Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 08:08 PM EDT

PDB ID	:	2OYQ
Title	:	Crystal structure of RB69 gp43 in complex with DNA with 5-NIMP opposite an abasic site analog
Authors	:	Zahn, K.E.; Belrhali, H.; Wallace, S.S.; Doublie, S.
Deposited on	:	2007-02-22
Resolution	:	2.86 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:

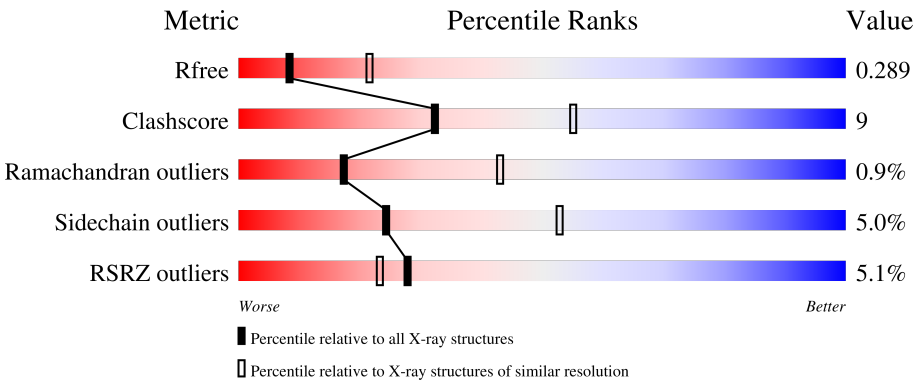
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.86 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	E	21	24% 52% 24%
1	G	21	19% 38% 14% 48%
1	I	21	10% 57% 29% 10% 5%
1	K	21	38% 19% 43%
2	F	15	47% 40% 13%

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Mol	Chain	Length	Quality of chain
2	H	15	47% 27% 33% 33% 7%
2	J	15	33% 47% 20%
2	L	15	7% 7% 67% 13% 13%
3	A	903	% 73% 19% • 6%
3	B	903	3% 62% 20% • 16%
3	C	903	3% 77% 19% • •
3	D	903	11% 74% 14% • 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 28889 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	16	314	150	56	93	15	0	0	0
1	G	11	223	106	44	63	10	0	0	0
1	I	20	395	188	72	116	19	0	0	0
1	K	12	244	116	49	68	11	0	0	0

- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	15	310	150	57	89	14	0	0	0
2	H	14	287	137	55	82	13	0	0	0
2	J	15	310	150	57	89	14	0	0	0
2	L	13	265	127	50	76	12	0	0	0

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	848	6877	4423	1143	1280	31	0	0	0
3	B	756	6045	3883	1001	1134	27	0	0	0
3	C	891	7150	4583	1182	1352	33	0	0	0
3	D	807	5688	3586	953	1125	24	0	0	0

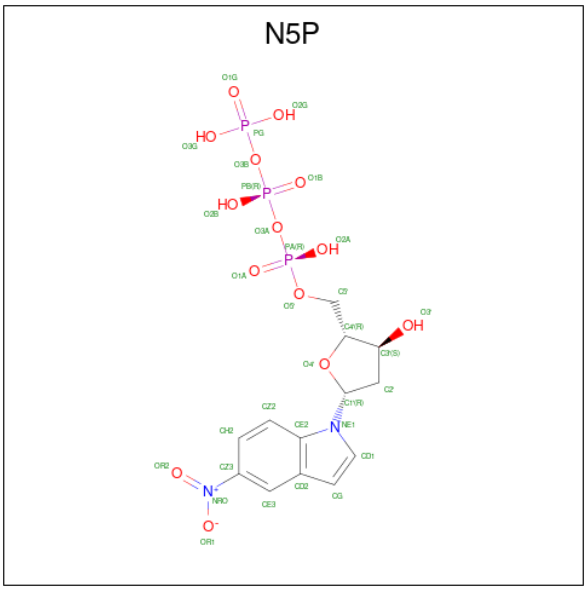
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Mg			
4	I	1	1	1		0	0
			Total	Mg			
4	K	1	1	1		0	0

- Molecule 5 is 1-{2-DEOXY-5-O-[(R)-HYDROXY{[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}PHOSPHORYL]-BETA-D-ERYTHRO-PENTOFURANOSYL}-5-NITRO -1H-INDOLE (three-letter code: N5P) (formula: $C_{13}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	I	1	32	13	2	14	3	0	0
			Total	C	N	O	P		
5	A	1	32	13	2	14	3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	32	13	2	14	3	0	0
5	C	1	32	13	2	14	3	0	0

- Molecule 6 is water.

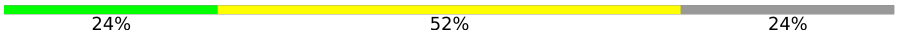
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	E	5	5	5	0	0
6	F	8	8	8	0	0
6	G	2	2	2	0	0
6	H	3	3	3	0	0
6	I	22	22	22	0	0
6	J	19	19	19	0	0
6	K	3	3	3	0	0
6	L	3	3	3	0	0
6	A	235	235	235	0	0
6	B	125	125	125	0	0
6	C	185	185	185	0	0
6	D	41	41	41	0	0

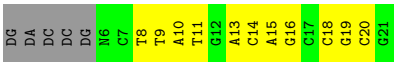
3 Residue-property plots (i)

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: Template DNA

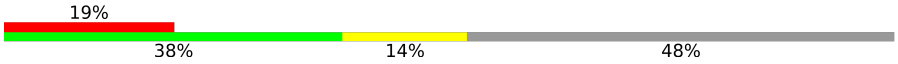
Chain E:

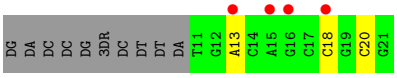




- Molecule 1: Template DNA

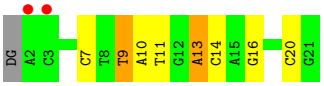
Chain G:





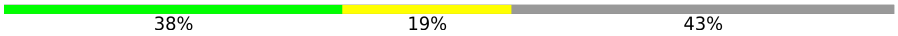
- Molecule 1: Template DNA

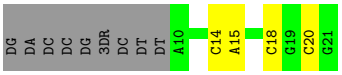
Chain I:



- Molecule 1: Template DNA

Chain K:



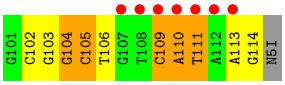


- Molecule 2: Primer DNA

Chain F:

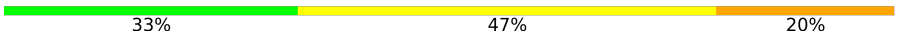
- Molecule 2: Primer DNA

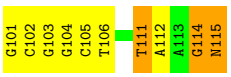
Chain H:



• Molecule 2: Primer DNA

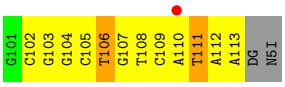
Chain J:





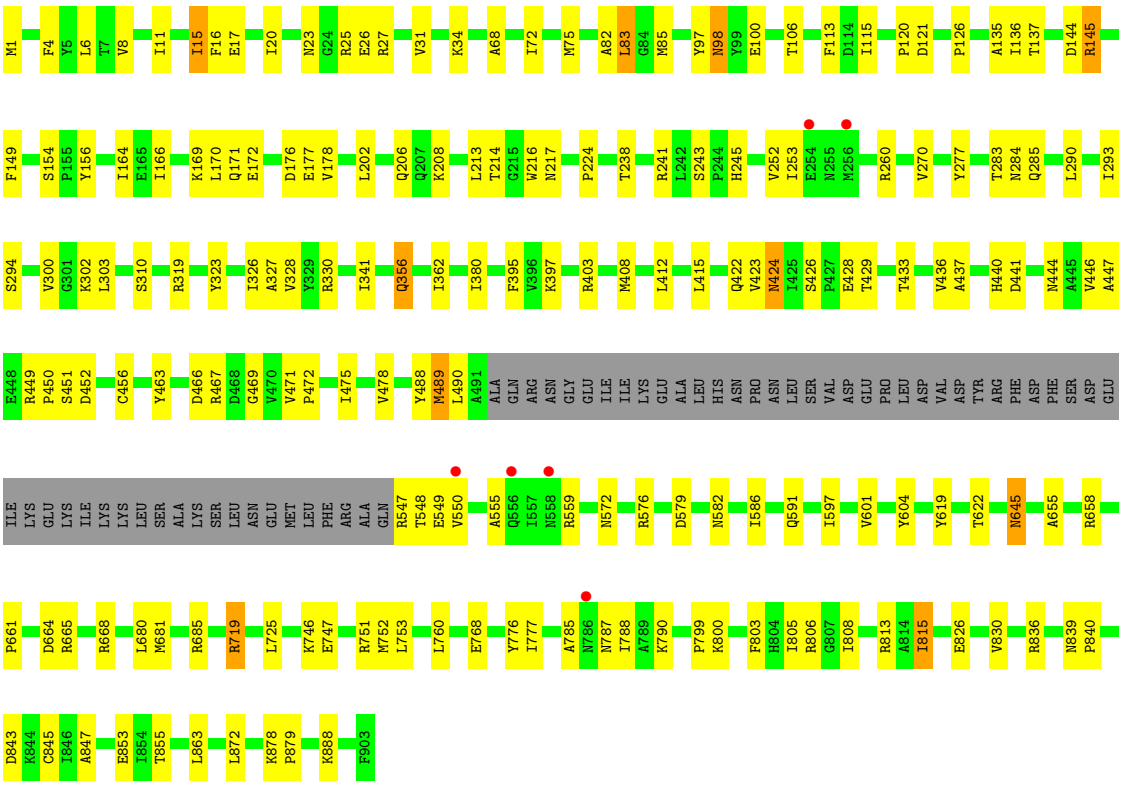
• Molecule 2: Primer DNA

Chain L:



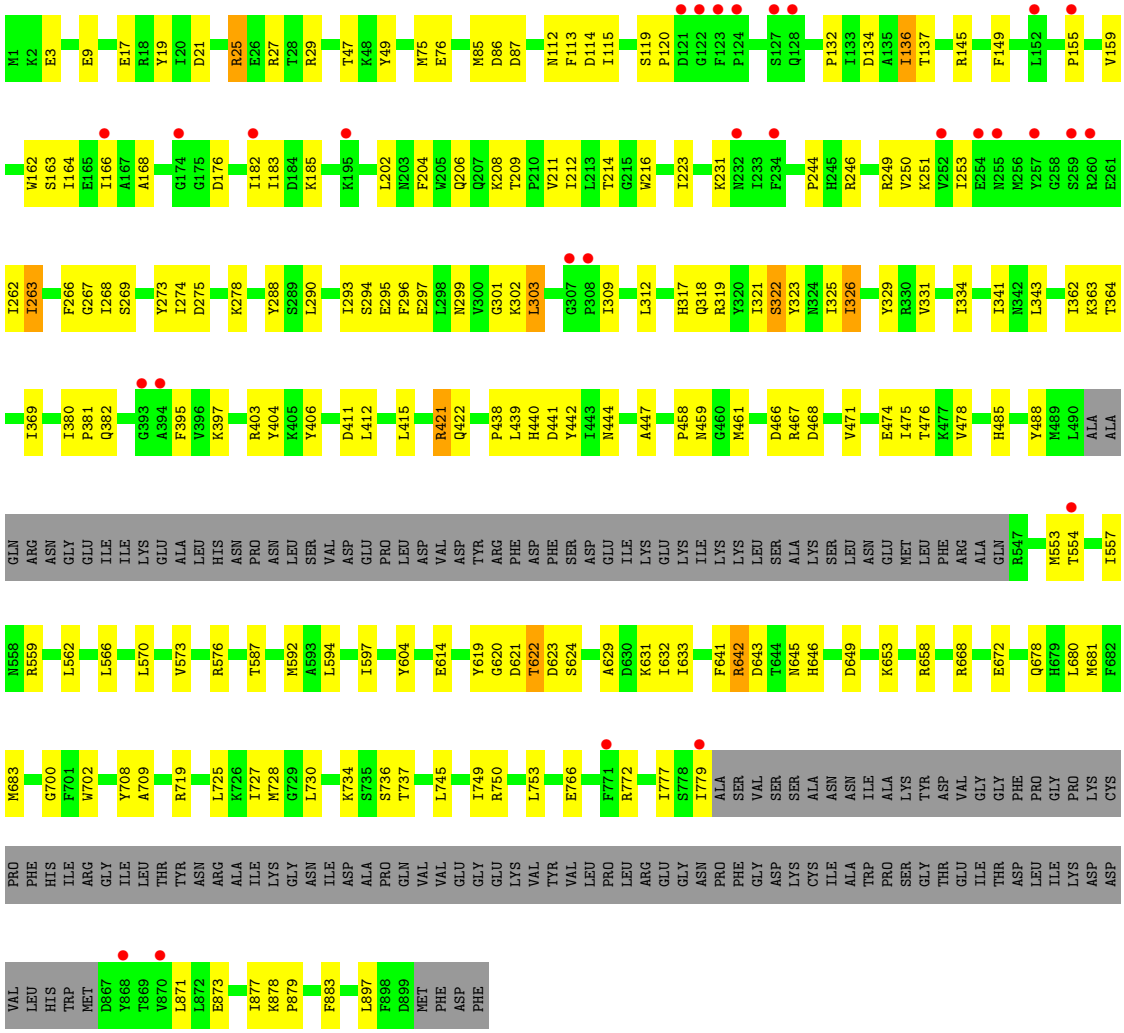
• Molecule 3: DNA polymerase

Chain A:



