



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:12 PM UTC

PDB ID : 1Q9X / pdb_00001q9x
Title : Crystal structure of Enterobacteria phage RB69 gp43 DNA polymerase complexed with tetrahydrofuran containing DNA
Authors : Freisinger, E.; Grollman, A.P.; Miller, H.; Kisker, C.
Deposited on : 2003-08-26
Resolution : 2.69 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

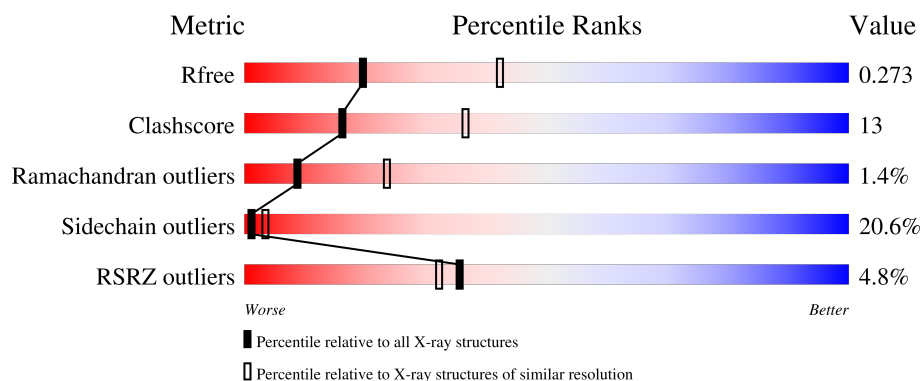
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	E	18	17% 33% 56% 11%
1	F	18	11% 33% 61% 6%
1	G	18	6% 39% 50% 11%
1	H	18	11% 56% 33% 11%
2	I	13	8% 15% 69% 15%

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Mol	Chain	Length	Quality of chain
2	J	13	54% 23% 23%
2	K	13	31% 62% 8%
2	L	13	46% 54%
3	A	903	10% 59% 33% 8%
3	B	903	5% 64% 29% 6%
3	C	903	2% 65% 27% 8%
3	D	903	2% 62% 30% 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called 5'-GCGGACTGCTTAC(dideoxycytidine)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	18	Total	C	N	O	P	0	0	0
			370	175	74	104	17			
1	F	18	Total	C	N	O	P	0	0	0
			370	175	74	104	17			
1	G	18	Total	C	N	O	P	0	0	0
			370	175	74	104	17			
1	H	18	Total	C	N	O	P	0	0	0
			370	175	74	104	17			

- Molecule 2 is a DNA chain called 5'-AC(tetrahydrofuran)GGTAAGCAGTCCGCGG-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			
2	J	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			
2	K	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			
2	L	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			

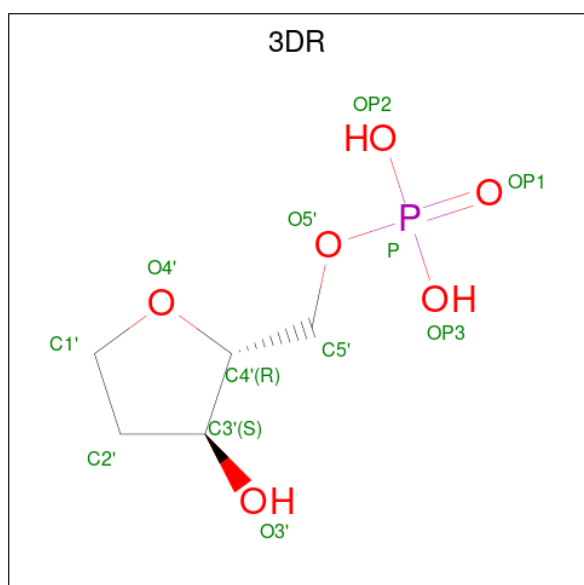
- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	903	Total	C	N	O	S	0	0	0
			7365	4730	1226	1376	33			
3	B	903	Total	C	N	O	S	0	0	0
			7365	4730	1226	1376	33			
3	C	903	Total	C	N	O	S	0	0	0
			7365	4730	1226	1376	33			
3	D	903	Total	C	N	O	S	0	0	0
			7365	4730	1226	1376	33			

There are 8 discrepancies between the modelled and reference sequences:

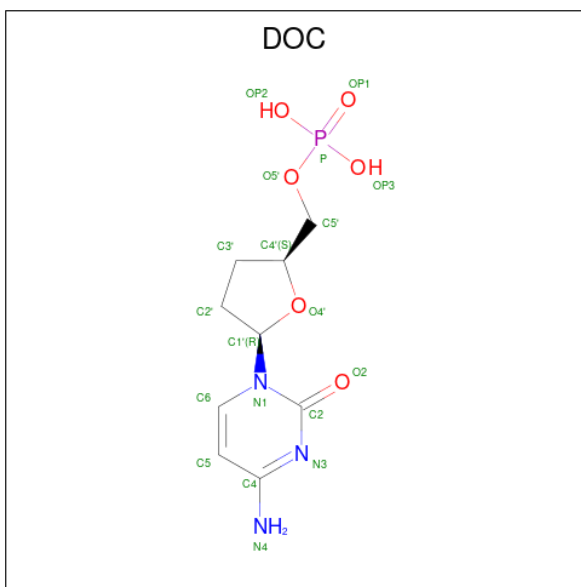
Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation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

- Molecule 4 is 1',2'-DIDEOXYRIBOFURANOSE-5'-PHOSPHATE (CCD ID: 3DR) (formula: $C_5H_{11}O_6P$).



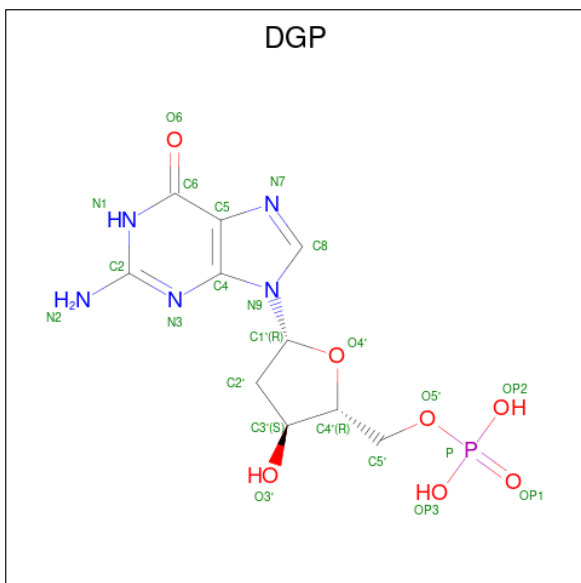
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	O	P	0	0
			11	5	5	1		
4	F	1	Total	C	O	P	0	0
			11	5	5	1		
4	G	1	Total	C	O	P	0	0
			11	5	5	1		
4	H	1	Total	C	O	P	0	0
			11	5	5	1		

- Molecule 5 is 2',3'-Dideoxycytidine-5'-monophosphate (CCD ID: DOC) (formula: $C_9H_{14}N_3O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	I	1	Total	C	N	O	P	0	0
			18	9	3	5	1		
5	J	1	Total	C	N	O	P	0	0
			18	9	3	5	1		
5	K	1	Total	C	N	O	P	0	0
			18	9	3	5	1		
5	L	1	Total	C	N	O	P	0	0
			18	9	3	5	1		

- Molecule 6 is 2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE (CCD ID: DGP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C N O 19 10 5 4	0	0
6	G	1	Total O 1 1	0	0
6	G	1	Total C N O P 22 10 5 6 1	0	0
6	K	1	Total C N O P 22 10 5 6 1	0	0
6	H	1	Total C N O 19 10 5 4	0	0
6	L	1	Total C N O P 22 10 5 6 1	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Ca 2 2	0	0
7	B	2	Total Ca 2 2	0	0
7	C	2	Total Ca 2 2	0	0
7	D	2	Total Ca 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	11	Total O 11 11	0	0
8	I	11	Total O 11 11	0	0
8	F	8	Total O 8 8	0	0
8	J	6	Total O 6 6	0	0
8	G	7	Total O 7 7	0	0
8	K	3	Total O 3 3	0	0
8	H	8	Total O 8 8	0	0
8	L	3	Total O 3 3	0	0

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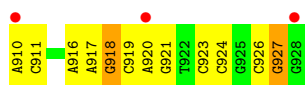
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	112	Total 112	O 112	0	0
8	B	129	Total 129	O 129	0	0
8	C	126	Total 126	O 126	0	0
8	D	111	Total 111	O 111	0	0

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.

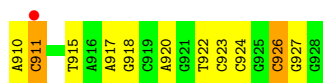
- Molecule 1: 5'-GCGGACTGCTTAC(dideoxycytidine)-3'



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- Molecule 1: 5'-GCGGACTGCTTAC(dideoxycytidine)-3'



- Molecule 2: 5'-AC(tetrahydrofuran)GGTAAGCAGTCCGCGG-3'

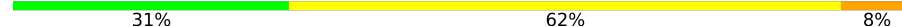


- Molecule 2: 5'-AC(tetrahydrofuran)GGTAAGCAGTCCGCGG-3'

Chain J: 

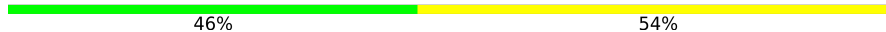


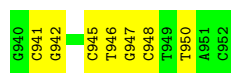
- Molecule 2: 5'-AC(tetrahydrofuran)GGTAAGCAGTCCGCGG-3'

Chain K: 



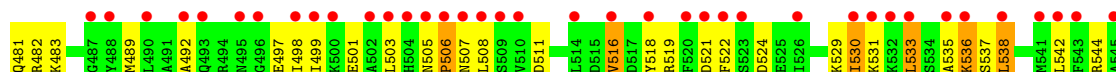
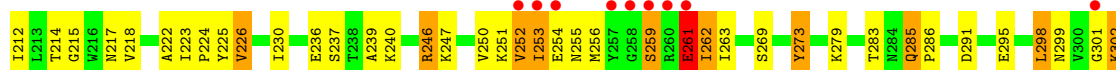
- Molecule 2: 5'-AC(tetrahydrofuran)GGTAAGCAGTCCGCGG-3'

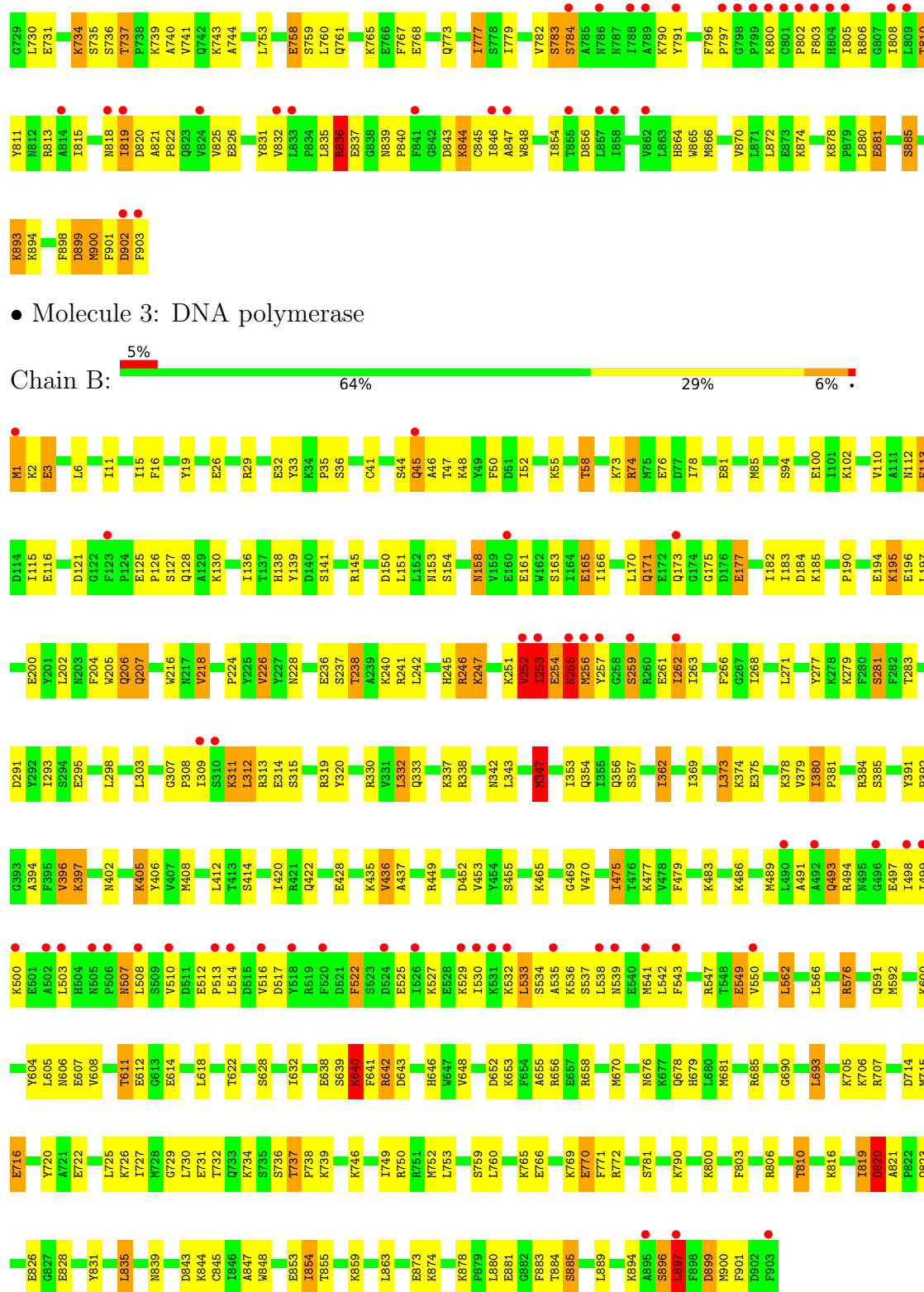
Chain L: 



- Molecule 3: DNA polymerase

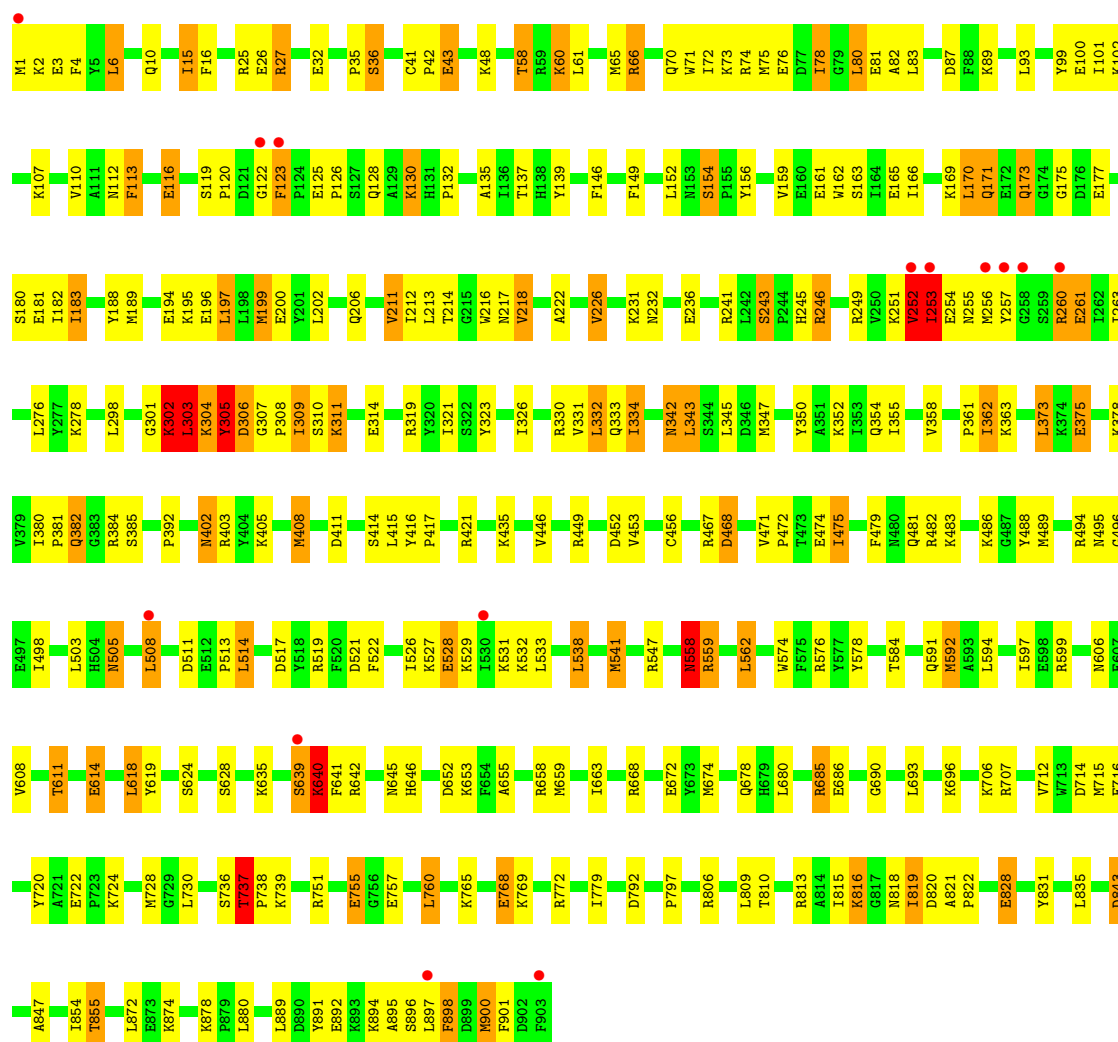
Chain A: 



