Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 09:53 PM EDT

PDB ID	:	6OY5
Title	:	X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter at 3 min
Authors	:	Shin, Y.; Murakami, K.S.
Deposited on	:	2019-05-14
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

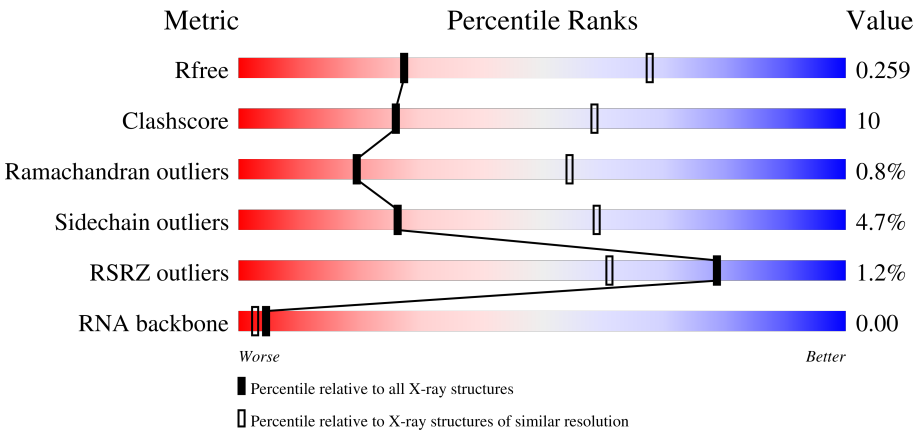
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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	315	54% 17% • 28%
1	B	315	52% 18% • 29%
2	C	1119	.% 71% 27% ••
3	D	1524	.% 70% 25% • •

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Mol	Chain	Length	Quality of chain
4	E	99	74% 20% • 5%
5	F	423	4% 60% 19% • 18%
6	G	22	23% 27% 36% 14%
7	H	27	22% 48% 11% 19%
8	I	2	50% 50%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28534 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-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	1782	1138	310	332	2	0	0	0
1	B	224	1767	1129	307	329	2	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1111	8764	5545	1561	1634	24	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1484	11722	7431	2065	2191	35	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	94	761	486	132	139	4	0	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	346	2807	1770	509	524	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P*CP*CP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*AP*AP*AP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	19	386	183	75	109	19	0	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*CP*TP*CP*TP*GP*AP*TP*GP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	H	22	453	216	87	129	21	0	0	0

- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	2	55	20	10	21	4	0	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

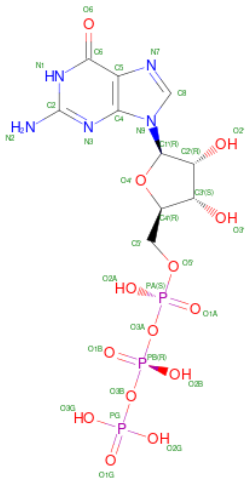
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
9	B	1	1	1	0	0
9	D	2	2	2	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
10	D	2	2	2	0	0

- Molecule 11 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



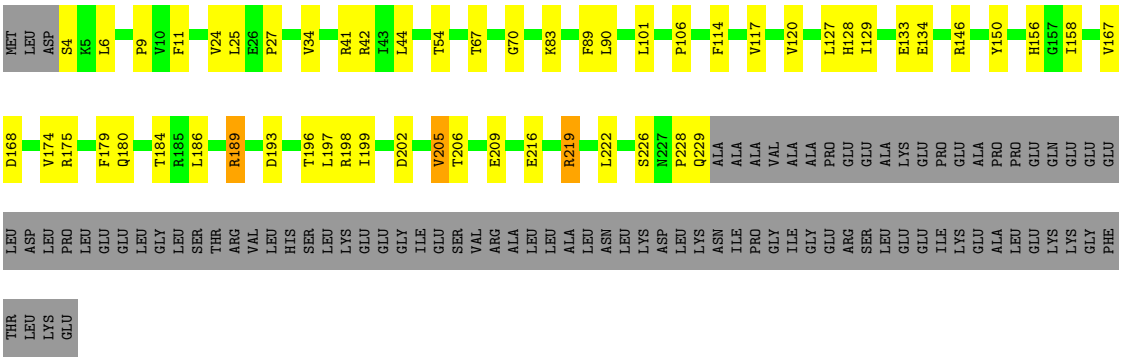
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	D	1	32	10	5	14	3	0	0

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.

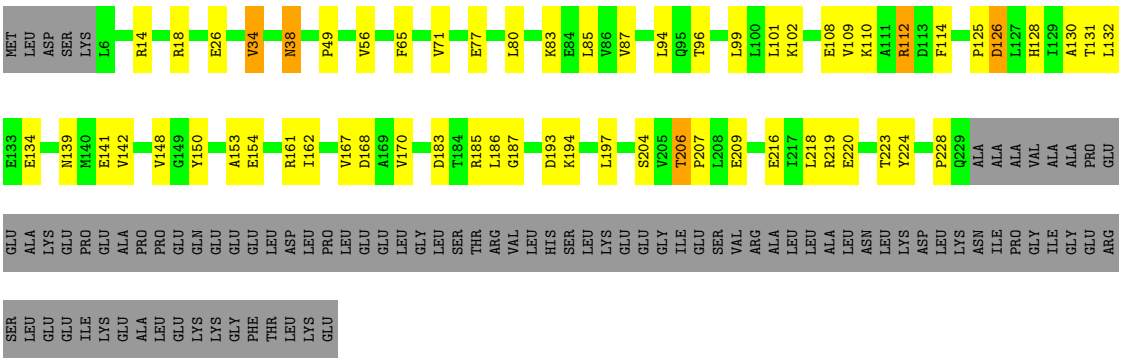
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



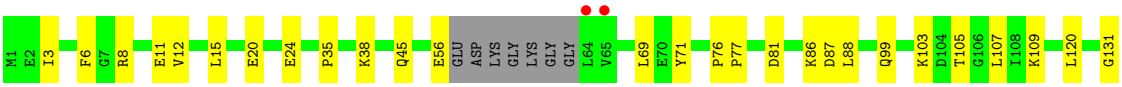
• Molecule 1: DNA-directed RNA polymerase subunit alpha

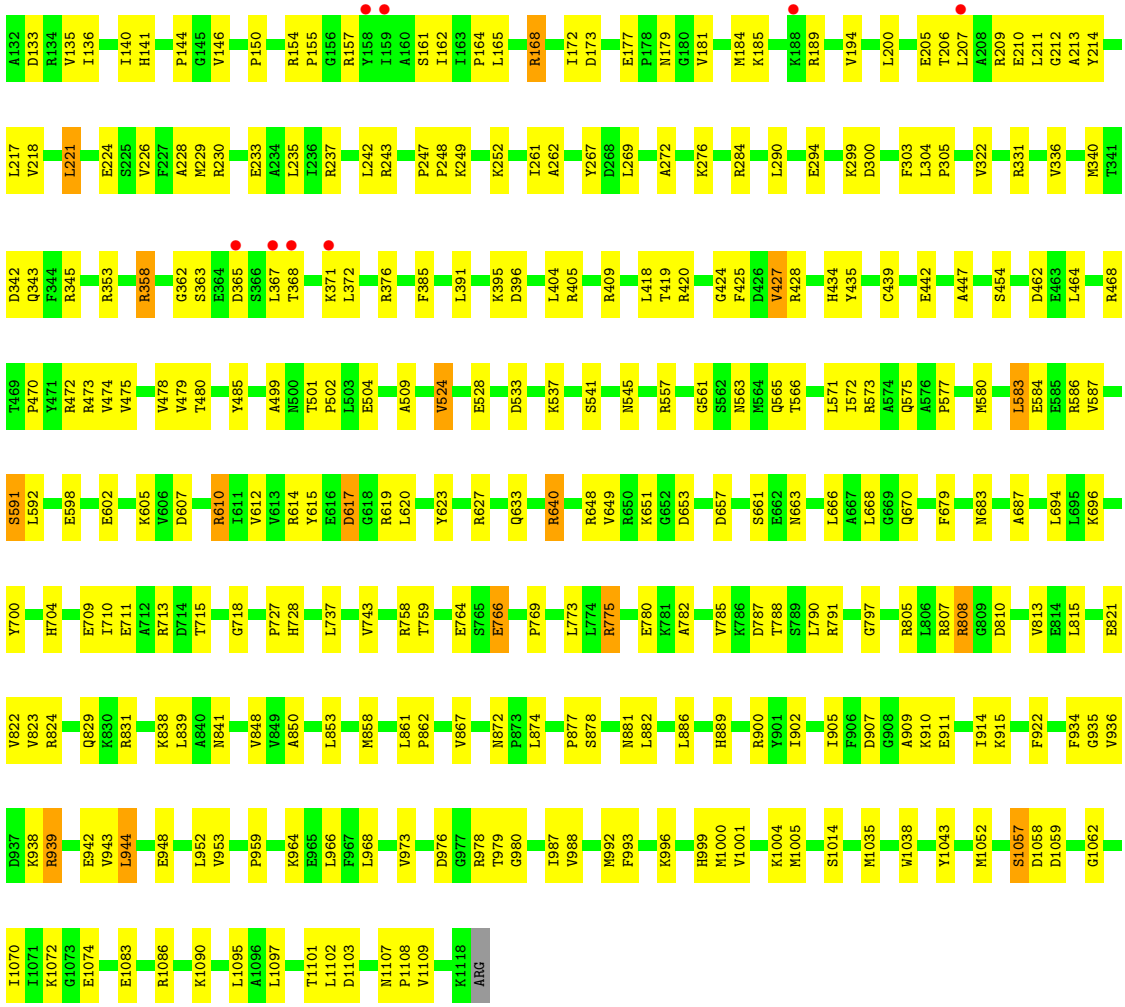
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