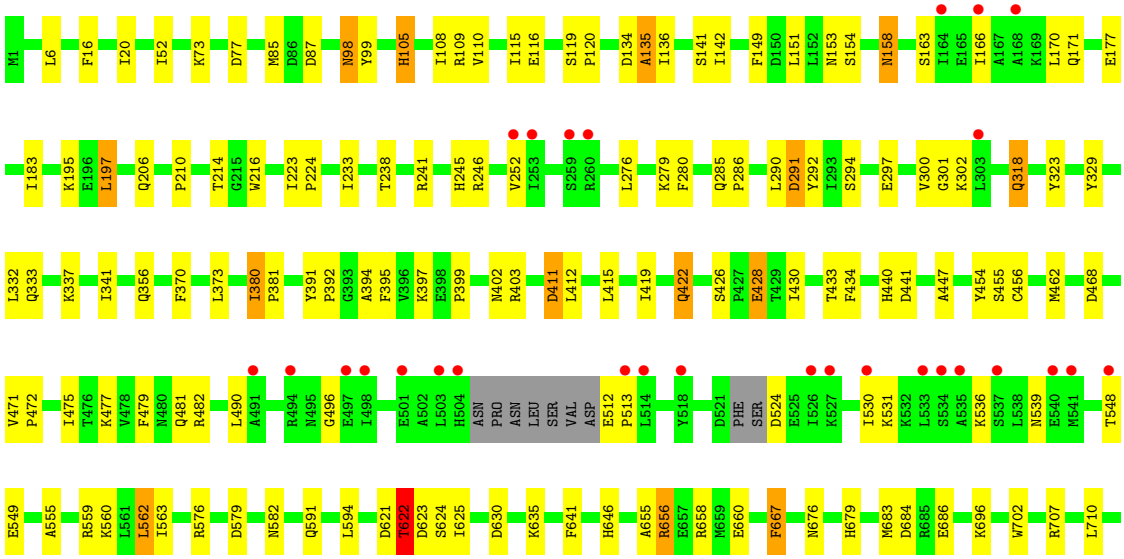
• Molecule 3: DNA polymerase

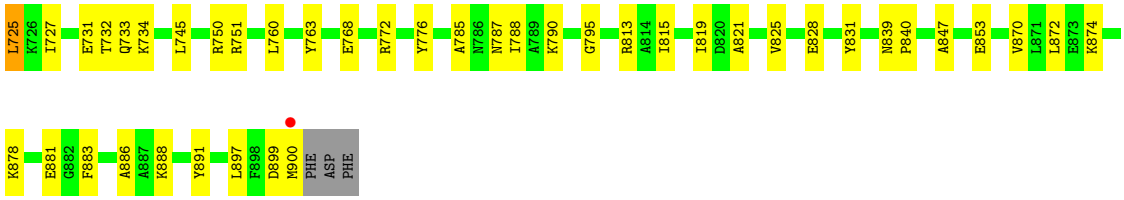
Chain B:



- Molecule 3: DNA polymerase

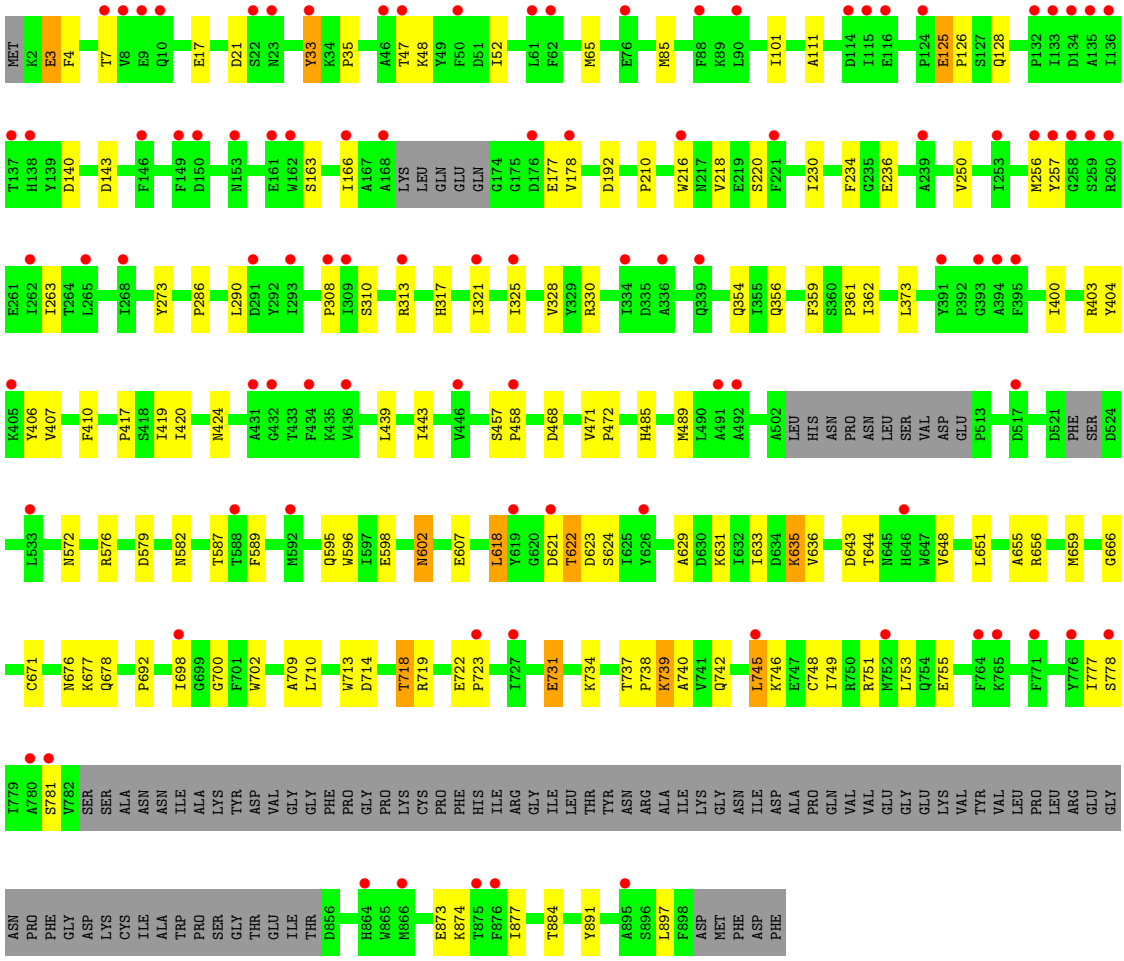
Chain C:





• Molecule 3: DNA polymerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	132.59Å 123.48Å 164.33Å 90.00° 96.22° 90.00°	Depositor
Resolution (Å)	30.00 – 2.86 49.82 – 2.85	Depositor EDS
% Data completeness (in resolution range)	91.2 (30.00-2.86) 96.3 (49.82-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.228 , 0.294 0.231 , 0.289	Depositor DCC
R_{free} test set	23125 reflections (9.68%)	wwPDB-VP
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	28889	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: N5I, N5P, MG, 3DR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	E	0.55	0/342	1.04	0/525
1	G	0.76	0/250	1.23	2/384 (0.5%)
1	I	0.77	0/429	1.45	5/657 (0.8%)
1	K	0.68	0/274	1.31	3/421 (0.7%)
2	F	0.69	0/322	1.42	4/496 (0.8%)
2	H	0.75	0/322	1.44	7/496 (1.4%)
2	J	0.66	0/322	1.41	9/496 (1.8%)
2	L	0.74	0/297	1.41	4/457 (0.9%)
3	A	0.42	0/7049	0.55	0/9536
3	B	0.40	0/6193	0.52	0/8393
3	C	0.40	0/7324	0.53	0/9912
3	D	0.34	0/5812	0.47	0/7955
All	All	0.43	0/28936	0.65	34/39728 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	7	DC	O4'-C1'-N1	9.80	114.86	108.00
2	H	105	DC	O4'-C1'-N1	7.96	113.57	108.00
1	I	20	DC	O4'-C1'-N1	7.69	113.38	108.00
2	F	113	DA	O4'-C1'-N9	7.59	113.32	108.00
1	K	20	DC	O4'-C1'-N1	7.59	113.32	108.00
2	J	114	DG	O4'-C4'-C3'	-7.53	101.48	106.00
2	L	106	DT	O4'-C1'-N1	7.31	113.12	108.00
2	H	110	DA	O4'-C1'-N9	7.23	113.06	108.00
2	F	105	DC	O4'-C1'-N1	7.02	112.91	108.00
2	J	102	DC	C1'-O4'-C4'	-6.67	103.43	110.10
2	J	102	DC	O4'-C1'-N1	6.64	112.65	108.00
2	H	109	DC	O4'-C1'-N1	6.31	112.42	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	111	DT	O4'-C1'-N1	6.17	112.31	108.00
1	G	20	DC	O4'-C1'-N1	6.10	112.27	108.00
2	L	105	DC	O4'-C1'-N1	6.06	112.24	108.00
1	K	18	DC	O4'-C1'-N1	5.99	112.19	108.00
2	H	104	DG	O4'-C1'-N9	5.85	112.09	108.00
2	J	101	DG	O4'-C1'-N9	5.81	112.07	108.00
2	J	114	DG	O4'-C1'-N9	5.73	112.01	108.00
1	K	20	DC	C3'-C2'-C1'	-5.62	95.76	102.50
1	I	13	DA	O4'-C1'-N9	-5.61	104.07	108.00
2	F	103	DG	P-O3'-C3'	5.51	126.32	119.70
2	H	111	DT	C4-C5-C7	5.45	122.27	119.00
2	J	111	DT	C1'-O4'-C4'	-5.41	104.69	110.10
2	F	113	DA	C1'-O4'-C4'	-5.41	104.69	110.10
2	H	102	DC	O4'-C1'-N1	5.40	111.78	108.00
2	J	114	DG	C1'-O4'-C4'	-5.39	104.71	110.10
1	G	13	DA	O4'-C1'-N9	5.38	111.77	108.00
2	H	106	DT	O4'-C1'-N1	5.34	111.74	108.00
2	J	114	DG	C4'-C3'-C2'	-5.22	98.41	103.10
2	L	110	DA	O4'-C1'-N9	5.18	111.63	108.00
1	I	9	DT	O4'-C1'-N1	5.13	111.59	108.00
2	J	102	DC	O4'-C1'-C2'	-5.10	101.82	105.90
1	I	16	DG	P-O3'-C3'	5.03	125.73	119.70

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	E	314	0	177	20	0
1	G	223	0	124	2	0
1	I	395	0	222	4	0
1	K	244	0	135	3	0
2	F	310	0	171	6	0
2	H	287	0	159	11	0
2	J	310	0	171	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	265	0	148	6	0
3	A	6877	0	6731	115	0
3	B	6045	0	5799	124	0
3	C	7150	0	6884	116	0
3	D	5688	0	4707	64	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	A	64	0	26	1	0
5	C	32	0	13	0	0
5	I	32	0	13	0	0
6	A	235	0	0	4	0
6	B	125	0	0	7	0
6	C	185	0	0	2	0
6	D	41	0	0	1	0
6	E	5	0	0	2	0
6	F	8	0	0	1	0
6	G	2	0	0	0	0
6	H	3	0	0	1	0
6	I	22	0	0	1	0
6	J	19	0	0	0	0
6	K	3	0	0	0	0
6	L	3	0	0	0	0
All	All	28889	0	25480	469	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 9.

