



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:44 AM UTC

PDB ID : 8DH4 / pdb_00008dh4
Title : T7 RNA polymerase elongation complex with unnatural base dPa-DsTP pair
Authors : Oh, J.; Wang, D.
Deposited on : 2022-06-24
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

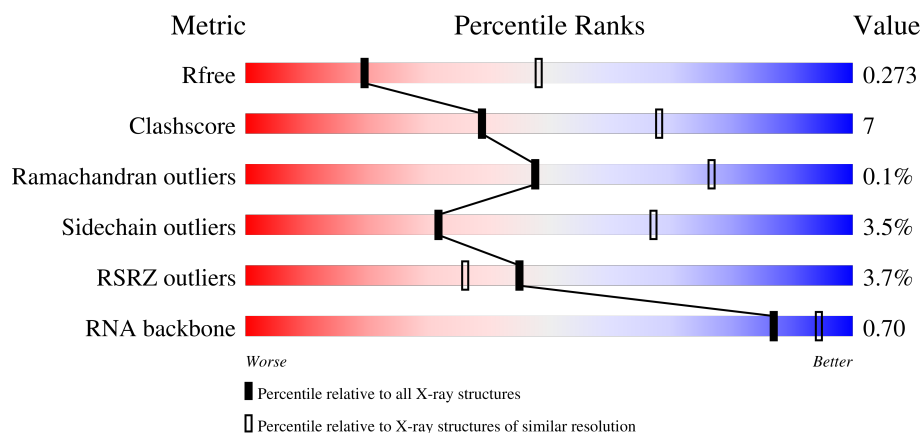
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



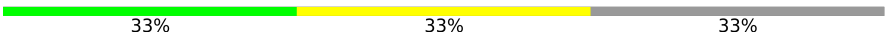
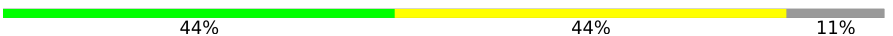
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	B	883	2% 82% 15% ••
1	E	883	3% 76% 16% 7%
1	I	883	5% 73% 20% 7%
1	M	883	4% 71% 21% 7%

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Mol	Chain	Length	Quality of chain
2	A	18	
2	F	18	
2	J	18	
2	N	18	
3	C	12	
3	G	12	
3	K	12	
3	O	12	
4	D	9	
4	H	9	
4	L	9	
4	P	9	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28446 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 T7 RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	856	Total	C	N	O	S	0	0	0
			6728	4284	1169	1239	36			
1	E	819	Total	C	N	O	S	0	0	0
			6397	4086	1097	1181	33			
1	I	821	Total	C	N	O	S	0	0	0
			6429	4106	1112	1176	35			
1	M	819	Total	C	N	O	S	0	0	0
			6409	4090	1111	1176	32			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	15	Total	C	N	O	P	0	0	0
			303	145	55	88	15			
2	F	17	Total	C	N	O	P	0	0	0
			344	165	65	98	16			
2	J	14	Total	C	N	O	P	0	0	0
			282	135	50	83	14			
2	N	15	Total	C	N	O	P	0	0	0
			303	145	55	88	15			

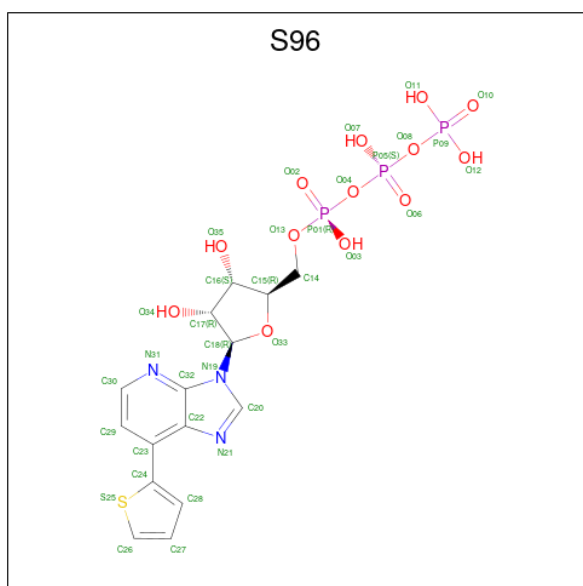
- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	P	0	0	0
			193	86	35	63	9			
3	G	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			
3	K	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			
3	O	8	Total	C	N	O	P	0	0	0
			173	77	33	55	8			

- Molecule 4 is a DNA chain called Non-template strand DNA.

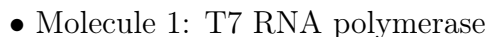
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	P	0	0	0
			122	59	19	38	6			
4	H	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			
4	L	3	Total	C	N	O	P	0	0	0
			63	30	12	18	3			
4	P	6	Total	C	N	O	P	0	0	0
			122	59	19	38	6			

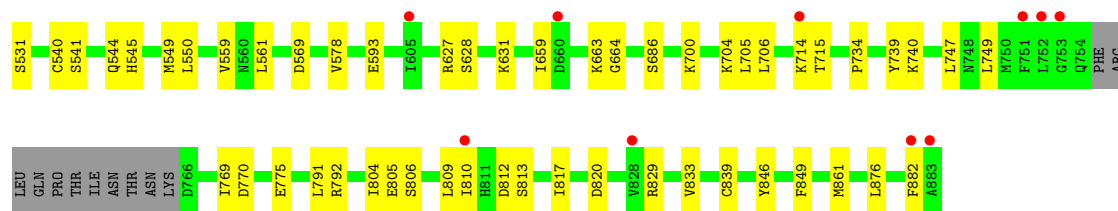
- Molecule 5 is (7P)-3-{5-O-[(R)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-D-ribofuranosyl}-7-(thiophen-2-yl)-3H-imidazo[4,5-b]pyridine (CCD ID: S96) (formula: C₁₅H₁₈N₃O₁₃P₃S) (labeled as "Ligand of Interest" by depositor).



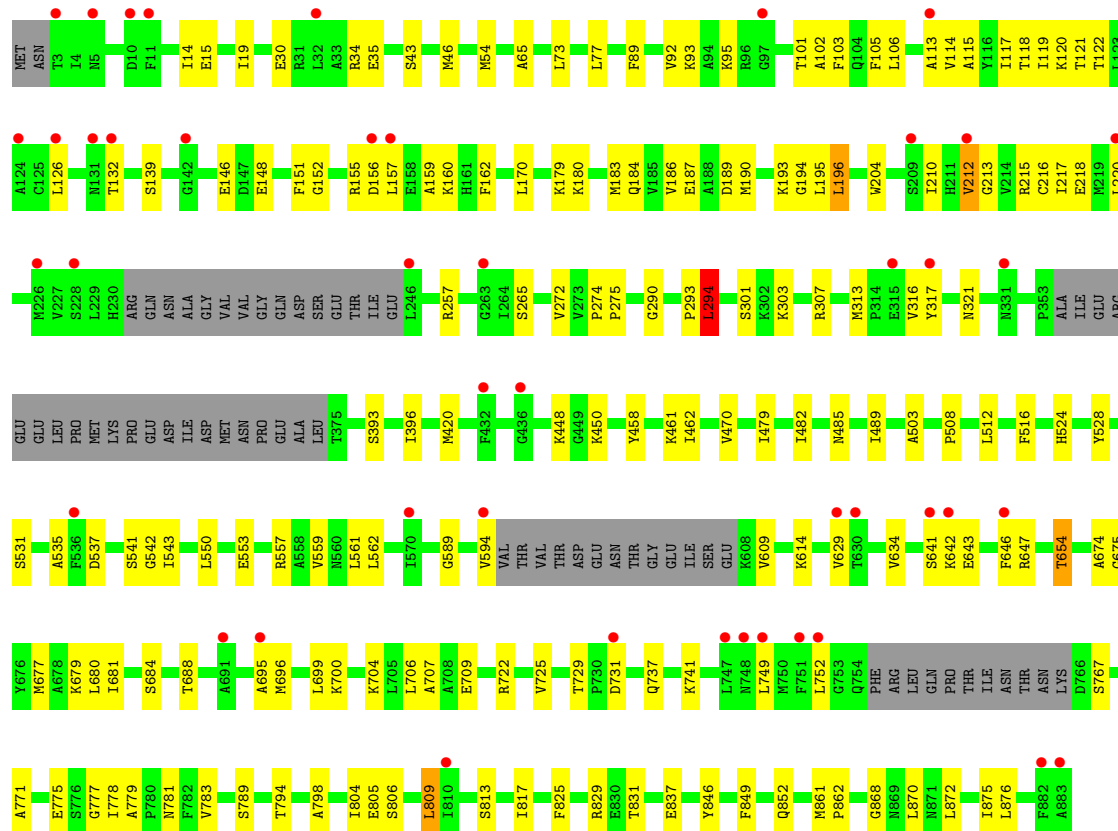
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- Molecule 1: T7 RNA polymerase

