Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:19 AM GMT

PDB ID	:	2GIE
Title	:	HincII bound to cognate DNA GTTAAC
Authors	:	Horton, N.C.; Joshi, H.K.; Etzkorn, C.; Chatwell, L.; Bitinaite, J.
Deposited on	:	2006-03-28
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

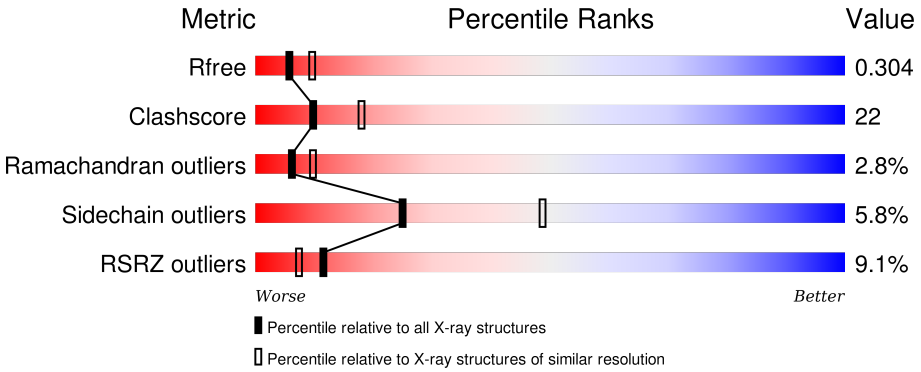
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	E	13	31% 62% 8%
1	F	13	31% 54% 15%
1	G	13	8% 38% 46% 15%
1	H	13	8% 31% 62% 8%
2	A	257	2% 64% 33% •

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Mol	Chain	Length	Quality of chain
2	B	257	2% 65% 30% 5%
2	C	257	21% 50% 47%
2	D	257	12% 54% 40% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9798 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 DNA chain called 5'-D(*GP*CP*CP*GP*GP*TP*TP*AP*AP*CP*CP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	13	Total	C	N	O	P	0	0	0
			265	126	51	76	12			
1	F	13	Total	C	N	O	P	0	0	0
			265	126	51	76	12			
1	G	13	Total	C	N	O	P	0	0	0
			265	126	51	76	12			
1	H	13	Total	C	N	O	P	0	0	0
			265	126	51	76	12			

- Molecule 2 is a protein called Type II restriction enzyme HincII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	257	Total	C	N	O	S	0	0	0
			2075	1344	337	388	6			
2	B	256	Total	C	N	O	S	0	0	0
			2081	1350	337	388	6			
2	C	257	Total	C	N	O	S	0	0	0
			2023	1311	330	376	6			
2	D	256	Total	C	N	O	S	0	0	0
			2050	1328	330	386	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	THR	ARG	CONFLICT	UNP P44413
A	173	TRP	SER	CONFLICT	UNP P44413
B	130	THR	ARG	CONFLICT	UNP P44413
B	173	TRP	SER	CONFLICT	UNP P44413
C	130	THR	ARG	CONFLICT	UNP P44413
C	173	TRP	SER	CONFLICT	UNP P44413
D	130	THR	ARG	CONFLICT	UNP P44413
D	173	TRP	SER	CONFLICT	UNP P44413

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	175	Total O 175 175	0	0
4	B	130	Total O 130 130	0	0
4	C	43	Total O 43 43	0	0
4	D	59	Total O 59 59	0	0
4	E	39	Total O 39 39	0	0
4	F	27	Total O 27 27	0	0
4	G	21	Total O 21 21	0	0
4	H	14	Total O 14 14	0	0

3 Residue-property plots (i)

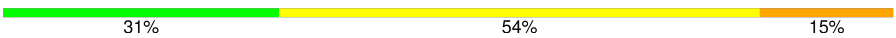
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

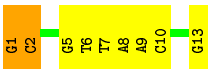
- Molecule 1: 5'-D(*GP*CP*CP*GP*GP*TP*TP*AP*AP*CP*CP*GP*G)-3'

Chain E:

- Molecule 1: 5'-D(*GP*CP*CP*GP*GP*TP*TP*AP*AP*CP*CP*GP*G)-3'

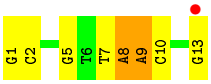
Chain F:





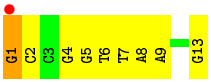
- Molecule 1: 5'-D(*GP*CP*CP*GP*GP*TP*TP*AP*AP*CP*CP*GP*G)-3'

Chain G:



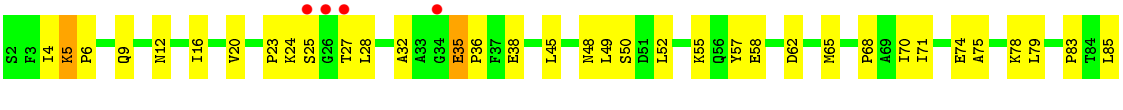
- Molecule 1: 5'-D(*GP*CP*CP*GP*GP*TP*TP*AP*AP*CP*CP*GP*G)-3'

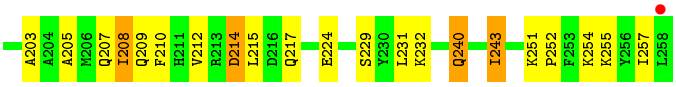
Chain H:



- Molecule 2: Type II restriction enzyme HincII

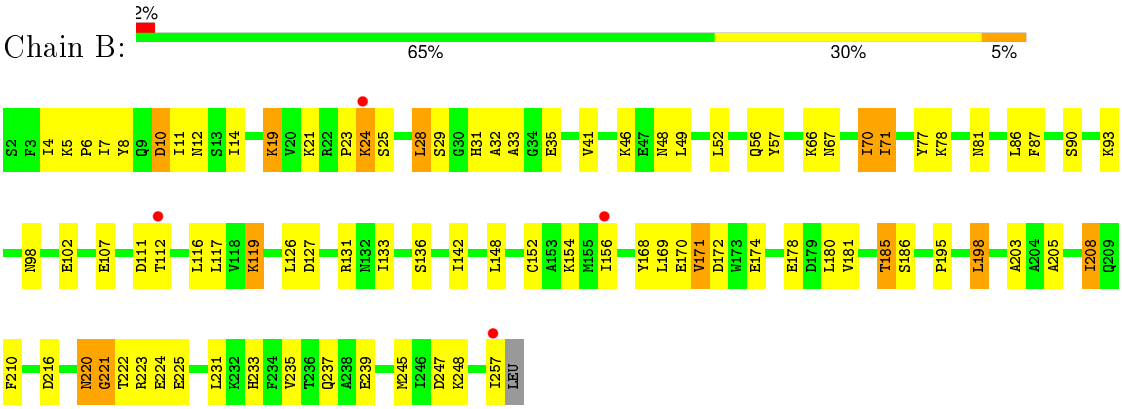
Chain A:





