WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:55 AM GMT

PDB ID	:	2V9W
Title	:	COMPLEX STRUCTURE OF SULFOLOBUS SOLFATARICUS DPO4 AND DNA DUPLEX CONTAINING A HYDROPHOBIC THYMINE ISOSTERE 2,4-DIFLUOROTOLUENE NUCLEOTIDE IN THE TEMPLATE STRAND
Authors	:	Irimia, A.; Pallan, P.S.; Egli, M.
Deposited on	:	2007-08-27
Resolution	:	3.00 Å(reported)

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

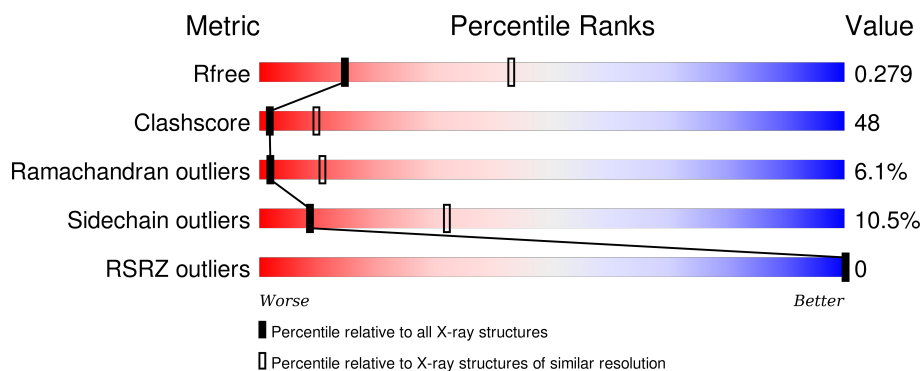|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.00 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.
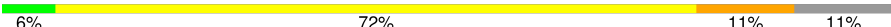
Metric	Percentile Ranks	Value
Rfree		0.279
Clashscore		48
Ramachandran outliers		6.1%
Sidechain outliers		10.5%
RSRZ outliers		0

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	A	358	32% 52% 10% · ·
1	B	358	39% 48% 8% ·
2	C	13	38% 62%
2	E	13	54% 46%
3	D	18	22% 78%

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Mol	Chain	Length	Quality of chain
3	F	18	6% 72% 11% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DCT	B	1346	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6961 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 DNA POLYMERASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total 2758	C 1768	N 475	O 508	S 7	0	18	1
1	B	343	Total 2764	C 1771	N 478	O 508	S 7	0	14	1

- Molecule 2 is a DNA chain called 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP *CP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total 275	C 129	N 60	O 74	P 12	0	0	0
2	E	13	Total 275	C 129	N 60	O 74	P 12	0	0	0

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

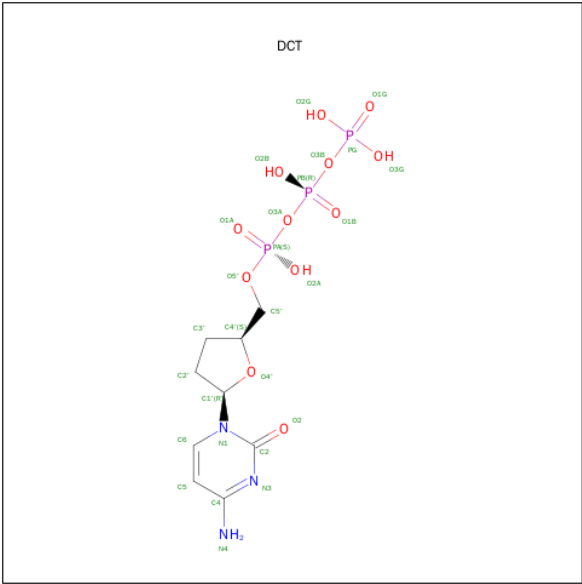| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	18	Total 355	C 174	F 2	N 54	O 108	P 17	0	2	0
3	F	16	Total 319	C 154	F 2	N 50	O 97	P 16	0	1	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Ca 2	0	0
4	A	2	Total 2	Ca 2	0	0

- Molecule 5 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (three-letter code: DCT)

(formula: $C_9H_{16}N_3O_{12}P_3$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 27	C 9	N 3	O 12	P 3	0	0
5	B	1	Total 27	C 9	N 3	O 12	P 3	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	59	Total 59	O 59	0	0
6	B	48	Total 48	O 48	0	0
6	C	14	Total 14	O 14	0	0
6	D	9	Total 9	O 9	0	0
6	E	12	Total 12	O 12	0	0
6	F	15	Total 15	O 15	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.

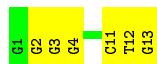- Molecule 1: DNA POLYMERASE IV
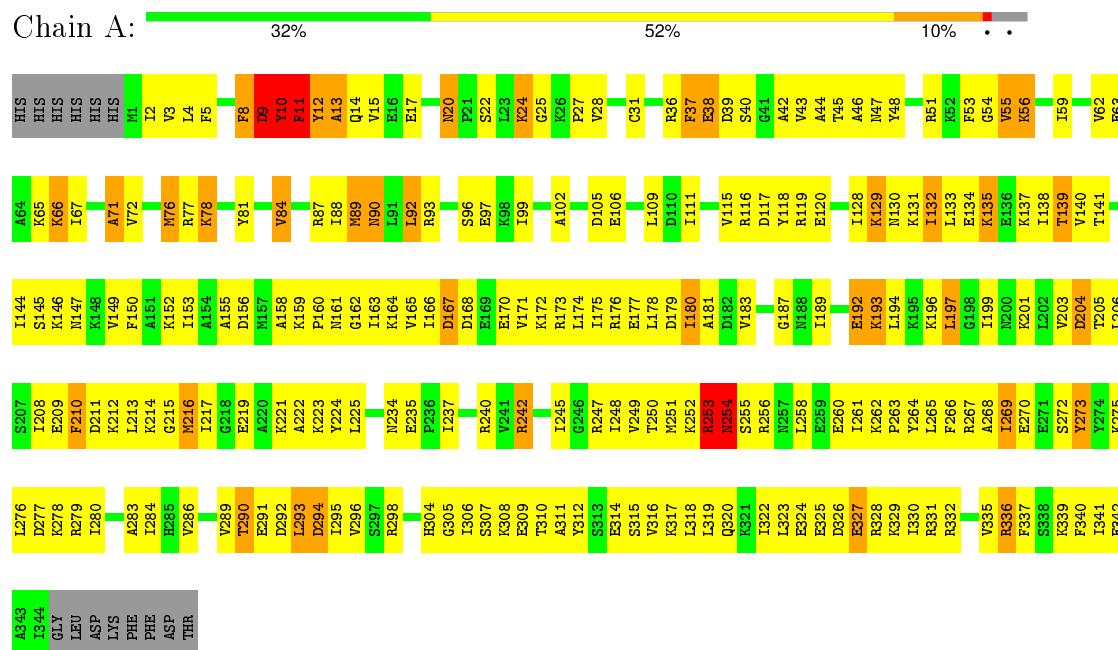
- Molecule 1: DNA POLYMERASE IV
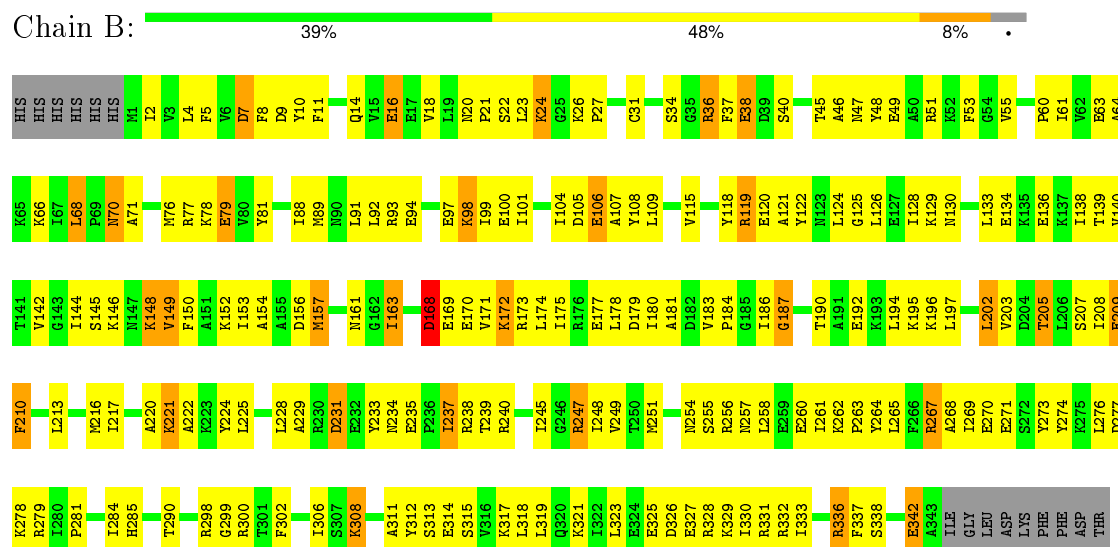
• Molecule 2: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP *CP*TP*G)-3'