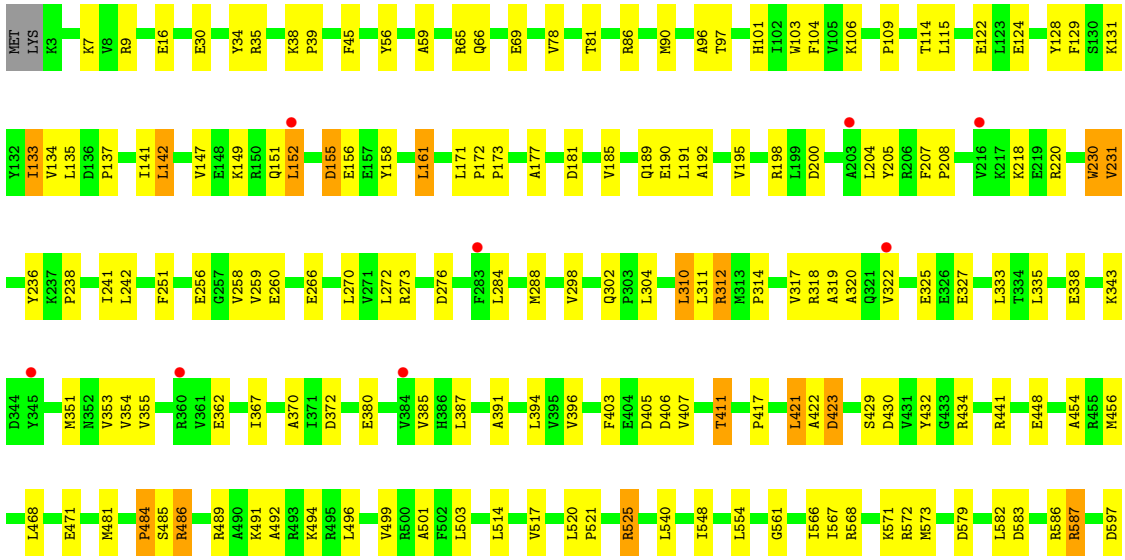
Chain C:

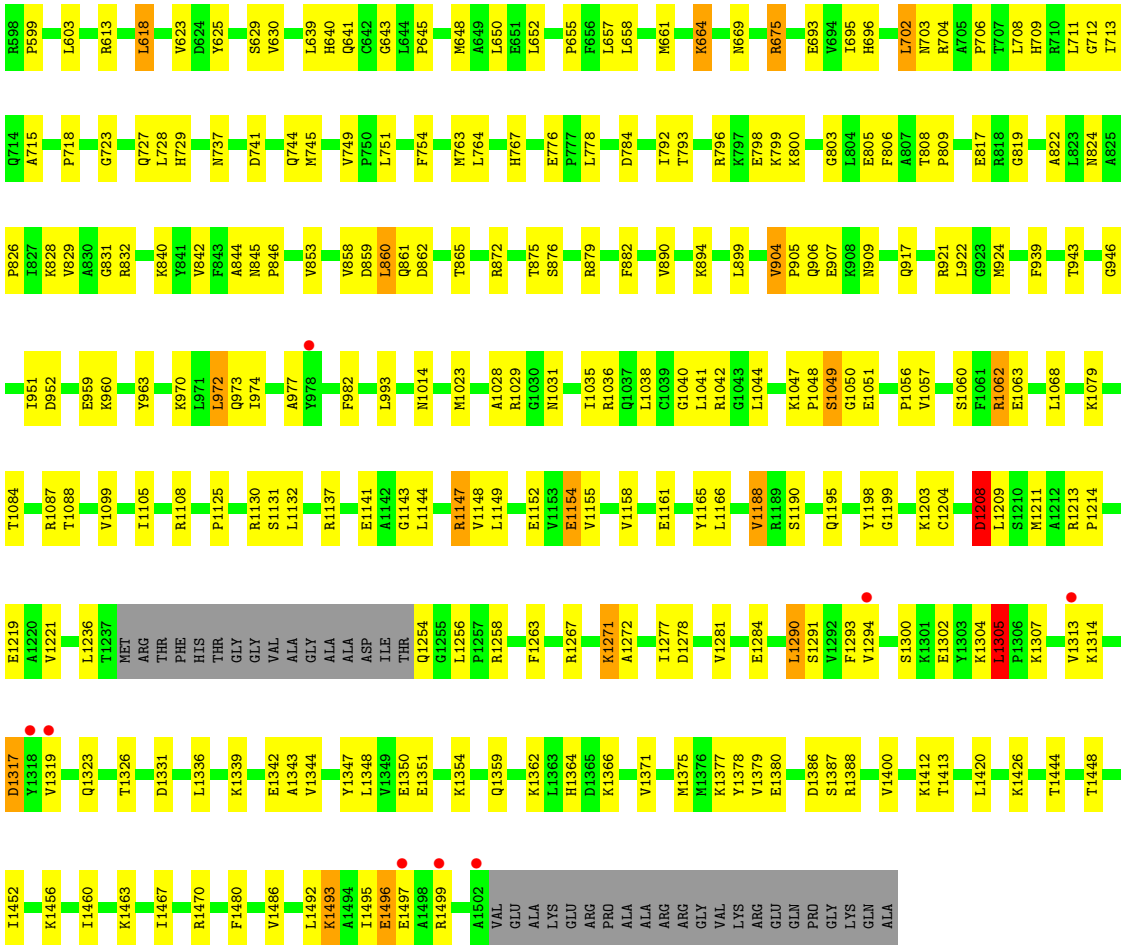




- Molecule 3: DNA-directed RNA polymerase subunit beta'

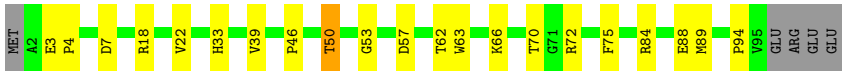
Chain D:





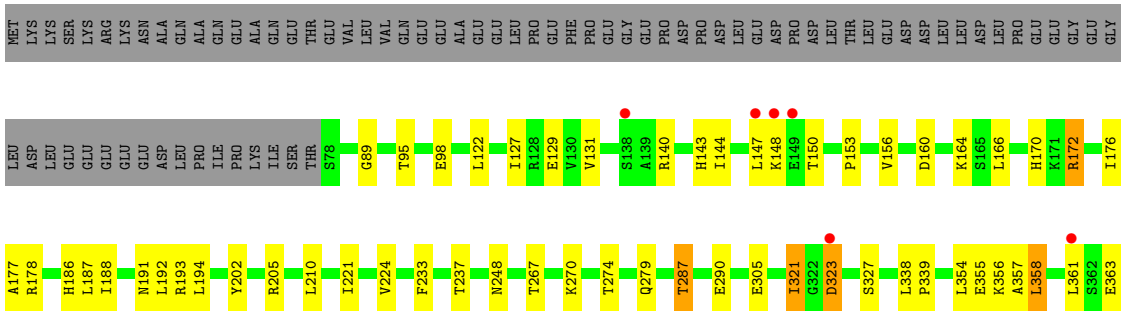
- Molecule 4: DNA-directed RNA polymerase subunit omega

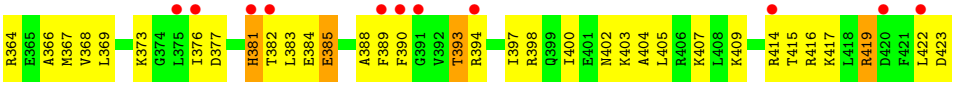
Chain E:



- Molecule 5: RNA polymerase sigma factor SigA

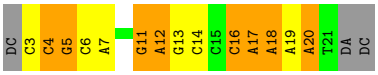
Chain F:





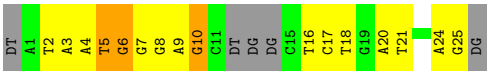
• Molecule 6: DNA (5'-D(P*CP*CP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*AP*AP*AP*AP*T)-3')

Chain G: 23% 27% 36% 14%



• Molecule 7: DNA (5'-D(*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*CP*TP*CP*TP*GP*AP*TP*GP*CP*AP*G)-3')

Chain H: 22% 48% 11% 19%



• Molecule 8: RNA (5'-D(*(GTP))-R(P*G)-3')

Chain I: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	186.11Å 102.42Å 297.24Å 90.00° 99.00° 90.00°	Depositor
Resolution (Å)	43.92 – 3.10 43.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.3 (43.92-3.10) 91.3 (43.92-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.207 , 0.259 0.207 , 0.259	Depositor DCC
R_{free} test set	1837 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	101.2	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28534	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, GTP

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	0/1814	0.81	3/2466 (0.1%)
1	B	0.55	0/1799	0.79	0/2447
2	C	0.51	0/8931	0.80	3/12080 (0.0%)
3	D	0.55	2/11928 (0.0%)	0.82	11/16127 (0.1%)
4	E	0.51	0/775	0.70	0/1045
5	F	0.50	0/2852	0.82	4/3837 (0.1%)
6	G	1.19	2/433 (0.5%)	1.61	12/664 (1.8%)
7	H	1.11	1/508 (0.2%)	1.18	2/781 (0.3%)
8	I	0.51	0/25	1.25	0/37
All	All	0.56	5/29065 (0.0%)	0.84	35/39484 (0.1%)