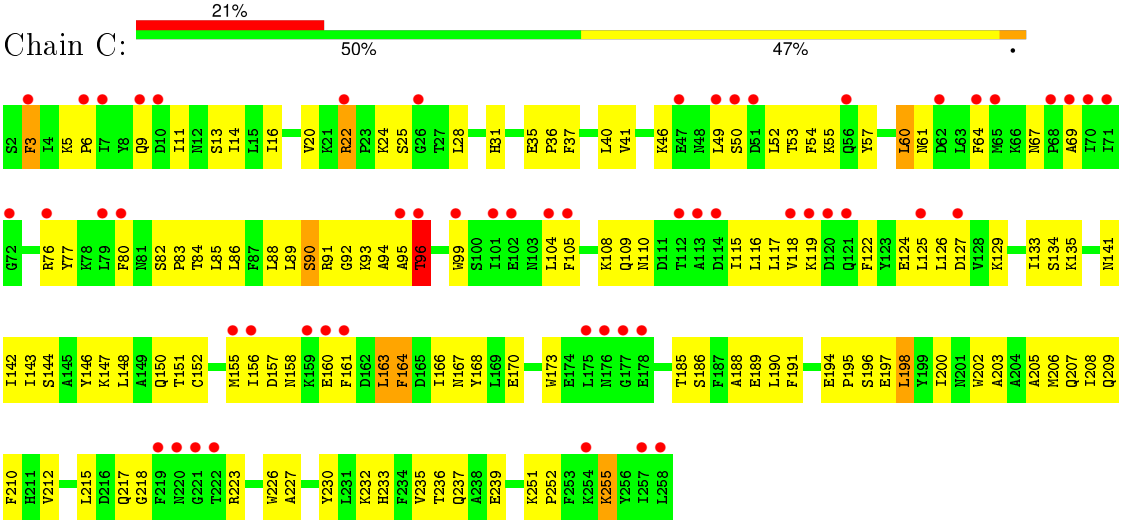
• Molecule 2: Type II restriction enzyme HincII

Chain B:



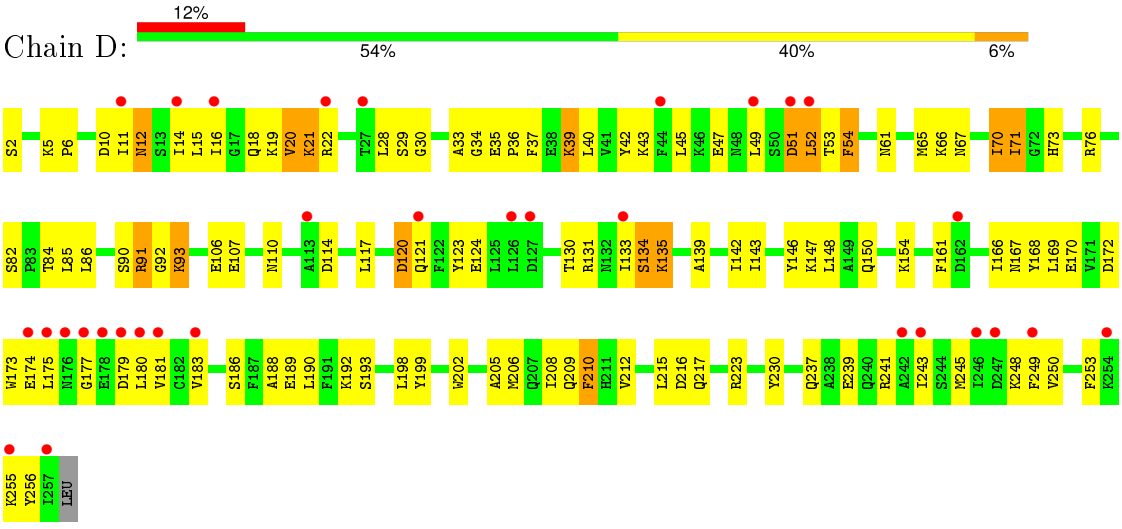
• Molecule 2: Type II restriction enzyme HincII

Chain C:



• Molecule 2: Type II restriction enzyme HincII

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.24Å 175.47Å 253.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 28.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.60) 97.1 (28.87-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.306 0.238 , 0.304	Depositor DCC
R_{free} test set	2269 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 74.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 45242 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9798	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA

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	E	0.52	0/297	0.81	0/457
1	F	0.55	0/297	0.90	0/457
1	G	0.40	0/297	0.76	0/457
1	H	0.40	0/297	0.76	0/457
2	A	0.40	0/2123	0.63	0/2873
2	B	0.43	0/2129	0.65	0/2875
2	C	0.32	0/2070	0.51	0/2811
2	D	0.35	0/2098	0.56	0/2844
All	All	0.39	0/9608	0.62	0/13231

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	E	0	3
1	F	0	5
1	G	0	3
1	H	0	4
All	All	0	15

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	7	DT	Sidechain

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Mol	Chain	Res	Type	Group
1	E	8	DA	Sidechain
1	E	9	DA	Sidechain
1	F	1	DG	Sidechain
1	F	2	DC	Sidechain
1	F	7	DT	Sidechain
1	F	8	DA	Sidechain
1	F	9	DA	Sidechain
1	G	10	DC	Sidechain
1	G	8	DA	Sidechain
1	G	9	DA	Sidechain
1	H	1	DG	Sidechain
1	H	7	DT	Sidechain
1	H	8	DA	Sidechain
1	H	9	DA	Sidechain

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	E	265	0	147	11	0
1	F	265	0	147	11	0
1	G	265	0	147	7	0
1	H	265	0	147	10	0
2	A	2075	0	2020	81	1
2	B	2081	0	2056	79	0
2	C	2023	0	1933	118	0
2	D	2050	0	1971	108	0
3	B	1	0	0	0	0
4	A	175	0	0	9	0
4	B	130	0	0	4	0
4	C	43	0	0	5	0
4	D	59	0	0	4	0
4	E	39	0	0	0	0
4	F	27	0	0	0	1
4	G	21	0	0	0	0
4	H	14	0	0	1	0
All	All	9798	0	8568	396	2

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 22.