Chain C:
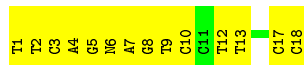
• Molecule 2: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP *CP*TP*G)-3'

Chain E:

• Molecule 3: 5'-D(*TP*TP*CP*AP*GP*DFTP*AP*GP*TP*CP*CP *TP*TP*CP*CP*CP*C P*C)-3'

Chain D:

• Molecule 3: 5'-D(*TP*TP*CP*AP*GP*DFTP*AP*GP*TP*CP*CP *TP*TP*CP*CP*CP*C P*C)-3'

Chain F:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.70Å 186.74Å 52.73Å 90.00° 110.06° 90.00°	Depositor
Resolution (Å)	49.51 – 3.00 49.51 – 2.94	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.51-3.00) 86.0 (49.51-2.94)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.59 (at 2.96Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.290 0.209 , 0.279	Depositor DCC
R_{free} test set	813 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.0	EDS
Estimated twinning fraction	0.206 for l,-k,h	Xtriage
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Outliers	1 of 17454 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6961	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DFT, CA, DCT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.54	0/2797	0.72	3/3757 (0.1%)
1	B	0.49	0/2803	0.63	0/3764
2	C	0.66	0/311	0.80	0/481
2	E	0.42	0/311	0.68	0/481
3	D	0.44	0/371	0.73	0/566
3	F	0.85	1/331 (0.3%)	0.84	1/502 (0.2%)
All	All	0.53	1/6924 (0.0%)	0.70	4/9551 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3[A]	DC	OP3-P	-6.67	1.53	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	TYR	CB-CG-CD1	-5.98	117.41	121.00
3	F	7	DA	C5'-C4'-O4'	5.74	120.20	109.30
1	A	9	ASP	C-N-CA	-5.42	108.14	121.70
1	A	11	PHE	N-CA-C	5.21	125.06	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2758	0	2867	324	0
1	B	2764	0	2881	221	0
2	C	275	0	146	36	0
2	E	275	0	146	18	0
3	D	355	0	196	18	0
3	F	319	0	177	36	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	27	0	12	5	0
5	B	27	0	12	13	0
6	A	59	0	0	16	0
6	B	48	0	0	4	0
6	C	14	0	0	6	0
6	D	9	0	0	1	0
6	E	12	0	0	4	0
6	F	15	0	0	6	0
All	All	6961	0	6437	644	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 48.