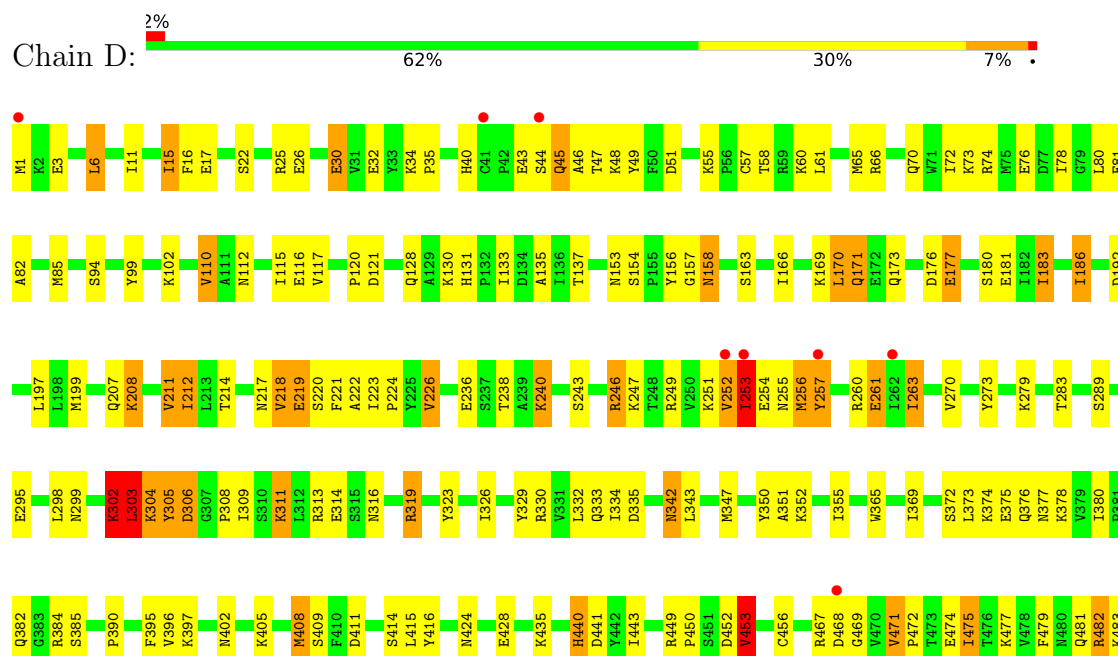


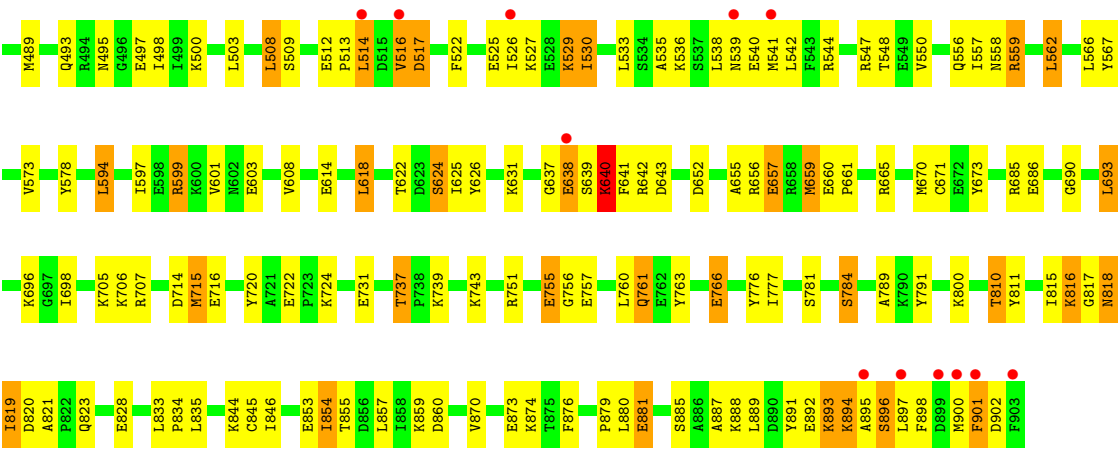
• Molecule 3: DNA polymerase





• Molecule 3: DNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.95Å 122.24Å 165.36Å 90.00° 96.85° 90.00°	Depositor
Resolution (Å)	47.00 – 2.69 47.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.7 (47.00-2.69) 95.1 (47.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.215 , 0.288 0.208 , 0.273	Depositor DCC
R_{free} test set	6757 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32756	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: 3DR, CA, DGP, DOC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	E	0.52	0/415	1.33	3/637 (0.5%)
1	F	0.50	0/415	1.23	2/637 (0.3%)
1	G	0.60	0/415	1.44	4/637 (0.6%)
1	H	0.62	0/415	1.24	2/637 (0.3%)
2	I	0.48	0/294	1.28	4/452 (0.9%)
2	J	0.51	0/294	1.31	3/452 (0.7%)
2	K	0.55	0/294	1.30	2/452 (0.4%)
2	L	0.55	0/294	1.32	1/452 (0.2%)
3	A	0.69	0/7545	1.01	10/10196 (0.1%)
3	B	0.74	2/7545 (0.0%)	1.02	13/10196 (0.1%)
3	C	0.79	3/7545 (0.0%)	1.06	12/10196 (0.1%)
3	D	0.72	2/7545 (0.0%)	1.01	8/10196 (0.1%)
All	All	0.72	7/33016 (0.0%)	1.06	64/45140 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	1
3	C	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	347	MET	SD-CE	8.32	2.00	1.79
3	C	1	MET	SD-CE	5.71	1.93	1.79
3	D	471	VAL	CA-CB	5.64	1.56	1.54
3	D	453	VAL	CA-CB	5.52	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	541	MET	SD-CE	-5.51	1.65	1.79
3	B	1	MET	SD-CE	5.42	1.93	1.79
3	C	489	MET	SD-CE	5.33	1.92	1.79

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	517	ASP	N-CA-C	9.44	124.42	109.50
3	C	211	VAL	N-CA-C	-9.27	102.86	111.67
1	G	911	DC	C1'-O4'-C4'	-8.49	96.96	109.70
3	B	897	LEU	N-CA-C	7.78	121.61	108.23
3	B	252	VAL	N-CA-C	7.70	118.44	108.12
3	B	253	ILE	N-CA-C	7.53	125.01	109.34
1	G	926	DC	P-O3'-C3'	7.31	131.16	120.20
3	A	261	GLU	N-CA-C	7.28	119.63	108.42
1	E	923	DC	P-O3'-C3'	6.71	130.26	120.20
1	F	924	DC	C4'-C3'-O3'	6.68	120.02	110.00
3	C	253	ILE	N-CA-C	6.67	123.22	109.34
3	B	74	ARG	N-CA-C	6.40	120.92	113.18
3	C	342	ASN	N-CA-C	6.37	119.04	111.33
1	H	911	DC	C1'-O4'-C4'	-6.23	100.35	109.70
3	A	451	SER	N-CA-C	6.19	118.58	108.55
3	B	648	VAL	N-CA-C	-6.19	104.47	110.72
2	L	945	DC	O5'-C5'-C4'	6.18	120.06	110.80
1	F	924	DC	P-O3'-C3'	6.15	129.42	120.20
3	C	456	CYS	N-CA-C	6.14	119.56	109.85
2	I	946	DT	N1-C1'-C2'	6.11	122.66	113.50
3	D	49	TYR	N-CA-C	6.04	118.37	108.52
3	C	592	MET	N-CA-C	-6.04	104.62	111.14
3	D	893	LYS	N-CA-C	-5.92	106.22	113.50
1	G	922	DT	N1-C1'-C2'	5.91	122.36	113.50
3	C	113	PHE	N-CA-C	5.90	118.14	109.24
3	A	837	GLU	N-CA-C	5.86	120.12	111.04
3	A	456	CYS	N-CA-C	5.82	119.05	109.85
3	B	380	ILE	N-CA-C	5.79	114.41	109.02
2	I	947	DG	P-O3'-C3'	5.79	128.88	120.20
1	H	917	DA	O3'-P-O5'	-5.75	95.38	104.00
2	J	944	DA	P-O3'-C3'	5.73	128.79	120.20
2	J	942	DG	P-O3'-C3'	5.72	128.78	120.20
3	A	302	LYS	N-CA-C	5.70	118.43	111.82
1	G	911	DC	O4'-C1'-N1	5.60	116.80	108.40
3	B	436	VAL	CB-CA-C	-5.50	104.01	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	255	ASN	N-CA-C	5.49	118.51	107.41
1	E	918	DG	O4'-C1'-N9	5.47	116.61	108.40
3	D	238	THR	N-CA-C	-5.46	107.17	113.88
3	A	536	LYS	N-CA-C	-5.45	108.41	114.62
3	B	113	PHE	N-CA-C	5.34	117.51	109.23
3	A	47	THR	CB-CA-C	-5.33	107.73	114.40
3	C	737	THR	CB-CA-C	5.33	116.09	108.68
3	D	211	VAL	N-CA-C	-5.32	106.98	111.56
2	I	946	DT	O4'-C1'-N1	-5.29	100.46	108.40
3	C	496	GLY	N-CA-C	-5.26	108.14	114.66
3	D	456	CYS	N-CA-C	5.22	118.08	109.72
3	C	712	VAL	N-CA-C	5.20	116.77	108.87
2	K	941	DC	P-O3'-C3'	5.19	127.99	120.20
2	J	943	DG	P-O3'-C3'	5.18	127.97	120.20
2	I	946	DT	P-O3'-C3'	5.17	127.96	120.20
3	B	771	PHE	N-CA-C	5.17	117.33	111.02
2	K	943	DG	O4'-C1'-N9	5.16	116.15	108.40
3	D	415	LEU	N-CA-C	5.15	117.56	111.33
3	C	468	ASP	N-CA-C	5.13	119.54	113.28
1	E	927	DG	P-O3'-C3'	5.12	127.88	120.20
3	C	474	GLU	N-CA-C	5.12	116.55	111.07
3	C	558	ASN	N-CA-CB	5.11	118.19	110.28
3	B	396	VAL	CA-C-N	-5.09	114.13	121.42
3	B	396	VAL	C-N-CA	-5.09	114.13	121.42
3	A	123	PHE	N-CA-C	-5.09	103.75	109.60
3	A	253	ILE	N-CA-C	5.04	117.65	110.09
3	D	342	ASN	N-CA-C	5.02	116.44	110.97
3	B	437	ALA	N-CA-C	-5.01	103.65	110.36
3	A	530	ILE	N-CA-C	-5.00	107.07	113.22

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	640	LYS	Peptide
3	C	252	VAL	Peptide

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	E	370	0	202	16	0
1	F	370	0	202	13	0
1	G	370	0	202	11	0
1	H	370	0	202	10	0
2	I	263	0	147	16	0
2	J	263	0	147	9	0
2	K	263	0	147	6	0
2	L	263	0	147	4	0
3	A	7365	0	7257	203	0
3	B	7365	0	7258	168	0
3	C	7365	0	7258	188	0
3	D	7365	0	7258	199	0
4	E	11	0	8	1	0
4	F	11	0	8	3	0
4	G	11	0	8	3	0
4	H	11	0	8	0	0
5	I	18	0	12	2	0
5	J	18	0	12	1	0
5	K	18	0	12	2	0
5	L	18	0	12	0	0
6	F	19	0	12	0	0
6	G	23	0	12	2	0
6	H	19	0	12	3	0
6	K	22	0	12	1	0
6	L	22	0	12	1	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
8	A	112	0	0	17	0
8	B	129	0	0	18	0
8	C	126	0	0	21	0
8	D	111	0	0	17	0
8	E	11	0	0	3	0
8	F	8	0	0	0	0
8	G	7	0	0	2	0
8	H	8	0	0	2	0
8	I	11	0	0	3	0
8	J	6	0	0	0	0
8	K	3	0	0	0	0
8	L	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	32756	0	30567	818	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 13.