All (396) 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)
2:C:142:ILE:HD11	2:C:208:ILE:HG23	1.49	0.94
1:G:7:DT:H2"	1:G:8:DA:H5'	1.51	0.93
2:D:70:ILE:HD11	2:D:76:ARG:HA	1.51	0.91
2:B:70:ILE:HG23	2:B:71:ILE:H	1.38	0.89
2:D:20:VAL:HG23	2:D:21:LYS:H	1.39	0.88
2:B:70:ILE:HG23	2:B:71:ILE:N	1.88	0.86
1:H:13:DG:H5"	2:D:92:GLY:HA2	1.54	0.86
2:C:142:ILE:HG13	2:C:143:ILE:H	1.40	0.84
2:B:28:LEU:HB3	2:B:33:ALA:HA	1.60	0.82
2:C:142:ILE:HG13	2:C:143:ILE:N	1.95	0.82
2:C:125:LEU:HB2	2:C:166:ILE:HG22	1.61	0.81
2:D:134:SER:HB2	2:D:174:GLU:HB2	1.64	0.79
2:D:142:ILE:HB	2:D:208:ILE:HG13	1.65	0.78
2:C:198:LEU:HB3	2:C:208:ILE:HD11	1.65	0.77
2:C:20:VAL:HG11	2:C:36:PRO:HB2	1.66	0.76
2:A:70:ILE:HD11	2:A:79:LEU:HD11	1.68	0.76
2:B:4:ILE:CD1	2:B:126:LEU:HD22	2.16	0.75
2:C:185:THR:HG22	2:C:186:SER:H	1.52	0.74
2:C:255:LYS:HD2	2:C:255:LYS:H	1.50	0.74
2:B:222:THR:O	2:B:224:GLU:N	2.20	0.74
2:B:70:ILE:CG2	2:B:71:ILE:H	1.99	0.74
1:F:1:DG:H2"	1:F:2:DC:H5'	1.70	0.74
1:F:5:DG:H2"	1:F:6:DT:H5'	1.70	0.74
2:D:188:ALA:HB1	2:D:215:LEU:HD23	1.68	0.73
1:G:13:DG:H3'	2:C:92:GLY:HA2	1.70	0.73
2:A:115:ILE:HG13	2:A:126:LEU:HB3	1.69	0.73
2:A:198:LEU:HG	2:A:208:ILE:CD1	2.19	0.72
2:D:170:GLU:HB3	2:D:186:SER:HB2	1.70	0.72
2:D:175:LEU:HD13	2:D:180:LEU:HD23	1.72	0.71
2:C:142:ILE:HD13	2:C:210:PHE:CE2	2.26	0.71
2:C:198:LEU:CB	2:C:208:ILE:HD11	2.21	0.71
2:C:170:GLU:HB2	2:C:212:VAL:HB	1.74	0.70
2:A:257:ILE:HD11	2:B:235:VAL:HG21	1.73	0.70
2:B:208:ILE:HD11	2:B:210:PHE:CE2	2.26	0.69
2:C:156:ILE:HD11	2:D:256:TYR:HE2	1.58	0.69
2:A:52:LEU:O	2:A:117:LEU:HA	1.93	0.69
2:C:142:ILE:HG12	4:C:284:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:LEU:HB2	2:D:124:GLU:HB3	1.75	0.68
2:C:188:ALA:HB1	2:C:217:GLN:NE2	2.08	0.68
2:B:119:LYS:HA	2:B:119:LYS:HE3	1.76	0.68
2:B:208:ILE:HD11	2:B:210:PHE:HE2	1.58	0.67
2:B:8:TYR:OH	2:B:185:THR:HG22	1.95	0.67
2:D:39:LYS:HE3	2:D:39:LYS:HA	1.75	0.67
2:A:4:ILE:HD13	2:A:117:LEU:HD11	1.76	0.67
2:C:202:TRP:HA	2:C:206:MET:HA	1.76	0.67
2:C:109:GLN:OE1	2:D:29:SER:HB2	1.95	0.67
1:G:1:DG:H2"	1:G:2:DC:O5'	1.94	0.67
2:C:144:SER:HB3	2:C:147:LYS:HB3	1.77	0.66
1:E:6:DT:H2'	4:B:662:HOH:O	1.95	0.66
2:A:70:ILE:HD11	2:A:79:LEU:CD1	2.26	0.66
1:E:4:DG:C6	2:A:138:GLN:HG3	2.31	0.65
2:C:235:VAL:HG13	2:D:250:VAL:HG13	1.77	0.65
2:C:55:LYS:HD2	2:C:57:TYR:HE1	1.60	0.65
2:A:229:SER:HA	2:A:232:LYS:NZ	2.12	0.64
2:C:185:THR:HG22	2:C:186:SER:N	2.11	0.64
2:D:11:ILE:HA	2:D:14:ILE:HD12	1.79	0.64
2:B:233:HIS:O	2:B:237:GLN:HG2	1.96	0.64
2:C:115:ILE:HG23	2:C:126:LEU:HB3	1.80	0.64
2:C:161:PHE:HB3	2:C:223:ARG:HB3	1.78	0.64
2:B:4:ILE:HD13	2:B:126:LEU:HD22	1.79	0.64
2:A:189:GLU:HB2	2:A:192:LYS:HB2	1.81	0.63
2:D:189:GLU:HB2	2:D:192:LYS:HB3	1.80	0.63
2:D:82:SER:HB3	2:D:85:LEU:HB2	1.81	0.63
2:B:23:PRO:HG2	2:B:28:LEU:HD12	1.81	0.63
1:E:10:DC:H2'	4:B:674:HOH:O	1.98	0.63
2:D:20:VAL:HG23	2:D:21:LYS:N	2.11	0.62
1:F:1:DG:H5'	1:F:1:DG:H8	1.65	0.62
2:B:24:LYS:NZ	2:B:25:SER:H	1.98	0.62
2:C:127:ASP:HB3	2:C:168:TYR:CD1	2.35	0.62
2:B:12:ASN:ND2	2:B:185:THR:HB	2.15	0.61
2:D:82:SER:OG	2:D:84:THR:HG22	2.01	0.60
2:C:37:PHE:O	2:C:41:VAL:HG23	2.01	0.60
2:B:57:TYR:CE2	2:B:107:GLU:HB3	2.37	0.60
2:B:5:LYS:HB3	2:B:6:PRO:HD3	1.84	0.60
2:C:115:ILE:CG2	2:C:126:LEU:HB3	2.32	0.60
2:C:52:LEU:O	2:C:117:LEU:HA	2.02	0.59
2:B:70:ILE:CG2	2:B:71:ILE:N	2.56	0.59
2:A:70:ILE:HD11	2:A:79:LEU:CG	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:LEU:O	2:D:199:TYR:HB3	2.02	0.59
2:D:20:VAL:O	2:D:21:LYS:HB2	2.00	0.59
2:B:98:ASN:HD22	2:B:98:ASN:N	2.00	0.59
2:C:31:HIS:CD2	2:D:30:GLY:HA3	2.37	0.59
2:A:251:LYS:HB2	2:A:252:PRO:HD3	1.84	0.59
4:H:313:HOH:O	2:D:110:ASN:HB2	2.01	0.59
1:E:1:DG:H1'	1:E:2:DC:H5"	1.84	0.59
2:A:119:LYS:O	2:A:120:ASP:HB2	2.01	0.59
2:D:189:GLU:H	2:D:217:GLN:HE22	1.48	0.59
2:A:91:ARG:HD2	4:A:427:HOH:O	2.03	0.58
2:B:248:LYS:NZ	2:B:248:LYS:HB3	2.18	0.58
2:A:198:LEU:HG	2:A:208:ILE:HD12	1.84	0.58
2:A:127:ASP:HB3	2:A:168:TYR:CE1	2.38	0.58
2:D:170:GLU:HB2	2:D:212:VAL:HB	1.85	0.58
2:D:146:TYR:O	2:D:150:GLN:HG3	2.03	0.58
2:C:83:PRO:HD2	2:C:158:ASN:OD1	2.02	0.58
1:F:1:DG:H2"	1:F:2:DC:C5'	2.33	0.58
2:D:35:GLU:HB3	2:D:36:PRO:HD3	1.86	0.57
2:A:161:PHE:CG	2:A:224:GLU:HG2	2.38	0.57