All (469) 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:E:13:DA:H2"	1:E:14:DC:H5"	1.29	1.07
3:A:356:GLN:H	3:A:356:GLN:HE21	1.02	0.98
1:E:8:DT:O4	2:F:113:DA:N6	2.03	0.91
1:E:13:DA:C2'	1:E:14:DC:H5"	2.00	0.91
1:E:8:DT:H4'	1:E:9:DT:OP1	1.70	0.91
3:A:395:PHE:HB2	3:A:591:GLN:HG3	1.55	0.88
3:B:442:TYR:HB3	3:B:592:MET:HE2	1.56	0.88
1:E:13:DA:H2"	1:E:14:DC:C5'	2.04	0.86
3:D:700:GLY:H	3:D:753:LEU:HD22	1.42	0.85
3:A:208:LYS:HG3	6:A:924:HOH:O	1.78	0.83
3:C:656:ARG:HH11	3:C:656:ARG:HG3	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:DT:H73	6:E:210:HOH:O	1.78	0.82
3:C:394:ALA:HB1	3:C:622:THR:HB	1.62	0.82
2:J:105:DC:H5'	2:J:105:DC:H6	1.45	0.81
3:B:317:HIS:CE1	3:B:321:ILE:HD11	2.15	0.81
3:D:655:ALA:HA	3:D:659:MET:HB2	1.63	0.81
3:B:441:ASP:HB3	3:B:447:ALA:HB2	1.61	0.81
3:B:734:LYS:HB3	3:B:737:THR:HG22	1.62	0.80
3:B:442:TYR:HB3	3:B:592:MET:CE	2.13	0.79
3:A:441:ASP:HB3	3:A:447:ALA:HB2	1.64	0.78
3:A:813:ARG:HG3	3:A:813:ARG:HH11	1.50	0.77
2:H:105:DC:N4	6:H:380:HOH:O	2.17	0.77
3:C:825:VAL:HB	3:C:828:GLU:HG3	1.67	0.77
2:J:105:DC:H2"	2:J:106:DT:H5'	1.67	0.76
3:A:303:LEU:HD13	3:A:326:ILE:HG13	1.67	0.76
3:A:408:MET:HE2	3:A:685:ARG:HD2	1.67	0.76
3:C:395:PHE:HB2	3:C:591:GLN:HG3	1.67	0.75
3:A:23:ASN:HD22	3:A:25:ARG:NH2	1.85	0.74
3:A:8:VAL:HG23	3:A:15:ILE:HD11	1.68	0.74
3:B:362:ILE:HD13	6:B:1161:HOH:O	1.88	0.73
3:C:151:LEU:HD21	3:C:154:SER:HB3	1.71	0.73
1:I:9:DT:H2"	1:I:10:DA:H5"	1.71	0.72
3:D:403:ARG:HB2	3:D:698:ILE:HG21	1.70	0.72
3:B:597:ILE:HG21	3:B:683:MET:HE3	1.71	0.72
6:I:818:HOH:O	3:C:707:ARG:HD3	1.90	0.71
3:D:656:ARG:HB3	6:D:925:HOH:O	1.92	0.70
3:A:356:GLN:H	3:A:356:GLN:NE2	1.84	0.70
3:A:422:GLN:NE2	3:A:680:LEU:H	1.90	0.70
3:A:582:ASN:O	3:A:586:ILE:HD12	1.92	0.70
3:C:370:PHE:HB2	3:C:380:ILE:HD11	1.74	0.69
3:C:411:ASP:HB2	3:C:686:GLU:HG2	1.73	0.69
3:B:614:GLU:OE2	3:B:631:LYS:HE2	1.93	0.69
3:C:641:PHE:HD1	3:C:646:HIS:HD1	1.41	0.69
3:A:422:GLN:HE22	3:A:681:MET:HG2	1.58	0.68
1:E:9:DT:H1'	1:E:10:DA:H5'	1.74	0.68
3:C:110:VAL:H	3:C:141:SER:HB3	1.59	0.68
2:J:105:DC:H5'	2:J:105:DC:C6	2.27	0.68
3:B:362:ILE:H	3:B:362:ILE:HD12	1.58	0.68
3:A:548:THR:C	3:A:550:VAL:H	1.96	0.67
3:C:471:VAL:HB	3:C:472:PRO:HD3	1.76	0.67
1:G:18:DC:H42	2:H:103:DG:H1	1.42	0.67
1:E:10:DA:H2"	1:E:11:DT:OP2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:DG:H2"	1:E:20:DC:H5"	1.76	0.67
3:C:477:LYS:HG2	3:C:481:GLN:HE21	1.60	0.67
1:I:13:DA:H2"	1:I:14:DC:O5'	1.96	0.66
3:A:785:ALA:HB2	3:A:808:ILE:HD11	1.77	0.65
3:B:115:ILE:HG22	3:B:136:ILE:HD13	1.78	0.65
3:B:206:GLN:HE22	3:B:246:ARG:HH22	1.42	0.65
3:C:395:PHE:HD2	3:C:594:LEU:HD23	1.61	0.65
2:H:110:DA:H2"	2:H:111:DT:O5'	1.97	0.65
3:B:168:ALA:HB2	3:B:183:ILE:HG21	1.79	0.65
3:A:579:ASP:OD2	6:A:985:HOH:O	2.15	0.65
2:H:114:DG:OP1	3:B:290:LEU:HB2	1.97	0.64
3:B:211:VAL:HG12	3:B:212:ILE:HD12	1.78	0.64
3:C:85:MET:HE2	3:C:87:ASP:H	1.60	0.64
3:A:356:GLN:HE21	3:A:356:GLN:N	1.85	0.64
2:F:113:DA:H5"	6:F:118:HOH:O	1.97	0.64
3:D:579:ASP:HB3	3:D:582:ASN:HB2	1.80	0.63
3:B:214:THR:HG21	3:B:341:ILE:HD11	1.80	0.63
3:B:312:LEU:HD11	3:B:319:ARG:HG2	1.79	0.63
3:D:740:ALA:HB2	3:D:778:SER:HB2	1.81	0.63
3:B:322:SER:HA	3:B:325:ILE:HD12	1.81	0.63
3:B:76:GLU:HG2	3:B:382:GLN:HE22	1.64	0.62
3:A:768:GLU:HG3	3:A:872:LEU:HD21	1.80	0.62
3:D:419:ILE:HD12	3:D:589:PHE:HD2	1.65	0.62
2:J:104:DG:H1'	2:J:105:DC:H5"	1.81	0.62
1:I:11:DT:H4'	3:C:707:ARG:HD2	1.82	0.62
3:B:653:LYS:NZ	6:B:1097:HOH:O	2.33	0.62
3:D:700:GLY:HA3	3:D:710:LEU:HD23	1.79	0.61
2:L:103:DG:H2'	2:L:104:DG:C8	2.36	0.61
3:A:408:MET:HE1	3:A:655:ALA:HB2	1.81	0.61
3:A:113:PHE:CE1	3:A:213:LEU:HD11	2.35	0.61
3:A:126:PRO:HB2	3:A:224:PRO:HB2	1.82	0.60
2:J:105:DC:C2'	2:J:106:DT:H5'	2.31	0.60
3:B:159:VAL:HG11	3:B:317:HIS:HB2	1.83	0.60
2:L:108:DT:H2"	2:L:109:DC:O4'	2.00	0.60
3:D:417:PRO:HA	3:D:420:ILE:HD12	1.83	0.60
3:C:825:VAL:HB	3:C:828:GLU:CG	2.31	0.60
2:L:102:DC:H2"	2:L:103:DG:H5"	1.82	0.60
2:H:109:DC:H2"	2:H:110:DA:C8	2.37	0.60
3:B:290:LEU:HD13	3:B:302:LYS:HE3	1.82	0.60
3:C:732:THR:HG23	3:C:733:GLN:OE1	2.02	0.60
2:J:111:DT:H2"	2:J:112:DA:H8	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:294:SER:HB2	3:B:301:GLY:HA2	1.84	0.60
3:C:667:PHE:HB3	3:C:679:HIS:HE1	1.67	0.60
3:C:116:GLU:HB2	3:C:135:ALA:HB3	1.82	0.59
3:C:579:ASP:HB3	3:C:582:ASN:HB2	1.85	0.59
3:D:35:PRO:HG2	3:D:65:MET:HA	1.85	0.59
3:A:245:HIS:HE1	6:A:973:HOH:O	1.85	0.59
3:C:727:ILE:HG21	3:C:732:THR:HG21	1.85	0.59
3:A:449:ARG:HH12	3:A:452:ASP:HB3	1.68	0.58
3:B:249:ARG:HD2	3:B:251:LYS:HE3	1.83	0.58
3:A:604:TYR:OH	3:A:658:ARG:HB3	2.04	0.58
3:A:664:ASP:O	3:A:668:ARG:HG3	2.02	0.58
3:A:449:ARG:NH1	3:A:452:ASP:HB3	2.17	0.58
3:A:555:ALA:O	3:A:559:ARG:HG2	2.05	0.57
3:D:739:LYS:HA	3:D:742:GLN:HE21	1.69	0.57
3:C:702:TRP:CH2	3:C:710:LEU:HD21	2.39	0.57
3:B:288:TYR:HA	3:B:293:ILE:HD11	1.87	0.57
3:B:204:PHE:CE1	3:B:208:LYS:HD2	2.40	0.56
3:C:6:LEU:HD11	3:C:20:ILE:CD1	2.35	0.56
2:H:104:DG:H2"	2:H:105:DC:O5'	2.05	0.56
3:A:466:ASP:OD1	3:A:467:ARG:NH1	2.38	0.56
3:A:294:SER:OG	3:A:330:ARG:HG3	2.06	0.56
3:A:878:LYS:HB3	3:A:879:PRO:HD3	1.87	0.56
3:C:297:GLU:O	3:C:337:LYS:HE3	2.05	0.56
3:C:731:GLU:CD	3:C:731:GLU:H	2.09	0.56
3:A:214:THR:HG21	3:A:341:ILE:HD11	1.88	0.56
3:A:17:GLU:OE2	3:A:97:TYR:OH	2.17	0.56
3:A:422:GLN:HE21	3:A:680:LEU:H	1.54	0.56
3:C:477:LYS:HG2	3:C:481:GLN:NE2	2.20	0.56
3:B:209:THR:HG21	3:B:244:PRO:HG3	1.88	0.55
3:D:738:PRO:HD3	3:D:781:SER:HB2	1.87	0.55
3:C:394:ALA:CB	3:C:622:THR:HB	2.34	0.55
3:D:407:VAL:HG11	3:D:710:LEU:HD22	1.87	0.55
1:E:18:DC:H2"	1:E:19:DG:H5'	1.89	0.55
3:D:731:GLU:HG3	3:D:734:LYS:HG3	1.88	0.55
3:B:303:LEU:HD23	3:B:326:ILE:HD13	1.89	0.55
3:C:656:ARG:HG3	3:C:656:ARG:NH1	2.13	0.55
3:D:749:ILE:O	3:D:753:LEU:HG	2.06	0.55
3:B:727:ILE:HG23	3:B:730:LEU:HD12	1.89	0.54
3:A:120:PRO:HG3	3:A:156:TYR:CE1	2.41	0.54
3:D:714:ASP:HA	3:D:718:THR:O	2.07	0.54
3:B:700:GLY:N	3:B:753:LEU:HD22	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:329:TYR:O	3:C:333:GLN:HG3	2.08	0.54
3:D:631:LYS:O	3:D:635:LYS:HB2	2.07	0.54
3:C:411:ASP:O	3:C:683:MET:HA	2.08	0.54
3:D:884:THR:HG21	3:D:891:TYR:HB3	1.90	0.54
3:A:15:ILE:HG22	3:A:31:VAL:O	2.08	0.54
3:A:777:ILE:HD11	3:A:853:GLU:HA	1.89	0.53
3:C:870:VAL:O	3:C:874:LYS:HB2	2.08	0.53
3:A:422:GLN:NE2	3:A:681:MET:HG2	2.22	0.53
3:B:223:ILE:HG22	3:B:263:ILE:HD11	1.89	0.53
3:B:395:PHE:HD2	3:B:594:LEU:HD23	1.72	0.53
3:B:702:TRP:CD1	3:B:708:TYR:HB3	2.43	0.53
3:B:730:LEU:HB3	3:B:883:PHE:CE1	2.43	0.53
3:A:788:ILE:HD13	3:A:826:GLU:HA	1.91	0.53
3:B:3:GLU:HG2	3:B:21:ASP:HA	1.90	0.53
3:C:170:LEU:HA	3:C:177:GLU:HG3	1.91	0.53
2:J:111:DT:H2"	2:J:112:DA:C8	2.44	0.53
2:L:112:DA:H2'	2:L:113:DA:C8	2.44	0.53
3:B:87:ASP:OD2	3:B:363:LYS:HE3	2.09	0.53
2:F:103:DG:H2"	2:F:104:DG:OP2	2.09	0.52
3:B:897:LEU:HD13	3:D:636:VAL:HG21	1.91	0.52
1:E:9:DT:C7	6:E:210:HOH:O	2.45	0.52
3:A:830:VAL:CG1	3:A:847:ALA:HB1	2.39	0.52
3:C:110:VAL:HB	3:C:141:SER:HB2	1.91	0.52
1:E:8:DT:H2"	1:E:9:DT:H71	1.90	0.52