All (818) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:253:ILE:HG22	3:A:261:GLU:HB3	1.28	1.13
3:C:171:GLN:NE2	3:C:177:GLU:HB2	1.66	1.10
3:C:89:LYS:HE2	3:C:354:GLN:HE22	1.13	1.06
3:C:514:LEU:H	3:C:541:MET:HE2	1.19	1.04
3:A:253:ILE:HG22	3:A:261:GLU:CB	1.91	1.01
3:C:171:GLN:HE22	3:C:177:GLU:HB2	0.86	1.01
3:B:897:LEU:HD21	3:B:899:ASP:HB3	1.42	1.00
3:C:898:PHE:O	3:C:898:PHE:HD1	1.45	0.99
3:B:897:LEU:HD22	3:B:899:ASP:H	1.21	0.99
3:D:513:PRO:HA	3:D:541:MET:HE2	1.42	0.98
3:C:302:LYS:O	3:C:303:LEU:HB2	1.63	0.98
3:C:171:GLN:HE22	3:C:177:GLU:CB	1.76	0.98
3:A:192:ASP:OD1	8:A:1101:HOH:O	1.82	0.97
3:C:639:SER:C	3:C:641:PHE:H	1.72	0.97
3:C:89:LYS:CE	3:C:354:GLN:HE22	1.78	0.96
2:K:951:DA:H2''	2:K:952:DC:H5'	1.48	0.95
3:D:639:SER:HA	8:D:1094:HOH:O	1.67	0.94
3:C:89:LYS:HE2	3:C:354:GLN:NE2	1.81	0.94
3:C:896:SER:O	3:C:898:PHE:N	2.00	0.94
3:C:408:MET:HE1	3:C:655:ALA:HB2	1.50	0.92
3:A:319:ARG:HG2	3:A:319:ARG:HH11	1.32	0.92
3:A:251:LYS:HB3	3:A:262:ILE:HD13	1.52	0.91
3:D:533:LEU:HD13	3:D:541:MET:HE1	1.49	0.91
3:D:408:MET:HE2	3:D:655:ALA:HB2	1.54	0.89
3:A:70:GLN:NE2	8:A:1104:HOH:O	2.06	0.89
3:C:639:SER:O	3:C:641:PHE:N	2.05	0.88
3:D:253:ILE:HG23	3:D:261:GLU:HB3	1.56	0.88
3:A:74:ARG:O	3:A:78:ILE:HG13	1.74	0.87
3:D:308:PRO:O	3:D:311:LYS:NZ	2.07	0.87
3:B:330:ARG:HH11	3:B:333:GLN:HE22	1.17	0.87
3:B:881:GLU:O	3:B:885:SER:HB2	1.75	0.86
3:A:642:ARG:H	3:A:646:HIS:HD2	1.24	0.86
3:A:731:GLU:O	3:A:737:THR:HG21	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:TYR:HD2	3:C:323:TYR:HE1	1.20	0.85
3:D:860:ASP:HB3	8:D:1070:HOH:O	1.74	0.85
3:C:305:TYR:HD2	3:C:323:TYR:CE1	1.95	0.85
3:D:640:LYS:HA	8:D:1116:HOH:O	1.76	0.83
3:B:81:GLU:HG3	3:B:384:ARG:NH2	1.94	0.83
3:B:428:GLU:OE2	3:B:469:GLY:HA2	1.78	0.83
3:D:253:ILE:CG2	3:D:261:GLU:HB3	2.08	0.83
3:D:533:LEU:CD1	3:D:541:MET:HE1	2.06	0.83
3:A:196:GLU:OE2	8:A:1101:HOH:O	1.96	0.83
3:A:639:SER:C	3:A:641:PHE:H	1.88	0.82
3:B:731:GLU:O	3:B:737:THR:HG21	1.79	0.82
3:A:899:ASP:O	3:A:900:MET:HB2	1.80	0.81
3:C:305:TYR:CD2	3:C:323:TYR:HE1	1.99	0.81
3:B:347:MET:SD	3:B:562:LEU:CD1	2.69	0.81
3:B:897:LEU:CD2	3:B:899:ASP:HB3	2.11	0.81
3:B:253:ILE:HB	3:B:255:ASN:HD22	1.45	0.80
3:C:305:TYR:HD1	3:C:306:ASP:N	1.80	0.80
3:D:170:LEU:HD23	3:D:173:GLN:HE22	1.45	0.80
3:A:736:SER:HA	3:A:782:VAL:HB	1.63	0.79
3:B:127:SER:HB3	3:B:259:SER:HB3	1.64	0.79
3:C:514:LEU:N	3:C:541:MET:HE2	1.97	0.79
3:B:251:LYS:HB3	3:B:262:ILE:HD13	1.64	0.78
1:G:926:DC:H2''	1:G:927:DG:O5'	1.82	0.78
3:C:898:PHE:O	3:C:898:PHE:CD1	2.33	0.78
3:C:828:GLU:HG2	8:C:1030:HOH:O	1.83	0.77
3:B:606:ASN:OD1	3:B:611:THR:HG22	1.84	0.77
3:D:183:ILE:HD11	8:D:1099:HOH:O	1.85	0.77
3:C:508:LEU:HD23	3:C:508:LEU:H	1.48	0.77
3:C:66:ARG:HD2	3:C:70:GLN:OE1	1.85	0.76
3:A:251:LYS:HB3	3:A:262:ILE:CD1	2.16	0.76
1:H:910:DA:H2''	1:H:911:DC:H5'	1.68	0.75
3:D:44:SER:O	3:D:46:ALA:N	2.19	0.75
3:C:27:ARG:HD3	8:C:1079:HOH:O	1.87	0.75
3:D:751:ARG:O	3:D:755:GLU:O	2.05	0.75
3:B:347:MET:SD	3:B:562:LEU:HD13	2.26	0.75
1:H:927:DG:C8	8:H:109:HOH:O	2.40	0.75
3:C:505:ASN:O	8:C:1110:HOH:O	2.05	0.74
3:A:253:ILE:CG2	3:A:261:GLU:HB3	2.15	0.74
3:C:896:SER:C	3:C:898:PHE:H	1.96	0.74
3:D:369:ILE:HG12	3:D:474:GLU:HG3	1.69	0.74
3:B:277:TYR:O	3:B:281:SER:HB3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:892:GLU:HB3	3:D:894:LYS:HG2	1.70	0.74
3:D:396:VAL:O	3:D:705:LYS:HD3	1.88	0.74
3:A:836:ARG:O	3:A:839:ASN:ND2	2.21	0.74
3:C:751:ARG:O	3:C:755:GLU:O	2.06	0.73
3:A:685:ARG:NH2	3:A:714:ASP:OD1	2.21	0.73
3:B:347:MET:SD	3:B:562:LEU:HD11	2.29	0.72
3:D:761:GLN:NE2	3:D:893:LYS:HB2	2.03	0.72
3:C:305:TYR:CD1	3:C:305:TYR:C	2.66	0.72
4:F:912:3DR:H5''	3:B:362:ILE:HD12	1.70	0.72
2:K:942:DG:H2''	2:K:943:DG:OP2	1.90	0.71
3:B:766:GLU:O	3:B:770:GLU:HG2	1.90	0.71
3:D:533:LEU:HD13	3:D:541:MET:CE	2.20	0.71
3:B:330:ARG:HH11	3:B:333:GLN:NE2	1.86	0.71
3:C:408:MET:CE	3:C:655:ALA:HB2	2.20	0.71
3:D:408:MET:CE	3:D:655:ALA:HB2	2.20	0.71
3:C:385:SER:HA	8:C:1047:HOH:O	1.90	0.71
3:D:731:GLU:O	3:D:737:THR:HG21	1.90	0.71
3:A:638:GLU:O	3:A:639:SER:HB3	1.90	0.70
3:C:41:CYS:HB3	3:C:58:THR:HG22	1.73	0.70
3:C:685:ARG:NH2	3:C:714:ASP:OD1	2.19	0.70
1:H:917:DA:H4'	3:D:707:ARG:HD2	1.72	0.70
3:A:170:LEU:O	3:A:173:GLN:NE2	2.24	0.70
3:C:517:ASP:HB3	8:C:1026:HOH:O	1.91	0.70
3:A:402:ASN:HD22	3:A:403:ARG:H	1.38	0.70
3:A:758:GLU:HG2	8:A:1103:HOH:O	1.90	0.70
3:B:163:SER:HA	8:B:1066:HOH:O	1.91	0.70
3:B:311:LYS:HG2	3:B:311:LYS:O	1.90	0.70
3:C:640:LYS:O	3:C:646:HIS:ND1	2.24	0.70
3:B:639:SER:O	3:B:641:PHE:N	2.25	0.69
3:B:640:LYS:O	3:B:640:LYS:HG2	1.90	0.69
3:B:115:ILE:HG22	3:B:136:ILE:HG12	1.75	0.69
3:C:183:ILE:HG13	8:C:1127:HOH:O	1.91	0.69
3:B:884:THR:HB	3:B:889:LEU:O	1.92	0.69
3:B:171:GLN:HE22	3:B:177:GLU:HB2	1.58	0.69
3:A:246:ARG:HG3	3:A:246:ARG:HH11	1.57	0.69
2:I:941:DC:H2''	2:I:942:DG:O5'	1.92	0.68
2:I:950:DT:OP1	3:A:783:SER:HA	1.93	0.68
3:A:262:ILE:HD12	3:A:262:ILE:H	1.59	0.68
3:C:82:ALA:O	3:C:382:GLN:HB2	1.92	0.68
3:B:766:GLU:HG3	8:B:1074:HOH:O	1.94	0.68
5:I:953:DOC:H2''	3:A:622:THR:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:251:LYS:HB3	3:B:262:ILE:CD1	2.23	0.67
3:B:252:VAL:HG12	3:B:253:ILE:HG12	1.75	0.67
3:C:303:LEU:HD11	3:C:326:ILE:HG21	1.76	0.67
3:D:304:LYS:O	3:D:305:TYR:HB3	1.93	0.67
3:B:639:SER:O	3:B:640:LYS:C	2.38	0.67
3:D:253:ILE:HD13	3:D:253:ILE:H	1.59	0.67
3:A:642:ARG:H	3:A:646:HIS:CD2	2.12	0.66
3:A:319:ARG:HG2	3:A:319:ARG:NH1	2.01	0.66
3:C:81:GLU:HG2	3:C:83:LEU:HG	1.77	0.66
3:D:395:PHE:O	8:D:1109:HOH:O	2.13	0.66
3:B:483:LYS:HB2	8:B:1086:HOH:O	1.94	0.66
3:D:514:LEU:HD11	3:D:529:LYS:HD3	1.76	0.66
3:D:652:ASP:CG	3:D:656:ARG:HH21	2.04	0.66
3:D:219:GLU:HG3	3:D:270:VAL:HG11	1.78	0.66
3:B:449:ARG:NH2	3:B:452:ASP:OD1	2.28	0.66
3:B:405:LYS:HG2	3:B:406:TYR:CE1	2.32	0.65
3:C:449:ARG:NH2	3:C:452:ASP:OD1	2.29	0.65
3:D:171:GLN:NE2	3:D:177:GLU:OE2	2.27	0.65
3:C:183:ILE:HB	8:C:1127:HOH:O	1.97	0.65
3:C:639:SER:C	3:C:641:PHE:N	2.39	0.65
2:I:952:DC:H2''	5:I:953:DOC:H5'	1.77	0.65
3:A:1:MET:HB3	8:A:1088:HOH:O	1.96	0.65
3:D:516:VAL:HG13	3:D:517:ASP:N	2.11	0.65
3:A:87:ASP:OD2	3:A:363:LYS:NZ	2.30	0.65
3:A:199:MET:HE3	3:A:199:MET:HA	1.78	0.65
3:A:347:MET:SD	3:A:562:LEU:HD13	2.37	0.65
3:A:639:SER:C	3:A:641:PHE:N	2.53	0.65
3:B:831:TYR:O	3:B:847:ALA:HA	1.96	0.64
3:D:390:PRO:HD2	8:D:1112:HOH:O	1.97	0.64
3:D:876:PHE:O	3:D:879:PRO:HD2	1.98	0.64
6:H:908:DGP:H2'	3:D:416:TYR:CD2	2.33	0.64
3:B:725:LEU:HD11	3:B:750:ARG:HB2	1.80	0.64
3:B:354:GLN:HG3	8:B:1065:HOH:O	1.96	0.64
3:C:305:TYR:HB3	3:C:323:TYR:OH	1.97	0.63
3:D:343:LEU:HD22	3:D:558:ASN:HB3	1.80	0.63
3:C:305:TYR:CD1	3:C:306:ASP:N	2.64	0.63
3:A:312:LEU:HD23	3:A:320:TYR:HD1	1.63	0.63
3:C:898:PHE:HB2	3:C:901:PHE:CD2	2.34	0.63
3:A:44:SER:C	3:A:46:ALA:H	2.07	0.63
3:C:533:LEU:HB2	3:C:538:LEU:HD13	1.80	0.63
3:D:652:ASP:OD2	3:D:656:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:206:GLN:OE1	3:B:246:ARG:NH2	2.30	0.62
3:B:271:LEU:HD21	3:B:356:GLN:HA	1.81	0.62
3:A:899:ASP:O	3:A:900:MET:CB	2.48	0.62
2:K:943:DG:H4'	2:K:944:DA:OP1	2.00	0.62
3:B:330:ARG:NH1	3:B:333:GLN:HE22	1.94	0.62
3:C:559:ARG:NH1	8:C:1096:HOH:O	2.33	0.62
3:D:11:ILE:HD12	3:D:16:PHE:CD2	2.35	0.62
3:D:898:PHE:CD1	3:D:898:PHE:C	2.78	0.62
3:C:206:GLN:OE1	3:C:246:ARG:NH2	2.33	0.61
3:A:298:LEU:HD11	3:A:333:GLN:HB3	1.82	0.61
1:E:917:DA:H1'	8:E:400:HOH:O	1.99	0.61
1:E:918:DG:H2''	1:E:919:DC:C6	2.35	0.61
3:A:199:MET:HA	3:A:199:MET:CE	2.30	0.61
3:C:183:ILE:CB	8:C:1127:HOH:O	2.46	0.61
3:D:516:VAL:HG13	3:D:517:ASP:H	1.64	0.61
3:D:898:PHE:CE1	3:D:900:MET:HG2	2.35	0.61
3:B:685:ARG:NH2	3:B:714:ASP:OD1	2.27	0.61
3:B:591:GLN:NE2	8:B:1017:HOH:O	2.30	0.61
3:C:373:LEU:HD23	3:C:380:ILE:HG22	1.83	0.61
1:H:916:DA:H5''	3:D:705:LYS:HD2	1.83	0.61
3:A:157:GLY:O	3:A:313:ARG:NH2	2.33	0.61
3:A:598:GLU:HG2	3:A:617:VAL:HG11	1.83	0.61
3:D:481:GLN:HE21	3:D:559:ARG:HD2	1.65	0.61
3:D:514:LEU:HD21	3:D:529:LYS:HB3	1.83	0.61
3:C:514:LEU:HD22	3:C:541:MET:HE1	1.81	0.61
3:D:776:TYR:OH	3:D:853:GLU:HB3	2.01	0.61
4:G:912:3DR:OP1	3:C:361:PRO:HD2	2.01	0.60
3:D:881:GLU:O	3:D:885:SER:HB2	2.00	0.60
3:C:252:VAL:C	3:C:253:ILE:HG13	2.25	0.60
3:D:535:ALA:O	3:D:539:ASN:ND2	2.33	0.60
3:A:212:ILE:HD11	3:A:345:LEU:HD21	1.83	0.60
3:A:314:GLU:HG3	8:A:1050:HOH:O	2.01	0.60
5:K:953:DOC:OP2	3:C:728:MET:HE2	2.01	0.60
3:B:247:LYS:HD3	3:B:266:PHE:CD1	2.36	0.60
3:B:604:TYR:OH	3:B:658:ARG:HB3	2.01	0.60
3:C:305:TYR:HD1	3:C:305:TYR:C	2.05	0.60
3:A:449:ARG:NH1	3:A:672:GLU:O	2.31	0.60
3:D:411:ASP:OD2	3:D:624:SER:HB3	2.02	0.60
3:D:685:ARG:HD3	8:D:1031:HOH:O	2.01	0.60
3:C:640:LYS:O	3:C:646:HIS:CE1	2.54	0.60
3:D:249:ARG:HD2	3:D:251:LYS:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:311:LYS:HZ2	3:B:311:LYS:H	1.49	0.59
3:D:326:ILE:O	3:D:330:ARG:HG2	2.02	0.59
3:C:218:VAL:HG23	3:C:222:ALA:HB3	1.83	0.59
3:D:637:GLY:O	3:D:639:SER:N	2.35	0.59
3:D:453:VAL:HA	8:D:1115:HOH:O	2.01	0.59
3:C:591:GLN:HG3	8:C:1121:HOH:O	2.02	0.59
3:D:516:VAL:HG11	3:D:526:ILE:HD13	1.84	0.59
1:G:918:DG:H2''	8:G:537:HOH:O	2.01	0.59
3:A:44:SER:O	3:A:46:ALA:N	2.34	0.59
3:C:375:GLU:O	3:C:375:GLU:HG3	2.01	0.59
3:B:81:GLU:HG3	3:B:384:ARG:HH21	1.66	0.59
3:A:298:LEU:HD11	3:A:333:GLN:CB	2.33	0.59
1:E:924:DC:H42	2:I:942:DG:H1	1.51	0.58
1:H:910:DA:H2''	1:H:911:DC:C5'	2.31	0.58
3:B:507:ASN:HB3	3:B:534:SER:HA	1.85	0.58
4:F:912:3DR:C5'	3:B:362:ILE:HD12	2.32	0.58
3:B:373:LEU:HD23	3:B:380:ILE:HG22	1.84	0.58
3:C:130:LYS:HG2	8:C:1043:HOH:O	2.03	0.58
3:C:797:PRO:HG2	3:C:806:ARG:NH1	2.18	0.58
3:A:330:ARG:HA	3:A:333:GLN:HE21	1.67	0.58
3:C:514:LEU:H	3:C:541:MET:CE	2.06	0.58
3:C:343:LEU:HD22	3:C:558:ASN:ND2	2.19	0.58
3:A:139:TYR:OH	3:A:144:ASP:OD1	2.17	0.58
3:B:85:MET:HA	3:B:380:ILE:HD11	1.85	0.58
3:C:166:ILE:O	3:C:175:GLY:HA2	2.03	0.58
3:A:533:LEU:HD22	3:A:537:SER:HB2	1.85	0.57
3:C:173:GLN:NE2	8:C:1091:HOH:O	1.93	0.57
3:B:226:VAL:HG23	3:B:242:LEU:HD11	1.87	0.57
1:F:927:DG:N1	2:J:940:DG:C6	2.72	0.57
3:B:894:LYS:HG3	3:B:897:LEU:HG	1.86	0.57
1:E:910:DA:H1'	1:E:911:DC:H5'	1.87	0.57
3:D:170:LEU:HB2	3:D:173:GLN:OE1	2.04	0.57
3:C:411:ASP:OD2	3:C:624:SER:OG	2.23	0.57
3:D:409:SER:OG	3:D:686:GLU:HB3	2.04	0.57
3:A:6:LEU:HG	3:A:211:VAL:HG21	1.86	0.56
3:C:449:ARG:NH1	3:C:672:GLU:O	2.36	0.56
3:D:302:LYS:O	3:D:303:LEU:HB2	2.05	0.56
2:J:942:DG:H2''	2:J:943:DG:OP2	2.05	0.56
3:A:402:ASN:ND2	3:A:403:ARG:H	2.01	0.56
3:B:369:ILE:HG22	3:B:373:LEU:HD22	1.86	0.56
1:F:927:DG:H2''	1:F:928:DG:O5'	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:262:ILE:HD12	3:B:262:ILE:H	1.71	0.56
3:B:308:PRO:HG2	3:B:820:ASP:OD2	2.05	0.56
3:B:422:GLN:HG3	3:B:678:GLN:O	2.06	0.56
3:B:897:LEU:HD23	8:B:1081:HOH:O	2.06	0.56
3:C:668:ARG:HD2	8:C:1027:HOH:O	2.05	0.56
3:D:82:ALA:O	3:D:382:GLN:HB2	2.05	0.56
3:A:609:CYS:HA	3:A:635:LYS:HE2	1.87	0.56
2:I:942:DG:H3'	8:I:53:HOH:O	2.06	0.56
1:H:927:DG:H8	8:H:109:HOH:O	1.82	0.56
3:A:253:ILE:HG22	3:A:261:GLU:HB2	1.83	0.56
3:A:402:ASN:HD22	3:A:403:ARG:N	2.04	0.56
3:D:176:ASP:OD1	3:D:319:ARG:HD3	2.06	0.56
3:A:805:ILE:HD13	3:A:808:ILE:HD12	1.88	0.55
3:C:216:TRP:O	3:C:217:ASN:HB2	2.05	0.55
1:E:916:DA:H5''	3:A:705:LYS:HD3	1.88	0.55
3:C:199:MET:HE1	3:C:241:ARG:HH21	1.70	0.55
3:D:319:ARG:NH1	3:D:323:TYR:OH	2.40	0.55
3:A:507:ASN:HB2	8:A:1098:HOH:O	2.06	0.55
3:A:898:PHE:O	3:A:899:ASP:CG	2.49	0.55
3:A:38:PHE:CE2	3:A:59:ARG:HG3	2.41	0.55
3:A:165:GLU:CD	3:A:165:GLU:H	2.15	0.55
3:B:330:ARG:HD3	3:B:333:GLN:NE2	2.21	0.55
3:D:513:PRO:CA	3:D:541:MET:HE2	2.27	0.55
3:A:777:ILE:CD1	3:A:848:TRP:HZ2	2.20	0.55
3:B:408:MET:HE1	3:B:655:ALA:HB2	1.89	0.55
1:E:911:DC:H2''	3:A:360:SER:OG	2.06	0.55
3:A:395:PHE:O	3:A:591:GLN:NE2	2.40	0.55
3:C:606:ASN:OD1	3:C:611:THR:HB	2.07	0.55
3:D:253:ILE:HG22	3:D:260:ARG:C	2.31	0.55
3:D:253:ILE:HG22	3:D:261:GLU:HB3	1.88	0.55
3:B:125:GLU:HA	3:B:125:GLU:OE1	2.07	0.55
3:D:6:LEU:HG	3:D:211:VAL:HG21	1.89	0.55
3:B:749:ILE:O	3:B:753:LEU:HG	2.07	0.55
3:C:15:ILE:HD12	3:C:65:MET:HE1	1.89	0.55
3:B:422:GLN:OE1	3:B:681:MET:HG2	2.06	0.55
3:C:6:LEU:HG	3:C:211:VAL:HG21	1.89	0.54
3:D:298:LEU:HD11	3:D:333:GLN:HB2	1.87	0.54
1:E:916:DA:H8	8:E:458:HOH:O	1.90	0.54
3:C:495:ASN:HD21	3:C:522:PHE:H	1.55	0.54
3:A:101:ILE:HG21	3:A:349:TYR:CD1	2.43	0.54
3:D:657:GLU:HG3	8:D:1079:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:638:GLU:N	3:B:638:GLU:OE1	2.40	0.54
3:B:381:PRO:O	3:B:576:ARG:HD3	2.08	0.54
3:C:199:MET:HE1	3:C:241:ARG:NH2	2.23	0.54
3:D:638:GLU:O	8:D:1094:HOH:O	2.18	0.53
3:A:222:ALA:O	3:A:226:VAL:HG13	2.07	0.53
3:C:173:GLN:O	3:C:173:GLN:HG2	2.07	0.53
2:J:942:DG:H1'	2:J:943:DG:C8	2.43	0.53
3:B:116:GLU:HB3	3:B:320:TYR:OH	2.09	0.53
3:C:112:ASN:HD22	3:C:214:THR:HG23	1.74	0.53
3:C:330:ARG:HH11	3:C:333:GLN:HE22	1.57	0.53
3:D:471:VAL:O	3:D:475:ILE:HG13	2.08	0.53
3:D:643:ASP:HA	3:D:693:LEU:HD12	1.89	0.53
3:A:391:TYR:HB2	3:A:392:PRO:HD2	1.90	0.53
3:C:305:TYR:HE1	3:C:307:GLY:O	1.91	0.53
3:A:652:ASP:OD2	3:A:656:ARG:NH2	2.29	0.53
3:B:605:LEU:HD22	3:B:632:ILE:HD11	1.91	0.53
3:C:183:ILE:CG1	8:C:1127:HOH:O	2.54	0.53
3:B:216:TRP:CH2	3:B:293:ILE:HG21	2.44	0.53
3:A:392:PRO:HD2	3:A:584:THR:HG23	1.91	0.53
1:E:916:DA:H2''	1:E:917:DA:C8	2.44	0.53
4:F:912:3DR:H5''	3:B:362:ILE:CD1	2.39	0.53
3:A:566:LEU:O	3:A:567:TYR:C	2.51	0.53
3:A:736:SER:CB	3:A:782:VAL:O	2.57	0.53
3:D:870:VAL:HG13	3:D:874:LYS:HD3	1.91	0.53
3:A:2:LYS:HD3	3:A:3:GLU:H	1.74	0.53
3:D:99:TYR:O	3:D:352:LYS:NZ	2.42	0.52
2:K:950:DT:H5''	3:C:736:SER:HB3	1.90	0.52
3:A:806:ARG:O	3:A:810:THR:HG22	2.09	0.52
3:C:222:ALA:O	3:C:226:VAL:HG13	2.09	0.52
1:F:924:DC:H42	2:J:942:DG:H1	1.57	0.52
3:B:47:THR:HB	8:B:1129:HOH:O	2.10	0.52
3:B:163:SER:HB2	3:B:165:GLU:HG2	1.92	0.52
3:B:165:GLU:H	3:B:165:GLU:CD	2.16	0.52
3:B:642:ARG:H	3:B:646:HIS:HD2	1.56	0.52
3:D:639:SER:C	3:D:641:PHE:H	2.18	0.52
3:A:881:GLU:O	3:A:885:SER:HB2	2.10	0.52
3:C:508:LEU:HD23	3:C:508:LEU:N	2.21	0.52
3:D:686:GLU:OE1	3:D:716:GLU:HG3	2.09	0.52
3:A:440:HIS:C	3:A:440:HIS:CD2	2.88	0.52
3:A:303:LEU:HD12	3:A:323:TYR:CE2	2.45	0.52
3:A:803:PHE:HE1	3:A:844:LYS:HE3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:330:ARG:HA	3:B:333:GLN:HE21	1.74	0.52
3:C:171:GLN:NE2	3:C:171:GLN:H	2.08	0.52
3:C:253:ILE:HG22	3:C:261:GLU:HB3	1.91	0.52
3:A:702:TRP:CZ3	3:A:710:LEU:HD21	2.45	0.52
3:B:166:ILE:O	3:B:166:ILE:HG22	2.09	0.52
3:B:749:ILE:HA	3:B:752:MET:HE3	1.90	0.52
3:C:818:ASN:ND2	3:C:821:ALA:HB2	2.25	0.52
3:D:218:VAL:HG13	3:D:223:ILE:CD1	2.40	0.52
3:D:731:GLU:O	3:D:737:THR:CG2	2.58	0.52
3:A:362:ILE:HD11	3:A:572:ASN:HB3	1.91	0.51
3:D:685:ARG:NH2	3:D:714:ASP:OD1	2.43	0.51
2:I:943:DG:C6	2:I:944:DA:C6	2.98	0.51
3:D:533:LEU:HD11	3:D:541:MET:HE1	1.92	0.51
3:B:44:SER:C	3:B:46:ALA:H	2.19	0.51
3:C:304:LYS:N	8:C:1118:HOH:O	2.44	0.51
3:C:343:LEU:HD22	3:C:558:ASN:HD22	1.76	0.51
3:C:479:PHE:HD2	8:C:1017:HOH:O	1.93	0.51
3:D:40:HIS:CE1	3:D:51:ASP:OD2	2.63	0.51
3:D:671:CYS:HB2	8:D:1012:HOH:O	2.11	0.51
3:D:898:PHE:HE1	3:D:900:MET:HG2	1.73	0.51
3:D:893:LYS:O	3:D:896:SER:HB2	2.11	0.51
3:D:573:VAL:HG22	8:D:1035:HOH:O	2.11	0.51
3:A:591:GLN:OE1	3:A:591:GLN:HA	2.10	0.51
3:A:417:PRO:HA	3:A:420:ILE:HD12	1.92	0.51
3:B:652:ASP:OD1	3:B:685:ARG:NH1	2.44	0.51
3:D:816:LYS:O	3:D:818:ASN:N	2.41	0.51
3:C:707:ARG:HG2	3:C:730:LEU:HD23	1.92	0.51
2:I:950:DT:OP2	3:A:784:SER:HB2	2.10	0.50
3:C:611:THR:HG21	3:C:614:GLU:HB2	1.92	0.50
3:D:428:GLU:OE1	3:D:428:GLU:N	2.34	0.50
2:J:951:DA:H5'	3:B:734:LYS:HG2	1.93	0.50
3:A:170:LEU:N	3:A:173:GLN:NE2	2.59	0.50
3:A:629:ALA:HA	3:A:632:ILE:HD12	1.94	0.50
3:A:236:GLU:O	3:A:240:LYS:HG2	2.11	0.50
3:A:355:ILE:O	3:A:358:VAL:HG13	2.11	0.50
3:A:898:PHE:CD1	3:A:898:PHE:N	2.79	0.50
3:D:212:ILE:HD11	3:D:355:ILE:HG21	1.93	0.50
3:A:369:ILE:HG12	3:A:474:GLU:HG3	1.92	0.50
3:C:813:ARG:O	3:C:816:LYS:HB2	2.11	0.50
3:D:639:SER:CA	8:D:1094:HOH:O	2.41	0.50
3:D:757:GLU:HG3	3:D:889:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:921:DG:N2	8:E:225:HOH:O	2.44	0.50
3:B:483:LYS:HE2	8:B:1086:HOH:O	2.11	0.50
3:B:734:LYS:O	3:B:737:THR:HG23	2.11	0.50
3:C:488:TYR:HB3	3:C:519:ARG:HG2	1.94	0.50
3:D:94:SER:OG	3:D:374:LYS:HE3	2.11	0.50
1:G:918:DG:OP1	3:C:707:ARG:NH1	2.45	0.50
2:K:946:DT:H2''	2:K:947:DG:C8	2.46	0.50
3:A:303:LEU:HD21	3:A:330:ARG:HE	1.76	0.50
3:A:699:GLY:C	3:A:753:LEU:HD22	2.37	0.50
3:C:822:PRO:HD2	3:C:855:THR:HG23	1.93	0.50
2:I:945:DC:H4'	8:I:105:HOH:O	2.11	0.50
3:A:703:THR:HG21	3:A:707:ARG:CZ	2.41	0.50
3:B:592:MET:HE3	3:B:670:MET:SD	2.52	0.50
1:G:920:DA:OP2	8:G:443:HOH:O	2.19	0.49
3:C:513:PRO:HA	3:C:541:MET:HE2	1.94	0.49
1:E:916:DA:H5''	3:A:705:LYS:CD	2.41	0.49
3:B:236:GLU:O	3:B:240:LYS:HG2	2.12	0.49
3:C:146:PHE:CE1	3:C:182:ILE:HB	2.46	0.49
3:D:761:GLN:HG3	3:D:891:TYR:O	2.11	0.49
2:L:946:DT:H2''	2:L:947:DG:OP2	2.11	0.49
3:A:681:MET:HE2	3:A:681:MET:HA	1.93	0.49
3:A:840:PRO:HD3	3:A:865:TRP:NE1	2.27	0.49
3:B:312:LEU:HG	3:B:312:LEU:O	2.13	0.49
3:A:303:LEU:HD11	3:A:326:ILE:HG21	1.94	0.49
3:A:402:ASN:ND2	3:A:403:ARG:N	2.59	0.49
3:A:408:MET:HE2	3:A:685:ARG:HD2	1.94	0.49
3:A:740:ALA:HB3	3:A:779:ILE:HG22	1.94	0.49
3:D:469:GLY:C	3:D:472:PRO:HD2	2.38	0.49
2:K:951:DA:H2''	2:K:952:DC:C5'	2.31	0.49
3:A:273:TYR:OH	3:A:340:PHE:HB2	2.13	0.49
3:A:481:GLN:HB3	3:A:559:ARG:HD2	1.95	0.49
3:A:663:ILE:HG21	3:A:683:MET:HB3	1.95	0.49
3:B:16:PHE:HB3	3:B:245:HIS:CE1	2.47	0.49
3:C:99:TYR:O	3:C:352:LYS:NZ	2.43	0.49
3:C:308:PRO:O	3:C:310:SER:N	2.45	0.49
3:C:686:GLU:OE1	3:C:716:GLU:CD	2.55	0.49
3:A:640:LYS:O	3:A:646:HIS:CD2	2.66	0.49
3:A:831:TYR:O	3:A:847:ALA:HA	2.13	0.49
3:A:806:ARG:NH2	8:A:1096:HOH:O	2.45	0.49
3:D:405:LYS:O	3:D:690:GLY:HA2	2.13	0.49
3:A:420:ILE:HA	3:A:425:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:768:GLU:HG2	3:A:872:LEU:HD21	1.94	0.49
3:B:513:PRO:HG3	3:B:537:SER:HA	1.94	0.49
3:A:262:ILE:CD1	3:A:262:ILE:H	2.19	0.49
3:A:648:VAL:HG13	3:A:688:ILE:HG21	1.95	0.49
3:C:645:ASN:HB2	8:C:1013:HOH:O	2.12	0.49
3:D:117:VAL:HG22	3:D:133:ILE:HA	1.94	0.49
3:D:517:ASP:HB3	8:D:1018:HOH:O	2.12	0.49
1:F:910:DA:H2''	1:F:911:DC:H5'	1.95	0.48