2:D:37:PHE:HA	2:D:40:LEU:HD12	1.84	0.57
2:D:193:SER:HB2	2:D:216:ASP:OD2	2.05	0.57
2:A:224:GLU:HG3	4:A:283:HOH:O	2.04	0.57
2:A:35:GLU:HB3	2:A:36:PRO:HD3	1.85	0.57
2:C:232:LYS:O	2:C:236:THR:HG23	2.03	0.57
2:B:28:LEU:HD22	2:B:28:LEU:H	1.70	0.57
1:F:1:DG:H2'	1:F:2:DC:C6	2.39	0.57
2:C:233:HIS:O	2:C:237:GLN:HG2	2.05	0.57
1:F:1:DG:H2'	1:F:2:DC:H6	1.70	0.56
2:B:24:LYS:HA	2:B:24:LYS:HE2	1.87	0.56
1:E:1:DG:C2'	1:E:2:DC:H5"	2.36	0.56
2:C:251:LYS:HB3	2:C:252:PRO:HD3	1.87	0.56
2:D:142:ILE:HB	2:D:208:ILE:O	2.06	0.56
2:C:156:ILE:HG22	2:C:161:PHE:HE1	1.70	0.56
2:C:218:GLY:HA3	4:C:299:HOH:O	2.04	0.56
2:C:170:GLU:HB3	2:C:186:SER:HB3	1.86	0.56
2:C:3:PHE:HB3	2:C:124:GLU:OE2	2.04	0.56
2:C:61:ASN:HD21	2:C:104:LEU:HB2	1.70	0.56
2:A:65:MET:O	2:A:68:PRO:HD3	2.05	0.56
2:C:5:LYS:HB3	2:C:6:PRO:HD3	1.87	0.56
1:E:1:DG:H2"	1:E:2:DC:H5"	1.87	0.56
2:B:66:LYS:HE3	4:B:690:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:127:ASP:OD1	2:A:129:LYS:HE3	2.06	0.55
2:D:34:GLY:HA3	2:D:130:THR:HG21	1.87	0.55
2:D:134:SER:HB2	2:D:174:GLU:CB	2.36	0.55
2:B:10:ASP:O	2:B:14:ILE:HG22	2.06	0.55
2:C:52:LEU:HD23	2:C:52:LEU:N	2.21	0.55
2:B:152:CYS:O	2:B:156:ILE:HG22	2.06	0.55
2:C:88:LEU:C	2:C:89:LEU:HD12	2.27	0.55
2:A:109:GLN:CD	2:B:29:SER:HB3	2.27	0.55
2:A:192:LYS:O	2:A:217:GLN:HA	2.07	0.54
2:A:195:PRO:HA	2:A:198:LEU:HD22	1.89	0.54
2:C:86:LEU:HD12	2:C:90:SER:HB3	1.89	0.54
2:C:116:LEU:HA	2:C:124:GLU:O	2.07	0.54
2:C:146:TYR:O	2:C:150:GLN:HG3	2.07	0.54
2:C:91:ARG:NH2	2:C:108:LYS:HB2	2.23	0.54
2:D:91:ARG:NH2	2:D:106:GLU:O	2.41	0.54
2:C:61:ASN:HD22	2:C:105:PHE:HB2	1.73	0.54
2:D:237:GLN:HG3	4:D:302:HOH:O	2.08	0.54
2:A:161:PHE:CD2	2:A:224:GLU:HG2	2.43	0.54
2:B:220:ASN:O	2:B:221:GLY:O	2.26	0.53
2:C:35:GLU:N	2:C:36:PRO:HD2	2.22	0.53
2:C:11:ILE:HA	2:C:14:ILE:HG22	1.90	0.53
1:G:7:DT:H2"	1:G:8:DA:C5'	2.33	0.53
2:A:210:PHE:CZ	2:A:215:LEU:HD22	2.43	0.53
2:A:85:LEU:HD21	2:A:123:TYR:CE1	2.43	0.53
2:C:76:ARG:HH22	2:C:99:TRP:HB3	1.73	0.53
2:C:108:LYS:HE3	2:C:110:ASN:OD1	2.08	0.53
2:B:8:TYR:O	2:B:11:ILE:HG22	2.09	0.53
2:B:98:ASN:N	2:B:98:ASN:ND2	2.55	0.53
2:A:127:ASP:HB3	2:A:168:TYR:CD1	2.44	0.53
2:C:122:PHE:HA	2:C:163:LEU:O	2.08	0.53
2:C:126:LEU:HD12	2:C:167:ASN:O	2.09	0.53
2:D:52:LEU:HD23	2:D:117:LEU:HD22	1.90	0.53
2:C:118:VAL:O	2:C:119:LYS:HG2	2.09	0.53
2:D:133:ILE:C	2:D:135:LYS:H	2.13	0.52
2:D:188:ALA:CB	2:D:215:LEU:HD23	2.36	0.52
1:H:4:DG:H2'	2:D:199:TYR:OH	2.10	0.52
2:B:222:THR:C	4:B:723:HOH:O	2.47	0.52
2:B:169:LEU:HD12	2:B:186:SER:O	2.09	0.52
2:A:115:ILE:CD1	2:A:117:LEU:HG	2.40	0.52
2:B:170:GLU:HB3	2:B:186:SER:OG	2.10	0.52
2:D:166:ILE:HG23	2:D:190:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:O	2:B:19:LYS:HD2	2.10	0.52
2:B:4:ILE:HD11	2:B:126:LEU:HD22	1.88	0.52
2:D:239:GLU:O	2:D:243:ILE:HG12	2.10	0.52
1:F:13:DG:H2'	2:B:77:TYR:OH	2.10	0.52
2:D:133:ILE:HG22	2:D:173:TRP:O	2.09	0.52
2:A:214:ASP:OD2	2:A:214:ASP:N	2.42	0.52
2:D:22:ARG:HH21	2:D:28:LEU:HD11	1.74	0.52
2:D:2:SER:HA	2:D:124:GLU:CD	2.30	0.51
2:C:148:LEU:HD23	2:C:230:TYR:CZ	2.45	0.51
2:A:123:TYR:O	2:A:164:PHE:HA	2.09	0.51
2:C:57:TYR:O	2:C:61:ASN:HB2	2.11	0.51
2:B:56:GLN:HA	2:B:116:LEU:HD12	1.93	0.51
2:A:70:ILE:HD11	2:A:79:LEU:HG	1.92	0.51
2:B:185:THR:CG2	2:B:186:SER:N	2.73	0.51
1:H:5:DG:H2"	1:H:6:DT:H5'	1.92	0.51
4:A:386:HOH:O	2:B:35:GLU:HB3	2.09	0.51
2:D:5:LYS:N	2:D:6:PRO:HD2	2.26	0.51
2:C:166:ILE:HG12	2:C:191:PHE:CE1	2.46	0.50
2:A:146:TYR:CE2	2:A:150:GLN:NE2	2.79	0.50
2:D:86:LEU:O	2:D:90:SER:HB2	2.11	0.50
2:A:251:LYS:HB3	4:A:285:HOH:O	2.11	0.50
1:E:7:DT:O2	2:B:31:HIS:HE1	1.93	0.50
2:C:22:ARG:O	2:C:22:ARG:HD3	2.10	0.50
2:C:151:THR:O	2:C:155:MET:HG3	2.12	0.50
2:D:169:LEU:HD12	2:D:186:SER:O	2.11	0.50
2:B:24:LYS:HG3	2:B:25:SER:N	2.25	0.50
1:H:5:DG:OP1	2:D:248:LYS:HE2	2.12	0.50
2:A:83:PRO:HG2	2:A:158:ASN:OD1	2.11	0.50
2:C:88:LEU:HD21	2:C:151:THR:OG1	2.11	0.50
2:A:115:ILE:HD12	2:A:115:ILE:C	2.31	0.50
2:D:12:ASN:O	2:D:16:ILE:HG12	2.12	0.50
2:C:125:LEU:HD13	2:C:164:PHE:HD1	1.76	0.50
2:C:196:SER:HA	2:C:233:HIS:HB2	1.94	0.50
2:D:16:ILE:HD12	2:D:183:VAL:O	2.11	0.50
2:C:142:ILE:CG1	2:C:143:ILE:H	2.17	0.50
2:C:141:ASN:HB3	2:C:207:GLN:OE1	2.11	0.50
2:A:71:ILE:HD12	2:A:71:ILE:C	2.32	0.50