3:A:115:ILE:HG22	3:A:136:ILE:HG12	1.90	0.52
3:C:73:LYS:O	3:C:77:ASP:HB2	2.08	0.52
3:C:621:ASP:O	3:C:623:ASP:N	2.43	0.52
3:B:468:ASP:HA	6:B:1154:HOH:O	2.09	0.52
2:H:114:DG:H5'	3:B:216:TRP:HD1	1.75	0.51
3:A:440:HIS:CE1	3:A:444:ASN:ND2	2.78	0.51
3:D:359:PHE:O	3:D:361:PRO:HD3	2.10	0.51
3:B:422:GLN:HG3	3:B:678:GLN:O	2.11	0.51
3:B:439:LEU:HD11	3:B:592:MET:HB2	1.91	0.51
3:C:85:MET:HE2	3:C:87:ASP:HB3	1.91	0.51
3:D:400:ILE:HG13	3:D:404:TYR:OH	2.10	0.51
3:C:555:ALA:O	3:C:559:ARG:HD3	2.10	0.51
3:A:166:ILE:HA	3:A:169:LYS:HE2	1.93	0.51
3:A:645:ASN:HD21	3:A:719:ARG:HE	1.59	0.51
3:C:402:ASN:HA	3:C:886:ALA:O	2.11	0.51
3:C:646:HIS:HD2	6:C:1057:HOH:O	1.93	0.51
3:B:749:ILE:O	3:B:753:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:33:TYR:O	3:D:35:PRO:HD3	2.11	0.51
3:B:629:ALA:HA	3:B:632:ILE:HD12	1.92	0.51
3:C:785:ALA:HB1	3:C:788:ILE:HD11	1.94	0.50
3:B:132:PRO:HG2	3:B:155:PRO:HD2	1.92	0.50
3:A:170:LEU:HA	3:A:177:GLU:HG2	1.93	0.50
3:A:283:THR:O	3:A:285:GLN:HG2	2.10	0.50
3:B:597:ILE:HG21	3:B:683:MET:CE	2.38	0.50
3:C:329:TYR:HA	3:C:332:LEU:HD12	1.93	0.50
2:J:112:DA:H5'	3:C:734:LYS:HG2	1.93	0.50
3:B:440:HIS:CE1	3:B:444:ASN:HD21	2.29	0.50
3:C:787:ASN:HB3	3:C:790:LYS:HB3	1.92	0.50
3:D:419:ILE:HD12	3:D:589:PHE:CD2	2.47	0.50
2:J:114:DG:H4'	3:C:622:THR:HG23	1.94	0.50
3:A:645:ASN:ND2	3:A:719:ARG:HE	2.09	0.50
3:B:296:PHE:HD1	3:B:297:GLU:HG2	1.77	0.50
3:B:397:LYS:HD3	3:B:619:TYR:HA	1.94	0.50
3:B:441:ASP:CB	3:B:447:ALA:HB2	2.36	0.50
3:A:787:ASN:HB3	3:A:790:LYS:CB	2.42	0.49
3:C:831:TYR:O	3:C:847:ALA:HA	2.11	0.49
3:A:436:VAL:HG12	3:A:437:ALA:O	2.12	0.49
3:B:622:THR:HG23	3:B:623:ASP:H	1.76	0.49
3:C:214:THR:HG21	3:C:341:ILE:HD11	1.94	0.49
3:D:250:VAL:HA	3:D:263:ILE:HA	1.95	0.49
1:E:19:DG:C6	1:E:20:DC:N4	2.80	0.49
3:A:11:ILE:HD12	3:A:16:PHE:CD1	2.47	0.49
3:C:294:SER:HB2	3:C:301:GLY:HA2	1.94	0.49
3:A:547:ARG:HG3	3:A:548:THR:N	2.27	0.49
3:B:412:LEU:HD13	3:B:415:LEU:HD13	1.94	0.49
3:B:421:ARG:HB3	3:B:680:LEU:HD12	1.95	0.49
3:A:178:VAL:HA	3:A:326:ILE:HD11	1.93	0.49
3:A:548:THR:C	3:A:550:VAL:N	2.66	0.49
3:B:145:ARG:NH1	3:B:185:LYS:HA	2.27	0.49
3:C:380:ILE:HG23	3:C:381:PRO:O	2.13	0.49
3:C:621:ASP:OD1	3:C:622:THR:HG22	2.13	0.49
3:B:471:VAL:HG11	3:B:570:LEU:HD11	1.94	0.49
3:B:642:ARG:H	3:B:646:HIS:HD2	1.60	0.49
3:D:3:GLU:HG3	3:D:21:ASP:HA	1.94	0.49
3:A:83:LEU:H	3:A:83:LEU:HD23	1.77	0.49
3:B:47:THR:HG23	3:B:49:TYR:H	1.77	0.49
2:F:101:DG:H4'	2:F:102:DC:H5'	1.95	0.48
3:B:700:GLY:H	3:B:753:LEU:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:433:THR:O	3:C:462:MET:HE1	2.12	0.48
3:D:4:PHE:HA	3:D:101:ILE:HD11	1.95	0.48
3:A:238:THR:HA	3:A:241:ARG:HH21	1.78	0.48
3:A:547:ARG:HG3	3:A:548:THR:H	1.78	0.48
3:C:412:LEU:HD13	3:C:415:LEU:HD13	1.96	0.48
3:D:140:ASP:HB2	3:D:143:ASP:HB2	1.96	0.48
3:B:182:ILE:HD11	3:B:329:TYR:CD2	2.49	0.48
3:B:331:VAL:HA	3:B:334:ILE:HD12	1.95	0.48
3:C:105:HIS:HA	3:C:108:ILE:HG13	1.96	0.48
3:B:381:PRO:HG2	3:B:576:ARG:HG2	1.96	0.48
3:B:421:ARG:HD2	3:B:476:THR:OG1	2.12	0.48
3:C:115:ILE:HG22	3:C:136:ILE:HG12	1.94	0.48
3:D:622:THR:HG23	3:D:623:ASP:H	1.78	0.48
2:J:103:DG:H2"	2:J:104:DG:C8	2.49	0.48
3:B:421:ARG:HB3	3:B:680:LEU:CD1	2.44	0.48
3:B:641:PHE:HA	3:B:646:HIS:HD2	1.79	0.48
3:D:648:VAL:HB	3:D:719:ARG:NH2	2.29	0.48
3:D:111:ALA:HB3	3:D:210:PRO:HB3	1.96	0.47
3:D:873:GLU:HA	3:D:877:ILE:HB	1.96	0.47
3:A:813:ARG:HH11	3:A:813:ARG:CG	2.21	0.47
3:C:815:ILE:HG23	3:C:821:ALA:HB3	1.96	0.47
3:A:121:ASP:N	3:A:121:ASP:OD1	2.48	0.47
3:A:412:LEU:HD13	3:A:415:LEU:HD13	1.96	0.47
3:B:466:ASP:OD2	3:B:467:ARG:HG3	2.13	0.47
3:C:285:GLN:HG3	3:C:286:PRO:HD2	1.95	0.47
2:H:113:DA:OP1	3:B:288:TYR:HB2	2.14	0.47
3:A:426:SER:HB2	3:A:472:PRO:HD3	1.96	0.47
3:B:397:LYS:HB3	3:B:620:GLY:H	1.78	0.47
3:C:900:MET:SD	3:C:900:MET:N	2.88	0.47
3:B:643:ASP:HB2	6:B:1157:HOH:O	2.13	0.47
3:C:52:ILE:HD12	3:C:428:GLU:HG2	1.97	0.47
3:C:151:LEU:CD2	3:C:154:SER:HB3	2.43	0.47
3:C:163:SER:HB3	3:C:166:ILE:HD12	1.97	0.47
3:D:216:TRP:CD2	3:D:290:LEU:HD13	2.50	0.47
3:D:629:ALA:HB1	3:D:651:LEU:HD21	1.96	0.47
3:A:428:GLU:OE2	3:A:469:GLY:HA2	2.15	0.47
3:B:668:ARG:O	3:B:672:GLU:HG3	2.14	0.47
3:C:136:ILE:HB	3:C:149:PHE:HB2	1.97	0.47
3:A:803:PHE:CZ	3:A:845:CYS:HB3	2.50	0.47
3:D:485:HIS:O	3:D:489:MET:HB2	2.15	0.47
3:B:458:PRO:HG3	3:B:592:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:291:ASP:OD2	3:C:302:LYS:HB2	2.15	0.46
3:A:75:MET:HG2	3:A:82:ALA:HB2	1.97	0.46
3:C:433:THR:HG22	3:C:434:PHE:N	2.30	0.46
3:C:454:TYR:HB3	3:C:462:MET:HB3	1.97	0.46
2:H:103:DG:H2"	2:H:104:DG:C8	2.50	0.46
1:I:14:DC:OP1	3:C:874:LYS:HD3	2.15	0.46
3:A:176:ASP:O	3:A:303:LEU:HD11	2.15	0.46
3:A:725:LEU:HD22	3:A:753:LEU:HD12	1.98	0.46
1:K:14:DC:H2"	1:K:15:DA:C8	2.50	0.46
3:A:395:PHE:CB	3:A:591:GLN:HG3	2.36	0.46
3:A:423:VAL:O	3:A:424:ASN:CB	2.62	0.46
3:D:745:LEU:HA	3:D:748:CYS:HB2	1.97	0.46
3:A:787:ASN:HB3	3:A:790:LYS:HB3	1.97	0.46
3:C:881:GLU:HG2	3:C:891:TYR:CE2	2.51	0.46
3:D:739:LYS:HA	3:D:742:GLN:HB2	1.98	0.46
3:A:471:VAL:HB	3:A:472:PRO:HD3	1.98	0.46
3:A:597:ILE:O	3:A:601:VAL:HG23	2.16	0.46
3:A:788:ILE:H	3:A:788:ILE:HD12	1.79	0.46
3:C:380:ILE:HG23	3:C:576:ARG:HD3	1.97	0.46
1:E:8:DT:O4	2:F:113:DA:C6	2.68	0.46
3:A:429:THR:HG22	3:A:463:TYR:HB3	1.98	0.46
3:A:488:TYR:C	3:A:490:LEU:H	2.19	0.46
3:A:302:LYS:HE3	3:A:327:ALA:HB2	1.98	0.46
3:A:661:PRO:O	3:A:665:ARG:HB2	2.15	0.46
3:C:223:ILE:HB	3:C:224:PRO:HD3	1.98	0.46
3:D:410:PHE:O	3:D:624:SER:HA	2.15	0.46
3:B:458:PRO:HG3	3:B:592:MET:CE	2.46	0.46
3:D:230:ILE:O	3:D:234:PHE:N	2.46	0.46
3:D:407:VAL:HG23	3:D:618:LEU:HD21	1.98	0.46
3:B:421:ARG:HD3	3:B:475:ILE:HG23	1.97	0.45
3:C:482:ARG:CZ	3:C:560:LYS:HB2	2.46	0.45
3:C:134:ASP:O	3:C:135:ALA:HB2	2.17	0.45
3:A:68:ALA:O	3:A:72:ILE:HG13	2.16	0.45
3:C:391:TYR:HB2	3:C:392:PRO:HD2	1.99	0.45
3:C:434:PHE:HE2	3:C:456:CYS:HB3	1.82	0.45
3:B:404:TYR:HA	6:B:1043:HOH:O	2.17	0.45
3:B:745:LEU:HD22	3:B:883:PHE:HE2	1.82	0.45
3:D:439:LEU:O	3:D:443:ILE:HG12	2.15	0.45
3:B:162:TRP:HB2	3:B:321:ILE:CD1	2.47	0.45
3:C:562:LEU:HD12	3:C:562:LEU:HA	1.85	0.45
3:C:667:PHE:HB3	3:C:679:HIS:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:440:HIS:CE1	3:A:444:ASN:HD21	2.35	0.45
3:B:725:LEU:HD11	3:B:750:ARG:HB2	1.98	0.45
3:C:302:LYS:HD3	3:C:323:TYR:CE1	2.52	0.45
3:A:472:PRO:HA	3:A:475:ILE:HG22	1.98	0.45
3:A:752:MET:HG3	3:A:760:LEU:HD13	1.99	0.44
3:C:276:LEU:HD12	3:C:276:LEU:HA	1.83	0.44
3:C:300:VAL:HG13	3:C:301:GLY:H	1.82	0.44
1:E:10:DA:N1	2:F:112:DA:C6	2.86	0.44
1:E:15:DA:C6	1:E:16:DG:C6	3.05	0.44
1:E:18:DC:H2"	1:E:19:DG:C5'	2.47	0.44
2:H:113:DA:P	3:B:288:TYR:H	2.40	0.44
1:K:14:DC:P	3:D:874:LYS:HD3	2.57	0.44
3:C:641:PHE:HD1	3:C:646:HIS:ND1	2.12	0.44
3:C:776:TYR:OH	3:C:853:GLU:OE1	2.27	0.44
3:A:839:ASN:HB2	3:A:840:PRO:HD2	1.99	0.44
3:B:85:MET:HA	3:B:380:ILE:HD11	1.99	0.44
3:B:302:LYS:HD3	3:B:323:TYR:OH	2.17	0.44
3:B:406:TYR:CD2	3:B:633:ILE:HG13	2.52	0.44
3:A:785:ALA:HB1	3:A:788:ILE:HD11	1.98	0.44