1:G:910:DA:H1'	3:C:574:TRP:CD2	2.48	0.48
3:A:468:ASP:HB3	3:A:677:LYS:HZ3	1.78	0.48
3:D:15:ILE:HD12	3:D:65:MET:HE1	1.95	0.48
1:E:920:DA:C5	1:E:921:DG:N7	2.81	0.48
1:G:918:DG:OP1	3:C:707:ARG:CZ	2.61	0.48
2:L:950:DT:OP2	3:D:784:SER:HB2	2.12	0.48
3:A:246:ARG:HG3	3:A:246:ARG:NH1	2.25	0.48
3:A:262:ILE:HD12	3:A:262:ILE:N	2.28	0.48
3:D:218:VAL:HG13	3:D:223:ILE:HD11	1.93	0.48
1:F:917:DA:H2'	1:F:918:DG:C8	2.47	0.48
3:A:373:LEU:HD23	3:A:380:ILE:HG22	1.95	0.48
3:B:207:GLN:HG2	8:B:1021:HOH:O	2.13	0.48
3:D:110:VAL:HB	3:D:212:ILE:HB	1.95	0.48
2:I:941:DC:C2'	2:I:942:DG:O5'	2.60	0.48
3:A:727:ILE:HG23	3:A:730:LEU:HD12	1.96	0.48
3:C:218:VAL:CG2	3:C:222:ALA:HB3	2.43	0.48
3:D:116:GLU:HB2	3:D:135:ALA:HB3	1.96	0.48
3:D:319:ARG:HG3	3:D:323:TYR:CZ	2.48	0.48
3:D:343:LEU:HD21	3:D:557:ILE:HG22	1.95	0.48
3:D:639:SER:C	3:D:641:PHE:N	2.66	0.48
3:D:273:TYR:OH	3:D:335:ASP:HA	2.14	0.48
3:D:655:ALA:HA	3:D:659:MET:HB2	1.95	0.48
3:A:250:VAL:HG22	3:A:263:ILE:HD12	1.94	0.48
3:B:171:GLN:CD	3:B:171:GLN:H	2.20	0.48
3:D:343:LEU:CD2	3:D:558:ASN:HB3	2.42	0.48
3:A:369:ILE:HG22	3:A:373:LEU:HD22	1.96	0.48
3:A:414:SER:O	3:A:415:LEU:C	2.56	0.48
3:C:308:PRO:HG2	3:C:311:LYS:HZ3	1.78	0.48
3:A:196:GLU:CD	8:A:1101:HOH:O	2.52	0.48
3:A:455:SER:OG	3:A:676:ASN:HA	2.14	0.48
3:A:641:PHE:HA	3:A:646:HIS:CD2	2.49	0.48
3:B:50:PHE:O	3:B:379:VAL:N	2.47	0.48
3:C:171:GLN:H	3:C:171:GLN:HE21	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:GLN:HA	8:C:1048:HOH:O	2.12	0.48
3:D:516:VAL:CG1	3:D:517:ASP:N	2.76	0.48
3:A:66:ARG:O	3:A:70:GLN:HG3	2.14	0.48
3:A:181:GLU:CD	3:A:181:GLU:H	2.22	0.48
3:B:200:GLU:OE2	3:B:200:GLU:HA	2.14	0.48
3:C:792:ASP:HB2	3:C:809:LEU:HD21	1.96	0.48
6:G:908:DGP:H2'	3:C:416:TYR:CD2	2.49	0.47
3:B:643:ASP:HA	3:B:693:LEU:HD12	1.95	0.47
3:B:772:ARG:HG3	8:B:1007:HOH:O	2.13	0.47
3:D:153:ASN:ND2	3:D:158:ASN:OD1	2.41	0.47
3:D:257:TYR:CE1	3:D:789:ALA:HB1	2.50	0.47
6:H:908:DGP:H2'	3:D:416:TYR:CG	2.50	0.47
3:B:11:ILE:HG12	3:B:247:LYS:HD2	1.97	0.47
3:D:302:LYS:O	3:D:303:LEU:CB	2.61	0.47
1:E:926:DC:C2	1:E:927:DG:C8	3.02	0.47
3:A:361:PRO:HB3	3:A:565:SER:HB2	1.97	0.47
3:D:263:ILE:O	3:D:263:ILE:HG22	2.13	0.47
3:A:806:ARG:HB3	3:A:845:CYS:SG	2.55	0.47
3:A:791:TYR:CE1	3:A:802:PRO:HD3	2.49	0.47
3:C:513:PRO:HA	3:C:541:MET:CE	2.44	0.47
3:B:391:TYR:HB2	3:B:392:PRO:HD2	1.97	0.47
3:C:152:LEU:HD22	3:C:159:VAL:O	2.15	0.47
3:D:311:LYS:N	3:D:311:LYS:HZ2	2.13	0.47
3:D:376:GLN:O	3:D:377:ASN:HB2	2.14	0.47
3:D:559:ARG:HA	3:D:559:ARG:HD3	1.66	0.47
3:D:898:PHE:C	3:D:898:PHE:HD1	2.23	0.47
1:F:925:DG:H2''	1:F:926:DC:OP2	2.15	0.47
1:G:911:DC:H4'	4:G:912:3DR:OP2	2.14	0.47
1:H:910:DA:C2'	1:H:911:DC:H5'	2.43	0.47
1:H:923:DC:H2''	1:H:924:DC:H5'	1.96	0.47
3:A:199:MET:HE3	3:A:199:MET:CA	2.44	0.47
3:A:518:TYR:HB3	8:A:1065:HOH:O	2.15	0.47
3:A:592:MET:HE2	3:A:592:MET:HB3	1.73	0.47
3:A:777:ILE:HD12	3:A:848:TRP:HZ2	1.78	0.47
3:B:262:ILE:CD1	3:B:262:ILE:H	2.26	0.47
3:B:679:HIS:HD2	8:B:1119:HOH:O	1.96	0.47
3:C:16:PHE:HB3	3:C:245:HIS:CE1	2.50	0.47
3:D:166:ILE:HA	3:D:169:LYS:HD2	1.96	0.47
3:A:736:SER:HB3	3:A:782:VAL:O	2.15	0.47
3:B:397:LYS:HE3	8:B:1121:HOH:O	2.15	0.47
3:B:489:MET:O	3:B:493:GLN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:392:PRO:HD2	3:C:584:THR:HG23	1.97	0.47
3:C:738:PRO:HB3	3:C:779:ILE:HA	1.97	0.47
3:A:744:ALA:HB2	3:A:767:PHE:CE2	2.49	0.47
3:C:162:TRP:HB3	3:C:188:TYR:CZ	2.50	0.47
3:D:157:GLY:O	3:D:313:ARG:NH2	2.46	0.47
3:D:639:SER:O	3:D:641:PHE:N	2.47	0.47
3:B:835:LEU:HB3	3:B:839:ASN:ND2	2.29	0.47
3:D:698:ILE:HD13	3:D:887:ALA:HB1	1.96	0.47
3:A:492:ALA:HA	8:A:1065:HOH:O	2.15	0.46
3:A:132:PRO:HD2	8:A:1074:HOH:O	2.15	0.46
3:B:420:ILE:HG21	3:B:475:ILE:HD11	1.97	0.46
3:C:162:TRP:CD1	3:C:321:ILE:HB	2.51	0.46
3:D:715:MET:HE3	3:D:715:MET:HB2	1.91	0.46
3:C:652:ASP:OD1	3:C:685:ARG:NH1	2.47	0.46
3:D:895:ALA:O	3:D:896:SER:C	2.58	0.46
3:B:311:LYS:HZ2	3:B:311:LYS:N	2.13	0.46
3:C:355:ILE:O	3:C:358:VAL:HG13	2.14	0.46
3:D:85:MET:HA	3:D:380:ILE:HD11	1.97	0.46
3:D:411:ASP:OD2	3:D:624:SER:CB	2.63	0.46
2:I:951:DA:H3'	8:I:3:HOH:O	2.15	0.46
3:B:897:LEU:HD23	3:B:897:LEU:HA	1.51	0.46
3:C:472:PRO:HA	3:C:475:ILE:HD11	1.98	0.46
2:L:948:DC:OP1	3:D:791:TYR:OH	2.32	0.46
3:B:150:ASP:O	3:B:190:PRO:HA	2.16	0.46
3:A:901:PHE:O	3:A:902:ASP:CB	2.63	0.46
3:C:343:LEU:CD2	3:C:558:ASN:ND2	2.79	0.46
3:D:308:PRO:HD2	3:D:311:LYS:HE2	1.97	0.46
3:D:599:ARG:HD2	3:D:603:GLU:OE2	2.15	0.46
4:E:912:3DR:P	3:A:361:PRO:HD2	2.55	0.46
3:B:253:ILE:HD12	3:B:255:ASN:HB2	1.97	0.46
3:B:394:ALA:C	3:B:591:GLN:OE1	2.59	0.46
3:B:790:LYS:N	8:B:1075:HOH:O	2.47	0.46
3:C:720:TYR:HB3	3:C:722:GLU:O	2.16	0.46
3:D:365:TRP:CE2	3:D:566:LEU:HD13	2.51	0.46
3:D:514:LEU:H	3:D:541:MET:HE2	1.81	0.46
1:G:915:DT:O2	3:C:706:LYS:HE3	2.15	0.46
3:A:153:ASN:HD22	3:A:158:ASN:ND2	2.13	0.46
3:A:819:ILE:H	3:A:819:ILE:HG12	1.43	0.46
3:B:238:THR:O	3:B:241:ARG:HB2	2.16	0.45
3:C:169:LYS:C	3:C:175:GLY:HA3	2.40	0.45
3:D:222:ALA:O	3:D:226:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ILE:HG22	3:C:80:LEU:HB2	1.97	0.45
3:D:221:PHE:O	3:D:224:PRO:HG2	2.17	0.45
3:D:495:ASN:HA	3:D:498:ILE:HD12	1.98	0.45
3:D:819:ILE:O	3:D:821:ALA:N	2.36	0.45
3:A:819:ILE:C	3:A:821:ALA:H	2.23	0.45
3:B:113:PHE:CE1	3:B:218:VAL:HG22	2.52	0.45
3:B:641:PHE:HA	3:B:646:HIS:CD2	2.52	0.45
3:D:121:ASP:HA	3:D:819:ILE:HG21	1.98	0.45
3:D:901:PHE:O	3:D:902:ASP:C	2.58	0.45
2:I:946:DT:H1'	2:I:947:DG:H5'	1.99	0.45
3:C:416:TYR:O	3:C:417:PRO:C	2.60	0.45
3:A:121:ASP:HB2	3:A:122:GLY:H	1.59	0.45
3:A:900:MET:HB2	3:A:900:MET:HE2	1.85	0.45
3:D:329:TYR:O	3:D:333:GLN:HG3	2.16	0.45
3:B:606:ASN:OD1	3:B:611:THR:CG2	2.61	0.45
3:D:350:TYR:OH	3:D:481:GLN:NE2	2.31	0.45
4:G:912:3DR:O5'	3:C:362:ILE:HD12	2.17	0.45
3:A:70:GLN:O	3:A:74:ARG:HG3	2.16	0.45
3:A:192:ASP:CG	8:A:1101:HOH:O	2.49	0.45
3:A:408:MET:HE3	3:A:688:ILE:HG12	1.98	0.45
3:D:16:PHE:CE1	3:D:30:GLU:HG3	2.52	0.45
3:D:896:SER:C	3:D:898:PHE:H	2.24	0.45
3:A:902:ASP:O	3:A:903:PHE:CB	2.64	0.45
3:D:471:VAL:HB	3:D:472:PRO:HD3	1.98	0.45
3:D:870:VAL:CG1	3:D:874:LYS:HD3	2.46	0.45
1:G:917:DA:H4'	3:C:707:ARG:HD2	1.99	0.45
3:A:71:TRP:CZ2	3:A:75:MET:HE2	2.52	0.45
3:C:132:PRO:HA	3:C:194:GLU:OE1	2.17	0.45
3:A:127:SER:OG	3:A:259:SER:O	2.34	0.45
3:A:506:PRO:HB2	3:A:507:ASN:H	1.59	0.45
3:B:455:SER:OG	3:B:676:ASN:HA	2.17	0.45
1:F:925:DG:C5	1:F:926:DC:C4	3.05	0.44
3:A:703:THR:HG21	3:A:707:ARG:NH1	2.32	0.44
3:A:731:GLU:O	3:A:737:THR:CG2	2.58	0.44
3:C:113:PHE:HB2	3:C:137:THR:O	2.17	0.44
3:D:223:ILE:N	3:D:224:PRO:HD2	2.32	0.44
3:D:720:TYR:CZ	3:D:724:LYS:HD2	2.51	0.44
3:B:810:THR:HG21	3:B:845:CYS:O	2.17	0.44
3:C:421:ARG:HG3	3:C:475:ILE:HD13	1.99	0.44
3:D:40:HIS:HE1	3:D:51:ASP:OD2	2.00	0.44
3:A:647:TRP:O	3:A:650:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:171:GLN:OE1	3:B:177:GLU:HG3	2.17	0.44
3:B:408:MET:HE2	3:B:408:MET:HB3	1.79	0.44
3:C:659:MET:O	3:C:663:ILE:HG13	2.17	0.44
3:D:115:ILE:HD12	3:D:117:VAL:HG23	1.99	0.44
3:D:449:ARG:NH2	3:D:452:ASP:OD1	2.50	0.44
2:I:952:DC:OP1	3:A:728:MET:HE3	2.18	0.44
3:B:253:ILE:CB	3:B:255:ASN:HD22	2.24	0.44
3:B:483:LYS:HB2	3:B:483:LYS:HE2	1.89	0.44
3:B:491:ALA:HA	3:B:494:ARG:HH12	1.81	0.44
3:B:731:GLU:O	3:B:737:THR:CG2	2.60	0.44
3:C:87:ASP:OD1	3:C:87:ASP:C	2.61	0.44
3:C:149:PHE:CD1	3:C:149:PHE:N	2.86	0.44
3:C:402:ASN:HD22	3:C:403:ARG:H	1.65	0.44
3:C:831:TYR:O	3:C:847:ALA:HA	2.17	0.44
1:E:917:DA:H2''	1:E:918:DG:O5'	2.18	0.44
3:A:864:HIS:HD2	3:A:865:TRP:CD1	2.36	0.44
3:B:125:GLU:HA	3:B:126:PRO:HD3	1.83	0.44
3:B:166:ILE:O	3:B:175:GLY:HA2	2.17	0.44
3:C:639:SER:O	3:C:640:LYS:C	2.60	0.44
1:F:926:DC:H2''	1:F:927:DG:OP2	2.17	0.44
3:A:354:GLN:O	3:A:355:ILE:C	2.59	0.44
3:A:505:ASN:HA	3:A:506:PRO:HD3	1.80	0.44
3:C:42:PRO:HG3	8:C:1045:HOH:O	2.17	0.44
3:D:256:MET:HE2	3:D:256:MET:HB2	1.94	0.44
1:F:926:DC:H6	1:F:926:DC:H2'	1.51	0.44
6:H:908:DGP:H8	3:D:567:TYR:CD2	2.52	0.44
3:B:819:ILE:C	3:B:821:ALA:H	2.26	0.44
3:C:528:GLU:HG3	8:C:1064:HOH:O	2.16	0.44
3:C:170:LEU:O	3:C:173:GLN:OE1	2.36	0.44
3:C:305:TYR:CE1	3:C:307:GLY:O	2.71	0.44
3:C:685:ARG:HG2	3:C:686:GLU:N	2.32	0.44
3:A:38:PHE:CZ	3:A:59:ARG:HG3	2.53	0.44
3:A:223:ILE:N	3:A:224:PRO:HD2	2.33	0.44
3:B:153:ASN:HD22	3:B:158:ASN:CG	2.26	0.44
3:B:494:ARG:O	3:B:494:ARG:HG2	2.18	0.44
2:J:943:DG:H2''	2:J:944:DA:C8	2.53	0.43
3:A:230:ILE:HG22	3:A:239:ALA:HB2	1.99	0.43
3:B:535:ALA:O	3:B:539:ASN:HB2	2.18	0.43
3:B:848:TRP:CG	3:B:854:ILE:HG23	2.53	0.43
3:C:347:MET:HE1	3:C:562:LEU:HD22	2.00	0.43
3:C:414:SER:O	3:C:415:LEU:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:942:DG:H2''	2:I:943:DG:OP2	2.18	0.43
3:A:658:ARG:C	3:A:661:PRO:HD2	2.43	0.43
3:C:819:ILE:H	3:C:819:ILE:HG12	1.51	0.43
3:D:94:SER:OG	3:D:374:LYS:CE	2.66	0.43
3:D:594:LEU:HD21	3:D:625:ILE:HG23	2.00	0.43
3:D:891:TYR:CE2	3:D:892:GLU:HG2	2.52	0.43
3:D:894:LYS:C	3:D:896:SER:H	2.25	0.43
3:A:414:SER:O	3:A:417:PRO:HD2	2.17	0.43
3:B:151:LEU:O	3:B:313:ARG:NH1	2.51	0.43
3:D:475:ILE:HG13	3:D:475:ILE:H	1.63	0.43
3:D:482:ARG:HD3	8:D:1088:HOH:O	2.18	0.43
3:C:306:ASP:HB2	8:C:1011:HOH:O	2.19	0.43
3:C:618:LEU:HD22	3:C:619:TYR:HB3	2.00	0.43
3:C:678:GLN:HG2	3:C:680:LEU:HG	2.00	0.43
3:D:47:THR:HG21	3:D:57:CYS:O	2.18	0.43
3:C:71:TRP:CZ2	3:C:75:MET:HE2	2.53	0.43
3:C:251:LYS:O	3:C:253:ILE:N	2.48	0.43
3:C:405:LYS:O	3:C:690:GLY:HA2	2.18	0.43
3:D:597:ILE:O	3:D:601:VAL:HG23	2.18	0.43
3:B:138:HIS:CD2	3:B:204:PHE:HE2	2.36	0.43
3:C:35:PRO:CG	3:C:65:MET:HG2	2.49	0.43
3:D:183:ILE:HA	3:D:186:ILE:HG13	2.00	0.43
3:D:424:ASN:OD1	3:D:468:ASP:O	2.35	0.43
3:D:578:TYR:CD1	3:D:578:TYR:C	2.96	0.43
3:D:761:GLN:CD	3:D:893:LYS:HB2	2.44	0.43
3:D:876:PHE:C	3:D:879:PRO:HD2	2.42	0.43
1:H:927:DG:H2''	6:L:955:DGP:N1	2.34	0.43
2:L:941:DC:H2''	2:L:942:DG:C8	2.53	0.43
3:B:251:LYS:HA	8:B:1131:HOH:O	2.17	0.43
3:B:522:PHE:HD1	3:B:522:PHE:HA	1.77	0.43
3:B:639:SER:C	3:B:641:PHE:N	2.77	0.43
3:B:706:LYS:O	3:B:729:GLY:HA3	2.18	0.43
3:C:381:PRO:O	3:C:576:ARG:HD3	2.19	0.43
3:C:592:MET:HE1	3:C:674:MET:HG3	2.00	0.43
3:D:351:ALA:O	3:D:352:LYS:HB2	2.19	0.43
3:D:482:ARG:HE	3:D:556:GLN:HE21	1.66	0.43
3:D:618:LEU:HB2	3:D:626:TYR:O	2.17	0.43
3:A:582:ASN:O	3:A:585:ALA:HB3	2.19	0.43
3:D:218:VAL:CG1	3:D:223:ILE:HD11	2.49	0.43
3:D:901:PHE:HD1	3:D:902:ASP:H	1.66	0.43
3:B:224:PRO:O	3:B:228:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:495:ASN:HD21	3:D:522:PHE:H	1.67	0.43
3:D:508:LEU:HD12	3:D:508:LEU:H	1.82	0.43
3:D:670:MET:O	3:D:673:TYR:HB3	2.19	0.43
3:B:475:ILE:HG23	3:B:566:LEU:HD22	2.01	0.43
3:B:737:THR:HA	3:B:738:PRO:HD3	1.95	0.43
3:C:533:LEU:HB2	3:C:538:LEU:CD1	2.47	0.43
3:D:131:HIS:HD2	3:D:156:TYR:CE2	2.37	0.43
3:D:525:GLU:O	3:D:529:LYS:HB2	2.19	0.43
1:E:927:DG:H1'	2:I:940:DG:N2	2.34	0.42
1:F:916:DA:H5''	3:B:705:LYS:HD3	1.99	0.42
3:A:125:GLU:HA	3:A:126:PRO:HD3	1.87	0.42
3:A:507:ASN:HB3	3:A:535:ALA:H	1.83	0.42
3:A:549:GLU:O	3:A:553:MET:HB2	2.19	0.42
3:A:618:LEU:HD13	3:A:626:TYR:O	2.19	0.42
3:B:3:GLU:H	3:B:3:GLU:HG2	1.62	0.42
3:B:166:ILE:O	3:B:166:ILE:CG2	2.67	0.42
3:C:36:SER:HA	3:C:60:LYS:O	2.19	0.42
3:C:330:ARG:O	3:C:334:ILE:HD12	2.19	0.42
3:D:540:GLU:HB2	8:D:1095:HOH:O	2.17	0.42
3:D:594:LEU:CD2	3:D:625:ILE:HG23	2.49	0.42
2:J:943:DG:H4'	2:J:944:DA:OP1	2.18	0.42
3:A:214:THR:OG1	3:A:215:GLY:N	2.51	0.42
3:B:707:ARG:HH22	3:B:731:GLU:CD	2.27	0.42
3:A:90:LEU:O	3:A:94:SER:HB2	2.19	0.42
3:A:104:ASP:OD1	3:A:104:ASP:C	2.61	0.42
3:A:806:ARG:O	3:A:810:THR:CG2	2.68	0.42
3:A:831:TYR:N	3:A:848:TRP:O	2.44	0.42
3:A:836:ARG:HD3	3:A:865:TRP:HE3	1.83	0.42
3:B:803:PHE:CE1	3:B:844:LYS:HE3	2.53	0.42
3:C:15:ILE:HD12	3:C:65:MET:CE	2.49	0.42
3:D:15:ILE:HD12	3:D:65:MET:CE	2.48	0.42
3:D:304:LYS:O	3:D:305:TYR:CB	2.65	0.42
3:D:347:MET:HE1	3:D:562:LEU:HD13	2.01	0.42
1:F:925:DG:C6	1:F:926:DC:N3	2.88	0.42
1:G:927:DG:C2	6:K:955:DGP:H1'	2.53	0.42
3:A:478:VAL:HG13	3:A:559:ARG:HD3	2.00	0.42
3:A:836:ARG:HD3	3:A:865:TRP:CE3	2.53	0.42
3:C:494:ARG:NH1	3:C:521:ASP:OD2	2.53	0.42
3:D:854:ILE:H	3:D:854:ILE:HG12	1.54	0.42
3:A:779:ILE:O	3:A:779:ILE:HG13	2.19	0.42
3:B:33:TYR:O	3:B:35:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:737:THR:HA	3:C:738:PRO:HD3	1.87	0.42
3:D:35:PRO:HG3	3:D:65:MET:HG2	2.00	0.42
3:D:376:GLN:HB3	3:D:378:LYS:HG2	2.01	0.42
1:H:915:DT:O2	3:D:706:LYS:HE3	2.20	0.42
3:A:90:LEU:HD11	3:A:363:LYS:HD2	2.02	0.42
3:A:170:LEU:C	3:A:173:GLN:HE21	2.27	0.42
3:C:125:GLU:HA	3:C:126:PRO:HD3	1.88	0.42
3:C:768:GLU:HG2	3:C:872:LEU:HD21	2.00	0.42
3:D:440:HIS:HA	3:D:443:ILE:HD12	2.00	0.42
1:F:913:DG:N2	5:J:953:DOC:O2	2.41	0.42
6:G:907:DGP:O3'	5:K:953:DOC:H2'	2.20	0.42
3:A:21:ASP:O	3:A:23:ASN:N	2.53	0.42
3:B:493:GLN:HA	3:B:549:GLU:HG3	2.01	0.42
3:B:512:GLU:O	3:B:533:LEU:HD21	2.19	0.42
3:C:116:GLU:HB2	3:C:135:ALA:HB3	2.01	0.42
3:C:171:GLN:HE21	3:C:171:GLN:N	2.17	0.42
3:C:243:SER:O	3:C:246:ARG:NH1	2.52	0.42
3:D:833:LEU:HA	3:D:834:PRO:HD3	1.91	0.42
3:B:820:ASP:O	3:B:820:ASP:CG	2.63	0.42
3:D:495:ASN:HD22	3:D:498:ILE:HD12	1.85	0.42
2:I:944:DA:H2''	2:I:945:DC:OP2	2.19	0.42
3:A:429:THR:O	3:A:463:TYR:HA	2.19	0.42
3:A:468:ASP:HB3	3:A:677:LYS:NZ	2.34	0.42
3:A:761:GLN:NE2	3:A:893:LYS:HD3	2.35	0.42
3:A:811:TYR:OH	3:A:822:PRO:O	2.20	0.42
3:B:19:TYR:HE1	3:B:29:ARG:HG2	1.84	0.42
3:B:161:GLU:OE2	3:B:190:PRO:HG3	2.20	0.42
3:B:900:MET:O	3:B:901:PHE:HB2	2.20	0.42
3:C:301:GLY:O	3:C:303:LEU:N	2.52	0.42
3:C:350:TYR:OH	3:C:481:GLN:NE2	2.49	0.42
3:D:542:LEU:HD12	3:D:542:LEU:HA	1.87	0.42
2:J:951:DA:H5'	3:B:734:LYS:HA	2.02	0.42
3:D:112:ASN:ND2	3:D:214:THR:HG23	2.35	0.42
3:D:530:ILE:HG13	3:D:533:LEU:HD12	2.01	0.42
3:D:660:GLU:N	3:D:661:PRO:CD	2.83	0.42
3:B:145:ARG:HB3	8:B:1124:HOH:O	2.20	0.41
3:B:194:GLU:O	3:B:195:LYS:C	2.62	0.41
3:C:119:SER:HA	3:C:120:PRO:HD2	1.91	0.41
3:C:139:TYR:CD1	3:C:332:LEU:HD21	2.55	0.41
3:D:696:LYS:O	3:D:756:GLY:HA2	2.20	0.41
1:F:921:DG:N2	2:J:946:DT:O2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:516:VAL:HB	3:A:522:PHE:CE1	2.55	0.41
3:A:533:LEU:HD13	3:A:538:LEU:HD13	2.01	0.41
3:A:864:HIS:HA	8:A:1078:HOH:O	2.20	0.41
3:B:499:ILE:HB	3:B:542:LEU:HD13	2.01	0.41
3:C:4:PHE:HB3	3:C:101:ILE:HG23	2.02	0.41
3:C:276:LEU:HD23	3:C:276:LEU:HA	1.90	0.41
3:C:304:LYS:C	3:C:323:TYR:HH	2.28	0.41
3:D:120:PRO:HD2	3:D:131:HIS:CD2	2.55	0.41
3:A:405:LYS:O	3:A:690:GLY:HA2	2.20	0.41
3:C:154:SER:C	3:C:156:TYR:H	2.28	0.41
3:C:304:LYS:O	3:C:323:TYR:OH	2.30	0.41
3:A:408:MET:CE	3:A:685:ARG:HD2	2.49	0.41
3:C:578:TYR:CD1	3:C:578:TYR:C	2.98	0.41
3:C:760:LEU:HD13	3:C:891:TYR:HA	2.01	0.41
3:D:219:GLU:HG3	3:D:270:VAL:CG1	2.49	0.41
3:D:251:LYS:O	3:D:252:VAL:C	2.62	0.41
1:E:910:DA:H8	1:E:911:DC:O2	2.03	0.41
3:C:197:LEU:HD12	3:C:197:LEU:C	2.46	0.41
3:C:472:PRO:HA	3:C:475:ILE:CD1	2.50	0.41
3:D:449:ARG:HA	3:D:450:PRO:HD2	1.92	0.41
3:A:305:TYR:HA	8:A:1079:HOH:O	2.19	0.41
3:A:734:LYS:HB3	3:A:737:THR:HG22	2.02	0.41
3:B:41:CYS:HB3	3:B:58:THR:HG22	2.02	0.41
3:B:52:ILE:HG12	8:B:1034:HOH:O	2.20	0.41
3:B:611:THR:CG2	3:B:612:GLU:N	2.83	0.41
3:B:720:TYR:HB3	3:B:722:GLU:O	2.21	0.41
3:C:894:LYS:O	3:C:895:ALA:C	2.61	0.41
3:D:316:ASN:CG	3:D:319:ARG:HB2	2.45	0.41
3:A:126:PRO:HA	3:A:225:TYR:CD2	2.56	0.41
3:A:176:ASP:OD1	3:A:319:ARG:HD3	2.21	0.41
3:B:727:ILE:HG21	3:B:732:THR:OG1	2.20	0.41
3:D:811:TYR:O	3:D:815:ILE:HG13	2.20	0.41
3:A:652:ASP:OD1	3:A:685:ARG:NH1	2.54	0.41
3:A:811:TYR:O	3:A:815:ILE:HG13	2.20	0.41
3:B:202:LEU:HD23	3:B:202:LEU:HA	1.88	0.41
3:B:405:LYS:O	3:B:690:GLY:HA2	2.21	0.41
3:C:93:LEU:HD23	3:C:93:LEU:HA	1.90	0.41
3:C:508:LEU:H	3:C:508:LEU:CD2	2.27	0.41
3:D:306:ASP:OD2	3:D:306:ASP:N	2.53	0.41
3:D:763:TYR:O	3:D:766:GLU:HB2	2.21	0.41
3:A:65:MET:HE3	3:A:65:MET:HB2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:180:SER:O	3:A:183:ILE:HG22	2.21	0.41
3:A:417:PRO:HB3	3:A:475:ILE:HG21	2.02	0.41
3:A:438:PRO:O	3:A:441:ASP:HB2	2.20	0.41
3:A:464:TYR:HB3	3:A:466:ASP:OD2	2.20	0.41
3:A:614:GLU:HB2	8:A:1114:HOH:O	2.21	0.41
3:B:184:ASP:HB2	8:B:1020:HOH:O	2.20	0.41
3:B:396:VAL:HA	8:B:1009:HOH:O	2.20	0.41
3:B:475:ILE:H	3:B:475:ILE:HG12	1.67	0.41
3:B:897:LEU:HD13	3:B:900:MET:HG2	2.02	0.41
3:C:212:ILE:CD1	3:C:345:LEU:HD21	2.51	0.41
3:C:815:ILE:O	3:C:816:LYS:C	2.64	0.41
3:D:80:LEU:HD23	3:D:80:LEU:HA	1.93	0.41
3:A:44:SER:C	3:A:46:ALA:N	2.76	0.41
3:A:575:PHE:O	3:A:576:ARG:C	2.63	0.41
3:A:639:SER:O	3:A:641:PHE:N	2.53	0.41
3:A:796:PHE:HB3	3:A:797:PRO:HD2	2.02	0.41
3:B:205:TRP:NE1	3:B:242:LEU:O	2.54	0.41
3:D:236:GLU:O	3:D:240:LYS:HG2	2.20	0.41
3:D:685:ARG:HG2	3:D:686:GLU:N	2.35	0.41
3:B:859:LYS:O	3:B:863:LEU:HG	2.21	0.40
3:C:112:ASN:HD21	3:C:331:VAL:HG11	1.87	0.40
3:D:246:ARG:HG2	8:D:1054:HOH:O	2.20	0.40
3:D:810:THR:HG21	3:D:845:CYS:O	2.20	0.40
1:G:923:DC:H1'	1:G:924:DC:H5'	2.02	0.40
3:A:285:GLN:HA	3:A:286:PRO:HD3	1.97	0.40
3:B:806:ARG:O	3:B:810:THR:HG22	2.20	0.40
3:C:128:GLN:O	3:C:232:ASN:ND2	2.54	0.40
3:C:130:LYS:HG2	3:C:130:LYS:H	1.77	0.40
3:C:806:ARG:HD3	3:C:843:ASP:OD1	2.21	0.40
3:D:78:ILE:HG22	3:D:78:ILE:O	2.20	0.40
1:E:920:DA:C2	2:I:947:DG:C2	3.09	0.40
3:A:3:GLU:HG2	3:A:21:ASP:HA	2.03	0.40
3:A:608:VAL:HG12	3:A:609:CYS:N	2.36	0.40
3:B:640:LYS:O	3:B:640:LYS:CG	2.65	0.40
3:C:757:GLU:HB2	3:C:889:LEU:HD22	2.03	0.40
3:A:246:ARG:HD3	8:A:1042:HOH:O	2.21	0.40
3:A:253:ILE:HD12	3:A:255:ASN:HD21	1.86	0.40
3:B:254:GLU:O	3:B:256:MET:HE2	2.21	0.40
3:B:347:MET:O	3:B:347:MET:HG3	2.21	0.40
3:B:514:LEU:HD11	3:B:529:LYS:HD3	2.03	0.40
3:C:260:ARG:HE	3:C:260:ARG:HB2	1.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:207:GLN:HG2	3:D:208:LYS:HG2	2.04	0.40
3:A:434:PHE:HD2	3:A:435:LYS:O	2.04	0.40
3:B:139:TYR:CG	3:B:332:LEU:HD21	2.57	0.40
3:B:730:LEU:HD13	3:B:883:PHE:CE1	2.55	0.40
3:C:122:GLY:O	3:C:123:PHE:C	2.63	0.40
3:C:471:VAL:N	3:C:472:PRO:CD	2.83	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	901/903 (100%)	805 (89%)	81 (9%)	15 (2%)	7	19
3	B	901/903 (100%)	830 (92%)	62 (7%)	9 (1%)	12	32
3	C	901/903 (100%)	827 (92%)	60 (7%)	14 (2%)	7	20
3	D	901/903 (100%)	823 (91%)	64 (7%)	14 (2%)	7	20
All	All	3604/3612 (100%)	3285 (91%)	267 (7%)	52 (1%)	9	23