1:H:1:DG:H8	1:H:1:DG:HO5'	1.59	0.50
2:C:13:SER:HA	2:C:16:ILE:HG12	1.94	0.50
2:D:20:VAL:CG2	2:D:21:LYS:H	2.12	0.49
2:C:88:LEU:HD11	2:C:151:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:205:ALA:O	2:A:207:GLN:HG2	2.12	0.49
2:A:12:ASN:O	2:A:16:ILE:HG22	2.12	0.49
2:D:142:ILE:HG13	2:D:210:PHE:CD2	2.47	0.49
2:D:28:LEU:N	2:D:28:LEU:HD12	2.27	0.49
2:C:160:GLU:HB2	4:C:285:HOH:O	2.12	0.49
2:B:222:THR:O	2:B:225:GLU:N	2.41	0.49
1:H:4:DG:H8	2:D:199:TYR:HH	1.61	0.49
2:D:148:LEU:HD22	2:D:230:TYR:CE2	2.47	0.49
2:C:116:LEU:HD12	2:C:125:LEU:HG	1.95	0.49
2:A:70:ILE:O	2:A:70:ILE:HG13	2.12	0.49
2:C:210:PHE:CD1	2:C:210:PHE:C	2.86	0.49
2:B:171:VAL:HG22	2:B:171:VAL:O	2.12	0.49
2:B:231:LEU:O	2:B:235:VAL:HG23	2.13	0.49
2:D:173:TRP:CZ3	2:D:180:LEU:HD22	2.48	0.49
2:B:28:LEU:HD13	2:B:28:LEU:N	2.28	0.49
2:C:88:LEU:HD11	2:C:151:THR:CG2	2.42	0.49
2:D:150:GLN:O	2:D:154:LYS:HG3	2.12	0.48
2:D:202:TRP:HA	2:D:206:MET:HA	1.95	0.48
2:B:11:ILE:HD11	2:B:41:VAL:HG13	1.95	0.48
2:A:229:SER:HA	2:A:232:LYS:HZ1	1.79	0.48
2:D:22:ARG:NH2	2:D:28:LEU:HD11	2.28	0.48
1:F:10:DC:H2'	4:A:394:HOH:O	2.12	0.48
2:A:243:ILE:C	2:A:243:ILE:HD13	2.33	0.48
2:C:170:GLU:HB2	2:C:212:VAL:CB	2.42	0.48
2:D:209:GLN:O	2:D:210:PHE:HB3	2.13	0.48
2:C:255:LYS:HD2	2:C:255:LYS:N	2.24	0.48
2:A:16:ILE:HG23	4:A:414:HOH:O	2.13	0.48
2:A:28:LEU:HA	2:A:32:ALA:O	2.13	0.48
1:F:5:DG:H2"	1:F:6:DT:C5'	2.43	0.48
2:D:11:ILE:O	2:D:15:LEU:HG	2.14	0.48
2:A:151:THR:O	2:A:155:MET:HG3	2.13	0.48
2:B:235:VAL:O	2:B:239:GLU:HG3	2.14	0.48
2:D:210:PHE:C	2:D:210:PHE:CD1	2.87	0.48
2:C:36:PRO:O	2:C:40:LEU:HB2	2.14	0.47
2:A:27:THR:O	2:A:28:LEU:HB2	2.13	0.47
2:C:205:ALA:HB3	2:C:207:GLN:HG2	1.96	0.47
2:A:203:ALA:O	2:B:205:ALA:HA	2.13	0.47
2:A:141:ASN:HA	2:A:209:GLN:HG2	1.97	0.47
2:C:95:ALA:O	2:C:96:THR:HG23	2.13	0.47
2:B:67:ASN:O	2:B:70:ILE:HG22	2.15	0.47
2:C:89:LEU:N	2:C:89:LEU:HD12	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:185:THR:CG2	2:C:186:SER:H	2.24	0.47
2:B:142:ILE:HB	2:B:208:ILE:HG12	1.95	0.47
2:D:208:ILE:HG13	2:D:208:ILE:O	2.15	0.47
2:C:203:ALA:O	2:D:205:ALA:HA	2.14	0.47
2:D:241:ARG:O	2:D:245:MET:HG3	2.15	0.47
2:D:61:ASN:HB3	2:D:65:MET:CE	2.44	0.47
2:D:10:ASP:O	2:D:14:ILE:HG13	2.14	0.47
2:A:101:ILE:HG22	4:A:367:HOH:O	2.15	0.47
2:B:28:LEU:HA	2:B:32:ALA:O	2.14	0.47
2:A:210:PHE:CD1	2:A:210:PHE:C	2.88	0.47
2:C:156:ILE:HD11	2:D:256:TYR:CE2	2.45	0.47
2:D:42:TYR:HE1	2:D:54:PHE:HA	1.79	0.47
2:A:117:LEU:HB2	2:A:124:GLU:HB3	1.97	0.47
2:C:117:LEU:N	2:C:117:LEU:HD12	2.30	0.46
2:C:77:TYR:HB3	4:C:266:HOH:O	2.14	0.46
2:D:73:HIS:CG	2:D:93:LYS:HG3	2.51	0.46
2:A:116:LEU:CD2	2:A:125:LEU:HD12	2.45	0.46
2:B:127:ASP:HB3	2:B:168:TYR:CD1	2.50	0.46
2:D:35:GLU:N	2:D:36:PRO:CD	2.78	0.46
2:C:85:LEU:HD22	2:C:163:LEU:HD21	1.96	0.46
2:B:195:PRO:HA	2:B:198:LEU:CD2	2.45	0.46
1:H:4:DG:H4'	1:H:5:DG:OP1	2.15	0.46
2:B:21:LYS:HE3	2:B:178:GLU:OE2	2.15	0.46
2:D:71:ILE:HD13	2:D:71:ILE:H	1.80	0.46
2:A:199:TYR:O	2:A:208:ILE:HA	2.15	0.46
2:C:64:PHE:CE2	2:C:76:ARG:HD3	2.51	0.46
2:C:239:GLU:OE1	2:D:250:VAL:HG21	2.15	0.46
2:C:127:ASP:HB3	2:C:168:TYR:HD1	1.78	0.45
2:C:28:LEU:HD13	2:C:173:TRP:CH2	2.50	0.45
4:A:405:HOH:O	2:B:29:SER:HA	2.15	0.45
2:A:91:ARG:HA	2:A:91:ARG:HD3	1.80	0.45
2:A:20:VAL:HG23	2:A:20:VAL:O	2.16	0.45
2:A:210:PHE:CE1	2:A:215:LEU:HD22	2.52	0.45
2:D:12:ASN:HD21	2:D:16:ILE:HD11	1.82	0.45
2:B:133:ILE:HA	2:B:133:ILE:HD12	1.84	0.45
2:B:7:ILE:HG13	2:B:7:ILE:O	2.16	0.45
2:D:71:ILE:HD11	4:D:260:HOH:O	2.15	0.45
2:A:170:GLU:HB2	2:A:212:VAL:HB	1.99	0.45
2:D:2:SER:HB2	2:D:167:ASN:HD21	1.82	0.45
2:A:55:LYS:HG2	2:A:57:TYR:CE1	2.52	0.45
2:C:52:LEU:HD13	2:C:119:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:ILE:HG22	2:D:208:ILE:HD11	1.98	0.45
2:D:20:VAL:HG22	2:D:180:LEU:O	2.17	0.44
1:H:13:DG:C5'	2:D:92:GLY:HA2	2.35	0.44
2:D:19:LYS:CB	2:D:179:ASP:HB3	2.47	0.44
2:D:131:ARG:HD3	2:D:172:ASP:OD1	2.16	0.44
2:D:66:LYS:HE3	4:D:265:HOH:O	2.17	0.44
2:B:248:LYS:HZ2	2:B:248:LYS:HB3	1.82	0.44
1:G:9:DA:H5"	2:D:33:ALA:HB3	1.98	0.44
2:C:200:ILE:HA	2:C:208:ILE:HA	1.99	0.44
2:C:116:LEU:C	2:C:116:LEU:HD23	2.37	0.44
2:A:208:ILE:HD11	2:A:210:PHE:HE2	1.82	0.44
2:C:127:ASP:HB3	2:C:168:TYR:CE1	2.53	0.44
2:A:205:ALA:HA	2:B:203:ALA:O	2.18	0.44