3:B:176:ASP:OD2	3:B:318:GLN:HG3	2.16	0.44
3:D:471:VAL:HB	3:D:472:PRO:HD3	2.00	0.44
3:A:330:ARG:HD2	3:A:330:ARG:HA	1.85	0.44
3:C:454:TYR:CB	3:C:462:MET:HB3	2.46	0.44
3:B:9:GLU:OE1	3:B:267:GLY:N	2.43	0.44
3:B:485:HIS:HA	3:B:488:TYR:CD2	2.53	0.44
3:B:553:MET:O	3:B:557:ILE:HG12	2.18	0.44
3:B:649:ASP:OD1	3:B:719:ARG:NH2	2.48	0.44
3:B:672:GLU:HB3	6:B:1122:HOH:O	2.17	0.44
3:C:655:ALA:O	3:C:660:GLU:HG3	2.17	0.44
2:J:114:DG:H2'	2:J:115:N5I:HD1	1.99	0.44
3:C:16:PHE:HB3	3:C:245:HIS:CE1	2.53	0.44
3:C:881:GLU:HG2	3:C:891:TYR:HE2	1.81	0.44
3:B:730:LEU:HB3	3:B:883:PHE:HE1	1.82	0.44
2:L:106:DT:H2"	2:L:107:DG:H5'	1.99	0.43
3:A:813:ARG:HG3	3:A:813:ARG:NH1	2.27	0.43
3:D:325:ILE:O	3:D:328:VAL:HG22	2.17	0.43
3:A:290:LEU:HD11	3:A:330:ARG:HB3	2.00	0.43
3:B:411:ASP:O	3:B:683:MET:HA	2.18	0.43
3:D:596:TRP:NE1	3:D:666:GLY:O	2.45	0.43
3:D:598:GLU:O	3:D:602:ASN:HB2	2.19	0.43
3:A:449:ARG:HA	3:A:450:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:17:GLU:OE1	3:B:29:ARG:NH1	2.49	0.43
3:B:119:SER:HA	3:B:120:PRO:HD2	1.92	0.43
3:C:725:LEU:HD21	3:C:750:ARG:HB2	2.00	0.43
3:A:362:ILE:HD11	3:A:572:ASN:HB3	2.01	0.43
3:B:274:ILE:HG23	3:B:275:ASP:N	2.33	0.43
3:C:768:GLU:HG2	3:C:872:LEU:HD21	2.00	0.43
3:A:4:PHE:CZ	3:A:20:ILE:HG13	2.54	0.43
3:B:478:VAL:HG13	3:B:559:ARG:HG3	2.01	0.43
3:B:459:ASN:HD21	3:B:461:MET:HG2	1.84	0.43
3:B:645:ASN:OD1	3:B:719:ARG:NH1	2.52	0.43
3:C:216:TRP:CD2	3:C:290:LEU:HD23	2.54	0.43
3:C:455:SER:OG	3:C:676:ASN:HA	2.19	0.43
3:C:795:GLY:O	3:C:813:ARG:NH1	2.52	0.43
2:J:104:DG:C1'	2:J:105:DC:H5"	2.47	0.43
3:A:815:ILE:HD12	3:A:815:ILE:HA	1.83	0.43
3:C:751:ARG:CZ	3:C:763:TYR:HB2	2.49	0.43
3:D:47:THR:HB	3:D:48:LYS:H	1.64	0.43
3:D:777:ILE:HG13	3:D:778:SER:N	2.33	0.43
3:A:277:TYR:CE2	3:A:293:ILE:HD12	2.54	0.43
3:A:424:ASN:O	3:A:429:THR:HG21	2.19	0.43
3:B:362:ILE:H	3:B:362:ILE:CD1	2.30	0.43
3:B:878:LYS:N	3:B:879:PRO:HD2	2.34	0.43
3:B:604:TYR:OH	3:B:658:ARG:HB3	2.19	0.43
3:C:163:SER:HB3	3:C:318:GLN:OE1	2.19	0.43
3:C:426:SER:C	3:C:582:ASN:HD21	2.22	0.43
3:D:218:VAL:C	3:D:220:SER:H	2.22	0.43
3:C:98:ASN:HD22	3:C:98:ASN:H	1.66	0.43
3:B:317:HIS:CE1	3:B:321:ILE:CD1	2.96	0.42
3:C:475:ILE:HD11	3:C:563:ILE:HA	2.00	0.42
3:A:172:GLU:H	3:A:172:GLU:CD	2.22	0.42
3:A:478:VAL:HG13	3:A:559:ARG:HD2	2.02	0.42
3:A:813:ARG:CG	3:A:813:ARG:NH1	2.82	0.42
3:C:216:TRP:CE3	3:C:290:LEU:HD23	2.53	0.42
3:D:125:GLU:HA	3:D:126:PRO:HD3	1.87	0.42
3:D:457:SER:OG	3:D:458:PRO:HD2	2.19	0.42
3:A:836:ARG:NH1	3:A:836:ARG:HB2	2.34	0.42
3:A:135:ALA:HA	3:A:149:PHE:O	2.20	0.42
3:B:268:ILE:HG22	3:B:269:SER:N	2.34	0.42
3:B:438:PRO:HG2	3:B:441:ASP:OD2	2.19	0.42
3:B:873:GLU:HA	3:B:877:ILE:HB	2.00	0.42
3:C:109:ARG:HG2	3:C:210:PRO:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:177:GLU:HB3	3:D:178:VAL:H	1.53	0.42
3:D:621:ASP:O	3:D:623:ASP:N	2.52	0.42
1:E:13:DA:C3'	1:E:14:DC:H5"	2.46	0.42
3:A:98:ASN:H	3:A:98:ASN:HD22	1.68	0.42
3:A:144:ASP:O	3:A:145:ARG:HD3	2.19	0.42
3:C:290:LEU:HD12	3:C:302:LYS:CE	2.50	0.42
3:A:113:PHE:CD1	3:A:213:LEU:HD11	2.54	0.42
3:B:364:THR:CG2	3:B:562:LEU:HD21	2.50	0.42
3:C:397:LYS:O	3:C:399:PRO:HD3	2.19	0.42
3:D:443:ILE:HD12	3:D:595:GLN:HB2	2.01	0.42
3:A:176:ASP:HA	3:A:319:ARG:HH21	1.84	0.42
3:B:573:VAL:HG22	6:B:1058:HOH:O	2.18	0.42
3:D:407:VAL:HG11	3:D:710:LEU:CD2	2.50	0.42
1:G:18:DC:N4	2:H:103:DG:H1	2.14	0.42
3:B:700:GLY:HA2	3:B:709:ALA:O	2.20	0.42
3:D:424:ASN:HD21	3:D:468:ASP:HA	1.85	0.42
3:A:137:THR:HG22	3:A:328:VAL:HG21	2.02	0.42
3:A:747:GLU:HG3	3:A:751:ARG:HD2	2.01	0.42
3:A:776:TYR:CD1	3:A:863:LEU:HD11	2.55	0.42
3:B:164:ILE:H	3:B:164:ILE:HG13	1.67	0.42
3:B:295:GLU:O	3:B:299:ASN:HA	2.20	0.42
3:D:406:TYR:CE2	3:D:633:ILE:HG21	2.55	0.42
1:E:19:DG:C5	1:E:20:DC:C4	3.07	0.41
3:A:252:VAL:HA	3:A:260:ARG:O	2.20	0.41
3:C:415:LEU:O	3:C:419:ILE:HG13	2.19	0.41
3:D:621:ASP:O	3:D:624:SER:N	2.53	0.41
2:J:104:DG:C2'	2:J:105:DC:H5"	2.50	0.41
3:C:149:PHE:HB3	3:C:197:LEU:CD2	2.50	0.41
3:B:163:SER:HB3	3:B:166:ILE:HB	2.03	0.41
3:B:597:ILE:HG12	3:B:683:MET:HE3	2.02	0.41
3:C:183:ILE:H	3:C:183:ILE:HG13	1.69	0.41
3:D:751:ARG:HB2	3:D:755:GLU:HB2	2.02	0.41
3:A:426:SER:HB3	3:A:429:THR:OG1	2.20	0.41
3:A:451:SER:HB3	3:A:456:CYS:SG	2.60	0.41
3:B:25:ARG:HA	3:B:25:ARG:HD2	1.78	0.41
3:B:302:LYS:HB3	3:B:323:TYR:HE1	1.85	0.41
3:B:369:ILE:HG12	3:B:474:GLU:HG3	2.01	0.41
3:C:403:ARG:NH2	3:C:888:LYS:O	2.53	0.41
3:D:700:GLY:HA2	3:D:709:ALA:O	2.21	0.41
3:A:6:LEU:CD1	3:A:26:GLU:HG3	2.51	0.41
3:B:621:ASP:OD1	3:B:622:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:737:THR:HA	3:D:738:PRO:HD2	1.81	0.41
3:A:216:TRP:O	3:A:217:ASN:HB2	2.20	0.41
3:A:270:VAL:HB	6:A:916:HOH:O	2.21	0.41
3:B:9:GLU:HG3	3:B:266:PHE:CD2	2.55	0.41
3:C:471:VAL:HB	3:C:472:PRO:CD	2.48	0.41
3:A:98:ASN:H	3:A:98:ASN:ND2	2.18	0.41
3:B:641:PHE:HA	3:B:646:HIS:CD2	2.55	0.41
3:C:206:GLN:NE2	3:C:241:ARG:HB3	2.35	0.41
3:A:202:LEU:O	3:A:206:GLN:HG2	2.21	0.41
3:B:162:TRP:HB2	3:B:321:ILE:HD13	2.03	0.41
3:C:153:ASN:HA	3:C:158:ASN:HA	2.03	0.41
3:C:195:LYS:HE2	3:C:233:ILE:HG23	2.03	0.41
3:C:512:GLU:HA	3:C:513:PRO:HD3	1.86	0.41
3:D:317:HIS:O	3:D:321:ILE:HD12	2.20	0.41
3:D:644:THR:CG2	3:D:692:PRO:HA	2.51	0.41
3:A:302:LYS:HE2	3:A:323:TYR:CZ	2.56	0.41
3:A:799:PRO:O	3:A:800:LYS:HB2	2.21	0.41
3:B:251:LYS:HB3	3:B:253:ILE:HG12	2.03	0.41
3:C:745:LEU:HD22	3:C:883:PHE:CE2	2.56	0.41
3:D:713:TRP:CH2	3:D:723:PRO:HD3	2.56	0.41
3:A:34:LYS:HB2	5:A:905:N5P:O3'	2.21	0.41
3:B:364:THR:HG22	3:B:562:LEU:HD21	2.03	0.41
3:B:725:LEU:HD22	3:B:753:LEU:HD12	2.03	0.41
2:L:111:DT:H2"	2:L:112:DA:C8	2.56	0.40
3:A:785:ALA:CB	3:A:808:ILE:HD11	2.48	0.40
3:B:136:ILE:HB	3:B:149:PHE:HB2	2.04	0.40
3:B:475:ILE:HD13	3:B:566:LEU:HD22	2.02	0.40
3:B:622:THR:HG23	3:B:623:ASP:N	2.36	0.40
3:C:109:ARG:HD3	3:C:142:ILE:HD12	2.03	0.40
3:C:291:ASP:OD1	3:C:291:ASP:N	2.53	0.40
3:C:441:ASP:HB3	3:C:447:ALA:HB2	2.03	0.40
1:K:14:DC:H2"	1:K:15:DA:H8	1.86	0.40
3:B:9:GLU:CG	3:B:266:PHE:CD2	3.04	0.40
3:C:286:PRO:HD2	3:C:292:TYR:HE2	1.86	0.40
3:B:19:TYR:CE1	3:B:27:ARG:HB2	2.56	0.40
3:B:263:ILE:N	3:B:263:ILE:HD13	2.36	0.40
3:B:274:ILE:O	3:B:278:LYS:HB2	2.21	0.40
3:C:119:SER:HA	3:C:120:PRO:HD2	1.99	0.40
3:C:594:LEU:HD11	3:C:624:SER:O	2.22	0.40
3:D:671:CYS:SG	3:D:676:ASN:HB2	2.62	0.40
3:A:380:ILE:HD12	3:A:576:ARG:NE	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:397:LYS:HD3	3:A:619:TYR:HA	2.03	0.40
3:B:343:LEU:HD12	3:B:554:THR:HG23	2.03	0.40
3:C:839:ASN:HB2	3:C:840:PRO:HD2	2.02	0.40
1:E:9:DT:H6	1:E:9:DT:H2'	1.64	0.40
3:C:279:LYS:HD3	3:C:280:PHE:CZ	2.57	0.40
3:C:422:GLN:HE21	3:C:422:GLN:HB3	1.60	0.40
3:C:772:ARG:NH2	6:C:1041:HOH:O	2.52	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
3	A	844/903 (94%)	794 (94%)	45 (5%)	5 (1%)	25 53
3	B	750/903 (83%)	697 (93%)	49 (6%)	4 (0%)	29 57
3	C	885/903 (98%)	817 (92%)	61 (7%)	7 (1%)	19 46
3	D	797/903 (88%)	701 (88%)	83 (10%)	13 (2%)	9 28
All	All	3276/3612 (91%)	3009 (92%)	238 (7%)	29 (1%)	17 43