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	22	SER
3	A	45	GLN
3	A	639	SER
3	A	640	LYS
3	A	902	ASP
3	B	253	ILE
3	B	640	LYS
3	C	304	LYS
3	C	305	TYR

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Mol	Chain	Res	Type
3	C	309	ILE
3	C	640	LYS
3	C	897	LEU
3	D	45	GLN
3	D	253	ILE
3	D	638	GLU
3	D	820	ASP
3	D	901	PHE
3	A	252	VAL
3	A	259	SER
3	A	301	GLY
3	A	506	PRO
3	B	622	THR
3	C	253	ILE
3	C	302	LYS
3	C	900	MET
3	D	252	VAL
3	D	305	TYR
3	D	817	GLY
3	D	818	ASN
3	A	638	GLU
3	A	836	ARG
3	B	896	SER
3	C	43	GLU
3	C	639	SER
3	D	302	LYS
3	D	622	THR
3	D	640	LYS
3	D	896	SER
3	A	44	SER
3	A	388	VAL
3	A	820	ASP
3	B	45	GLN
3	B	121	ASP
3	C	252	VAL
3	C	303	LEU
3	C	306	ASP
3	A	899	ASP
3	B	307	GLY
3	B	716	GLU
3	B	820	ASP
3	D	303	LEU