1:E:4:DG:O6	2:A:138:GLN:HG3	2.16	0.44
2:D:85:LEU:HD11	2:D:123:TYR:CD1	2.52	0.44
2:D:166:ILE:HG23	2:D:190:LEU:CB	2.47	0.44
2:C:152:CYS:SG	2:C:227:ALA:HA	2.58	0.44
2:A:161:PHE:CD1	2:A:224:GLU:HG2	2.52	0.44
2:C:80:PHE:HB2	2:C:86:LEU:HD13	1.98	0.44
2:C:84:THR:HG21	2:C:155:MET:CG	2.48	0.44
2:D:19:LYS:CB	2:D:181:VAL:HG22	2.48	0.44
1:E:1:DG:H2"	1:E:2:DC:C5'	2.48	0.44
2:D:18:GLN:O	2:D:181:VAL:HA	2.17	0.44
2:D:20:VAL:CG2	2:D:21:LYS:N	2.78	0.44
2:C:11:ILE:O	2:C:14:ILE:HG22	2.18	0.43
2:A:152:CYS:HA	2:A:155:MET:CE	2.48	0.43
2:D:139:ALA:HB1	2:D:210:PHE:N	2.33	0.43
1:E:1:DG:C1'	1:E:2:DC:H5"	2.47	0.43
2:D:189:GLU:H	2:D:217:GLN:NE2	2.16	0.43
2:C:89:LEU:HD11	2:C:125:LEU:HD21	1.99	0.43
2:D:199:TYR:HA	4:D:302:HOH:O	2.17	0.43
2:C:146:TYR:CD1	2:D:249:PHE:HD1	2.37	0.43
2:C:157:ASP:C	2:C:158:ASN:HD22	2.22	0.43
2:C:86:LEU:CD1	2:C:90:SER:HB3	2.48	0.43
2:A:115:ILE:HD11	2:A:117:LEU:HG	2.00	0.43
2:C:35:GLU:H	2:C:36:PRO:HD2	1.83	0.43
2:D:73:HIS:CD2	2:D:93:LYS:HG3	2.54	0.43
2:A:143:ILE:HD13	4:A:332:HOH:O	2.18	0.43
2:C:67:ASN:C	2:C:69:ALA:H	2.22	0.43
2:D:142:ILE:HG13	2:D:210:PHE:CE2	2.54	0.43
2:C:60:LEU:HB3	2:C:80:PHE:HZ	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ASN:O	2:B:49:LEU:HD23	2.17	0.43
2:B:70:ILE:O	2:B:71:ILE:O	2.36	0.43
2:B:4:ILE:O	2:B:7:ILE:HG22	2.19	0.43
2:D:253:PHE:C	2:D:255:LYS:H	2.22	0.43
1:F:1:DG:H5'	1:F:1:DG:C8	2.50	0.42
2:A:5:LYS:N	2:A:6:PRO:CD	2.82	0.42
2:B:257:ILE:O	2:B:257:ILE:HG22	2.17	0.42
2:B:4:ILE:HD11	2:B:117:LEU:HD11	2.00	0.42
2:C:188:ALA:HB1	2:C:215:LEU:HD23	2.01	0.42
2:B:52:LEU:HG	2:B:119:LYS:HB2	2.01	0.42
2:D:148:LEU:HD22	2:D:230:TYR:CD2	2.54	0.42
2:D:120:ASP:O	2:D:121:GLN:HB2	2.20	0.42
2:A:55:LYS:O	2:A:58:GLU:HB3	2.20	0.42
2:D:161:PHE:HB3	2:D:223:ARG:HB3	2.00	0.42
2:B:152:CYS:HB3	2:B:231:LEU:HD21	2.00	0.42
2:D:86:LEU:O	2:D:90:SER:CB	2.67	0.42
2:B:174:GLU:O	2:B:181:VAL:HG12	2.19	0.42
2:C:84:THR:HG21	2:C:155:MET:HG3	2.01	0.42
1:F:13:DG:C8	2:B:93:LYS:HB3	2.54	0.42
2:C:195:PRO:HD3	2:C:226:TRP:CE3	2.55	0.42
2:B:14:ILE:HD12	2:B:14:ILE:O	2.20	0.42
2:C:77:TYR:CD2	2:C:86:LEU:HD21	2.55	0.42
2:B:19:LYS:HA	2:B:180:LEU:O	2.19	0.42
2:A:9:GLN:HE21	2:A:9:GLN:HA	1.84	0.42
2:C:209:GLN:HA	4:C:284:HOH:O	2.19	0.42
2:C:166:ILE:HD11	2:C:190:LEU:HD23	2.01	0.42
1:G:13:DG:H2'	2:C:93:LYS:N	2.35	0.42
2:B:198:LEU:HG	2:B:208:ILE:HD12	2.00	0.42
2:C:52:LEU:HD13	2:C:119:LYS:CG	2.48	0.42
2:A:74:GLU:O	2:A:78:LYS:HG3	2.20	0.42
2:B:86:LEU:HD23	2:B:90:SER:OG	2.20	0.42
2:C:197:GLU:O	2:C:198:LEU:C	2.59	0.42
2:A:70:ILE:HD12	2:A:75:ALA:O	2.20	0.42
2:A:240:GLN:O	2:A:243:ILE:HG23	2.20	0.42
2:A:28:LEU:N	2:A:28:LEU:HD22	2.35	0.42
2:D:45:LEU:HB3	2:D:53:THR:HG21	2.02	0.42
2:A:23:PRO:C	2:A:25:SER:H	2.23	0.42
2:C:208:ILE:HG23	2:C:208:ILE:O	2.19	0.41
1:G:5:DG:OP2	2:C:203:ALA:HB2	2.20	0.41
2:B:87:PHE:CG	2:B:154:LYS:HE3	2.55	0.41
2:D:12:ASN:HD22	2:D:12:ASN:C	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:DG:H2"	1:H:2:DC:C6	2.55	0.41
2:A:257:ILE:HD11	2:B:235:VAL:CG2	2.45	0.41
2:B:24:LYS:HZ3	2:B:25:SER:H	1.64	0.41
2:A:9:GLN:NE2	2:A:9:GLN:HA	2.36	0.41
2:A:208:ILE:HD11	2:A:210:PHE:CE2	2.55	0.41
2:A:85:LEU:HD21	2:A:123:TYR:CZ	2.56	0.41
2:C:148:LEU:HB3	2:C:230:TYR:OH	2.20	0.41
2:D:18:GLN:C	2:D:181:VAL:HG13	2.41	0.41
2:C:46:LYS:HA	2:C:53:THR:OG1	2.19	0.41
2:C:129:LYS:NZ	2:C:142:ILE:HA	2.36	0.41
2:C:167:ASN:OD1	2:C:189:GLU:HB3	2.20	0.41
2:D:67:ASN:O	2:D:70:ILE:HG23	2.20	0.41
2:C:52:LEU:HD12	2:C:118:VAL:N	2.35	0.41
2:A:161:PHE:CE1	2:A:224:GLU:HA	2.56	0.41
2:A:152:CYS:HA	2:A:155:MET:HE2	2.03	0.41
1:E:11:DC:H6	2:B:136:SER:O	2.03	0.41
2:C:156:ILE:HG22	2:C:161:PHE:CE1	2.53	0.41
2:A:48:ASN:O	2:A:49:LEU:HD23	2.21	0.41
2:C:24:LYS:O	2:C:25:SER:HB3	2.21	0.41
2:C:133:ILE:C	2:C:135:LYS:H	2.25	0.41
2:B:245:MET:O	2:B:248:LYS:O	2.39	0.40
2:D:43:LYS:O	2:D:47:GLU:HG3	2.21	0.40
2:D:189:GLU:HB2	2:D:192:LYS:CB	2.49	0.40
2:A:38:GLU:HG2	2:A:128:VAL:HG11	2.03	0.40
2:D:147:LYS:HG2	2:D:147:LYS:O	2.21	0.40
1:H:4:DG:H8	2:D:199:TYR:OH	2.04	0.40
2:B:248:LYS:CB	2:B:248:LYS:NZ	2.85	0.40
2:D:49:LEU:N	2:D:49:LEU:HD12	2.37	0.40
2:D:142:ILE:HG23	2:D:168:TYR:CE2	2.57	0.40
2:B:170:GLU:OE1	2:B:172:ASP:OD1	2.38	0.40
2:D:82:SER:CB	2:D:85:LEU:HB2	2.50	0.40