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	622	THR
3	B	736	SER
3	C	622	THR
3	D	622	THR
3	A	549	GLU
3	B	262	ILE
3	B	777	ILE
3	D	33	TYR

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Mol	Chain	Res	Type
3	D	286	PRO
3	D	308	PRO
3	D	897	LEU
3	A	300	VAL
3	A	622	THR
3	C	496	GLY
3	C	531	LYS
3	D	310	SER
3	A	424	ASN
3	C	135	ALA
3	C	430	ILE
3	D	163	SER
3	D	256	MET
3	D	718	THR
3	A	489	MET
3	C	252	VAL
3	D	354	GLN
3	D	677	LYS
3	D	731	GLU
3	C	99	TYR
3	D	166	ILE

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	
3	A	738/800 (92%)	708 (96%)	30 (4%)	30	61
3	B	634/800 (79%)	605 (95%)	29 (5%)	27	56
3	C	755/800 (94%)	714 (95%)	41 (5%)	22	49
3	D	483/800 (60%)	453 (94%)	30 (6%)	18	43
All	All	2610/3200 (82%)	2480 (95%)	130 (5%)	24	53

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	MET
3	A	15	ILE
3	A	27	ARG
3	A	83	LEU
3	A	85	MET
3	A	98	ASN
3	A	100	GLU
3	A	106	THR
3	A	145	ARG
3	A	154	SER
3	A	164	ILE
3	A	171	GLN
3	A	243	SER
3	A	253	ILE
3	A	284	ASN
3	A	310	SER
3	A	356	GLN
3	A	403	ARG
3	A	433	THR
3	A	446	VAL
3	A	489	MET
3	A	645	ASN
3	A	719	ARG
3	A	746	LYS
3	A	805	ILE
3	A	806	ARG
3	A	815	ILE
3	A	843	ASP
3	A	855	THR
3	A	888	LYS
3	B	25	ARG
3	B	75	MET
3	B	86	ASP
3	B	112	ASN
3	B	113	PHE
3	B	114	ASP
3	B	134	ASP
3	B	136	ILE
3	B	137	THR
3	B	202	LEU
3	B	231	LYS
3	B	250	VAL
3	B	263	ILE

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Mol	Chain	Res	Type
3	B	273	TYR
3	B	303	LEU
3	B	309	ILE
3	B	322	SER
3	B	326	ILE
3	B	403	ARG
3	B	421	ARG
3	B	587	THR
3	B	624	SER
3	B	642	ARG
3	B	681	MET
3	B	728	MET
3	B	766	GLU
3	B	772	ARG
3	B	779	ILE
3	B	871	LEU
3	C	98	ASN
3	C	105	HIS
3	C	158	ASN
3	C	171	GLN
3	C	197	LEU
3	C	238	THR
3	C	246	ARG
3	C	291	ASP
3	C	318	GLN
3	C	356	GLN
3	C	373	LEU
3	C	380	ILE
3	C	411	ASP
3	C	422	GLN
3	C	428	GLU
3	C	440	HIS
3	C	468	ASP
3	C	479	PHE
3	C	490	LEU
3	C	524	ASP
3	C	530	ILE
3	C	536	LYS
3	C	539	ASN
3	C	548	THR
3	C	549	GLU
3	C	562	LEU

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Mol	Chain	Res	Type
3	C	622	THR
3	C	625	ILE
3	C	630	ASP
3	C	635	LYS
3	C	656	ARG
3	C	658	ARG
3	C	667	PHE
3	C	684	ASP
3	C	696	LYS
3	C	725	LEU
3	C	760	LEU
3	C	819	ILE
3	C	878	LYS
3	C	897	LEU
3	C	899	ASP
3	D	3	GLU
3	D	7	THR
3	D	17	GLU
3	D	52	ILE
3	D	85	MET
3	D	125	GLU
3	D	128	GLN
3	D	192	ASP
3	D	236	GLU
3	D	257	TYR
3	D	273	TYR
3	D	313	ARG
3	D	330	ARG
3	D	356	GLN
3	D	362	ILE
3	D	373	LEU
3	D	572	ASN
3	D	576	ARG
3	D	587	THR
3	D	602	ASN
3	D	607	GLU
3	D	618	LEU
3	D	635	LYS
3	D	643	ASP
3	D	678	GLN
3	D	702	TRP
3	D	722	GLU

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Mol	Chain	Res	Type
3	D	739	LYS
3	D	745	LEU
3	D	746	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	ASN
3	A	45	GLN
3	A	98	ASN
3	A	128	GLN
3	A	217	ASN
3	A	228	ASN
3	A	356	GLN
3	A	386	HIS
3	A	422	GLN
3	A	645	ASN
3	B	70	GLN
3	B	153	ASN
3	B	285	GLN
3	B	317	HIS
3	B	324	ASN
3	B	444	ASN
3	B	646	HIS
3	B	678	GLN
3	C	98	ASN
3	C	228	ASN
3	C	324	ASN
3	C	480	ASN
3	C	481	GLN
3	C	539	ASN
3	C	556	GLN
3	C	558	ASN
3	C	564	ASN
3	C	572	ASN
3	C	591	GLN
3	C	595	GLN
3	C	645	ASN
3	D	556	GLN
3	D	572	ASN
3	D	595	GLN
3	D	645	ASN

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Mol	Chain	Res	Type
3	D	678	GLN
3	D	742	GLN
3	D	754	GLN
3	D	761	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)

4 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	$\#\|Z\| > 2$
2	N5I	F	115	2	20,25,26	0.60	0	25,36,39	0.98	1 (4%)
1	3DR	E	6	1	8,8,12	0.41	0	9,10,17	0.77	0
2	N5I	J	115	2	20,25,26	0.56	0	25,36,39	1.09	1 (4%)
1	3DR	I	6	1	8,11,12	0.50	0	9,14,17	0.74	0

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
2	N5I	F	115	2	-	0/5/25/26	0/3/3/3
1	3DR	E	6	1	-	2/2/12/16	0/1/1/1
2	N5I	J	115	2	-	0/5/25/26	0/3/3/3
1	3DR	I	6	1	-	2/3/15/16	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	115	N5I	CD1-NE1-C1'	-2.86	122.57	125.40
2	F	115	N5I	CD1-NE1-C1'	-2.26	123.16	125.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	6	3DR	C3'-C4'-C5'-O5'
1	E	6	3DR	O4'-C4'-C5'-O5'
1	I	6	3DR	C3'-C4'-C5'-O5'
1	I	6	3DR	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	115	N5I	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	N5P	A	905	4	28,34,34	0.53	0	38,53,53	1.16	2 (5%)
5	N5P	C	904	-	28,34,34	0.56	0	38,53,53	1.15	3 (7%)
5	N5P	I	704	4	28,34,34	0.54	0	38,53,53	1.17	2 (5%)
5	N5P	A	904	-	28,34,34	0.59	0	38,53,53	1.16	2 (5%)

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	N5P	A	905	4	-	4/20/38/38	0/3/3/3
5	N5P	C	904	-	-	0/20/38/38	0/3/3/3
5	N5P	I	704	4	-	4/20/38/38	0/3/3/3
5	N5P	A	904	-	-	4/20/38/38	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	904	N5P	PB-O3A-PA	-3.43	121.04	132.83
5	I	704	N5P	PB-O3B-PG	-3.02	122.48	132.83
5	I	704	N5P	PB-O3A-PA	-3.00	122.54	132.83
5	A	905	N5P	PB-O3B-PG	-2.92	122.82	132.83
5	C	904	N5P	PB-O3A-PA	-2.85	123.06	132.83
5	C	904	N5P	CD1-NE1-C1'	-2.72	122.71	125.40
5	C	904	N5P	PB-O3B-PG	-2.59	123.92	132.83
5	A	904	N5P	PB-O3B-PG	-2.51	124.22	132.83
5	A	905	N5P	PB-O3A-PA	-2.31	124.88	132.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	904	N5P	O4'-C4'-C5'-O5'
5	A	904	N5P	C3'-C4'-C5'-O5'
5	I	704	N5P	PA-O3A-PB-O1B
5	A	905	N5P	PA-O3A-PB-O1B
5	A	905	N5P	PB-O3A-PA-O1A
5	I	704	N5P	PA-O3A-PB-O2B
5	A	905	N5P	PB-O3A-PA-O2A
5	A	905	N5P	PA-O3A-PB-O2B
5	I	704	N5P	PB-O3A-PA-O1A
5	I	704	N5P	PB-O3A-PA-O2A
5	A	904	N5P	PB-O3A-PA-O1A
5	A	904	N5P	PB-O3A-PA-O2A