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
2	C	0	1
5	F	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	12	DA	C3'-O3'	-5.91	1.36	1.44
6	G	14	DC	C3'-O3'	-5.81	1.36	1.44
3	D	1213	ARG	CB-CG	-5.61	1.37	1.52
3	D	16	GLU	CG-CD	5.47	1.60	1.51
7	H	6	DG	N9-C4	-5.17	1.33	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	16	DC	O5'-P-OP2	-12.56	94.40	105.70
6	G	20	DA	O4'-C1'-N9	9.38	114.57	108.00
6	G	18	DA	O4'-C4'-C3'	-9.33	100.40	106.00
6	G	17	DA	O4'-C1'-N9	9.06	114.34	108.00
6	G	11	DG	O4'-C1'-N9	8.52	113.96	108.00
1	A	205	VAL	C-N-CA	7.47	140.37	121.70
5	F	383	LEU	CA-CB-CG	7.44	132.40	115.30
2	C	944	LEU	CB-CG-CD2	-7.15	98.84	111.00
6	G	14	DC	O4'-C4'-C3'	-6.73	101.81	104.50
7	H	5	DT	O4'-C1'-N1	6.58	112.60	108.00
3	D	1305	LEU	CA-CB-CG	6.48	130.20	115.30
6	G	14	DC	O5'-P-OP1	-6.44	99.91	105.70
6	G	13	DG	O4'-C4'-C3'	-6.22	102.01	104.50
3	D	152	LEU	CA-CB-CG	6.19	129.54	115.30
2	C	235	LEU	CA-CB-CG	6.11	129.35	115.30
5	F	172	ARG	CA-CB-CG	6.10	126.82	113.40
5	F	358	LEU	CA-CB-CG	6.10	129.32	115.30
3	D	310	LEU	CA-CB-CG	6.07	129.26	115.30
7	H	10	DG	O4'-C4'-C3'	-6.04	102.08	104.50
3	D	1208	ASP	CB-CG-OD1	6.02	123.72	118.30
3	D	583	ASP	CB-CG-OD2	-5.98	112.91	118.30
3	D	728	LEU	CB-CG-CD2	-5.92	100.93	111.00
3	D	1147	ARG	CG-CD-NE	-5.61	100.01	111.80
6	G	4	DC	O4'-C1'-N1	-5.44	104.19	108.00
6	G	16	DC	OP1-P-OP2	5.38	127.67	119.60
3	D	711	LEU	CA-CB-CG	-5.36	102.98	115.30
6	G	13	DG	O5'-P-OP1	5.33	117.09	110.70
3	D	115	LEU	CA-CB-CG	5.31	127.50	115.30
1	A	127	LEU	CA-CB-CG	5.26	127.40	115.30
6	G	5	DG	O4'-C1'-N9	5.25	111.68	108.00
2	C	284	ARG	CB-CG-CD	5.23	125.20	111.60
1	A	41	ARG	NE-CZ-NH1	-5.21	117.69	120.30
3	D	702	LEU	CB-CG-CD2	-5.13	102.27	111.00
3	D	840	LYS	CD-CE-NZ	5.10	123.44	111.70
5	F	419	ARG	CA-CB-CG	5.05	124.52	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	766	GLU	Peptide
5	F	389	PHE	Peptide

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	1782	0	1834	33	0
1	B	1767	0	1816	42	0
2	C	8764	0	8863	203	0
3	D	11722	0	11950	257	1
4	E	761	0	778	16	0
5	F	2807	0	2882	77	0
6	G	386	0	212	19	0
7	H	453	0	250	35	0
8	I	55	0	22	1	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
10	D	2	0	0	0	0
11	D	32	0	12	1	0
All	All	28534	0	28619	596	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 10.