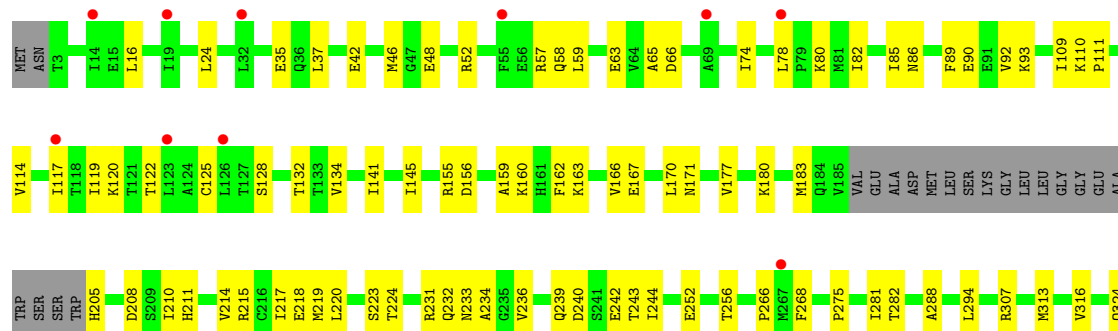


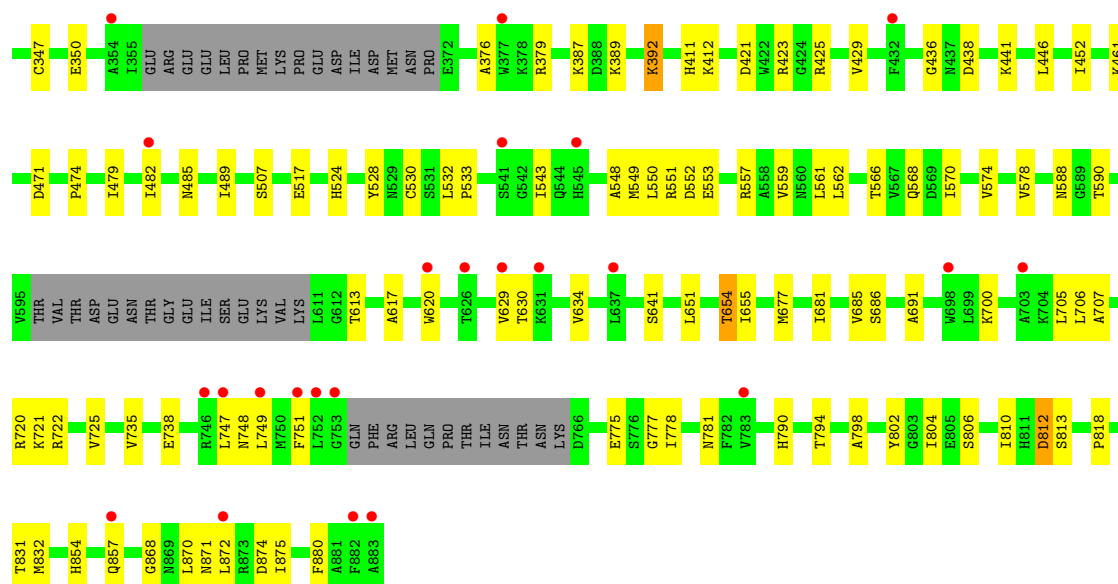


• Molecule 1: T7 RNA polymerase



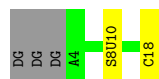
• Molecule 1: T7 RNA polymerase





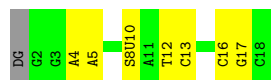
- Molecule 2: Template strand DNA

Chain A: 72% 11% 17%



- Molecule 2: Template strand DNA

Chain F: 56% 39% 6%



- Molecule 2: Template strand DNA

Chain J: 50% 28% 22%



- Molecule 2: Template strand DNA

Chain N: 61% 22% 17%



- Molecule 3: RNA

Chain C: 75% 25%



- Molecule 3: RNA



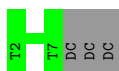
- Molecule 3: RNA



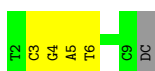
- Molecule 3: RNA



- Molecule 4: Non-template strand DNA



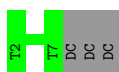
- Molecule 4: Non-template strand DNA



- Molecule 4: Non-template strand DNA



- Molecule 4: Non-template strand DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.78Å 86.23Å 201.46Å 89.85° 85.39° 69.59°	Depositor
Resolution (Å)	43.20 – 2.80 43.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (43.20-2.80) 97.7 (43.20-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.233 , 0.275 0.233 , 0.273	Depositor DCC
R_{free} test set	2002 reflections (1.56%)	wwPDB-VP
Wilson B-factor (Å ²)	82.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28446	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, S96, S8U

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	B	0.17	0/6878	0.39	1/9304 (0.0%)
1	E	0.17	0/6542	0.40	0/8859
1	I	0.21	0/6575	0.46	0/8894
1	M	0.20	0/6553	0.45	0/8870
2	A	0.16	0/318	0.32	0/485
2	F	0.16	0/365	0.36	0/559
2	J	0.15	0/294	0.35	0/448
2	N	0.17	0/318	0.39	0/485
3	C	0.11	0/215	0.26	0/333
3	G	0.09	0/193	0.21	0/299
3	K	0.07	0/193	0.17	0/299
3	O	0.10	0/193	0.26	0/299
4	D	0.13	0/135	0.33	0/206
4	H	0.26	0/177	0.52	0/270
4	L	0.13	0/70	0.30	0/106
4	P	0.26	0/135	0.50	0/206
All	All	0.19	0/29154	0.42	1/39922 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	LEU	CB-CG-CD2	-6.95	89.86	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6728	0	6694	77	0
1	E	6397	0	6304	73	0
1	I	6429	0	6372	105	0
1	M	6409	0	6347	113	0
2	A	303	0	157	1	0
2	F	344	0	180	4	0
2	J	282	0	146	3	0
2	N	303	0	157	2	0
3	C	193	0	96	0	0
3	G	173	0	86	0	0
3	K	173	0	86	0	0
3	O	173	0	86	2	0
4	D	122	0	70	0	0
4	H	160	0	92	3	0
4	L	63	0	35	2	0
4	P	122	0	70	0	0
5	B	35	0	0	1	0
5	E	35	0	0	2	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
All	All	28446	0	26978	378	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 7.