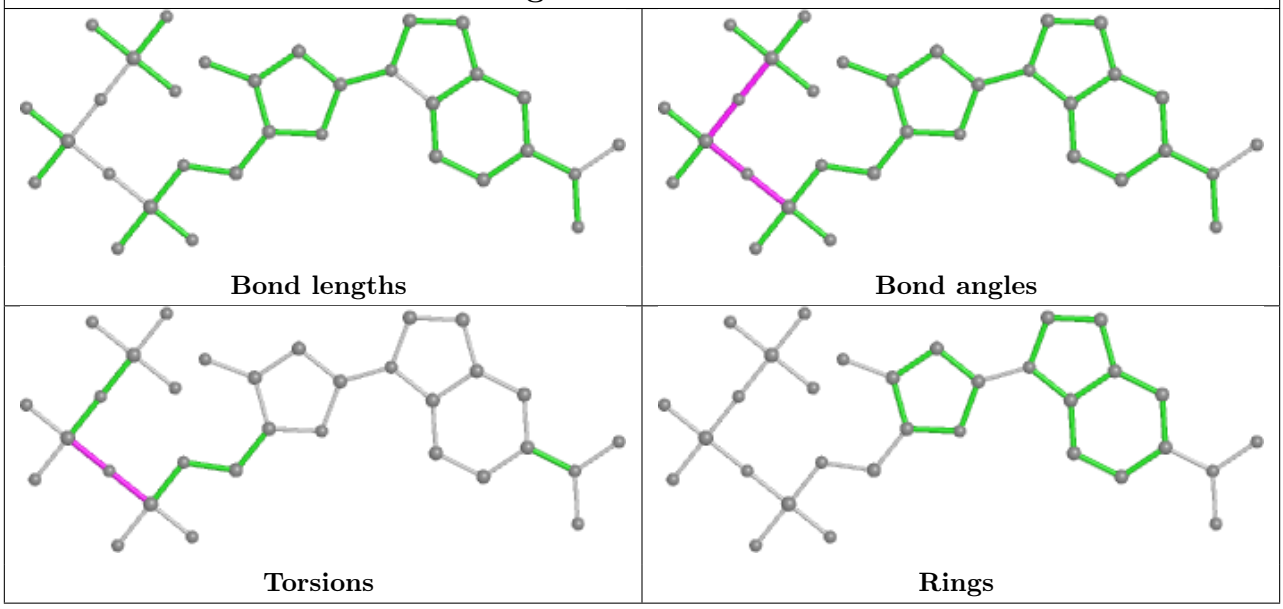
There are no ring outliers.

1 monomer is involved in 1 short contact:

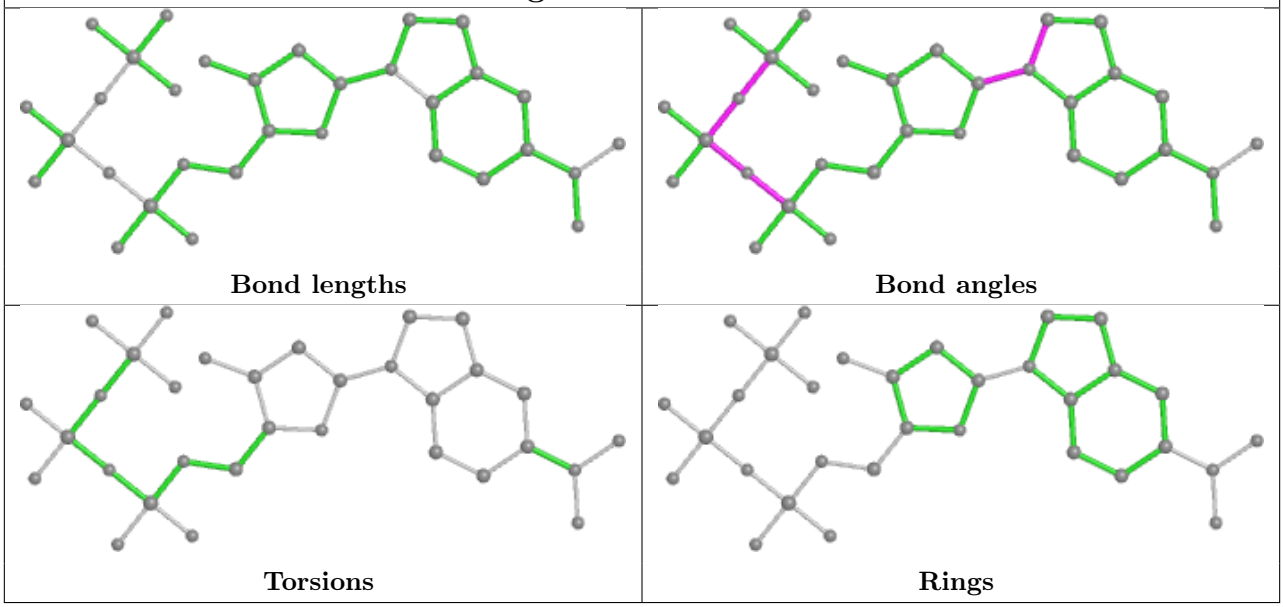
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	905	N5P	1	0

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.