All (596) 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)
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.44	0.97
6:G:18:DA:H2'	6:G:19:DA:H5'	1.46	0.94
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.56	0.86
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.57	0.85
2:C:211:LEU:O	2:C:213:ALA:N	2.08	0.85
3:D:1267:ARG:NH1	3:D:1331:ASP:OD2	2.12	0.82
3:D:34:TYR:OH	3:D:35:ARG:NH1	2.13	0.82
3:D:669:ASN:HB3	5:F:417:LYS:HE2	1.62	0.80
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.64	0.79
2:C:367:LEU:HA	2:C:371:LYS:HE2	1.65	0.78
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.63	0.78
6:G:16:DC:H2'	6:G:17:DA:H8	1.47	0.78
1:B:206:THR:HG22	1:B:209:GLU:H	1.47	0.78
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:358:LEU:HB3	5:F:366:ALA:HB1	1.66	0.77
3:D:669:ASN:HD22	5:F:417:LYS:HG2	1.50	0.76
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.68	0.75
2:C:331:ARG:HH22	2:C:427:VAL:HG12	1.50	0.75
3:D:675:ARG:HH12	5:F:423:ASP:HA	1.52	0.75
3:D:1294:VAL:O	3:D:1300:SER:HB2	1.87	0.74
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.68	0.74
2:C:243:ARG:NH1	7:H:10:DG:H1	1.85	0.73
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.70	0.73
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.24	0.72
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.70	0.72
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.72	0.72
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.72	0.72
3:D:1209:LEU:HD11	3:D:1364:HIS:HD2	1.54	0.71
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.22	0.71
5:F:193:ARG:HB3	7:H:7:DG:H5"	1.71	0.71
2:C:911:GLU:OE2	3:D:1062:ARG:NH1	2.24	0.71
3:D:97:THR:HG23	3:D:554:LEU:HD21	1.73	0.70
3:D:134:VAL:HG22	3:D:151:GLN:H	1.57	0.70
5:F:129:GLU:HG3	5:F:147:LEU:HD21	1.74	0.70
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.74	0.70
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.26	0.68
3:D:1254:GLN:HB2	3:D:1258:ARG:HB2	1.76	0.68
2:C:1059:ASP:OD1	2:C:1062:GLY:HA3	1.93	0.68
3:D:800:LYS:NZ	3:D:819:GLY:O	2.26	0.68
2:C:758:ARG:HH21	2:C:788:THR:HB	1.58	0.68
5:F:237:THR:HG21	7:H:3:DA:H5"	1.76	0.68
1:B:110:LYS:HB2	1:B:112:ARG:HH21	1.59	0.68
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.76	0.67
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.77	0.67
2:C:243:ARG:HH12	7:H:10:DG:H1	1.40	0.67
3:D:776:GLU:OE2	3:D:1362:LYS:HD3	1.95	0.67
2:C:207:LEU:HD13	2:C:221:LEU:HD11	1.76	0.67
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.75	0.66
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.76	0.66
5:F:393:THR:HG22	5:F:394:ARG:HG2	1.78	0.66
2:C:853:LEU:HB2	2:C:858:MET:CE	2.26	0.65
2:C:243:ARG:HH21	7:H:9:DA:H61	1.44	0.65
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.30	0.65
2:C:189:ARG:NH1	2:C:242:LEU:O	2.30	0.65
3:D:133:ILE:HD12	3:D:152:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:237:THR:HA	7:H:5:DT:C7	2.27	0.65
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.80	0.64
3:D:1137:ARG:O	3:D:1141:GLU:HG3	1.97	0.64
1:B:18:ARG:O	1:B:207:PRO:HD3	1.96	0.64
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.79	0.64
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.31	0.64
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.30	0.64
3:D:156:GLU:N	3:D:156:GLU:OE2	2.27	0.64
3:D:181:ASP:HB2	3:D:205:TYR:CG	2.32	0.64
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.80	0.64
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.33	0.63
2:C:728:HIS:HE1	5:F:422:LEU:HD22	1.62	0.63
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.79	0.63
3:D:960:LYS:NZ	3:D:1063:GLU:OE1	2.31	0.63
3:D:1281:VAL:HG22	3:D:1317:ASP:H	1.63	0.63
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.32	0.63
2:C:428:ARG:NH2	2:C:447:ALA:O	2.31	0.63
5:F:397:ILE:HD13	5:F:400:ILE:HD11	1.80	0.63
3:D:973:GLN:HG2	3:D:974:ILE:HD13	1.80	0.63
4:E:50:THR:HG23	4:E:53:GLY:O	1.99	0.63
2:C:1095:LEU:HG	3:D:603:LEU:HD23	1.80	0.63
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.80	0.63
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.64	0.62
5:F:368:VAL:HG13	5:F:390:PHE:HD2	1.63	0.62
2:C:294:GLU:HB3	2:C:299:LYS:HD2	1.82	0.62
2:C:571:LEU:CD2	2:C:700:TYR:HA	2.30	0.62
2:C:649:VAL:HG13	2:C:653:ASP:HB2	1.82	0.62
5:F:191:ASN:HA	7:H:6:DG:N2	2.14	0.62
3:D:122:GLU:HG2	3:D:152:LEU:HD11	1.82	0.61
3:D:514:LEU:HD13	3:D:517:VAL:HG22	1.82	0.61
5:F:414:ARG:HB3	5:F:414:ARG:HH11	1.65	0.61
3:D:1152:GLU:OE1	3:D:1161:GLU:HA	2.00	0.61
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.82	0.61
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.82	0.61
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.82	0.61
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.35	0.61
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.81	0.61
3:D:1047:LYS:HD2	3:D:1051:GLU:HG3	1.82	0.61
2:C:206:THR:HG23	2:C:209:ARG:NH1	2.16	0.61
2:C:727:PRO:HB2	2:C:728:HIS:HD2	1.65	0.61
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:16:DC:O2	8:I:7:GTP:N2	2.17	0.61
5:F:144:ILE:HB	5:F:147:LEU:HD22	1.84	0.60
3:D:640:HIS:CE1	3:D:641:GLN:HE21	2.19	0.60
5:F:172:ARG:O	5:F:176:ILE:HG12	2.02	0.60
2:C:424:GLY:O	2:C:427:VAL:HG23	2.01	0.60
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.36	0.60
2:C:769:PRO:HD2	3:D:65:ARG:HH21	1.65	0.60
3:D:241:ILE:HG12	3:D:312:ARG:HH12	1.67	0.60
2:C:243:ARG:NH2	7:H:9:DA:H61	2.00	0.60
2:C:214:TYR:HB3	2:C:217:LEU:HD12	1.84	0.59
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.83	0.59
3:D:1254:GLN:CB	3:D:1258:ARG:HB2	2.32	0.59
6:G:20:DA:H4'	6:G:20:DA:OP1	2.01	0.59
3:D:669:ASN:ND2	5:F:417:LYS:HG2	2.14	0.59
2:C:418:LEU:H	2:C:418:LEU:HD12	1.67	0.59
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.84	0.59
1:B:101:LEU:HB2	1:B:114:PHE:CE2	2.36	0.59
2:C:764:GLU:C	2:C:766:GLU:H	2.05	0.59
2:C:948:GLU:HG2	2:C:953:VAL:HG23	1.85	0.59
5:F:398:ARG:O	5:F:402:ASN:ND2	2.34	0.59
2:C:573:ARG:HB2	2:C:670:GLN:NE2	2.18	0.58
2:C:184:MET:HE1	2:C:303:PHE:HE2	1.68	0.58
2:C:602:GLU:HB2	2:C:648:ARG:HH11	1.67	0.58
5:F:270:LYS:O	5:F:274:THR:OG1	2.19	0.58
2:C:1052:MET:HG3	3:D:623:VAL:HG11	1.85	0.58
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.85	0.58
3:D:658:LEU:HA	3:D:661:MET:HE3	1.85	0.58
5:F:237:THR:HA	7:H:5:DT:H72	1.85	0.58
5:F:358:LEU:HB3	5:F:366:ALA:CB	2.33	0.58
1:B:102:LYS:HG2	1:B:139:ASN:OD1	2.04	0.58
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.86	0.58
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.19	0.58
1:A:4:SER:HB3	1:A:189:ARG:HH21	1.68	0.57
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.87	0.57
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.86	0.57
1:B:101:LEU:HB2	1:B:114:PHE:HD2	1.69	0.57
3:D:645:PRO:HB3	3:D:723:GLY:O	2.04	0.57
3:D:561:GLY:HA2	5:F:140:ARG:HH11	1.69	0.57
6:G:6:DC:H2"	6:G:7:DA:H8	1.69	0.57
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.20	0.57
3:D:241:ILE:HG12	3:D:312:ARG:NH1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.40	0.56
2:C:45:GLN:HG2	2:C:71:TYR:HE2	1.69	0.56
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.86	0.56
2:C:229:MET:HE1	2:C:237:ARG:HH21	1.70	0.56
3:D:241:ILE:HD13	3:D:310:LEU:HD22	1.87	0.56
6:G:18:DA:H2'	6:G:19:DA:C5'	2.27	0.56
3:D:411:THR:HG22	5:F:178:ARG:HB3	1.88	0.56
1:B:161:ARG:HG3	1:B:162:ILE:O	2.06	0.56
6:G:6:DC:H2"	6:G:7:DA:C8	2.41	0.56
6:G:16:DC:H2'	6:G:17:DA:C8	2.35	0.56
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.41	0.56
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.87	0.56
3:D:737:ASN:ND2	11:D:2004:GTP:O3'	2.39	0.56
2:C:11:GLU:OE2	2:C:537:LYS:HE2	2.06	0.56
5:F:194:LEU:HB2	7:H:6:DG:C2	2.41	0.56
1:B:185:ARG:NH1	1:B:187:GLY:O	2.39	0.56
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.88	0.56
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.88	0.56
3:D:1444:THR:O	3:D:1448:THR:HG23	2.07	0.55
3:D:1198:TYR:CZ	3:D:1460:ILE:HD13	2.40	0.55
5:F:368:VAL:HG13	5:F:390:PHE:CD2	2.41	0.55
3:D:586:ARG:O	3:D:586:ARG:NH1	2.40	0.55
2:C:206:THR:HG23	2:C:209:ARG:HH12	1.72	0.55
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.31	0.55
4:E:39:VAL:HG21	4:E:72:ARG:HB2	1.88	0.55
1:A:70:GLY:N	2:C:607:ASP:OD1	2.39	0.55
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.36	0.55
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.89	0.55
2:C:1072:LYS:HD3	2:C:1074:GLU:OE2	2.06	0.55
3:D:1131:SER:OG	3:D:1132:LEU:N	2.36	0.55
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.89	0.55
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.87	0.54
2:C:214:TYR:O	2:C:218:VAL:HG23	2.07	0.54
3:D:1209:LEU:HD11	3:D:1364:HIS:CD2	2.39	0.54
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.07	0.54
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.42	0.54
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.21	0.54
3:D:1281:VAL:CG2	3:D:1317:ASP:H	2.21	0.54
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.89	0.54
3:D:97:THR:HG21	3:D:571:LYS:HE3	1.89	0.54
3:D:1290:LEU:HD23	3:D:1307:LYS:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:405:LEU:O	5:F:409:LYS:HG3	2.08	0.54
3:D:258:VAL:HG12	3:D:273:ARG:O	2.08	0.54
1:B:110:LYS:HD2	1:B:128:HIS:HA	1.89	0.54
2:C:607:ASP:HB3	2:C:610:ARG:H	1.73	0.54
2:C:769:PRO:HD2	3:D:65:ARG:NH2	2.23	0.54
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.90	0.54
6:G:4:DC:H42	7:H:24:DA:H61	1.53	0.54
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.90	0.54
3:D:1277:ILE:HG13	3:D:1278:ASP:H	1.72	0.54
3:D:259:VAL:HG13	3:D:270:LEU:HD21	1.89	0.53
3:D:351:MET:HG2	3:D:370:ALA:HB2	1.88	0.53
6:G:19:DA:H4'	6:G:20:DA:O5'	2.07	0.53