All (644) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LYS:HE3	1:A:266:PHE:CE1	1.71	1.26
5:B:1346:DCT:C5'	2:E:13:DG:H2"	1.69	1.23
5:B:1346:DCT:H5'	2:E:13:DG:C2'	1.74	1.15
2:C:12:DT:H5'	2:C:13:DG:N7	1.61	1.14
1:A:180:ILE:HG22	1:A:181:ALA:H	1.14	1.10
5:B:1346:DCT:H6	5:B:1346:DCT:H5"	1.39	1.04
1:A:137:LYS:HD3	6:A:2024:HOH:O	1.58	1.02
1:A:62:VAL:O	1:A:66:LYS:HD2	1.62	0.99
6:A:2054:HOH:O	3:D:2[A]:DT:H72	1.63	0.96
1:A:180:ILE:HG22	1:A:181:ALA:N	1.78	0.96
3:D:17:DC:H2"	3:D:18:DC:C5	1.99	0.96
1:B:60:PRO:HB2	1:B:63:GLU:HG2	1.47	0.94
2:C:12:DT:C5'	2:C:13:DG:N7	2.31	0.93
1:A:308:LYS:HG2	6:A:2041:HOH:O	1.68	0.91
1:A:208:ILE:HG22	1:A:209:GLU:H	1.33	0.91
1:A:45:THR:HG22	1:A:46:ALA:H	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LYS:CE	1:A:266:PHE:CE1	2.54	0.90
1:B:20:ASN:HD22	1:B:23:LEU:HG	1.37	0.90
1:A:199:ILE:HD12	1:A:199:ILE:H	1.36	0.89
1:B:148:LYS:HB2	1:B:148:LYS:HZ3	1.37	0.89
1:B:60:PRO:HD2	1:B:63:GLU:HG3	1.53	0.88
5:B:1346:DCT:H6	5:B:1346:DCT:C5'	2.04	0.87
1:A:253:ARG:HA	1:A:253:ARG:CZ	2.05	0.87
1:B:97:GLU:HG2	1:B:98:LYS:HD3	1.55	0.86
1:B:148:LYS:NZ	1:B:148:LYS:HB2	1.91	0.85
1:A:56:LYS:HZ2	1:A:59:ILE:HG23	1.39	0.85
1:A:45:THR:HG22	1:A:46:ALA:N	1.91	0.85
1:A:9:ASP:HB3	1:A:10:TYR:CD2	2.13	0.83
2:C:12:DT:H2"	2:C:13:DG:H5'	1.60	0.83
1:A:9:ASP:HB3	1:A:10:TYR:HD2	1.44	0.83
3:F:18:DC:H2'	6:F:2015:HOH:O	1.78	0.83
3:F:3[A]:DC:H2"	3:F:4:DA:C5'	2.09	0.83
1:A:258:LEU:HD21	6:A:2038:HOH:O	1.79	0.82
1:B:36:ARG:HG2	1:B:37:PHE:H	1.44	0.82
2:C:12:DT:H2'	2:C:13:DG:O4'	1.78	0.82
3:F:3[A]:DC:H2"	3:F:4:DA:H5'	1.62	0.82
1:B:332:ARG:NH2	3:F:6:DFT:H71	1.95	0.82
1:B:265:LEU:HD11	1:B:315:SER:OG	1.80	0.81
1:A:252:LYS:HD2	1:A:264:TYR:OH	1.80	0.81
1:A:253:ARG:O	1:A:254:ASN:HB2	1.81	0.81
1:A:9:ASP:O	1:A:10:TYR:HB3	1.79	0.81
2:C:12:DT:H2"	2:C:13:DG:C5'	2.11	0.80
1:B:21:PRO:O	1:B:24[A]:LYS:HG3	1.81	0.80
1:A:258:LEU:HD12	1:A:262:LYS:HB2	1.64	0.80
6:A:2046:HOH:O	2:C:7:DA:H8	1.65	0.80
2:C:11:DC:H1'	2:C:12:DT:H5"	1.63	0.80
5:B:1346:DCT:H5'	2:E:13:DG:H2"	0.85	0.79
1:B:192:GLU:HA	1:B:192:GLU:OE2	1.81	0.79
2:C:12:DT:H3'	2:C:13:DG:H8	1.48	0.79
1:B:271:GLU:O	1:B:274:TYR:HB3	1.83	0.78
1:A:266:PHE:O	1:A:270:GLU:HG2	1.83	0.78
2:C:12:DT:H5'	2:C:13:DG:C8	2.17	0.78
1:A:147:ASN:HD21	1:A:150:PHE:HD1	1.31	0.78
2:C:12:DT:C5'	2:C:13:DG:C8	2.68	0.77
1:B:49:GLU:OE2	1:B:49:GLU:N	2.18	0.77
1:B:133:LEU:HD22	6:B:2021:HOH:O	1.85	0.76
3:F:5:DG:H2"	3:F:6:DFT:H5"	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LEU:O	1:B:269:ILE:HG13	1.85	0.75
1:B:5:PHE:CZ	1:B:106:GLU:HG2	2.21	0.75
1:A:131:LYS:HE2	1:A:135:LYS:HZ3	1.52	0.75
2:C:12:DT:H2'	2:C:13:DG:C8	2.22	0.74
1:A:66:LYS:HE3	1:A:66:LYS:HA	1.70	0.74
1:A:273:TYR:OH	1:A:306:ILE:HG22	1.88	0.73
1:A:258:LEU:CD1	1:A:262:LYS:HB2	2.17	0.73
1:A:265:LEU:O	1:A:269:ILE:HG13	1.89	0.73
3:D:3[A]:DC:H5	6:D:2005:HOH:O	1.70	0.73
1:A:14:GLN:HE22	1:A:139:THR:H	1.35	0.73
1:B:40:SER:HB2	3:F:4:DA:OP1	1.90	0.72
2:E:12:DT:H71	6:E:2011:HOH:O	1.88	0.72
1:A:265:LEU:HG	1:A:269:ILE:HD11	1.71	0.72
1:A:105:ASP:OD2	5:A:1347:DCT:H5'	1.90	0.72
2:C:12:DT:C3'	2:C:13:DG:H8	2.02	0.72
1:B:97:GLU:HG2	1:B:98:LYS:CD	2.18	0.72
1:A:180:ILE:O	1:A:183:VAL:HG23	1.89	0.71
1:A:331:ARG:HG2	1:A:332:ARG:HG3	1.73	0.71
1:A:56:LYS:NZ	1:A:59:ILE:CG2	2.54	0.71
1:A:63:GLU:O	1:A:66:LYS:HB2	1.89	0.71
1:A:309:GLU:HA	1:A:312:TYR:HD1	1.56	0.71
1:A:45:THR:CG2	1:A:46:ALA:H	2.02	0.71
1:A:258:LEU:HD11	1:A:262:LYS:HD3	1.73	0.70
1:A:292:ASP:O	1:A:293:LEU:HG	1.91	0.70
3:F:9:DT:H2"	3:F:10:DC:C6	2.27	0.70
1:A:309:GLU:HA	1:A:312:TYR:CD1	2.27	0.70
1:A:139:THR:HG21	6:A:2025:HOH:O	1.90	0.70
1:B:285:HIS:CD2	1:B:299:GLY:HA3	2.27	0.69
1:B:217:ILE:HD12	1:B:221:LYS:HB3	1.75	0.69
1:A:133:LEU:O	1:A:137:LYS:HA	1.92	0.69
1:A:56:LYS:HZ2	1:A:59:ILE:CG2	2.06	0.69
1:B:152:LYS:HE2	6:B:2011:HOH:O	1.92	0.69
1:A:309:GLU:CD	1:A:309:GLU:H	1.94	0.68
1:B:36:ARG:HG2	1:B:37:PHE:N	2.07	0.68
1:B:70:ASN:C	1:B:70:ASN:HD22	1.96	0.68
1:B:336:ARG:HH22	3:F:7:DA:H2"	1.58	0.68
5:B:1346:DCT:C6	5:B:1346:DCT:H5"	2.21	0.68
2:C:11:DC:H1'	6:C:2011:HOH:O	1.92	0.67
1:A:14:GLN:NE2	1:A:139:THR:HG23	2.08	0.67
1:B:14:GLN:NE2	1:B:139:THR:H	1.93	0.67
1:B:186:ILE:HG13	1:B:225:LEU:HD21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:HD12	1:B:144:ILE:HG12	1.77	0.67
1:A:254:ASN:HA	1:A:330:ILE:O	1.94	0.67
1:A:258:LEU:HD12	1:A:258:LEU:O	1.95	0.67
1:A:66:LYS:CA	1:A:66:LYS:HE3	2.25	0.67
1:A:8:PHE:CD1	1:A:8:PHE:N	2.60	0.67
1:A:131:LYS:HE2	1:A:135:LYS:NZ	2.09	0.66
1:A:208:ILE:HG22	1:A:209:GLU:N	2.08	0.66
1:B:336:ARG:NH2	3:F:7:DA:H2"	2.09	0.66
1:A:8:PHE:HD1	1:A:8:PHE:N	1.94	0.66
1:B:254:ASN:HB3	1:B:329:LYS:HB3	1.77	0.66
1:B:302:PHE:HZ	1:B:314[A]:GLU:HG2	1.61	0.66
1:A:318:LEU:O	1:A:322:ILE:HG13	1.96	0.66
2:C:5:DG:N2	6:C:2003:HOH:O	2.23	0.66
2:C:11:DC:C6	2:C:12:DT:H71	2.31	0.66
1:A:132:ILE:HG22	1:A:133:LEU:N	2.11	0.66
1:B:163:ILE:O	1:B:163:ILE:HG23	1.95	0.65
1:B:115:VAL:HG13	1:B:120:GLU:HB2	1.76	0.65
1:A:179:ASP:HA	1:A:201:LYS:HA	1.77	0.65
1:B:14:GLN:HG2	1:B:138:ILE:CD1	2.27	0.65
1:B:14:GLN:HG2	1:B:138:ILE:HD13	1.79	0.65
1:A:118:TYR:HE1	1:A:167:ASP:HA	1.62	0.65
1:A:24:LYS:HD3	1:A:25:GLY:H	1.61	0.65
1:B:148:LYS:NZ	1:B:148:LYS:CB	2.60	0.64
1:A:279:ARG:HH11	1:A:279:ARG:HG2	1.63	0.64
2:E:11:DC:H2"	2:E:12:DT:OP2	1.97	0.64
1:A:128:ILE:O	1:A:130:ASN:N	2.30	0.64
1:A:45:THR:CG2	1:A:46:ALA:N	2.60	0.64
1:A:262:LYS:HE2	6:A:2014:HOH:O	1.98	0.64
1:B:332:ARG:HH22	3:F:6:DFT:H71	1.61	0.64
1:A:192:GLU:OE2	1:A:193:LYS:HG2	1.98	0.64
1:A:9:ASP:OD2	1:A:161:ASN:N	2.29	0.63
1:B:99:ILE:HG12	1:B:100:GLU:N	2.13	0.63
2:C:12:DT:C3'	2:C:13:DG:C8	2.81	0.63
1:B:237:ILE:O	1:B:237:ILE:HG22	1.97	0.63
1:A:264:TYR:HA	1:A:267:ARG:HD2	1.79	0.63
1:B:97:GLU:CD	1:B:97:GLU:H	2.00	0.63
1:A:314:GLU:HA	1:A:317:LYS:NZ	2.13	0.63
1:A:116:ARG:HB3	1:A:120:GLU:OE2	1.99	0.63
1:A:251:MET:C	1:A:253:ARG:H	2.02	0.63
1:A:251:MET:HE2	1:A:330:ILE:HG22	1.80	0.63
1:A:145:SER:OG	1:A:146:LYS:N	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:OG1	1:A:332:ARG:HG2	1.99	0.63
1:B:4:LEU:HD11	1:B:142:VAL:HG11	1.80	0.63
1:B:308:LYS:O	1:B:311:ALA:HB3	1.98	0.63
1:A:36:ARG:NH2	1:A:251:MET:O	2.32	0.62
1:B:262:LYS:N	1:B:263:PRO:HD2	2.13	0.62
2:C:8:DG:H4'	6:C:2006:HOH:O	1.97	0.62
1:B:122:TYR:HE2	1:B:126:LEU:HD11	1.64	0.62
1:B:221:LYS:O	1:B:224:TYR:HB3	1.99	0.62
1:B:302:PHE:CD1	1:B:306:ILE:HD11	2.35	0.62
1:A:28:VAL:H	1:A:47:ASN:HD21	1.45	0.62
1:A:180:ILE:CG2	1:A:181:ALA:N	2.51	0.61
1:A:209:GLU:O	1:A:211:ASP:N	2.33	0.61
1:A:89:MET:HA	1:A:92:LEU:HD12	1.81	0.61
1:B:326:ASP:OD2	1:B:328:ARG:HD2	2.00	0.61
1:A:251:MET:HA	1:A:264:TYR:CZ	2.35	0.61
1:A:317:LYS:HB2	1:A:317:LYS:NZ	2.14	0.61
1:A:137:LYS:NZ	6:A:2023:HOH:O	2.23	0.61