All (378) 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)
5:E:901:S96:C18	5:E:901:S96:O33	1.66	1.16
5:B:901:S96:C18	5:B:901:S96:O33	1.66	1.15
1:M:80:LYS:NZ	1:M:223:SER:O	1.96	0.99
1:B:78:LEU:HD21	1:B:746:ARG:HH12	1.47	0.78
1:E:700:LYS:HG2	1:E:775:GLU:HB2	1.67	0.76
1:B:226:MET:HG2	1:B:227:VAL:HG23	1.69	0.75
1:M:561:LEU:HD22	1:M:875:ILE:HG12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:281:ILE:HD12	1:M:282:THR:HG23	1.72	0.71
1:M:57:ARG:HH12	2:N:17:DG:H5''	1.57	0.70
1:M:548:ALA:O	1:M:551:ARG:NH1	2.25	0.69
1:M:236:VAL:HB	1:M:239:GLN:HG2	1.74	0.69
1:E:421:ASP:OD2	1:E:423:ARG:NH1	2.25	0.69
1:M:86:ASN:HA	1:M:89:PHE:HB2	1.76	0.68
1:M:376:ALA:HA	1:M:379:ARG:HE	1.58	0.68
1:B:715:THR:HG23	1:B:717:GLU:H	1.59	0.68
1:I:184:GLN:HA	1:I:187:GLU:HB3	1.77	0.67
1:M:85:ILE:HD13	1:M:111:PRO:HB2	1.77	0.67
1:M:436:GLY:O	1:M:441:LYS:NZ	2.28	0.66
1:E:36:GLN:HG3	1:E:273:VAL:HG12	1.79	0.65
1:B:46:MET:SD	1:B:269:GLN:NE2	2.71	0.64
1:I:706:LEU:HD12	1:I:725:VAL:HG12	1.79	0.64
1:I:825:PHE:O	1:I:829:ARG:NH1	2.30	0.63
1:B:126:LEU:HD13	1:B:246:LEU:HB2	1.80	0.63
1:M:700:LYS:HG3	1:M:775:GLU:HB2	1.81	0.62
1:B:798:ALA:HB1	1:B:804:ILE:HD12	1.82	0.62
1:B:310:ASP:OD2	1:I:307:ARG:NE	2.33	0.61
1:M:171:ASN:HB3	3:O:3:G:H5'	1.82	0.61
1:E:705:LEU:HD12	1:E:861:MET:HG2	1.82	0.61
1:M:163:LYS:HA	1:M:166:VAL:HB	1.82	0.61
1:I:629:VAL:HG13	1:I:654:THR:HG21	1.83	0.60
1:I:707:ALA:O	1:I:722:ARG:NH1	2.32	0.60
1:M:578:VAL:HG11	1:M:677:MET:HE1	1.84	0.60
1:I:14:ILE:HG22	1:I:290:GLY:HA2	1.84	0.60
1:I:542:GLY:HA2	1:I:783:VAL:HG21	1.82	0.60
1:M:721:LYS:HE3	1:M:722:ARG:H	1.68	0.59
1:I:316:VAL:HG12	1:I:731:ASP:OD2	2.02	0.59
1:I:186:VAL:HG13	1:I:190:MET:HE3	1.85	0.58
1:I:448:LYS:NZ	1:I:805:GLU:OE2	2.36	0.58
1:I:461:LYS:HE2	1:I:479:ILE:HG23	1.86	0.58
1:I:696:MET:HG2	1:I:779:ALA:HB1	1.86	0.58
1:M:812:ASP:N	1:M:812:ASP:OD1	2.37	0.58
1:B:227:VAL:HG13	1:B:244:ILE:HD11	1.86	0.58
1:E:544:GLN:HG2	1:E:561:LEU:HD21	1.86	0.57
1:B:163:LYS:HA	1:B:166:VAL:HG22	1.84	0.57
1:I:317:TYR:O	1:I:321:ASN:ND2	2.37	0.57
1:B:159:ALA:O	1:B:163:LYS:N	2.33	0.57
1:E:791:LEU:HD21	1:E:809:LEU:HD13	1.86	0.57
2:F:5:DA:H61	4:H:6:DT:H3	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:ASP:C	1:I:160:LYS:HZ2	2.12	0.57
1:E:345:LYS:NZ	1:E:351:ASP:O	2.36	0.57
1:M:232:GLN:O	1:M:233:ASN:ND2	2.38	0.57
1:M:160:LYS:HG3	1:M:163:LYS:HZ1	1.69	0.57
1:M:307:ARG:NH1	1:M:738:GLU:OE1	2.35	0.57
1:E:36:GLN:NE2	1:E:271:CYS:SG	2.78	0.56
1:B:57:ARG:NH1	2:A:18:DC:OP2	2.39	0.56
1:B:334:VAL:HG23	1:B:443:LEU:HD23	1.88	0.55
1:B:663:LYS:HA	1:B:663:LYS:HE2	1.88	0.55
1:B:298:ARG:NH1	1:B:419:ASN:OD1	2.39	0.55
1:E:740:LYS:HA	1:E:769:ILE:HA	1.87	0.55
1:B:24:LEU:HD21	1:B:273:VAL:HG21	1.87	0.55
1:I:709:GLU:HG3	1:I:722:ARG:HG3	1.88	0.55
1:B:541:SER:HA	1:B:544:GLN:HB2	1.88	0.55
1:E:46:MET:HB3	1:E:267:MET:HE3	1.87	0.55
1:I:677:MET:HG3	1:I:681:ILE:HD11	1.89	0.55
1:E:706:LEU:HD11	1:E:849:PHE:HB2	1.88	0.55
1:I:543:ILE:HB	1:I:559:VAL:HG11	1.88	0.55
1:M:425:ARG:NH2	3:O:8:U:O2'	2.40	0.55
1:M:798:ALA:HB1	1:M:804:ILE:HD12	1.88	0.55
1:B:85:ILE:HD11	1:B:111:PRO:HB3	1.89	0.55
1:I:313:MET:HE2	1:I:316:VAL:HG21	1.89	0.55
1:B:226:MET:CG	1:B:227:VAL:HG23	2.37	0.54
1:E:804:ILE:HG12	1:E:820:ASP:HB3	1.88	0.54
1:I:35:GLU:HG2	1:I:272:VAL:HG21	1.89	0.54
1:M:471:ASP:N	1:M:471:ASP:OD1	2.40	0.54
1:E:347:CYS:HB3	1:E:350:GLU:HB2	1.89	0.54
1:M:590:THR:HG22	1:M:613:THR:HG23	1.90	0.54
1:I:180:LYS:HE3	1:I:184:GLN:HE22	1.73	0.54
1:B:78:LEU:HD21	1:B:746:ARG:NH1	2.21	0.54
1:I:594:VAL:HA	1:I:609:VAL:HA	1.89	0.54
1:M:421:ASP:OD2	1:M:423:ARG:NH1	2.40	0.54
1:I:43:SER:HA	1:I:46:MET:HE2	1.90	0.54
1:B:78:LEU:HD23	1:B:79:PRO:HD3	1.90	0.53
1:I:503:ALA:HA	1:I:508:PRO:HB3	1.90	0.53
1:B:466:ASN:OD1	1:B:478:ARG:NH1	2.41	0.53
1:M:530:CYS:HB3	1:M:818:PRO:HG2	1.89	0.53
1:M:217:ILE:HA	1:M:220:LEU:HD12	1.90	0.53
1:E:118:THR:HG22	1:E:141:ILE:HD13	1.91	0.53
1:M:707:ALA:O	1:M:722:ARG:NH1	2.42	0.53
1:B:810:ILE:O	1:B:812:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:461:LYS:HB3	1:I:482:ILE:HG13	1.91	0.53
1:M:651:LEU:HA	1:M:655:ILE:HB	1.91	0.53
1:B:73:LEU:HD11	1:B:250:TYR:HD1	1.74	0.53
1:I:160:LYS:HE2	1:I:160:LYS:N	2.23	0.53
1:I:152:GLY:O	1:I:155:ARG:N	2.41	0.53
1:M:205:HIS:HB3	1:M:208:ASP:HB2	1.91	0.53
1:B:578:VAL:HG11	1:B:677:MET:HE1	1.91	0.53
1:I:115:ALA:O	1:I:118:THR:OG1	2.24	0.52
1:I:794:THR:HA	1:I:831:THR:HG21	1.92	0.52
1:E:329:LYS:HG2	1:E:447:ALA:HA	1.91	0.52
1:I:557:ARG:HG2	1:I:562:LEU:HD13	1.90	0.52
1:M:231:ARG:HB3	1:M:242:GLU:HA	1.90	0.52
1:B:446:LEU:HD13	1:B:806:SER:HB3	1.92	0.52
1:E:349:VAL:HG11	1:E:508:PRO:HG3	1.91	0.52
1:E:475:PHE:HA	1:E:478:ARG:HG3	1.90	0.52
1:E:569:ASP:OD2	1:E:627:ARG:NH1	2.43	0.52
1:B:859:ASP:HB2	1:B:860:LYS:HE2	1.92	0.52
1:I:561:LEU:HD22	1:I:875:ILE:HD13	1.92	0.52
1:M:524:HIS:HB2	1:M:528:TYR:HB2	1.91	0.52
1:M:275:PRO:HG2	1:M:324:GLN:HB3	1.92	0.52
1:M:59:LEU:O	1:M:128:SER:OG	2.28	0.51
1:E:524:HIS:HB2	1:E:528:TYR:HB2	1.92	0.51
1:M:790:HIS:O	1:M:794:THR:OG1	2.25	0.51
1:B:109:ILE:HD12	1:B:145:ILE:HG23	1.92	0.51
1:M:376:ALA:HA	1:M:379:ARG:NE	2.24	0.51
1:E:304:ALA:HA	1:E:307:ARG:HD2	1.92	0.51
1:E:150:ARG:HH21	1:E:187:GLU:HG2	1.76	0.51
1:B:93:LYS:HA	1:B:99:ARG:HH21	1.76	0.51
1:B:468:ALA:HA	1:B:505:GLN:HG3	1.92	0.50
1:M:553:GLU:HG3	1:M:870:LEU:HA	1.93	0.50
1:B:3:THR:OG1	1:B:52:ARG:NH1	2.44	0.50
1:E:85:ILE:HD13	1:E:219:MET:HE2	1.93	0.50
1:E:810:ILE:HB	1:E:813:SER:HB2	1.92	0.50
1:I:155:ARG:HG2	1:I:749:LEU:HD11	1.92	0.50
1:E:419:ASN:N	1:E:427:TYR:O	2.42	0.50
1:I:148:GLU:OE2	1:I:155:ARG:NH2	2.43	0.50
1:E:311:VAL:HG11	1:E:734:PRO:HG3	1.94	0.50
1:M:65:ALA:HB3	1:M:120:LYS:HE3	1.92	0.50