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.18	0.53
1:B:77:GLU:HG2	3:D:872:ARG:HH11	1.73	0.53
3:D:977:ALA:HA	3:D:982:PHE:HD2	1.72	0.53
6:G:18:DA:N6	6:G:19:DA:N1	2.56	0.53
3:D:652:LEU:HB3	3:D:749:VAL:HG21	1.91	0.53
2:C:358:ARG:HB3	2:C:372:LEU:HD12	1.91	0.53
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.35	0.53
2:C:243:ARG:NH2	7:H:9:DA:N6	2.56	0.53
3:D:798:GLU:OE2	3:D:824:ASN:ND2	2.31	0.53
3:D:1149:LEU:HG	3:D:1166:LEU:HD21	1.91	0.53
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.89	0.53
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.33	0.53
1:B:94:LEU:HD11	1:B:96:THR:O	2.09	0.53
3:D:1364:HIS:CD2	3:D:1366:LYS:HE3	2.44	0.53
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.44	0.53
2:C:35:PRO:HG2	2:C:38:LYS:HB2	1.91	0.52
2:C:886:LEU:HD21	3:D:951:ILE:HG12	1.91	0.52
6:G:4:DC:H42	7:H:24:DA:N6	2.06	0.52
1:B:56:VAL:HG23	1:B:142:VAL:HG12	1.92	0.52
2:C:715:THR:OG1	2:C:718:GLY:O	2.27	0.52
5:F:358:LEU:O	5:F:366:ALA:HB2	2.09	0.52
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.24	0.52
3:D:204:LEU:HD22	3:D:441:ARG:CZ	2.39	0.52
3:D:251:PHE:CE2	3:D:304:LEU:HD12	2.45	0.52
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.24	0.52
3:D:629:SER:OG	3:D:630:VAL:N	2.42	0.52
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.90	0.52
2:C:874:LEU:HD12	3:D:784:ASP:OD1	2.10	0.52
4:E:57:ASP:O	4:E:63:TRP:NE1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.92	0.52
3:D:1105:ILE:HD12	3:D:1199:GLY:HA2	1.92	0.52
2:C:839:LEU:HD23	2:C:996:LYS:HA	1.92	0.52
3:D:109:PRO:HD3	7:H:21:DT:H5"	1.92	0.52
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.45	0.52
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.09	0.52
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.92	0.52
2:C:775:ARG:HG3	2:C:780:GLU:O	2.09	0.51
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.92	0.51
3:D:1125:PRO:HA	3:D:1132:LEU:HD23	1.92	0.51
2:C:230:ARG:HG3	2:C:233:GLU:HG3	1.92	0.51
3:D:1387:SER:OG	3:D:1388:ARG:N	2.42	0.51
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.93	0.51
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.91	0.51
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.43	0.51
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.92	0.51
6:G:18:DA:N6	6:G:19:DA:C6	2.79	0.51
3:D:251:PHE:HE2	3:D:304:LEU:HD12	1.74	0.51
3:D:284:LEU:HD22	3:D:288:MET:HE2	1.92	0.51
3:D:492:ALA:O	3:D:496:LEU:HB2	2.11	0.51
1:A:89:PHE:HB2	1:A:146:ARG:HH22	1.76	0.51
3:D:561:GLY:HA2	5:F:140:ARG:NH1	2.26	0.51
5:F:237:THR:OG1	7:H:4:DA:H8	1.93	0.51
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.91	0.51
2:C:679:PHE:HA	3:D:943:THR:HG23	1.93	0.51
5:F:363:GLU:O	5:F:367:MET:N	2.40	0.51
6:G:5:DG:C3'	6:G:6:DC:H5"	2.41	0.50
3:D:703:ASN:HA	3:D:712:GLY:O	2.12	0.50
5:F:95:THR:HB	5:F:98:GLU:HG3	1.92	0.50
1:A:198:ARG:O	1:A:199:ILE:HD13	2.11	0.50
3:D:860:LEU:O	3:D:876:SER:HB2	2.12	0.50
1:B:85:LEU:HG	1:B:87:VAL:HG23	1.93	0.50
7:H:17:DC:H2"	7:H:18:DT:H5'	1.93	0.50
2:C:615:TYR:OH	2:C:623:TYR:OH	2.14	0.50
3:D:129:PHE:CD2	3:D:456:MET:HB3	2.47	0.50
5:F:127:ILE:O	5:F:131:VAL:HG23	2.12	0.50
3:D:208:PRO:HG3	3:D:387:LEU:HD22	1.94	0.50
7:H:10:DG:H8	7:H:10:DG:OP2	1.94	0.50
3:D:806:PHE:O	3:D:829:VAL:HA	2.12	0.50
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.12	0.50
2:C:939:ARG:NH1	2:C:980:GLY:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:171:LEU:HD21	3:D:177:ALA:HB2	1.94	0.50
3:D:805:GLU:HG3	3:D:828:LYS:HB2	1.93	0.50
4:E:70:THR:OG1	4:E:72:ARG:HG3	2.12	0.50
2:C:858:MET:HG2	2:C:867:VAL:O	2.11	0.49
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.93	0.49
3:D:1084:THR:O	3:D:1088:THR:HG23	2.11	0.49
3:D:1087:ARG:HG3	3:D:1256:LEU:HD23	1.93	0.49
5:F:233:PHE:CE2	7:H:2:DT:H2"	2.47	0.49
1:B:38:ASN:OD1	2:C:979:THR:HG22	2.12	0.49
2:C:878:SER:OG	3:D:1029:ARG:HD2	2.12	0.49
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.45	0.49
2:C:12:VAL:HG11	2:C:472:ARG:HD3	1.94	0.49
2:C:272:ALA:HA	2:C:464:LEU:HD13	1.93	0.49
3:D:501:ALA:HB1	3:D:1452:ILE:HG22	1.94	0.49
1:B:112:ARG:HG3	1:B:125:PRO:O	2.12	0.49
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	1.93	0.49
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.94	0.49
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.46	0.49
3:D:38:LYS:HB3	3:D:39:PRO:HD2	1.95	0.49
3:D:1319:VAL:HG12	3:D:1323:GLN:NE2	2.28	0.49
3:D:1386:ASP:HB2	3:D:1412:LYS:HB3	1.93	0.49
5:F:369:LEU:HD22	5:F:404:ALA:HB1	1.94	0.49
2:C:910:LYS:O	2:C:914:ILE:HG13	2.13	0.49
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.93	0.49
2:C:224:GLU:CD	2:C:224:GLU:H	2.16	0.49
2:C:1005:MET:SD	3:D:648:MET:HG3	2.53	0.49
3:D:66:GLN:HB3	5:F:376:ILE:HG22	1.94	0.49
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.95	0.49
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.28	0.49
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.51	0.49
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.42	0.49
5:F:415:THR:O	5:F:417:LYS:N	2.43	0.49
2:C:405:ARG:HD2	2:C:442:GLU:OE1	2.13	0.49
5:F:191:ASN:CA	7:H:6:DG:H22	2.25	0.49
1:A:9:PRO:HB3	1:A:27:PRO:O	2.12	0.48
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.46	0.48
1:B:220:GLU:O	1:B:223:THR:OG1	2.20	0.48
2:C:807:ARG:HG2	2:C:821:GLU:HB3	1.93	0.48
3:D:1263:PHE:O	3:D:1375:MET:HE2	2.13	0.48
1:B:141:GLU:OE1	1:B:161:ARG:NH2	2.47	0.48
2:C:472:ARG:HD2	2:C:480:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:695:ILE:HD12	3:D:718:PRO:HG2	1.94	0.48
5:F:414:ARG:HB3	5:F:414:ARG:NH1	2.27	0.48
2:C:563:ASN:O	2:C:566:THR:HB	2.12	0.48
2:C:807:ARG:HB2	2:C:810:ASP:OD2	2.14	0.48
1:B:80:LEU:HD22	3:D:844:ALA:HA	1.95	0.48
4:E:66:LYS:HD2	4:E:66:LYS:N	2.29	0.48
6:G:19:DA:H1'	6:G:20:DA:OP2	2.13	0.48
1:B:18:ARG:NH1	1:B:204:SER:O	2.47	0.48
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.95	0.48
3:D:625:TYR:CD2	3:D:751:LEU:HD11	2.48	0.48
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.48	0.48
5:F:287:THR:OG1	5:F:290:GLU:OE2	2.31	0.48
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.95	0.48
2:C:614:ARG:HE	2:C:620:LEU:HD13	1.78	0.48
5:F:89:GLY:HA3	7:H:7:DG:C6	2.48	0.48
6:G:5:DG:H2"	6:G:6:DC:H5"	1.96	0.48
2:C:473:ARG:HB3	2:C:480:THR:OG1	2.13	0.48
3:D:468:LEU:HA	3:D:468:LEU:HD23	1.68	0.48
2:C:168:ARG:NH1	2:C:345:ARG:HD3	2.29	0.48
2:C:580:MET:HB3	2:C:584:GLU:CD	2.34	0.48
3:D:131:LYS:N	3:D:456:MET:HE2	2.29	0.48
3:D:231:VAL:O	3:D:236:TYR:OH	2.31	0.48
3:D:417:PRO:HB3	3:D:430:ASP:O	2.14	0.48
3:D:1486:VAL:HG22	4:E:22:VAL:HG13	1.96	0.48
3:D:1492:LEU:O	3:D:1496:GLU:HB2	2.14	0.48
3:D:135:LEU:O	3:D:149:LYS:HG3	2.13	0.47
2:C:249:LYS:HB3	2:C:252:LYS:HB2	1.96	0.47
2:C:267:TYR:CE1	2:C:290:LEU:HG	2.49	0.47
2:C:775:ARG:HE	2:C:782:ALA:HA	1.79	0.47
3:D:876:SER:OG	3:D:879:ARG:HG3	2.13	0.47
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.97	0.47
2:C:168:ARG:O	2:C:267:TYR:HA	2.14	0.47
3:D:471:GLU:H	3:D:471:GLU:HG2	1.50	0.47
2:C:573:ARG:HB2	2:C:670:GLN:HE21	1.79	0.47
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.96	0.47
1:B:108:GLU:HA	1:B:131:THR:HA	1.97	0.47
3:D:907:GLU:OE2	3:D:909:ASN:HB2	2.15	0.47
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.96	0.47
3:D:1348:LEU:HD23	3:D:1348:LEU:HA	1.75	0.47
5:F:191:ASN:HA	7:H:6:DG:H22	1.79	0.47
1:A:106:PRO:CG	1:A:134:GLU:HG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:HIS:O	1:A:129:ILE:HD13	2.14	0.47
1:A:179:PHE:CB	1:A:197:LEU:HD23	2.42	0.47
3:D:573:MET:SD	5:F:210:LEU:HB3	2.54	0.47
3:D:899:LEU:HD21	3:D:921:ARG:HD3	1.96	0.47
5:F:237:THR:HA	7:H:5:DT:H73	1.95	0.47
2:C:598:GLU:O	2:C:651:LYS:HG3	2.14	0.47
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.96	0.47
2:C:425:PHE:CD1	3:D:1079:LYS:HE3	2.49	0.46
3:D:432:TYR:O	3:D:448:GLU:HA	2.15	0.46
3:D:842:VAL:HG22	3:D:865:THR:HB	1.96	0.46
3:D:924:MET:HG2	4:E:7:ASP:OD1	2.14	0.46
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.16	0.46
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.97	0.46
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.50	0.46
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.97	0.46
3:D:481:MET:O	3:D:489:ARG:HG2	2.15	0.46
3:D:1499:ARG:CZ	4:E:84:ARG:HG2	2.45	0.46
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.97	0.46
3:D:322:VAL:HG22	3:D:335:LEU:CD2	2.45	0.46
3:D:1314:LYS:H	3:D:1314:LYS:HD2	1.81	0.46
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.98	0.46
3:D:45:PHE:O	3:D:86:ARG:NH2	2.48	0.46
3:D:1038:LEU:O	3:D:1060:SER:HB2	2.16	0.46
1:B:197:LEU:HA	1:B:197:LEU:HD23	1.58	0.46
3:D:354:VAL:HG22	3:D:367:ILE:O	2.15	0.46
1:B:65:PHE:CD2	3:D:809:PRO:HB2	2.50	0.46
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.69	0.46
2:C:210:GLU:HB3	2:C:211:LEU:HD12	1.97	0.46
2:C:1038:TRP:NE1	3:D:1099:VAL:HG11	2.30	0.46
5:F:397:ILE:CD1	5:F:400:ILE:HD11	2.44	0.46
3:D:56:TYR:HE1	3:D:69:GLU:HG3	1.81	0.46
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.97	0.46
3:D:853:VAL:HG22	3:D:858:VAL:HG23	1.97	0.46
3:D:972:LEU:HD13	3:D:972:LEU:HA	1.54	0.46
3:D:1271:LYS:HD3	3:D:1331:ASP:HB2	1.98	0.46
5:F:361:LEU:HD13	5:F:407:LYS:HB3	1.98	0.46
1:A:206:THR:HG22	1:A:209:GLU:H	1.81	0.46
1:B:110:LYS:HB2	1:B:112:ARG:NH2	2.28	0.46
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.98	0.46
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.97	0.46
3:D:491:LYS:NZ	3:D:494:LYS:HE3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.76	0.46
5:F:160:ASP:OD2	5:F:164:LYS:HE3	2.16	0.46
2:C:1103:ASP:OD2	2:C:1107:ASN:HB2	2.16	0.45
3:D:613:ARG:HG3	3:D:618:LEU:HD23	1.98	0.45
3:D:618:LEU:HD12	3:D:1467:ILE:HG23	1.97	0.45
3:D:103:TRP:CZ2	3:D:1444:THR:HG22	2.52	0.45
3:D:207:PHE:HB2	3:D:391:ALA:HB2	1.98	0.45