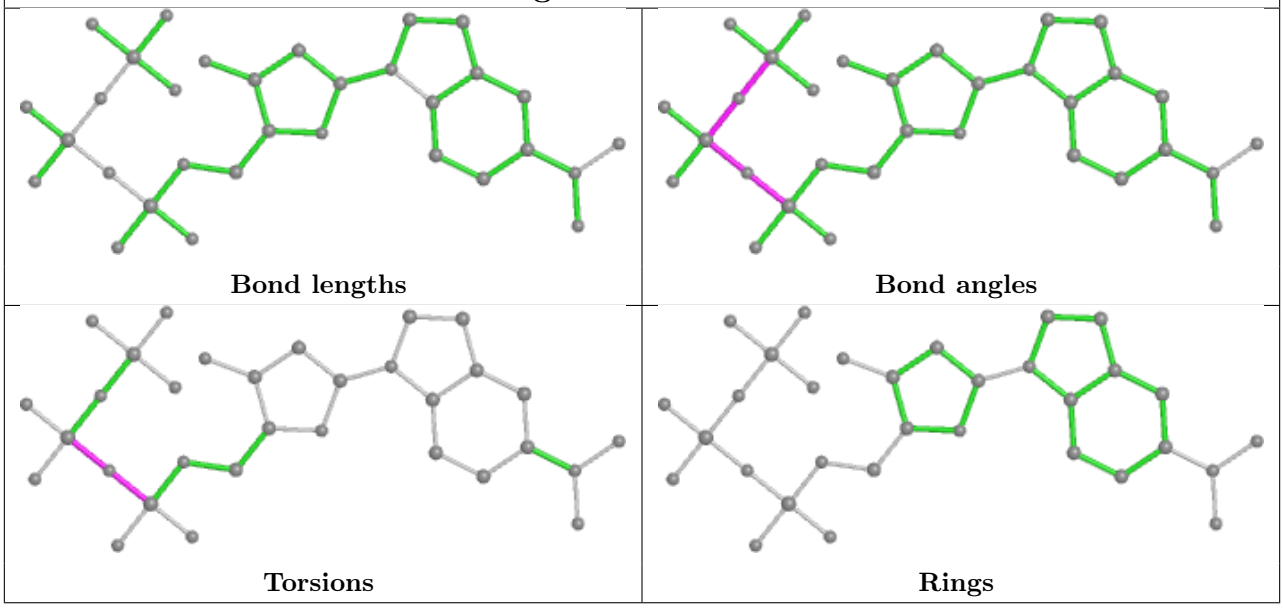
Ligand N5P A 905



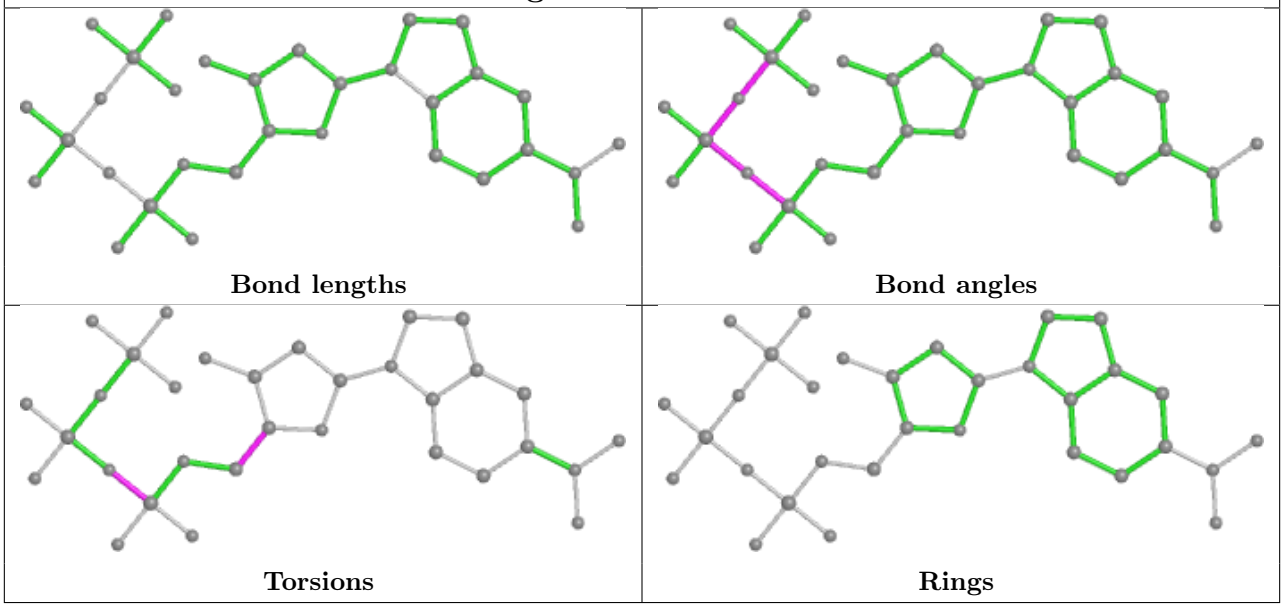
Ligand N5P C 904



Ligand N5P I 704



Ligand N5P A 904



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	E	15/21 (71%)	0.12	0 100 100	58, 78, 115, 119	0
1	G	11/21 (52%)	1.39	4 (36%) 0 0	62, 115, 126, 132	0
1	I	19/21 (90%)	0.01	2 (10%) 6 4	43, 56, 138, 144	0
1	K	12/21 (57%)	-0.18	0 100 100	42, 94, 107, 115	0
2	F	14/15 (93%)	-0.02	0 100 100	73, 106, 124, 126	0
2	H	14/15 (93%)	1.92	7 (50%) 0 0	102, 129, 134, 137	0
2	J	14/15 (93%)	-0.39	0 100 100	44, 68, 85, 88	0
2	L	13/15 (86%)	0.64	1 (7%) 13 10	85, 108, 113, 113	0
3	A	848/903 (93%)	0.04	6 (0%) 87 87	36, 53, 79, 96	0
3	B	756/903 (83%)	0.21	29 (3%) 40 35	44, 68, 105, 116	0
3	C	891/903 (98%)	0.25	29 (3%) 46 41	36, 63, 110, 135	0
3	D	807/903 (89%)	0.71	96 (11%) 4 3	105, 121, 145, 147	0
All	All	3414/3756 (90%)	0.30	174 (5%) 28 23	36, 69, 138, 147	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	257	TYR	8.0
3	D	395	PHE	6.8
3	D	162	TRP	6.5
3	C	252	VAL	6.4
3	B	259	SER	5.9
3	D	321	ILE	5.7
3	D	394	ALA	5.7
3	D	134	ASP	5.6
3	D	178	VAL	5.6
3	D	47	THR	5.4
3	C	491	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
3	C	513	PRO	5.3
3	C	498	ILE	5.2
3	C	303	LEU	4.9
3	D	168	ALA	4.9
3	D	216	TRP	4.7
3	D	864	HIS	4.6
3	D	33	TYR	4.5
3	D	393	GLY	4.5
3	D	776	TYR	4.4
3	D	876	PHE	4.3
3	D	291	ASP	4.3
3	D	258	GLY	4.3
3	D	619	TYR	4.3
3	D	256	MET	4.2
3	D	752	MET	4.2
2	H	109	DC	4.1
3	D	325	ILE	4.1
3	B	174	GLY	4.1
3	D	8	VAL	4.1
3	D	221	PHE	4.1
3	D	308	PRO	3.9
3	D	265	LEU	3.9
3	D	875	THR	3.9
3	D	745	LEU	3.8
3	B	124	PRO	3.8
2	H	107	DG	3.8
3	D	765	LYS	3.8
3	B	255	ASN	3.8
3	D	136	ILE	3.8
1	I	2	DA	3.7
3	C	168	ALA	3.7
3	D	259	SER	3.6
3	D	161	GLU	3.5
3	D	781	SER	3.5
3	D	23	ASN	3.4
3	B	254	GLU	3.4
3	D	146	PHE	3.4
3	D	9	GLU	3.4
1	G	13	DA	3.3
3	B	127	SER	3.3
3	D	138	HIS	3.3
3	D	432	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	153	ASN	3.3
3	C	530	ILE	3.2
3	A	550	VAL	3.2
3	D	10	GLN	3.2
3	D	727	ILE	3.2
2	H	112	DA	3.2
3	C	504	HIS	3.2
3	D	313	ARG	3.1
3	C	518	TYR	3.1
3	D	88	PHE	3.1
3	D	592	MET	3.1
3	D	137	THR	3.1
3	D	446	VAL	3.1
3	D	723	PRO	3.1
3	B	394	ALA	3.0
3	B	123	PHE	3.0
3	B	260	ARG	3.0
3	D	866	MET	3.0
3	D	293	ILE	3.0
3	C	164	ILE	3.0
3	D	133	ILE	3.0
3	C	494	ARG	3.0
3	C	253	ILE	3.0
2	H	111	DT	3.0
2	H	113	DA	2.9
3	B	121	ASP	2.9
3	B	128	GLN	2.9
3	D	405	LYS	2.9
3	B	122	GLY	2.9
3	D	46	ALA	2.9
3	D	116	GLU	2.9
3	D	90	LEU	2.9
3	C	526	ILE	2.9
3	C	537	SER	2.8
3	C	259	SER	2.8
3	D	391	TYR	2.8
3	B	257	TYR	2.8
3	B	234	PHE	2.8
3	C	501	GLU	2.8
3	B	554	THR	2.8
3	B	868	TYR	2.8
3	C	527	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
3	B	779	ILE	2.7
3	C	541	MET	2.7
3	D	780	ALA	2.7
3	A	256	MET	2.7
3	D	22	SER	2.7
3	D	76	GLU	2.7
3	D	336	ALA	2.7
3	B	155	PRO	2.7
3	C	540	GLU	2.7
3	B	182	ILE	2.7
3	D	588	THR	2.7
3	D	132	PRO	2.7
3	D	491	ALA	2.6
3	C	535	ALA	2.6
3	D	7	THR	2.6
2	H	110	DA	2.6
3	D	176	ASP	2.6
3	A	558	ASN	2.6
3	B	393	GLY	2.6
3	D	114	ASP	2.5
3	D	339	GLN	2.5
3	C	166	ILE	2.5
3	D	253	ILE	2.5
3	D	61	LEU	2.5
3	D	895	ALA	2.5
3	D	492	ALA	2.5
3	D	150	ASP	2.4
3	D	431	ALA	2.4
1	G	15	DA	2.4
3	D	239	ALA	2.4
3	D	260	ARG	2.4
3	C	533	LEU	2.4
3	D	626	TYR	2.4
3	A	556	GLN	2.4
3	B	308	PRO	2.4
3	C	534	SER	2.4
1	G	16	DG	2.4
3	C	548	THR	2.4
3	B	252	VAL	2.3
3	D	434	PHE	2.3
3	A	254	GLU	2.3
3	C	497	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	533	LEU	2.3
3	D	698	ILE	2.3
3	D	621	ASP	2.3
3	B	152	LEU	2.3
3	B	195	LYS	2.3
3	D	764	PHE	2.3
3	D	771	PHE	2.3
1	G	18	DC	2.3
2	H	108	DT	2.3
3	D	646	HIS	2.3
3	D	115	ILE	2.2
3	D	124	PRO	2.2
3	C	503	LEU	2.2
3	D	135	ALA	2.2
3	D	166	ILE	2.2
3	B	870	VAL	2.2
3	D	62	PHE	2.2
3	D	262	ILE	2.2
3	D	334	ILE	2.2
3	B	307	GLY	2.2
3	D	458	PRO	2.2
2	L	110	DA	2.2
3	D	149	PHE	2.1
3	D	517	ASP	2.1
3	B	232	ASN	2.1
3	D	268	ILE	2.1
3	C	260	ARG	2.1
3	C	514	LEU	2.1
3	C	900	MET	2.1
3	D	436	VAL	2.1
3	D	778	SER	2.1
3	B	166	ILE	2.1
3	A	786	ASN	2.1
3	D	50	PHE	2.1
1	I	3	DC	2.0
3	D	309	ILE	2.0
3	B	771	PHE	2.0

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. 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
2	N5I	F	115	23/24	0.80	0.26	127,128,128,128	0
1	3DR	E	6	8/12	0.81	0.31	123,124,124,124	0
1	3DR	I	6	11/12	0.89	0.20	104,108,115,115	0
2	N5I	J	115	23/24	0.93	0.18	83,89,89,89	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

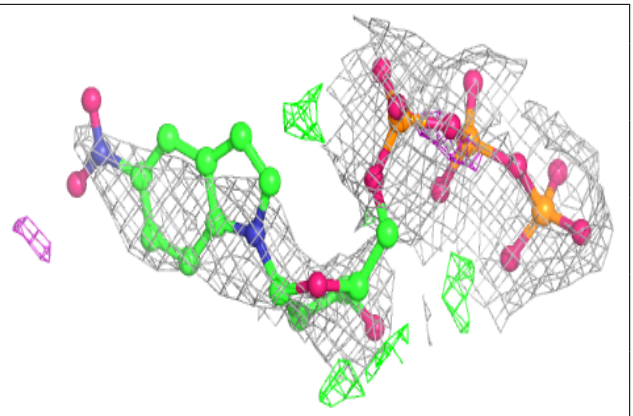
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

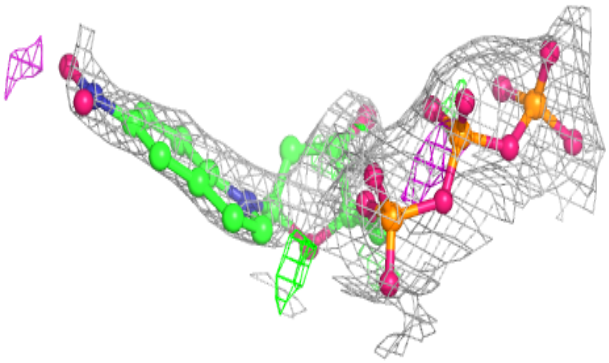
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	I	802	1/1	0.73	0.10	82,82,82,82	1
4	MG	K	801	1/1	0.80	0.24	67,67,67,67	1
5	N5P	C	904	32/32	0.80	0.29	79,81,83,83	32
5	N5P	A	904	32/32	0.86	0.20	74,76,88,88	32
5	N5P	I	704	32/32	0.87	0.28	78,80,84,84	32
5	N5P	A	905	32/32	0.92	0.22	61,65,75,76	32

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 N5P C 904:

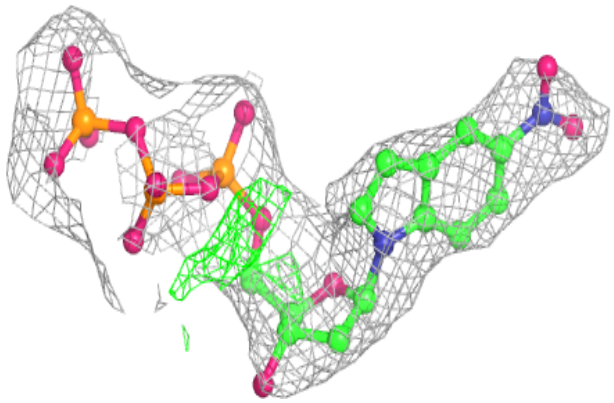
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

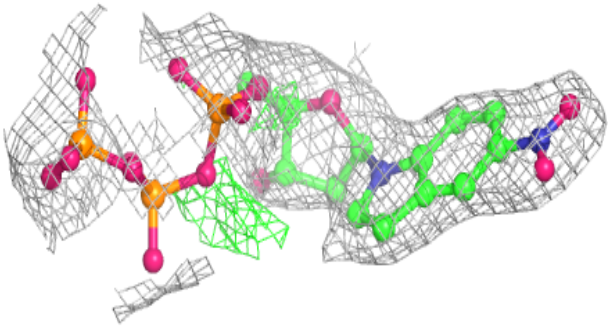


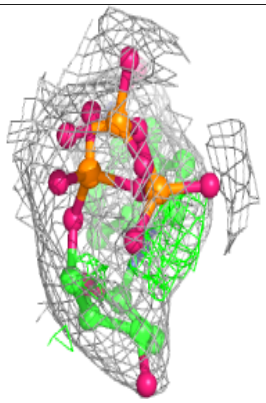


Electron density around N5P A 904:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

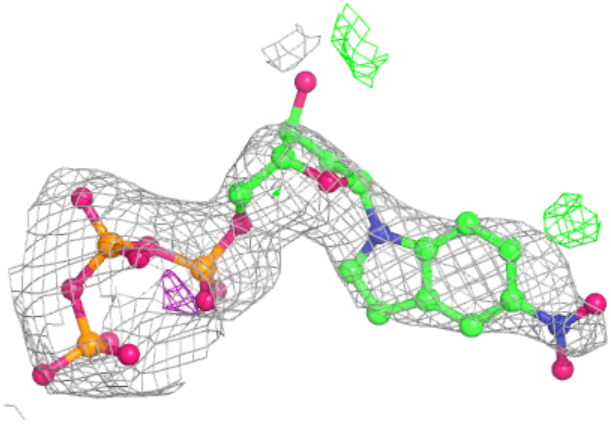


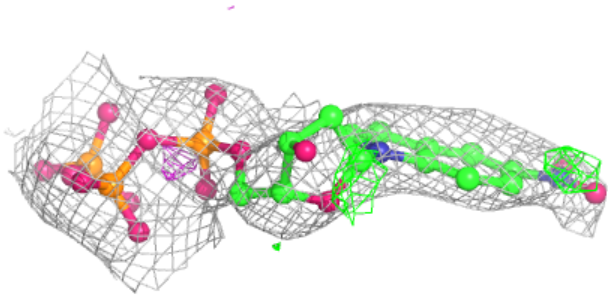


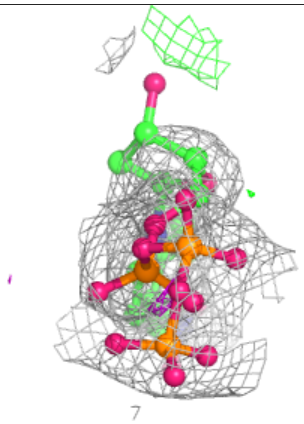


Electron density around N5P I 704:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

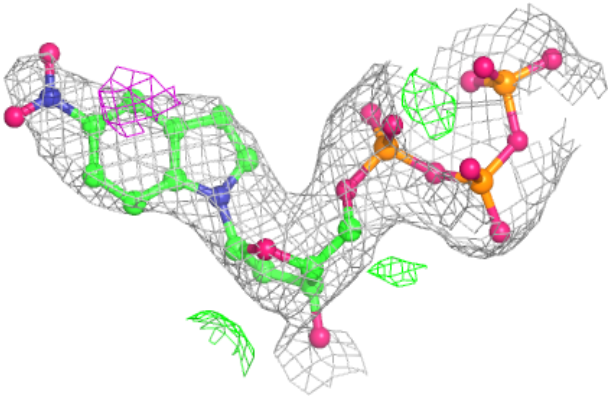


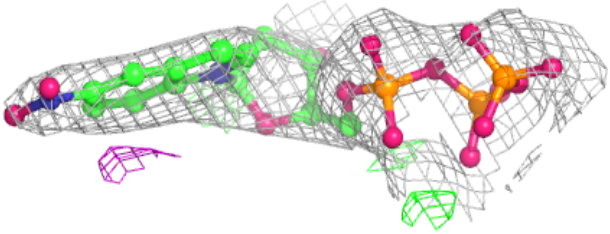


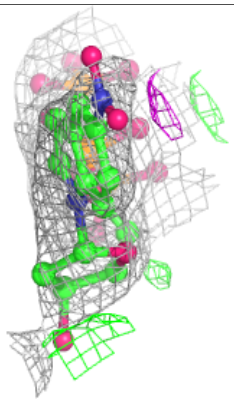


Electron density around N5P A 905:

$2mF_o$-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.