1:M:74:ILE:HD12	1:M:119:ILE:HD12	1.94	0.50
1:M:446:LEU:HG	1:M:533:PRO:HG3	1.93	0.50
1:M:557:ARG:HD3	1:M:562:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLU:O	1:B:46:MET:HG3	2.11	0.50
1:I:170:LEU:HD11	1:I:179:LYS:HB3	1.94	0.50
1:B:227:VAL:CG1	1:B:244:ILE:HD11	2.41	0.49
1:E:531:SER:HA	1:E:817:ILE:HD12	1.94	0.49
1:I:695:ALA:O	1:I:699:LEU:HD12	2.12	0.49
1:B:10:ASP:HB3	1:B:291:ARG:NH1	2.27	0.49
1:B:551:ARG:HA	1:B:870:LEU:HD23	1.94	0.49
1:I:19:ILE:HD12	1:I:19:ILE:H	1.77	0.49
1:I:151:PHE:HE1	1:I:184:GLN:HB3	1.76	0.49
1:M:617:ALA:O	1:M:620:TRP:N	2.45	0.49
1:M:588:ASN:OD1	1:M:588:ASN:N	2.46	0.49
1:B:692:ALA:O	1:B:696:MET:HG3	2.11	0.49
1:E:495:SER:OG	1:E:498:GLU:OE1	2.28	0.49
1:E:163:LYS:O	1:E:167:GLU:N	2.45	0.49
1:I:798:ALA:HB1	1:I:804:ILE:HD12	1.94	0.49
1:M:461:LYS:HD3	1:M:479:ILE:HD12	1.95	0.49
1:B:226:MET:HG2	1:B:227:VAL:CG2	2.41	0.48
1:E:219:MET:SD	1:E:219:MET:N	2.83	0.48
1:I:139:SER:HB3	1:I:210:ILE:HG13	1.95	0.48
1:I:643:GLU:HA	1:I:646:PHE:CD2	2.48	0.48
1:I:778:ILE:HD12	1:I:779:ALA:N	2.27	0.48
1:I:190:MET:O	1:I:194:GLY:N	2.46	0.48
1:I:537:ASP:OD1	1:I:813:SER:OG	2.22	0.48
1:E:10:ASP:CG	1:E:291:ARG:HE	2.21	0.48
1:E:151:PHE:HB3	1:E:749:LEU:HD11	1.96	0.48
1:B:190:MET:HE3	1:B:195:LEU:HB3	1.96	0.48
1:E:714:LYS:HA	1:E:714:LYS:HD3	1.64	0.48
1:E:631:LYS:NZ	5:E:901:S96:O11	2.46	0.48
1:B:7:ALA:HA	1:B:11:PHE:HB2	1.95	0.48
1:I:186:VAL:O	1:I:190:MET:HG2	2.13	0.48
1:I:115:ALA:O	1:I:119:ILE:HG13	2.14	0.48
1:I:393:SER:HA	1:I:396:ILE:HD12	1.96	0.48
1:M:706:LEU:HD12	1:M:725:VAL:HG22	1.96	0.48
1:E:419:ASN:HB2	1:E:429:VAL:HG22	1.96	0.47
1:B:247:ALA:HB3	1:B:250:TYR:HD2	1.80	0.47
1:B:350:GLU:OE1	1:B:391:ARG:NH2	2.46	0.47
1:I:675:GLY:O	1:I:679:LYS:N	2.36	0.47
2:J:7:DC:H42	4:L:4:DG:H1	1.60	0.47
1:I:771:ALA:O	1:I:775:GLU:HG3	2.14	0.47
1:M:122:THR:HG23	1:M:141:ILE:HD11	1.96	0.47
1:M:613:THR:O	1:M:617:ALA:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:810:ILE:HB	1:M:813:SER:HB3	1.95	0.47
1:E:739:TYR:O	1:E:770:ASP:N	2.48	0.47
1:I:162:PHE:CE2	1:I:190:MET:HE1	2.50	0.47
1:E:65:ALA:HB3	1:E:120:LYS:HG3	1.97	0.47
1:E:541:SER:HA	1:E:544:GLN:HB2	1.96	0.47
1:I:92:VAL:HA	1:I:95:LYS:HB3	1.97	0.47
1:I:704:LYS:HZ3	4:L:5:DA:H4'	1.80	0.47
1:E:160:LYS:O	1:E:164:LYS:N	2.47	0.47
1:I:829:ARG:HB3	1:I:876:LEU:HD13	1.97	0.47
1:M:854:HIS:HB3	1:M:857:GLN:HG3	1.97	0.47
1:I:152:GLY:O	1:I:155:ARG:HG3	2.15	0.46
1:I:589:GLY:HA3	1:I:614:LYS:HB3	1.96	0.46
1:M:452:ILE:HG13	1:M:818:PRO:HB2	1.97	0.46
1:E:468:ALA:HA	1:E:505:GLN:HB3	1.96	0.46
1:I:65:ALA:HB3	1:I:120:LYS:HG3	1.97	0.46
1:I:215:ARG:HD2	1:I:215:ARG:HA	1.65	0.46
1:M:78:LEU:O	1:M:82:ILE:HG12	2.15	0.46
1:M:629:VAL:HG12	1:M:654:THR:HG21	1.97	0.46
1:I:512:LEU:HG	1:I:516:PHE:HE1	1.80	0.46
1:I:837:GLU:HG3	1:I:872:LEU:HD22	1.97	0.46
1:M:550:LEU:O	1:M:868:GLY:N	2.48	0.46
1:B:550:LEU:HD21	1:B:842:LEU:HD12	1.96	0.46
1:E:67:ASN:OD1	1:E:68:ALA:N	2.48	0.46
1:E:8:LYS:HE3	1:E:8:LYS:HB3	1.48	0.46
1:I:113:ALA:O	1:I:117:ILE:HG13	2.15	0.46
1:M:63:GLU:O	1:M:66:ASP:N	2.46	0.46
1:M:705:LEU:O	1:M:720:ARG:NH2	2.48	0.46
1:B:550:LEU:HB2	1:B:691:ALA:HB1	1.98	0.46
1:I:105:PHE:CD2	1:I:212:VAL:HB	2.50	0.46
1:I:190:MET:HB3	1:I:196:LEU:HD23	1.98	0.46
1:B:118:THR:O	1:B:122:THR:OG1	2.23	0.46
1:E:416:PHE:HB2	1:E:418:TYR:HE1	1.78	0.46
1:I:102:ALA:HA	1:I:105:PHE:CE2	2.50	0.46
1:I:151:PHE:CD1	1:I:183:MET:HB3	2.50	0.46
1:E:298:ARG:HH21	1:E:419:ASN:HB3	1.80	0.46
1:I:684:SER:O	1:I:688:THR:OG1	2.28	0.46
1:M:412:LYS:H	1:M:412:LYS:HD2	1.79	0.46
1:E:36:GLN:HA	1:E:39:LEU:HG	1.97	0.45
1:M:134:VAL:HA	1:M:244:ILE:HD11	1.98	0.45
1:M:313:MET:HE2	1:M:316:VAL:HG11	1.97	0.45
1:M:871:ASN:ND2	1:M:874:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:146:GLU:HG3	1:I:204:TRP:CD2	2.52	0.45
1:I:777:GLY:O	1:I:781:ASN:ND2	2.49	0.45
1:B:688:THR:HG22	1:B:689:VAL:HG13	1.98	0.45
1:E:50:ARG:HB2	1:E:267:MET:HE2	1.99	0.45
1:I:700:LYS:HE2	1:I:775:GLU:HB3	1.98	0.45
1:M:387:LYS:HA	1:M:387:LYS:HD3	1.77	0.45
1:M:777:GLY:O	1:M:781:ASN:ND2	2.50	0.45
1:E:141:ILE:O	1:E:145:ILE:HG12	2.17	0.45
1:B:349:VAL:HG11	1:B:508:PRO:HG3	1.98	0.45
2:F:16:DC:H2'	2:F:17:DG:C8	2.52	0.45
1:I:93:LYS:HD2	1:I:93:LYS:HA	1.76	0.45
1:I:118:THR:HG21	1:I:216:CYS:HB3	1.98	0.45
1:M:35:GLU:OE2	1:M:411:HIS:NE2	2.43	0.45
1:M:85:ILE:HD12	1:M:86:ASN:N	2.31	0.45
1:M:214:VAL:HA	1:M:217:ILE:HD12	1.98	0.45
1:M:294:LEU:HD11	1:M:429:VAL:HG11	1.99	0.45
1:B:10:ASP:HB3	1:B:291:ARG:HH12	1.82	0.45
1:B:78:LEU:HD21	1:B:746:ARG:HH22	1.82	0.45
1:E:446:LEU:HD22	1:E:806:SER:HB3	1.99	0.45
1:M:543:ILE:HB	1:M:559:VAL:HG11	1.99	0.45
1:B:551:ARG:NE	1:B:872:LEU:HD11	2.32	0.45
1:M:132:THR:HG23	1:M:243:THR:HB	1.99	0.45
1:B:186:VAL:O	1:B:190:MET:HG3	2.18	0.44
1:I:89:PHE:HA	1:I:103:PHE:HE1	1.82	0.44
1:I:293:PRO:O	1:I:294:LEU:HB2	2.16	0.44
1:M:268:PHE:CD1	1:M:429:VAL:HG12	2.52	0.44
1:B:666:MET:HE3	1:B:666:MET:HB3	1.82	0.44
1:E:51:PHE:HE2	1:E:261:LEU:HB3	1.82	0.44
1:E:55:PHE:HA	1:E:58:GLN:HE21	1.82	0.44
1:B:19:ILE:HD12	1:B:19:ILE:H	1.81	0.44
1:B:611:LEU:HD11	1:B:669:GLN:HB2	1.99	0.44
1:I:30:GLU:OE2	1:I:34:ARG:NH2	2.51	0.44
1:M:132:THR:OG1	1:M:244:ILE:O	2.34	0.44
1:M:552:ASP:HB2	1:M:691:ALA:HB2	1.99	0.44
1:M:775:GLU:HA	1:M:778:ILE:HG22	2.00	0.44
1:B:73:LEU:HD11	1:B:250:TYR:CD1	2.52	0.44
1:B:190:MET:HE2	1:B:196:LEU:HG	2.00	0.44
1:I:180:LYS:HE3	1:I:184:GLN:NE2	2.31	0.44
1:I:213:GLY:O	1:I:217:ILE:HG13	2.18	0.44
1:I:420:MET:HE2	1:I:420:MET:HB3	1.91	0.44
1:M:85:ILE:HA	1:M:219:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:183:MET:HE3	1:M:183:MET:HA	1.99	0.44
4:H:5:DA:H2'	4:H:6:DT:C6	2.53	0.43
1:B:226:MET:HA	1:B:250:TYR:CD2	2.52	0.43