6:G:4:DC:N4	7:H:24:DA:H61	2.14	0.45
3:D:312:ARG:NH1	3:D:312:ARG:HB3	2.30	0.45
3:D:1198:TYR:CE2	3:D:1460:ILE:HD13	2.51	0.45
3:D:1236:LEU:HG	3:D:1359:GLN:HG3	1.98	0.45
4:E:46:PRO:HB2	4:E:57:ASP:HB2	1.97	0.45
4:E:62:THR:O	4:E:66:LYS:HD3	2.17	0.45
1:A:117:VAL:O	1:A:120:VAL:HG22	2.16	0.45
1:B:153:ALA:HB2	1:B:168:ASP:N	2.31	0.45
2:C:154:ARG:HH21	2:C:157:ARG:HG3	1.82	0.45
2:C:943:VAL:HG11	2:C:973:VAL:HG22	1.98	0.45
2:C:952:LEU:HA	2:C:952:LEU:HD23	1.73	0.45
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.98	0.45
5:F:355:GLU:C	5:F:357:ALA:H	2.20	0.45
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.97	0.45
5:F:122:LEU:HB2	5:F:127:ILE:HD11	1.98	0.45
2:C:1083:GLU:OE1	2:C:1086:ARG:NH1	2.49	0.45
3:D:1028:ALA:O	3:D:1029:ARG:HG2	2.17	0.45
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.17	0.45
2:C:797:GLY:O	2:C:829:GLN:NE2	2.50	0.45
3:D:343:LYS:NZ	3:D:380:GLU:OE2	2.41	0.45
5:F:193:ARG:HB3	7:H:7:DG:C5'	2.44	0.45
7:H:24:DA:H2"	7:H:25:DG:OP2	2.16	0.45
2:C:572:ILE:HG13	2:C:573:ARG:HG2	1.99	0.45
3:D:520:LEU:O	3:D:525:ARG:NH1	2.48	0.45
3:D:1209:LEU:HD23	3:D:1209:LEU:HA	1.76	0.45
2:C:211:LEU:HB2	2:C:218:VAL:HG11	1.98	0.45
2:C:226:VAL:O	2:C:229:MET:HG2	2.17	0.45
3:D:1290:LEU:HB3	3:D:1305:LEU:HD23	1.99	0.45
3:D:1291:SER:OG	3:D:1304:LYS:HG2	2.17	0.45
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.98	0.45
2:C:76:PRO:HG3	2:C:120:LEU:HD12	1.99	0.44
2:C:627:ARG:CZ	2:C:640:ARG:HG3	2.47	0.44
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.99	0.44
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:LEU:HD21	2:C:99:GLN:HE21	1.82	0.44
2:C:135:VAL:HG23	2:C:395:LYS:HG3	2.00	0.44
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.52	0.44
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.18	0.44
5:F:131:VAL:HG11	5:F:177:ALA:HB1	2.00	0.44
5:F:202:TYR:HE1	5:F:248:ASN:HD21	1.65	0.44
1:B:150:TYR:CE2	1:B:170:VAL:HG22	2.53	0.44
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.69	0.44
2:C:419:THR:HG22	2:C:420:ARG:H	1.83	0.44
2:C:1035:MET:HA	2:C:1038:TRP:CE3	2.53	0.44
5:F:191:ASN:CA	7:H:6:DG:N2	2.78	0.44
2:C:474:VAL:HG22	2:C:479:VAL:HG22	1.99	0.44
1:A:25:LEU:HD12	1:A:25:LEU:HA	1.81	0.44
3:D:882:PHE:CZ	3:D:906:GLN:HG3	2.52	0.44
2:C:561:GLY:O	2:C:565:GLN:HG3	2.18	0.44
2:C:591:SER:O	2:C:592:LEU:HB2	2.17	0.44
3:D:702:LEU:O	3:D:713:ILE:HA	2.18	0.44
3:D:1426:LYS:NZ	7:H:20:DA:OP1	2.49	0.44
1:A:180:GLN:NE2	2:C:935:GLY:O	2.51	0.44
3:D:993:LEU:HD22	3:D:1044:LEU:HD13	1.99	0.44
2:C:276:LYS:HE2	2:C:276:LYS:HB3	1.87	0.43
2:C:470:PRO:HD3	2:C:485:TYR:CE1	2.53	0.43
2:C:773:LEU:HD13	5:F:373:LYS:HG3	2.00	0.43
2:C:889:HIS:HE1	2:C:988:VAL:HG13	1.83	0.43
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	2.01	0.43
2:C:376:ARG:NH2	5:F:279:GLN:OE1	2.51	0.43
2:C:420:ARG:HH22	5:F:323:ASP:HB3	1.84	0.43
2:C:657:ASP:OD2	2:C:663:ASN:N	2.47	0.43
2:C:841:ASN:HD22	2:C:992:MET:CE	2.31	0.43
3:D:403:PHE:HB2	3:D:423:ASP:OD1	2.19	0.43
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.48	0.43
2:C:499:ALA:HB2	2:C:533:ASP:HB2	2.01	0.43
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.53	0.43
3:D:800:LYS:HB3	3:D:822:ALA:CB	2.41	0.43
3:D:1190:SER:O	3:D:1204:CYS:HB3	2.18	0.43
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.22	0.43
3:D:1386:ASP:OD2	3:D:1412:LYS:HD2	2.19	0.43
2:C:343:GLN:HG3	2:C:385:PHE:HB2	2.01	0.43
2:C:914:ILE:HD13	2:C:914:ILE:HG21	1.72	0.43
3:D:1154:GLU:HA	3:D:1158:VAL:O	2.17	0.43
5:F:89:GLY:HA3	7:H:7:DG:O6	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:799:LYS:NZ	3:D:1014:ASN:HA	2.34	0.43
2:C:524:VAL:HG23	2:C:528:GLU:HB2	2.00	0.43
2:C:838:LYS:HE3	3:D:741:ASP:O	2.19	0.43
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.84	0.43
4:E:33:HIS:HE2	4:E:89:MET:HB3	1.83	0.43
2:C:598:GLU:N	2:C:615:TYR:OH	2.48	0.43
2:C:881:ASN:OD1	2:C:881:ASN:N	2.50	0.43
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.54	0.43
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.37	0.43
3:D:484:PRO:C	3:D:486:ARG:H	2.22	0.43
3:D:1380:GLU:HB2	3:D:1420:LEU:HD22	2.00	0.43
5:F:143:HIS:HB2	5:F:150:THR:HG23	2.00	0.43
2:C:154:ARG:HA	2:C:155:PRO:HD2	1.93	0.42
2:C:261:ILE:HG22	2:C:262:ALA:N	2.34	0.42
2:C:877:PRO:HG3	3:D:1023:MET:HE1	2.00	0.42
3:D:353:VAL:HG12	3:D:355:VAL:H	1.84	0.42
3:D:597:ASP:O	3:D:599:PRO:HD3	2.19	0.42
5:F:369:LEU:HD22	5:F:404:ALA:CB	2.49	0.42
3:D:230:TRP:CZ3	3:D:333:LEU:HD21	2.53	0.42
3:D:259:VAL:HG13	3:D:270:LEU:CD2	2.48	0.42
4:E:46:PRO:HB2	4:E:57:ASP:CB	2.49	0.42
5:F:194:LEU:HD12	7:H:6:DG:H5'	2.00	0.42
2:C:20:GLU:O	2:C:24:GLU:HB2	2.19	0.42
2:C:45:GLN:HG2	2:C:71:TYR:CE2	2.52	0.42
1:A:44:LEU:O	1:A:174:VAL:HG21	2.19	0.42
2:C:501:THR:HA	2:C:502:PRO:HD3	1.94	0.42
3:D:204:LEU:HD23	3:D:204:LEU:HA	1.89	0.42
3:D:298:VAL:HA	3:D:302:GLN:OE1	2.19	0.42
2:C:1097:LEU:HD23	2:C:1097:LEU:HA	1.66	0.42
3:D:1023:MET:HB2	3:D:1023:MET:HE3	1.92	0.42
3:D:1386:ASP:OD2	3:D:1413:THR:HG22	2.18	0.42
3:D:405:ASP:CG	3:D:406:ASP:H	2.22	0.42
3:D:715:ALA:HB3	3:D:764:LEU:HA	2.02	0.42
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.32	0.42
3:D:1271:LYS:HG3	3:D:1272:ALA:O	2.19	0.42
5:F:188:ILE:HD13	5:F:221:ILE:HG12	2.01	0.42
5:F:393:THR:HG22	5:F:394:ARG:N	2.35	0.42
1:A:25:LEU:HD21	1:B:224:TYR:HB2	2.02	0.42
3:D:1377:LYS:HE3	3:D:1378:TYR:OH	2.19	0.42
2:C:882:LEU:HD23	2:C:882:LEU:HA	1.80	0.42
3:D:499:VAL:HG12	3:D:503:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1105:ILE:HG23	3:D:1199:GLY:HA2	2.02	0.42
1:A:90:LEU:HA	1:A:90:LEU:HD13	1.73	0.42
1:B:153:ALA:HB2	1:B:167:VAL:C	2.40	0.42
2:C:687:ALA:HB1	2:C:850:ALA:HB2	2.01	0.42
5:F:321:ILE:HG12	5:F:327:SER:OG	2.20	0.42
5:F:368:VAL:HG11	5:F:400:ILE:HG13	2.01	0.42
2:C:269:LEU:HD12	2:C:269:LEU:HA	1.90	0.42
2:C:475:VAL:O	2:C:478:VAL:HG12	2.19	0.42
3:D:90:MET:SD	3:D:521:PRO:HD3	2.60	0.42
3:D:172:PRO:HA	3:D:173:PRO:HD3	1.93	0.42
3:D:613:ARG:HG3	3:D:618:LEU:CD2	2.49	0.42
6:G:3:DC:H42	7:H:25:DG:H1	1.68	0.42
7:H:8:DG:H2"	7:H:9:DA:C8	2.54	0.42
3:D:192:ALA:HB3	3:D:195:VAL:HB	2.02	0.41
2:C:179:ASN:OD1	2:C:181:VAL:HG12	2.20	0.41
2:C:966:LEU:HD23	2:C:966:LEU:HA	1.91	0.41
5:F:381:HIS:ND1	5:F:385:GLU:HG3	2.35	0.41
5:F:415:THR:C	5:F:417:LYS:H	2.22	0.41
1:A:11:PHE:O	1:B:228:PRO:HA	2.19	0.41
1:B:109:VAL:N	1:B:130:ALA:O	2.41	0.41
2:C:144:PRO:HG2	2:C:165:LEU:HD23	2.02	0.41
2:C:161:SER:HA	2:C:172:ILE:O	2.20	0.41
3:D:185:VAL:HG13	3:D:189:GLN:HB3	2.01	0.41
3:D:1263:PHE:HD2	3:D:1375:MET:HE1	1.85	0.41
1:A:42:ARG:NH2	1:B:34:VAL:HG22	2.35	0.41
1:A:54:THR:HB	1:A:158:ILE:HD12	2.02	0.41
1:A:206:THR:HB	1:A:209:GLU:HG3	2.02	0.41
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.50	0.41
2:C:6:PHE:CD1	2:C:909:ALA:HB2	2.55	0.41
3:D:1293:PHE:CZ	3:D:1302:GLU:OE2	2.73	0.41
5:F:194:LEU:CD1	7:H:6:DG:H5'	2.50	0.41
1:A:175:ARG:HE	1:A:202:ASP:HB3	1.85	0.41
2:C:76:PRO:HA	2:C:77:PRO:HD3	1.95	0.41
2:C:164:PRO:HA	2:C:269:LEU:HD12	2.02	0.41
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.03	0.41
2:C:587:VAL:O	2:C:591:SER:HB3	2.20	0.41
2:C:905:ILE:C	2:C:907:ASP:H	2.24	0.41
6:G:11:DG:H2"	6:G:12:DA:O5'	2.20	0.41
1:B:83:LYS:HE2	1:B:168:ASP:HB2	2.03	0.41
1:B:110:LYS:HE3	1:B:126:ASP:O	2.21	0.41
3:D:540:LEU:HD23	3:D:540:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:657:LEU:HG	3:D:661:MET:HE2	2.02	0.41
3:D:1144:LEU:HD23	3:D:1144:LEU:HA	1.80	0.41
5:F:194:LEU:HB2	7:H:6:DG:N3	2.35	0.41
1:A:101:LEU:HB2	1:A:114:PHE:CE2	2.55	0.41
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.01	0.41
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.82	0.41
3:D:706:PRO:HB2	3:D:708:LEU:HD21	2.03	0.41
2:C:694:LEU:HD23	2:C:694:LEU:HA	1.93	0.41
2:C:759:THR:HB	2:C:785:VAL:HB	2.02	0.41
3:D:696:HIS:ND1	4:E:57:ASP:OD1	2.52	0.41
3:D:784:ASP:HB2	3:D:939:PHE:CE1	2.55	0.41
2:C:136:ILE:HB	2:C:336:VAL:HG13	2.03	0.41
2:C:439:CYS:CB	2:C:541:SER:HB3	2.50	0.41
2:C:713:ARG:CZ	2:C:715:THR:HG22	2.51	0.41
2:C:944:LEU:HA	2:C:944:LEU:HD23	1.79	0.41
3:D:96:ALA:HB3	3:D:554:LEU:HD23	2.03	0.41
3:D:1148:VAL:HG21	3:D:1203:LYS:HD3	2.02	0.41
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.59	0.41
3:D:1263:PHE:CE2	3:D:1371:VAL:HG11	2.55	0.41
1:B:49:PRO:CA	1:B:148:VAL:HG12	2.50	0.41
1:B:150:TYR:HE2	1:B:170:VAL:HG22	1.86	0.41
2:C:580:MET:HE2	2:C:902:ILE:HG12	2.02	0.41
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.21	0.41
3:D:394:LEU:HG	3:D:396:VAL:HG23	2.02	0.41
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.95	0.41
2:C:617:ASP:OD1	2:C:617:ASP:N	2.53	0.40
2:C:666:LEU:HD11	2:C:668:LEU:HD21	2.03	0.40
2:C:911:GLU:O	2:C:915:LYS:HG2	2.21	0.40
2:C:996:LYS:HE2	2:C:1000:MET:SD	2.62	0.40
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	2.03	0.40
2:C:140:ILE:HD13	2:C:331:ARG:HH11	1.85	0.40
2:C:737:LEU:HA	2:C:743:VAL:HA	2.04	0.40
3:D:298:VAL:HG12	3:D:302:GLN:NE2	2.37	0.40
3:D:567:ILE:HD12	3:D:567:ILE:HG23	1.89	0.40
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.56	0.40
5:F:267:THR:O	5:F:270:LYS:HB3	2.21	0.40
5:F:354:LEU:HD23	5:F:354:LEU:HA	1.86	0.40
1:A:83:LYS:HD2	1:A:168:ASP:HB2	2.03	0.40
1:A:156:HIS:NE2	1:A:167:VAL:O	2.46	0.40
1:B:99:LEU:HB2	1:B:142:VAL:HG22	2.03	0.40
2:C:243:ARG:HH21	7:H:9:DA:N6	2.12	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:155:ASP:OD1	3:D:568:ARG:NH1	2.34	0.40
3:D:1211:MET:HE2	3:D:1211:MET:HB2	1.95	0.40
7:H:16:DT:H4'	7:H:17:DC:OP1	2.22	0.40
3:D:796:ARG:NH1	3:D:862:ASP:OD1	2.54	0.40
1:A:226:SER:O	1:A:228:PRO:HD3	2.21	0.40
3:D:803:GLY:HA2	3:D:826:PRO:O	2.22	0.40
3:D:1068:LEU:HA	3:D:1068:LEU:HD12	1.75	0.40
3:D:1254:GLN:HB2	3:D:1258:ARG:CB	2.48	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)
3:D:34:TYR:OH	3:D:327:GLU:OE1[4_1159]	2.14	0.06