All (2) 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)
2:A:174:GLU:OE1	2:A:174:GLU:OE1[8_556]	1.90	0.30
4:F:448:HOH:O	4:F:448:HOH:O[6_655]	2.16	0.04

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
2	A	255/257 (99%)	221 (87%)	30 (12%)	4 (2%)	12 24
2	B	254/257 (99%)	223 (88%)	25 (10%)	6 (2%)	7 13
2	C	255/257 (99%)	196 (77%)	51 (20%)	8 (3%)	5 8
2	D	254/257 (99%)	211 (83%)	33 (13%)	10 (4%)	4 5
All	All	1018/1028 (99%)	851 (84%)	139 (14%)	28 (3%)	6 10

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	71	ILE
2	B	221	GLY
2	B	223	ARG
2	C	94	ALA
2	D	21	LYS
2	A	24	LYS
2	B	112	THR
2	C	90	SER
2	C	96	THR
2	C	163	LEU
2	D	20	VAL
2	A	50	SER
2	A	255	LYS
2	B	111	ASP
2	C	50	SER
2	C	198	LEU
2	D	135	LYS
2	C	82	SER
2	C	134	SER
2	D	52	LEU
2	D	120	ASP
2	D	210	PHE

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Mol	Chain	Res	Type
2	B	70	ILE
2	D	93	LYS
2	D	134	SER
2	D	177	GLY
2	A	35	GLU
2	D	51	ASP