1:E:24:LEU:HD12	1:E:24:LEU:HA	1.82	0.43
1:E:545:HIS:O	1:E:549:MET:HG3	2.18	0.43
1:B:707:ALA:O	1:B:722:ARG:HD3	2.19	0.43
1:I:118:THR:O	1:I:122:THR:HG23	2.18	0.43
2:N:8:DG:H2''	2:N:9:DA:N7	2.33	0.43
1:I:159:ALA:C	1:I:160:LYS:HE2	2.44	0.43
1:I:257:ARG:HD3	1:I:257:ARG:HA	1.74	0.43
1:M:790:HIS:CE1	1:M:832:MET:HB2	2.53	0.43
1:M:177:VAL:HA	1:M:180:LYS:HE3	2.00	0.43
1:B:69:ALA:HA	1:B:257:ARG:HG2	2.00	0.43
1:I:647:ARG:HB2	1:I:674:ALA:HB1	2.00	0.43
1:M:252:GLU:O	1:M:256:THR:HG23	2.18	0.43
1:M:266:PRO:HG2	1:M:268:PHE:HE2	1.84	0.43
1:B:378:LYS:HE3	1:E:377:TRP:CE2	2.54	0.43
1:E:704:LYS:HB3	1:E:704:LYS:HE2	1.70	0.43
1:I:809:LEU:HD13	1:I:809:LEU:HA	1.74	0.43
1:M:389:LYS:HD3	1:M:389:LYS:HA	1.79	0.43
1:B:159:ALA:HB2	1:B:190:MET:HE1	2.00	0.43
1:I:215:ARG:NE	1:I:218:GLU:OE1	2.52	0.43
1:B:766:ASP:OD1	1:B:766:ASP:N	2.52	0.43
1:M:208:ASP:HA	1:M:211:HIS:ND1	2.34	0.43
1:B:112:GLU:OE2	1:B:112:GLU:N	2.51	0.42
1:E:106:LEU:HD23	1:E:106:LEU:HA	1.90	0.42
2:F:12:DT:H2'	2:F:13:DC:C6	2.54	0.42
1:I:535:ALA:HB1	1:I:813:SER:HB3	2.01	0.42
1:M:234:ALA:HA	1:M:240:ASP:CG	2.44	0.42
2:J:7:DC:H2''	2:J:8:DG:C8	2.54	0.42
1:M:681:ILE:O	1:M:685:VAL:HG13	2.18	0.42
1:B:463:HIS:CD2	1:B:535:ALA:H	2.38	0.42
1:E:44:TYR:HA	1:E:266:PRO:HB3	2.01	0.42
1:I:105:PHE:HB2	1:I:106:LEU:HD23	2.00	0.42
1:M:42:GLU:O	1:M:46:MET:HG3	2.19	0.42
1:M:446:LEU:HD13	1:M:806:SER:HB3	2.01	0.42
1:M:485:ASN:O	1:M:489:ILE:HG13	2.19	0.42
1:M:748:ASN:OD1	1:M:749:LEU:N	2.53	0.42
1:I:313:MET:HG3	1:I:316:VAL:HG22	2.01	0.42
1:I:725:VAL:HG22	1:I:737:GLN:HB3	2.01	0.42
1:M:132:THR:OG1	1:M:132:THR:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:159:ALA:HB1	1:M:162:PHE:HD2	1.83	0.42
1:M:215:ARG:O	1:M:219:MET:HG3	2.19	0.42
1:E:163:LYS:HZ3	1:E:166:VAL:HG12	1.84	0.42
1:I:553:GLU:HG3	1:I:870:LEU:HA	2.01	0.42
1:M:461:LYS:HG2	1:M:482:ILE:HG21	2.02	0.42
1:E:663:LYS:HE2	1:E:663:LYS:HB3	1.76	0.42
1:I:450:LYS:HE2	1:I:817:ILE:HD11	2.01	0.42
1:I:741:LYS:HB3	1:I:741:LYS:HE2	1.86	0.42
1:I:861:MET:HE3	1:I:862:PRO:HD2	2.02	0.42
1:M:517:GLU:HG3	1:M:532:LEU:HB2	2.02	0.42
1:M:566:THR:O	1:M:568:GLN:NE2	2.51	0.42
1:B:189:ASP:O	1:B:192:SER:OG	2.31	0.42
1:B:829:ARG:NH2	1:B:882:PHE:H	2.17	0.42
1:E:329:LYS:HG3	1:E:445:THR:HG23	2.02	0.42
1:E:559:VAL:HG23	1:E:561:LEU:HG	2.01	0.42
1:I:120:LYS:HZ2	1:I:752:LEU:H	1.67	0.42
1:M:474:PRO:HA	1:M:880:PHE:CZ	2.54	0.42
1:B:230:HIS:HB2	1:B:243:THR:HG22	2.00	0.42
1:B:402:LEU:HD12	1:B:402:LEU:HA	1.89	0.42
1:B:650:VAL:HG21	1:B:677:MET:HB3	2.01	0.42
1:I:852:GLN:OE1	1:I:852:GLN:N	2.53	0.42
1:M:392:LYS:H	1:M:392:LYS:HG2	1.57	0.42
1:M:474:PRO:HA	1:M:880:PHE:HZ	1.85	0.42
1:B:153:ARG:O	1:B:157:LEU:HB2	2.20	0.42
1:B:345:LYS:NZ	1:B:351:ASP:O	2.37	0.42
1:E:109:ILE:HD11	1:E:149:ALA:HA	2.01	0.42
1:E:659:ILE:HD13	1:E:664:GLY:HA3	2.02	0.42
1:I:54:MET:HB3	1:I:54:MET:HE2	1.76	0.42
1:I:485:ASN:O	1:I:489:ILE:HG13	2.19	0.42
1:M:114:VAL:HG13	1:M:145:ILE:HD12	2.00	0.42
1:M:798:ALA:HA	1:M:802:TYR:HD2	1.83	0.42
1:M:802:TYR:HB2	1:M:804:ILE:HG13	2.02	0.42
1:E:494:LYS:HB3	1:E:494:LYS:HE2	1.72	0.41
1:I:189:ASP:O	1:I:193:LYS:HG2	2.19	0.41
1:M:266:PRO:HG2	1:M:268:PHE:CE2	2.55	0.41
1:E:420:MET:HE3	1:E:792:ARG:HD3	2.01	0.41
1:I:120:LYS:NZ	1:I:752:LEU:H	2.18	0.41
1:M:214:VAL:O	1:M:218:GLU:HG3	2.20	0.41
1:M:570:ILE:O	1:M:574:VAL:HG12	2.20	0.41
1:B:545:HIS:O	1:B:549:MET:HG3	2.20	0.41
1:M:163:LYS:O	1:M:167:GLU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:MET:HB2	1:E:550:LEU:HD22	2.02	0.41
1:E:700:LYS:HE3	1:E:775:GLU:HG3	2.02	0.41
1:M:794:THR:HA	1:M:831:THR:HG21	2.02	0.41
1:I:479:ILE:HD12	1:I:479:ILE:H	1.86	0.41
1:M:549:MET:HE3	1:M:549:MET:HB2	1.80	0.41
1:E:340:VAL:HG11	1:E:497:LEU:HD11	2.01	0.41
1:E:833:VAL:HG21	1:E:876:LEU:HG	2.02	0.41
2:F:4:DA:H2''	2:F:5:DA:H5'	2.02	0.41
1:E:6:ILE:H	1:E:6:ILE:HG13	1.32	0.41
1:E:846:TYR:HA	1:E:849:PHE:CE2	2.56	0.41
1:I:458:TYR:O	1:I:462:ILE:HG12	2.21	0.41
1:I:642:LYS:HA	1:I:642:LYS:HD3	1.83	0.41
1:M:90:GLU:HA	1:M:93:LYS:HD2	2.03	0.41
1:B:113:ALA:O	1:B:117:ILE:HD12	2.21	0.41
1:B:490:MET:HE3	1:B:490:MET:HB3	1.88	0.41
1:E:829:ARG:NH2	1:E:882:PHE:H	2.18	0.41
1:I:274:PRO:HA	1:I:275:PRO:HD3	1.91	0.41
1:I:846:TYR:HA	1:I:849:PHE:CE2	2.56	0.41
1:M:574:VAL:O	1:M:578:VAL:HG23	2.21	0.41
1:B:329:LYS:HG2	1:B:447:ALA:HA	2.03	0.41
1:E:37:LEU:HD13	1:E:288:ALA:HB2	2.03	0.41
1:I:14:ILE:HD12	1:I:15:GLU:N	2.36	0.41
1:M:37:LEU:HD22	1:M:288:ALA:HB2	2.02	0.41
1:M:48:GLU:O	1:M:52:ARG:HG2	2.21	0.41
1:I:550:LEU:O	1:I:868:GLY:N	2.54	0.40
1:I:729:THR:HB	1:I:789:SER:HB2	2.03	0.40
2:J:11:DA:H2'	2:J:12:DT:C6	2.56	0.40
1:M:117:ILE:HG23	1:M:751:PHE:HE2	1.86	0.40
1:M:677:MET:O	1:M:681:ILE:HG13	2.21	0.40
1:B:791:LEU:HA	1:B:814:PHE:HE1	1.86	0.40
1:E:451:PRO:HA	1:E:529:ASN:HA	2.03	0.40
1:I:524:HIS:HB2	1:I:528:TYR:HB2	2.02	0.40
1:M:155:ARG:HG2	1:M:163:LYS:HD2	2.03	0.40
1:M:347:CYS:HB2	1:M:350:GLU:HB2	2.04	0.40
1:B:574:VAL:HG13	1:B:684:SER:HB2	2.03	0.40
1:B:302:LYS:O	1:B:306:MET:HG2	2.21	0.40
1:B:461:LYS:HE3	1:B:479:ILE:HD12	2.02	0.40
1:E:161:HIS:HA	1:E:164:LYS:HD2	2.03	0.40
4:H:3:DC:H2''	4:H:4:DG:H5''	2.04	0.40
1:I:73:LEU:O	1:I:77:LEU:HG	2.21	0.40
1:M:110:LYS:HE3	1:M:156:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:629:VAL:HG23	1:M:630:THR:HG23	2.03	0.40
1:M:630:THR:O	1:M:634:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	850/883 (96%)	828 (97%)	21 (2%)	1 (0%)	48	77
1	E	809/883 (92%)	798 (99%)	11 (1%)	0	100	100
1	I	811/883 (92%)	796 (98%)	14 (2%)	1 (0%)	48	77
1	M	809/883 (92%)	797 (98%)	12 (2%)	0	100	100
All	All	3279/3532 (93%)	3219 (98%)	58 (2%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	811	HIS
1	I	294	LEU

