD12	1:B:134:LYS:N	2.37	0.40
1:C:18:GLU:O	1:C:39:GLN:NE2	2.50	0.40
1:C:129:VAL:HG13	1:C:130:ASP:N	2.37	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:B:179:ARG:O	1:C:144:GLN:HE22[4_555]	1.58	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	318/336 (95%)	282 (89%)	34 (11%)	2 (1%)	25 61
1	B	321/336 (96%)	282 (88%)	37 (12%)	2 (1%)	25 61
1	C	323/336 (96%)	279 (86%)	44 (14%)	0	100 100
1	D	305/336 (91%)	268 (88%)	35 (12%)	2 (1%)	22 59
2	E	90/105 (86%)	84 (93%)	6 (7%)	0	100 100
2	F	90/105 (86%)	80 (89%)	10 (11%)	0	100 100
All	All	1447/1554 (93%)	1275 (88%)	166 (12%)	6 (0%)	34 69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	GLN
1	D	288	LYS
1	D	132	PRO
1	A	289	HIS
1	A	290	PRO
1	B	27	GLU

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	272/280 (97%)	261 (96%)	11 (4%)	31 59
1	B	273/280 (98%)	271 (99%)	2 (1%)	84 91
1	C	275/280 (98%)	262 (95%)	13 (5%)	26 56
1	D	266/280 (95%)	259 (97%)	7 (3%)	46 69
2	E	82/89 (92%)	80 (98%)	2 (2%)	49 70
2	F	82/89 (92%)	80 (98%)	2 (2%)	49 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1250/1298 (96%)	1213 (97%)	37 (3%)	41 65

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	31	TRP
1	A	86	ARG
1	A	171	GLU
1	A	172	TRP
1	A	174	PHE
1	A	178	PHE
1	A	184	ASP
1	A	196	LEU
1	A	292	PHE
1	A	294	TYR
1	B	63	LEU
1	B	287	PHE
1	C	26	GLN
1	C	86	ARG
1	C	118	ASN
1	C	164	TRP
1	C	172	TRP
1	C	174	PHE
1	C	177	ARG
1	C	251	ARG
1	C	255	ARG
1	C	258	PHE
1	C	275	PHE
1	C	287	PHE
1	C	292	PHE
1	D	86	ARG
1	D	124	TYR
1	D	251	ARG
1	D	279	PHE
1	D	288	LYS
1	D	289	HIS
1	D	294	TYR
2	E	42	LEU
2	E	88	LYS
2	F	42	LEU
2	F	77	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	148	GLN
1	B	39	GLN
1	B	117	HIS
1	C	289	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	322/336 (95%)	0.02	8 (2%) 57 49	11, 43, 83, 107	0
1	B	323/336 (96%)	-0.11	3 (0%) 84 80	14, 38, 71, 100	0
1	C	325/336 (96%)	-0.15	4 (1%) 79 74	9, 30, 72, 120	0
1	D	313/336 (93%)	-0.22	2 (0%) 89 87	12, 32, 62, 79	0
2	E	92/105 (87%)	0.00	2 (2%) 62 55	22, 45, 73, 89	0
2	F	92/105 (87%)	-0.17	0 100 100	12, 43, 58, 62	0
3	G	26/36 (72%)	0.47	1 (3%) 40 33	41, 71, 105, 114	0
4	H	25/36 (69%)	0.30	0 100 100	38, 67, 88, 91	0
All	All	1518/1626 (93%)	-0.09	20 (1%) 77 72	9, 38, 77, 120	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	SER	4.6
1	B	289	HIS	3.7
1	D	30	SER	3.7
1	A	263	GLY	3.7
2	E	13	LYS	3.2
1	A	262	LEU	2.9
1	A	294	TYR	2.9
1	D	26	GLN	2.9
2	E	11	ALA	2.7
1	A	293	ASN	2.7
1	B	290	PRO	2.6
1	C	261	SER	2.4
1	B	277	GLY	2.3
1	C	26	GLN	2.3
1	A	175	THR	2.3
3	G	15	DC	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	180	ARG	2.2
1	A	176	GLY	2.2
1	A	296	CYS	2.0
1	C	263	GLY	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.