1:A:252:LYS:HD2	1:A:252:LYS:H	1.64	0.61
1:A:336:ARG:NH1	6:A:2056:HOH:O	2.32	0.61
1:A:9:ASP:O	1:A:10:TYR:CB	2.45	0.61
2:E:12:DT:C7	6:E:2011:HOH:O	2.47	0.61
1:A:199:ILE:H	1:A:199:ILE:CD1	2.11	0.61
5:B:1346:DCT:O1A	5:B:1346:DCT:O1G	2.18	0.60
3:F:5:DG:H2"	3:F:6:DFT:C5'	2.31	0.60
1:A:256:ARG:HG3	1:A:323:LEU:HD22	1.83	0.60
1:B:300[A]:ARG:HD3	1:B:302:PHE:CZ	2.35	0.60
1:A:116:ARG:HH11	1:A:116:ARG:HG3	1.64	0.60
1:A:197:LEU:HB2	1:A:199:ILE:CD1	2.31	0.60
1:B:14:GLN:HE22	1:B:139:THR:H	1.48	0.60
1:B:125:GLY:O	1:B:129:LYS:HG3	2.02	0.60
1:A:263:PRO:O	1:A:267:ARG:HG3	2.02	0.60
1:B:251:MET:HB3	1:B:264:TYR:CE2	2.36	0.60
1:A:329:LYS:NZ	6:A:2054:HOH:O	2.33	0.60
1:A:216:MET:HG3	1:A:217:ILE:HG23	1.84	0.60
1:A:262:LYS:N	1:A:263:PRO:HD2	2.17	0.60
1:B:47:ASN:HD21	1:B:49:GLU:HB2	1.67	0.60
1:A:279:ARG:HD3	1:A:340:PHE:CE2	2.37	0.60
1:A:251:MET:CE	1:A:330:ILE:HG22	2.32	0.59
1:A:176:ARG:HH11	1:A:176:ARG:HB3	1.66	0.59
1:A:147:ASN:ND2	1:A:150:PHE:HD1	1.99	0.59
1:A:119:ARG:NH1	6:A:2018:HOH:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LYS:NZ	1:A:316:VAL:HG23	2.17	0.59
1:A:245:ILE:HG21	1:A:275:LYS:HB2	1.85	0.59
1:A:181:ALA:C	1:A:183:VAL:H	2.06	0.59
1:B:60:PRO:HB2	1:B:63:GLU:CG	2.26	0.59
1:A:141:THR:HG21	1:A:155:ALA:O	2.01	0.59
1:A:269:ILE:HG12	1:A:335:VAL:HG21	1.84	0.59
1:A:31:CYS:HB3	1:A:43:VAL:HA	1.83	0.59
2:C:12:DT:C2'	2:C:13:DG:O4'	2.50	0.59
2:C:12:DT:C2'	2:C:13:DG:C8	2.86	0.58
1:B:146:LYS:HD2	1:B:171:VAL:HG21	1.84	0.58
1:A:280:ILE:CG2	1:A:305:GLY:HA3	2.33	0.58
1:A:149:VAL:O	1:A:153:ILE:HG13	2.04	0.58
1:A:51:ARG:HH11	1:A:51:ARG:HG3	1.67	0.58
3:F:17:DC:H5	6:F:2014:HOH:O	1.85	0.58
1:A:317:LYS:HB2	1:A:317:LYS:HZ3	1.68	0.58
1:A:28:VAL:H	1:A:47:ASN:ND2	2.01	0.58
1:A:4:LEU:HB3	1:A:109:LEU:HB2	1.86	0.58
1:B:92:LEU:HD23	1:B:92:LEU:N	2.18	0.58
1:A:251:MET:C	1:A:253:ARG:N	2.55	0.58
3:F:17:DC:H4'	6:F:2013:HOH:O	2.04	0.58
2:E:3:DG:H2"	2:E:4:DG:C8	2.38	0.58
1:B:88:ILE:HA	1:B:91:LEU:HD12	1.86	0.58
1:B:302:PHE:CZ	1:B:314[A]:GLU:HG2	2.39	0.58
1:A:316:VAL:CG1	1:A:320:GLN:HE21	2.17	0.57
1:A:280:ILE:HB	1:A:341:ILE:HD12	1.86	0.57
1:A:11:PHE:O	1:A:12:TYR:C	2.42	0.57
1:A:237:ILE:O	1:A:237:ILE:HG22	2.05	0.57
1:A:37:PHE:HB2	1:A:40:SER:HB2	1.85	0.57
1:A:210[A]:PHE:CE1	1:A:223:LYS:HG2	2.39	0.57
1:A:256:ARG:HH22	1:A:327:GLU:HA	1.68	0.57
1:A:280:ILE:HG22	1:A:305:GLY:HA3	1.86	0.57
1:A:277:ASP:CG	1:A:278:LYS:H	2.06	0.57
1:A:180:ILE:CG2	1:A:181:ALA:H	1.91	0.57
1:A:10:TYR:CE2	1:A:14:GLN:HG3	2.39	0.57
1:A:240[A]:ARG:HG2	1:A:242:ARG:NH2	2.19	0.57
1:A:88:ILE:CG2	1:A:132:ILE:HD11	2.35	0.57
1:A:56:LYS:NZ	1:A:59:ILE:HG22	2.19	0.57
1:A:90:ASN:O	1:A:93:ARG:HB3	2.04	0.57
1:A:279:ARG:HD3	1:A:340:PHE:CD2	2.40	0.57
2:E:2:DG:H2"	2:E:3:DG:OP2	2.03	0.57
1:B:77:ARG:O	1:B:79:GLU:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HD12	1:A:118:TYR:CD2	2.40	0.57
1:A:20:ASN:C	1:A:20:ASN:HD22	2.07	0.57
1:B:2:ILE:HD12	1:B:118[A]:TYR:CD1	2.40	0.56
1:A:54:GLY:O	1:A:56:LYS:N	2.38	0.56
1:A:199:ILE:N	1:A:199:ILE:HD12	2.12	0.56
1:B:323:LEU:O	1:B:327:GLU:HG2	2.05	0.56
1:A:130:ASN:ND2	6:A:2021:HOH:O	2.38	0.56
1:B:8:PHE:CE1	1:B:88:ILE:HG21	2.40	0.56
1:A:262:LYS:HZ2	1:A:316:VAL:HG23	1.70	0.56
1:B:140:VAL:O	1:B:161:ASN:HA	2.06	0.56
1:A:264:TYR:O	1:A:267:ARG:HB2	2.06	0.56
1:A:295:ILE:N	1:A:295:ILE:HD12	2.21	0.56
1:A:56:LYS:NZ	1:A:59:ILE:HG23	2.12	0.56
1:B:14:GLN:O	1:B:18:VAL:HG23	2.05	0.56
1:A:279:ARG:HG2	1:A:279:ARG:NH1	2.20	0.56
1:A:158:ALA:HB2	1:A:164:LYS:HB2	1.88	0.56
1:B:251:MET:CE	1:B:330:ILE:O	2.54	0.56
1:A:53:PHE:O	1:A:67:ILE:HG21	2.06	0.55
1:B:202:LEU:O	1:B:205:THR:HG23	2.05	0.55
1:B:31:CYS:HB3	1:B:61:ILE:HD11	1.87	0.55
1:A:167:ASP:O	1:A:171:VAL:HG23	2.06	0.55
1:B:150:PHE:CE1	1:B:171:VAL:HG13	2.42	0.55
1:B:174:LEU:O	1:B:178:LEU:HB3	2.07	0.55
1:A:316:VAL:HG12	1:A:320:GLN:HE21	1.72	0.55
1:B:8:PHE:CE2	1:B:105:ASP:HA	2.42	0.55
3:F:5:DG:C2'	3:F:6:DFT:H5"	2.37	0.55
2:C:12:DT:O5'	2:C:13:DG:N7	2.39	0.55
2:C:11:DC:H2'	6:C:2013:HOH:O	2.07	0.55
2:E:11:DC:H2"	6:E:2011:HOH:O	2.06	0.55
1:B:251:MET:HE1	1:B:330:ILE:O	2.07	0.55
1:A:268:ALA:O	1:A:270:GLU:N	2.40	0.55
1:A:48:TYR:OH	1:A:159:LYS:HD3	2.06	0.55
1:A:262:LYS:HZ1	1:A:266:PHE:HE1	1.53	0.55
1:A:3:VAL:HG12	1:A:4:LEU:N	2.22	0.55
1:A:164:LYS:HG2	1:A:165:VAL:N	2.22	0.55
1:B:92:LEU:C	1:B:94:GLU:H	2.11	0.54
3:D:1:DT:H2'	3:D:2[A]:DT:C6	2.42	0.54
1:B:261:ILE:HG21	1:B:319:LEU:HD21	1.89	0.54
1:B:342:GLU:C	1:B:342:GLU:CD	2.65	0.54
1:A:308:LYS:O	1:A:311:ALA:HB3	2.07	0.54
1:A:176:ARG:NH1	1:A:176:ARG:HB3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:DT:H5"	6:C:2011:HOH:O	2.06	0.54
1:B:168:ASP:C	1:B:170:GLU:H	2.11	0.54
1:B:4:LEU:HB3	1:B:109:LEU:HB2	1.89	0.54
1:A:214[A]:LYS:HE2	1:A:219[A]:GLU:HG3	1.90	0.54
1:A:76:MET:HE1	1:A:78:LYS:HB2	1.90	0.54
1:A:262:LYS:CE	1:A:266:PHE:HE1	2.19	0.54
1:A:10:TYR:N	1:A:10:TYR:CD2	2.75	0.54
1:A:130:ASN:O	1:A:131:LYS:C	2.46	0.54
1:A:2:ILE:HD12	1:A:118:TYR:CE2	2.43	0.54
1:B:173:ARG:HG2	1:B:177:GLU:OE1	2.08	0.54
1:B:149:VAL:HG21	1:B:233[A]:TYR:HD2	1.74	0.53
1:A:129:LYS:NZ	1:A:161:ASN:OD1	2.41	0.53
1:A:260:GLU:HG3	1:A:260:GLU:O	2.09	0.53
1:A:262:LYS:HE3	1:A:266:PHE:CD1	2.39	0.53
1:B:20:ASN:ND2	1:B:23:LEU:HG	2.15	0.53
1:A:174:LEU:HD22	1:A:178:LEU:HB2	1.89	0.53
1:A:187:GLY:HA3	2:C:11:DC:O5'	2.09	0.53
1:A:3:VAL:O	1:A:144:ILE:HG23	2.08	0.53
1:B:217:ILE:HD11	1:B:222:ALA:CA	2.39	0.53
1:B:2:ILE:HD12	1:B:118[A]:TYR:HD1	1.73	0.53
1:B:217:ILE:HD11	1:B:222:ALA:HA	1.90	0.53
1:B:277:ASP:OD1	1:B:278:LYS:HE2	2.09	0.53
1:A:106:GLU:OE2	1:A:152:LYS:HE2	2.08	0.53
1:A:111:ILE:HD12	1:A:115:VAL:HG21	1.90	0.53
1:A:179:ASP:HB3	1:A:201:LYS:HD3	1.91	0.53
1:B:8:PHE:HA	1:B:140:VAL:HG12	1.90	0.53
1:B:122:TYR:CE2	1:B:126:LEU:HD11	2.44	0.53
1:A:255:SER:OG	1:A:256:ARG:N	2.42	0.53
1:B:290:THR:HG21	1:B:328:ARG:HD3	1.91	0.53
1:A:194:LEU:HD23	1:A:216:MET:CE	2.39	0.53
1:A:256:ARG:NH2	1:A:327:GLU:HA	2.24	0.52
1:B:119[B]:ARG:HB3	1:B:119[B]:ARG:NH1	2.24	0.52
1:B:228:LEU:O	1:B:231:ASP:N	2.42	0.52
1:B:202:LEU:HD22	1:B:229:ALA:HB2	1.91	0.52
1:A:326:ASP:OD2	1:A:328:ARG:HG2	2.09	0.52
1:A:118:TYR:CE1	1:A:167:ASP:HA	2.44	0.52
1:A:262:LYS:NZ	1:A:266:PHE:HE1	2.06	0.52
1:B:136:GLU:O	1:B:138:ILE:HG12	2.10	0.52
1:A:280:ILE:HG22	1:A:305:GLY:CA	2.40	0.52
3:D:12:DT:H2"	3:D:13:DT:H71	1.90	0.52
5:A:1347:DCT:H5'	5:A:1347:DCT:O2B	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ASP:OD2	1:B:106:GLU:OE2	2.28	0.52
1:A:262:LYS:HE3	1:A:266:PHE:CZ	2.36	0.52
1:B:10:TYR:CD2	1:B:48:TYR:HE1	2.28	0.52
1:B:168:ASP:N	1:B:168:ASP:OD1	2.42	0.52
1:B:70:ASN:C	1:B:70:ASN:ND2	2.63	0.51
1:B:46:ALA:O	1:B:51:ARG:NH1	2.43	0.51
3:D:1:DT:H2'	3:D:2[A]:DT:C5	2.45	0.51
1:A:31:CYS:HB2	1:A:42:ALA:O	2.09	0.51