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	B	701/729 (96%)	677 (97%)	24 (3%)	32	68
1	E	660/729 (90%)	633 (96%)	27 (4%)	27	62
1	I	664/729 (91%)	640 (96%)	24 (4%)	31	66
1	M	662/729 (91%)	643 (97%)	19 (3%)	37	73
All	All	2687/2916 (92%)	2593 (96%)	94 (4%)	32	67

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	24	LEU
1	B	50	ARG
1	B	133	THR
1	B	203	SER
1	B	229	LEU
1	B	243	THR
1	B	301	SER
1	B	310	ASP
1	B	375	THR
1	B	426	VAL
1	B	470	VAL
1	B	507	SER
1	B	539	SER
1	B	540	CYS
1	B	578	VAL
1	B	606	SER
1	B	609	VAL
1	B	719	LEU
1	B	723	CYS
1	B	735	VAL
1	B	745	THR
1	B	813	SER
1	B	841	VAL
1	B	859	ASP
1	E	6	ILE
1	E	8	LYS
1	E	76	THR
1	E	78	LEU
1	E	90	GLU
1	E	114	VAL
1	E	130	ASP
1	E	174	VAL
1	E	177	VAL

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Mol	Chain	Res	Type
1	E	186	VAL
1	E	203	SER
1	E	220	LEU
1	E	294	LEU
1	E	315	GLU
1	E	320	ILE
1	E	379	ARG
1	E	470	VAL
1	E	540	CYS
1	E	578	VAL
1	E	593	GLU
1	E	628	SER
1	E	686	SER
1	E	715	THR
1	E	747	LEU
1	E	805	GLU
1	E	812	ASP
1	E	839	CYS
1	I	101	THR
1	I	114	VAL
1	I	121	THR
1	I	126	LEU
1	I	132	THR
1	I	157	LEU
1	I	195	LEU
1	I	196	LEU
1	I	212	VAL
1	I	220	LEU
1	I	265	SER
1	I	294	LEU
1	I	301	SER
1	I	303	LYS
1	I	470	VAL
1	I	531	SER
1	I	541	SER
1	I	634	VAL
1	I	641	SER
1	I	654	THR
1	I	680	LEU
1	I	767	SER
1	I	806	SER
1	I	809	LEU

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Mol	Chain	Res	Type
1	M	16	LEU
1	M	24	LEU
1	M	58	GLN
1	M	92	VAL
1	M	109	ILE
1	M	125	CYS
1	M	170	LEU
1	M	210	ILE
1	M	224	THR
1	M	392	LYS
1	M	438	ASP
1	M	507	SER
1	M	641	SER
1	M	654	THR
1	M	686	SER
1	M	735	VAL
1	M	747	LEU
1	M	812	ASP
1	M	872	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	22	ASN
1	B	232	GLN
1	B	463	HIS
1	B	499	ASN
1	B	601	ASN
1	B	811	HIS
1	E	36	GLN
1	E	58	GLN
1	E	107	GLN
1	E	131	ASN
1	E	346	HIS
1	E	463	HIS
1	E	601	ASN
1	E	726	HIS
1	E	781	ASN
1	E	848	GLN
1	E	869	ASN
1	I	22	ASN
1	I	131	ASN

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Mol	Chain	Res	Type
1	I	331	ASN
1	I	404	GLN
1	I	485	ASN
1	I	499	ASN
1	I	568	GLN
1	I	579	ASN
1	I	672	GLN
1	M	331	ASN
1	M	339	ASN
1	M	406	ASN
1	M	583	GLN
1	M	619	GLN
1	M	781	ASN
1	M	869	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	7/12 (58%)	0	0
3	G	6/12 (50%)	0	0
3	K	6/12 (50%)	0	0
3	O	6/12 (50%)	2 (33%)	0
All	All	25/48 (52%)	2 (8%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	O	2	C
3	O	4	G

There are no RNA pucker outliers to report.

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

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	S8U	F	10	2	15,19,20	4.66	8 (53%)	19,26,29	1.34	2 (10%)
2	S8U	N	10	2	15,19,20	4.66	8 (53%)	19,26,29	1.29	2 (10%)
2	S8U	A	10	2	15,19,20	4.66	8 (53%)	19,26,29	1.21	2 (10%)
2	S8U	J	10	2	15,19,20	4.66	8 (53%)	19,26,29	1.33	2 (10%)

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	S8U	F	10	2	-	2/9/23/24	0/2/2/2
2	S8U	N	10	2	-	2/9/23/24	0/2/2/2
2	S8U	A	10	2	-	2/9/23/24	0/2/2/2
2	S8U	J	10	2	-	3/9/23/24	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	10	S8U	C2'-C3'	-11.75	1.23	1.52
2	A	10	S8U	C2'-C3'	-11.74	1.23	1.52
2	N	10	S8U	C2'-C3'	-11.73	1.23	1.52
2	F	10	S8U	C2'-C3'	-11.71	1.23	1.52
2	F	10	S8U	O4'-C4'	-8.14	1.26	1.45
2	J	10	S8U	O4'-C4'	-8.12	1.26	1.45
2	N	10	S8U	O4'-C4'	-8.09	1.27	1.45
2	A	10	S8U	O4'-C4'	-8.09	1.27	1.45
2	A	10	S8U	C1'-N11	-5.66	1.33	1.48
2	F	10	S8U	C1'-N11	-5.65	1.33	1.48
2	N	10	S8U	C1'-N11	-5.63	1.33	1.48
2	J	10	S8U	C1'-N11	-5.62	1.33	1.48
2	A	10	S8U	C3'-C4'	5.33	1.67	1.53
2	N	10	S8U	C3'-C4'	5.30	1.66	1.53
2	F	10	S8U	C3'-C4'	5.29	1.66	1.53
2	J	10	S8U	C3'-C4'	5.22	1.66	1.53
2	N	10	S8U	C13-C12	4.48	1.52	1.44
2	J	10	S8U	C13-C12	4.47	1.52	1.44
2	F	10	S8U	C13-C12	4.46	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	10	S8U	C13-C12	4.42	1.52	1.44
2	N	10	S8U	O4'-C1'	4.14	1.51	1.42
2	F	10	S8U	O4'-C1'	4.13	1.51	1.42
2	J	10	S8U	O4'-C1'	4.12	1.51	1.42
2	A	10	S8U	O4'-C1'	4.11	1.51	1.42
2	A	10	S8U	O3'-C3'	3.27	1.50	1.43
2	F	10	S8U	O3'-C3'	3.27	1.50	1.43
2	N	10	S8U	O3'-C3'	3.24	1.50	1.43
2	J	10	S8U	O3'-C3'	3.18	1.50	1.43
2	J	10	S8U	O14-C13	-2.34	1.16	1.22
2	F	10	S8U	O14-C13	-2.31	1.16	1.22
2	N	10	S8U	O14-C13	-2.29	1.17	1.22
2	A	10	S8U	O14-C13	-2.28	1.17	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	10	S8U	O14-C13-C12	-2.88	119.98	126.63
2	N	10	S8U	O14-C13-C12	-2.87	120.01	126.63
2	A	10	S8U	O14-C13-C12	-2.84	120.07	126.63
2	F	10	S8U	O14-C13-C12	-2.84	120.09	126.63
2	J	10	S8U	C2'-C3'-C4'	2.73	108.35	102.80
2	F	10	S8U	C2'-C3'-C4'	2.70	108.27	102.80
2	N	10	S8U	C2'-C3'-C4'	2.69	108.27	102.80
2	A	10	S8U	C2'-C3'-C4'	2.26	107.39	102.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	10	S8U	C15-C12-C13-O14
2	A	10	S8U	N11-C12-C13-O14
2	N	10	S8U	C15-C12-C13-O14
2	N	10	S8U	N11-C12-C13-O14
2	F	10	S8U	N11-C12-C13-O14
2	J	10	S8U	N11-C12-C13-O14
2	F	10	S8U	O4'-C1'-N11-C17
2	J	10	S8U	O4'-C1'-N11-C17
2	J	10	S8U	C2'-C1'-N11-C17

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	S96	B	901	6	37,38,38	4.94	20 (54%)	54,59,59	1.89	11 (20%)
5	S96	E	901	6	37,38,38	4.94	20 (54%)	54,59,59	1.89	10 (18%)