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Mol	Chain	Res	Type
3	C	161	GLU

5.3.2 Protein sidechains ⓘ

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	798/800 (100%)	619 (78%)	179 (22%)	1	3
3	B	798/800 (100%)	631 (79%)	167 (21%)	1	3
3	C	798/800 (100%)	649 (81%)	149 (19%)	1	4
3	D	798/800 (100%)	637 (80%)	161 (20%)	1	4
All	All	3192/3200 (100%)	2536 (79%)	656 (21%)	1	3

All (656) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	MET
3	A	2	LYS
3	A	6	LEU
3	A	15	ILE
3	A	27	ARG
3	A	28	THR
3	A	34	LYS
3	A	43	GLU
3	A	48	LYS
3	A	55	LYS
3	A	58	THR
3	A	66	ARG
3	A	73	LYS
3	A	76	GLU
3	A	78	ILE
3	A	80	LEU
3	A	94	SER
3	A	98	ASN
3	A	100	GLU
3	A	101	ILE

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Mol	Chain	Res	Type
3	A	102	LYS
3	A	106	THR
3	A	107	LYS
3	A	110	VAL
3	A	112	ASN
3	A	121	ASP
3	A	128	GLN
3	A	142	ILE
3	A	160	GLU
3	A	163	SER
3	A	165	GLU
3	A	170	LEU
3	A	171	GLN
3	A	173	GLN
3	A	177	GLU
3	A	181	GLU
3	A	183	ILE
3	A	197	LEU
3	A	202	LEU
3	A	206	GLN
3	A	217	ASN
3	A	218	VAL
3	A	226	VAL
3	A	237	SER
3	A	246	ARG
3	A	247	LYS
3	A	252	VAL
3	A	254	GLU
3	A	256	MET
3	A	261	GLU
3	A	262	ILE
3	A	269	SER
3	A	273	TYR
3	A	279	LYS
3	A	283	THR
3	A	285	GLN
3	A	291	ASP
3	A	295	GLU
3	A	298	LEU
3	A	299	ASN
3	A	302	LYS
3	A	303	LEU

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Mol	Chain	Res	Type
3	A	304	LYS
3	A	309	ILE
3	A	314	GLU
3	A	315	SER
3	A	319	ARG
3	A	332	LEU
3	A	342	ASN
3	A	343	LEU
3	A	362	ILE
3	A	373	LEU
3	A	375	GLU
3	A	378	LYS
3	A	384	ARG
3	A	388	VAL
3	A	389	GLN
3	A	397	LYS
3	A	398	GLU
3	A	408	MET
3	A	423	VAL
3	A	426	SER
3	A	435	LYS
3	A	440	HIS
3	A	448	GLU
3	A	453	VAL
3	A	467	ARG
3	A	479	PHE
3	A	482	ARG
3	A	483	LYS
3	A	489	MET
3	A	497	GLU
3	A	498	ILE
3	A	499	ILE
3	A	501	GLU
3	A	503	LEU
3	A	508	LEU
3	A	511	ASP
3	A	516	VAL
3	A	519	ARG
3	A	521	ASP
3	A	524	ASP
3	A	529	LYS
3	A	530	ILE

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Mol	Chain	Res	Type
3	A	531	LYS
3	A	533	LEU
3	A	536	LYS
3	A	538	LEU
3	A	542	LEU
3	A	544	ARG
3	A	546	GLN
3	A	547	ARG
3	A	549	GLU
3	A	553	MET
3	A	554	THR
3	A	556	GLN
3	A	558	ASN
3	A	559	ARG
3	A	562	LEU
3	A	563	ILE
3	A	591	GLN
3	A	592	MET
3	A	594	LEU
3	A	598	GLU
3	A	603	GLU
3	A	607	GLU
3	A	608	VAL
3	A	618	LEU
3	A	624	SER
3	A	635	LYS
3	A	636	VAL
3	A	638	GLU
3	A	640	LYS
3	A	658	ARG
3	A	665	ARG
3	A	677	LYS
3	A	703	THR
3	A	724	LYS
3	A	725	LEU
3	A	734	LYS
3	A	735	SER
3	A	737	THR
3	A	739	LYS
3	A	741	VAL
3	A	743	LYS
3	A	758	GLU

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Mol	Chain	Res	Type
3	A	759	SER
3	A	760	LEU
3	A	765	LYS
3	A	773	GLN
3	A	777	ILE
3	A	783	SER
3	A	784	SER
3	A	790	LYS
3	A	800	LYS
3	A	810	THR
3	A	813	ARG
3	A	818	ASN
3	A	819	ILE
3	A	825	VAL
3	A	826	GLU
3	A	832	VAL
3	A	835	LEU
3	A	836	ARG
3	A	843	ASP
3	A	844	LYS
3	A	846	ILE
3	A	854	ILE
3	A	856	ASP
3	A	866	MET
3	A	870	VAL
3	A	874	LYS
3	A	878	LYS
3	A	880	LEU
3	A	881	GLU
3	A	885	SER
3	A	893	LYS
3	A	894	LYS
3	A	900	MET
3	B	1	MET
3	B	2	LYS
3	B	3	GLU
3	B	6	LEU
3	B	15	ILE
3	B	26	GLU
3	B	32	GLU
3	B	36	SER
3	B	45	GLN

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Mol	Chain	Res	Type
3	B	48	LYS
3	B	55	LYS
3	B	58	THR
3	B	73	LYS
3	B	74	ARG
3	B	76	GLU
3	B	78	ILE
3	B	94	SER
3	B	100	GLU
3	B	102	LYS
3	B	110	VAL
3	B	112	ASN
3	B	128	GLN
3	B	130	LYS
3	B	141	SER
3	B	154	SER
3	B	158	ASN
3	B	165	GLU
3	B	170	LEU
3	B	171	GLN
3	B	173	GLN
3	B	177	GLU
3	B	182	ILE
3	B	183	ILE
3	B	185	LYS
3	B	195	LYS
3	B	196	GLU
3	B	197	LEU
3	B	206	GLN
3	B	207	GLN
3	B	218	VAL
3	B	226	VAL
3	B	237	SER
3	B	238	THR
3	B	246	ARG
3	B	247	LYS
3	B	252	VAL
3	B	254	GLU
3	B	255	ASN
3	B	256	MET
3	B	257	TYR
3	B	259	SER

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Mol	Chain	Res	Type
3	B	261	GLU
3	B	262	ILE
3	B	263	ILE
3	B	268	ILE
3	B	279	LYS
3	B	281	SER
3	B	283	THR
3	B	291	ASP
3	B	295	GLU
3	B	298	LEU
3	B	303	LEU
3	B	309	ILE
3	B	311	LYS
3	B	312	LEU
3	B	314	GLU
3	B	315	SER
3	B	319	ARG
3	B	332	LEU
3	B	337	LYS
3	B	338	ARG
3	B	342	ASN
3	B	343	LEU
3	B	347	MET
3	B	353	ILE
3	B	357	SER
3	B	362	ILE
3	B	373	LEU
3	B	374	LYS
3	B	375	GLU
3	B	378	LYS
3	B	385	SER
3	B	397	LYS
3	B	402	ASN
3	B	405	LYS
3	B	412	LEU
3	B	414	SER
3	B	435	LYS
3	B	436	VAL
3	B	453	VAL
3	B	465	LYS
3	B	470	VAL
3	B	475	ILE

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Mol	Chain	Res	Type
3	B	477	LYS
3	B	479	PHE
3	B	486	LYS
3	B	493	GLN
3	B	497	GLU
3	B	498	ILE
3	B	500	LYS
3	B	503	LEU
3	B	507	ASN
3	B	508	LEU
3	B	510	VAL
3	B	516	VAL
3	B	517	ASP
3	B	522	PHE
3	B	525	GLU
3	B	527	LYS
3	B	530	ILE
3	B	532	LYS
3	B	533	LEU
3	B	536	LYS
3	B	538	LEU
3	B	541	MET
3	B	543	PHE
3	B	547	ARG
3	B	549	GLU
3	B	550	VAL
3	B	562	LEU
3	B	576	ARG
3	B	600	LYS
3	B	607	GLU
3	B	608	VAL
3	B	611	THR
3	B	614	GLU
3	B	618	LEU
3	B	628	SER
3	B	640	LYS
3	B	642	ARG
3	B	653	LYS
3	B	656	ARG
3	B	693	LEU
3	B	715	MET
3	B	716	GLU

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Mol	Chain	Res	Type
3	B	726	LYS
3	B	736	SER
3	B	737	THR
3	B	739	LYS
3	B	746	LYS
3	B	759	SER
3	B	760	LEU
3	B	765	LYS
3	B	769	LYS
3	B	770	GLU
3	B	781	SER
3	B	800	LYS
3	B	810	THR
3	B	816	LYS
3	B	819	ILE
3	B	820	ASP
3	B	823	GLN
3	B	826	GLU
3	B	828	GLU
3	B	835	LEU
3	B	843	ASP
3	B	853	GLU
3	B	854	ILE
3	B	855	THR
3	B	873	GLU
3	B	874	LYS
3	B	878	LYS
3	B	880	LEU
3	B	885	SER
3	B	896	SER
3	B	897	LEU
3	B	899	ASP
3	C	2	LYS
3	C	3	GLU
3	C	6	LEU
3	C	10	GLN
3	C	15	ILE
3	C	25	ARG
3	C	26	GLU
3	C	27	ARG
3	C	32	GLU
3	C	36	SER

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Mol	Chain	Res	Type
3	C	43	GLU
3	C	48	LYS
3	C	58	THR
3	C	60	LYS
3	C	61	LEU
3	C	66	ARG
3	C	72	ILE
3	C	73	LYS
3	C	74	ARG
3	C	76	GLU
3	C	78	ILE
3	C	80	LEU
3	C	100	GLU
3	C	102	LYS
3	C	107	LYS
3	C	110	VAL
3	C	116	GLU
3	C	123	PHE
3	C	130	LYS
3	C	154	SER
3	C	163	SER
3	C	165	GLU
3	C	170	LEU
3	C	171	GLN
3	C	173	GLN
3	C	180	SER
3	C	181	GLU
3	C	183	ILE
3	C	189	MET
3	C	195	LYS
3	C	196	GLU
3	C	197	LEU
3	C	199	MET
3	C	200	GLU
3	C	202	LEU
3	C	213	LEU
3	C	218	VAL
3	C	226	VAL
3	C	231	LYS
3	C	236	GLU
3	C	243	SER
3	C	246	ARG

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Mol	Chain	Res	Type
3	C	249	ARG
3	C	254	GLU
3	C	255	ASN
3	C	256	MET
3	C	257	TYR
3	C	260	ARG
3	C	261	GLU
3	C	263	ILE
3	C	278	LYS
3	C	298	LEU
3	C	302	LYS
3	C	303	LEU
3	C	305	TYR
3	C	309	ILE
3	C	311	LYS
3	C	314	GLU
3	C	319	ARG
3	C	332	LEU
3	C	334	ILE
3	C	342	ASN
3	C	343	LEU
3	C	362	ILE
3	C	363	LYS
3	C	373	LEU
3	C	375	GLU
3	C	378	LYS
3	C	382	GLN
3	C	384	ARG
3	C	402	ASN
3	C	408	MET
3	C	435	LYS
3	C	446	VAL
3	C	453	VAL
3	C	467	ARG
3	C	468	ASP
3	C	475	ILE
3	C	482	ARG
3	C	483	LYS
3	C	486	LYS
3	C	498	ILE
3	C	503	LEU
3	C	505	ASN

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Mol	Chain	Res	Type
3	C	508	LEU
3	C	511	ASP
3	C	514	LEU
3	C	526	ILE
3	C	527	LYS
3	C	528	GLU
3	C	529	LYS
3	C	531	LYS
3	C	532	LYS
3	C	538	LEU
3	C	547	ARG
3	C	558	ASN
3	C	559	ARG
3	C	562	LEU
3	C	594	LEU
3	C	597	ILE
3	C	599	ARG
3	C	608	VAL
3	C	611	THR
3	C	614	GLU
3	C	618	LEU
3	C	628	SER
3	C	635	LYS
3	C	640	LYS
3	C	642	ARG
3	C	653	LYS
3	C	658	ARG
3	C	685	ARG
3	C	693	LEU
3	C	696	LYS
3	C	715	MET
3	C	724	LYS
3	C	737	THR
3	C	739	LYS
3	C	755	GLU
3	C	760	LEU
3	C	765	LYS
3	C	768	GLU
3	C	769	LYS
3	C	772	ARG
3	C	810	THR
3	C	816	LYS

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Mol	Chain	Res	Type
3	C	819	ILE
3	C	820	ASP
3	C	828	GLU
3	C	835	LEU
3	C	843	ASP
3	C	854	ILE
3	C	855	THR
3	C	874	LYS
3	C	878	LYS
3	C	880	LEU
3	C	892	GLU
3	C	898	PHE
3	C	900	MET
3	D	1	MET
3	D	3	GLU
3	D	6	LEU
3	D	15	ILE
3	D	17	GLU
3	D	22	SER
3	D	25	ARG
3	D	26	GLU
3	D	30	GLU
3	D	32	GLU
3	D	34	LYS
3	D	43	GLU
3	D	45	GLN
3	D	48	LYS
3	D	55	LYS
3	D	58	THR
3	D	60	LYS
3	D	61	LEU
3	D	66	ARG
3	D	70	GLN
3	D	72	ILE
3	D	73	LYS
3	D	74	ARG
3	D	76	GLU
3	D	81	GLU
3	D	102	LYS
3	D	110	VAL
3	D	128	GLN
3	D	130	LYS

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Mol	Chain	Res	Type
3	D	137	THR
3	D	154	SER
3	D	158	ASN
3	D	163	SER
3	D	170	LEU
3	D	171	GLN
3	D	177	GLU
3	D	180	SER
3	D	181	GLU
3	D	183	ILE
3	D	186	ILE
3	D	192	ASP
3	D	197	LEU
3	D	199	MET
3	D	208	LYS
3	D	212	ILE
3	D	217	ASN
3	D	218	VAL
3	D	219	GLU
3	D	220	SER
3	D	226	VAL
3	D	240	LYS
3	D	243	SER
3	D	246	ARG
3	D	247	LYS
3	D	253	ILE
3	D	254	GLU
3	D	255	ASN
3	D	256	MET
3	D	257	TYR
3	D	261	GLU
3	D	263	ILE
3	D	279	LYS
3	D	283	THR
3	D	289	SER
3	D	295	GLU
3	D	299	ASN
3	D	302	LYS
3	D	303	LEU
3	D	304	LYS
3	D	306	ASP
3	D	309	ILE

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Mol	Chain	Res	Type
3	D	311	LYS
3	D	314	GLU
3	D	319	ARG
3	D	332	LEU
3	D	334	ILE
3	D	342	ASN
3	D	372	SER
3	D	373	LEU
3	D	375	GLU
3	D	384	ARG
3	D	385	SER
3	D	397	LYS
3	D	402	ASN
3	D	408	MET
3	D	414	SER
3	D	435	LYS
3	D	440	HIS
3	D	441	ASP
3	D	453	VAL
3	D	467	ARG
3	D	475	ILE
3	D	477	LYS
3	D	479	PHE
3	D	482	ARG
3	D	483	LYS
3	D	489	MET
3	D	493	GLN
3	D	497	GLU
3	D	500	LYS
3	D	503	LEU
3	D	508	LEU
3	D	509	SER
3	D	512	GLU
3	D	514	LEU
3	D	516	VAL
3	D	527	LYS
3	D	529	LYS
3	D	530	ILE
3	D	536	LYS
3	D	538	LEU
3	D	544	ARG
3	D	547	ARG