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	224/315 (71%)	220 (98%)	4 (2%)	0	100	100
1	B	222/315 (70%)	211 (95%)	10 (4%)	1 (0%)	29	64
2	C	1107/1119 (99%)	1062 (96%)	38 (3%)	7 (1%)	25	59
3	D	1480/1524 (97%)	1433 (97%)	39 (3%)	8 (0%)	29	64
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	14	46
5	F	344/423 (81%)	314 (91%)	20 (6%)	10 (3%)	4	24
All	All	3469/3795 (91%)	3329 (96%)	113 (3%)	27 (1%)	19	54

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	212	GLY
2	C	363	SER
3	D	484	PRO
3	D	486	ARG
3	D	664	LYS
5	F	388	ALA
2	C	228	ALA
5	F	323	ASP
5	F	384	GLU
5	F	385	GLU
5	F	416	ARG
2	C	362	GLY
2	C	391	LEU
3	D	485	SER
3	D	1049	SER
3	D	1050	GLY
5	F	356	LYS
1	B	154	GLU
2	C	105	THR
5	F	148	LYS
5	F	381	HIS
2	C	365	ASP
5	F	382	THR
3	D	320	ALA
5	F	393	THR
4	E	94	PRO
3	D	831	GLY

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	199/273 (73%)	189 (95%)	10 (5%)	24	57
1	B	197/273 (72%)	187 (95%)	10 (5%)	24	56
2	C	935/941 (99%)	892 (95%)	43 (5%)	27	59
3	D	1250/1279 (98%)	1184 (95%)	66 (5%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	83/88 (94%)	81 (98%)	2 (2%)	49	76
5	F	301/371 (81%)	294 (98%)	7 (2%)	50	77
All	All	2965/3225 (92%)	2827 (95%)	138 (5%)	26	59

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	67	THR
1	A	133	GLU
1	A	184	THR
1	A	186	LEU
1	A	189	ARG
1	A	205	VAL
1	A	219	ARG
1	A	229	GLN
1	B	14	ARG
1	B	34	VAL
1	B	38	ASN
1	B	112	ARG
1	B	126	ASP
1	B	134	GLU
1	B	183	ASP
1	B	186	LEU
1	B	193	ASP
1	B	206	THR
2	C	8	ARG
2	C	15	LEU
2	C	56	GLU
2	C	81	ASP
2	C	103	LYS
2	C	107	LEU
2	C	133	ASP
2	C	141	HIS
2	C	168	ARG
2	C	177	GLU
2	C	194	VAL
2	C	205	GLU
2	C	221	LEU
2	C	340	MET

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Mol	Chain	Res	Type
2	C	342	ASP
2	C	353	ARG
2	C	358	ARG
2	C	404	LEU
2	C	409	ARG
2	C	427	VAL
2	C	434	HIS
2	C	454	SER
2	C	524	VAL
2	C	557	ARG
2	C	575	GLN
2	C	583	LEU
2	C	586	ARG
2	C	591	SER
2	C	610	ARG
2	C	617	ASP
2	C	640	ARG
2	C	661	SER
2	C	775	ARG
2	C	808	ARG
2	C	813	VAL
2	C	815	LEU
2	C	848	VAL
2	C	939	ARG
2	C	942	GLU
2	C	968	LEU
2	C	1001	VAL
2	C	1014	SER
2	C	1057	SER
3	D	30	GLU
3	D	81	THR
3	D	106	LYS
3	D	114	THR
3	D	133	ILE
3	D	141	ILE
3	D	142	LEU
3	D	155	ASP
3	D	161	LEU
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	200	ASP

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Mol	Chain	Res	Type
3	D	220	ARG
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	272	LEU
3	D	276	ASP
3	D	312	ARG
3	D	325	GLU
3	D	362	GLU
3	D	372	ASP
3	D	411	THR
3	D	421	LEU
3	D	423	ASP
3	D	434	ARG
3	D	525	ARG
3	D	548	ILE
3	D	572	ARG
3	D	587	ARG
3	D	618	LEU
3	D	650	LEU
3	D	675	ARG
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	817	GLU
3	D	832	ARG
3	D	860	LEU
3	D	861	GLN
3	D	875	THR
3	D	894	LYS
3	D	904	VAL
3	D	970	LYS
3	D	972	LEU
3	D	1041	LEU
3	D	1062	ARG
3	D	1130	ARG
3	D	1154	GLU
3	D	1155	VAL
3	D	1188	VAL
3	D	1195	GLN
3	D	1208	ASP