1:B:180:ILE:CD1	1:B:194:LEU:HD13	2.41	0.51
1:A:262:LYS:HD3	6:A:2038:HOH:O	2.09	0.51
1:A:51:ARG:NH1	1:A:51:ARG:HG3	2.26	0.51
1:B:149:VAL:O	1:B:153:ILE:HG13	2.10	0.51
1:A:20:ASN:ND2	1:A:22:SER:OG	2.40	0.51
1:A:290:THR:O	1:A:331:ARG:HB3	2.11	0.51
1:B:9:ASP:HA	6:B:2048:HOH:O	2.09	0.51
3:D:9:DT:H2"	3:D:10:DC:C6	2.46	0.51
1:B:47:ASN:ND2	1:B:49:GLU:OE2	2.44	0.51
1:A:307:SER:O	1:A:308:LYS:C	2.49	0.51
5:B:1346:DCT:C5'	2:E:13:DG:C2'	2.59	0.51
1:A:9:ASP:CG	1:A:161:ASN:H	2.12	0.51
1:A:215:GLY:O	1:A:216:MET:HB3	2.10	0.51
3:F:16:DC:H4'	3:F:17:DC:OP1	2.11	0.51
1:B:76:MET:HG3	1:B:81:TYR:CE2	2.45	0.51
1:B:326:ASP:OD2	1:B:327:GLU:N	2.44	0.51
1:B:60:PRO:CD	1:B:63:GLU:HG3	2.33	0.50
1:A:197:LEU:N	1:A:197:LEU:HD23	2.26	0.50
1:A:84:VAL:O	1:A:87:ARG:N	2.40	0.50
1:B:153:ILE:HA	1:B:156[A]:ASP:OD2	2.10	0.50
1:A:36:ARG:NH2	1:A:331:ARG:HG3	2.27	0.50
1:A:128:ILE:C	1:A:130:ASN:N	2.63	0.50
1:A:298:ARG:NH1	2:C:7:DA:H3'	2.26	0.50
1:B:247:ARG:O	1:B:268:ALA:HB1	2.11	0.50
1:A:203:VAL:HG13	1:A:204:ASP:N	2.26	0.50
1:A:265:LEU:CD2	1:A:315:SER:HB3	2.41	0.50
1:B:97:GLU:OE2	1:B:97:GLU:N	2.33	0.50
1:B:92:LEU:C	1:B:94:GLU:N	2.65	0.50
1:B:130:ASN:O	1:B:134:GLU:HG2	2.11	0.50
1:B:247:ARG:HA	3:F:7:DA:OP2	2.12	0.50
1:B:101:ILE:HD12	1:B:101:ILE:N	2.26	0.50
1:A:291:GLU:OE2	1:A:329:LYS:HB2	2.11	0.50
1:B:281:PRO:HB3	1:B:337:PHE:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LYS:NZ	1:A:316:VAL:CG2	2.75	0.50
1:A:8:PHE:O	1:A:9:ASP:C	2.49	0.50
1:B:323:LEU:HD22	1:B:327:GLU:OE1	2.11	0.50
1:A:258:LEU:HD11	1:A:262:LYS:CD	2.41	0.50
1:A:221:LYS:O	1:A:224:TYR:HB3	2.12	0.50
1:A:336:ARG:HH22	3:D:7:DA:C2'	2.25	0.49
1:B:81:TYR:N	1:B:81:TYR:CD1	2.79	0.49
1:B:210:PHE:O	1:B:213:LEU:N	2.45	0.49
1:A:37:PHE:O	1:A:38[A]:GLU:HB2	2.10	0.49
1:A:132:ILE:CG2	1:A:133:LEU:N	2.75	0.49
1:B:331:ARG:NH2	3:F:4:DA:OP2	2.44	0.49
1:B:249:VAL:HG11	1:B:267:ARG:HH12	1.77	0.49
1:A:289:VAL:HB	1:A:332:ARG:HB2	1.94	0.49
1:A:179:ASP:CB	1:A:201:LYS:HD3	2.42	0.49
1:A:9:ASP:OD2	1:A:160:PRO:HB2	2.12	0.49
1:A:209:GLU:O	1:A:212:LYS:N	2.45	0.49
1:A:192:GLU:OE2	1:A:193:LYS:HE2	2.13	0.49
1:A:173:ARG:O	1:A:177:GLU:OE1	2.30	0.49
1:A:130:ASN:C	1:A:132:ILE:N	2.63	0.49
1:A:217:ILE:HD12	1:A:221:LYS:HG2	1.93	0.49
1:A:208:ILE:CG2	1:A:209:GLU:H	2.16	0.49
1:B:16:GLU:O	1:B:23:LEU:HD12	2.13	0.49
1:A:314:GLU:HG3	1:A:318:LEU:CD1	2.42	0.49
1:A:116:ARG:HG3	1:A:116:ARG:NH1	2.28	0.49
1:B:284:ILE:HD12	1:B:337:PHE:CE1	2.47	0.49
1:A:247:ARG:HB3	1:A:272:SER:OG	2.13	0.49
1:A:130:ASN:O	1:A:132:ILE:N	2.46	0.49
1:A:2:ILE:HD11	1:A:144:ILE:CG2	2.43	0.49
1:A:339:LYS:NZ	2:C:5:DG:OP2	2.41	0.49
1:B:245:ILE:HB	1:B:276:LEU:CD2	2.43	0.49
3:D:6:DFT:H2'	3:D:7:DA:O5'	2.13	0.48
1:A:128:ILE:C	1:A:130:ASN:H	2.17	0.48
1:A:269:ILE:HG22	1:A:269:ILE:O	2.13	0.48
2:C:12:DT:H72	2:C:13:DG:C6	2.48	0.48
5:B:1346:DCT:O5'	5:B:1346:DCT:O2B	2.32	0.48
1:A:284:ILE:HD12	1:A:337:PHE:HE1	1.78	0.48
1:B:92:LEU:O	1:B:94:GLU:N	2.47	0.48
1:B:38:GLU:HA	1:B:38:GLU:OE2	2.13	0.48
1:A:277:ASP:CG	1:A:278:LYS:N	2.67	0.48
5:B:1346:DCT:C4'	2:E:13:DG:H2''	2.41	0.48
1:A:5:PHE:CZ	1:A:106:GLU:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ALA:C	1:A:270:GLU:H	2.16	0.48
1:A:132:ILE:CG2	1:A:138:ILE:O	2.62	0.48
1:B:21:PRO:C	1:B:23:LEU:N	2.67	0.48
1:B:336:ARG:NH2	3:F:7:DA:C2'	2.77	0.48
1:A:4:LEU:HD21	1:A:128:ILE:HD12	1.96	0.48
1:B:5:PHE:CD2	1:B:152:LYS:HA	2.48	0.48
1:A:15:VAL:HG11	1:A:84:VAL:HG21	1.95	0.48
1:A:309:GLU:CA	1:A:312:TYR:HD1	2.26	0.47
1:A:12:TYR:O	1:A:14:GLN:N	2.47	0.47
1:A:3:VAL:CG1	1:A:4:LEU:N	2.77	0.47
3:F:13:DT:H2"	3:F:14:DC:C6	2.49	0.47
1:A:9:ASP:HB2	1:A:139:THR:OG1	2.14	0.47
1:B:145:SER:OG	1:B:146:LYS:N	2.45	0.47
1:A:2:ILE:HD11	1:A:144:ILE:HG21	1.97	0.47
1:B:21:PRO:C	1:B:23:LEU:H	2.17	0.47
1:B:207:SER:O	1:B:208:ILE:HD13	2.14	0.47
1:B:36:ARG:HB3	1:B:40:SER:OG	2.14	0.47
1:B:313:SER:O	1:B:317:LYS:HG2	2.14	0.47
1:A:164:LYS:HG2	1:A:165:VAL:H	1.80	0.47
1:B:248:ILE:HG22	6:F:2005:HOH:O	2.15	0.47
1:B:10:TYR:CD2	1:B:48:TYR:CE1	3.02	0.47
1:B:133:LEU:O	1:B:133:LEU:HD12	2.15	0.47
2:C:12:DT:H2'	2:C:13:DG:C1'	2.45	0.47
1:A:286:VAL:HG22	1:A:335:VAL:HG12	1.97	0.47
2:C:11:DC:C1'	2:C:12:DT:H5"	2.41	0.47
3:D:5:DG:N7	3:D:6:DFT:H72	2.30	0.47
5:B:1346:DCT:C6	5:B:1346:DCT:C5'	2.86	0.47
1:B:99:ILE:CG1	1:B:100:GLU:N	2.78	0.47
1:B:257:ASN:HB3	1:B:260:GLU:HB3	1.96	0.47
1:B:34:SER:HG	1:B:40:SER:HG	1.59	0.47
1:A:295:ILE:H	1:A:295:ILE:HD12	1.80	0.47
1:A:258:LEU:HD11	1:A:262:LYS:HB2	1.95	0.47
1:B:60:PRO:HB3	3:F:4:DA:H5"	1.97	0.46
1:A:268:ALA:C	1:A:270:GLU:N	2.69	0.46
1:B:98:LYS:O	1:B:237:ILE:HG21	2.14	0.46
1:A:134:GLU:HG3	6:A:2022:HOH:O	2.15	0.46
1:B:180:ILE:HG23	1:B:181:ALA:N	2.29	0.46
1:B:26:LYS:HB3	1:B:27:PRO:HD2	1.97	0.46
1:A:253:ARG:O	1:A:254:ASN:CB	2.59	0.46
1:A:172:LYS:O	1:A:176:ARG:HG3	2.15	0.46
1:A:119:ARG:HH11	1:A:119:ARG:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ASP:C	1:B:170:GLU:N	2.69	0.46
1:A:177:GLU:N	1:A:177:GLU:OE1	2.49	0.46
2:E:13:DG:H4'	2:E:13:DG:OP1	2.15	0.46
1:A:102:ALA:HA	1:A:240[A]:ARG:NH1	2.31	0.46
1:A:203:VAL:O	1:A:205:THR:N	2.49	0.46
1:A:291:GLU:CD	1:A:329:LYS:HB2	2.36	0.46
1:B:124:LEU:O	1:B:128:ILE:HG13	2.16	0.46
3:F:15:DC:H2"	3:F:16:DC:C5	2.51	0.46
2:E:13:DG:C4'	2:E:13:DG:OP1	2.64	0.45
1:B:221:LYS:O	1:B:224:TYR:N	2.49	0.45
1:A:210[A]:PHE:HE1	1:A:223:LYS:HG2	1.79	0.45
1:B:68:LEU:HD22	1:B:71:ALA:HB2	1.98	0.45
1:B:254:ASN:HB2	1:B:329:LYS:HD2	1.97	0.45
1:A:116:ARG:HB3	1:A:120:GLU:CD	2.37	0.45
1:A:242:ARG:HD2	1:A:242:ARG:H	1.80	0.45
1:B:273:TYR:HA	1:B:276:LEU:HG	1.98	0.45
1:A:262:LYS:HZ3	1:A:316:VAL:CG2	2.30	0.45
1:A:88:ILE:HG23	1:A:132:ILE:HD11	1.99	0.45
1:B:136:GLU:C	1:B:138:ILE:N	2.68	0.45
1:B:154:ALA:O	1:B:157:MET:HG3	2.16	0.45
2:C:12:DT:C4'	6:C:2011:HOH:O	2.64	0.45
1:B:175:ILE:HG23	1:B:229:ALA:HA	1.98	0.45
1:A:132:ILE:HD13	1:A:140:VAL:HG11	1.98	0.45
1:B:281:PRO:CB	1:B:337:PHE:HB3	2.47	0.45
1:B:4:LEU:CD1	1:B:144:ILE:HG12	2.45	0.45
1:B:5:PHE:O	1:B:142:VAL:HA	2.16	0.45
1:B:249:VAL:HG11	1:B:267:ARG:NH1	2.31	0.45
1:B:321:LYS:O	1:B:325:GLU:HG3	2.17	0.45
1:A:56:LYS:CE	1:A:59:ILE:CG2	2.95	0.45
1:A:283:ALA:HB3	1:A:339:LYS:HG3	1.99	0.45
1:A:175:ILE:O	1:A:175:ILE:HG22	2.17	0.45
1:A:331:ARG:CZ	3:D:5:DG:OP1	2.65	0.45
1:A:48:TYR:CZ	1:A:160:PRO:HB3	2.52	0.45
1:A:20:ASN:OD1	1:B:312:TYR:CD1	2.70	0.45
1:A:295:ILE:HG22	1:A:296:VAL:N	2.32	0.45
1:A:27:PRO:HG2	1:A:71:ALA:HA	1.98	0.45
1:B:208:ILE:O	1:B:210:PHE:N	2.50	0.45
3:D:17:DC:H2"	3:D:18:DC:C6	2.48	0.44
1:B:163:ILE:O	1:B:163:ILE:CG2	2.64	0.44
1:A:224:TYR:CD2	1:A:225:LEU:HD23	2.52	0.44
3:F:15:DC:H2"	3:F:16:DC:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLU:O	1:B:210:PHE:C	2.55	0.44
1:A:13:ALA:O	1:A:17:GLU:HG3	2.16	0.44