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	S96	B	901	6	-	3/26/42/42	0/4/4/4
5	S96	E	901	6	-	7/26/42/42	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	901	S96	C23-C22	12.49	1.58	1.41
5	B	901	S96	C23-C22	12.27	1.58	1.41
5	E	901	S96	C32-N31	11.85	1.56	1.34
5	B	901	S96	C32-N31	11.82	1.56	1.34
5	E	901	S96	O33-C18	10.68	1.66	1.42
5	B	901	S96	O33-C18	10.65	1.66	1.42
5	B	901	S96	P01-O04	10.41	1.70	1.59
5	E	901	S96	P01-O04	10.14	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	901	S96	C17-C18	-7.77	1.29	1.53
5	B	901	S96	C17-C18	-7.71	1.29	1.53
5	B	901	S96	P05-O04	7.24	1.67	1.59
5	E	901	S96	P05-O04	7.21	1.67	1.59
5	B	901	S96	C30-N31	6.71	1.48	1.34
5	E	901	S96	C30-N31	6.66	1.48	1.34
5	B	901	S96	O33-C15	-6.19	1.31	1.45
5	E	901	S96	C29-C30	6.05	1.50	1.38
5	B	901	S96	C29-C30	6.04	1.50	1.38
5	E	901	S96	O33-C15	-6.02	1.31	1.45
5	B	901	S96	C29-C23	5.50	1.48	1.39
5	E	901	S96	C29-C23	5.50	1.48	1.39
5	B	901	S96	C24-S25	-4.65	1.56	1.71
5	E	901	S96	C20-N21	4.64	1.40	1.31
5	E	901	S96	C24-S25	-4.62	1.56	1.71
5	B	901	S96	C20-N21	4.55	1.40	1.31
5	E	901	S96	C27-C28	3.88	1.61	1.42
5	B	901	S96	C27-C28	3.84	1.61	1.42
5	E	901	S96	O35-C16	-3.74	1.33	1.43
5	B	901	S96	O35-C16	-3.73	1.33	1.43
5	B	901	S96	C26-S25	-3.43	1.54	1.70
5	E	901	S96	C26-S25	-3.42	1.55	1.70
5	E	901	S96	O34-C17	2.85	1.50	1.43
5	B	901	S96	O34-C17	2.82	1.49	1.43
5	B	901	S96	C27-C26	2.71	1.44	1.34
5	E	901	S96	C27-C26	2.67	1.44	1.34
5	B	901	S96	P05-O08	2.56	1.62	1.59
5	E	901	S96	P05-O08	2.55	1.62	1.59
5	B	901	S96	P01-O13	2.04	1.67	1.59
5	B	901	S96	C23-C24	2.02	1.51	1.48
5	E	901	S96	P01-O13	2.02	1.67	1.59
5	E	901	S96	C23-C24	2.01	1.51	1.48

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	901	S96	C26-S25-C24	8.56	107.88	92.68
5	B	901	S96	C26-S25-C24	8.50	107.77	92.68
5	E	901	S96	C22-C32-N31	-4.82	120.08	126.72
5	B	901	S96	C22-C32-N31	-4.71	120.23	126.72
5	B	901	S96	N19-C20-N21	-4.04	108.20	113.94
5	E	901	S96	N19-C20-N21	-4.02	108.23	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	901	S96	C29-C30-N31	-3.53	119.64	123.97
5	B	901	S96	C29-C30-N31	-3.38	119.83	123.97
5	E	901	S96	C22-N21-C20	2.95	108.09	103.45
5	B	901	S96	C22-N21-C20	2.91	108.02	103.45
5	E	901	S96	N31-C32-N19	2.76	131.86	127.17
5	B	901	S96	N31-C32-N19	2.74	131.82	127.17
5	E	901	S96	C32-C22-N21	-2.38	107.86	110.58
5	E	901	S96	C30-N31-C32	2.38	120.44	115.05
5	B	901	S96	C32-C22-N21	-2.28	107.98	110.58
5	B	901	S96	C30-N31-C32	2.23	120.11	115.05
5	E	901	S96	C27-C26-S25	-2.09	107.92	113.02
5	E	901	S96	C22-C32-N19	2.07	108.07	105.81
5	B	901	S96	C23-C24-S25	2.06	126.06	121.88
5	B	901	S96	C27-C26-S25	-2.03	108.05	113.02
5	B	901	S96	C32-N19-C20	2.01	107.85	105.74

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	901	S96	C14-O13-P01-O03
5	E	901	S96	O13-C14-C15-O33
5	E	901	S96	C14-O13-P01-O03
5	E	901	S96	C14-O13-P01-O04
5	E	901	S96	O13-C14-C15-C16
5	E	901	S96	P05-O04-P01-O02
5	B	901	S96	C14-O13-P01-O02
5	B	901	S96	C14-O13-P01-O04
5	E	901	S96	C15-C14-O13-P01
5	E	901	S96	P09-O08-P05-O07

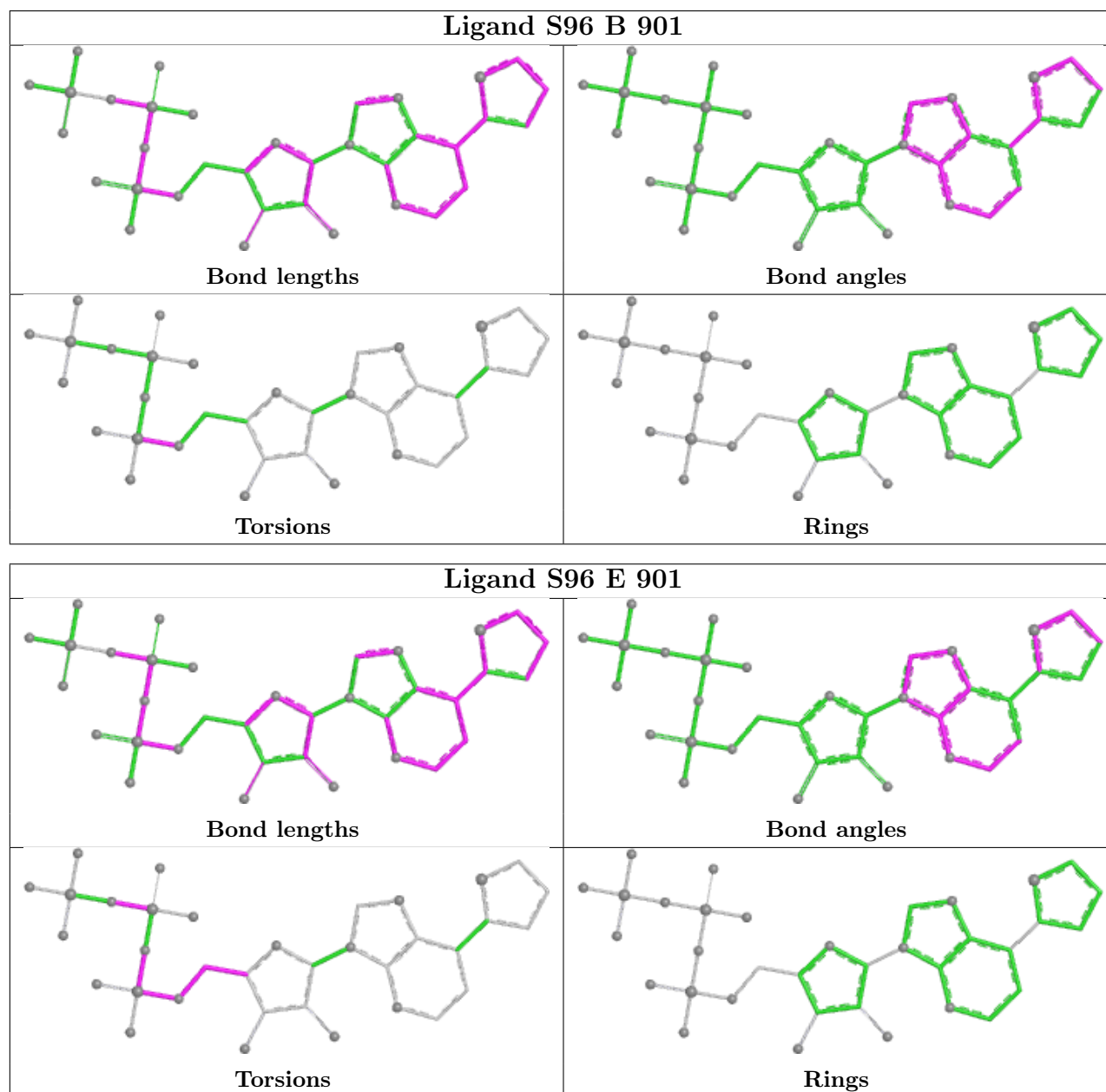
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	901	S96	1	0
5	E	901	S96	2	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 than 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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	856/883 (96%)	0.22	20 (2%) 61 51	46, 79, 149, 207	0
1	E	819/883 (92%)	0.35	28 (3%) 48 39	51, 91, 194, 254	0
1	I	821/883 (92%)	0.45	45 (5%) 30 23	65, 116, 181, 226	0
1	M	819/883 (92%)	0.43	34 (4%) 40 32	79, 130, 209, 268	0
2	A	14/18 (77%)	0.07	0 100 100	57, 83, 257, 270	0
2	F	16/18 (88%)	-0.05	0 100 100	74, 128, 257, 274	0
2	J	13/18 (72%)	0.05	0 100 100	82, 92, 293, 308	0
2	N	14/18 (77%)	0.08	0 100 100	102, 150, 228, 260	0
3	C	9/12 (75%)	-0.05	0 100 100	65, 75, 116, 168	0
3	G	8/12 (66%)	-0.13	0 100 100	77, 92, 140, 155	0
3	K	8/12 (66%)	-0.29	0 100 100	96, 100, 125, 152	0
3	O	8/12 (66%)	-0.18	0 100 100	114, 124, 185, 194	0
4	D	6/9 (66%)	0.49	0 100 100	217, 228, 252, 264	0
4	H	8/9 (88%)	0.34	0 100 100	224, 231, 239, 254	0
4	L	3/9 (33%)	0.83	0 100 100	251, 251, 273, 277	0
4	P	6/9 (66%)	0.25	0 100 100	244, 258, 263, 277	0
All	All	3428/3688 (92%)	0.35	127 (3%) 45 36	46, 106, 197, 308	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	545	HIS	4.6
1	B	158	GLU	4.6
1	M	883	ALA	4.5
1	I	642	LYS	4.1
1	I	752	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	752	LEU	3.8
1	I	883	ALA	3.7
1	M	747	LEU	3.7
1	I	126	LEU	3.6
1	M	541	SER	3.6
1	I	436	GLY	3.6
1	I	748	ASN	3.5
1	B	776	SER	3.5
1	M	749	LEU	3.4
1	I	315	GLU	3.2
1	E	212	VAL	3.2
1	B	752	LEU	3.1
1	E	102	ALA	3.1
1	I	142	GLY	3.1
1	I	10	ASP	3.1
1	B	165	ASN	3.1
1	M	354	ALA	3.1
1	B	134	VAL	3.1
1	M	32	LEU	3.1
1	E	109	ILE	3.0
1	M	123	LEU	3.0
1	I	695	ALA	3.0
1	B	540	CYS	2.9
1	I	691	ALA	2.9
1	E	393	SER	2.9
1	B	753	GLY	2.9
1	B	113	ALA	2.9
1	M	78	LEU	2.9
1	E	882	PHE	2.8
1	I	641	SER	2.8
1	E	182	PHE	2.8
1	I	3	THR	2.8
1	I	630	THR	2.8
1	E	186	VAL	2.8
1	E	883	ALA	2.8
1	I	747	LEU	2.8
1	E	605	ILE	2.7
1	I	432	PHE	2.7
1	M	637	LEU	2.7
1	B	567	VAL	2.7
1	E	220	LEU	2.7
1	B	857	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	181	ALA	2.6
1	B	388	ASP	2.6
1	B	754	GLN	2.6
1	I	246	LEU	2.6
1	E	418	TYR	2.6
1	E	714	LYS	2.5
1	M	872	LEU	2.5
1	E	123	LEU	2.5
1	M	14	ILE	2.5
1	M	19	ILE	2.5
1	I	629	VAL	2.5
1	M	626	THR	2.5
1	E	250	TYR	2.4
1	B	1	MET	2.4
1	E	810	ILE	2.4
1	I	97	GLY	2.4
1	M	753	GLY	2.4
1	M	126	LEU	2.4
1	E	74	ILE	2.4
1	I	570	ILE	2.4
1	E	173	ARG	2.4
1	M	620	TRP	2.4
1	I	131	ASN	2.4
1	M	857	GLN	2.4
1	I	226	MET	2.4
1	E	355	ILE	2.4
1	E	751	PHE	2.3
1	I	5	ASN	2.3
1	E	221	ILE	2.3
1	I	212	VAL	2.3
1	M	432	PHE	2.3
1	B	135	GLN	2.3
1	M	746	ARG	2.3
1	E	174	VAL	2.3
1	B	126	LEU	2.3
1	E	660	ASP	2.3
1	I	536	PHE	2.2
1	I	751	PHE	2.2
1	I	113	ALA	2.2
1	B	77	LEU	2.2
1	I	731	ASP	2.2
1	M	482	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	646	PHE	2.2
1	I	124	ALA	2.2
1	I	749	LEU	2.2
1	M	631	LYS	2.2
1	M	752	LEU	2.2
1	M	882	PHE	2.2
1	M	117	ILE	2.2
1	E	828	VAL	2.2
1	I	209	SER	2.2
1	I	317	TYR	2.2
1	I	882	PHE	2.2
1	B	4	ILE	2.2
1	I	156	ASP	2.2
1	M	629	VAL	2.2
1	M	698	TRP	2.2
1	I	11	PHE	2.2
1	I	594	VAL	2.1
1	B	510	CYS	2.1
1	I	810	ILE	2.1
1	I	331	ASN	2.1
1	I	263	GLY	2.1
1	M	377	TRP	2.1
1	B	341	ILE	2.1
1	I	228	SER	2.1
1	M	55	PHE	2.1
1	E	320	ILE	2.1
1	E	376	ALA	2.1
1	E	377	TRP	2.1
1	M	703	ALA	2.1
1	M	267	MET	2.0
1	I	32	LEU	2.0
1	I	157	LEU	2.0
1	M	751	PHE	2.0
1	I	132	THR	2.0
1	M	69	ALA	2.0
1	M	783	VAL	2.0
1	I	220	LEU	2.0
1	E	753	GLY	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	S8U	N	10	18/19	0.88	0.12	133,140,152,158	0
2	S8U	J	10	18/19	0.92	0.10	102,109,130,139	0
2	S8U	F	10	18/19	0.95	0.09	78,87,103,108	0
2	S8U	A	10	18/19	0.96	0.07	62,75,87,89	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