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Mol	Chain	Res	Type
3	D	1219	GLU
3	D	1221	VAL
3	D	1271	LYS
3	D	1284	GLU
3	D	1290	LEU
3	D	1305	LEU
3	D	1313	VAL
3	D	1317	ASP
3	D	1470	ARG
3	D	1493	LYS
3	D	1496	GLU
4	E	50	THR
4	E	75	PHE
5	F	186	HIS
5	F	205	ARG
5	F	287	THR
5	F	321	ILE
5	F	364	ARG
5	F	377	ASP
5	F	419	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	728	HIS
3	D	388	HIS
3	D	640	HIS
3	D	737	ASN
3	D	744	GLN
3	D	1075	HIS
3	D	1323	GLN
5	F	83	GLN
5	F	269	ASN
5	F	277	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	0/2	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
11	GTP	D	2004	9	26,34,34	1.09	2 (7%)	32,54,54	1.58	7 (21%)

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
11	GTP	D	2004	9	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2004	GTP	C5-C6	-3.13	1.41	1.47
11	D	2004	GTP	C2-N3	3.11	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	2004	GTP	C8-N7-C5	3.24	109.17	102.99
11	D	2004	GTP	PA-O3A-PB	-3.18	121.93	132.83
11	D	2004	GTP	C5-C6-N1	3.12	119.46	113.95
11	D	2004	GTP	C2-N1-C6	-3.08	119.42	125.10
11	D	2004	GTP	PB-O3B-PG	-3.08	122.26	132.83
11	D	2004	GTP	O3G-PG-O3B	2.59	113.31	104.64
11	D	2004	GTP	C2'-C3'-C4'	2.02	106.57	102.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	2004	GTP	C5'-O5'-PA-O3A
11	D	2004	GTP	O4'-C4'-C5'-O5'
11	D	2004	GTP	C3'-C4'-C5'-O5'
11	D	2004	GTP	PG-O3B-PB-O1B
11	D	2004	GTP	PA-O3A-PB-O1B
11	D	2004	GTP	C5'-O5'-PA-O1A

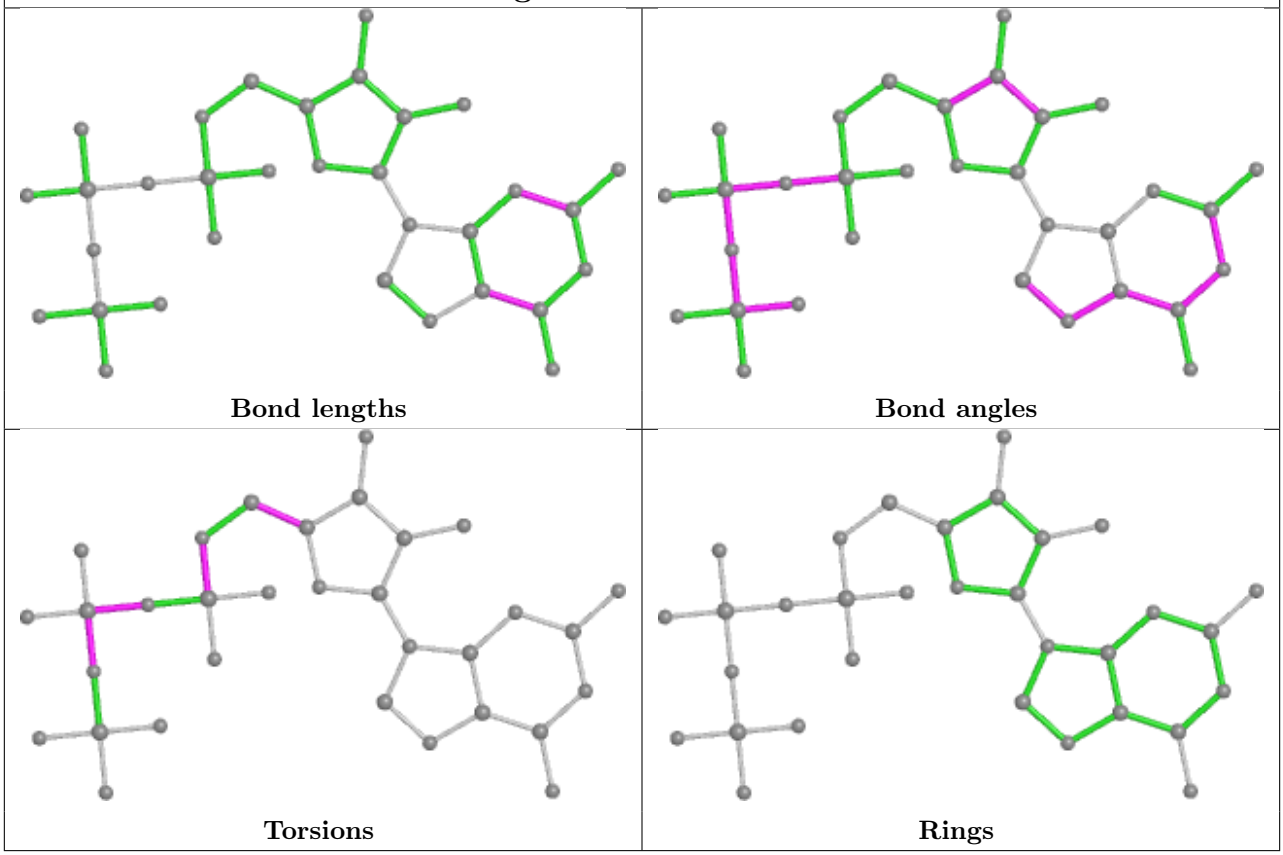
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2004	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP D 2004



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	226/315 (71%)	-0.35	0 100 100	86, 111, 134, 146	0
1	B	224/315 (71%)	-0.39	0 100 100	76, 112, 144, 158	0
2	C	1111/1119 (99%)	-0.19	10 (0%) 84 69	64, 111, 177, 210	0
3	D	1484/1524 (97%)	-0.17	16 (1%) 80 64	63, 102, 170, 219	0
4	E	94/99 (94%)	-0.37	0 100 100	78, 115, 158, 168	0
5	F	346/423 (81%)	-0.07	17 (4%) 29 14	78, 120, 206, 232	0
6	G	19/22 (86%)	-0.34	0 100 100	95, 130, 229, 231	0
7	H	22/27 (81%)	-0.59	0 100 100	102, 146, 235, 245	0
8	I	1/2 (50%)	-0.43	0 100 100	123, 123, 123, 123	0
All	All	3527/3846 (91%)	-0.20	43 (1%) 79 61	63, 110, 179, 245	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	390	PHE	5.9
2	C	207	LEU	4.5
5	F	375	LEU	4.2
5	F	391	GLY	3.9
5	F	382	THR	3.7
5	F	148	LYS	3.5
5	F	422	LEU	3.3
2	C	158	TYR	3.0
2	C	365	ASP	3.0
3	D	1319	VAL	2.8
5	F	147	LEU	2.7
3	D	1502	ALA	2.6
5	F	376	ILE	2.6
2	C	65	VAL	2.6
3	D	322	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	159	ILE	2.5
3	D	1318	TYR	2.5
5	F	394	ARG	2.5
5	F	149	GLU	2.5
5	F	389	PHE	2.5
3	D	216	VAL	2.5
5	F	414	ARG	2.4
5	F	361	LEU	2.4
2	C	368	THR	2.4
3	D	283	PHE	2.4
2	C	64	LEU	2.3
3	D	1499	ARG	2.3
3	D	152	LEU	2.3
5	F	420	ASP	2.2
3	D	1497	GLU	2.2
5	F	138	SER	2.2
2	C	367	LEU	2.2
3	D	1313	VAL	2.2
3	D	203	ALA	2.1
3	D	360	ARG	2.1
3	D	384	VAL	2.1
5	F	381	HIS	2.1
2	C	371	LYS	2.1
3	D	1294	VAL	2.0
3	D	978	TYR	2.0
3	D	345	TYR	2.0
2	C	188	LYS	2.0
5	F	323	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

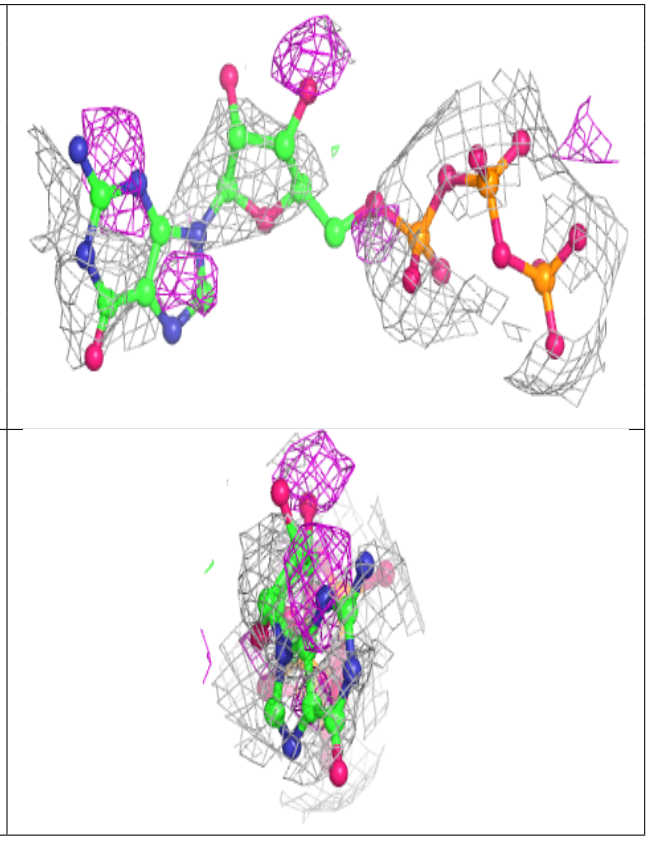
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	GTP	D	2004	32/32	0.82	0.31	93,120,128,141	32
9	MG	D	2005	1/1	0.84	0.30	104,104,104,104	0
9	MG	D	2001	1/1	0.94	0.30	77,77,77,77	0
10	ZN	D	2002	1/1	0.95	0.08	132,132,132,132	0
10	ZN	D	2003	1/1	0.98	0.29	118,118,118,118	0
9	MG	B	1001	1/1	0.98	0.51	81,81,81,81	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GTP D 2004:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.