1:B:237:ILE:O	1:B:237:ILE:CG2	2.64	0.44
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.82	0.44
1:B:180:ILE:HD11	1:B:194:LEU:HD13	2.00	0.44
1:A:55:VAL:O	1:A:55:VAL:HG12	2.16	0.44
1:B:5:PHE:CE1	1:B:106:GLU:HG2	2.51	0.44
1:B:217:ILE:HD11	1:B:222:ALA:N	2.33	0.44
1:B:172:LYS:N	1:B:172:LYS:HD2	2.31	0.44
1:A:254:ASN:O	1:A:329:LYS:HE2	2.17	0.44
1:A:176:ARG:HB2	1:A:177:GLU:OE1	2.18	0.44
1:B:258:LEU:O	1:B:262:LYS:HG3	2.17	0.44
1:A:304:HIS:CD2	1:A:305:GLY:O	2.70	0.44
1:B:10:TYR:CD1	1:B:47:ASN:HA	2.53	0.44
1:A:9:ASP:H	1:A:140:VAL:HA	1.83	0.44
1:A:214[A]:LYS:HE2	1:A:219[A]:GLU:CG	2.48	0.44
1:B:64:ALA:C	1:B:66:LYS:H	2.21	0.44
1:A:265:LEU:HD21	1:A:315:SER:HB3	1.98	0.44
3:D:5:DG:C8	3:D:6:DFT:H72	2.53	0.44
1:A:129:LYS:HE2	1:A:140:VAL:O	2.18	0.44
1:A:65:LYS:C	1:A:66:LYS:HE3	2.37	0.44
3:F:16:DC:H2"	3:F:17:DC:H6	1.83	0.44
1:A:266:PHE:CE1	1:A:312:TYR:HD2	2.35	0.44
1:A:189:ILE:O	1:A:192:GLU:HG3	2.18	0.44
1:B:262:LYS:N	1:B:263:PRO:CD	2.80	0.44
1:A:253:ARG:HA	1:A:253:ARG:NH1	2.33	0.44
1:B:36:ARG:NH1	1:B:331:ARG:NH1	2.66	0.44
1:B:108:TYR:CE2	1:B:148:LYS:HB3	2.53	0.44
1:B:270:GLU:OE1	1:B:308:LYS:HE2	2.18	0.44
3:F:13:DT:H2'	6:F:2010:HOH:O	2.17	0.44
1:A:31:CYS:HA	1:A:44:ALA:H	1.81	0.43
1:B:150:PHE:CD2	1:B:153:ILE:HD12	2.53	0.43
3:D:12:DT:C2'	3:D:13:DT:H71	2.48	0.43
1:A:166:ILE:O	1:A:166:ILE:HG22	2.18	0.43
1:B:168:ASP:O	1:B:170:GLU:N	2.52	0.43
1:A:187:GLY:H	2:C:11:DC:H5"	1.83	0.43
1:B:187:GLY:CA	2:E:11:DC:H3'	2.48	0.43
1:B:5:PHE:CE2	1:B:152:LYS:HG3	2.53	0.43
1:B:136:GLU:O	1:B:138:ILE:N	2.51	0.43
3:F:11:DC:H2'	3:F:12:DT:H72	2.00	0.43
1:A:336:ARG:NH2	3:D:8:DG:OP2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:O	1:A:204:ASP:C	2.56	0.43
1:B:333:ILE:O	1:B:333:ILE:HG23	2.18	0.43
1:A:269:ILE:HG22	6:A:2041:HOH:O	2.18	0.43
1:A:306:ILE:HG23	1:A:310:THR:HB	2.01	0.43
1:A:181:ALA:C	1:A:183:VAL:N	2.70	0.43
1:A:203:VAL:C	1:A:205:THR:N	2.72	0.43
5:B:1346:DCT:H6	5:B:1346:DCT:H5'	1.95	0.43
1:B:261:ILE:CG2	1:B:319:LEU:HD21	2.48	0.43
1:B:180:ILE:O	1:B:183:VAL:HG23	2.18	0.43
1:B:257:ASN:O	1:B:260:GLU:N	2.50	0.43
3:F:15:DC:C4	3:F:16:DC:N4	2.87	0.43
1:A:267:ARG:O	1:A:270:GLU:HB2	2.18	0.43
1:A:10:TYR:N	1:A:10:TYR:HD2	2.17	0.43
1:A:59:ILE:HD12	1:A:63:GLU:HB2	2.00	0.43
1:B:254:ASN:OD1	1:B:331:ARG:HA	2.19	0.43
1:A:264:TYR:CE1	1:A:267:ARG:NH1	2.87	0.43
2:E:12:DT:C5	2:E:13:DG:N1	2.86	0.43
1:B:7:ASP:OD2	1:B:106:GLU:OE2	2.36	0.43
1:B:225:LEU:O	1:B:228:LEU:HB2	2.18	0.43
1:A:213:LEU:HD23	1:A:222:ALA:HB1	1.99	0.43
2:C:11:DC:C5	2:C:12:DT:C7	3.02	0.43
5:A:1347:DCT:H3'1	5:A:1347:DCT:O2B	2.19	0.43
1:A:63:GLU:HA	1:A:63:GLU:OE1	2.18	0.43
1:A:66:LYS:HA	1:A:66:LYS:CE	2.43	0.43
1:B:148:LYS:CB	1:B:148:LYS:HZ3	2.16	0.43
1:A:294:ASP:HB3	1:A:328:ARG:HH12	1.83	0.43
1:A:213:LEU:O	1:A:216:MET:HG2	2.19	0.43
1:A:174:LEU:O	1:A:178:LEU:HB3	2.19	0.43
1:B:221:LYS:O	1:B:222:ALA:C	2.57	0.42
1:A:314:GLU:HA	1:A:317:LYS:HZ1	1.84	0.42
1:A:192:GLU:O	1:A:196:LYS:HE3	2.19	0.42
6:E:2001:HOH:O	3:F:13:DT:C7	2.67	0.42
1:B:100:GLU:O	1:B:107:ALA:HA	2.19	0.42
1:A:53:PHE:CD1	1:A:53:PHE:N	2.87	0.42
1:B:238:ARG:HD3	1:B:238:ARG:HA	1.80	0.42
1:A:99:ILE:HD12	1:A:109:LEU:HD22	2.00	0.42
1:A:96:SER:OG	1:A:109:LEU:CD1	2.67	0.42
1:A:66:LYS:HE3	1:A:66:LYS:N	2.34	0.42
1:B:36:ARG:NH1	1:B:331:ARG:HH12	2.16	0.42
1:A:194:LEU:HD23	1:A:216:MET:HE1	2.02	0.42
1:A:117:ASP:OD2	1:A:119:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ASP:HB3	1:B:278:LYS:H	1.53	0.42
1:A:256:ARG:HH22	1:A:327:GLU:CA	2.33	0.42
1:B:298:ARG:HD3	1:B:298:ARG:HA	1.83	0.42
2:C:12:DT:H3	3:D:7:DA:H2	1.68	0.42
1:A:96:SER:OG	1:A:109:LEU:HD13	2.19	0.42
1:A:76:MET:HE3	1:A:77:ARG:N	2.35	0.42
1:B:51:ARG:C	1:B:53:PHE:H	2.22	0.42
5:B:1346:DCT:O2G	6:B:2048:HOH:O	2.22	0.42
2:E:12:DT:C2'	2:E:13:DG:C8	3.03	0.42
5:A:1347:DCT:H2'	5:A:1347:DCT:O5'	2.18	0.42
2:E:12:DT:H2'	2:E:13:DG:C8	2.54	0.42
1:B:94:GLU:HA	1:B:94:GLU:OE2	2.19	0.42
1:A:76:MET:CE	1:A:78:LYS:N	2.83	0.42
1:B:321:LYS:HE2	1:B:321:LYS:HB3	1.91	0.42
1:B:255:SER:OG	1:B:256:ARG:N	2.51	0.42
1:B:187:GLY:HA3	2:E:11:DC:H3'	2.02	0.42
1:A:11:PHE:O	1:A:12:TYR:O	2.36	0.42
1:A:245:ILE:CG2	1:A:275:LYS:HB2	2.48	0.42
1:A:248:ILE:HG12	1:A:249:VAL:N	2.34	0.42
2:C:12:DT:O5'	2:C:13:DG:C8	2.73	0.42
1:A:129:LYS:HE2	1:A:162:GLY:O	2.19	0.41
1:A:177:GLU:O	1:A:201:LYS:HD2	2.20	0.41
1:B:21:PRO:O	1:B:23:LEU:N	2.52	0.41
1:B:2:ILE:HD11	1:B:121:ALA:CB	2.50	0.41
1:A:11:PHE:O	1:A:14:GLN:N	2.52	0.41
2:C:1:DG:H4'	2:C:2:DG:O5'	2.19	0.41
3:F:12:DT:H71	6:F:2008:HOH:O	2.18	0.41
1:B:76:MET:HG3	1:B:81:TYR:HE2	1.85	0.41
3:F:13:DT:H2"	3:F:14:DC:H6	1.86	0.41
1:A:307:SER:O	1:A:310:THR:N	2.53	0.41
3:F:16:DC:H2"	3:F:17:DC:C6	2.55	0.41
1:B:104:ILE:O	1:B:104:ILE:HG13	2.20	0.41
1:A:319:LEU:HD12	1:A:319:LEU:O	2.21	0.41
1:A:203:VAL:O	1:A:206:LEU:N	2.45	0.41
3:F:12:DT:H2"	3:F:13:DT:C6	2.55	0.41
1:A:14:GLN:NE2	1:A:139:THR:H	2.09	0.41
1:B:285:HIS:HA	1:B:299:GLY:HA2	2.03	0.41
1:B:77:ARG:C	1:B:79:GLU:H	2.23	0.41
1:B:60:PRO:CB	1:B:63:GLU:HG2	2.34	0.41
6:A:2046:HOH:O	2:C:7:DA:H2'	2.21	0.41
3:F:9:DT:H2"	3:F:10:DC:H6	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:NH1	1:A:119:ARG:HG2	2.36	0.41
1:B:45:THR:CG2	1:B:46:ALA:N	2.84	0.41
3:F:12:DT:C6	3:F:13:DT:H72	2.55	0.41
1:A:9:ASP:O	5:A:1347:DCT:O2G	2.39	0.41
1:A:138:ILE:HA	1:A:138:ILE:HD13	1.92	0.41
1:B:186:ILE:HG23	1:B:190:THR:CG2	2.51	0.41
1:B:261:ILE:C	1:B:263:PRO:HD2	2.40	0.41
1:A:141:THR:HG22	1:A:155:ALA:HB1	2.02	0.41
1:B:195:LYS:C	1:B:197:LEU:H	2.24	0.41
1:A:276:LEU:HA	1:A:276:LEU:HD23	1.88	0.41
1:B:9:ASP:C	1:B:10:TYR:CD2	2.94	0.40
1:A:12:TYR:O	1:A:13:ALA:C	2.58	0.40
1:A:293:LEU:O	1:A:294:ASP:O	2.40	0.40
1:B:51:ARG:C	1:B:53:PHE:N	2.75	0.40
1:A:203:VAL:CG1	1:A:204:ASP:N	2.83	0.40
1:A:179:ASP:O	1:A:180:ILE:O	2.40	0.40
1:A:197:LEU:HB2	1:A:199:ILE:HD13	2.02	0.40
1:B:186:ILE:O	1:B:186:ILE:HG22	2.21	0.40
3:F:11:DC:H2"	3:F:12:DT:C6	2.56	0.40
1:A:9:ASP:CB	1:A:139:THR:OG1	2.70	0.40
1:B:36:ARG:HH12	1:B:331:ARG:HH12	1.68	0.40
1:B:245:ILE:HD11	1:B:279:ARG:HE	1.87	0.40
2:C:12:DT:H2'	2:C:13:DG:N9	2.35	0.40
1:A:323:LEU:C	1:A:325:GLU:H	2.24	0.40
1:B:128:ILE:O	1:B:129:LYS:C	2.60	0.40
1:A:20:ASN:ND2	1:A:20:ASN:C	2.73	0.40
1:B:101:ILE:CD1	1:B:101:ILE:N	2.84	0.40
1:A:307:SER:OG	1:A:309:GLU:HG2	2.22	0.40
1:A:10:TYR:CZ	1:A:14:GLN:HG3	2.55	0.40
1:B:77:ARG:C	1:B:79:GLU:N	2.74	0.40
1:B:178:LEU:HD12	1:B:179:ASP:N	2.37	0.40
1:B:245:ILE:CD1	1:B:279:ARG:HE	2.34	0.40
1:B:276:LEU:HD13	1:B:281:PRO:HD3	2.03	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	342/358 (96%)	266 (78%)	52 (15%)	24 (7%)	1	7
1	B	342/358 (96%)	265 (78%)	59 (17%)	18 (5%)	2	14
All	All	684/716 (96%)	531 (78%)	111 (16%)	42 (6%)	2	11