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	
2	A	220/229 (96%)	207 (94%)	13 (6%)	24	47
2	B	224/229 (98%)	206 (92%)	18 (8%)	15	29
2	C	208/229 (91%)	198 (95%)	10 (5%)	31	58
2	D	215/229 (94%)	206 (96%)	9 (4%)	36	65
All	All	867/916 (95%)	817 (94%)	50 (6%)	25	49

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	LYS
2	A	45	LEU
2	A	62	ASP
2	A	107	GLU
2	A	128	VAL
2	A	148	LEU
2	A	198	LEU
2	A	208	ILE
2	A	214	ASP
2	A	231	LEU
2	A	240	GLN
2	A	243	ILE
2	A	254	LYS
2	B	10	ASP
2	B	19	LYS

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Mol	Chain	Res	Type
2	B	24	LYS
2	B	28	LEU
2	B	46	LYS
2	B	78	LYS
2	B	81	ASN
2	B	102	GLU
2	B	119	LYS
2	B	131	ARG
2	B	148	LEU
2	B	171	VAL
2	B	185	THR
2	B	198	LEU
2	B	208	ILE
2	B	216	ASP
2	B	220	ASN
2	B	247	ASP
2	C	3	PHE
2	C	9	GLN
2	C	22	ARG
2	C	49	LEU
2	C	54	PHE
2	C	60	LEU
2	C	96	THR
2	C	164	PHE
2	C	194	GLU
2	C	255	LYS
2	D	12	ASN
2	D	39	LYS
2	D	51	ASP
2	D	54	PHE
2	D	70	ILE
2	D	71	ILE
2	D	91	ARG
2	D	107	GLU
2	D	114	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	9	GLN
2	A	98	ASN
2	A	109	GLN

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Mol	Chain	Res	Type
2	A	150	GLN
2	A	211	HIS
2	A	237	GLN
2	A	240	GLN
2	B	31	HIS
2	B	81	ASN
2	B	98	ASN
2	C	31	HIS
2	C	61	ASN
2	C	121	GLN
2	C	138	GLN
2	C	150	GLN
2	C	237	GLN
2	D	12	ASN
2	D	18	GLN
2	D	109	GLN
2	D	132	ASN
2	D	217	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	E	13/13 (100%)	-0.19	0 100 100	19, 27, 64, 68	0
1	F	13/13 (100%)	-0.13	0 100 100	21, 29, 40, 73	0
1	G	13/13 (100%)	0.40	1 (7%) 16 11	39, 49, 85, 120	0
1	H	13/13 (100%)	0.53	1 (7%) 16 11	43, 48, 66, 85	0
2	A	257/257 (100%)	-0.05	5 (1%) 70 64	23, 45, 65, 79	0
2	B	256/257 (99%)	-0.01	4 (1%) 74 69	21, 44, 64, 89	0
2	C	257/257 (100%)	1.18	55 (21%) 1 0	46, 102, 143, 153	0
2	D	256/257 (99%)	0.60	32 (12%) 5 3	37, 78, 121, 139	0
All	All	1078/1080 (99%)	0.42	98 (9%) 11 7	19, 59, 127, 153	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	258	LEU	7.2
2	C	71	ILE	6.5
2	C	101	ILE	6.2
2	C	104	LEU	5.6
2	C	222	THR	5.2
2	C	70	ILE	4.9
2	C	221	GLY	4.6
2	C	49	LEU	4.6
2	C	64	PHE	4.4
2	D	254	LYS	4.3
2	C	159	LYS	4.2
2	B	156	ILE	4.1
2	C	6	PRO	4.1
2	A	258	LEU	4.0
2	D	176	ASN	3.9
2	C	113	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	178	GLU	3.7
2	C	7	ILE	3.7
2	A	27	THR	3.6
2	C	51	ASP	3.5
2	C	102	GLU	3.5
2	C	119	LYS	3.5
2	D	255	LYS	3.5
2	C	50	SER	3.4
2	D	247	ASP	3.4
2	C	257	ILE	3.4
2	C	10	ASP	3.3
2	D	180	LEU	3.2
2	C	219	PHE	3.2
2	C	76	ARG	3.1
2	C	105	PHE	3.1
2	C	175	LEU	3.1
2	C	156	ILE	3.1
2	C	22	ARG	3.1
2	C	26	GLY	3.1
2	D	121	GLN	3.1
1	H	1	DG	3.0
2	C	80	PHE	2.9
2	D	44	PHE	2.9
2	D	175	LEU	2.9
2	D	179	ASP	2.9
2	C	161	PHE	2.9
2	A	34	GLY	2.9
2	D	162	ASP	2.8
2	A	25	SER	2.8
2	D	174	GLU	2.8
2	C	254	LYS	2.7
2	C	47	GLU	2.7
2	C	114	ASP	2.7
2	D	11	ILE	2.7
2	B	257	ILE	2.7
2	C	56	GLN	2.6
2	D	183	VAL	2.6
2	C	220	ASN	2.6
2	C	68	PRO	2.6
2	D	22	ARG	2.6
2	C	160	GLU	2.6
2	D	243	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	177	GLY	2.5
2	B	24	LYS	2.5
2	D	52	LEU	2.5
2	C	62	ASP	2.4
2	C	79	LEU	2.4
2	D	126	LEU	2.4
2	C	96	THR	2.4
2	C	65	MET	2.4
2	D	133	ILE	2.4
2	D	242	ALA	2.4
2	D	246	ILE	2.4
2	D	51	ASP	2.4
2	D	49	LEU	2.4
2	C	118	VAL	2.4
1	G	13	DG	2.3
2	C	120	ASP	2.3
2	D	14	ILE	2.3
2	C	155	MET	2.3
2	D	16	ILE	2.3
2	C	99	TRP	2.3
2	C	72	GLY	2.3
2	C	178	GLU	2.3
2	C	69	ALA	2.2
2	D	113	ALA	2.2
2	C	177	GLY	2.2
2	C	176	ASN	2.2
2	C	112	THR	2.2
2	D	249	PHE	2.2
2	C	3	PHE	2.1
2	C	95	ALA	2.1
2	B	112	THR	2.1
2	A	26	GLY	2.1
2	C	127	ASP	2.1
2	D	127	ASP	2.1
2	C	121	GLN	2.1
2	C	125	LEU	2.1
2	D	27	THR	2.1
2	D	257	ILE	2.1
2	C	9	GLN	2.0
2	D	181	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	NA	B	601	1/1	0.94	0.11	-3.00	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.