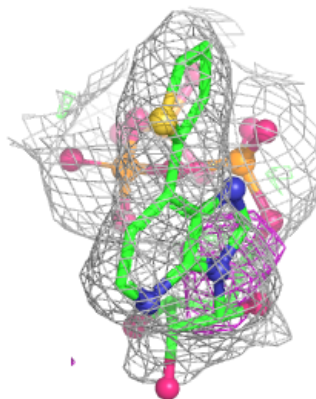
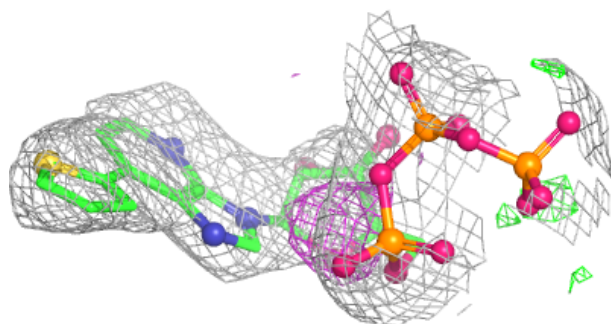
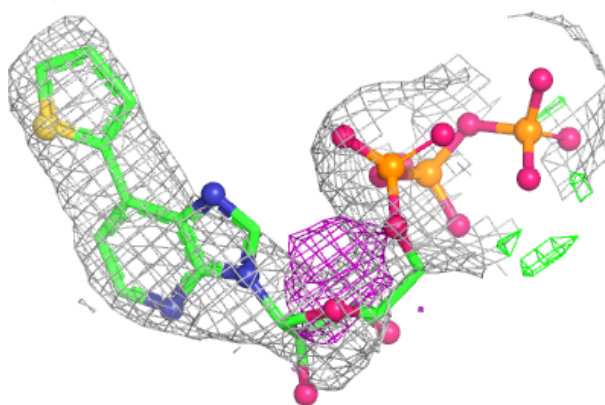
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	E	902	1/1	0.77	0.22	103,103,103,103	0
5	S96	E	901	35/35	0.81	0.12	76,122,135,140	0
6	MG	B	902	1/1	0.88	0.10	79,79,79,79	0
5	S96	B	901	35/35	0.88	0.10	68,102,129,134	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.

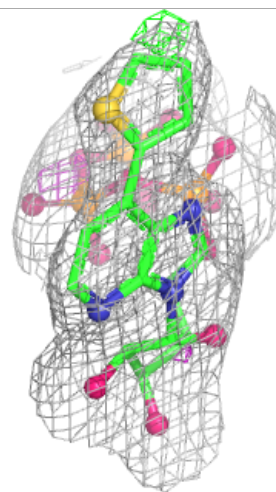
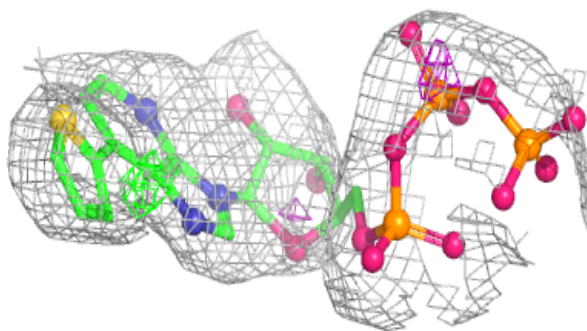
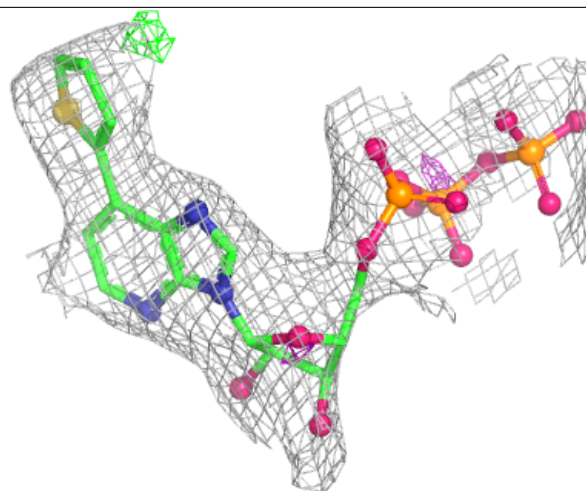
Electron density around S96 E 901:

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



Electron density around S96 B 901:

$2mF_o-DF_c$ (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.