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	12	TYR
1	A	38[A]	GLU
1	A	55	VAL
1	A	71	ALA
1	A	135	LYS
1	A	180	ILE
1	A	210[A]	PHE
1	A	216	MET
1	A	235	GLU
1	A	254	ASN
1	A	294	ASP
1	A	342	GLU
1	B	11	PHE
1	B	36	ARG
1	B	38	GLU
1	B	210	PHE
1	B	231	ASP
1	A	10	TYR
1	A	129	LYS
1	A	253	ARG
1	A	269	ILE
1	B	55	VAL
1	B	78	LYS
1	B	187	GLY

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Mol	Chain	Res	Type
1	A	24	LYS
1	A	290	THR
1	A	324	GLU
1	B	93	ARG
1	B	163	ILE
1	B	209	GLU
1	A	13	ALA
1	B	169	GLU
1	B	220	ALA
1	A	204	ASP
1	A	261	ILE
1	B	168	ASP
1	B	205	THR
1	B	216	MET
1	B	184	PRO
1	B	240	ARG
1	A	84	VAL

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	301/315 (96%)	268 (89%)	33 (11%)	8	30
1	B	302/315 (96%)	271 (90%)	31 (10%)	9	33
All	All	603/630 (96%)	539 (89%)	64 (11%)	8	31

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	9	ASP
1	A	10	TYR
1	A	11	PHE
1	A	20	ASN
1	A	37	PHE

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Mol	Chain	Res	Type
1	A	39[A]	ASP
1	A	56	LYS
1	A	66	LYS
1	A	72	VAL
1	A	76	MET
1	A	78	LYS
1	A	89	MET
1	A	90	ASN
1	A	92	LEU
1	A	132	ILE
1	A	139	THR
1	A	156	ASP
1	A	163	ILE
1	A	167	ASP
1	A	168	ASP
1	A	170	GLU
1	A	192	GLU
1	A	193	LYS
1	A	197	LEU
1	A	234	ASN
1	A	242	ARG
1	A	253	ARG
1	A	254	ASN
1	A	273	TYR
1	A	293	LEU
1	A	327	GLU
1	A	336	ARG
1	B	7	ASP
1	B	16	GLU
1	B	22	SER
1	B	24[A]	LYS
1	B	68	LEU
1	B	70	ASN
1	B	79	GLU
1	B	89	MET
1	B	98	LYS
1	B	106	GLU
1	B	119[A]	ARG
1	B	119[B]	ARG
1	B	148	LYS
1	B	149	VAL
1	B	157	MET

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Mol	Chain	Res	Type
1	B	168	ASP
1	B	172	LYS
1	B	196	LYS
1	B	202	LEU
1	B	203	VAL
1	B	221	LYS
1	B	234	ASN
1	B	235	GLU
1	B	237	ILE
1	B	239	THR
1	B	247	ARG
1	B	267	ARG
1	B	308	LYS
1	B	336	ARG
1	B	338	SER
1	B	342	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	20	ASN
1	A	130	ASN
1	A	200	ASN
1	A	234	ASN
1	A	304	HIS
1	A	320	GLN
1	B	14	GLN
1	B	20	ASN
1	B	70	ASN
1	B	82	GLN
1	B	83	GLN
1	B	285	HIS
1	B	320	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	#$|Z| > 2$
3	DFT	D	6	3	17,21,22	0.70	0	23,30,33	2.05	6 (26%)
3	DFT	F	6	3	17,21,22	0.92	0	23,30,33	2.78	9 (39%)

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
3	DFT	D	6	3	-	0/7/21/22	0/2/2/2
3	DFT	F	6	3	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	6	DFT	C5M-C5-C4	-5.72	118.40	121.68
3	F	6	DFT	C2'-C1'-C1	-5.29	107.14	114.79
3	D	6	DFT	C4'-O4'-C1'	-4.18	101.99	109.14
3	F	6	DFT	C3'-C2'-C1'	-3.68	99.19	102.69
3	D	6	DFT	C3-C2-C1	-3.31	120.25	123.78
3	F	6	DFT	O4'-C4'-C5'	-2.91	98.92	109.32
3	F	6	DFT	C3-C2-C1	-2.59	121.03	123.78
3	F	6	DFT	C2'-C3'-C4'	-2.20	98.21	102.77
3	D	6	DFT	C2'-C1'-C1	-2.07	111.80	114.79
3	F	6	DFT	C4-C3-C2	2.11	121.29	116.98
3	D	6	DFT	F4-C4-C5	2.64	120.33	117.83
3	D	6	DFT	C6-C1-C2	2.90	120.08	116.17
3	F	6	DFT	F4-C4-C5	3.60	121.24	117.83
3	D	6	DFT	C6-C5-C4	5.79	120.20	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	6	DFT	C6-C5-C4	7.09	121.15	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	6	DFT	3	0
3	F	6	DFT	5	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	DCT	A	1347	4	20,28,28	1.49	3 (15%)	29,43,43	1.97	6 (20%)
5	DCT	B	1346	4	20,28,28	1.49	3 (15%)	29,43,43	1.74	7 (24%)

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	DCT	A	1347	4	-	0/18/31/31	0/2/2/2
5	DCT	B	1346	4	-	0/18/31/31	0/2/2/2

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All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1346	DCT	C4-N3	2.66	1.40	1.35
5	A	1347	DCT	C4-N3	2.82	1.40	1.35
5	B	1346	DCT	PG-O1G	3.05	1.61	1.51
5	A	1347	DCT	PG-O1G	3.16	1.61	1.51
5	A	1347	DCT	C6-N1	3.25	1.40	1.35
5	B	1346	DCT	C6-N1	3.42	1.40	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1347	DCT	C3'-C2'-C1'	-5.22	96.87	102.71
5	B	1346	DCT	PB-O3A-PA	-4.75	119.38	132.73
5	A	1347	DCT	PB-O3A-PA	-4.18	120.98	132.73
5	A	1347	DCT	PB-O3B-PG	-3.54	120.81	132.67
5	B	1346	DCT	PB-O3B-PG	-3.17	122.02	132.67
5	A	1347	DCT	O4'-C1'-C2'	-2.82	103.62	106.67
5	B	1346	DCT	C2'-C3'-C4'	-2.73	97.25	102.59
5	B	1346	DCT	C3'-C4'-C5'	-2.07	107.61	116.05
5	B	1346	DCT	O3G-PG-O3B	2.02	114.27	105.09
5	B	1346	DCT	O4'-C1'-N1	2.49	112.02	107.72
5	B	1346	DCT	C2-N3-C4	2.99	119.83	115.61
5	A	1347	DCT	C2-N3-C4	3.13	120.02	115.61
5	A	1347	DCT	O4'-C1'-N1	3.30	113.44	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1347	DCT	5	0
5	B	1346	DCT	13	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	344/358 (96%)	-0.36	0	100	100	26, 53, 75, 81	18 (5%)
1	B	343/358 (95%)	-0.41	0	100	100	29, 52, 73, 81	13 (3%)
2	C	13/13 (100%)	-0.49	0	100	100	58, 68, 99, 104	0
2	E	13/13 (100%)	-0.55	0	100	100	58, 77, 98, 99	0
3	D	17/18 (94%)	-0.54	0	100	100	45, 76, 118, 124	1 (5%)
3	F	15/18 (83%)	-0.42	0	100	100	43, 79, 110, 113	1 (6%)
All	All	745/778 (95%)	-0.39	0	100	100	26, 53, 77, 124	33 (4%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	DFT	F	6	20/21	0.94	0.17	-	59,63,65,66	0
3	DFT	D	6	20/21	0.96	0.16	-	46,50,53,56	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
5	DCT	B	1346	27/27	0.94	0.15	-0.72	48,60,74,77	0
5	DCT	A	1347	27/27	0.94	0.15	-1.04	48,58,69,70	0
4	CA	B	1344	1/1	0.97	0.12	-1.06	55,55,55,55	0
4	CA	A	1346	1/1	0.96	0.06	-2.55	49,49,49,49	0
4	CA	B	1345	1/1	0.75	0.08	-	63,63,63,63	0
4	CA	A	1345	1/1	0.99	0.10	-	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.