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Mol	Chain	Res	Type
3	D	548	THR
3	D	550	VAL
3	D	559	ARG
3	D	562	LEU
3	D	594	LEU
3	D	599	ARG
3	D	608	VAL
3	D	614	GLU
3	D	618	LEU
3	D	624	SER
3	D	631	LYS
3	D	640	LYS
3	D	642	ARG
3	D	657	GLU
3	D	659	MET
3	D	665	ARG
3	D	693	LEU
3	D	715	MET
3	D	722	GLU
3	D	737	THR
3	D	739	LYS
3	D	743	LYS
3	D	755	GLU
3	D	760	LEU
3	D	761	GLN
3	D	766	GLU
3	D	777	ILE
3	D	781	SER
3	D	784	SER
3	D	800	LYS
3	D	810	THR
3	D	816	LYS
3	D	819	ILE
3	D	823	GLN
3	D	828	GLU
3	D	835	LEU
3	D	844	LYS
3	D	846	ILE
3	D	854	ILE
3	D	855	THR
3	D	857	LEU
3	D	859	LYS

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Mol	Chain	Res	Type
3	D	873	GLU
3	D	880	LEU
3	D	881	GLU
3	D	888	LYS
3	D	894	LYS
3	D	897	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	ASN
3	A	98	ASN
3	A	105	HIS
3	A	112	ASN
3	A	131	HIS
3	A	153	ASN
3	A	158	ASN
3	A	171	GLN
3	A	173	GLN
3	A	333	GLN
3	A	339	GLN
3	A	376	GLN
3	A	402	ASN
3	A	480	ASN
3	A	481	GLN
3	A	495	ASN
3	A	505	ASN
3	A	558	ASN
3	A	591	GLN
3	A	646	HIS
3	A	733	GLN
3	A	761	GLN
3	A	812	ASN
3	A	823	GLN
3	A	839	ASN
3	A	864	HIS
3	B	45	GLN
3	B	98	ASN
3	B	112	ASN
3	B	153	ASN
3	B	171	GLN
3	B	173	GLN

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Mol	Chain	Res	Type
3	B	255	ASN
3	B	333	GLN
3	B	339	GLN
3	B	354	GLN
3	B	376	GLN
3	B	382	GLN
3	B	386	HIS
3	B	402	ASN
3	B	424	ASN
3	B	440	HIS
3	B	480	ASN
3	B	505	ASN
3	B	507	ASN
3	B	539	ASN
3	B	546	GLN
3	B	646	HIS
3	B	679	HIS
3	B	733	GLN
3	B	787	ASN
3	B	823	GLN
3	C	98	ASN
3	C	112	ASN
3	C	131	HIS
3	C	153	ASN
3	C	158	ASN
3	C	171	GLN
3	C	245	HIS
3	C	333	GLN
3	C	354	GLN
3	C	376	GLN
3	C	402	ASN
3	C	440	HIS
3	C	480	ASN
3	C	495	ASN
3	C	505	ASN
3	C	546	GLN
3	C	558	ASN
3	C	591	GLN
3	C	679	HIS
3	C	818	ASN
3	C	823	GLN
3	D	40	HIS

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Mol	Chain	Res	Type
3	D	70	GLN
3	D	112	ASN
3	D	131	HIS
3	D	255	ASN
3	D	317	HIS
3	D	333	GLN
3	D	339	GLN
3	D	354	GLN
3	D	376	GLN
3	D	402	ASN
3	D	440	HIS
3	D	481	GLN
3	D	485	HIS
3	D	493	GLN
3	D	495	ASN
3	D	505	ASN
3	D	556	GLN
3	D	645	ASN
3	D	646	HIS
3	D	679	HIS
3	D	761	GLN
3	D	786	ASN
3	D	787	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 1 is modelled with single atom and 8 are monoatomic - leaving 13 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	$\# Z > 2$
4	3DR	H	912	1	8,11,12	0.65	0	7,14,17	0.81	0
5	DOC	J	953	2	16,19,20	0.61	0	20,26,29	1.20	2 (10%)
6	DGP	F	908	-	21,21,25	0.73	0	31,31,38	1.13	1 (3%)
6	DGP	K	955	-	21,24,25	0.66	0	30,35,38	1.36	3 (10%)
6	DGP	H	908	-	21,21,25	0.88	1 (4%)	31,31,38	1.30	3 (9%)
4	3DR	G	912	1	8,11,12	0.85	0	7,14,17	1.49	2 (28%)
4	3DR	F	912	1	8,11,12	0.50	0	7,14,17	0.85	0
6	DGP	G	908	6,7	21,24,25	0.82	1 (4%)	30,35,38	1.41	5 (16%)
5	DOC	L	953	2	16,19,20	0.46	0	20,26,29	1.09	1 (5%)
5	DOC	I	953	2	16,19,20	0.46	0	20,26,29	0.86	1 (5%)
4	3DR	E	912	1	8,11,12	0.64	0	7,14,17	0.91	0
5	DOC	K	953	2	16,19,20	0.46	0	20,26,29	1.91	3 (15%)
6	DGP	L	955	-	21,24,25	0.56	0	30,35,38	0.72	1 (3%)

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
4	3DR	H	912	1	-	2/3/15/16	0/1/1/1
5	DOC	J	953	2	-	0/7/18/19	0/2/2/2
6	DGP	F	908	-	-	4/6/18/22	0/3/3/3
6	DGP	K	955	-	-	1/7/21/22	0/3/3/3
6	DGP	H	908	-	-	2/6/18/22	0/3/3/3
4	3DR	G	912	1	-	2/3/15/16	0/1/1/1
4	3DR	F	912	1	-	0/3/15/16	0/1/1/1
6	DGP	G	908	6,7	-	2/7/21/22	0/3/3/3
5	DOC	L	953	2	-	0/7/18/19	0/2/2/2
5	DOC	I	953	2	-	2/7/18/19	0/2/2/2
4	3DR	E	912	1	-	2/3/15/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DOC	K	953	2	-	2/7/18/19	0/2/2/2
6	DGP	L	955	-	-	4/7/21/22	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	908	DGP	C4-N3	2.30	1.39	1.34
6	H	908	DGP	C4-N3	2.12	1.39	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	953	DOC	C4'-O4'-C1'	-7.11	103.09	109.81
6	K	955	DGP	O4'-C1'-N9	4.62	116.07	107.86
6	G	908	DGP	O4'-C1'-N9	3.73	114.48	107.86
6	H	908	DGP	O4'-C1'-N9	3.51	114.09	107.86
6	K	955	DGP	C4'-O4'-C1'	-3.28	101.71	109.51
5	J	953	DOC	C4'-O4'-C1'	-3.07	106.91	109.81
6	G	908	DGP	C1'-N9-C4	2.99	133.55	125.50
5	I	953	DOC	O4'-C1'-N1	2.88	112.97	107.86
6	G	908	DGP	C1'-N9-C8	-2.87	121.48	127.91
5	L	953	DOC	O4'-C1'-N1	2.69	112.63	107.86
5	K	953	DOC	O4'-C1'-C2'	-2.59	103.34	106.41
5	J	953	DOC	C3'-C2'-C1'	2.50	105.75	102.87
6	G	908	DGP	N9-C4-N3	2.48	130.91	125.95
6	H	908	DGP	C1'-N9-C8	-2.47	122.38	127.91
6	H	908	DGP	C1'-N9-C4	2.46	132.13	125.50
4	G	912	3DR	O4'-C4'-C3'	2.45	107.33	103.73
6	G	908	DGP	C5-C4-N3	-2.44	124.50	128.39
5	K	953	DOC	O4'-C4'-C3'	-2.29	101.03	104.81
6	F	908	DGP	O4'-C1'-C2'	-2.22	102.10	106.25
4	G	912	3DR	C1'-O4'-C4'	-2.13	105.01	108.37
6	K	955	DGP	O4'-C1'-C2'	-2.08	102.36	106.25
6	L	955	DGP	O4'-C1'-N9	2.04	111.48	107.86

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	953	DOC	C3'-C4'-C5'-O5'
5	I	953	DOC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	K	953	DOC	O4'-C4'-C5'-O5'
6	F	908	DGP	O4'-C1'-N9-C8
6	F	908	DGP	O4'-C1'-N9-C4
6	L	955	DGP	O4'-C1'-N9-C8
6	L	955	DGP	O4'-C1'-N9-C4
6	F	908	DGP	C3'-C4'-C5'-O5'
6	F	908	DGP	O4'-C4'-C5'-O5'
4	H	912	3DR	O4'-C4'-C5'-O5'
6	G	908	DGP	O4'-C4'-C5'-O5'
6	G	908	DGP	C3'-C4'-C5'-O5'
6	L	955	DGP	C4'-C5'-O5'-P
6	H	908	DGP	O4'-C1'-N9-C4
6	H	908	DGP	O4'-C1'-N9-C8
6	K	955	DGP	C4'-C5'-O5'-P
5	K	953	DOC	C3'-C4'-C5'-O5'
4	H	912	3DR	C4'-C5'-O5'-P
4	E	912	3DR	O4'-C4'-C5'-O5'
4	E	912	3DR	C3'-C4'-C5'-O5'
4	G	912	3DR	C3'-C4'-C5'-O5'
4	G	912	3DR	O4'-C4'-C5'-O5'
6	L	955	DGP	C3'-C4'-C5'-O5'

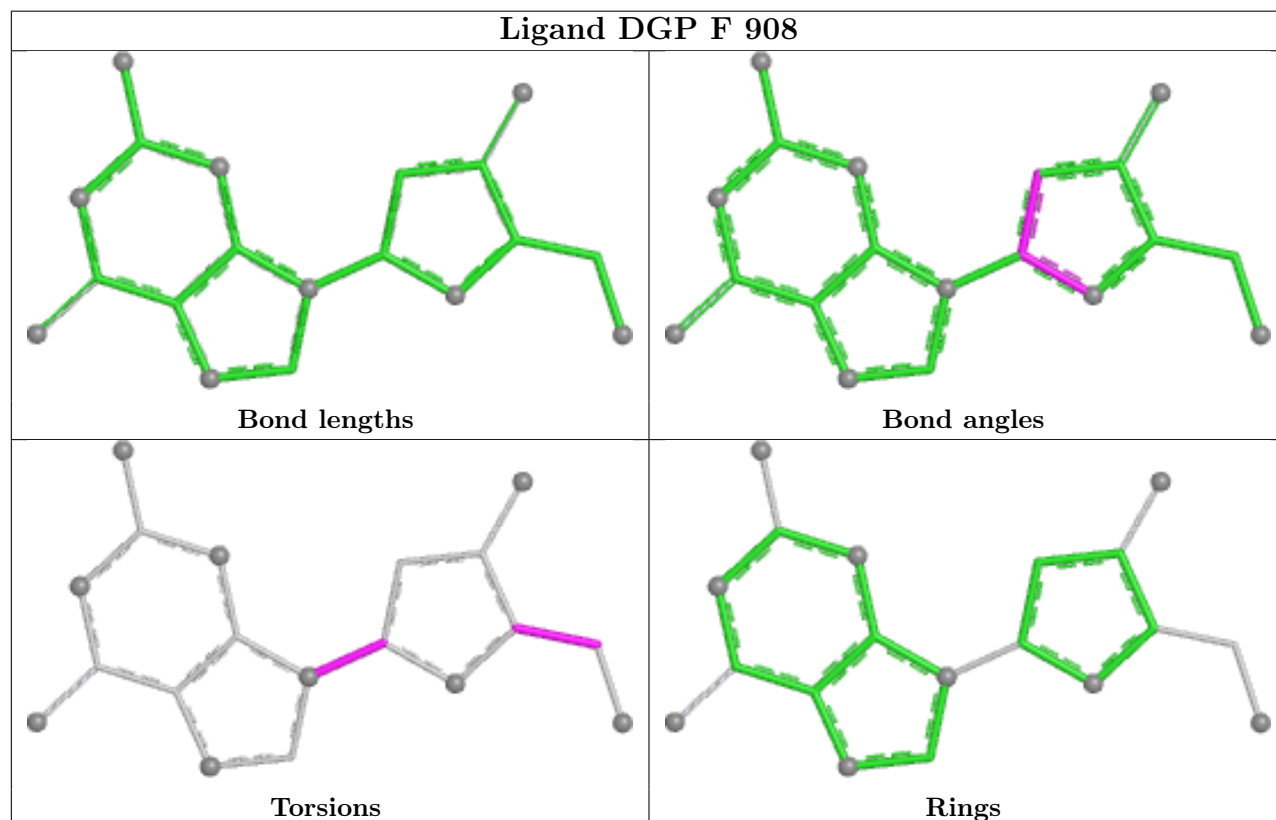
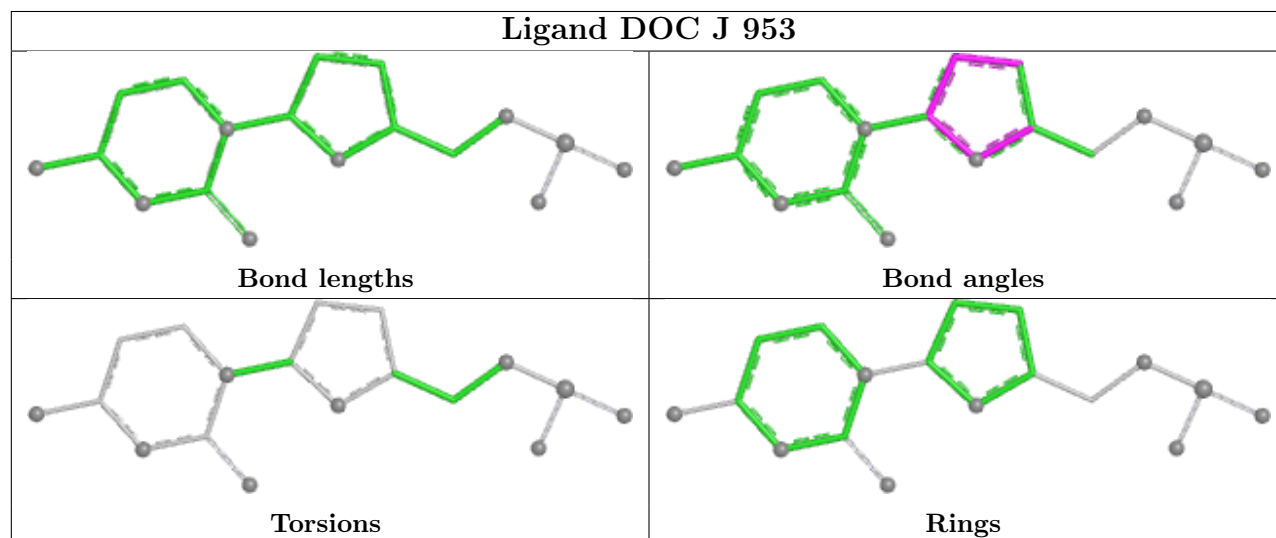
There are no ring outliers.

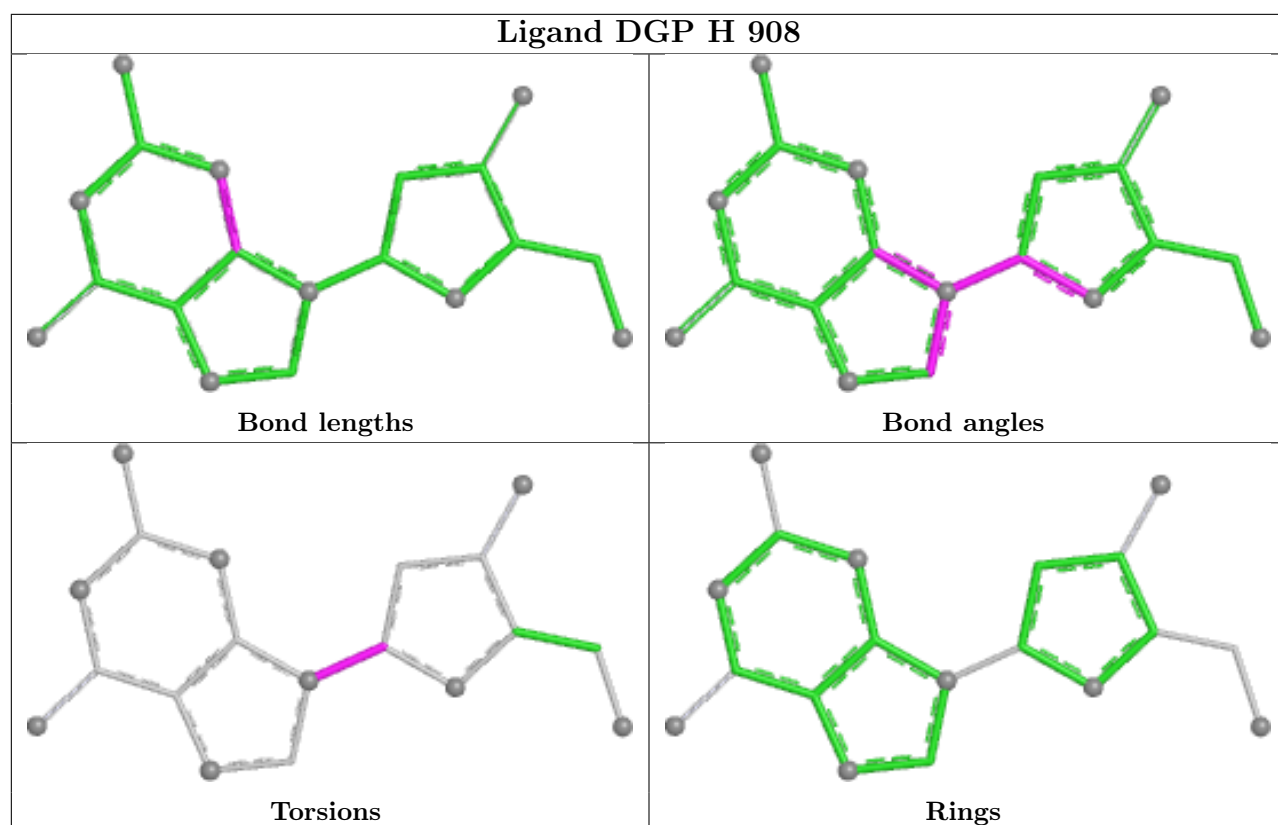
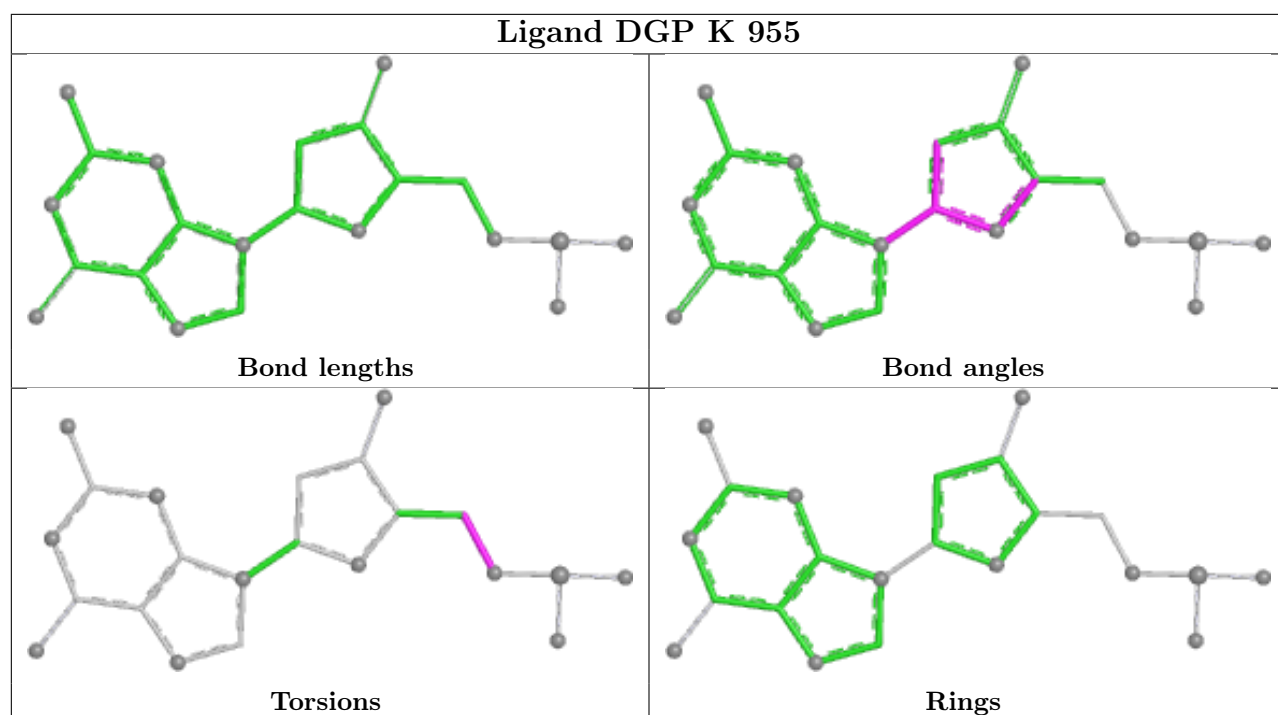
10 monomers are involved in 18 short contacts:

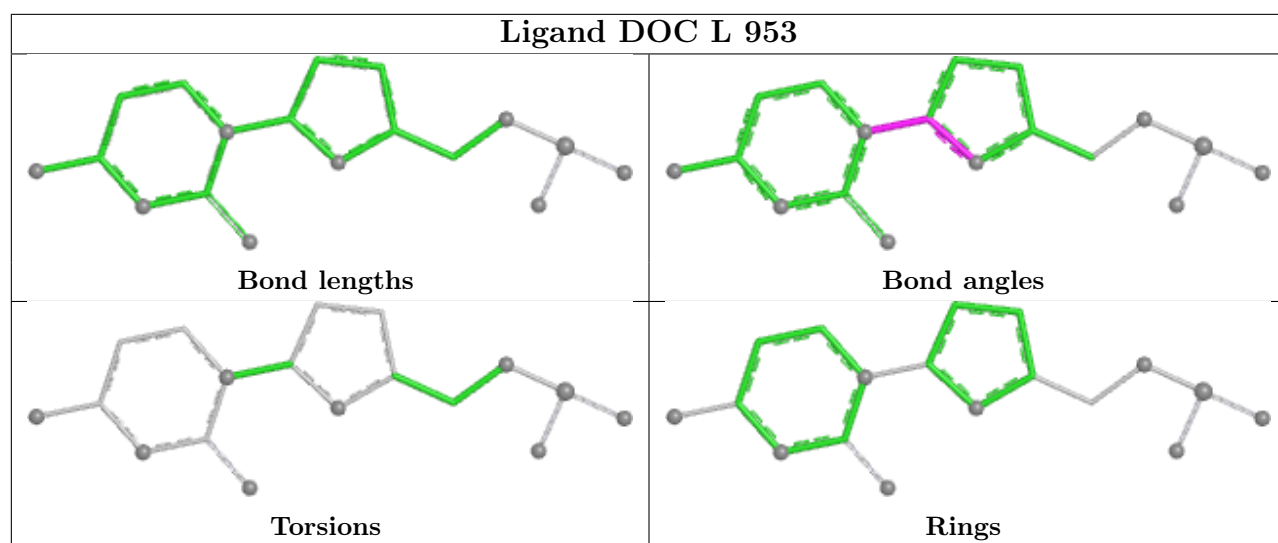
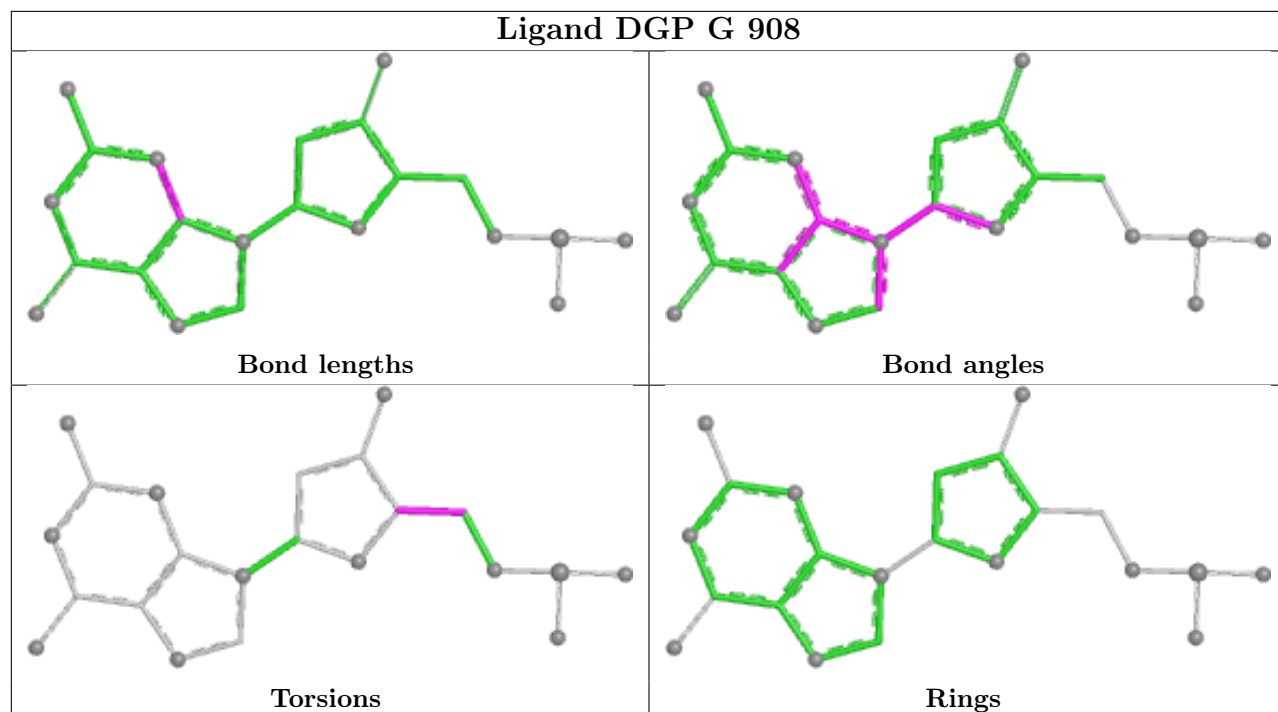
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	953	DOC	1	0
6	K	955	DGP	1	0
6	H	908	DGP	3	0
4	G	912	3DR	3	0
4	F	912	3DR	3	0
6	G	908	DGP	1	0
5	I	953	DOC	2	0
4	E	912	3DR	1	0
5	K	953	DOC	2	0
6	L	955	DGP	1	0

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 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.

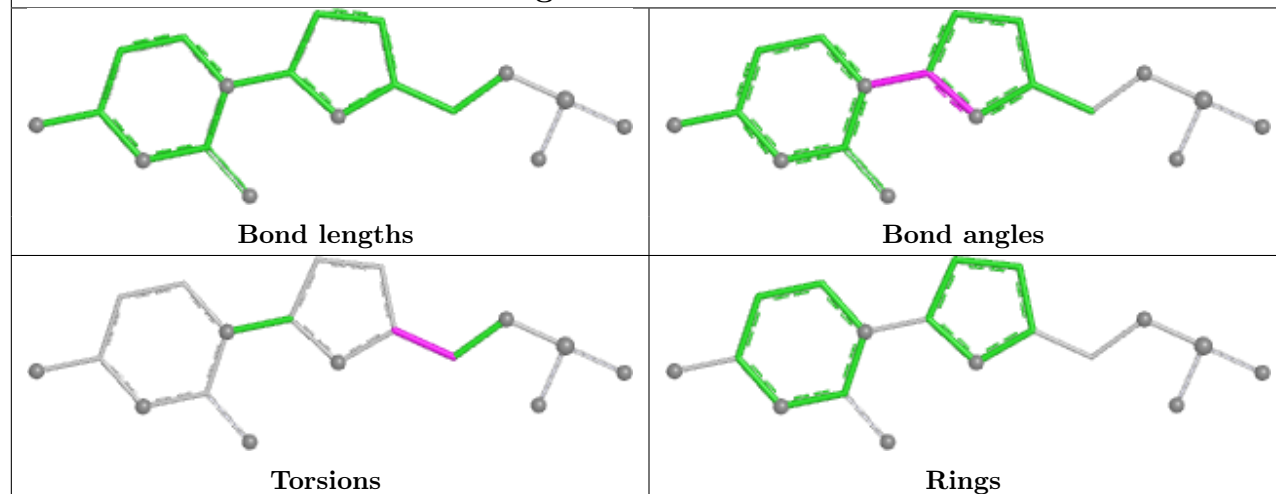
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



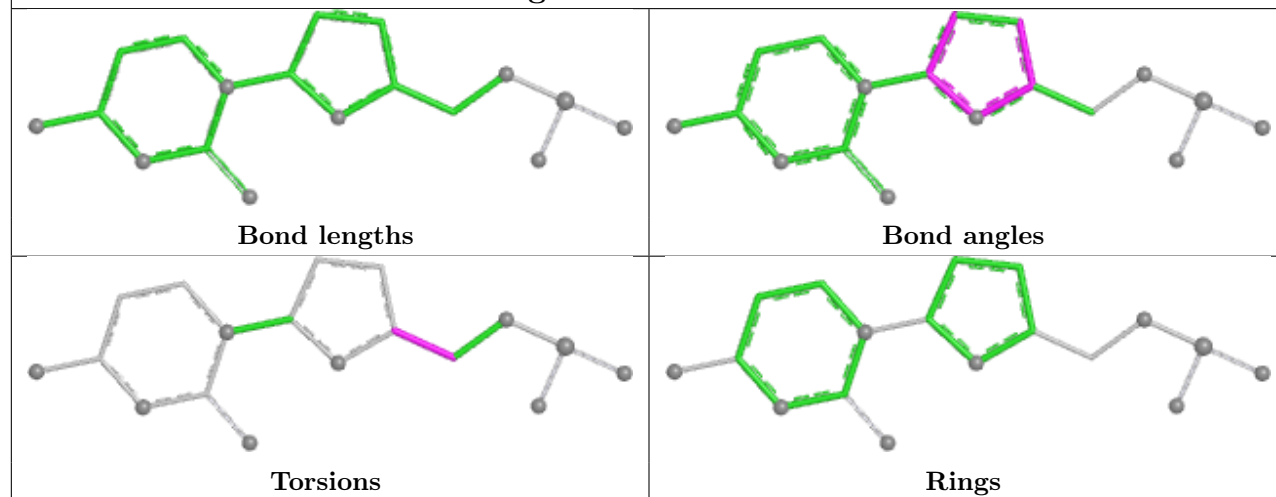


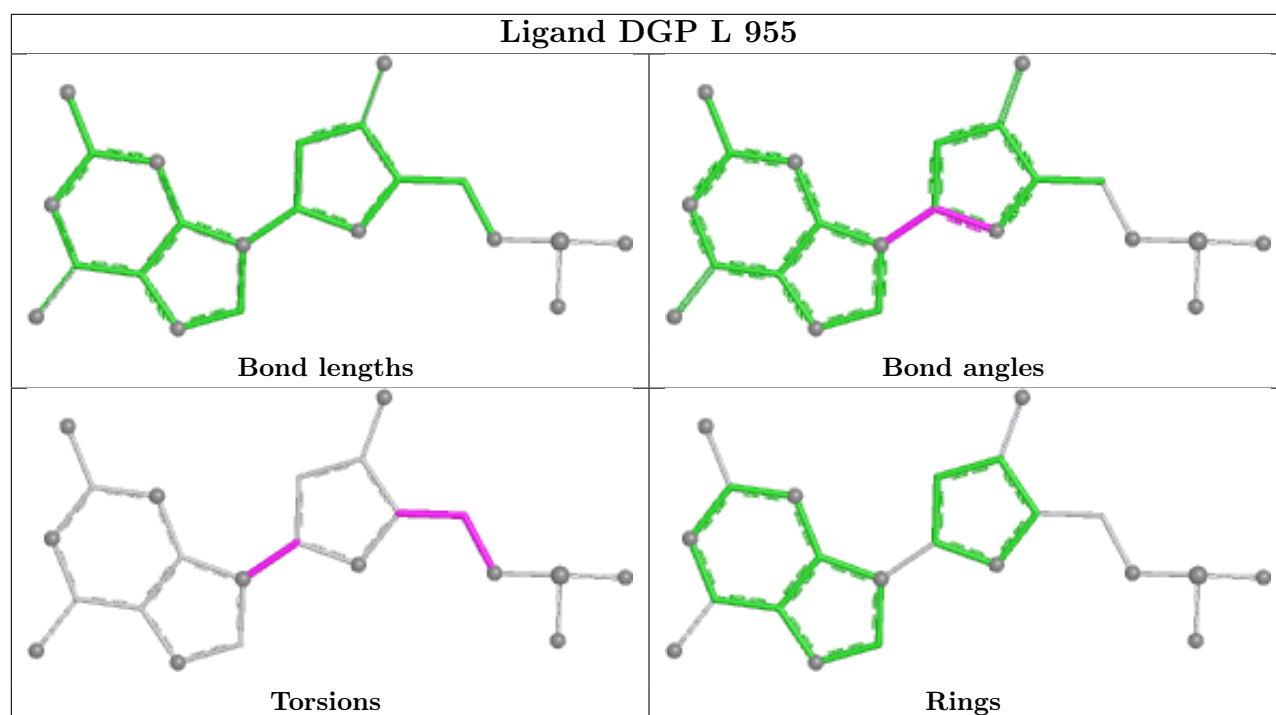


Ligand DOC I 953



Ligand DOC K 953





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1
1	G	1
1	E	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	911:DC	O3'	913:DG	P	7.44
1	G	911:DC	O3'	913:DG	P	6.78
1	E	911:DC	O3'	913:DG	P	6.67
1	F	911:DC	O3'	913:DG	P	6.67

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	E	18/18 (100%)	1.23	3 (16%) 4 3	76, 92, 130, 152	0
1	F	18/18 (100%)	0.66	2 (11%) 10 8	39, 75, 149, 176	0
1	G	18/18 (100%)	0.02	1 (5%) 30 26	36, 54, 90, 102	0
1	H	18/18 (100%)	0.48	2 (11%) 10 8	44, 67, 128, 131	0
2	I	13/13 (100%)	0.76	1 (7%) 19 17	77, 95, 100, 102	0
2	J	13/13 (100%)	-0.04	0 100 100	41, 68, 121, 135	0
2	K	13/13 (100%)	-0.33	0 100 100	36, 55, 77, 83	0
2	L	13/13 (100%)	-0.16	0 100 100	43, 65, 95, 102	0
3	A	903/903 (100%)	0.39	92 (10%) 12 10	30, 64, 147, 260	0
3	B	903/903 (100%)	0.01	46 (5%) 33 29	30, 53, 121, 222	0
3	C	903/903 (100%)	-0.20	14 (1%) 70 68	28, 47, 88, 138	0
3	D	903/903 (100%)	-0.06	20 (2%) 62 59	30, 57, 93, 170	0
All	All	3736/3736 (100%)	0.05	181 (4%) 35 32	28, 56, 113, 260	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	508	LEU	10.0
1	F	928	DG	8.8
3	C	903	PHE	6.0
3	A	554	THR	5.8
3	A	543	PHE	5.1
3	B	253	ILE	5.1
3	A	503	LEU	4.8
3	A	499	ILE	4.7
3	A	550	VAL	4.6
3	A	520	PHE	4.6
3	A	538	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
3	B	257	TYR	4.4
3	B	498	ILE	4.4
1	H	928	DG	4.2
3	A	847	ALA	4.2
3	A	542	LEU	4.1
3	A	498	ILE	4.1
3	A	507	ASN	4.0
3	B	530	ILE	4.0
3	A	530	ILE	4.0
3	A	846	ILE	4.0
3	A	803	PHE	4.0
3	A	514	LEU	3.9
3	A	547	ARG	3.9
3	A	502	ALA	3.9
3	A	253	ILE	3.8
3	A	522	PHE	3.8
3	A	799	PRO	3.8
3	A	545	ALA	3.8
3	B	508	LEU	3.7
3	A	798	GLY	3.7
3	B	895	ALA	3.6
1	G	911	DC	3.5
3	B	506	PRO	3.5
3	B	256	MET	3.5
3	A	488	TYR	3.4
3	C	257	TYR	3.4
3	A	492	ALA	3.4
3	A	259	SER	3.4
3	A	518	TYR	3.4
3	A	809	LEU	3.4
3	B	500	LYS	3.3
3	B	492	ALA	3.3
3	A	510	VAL	3.3
3	A	506	PRO	3.3
3	A	495	ASN	3.3
3	D	516	VAL	3.3
3	A	516	VAL	3.2
3	B	539	ASN	3.2
3	A	551	ALA	3.2
3	A	832	VAL	3.2
3	B	543	PHE	3.2
3	D	253	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	895	ALA	3.1
3	A	802	PRO	3.1
1	F	927	DG	3.1
3	A	526	ILE	3.1
3	D	901	PHE	3.1
3	A	395	PHE	3.0
3	B	255	ASN	3.0
3	B	538	LEU	3.0
3	A	504	HIS	3.0
3	A	532	LYS	3.0
3	D	903	PHE	3.0
3	A	858	ILE	3.0
3	A	903	PHE	3.0
3	C	252	VAL	2.9
3	A	500	LYS	2.9
3	A	855	THR	2.9
3	A	536	LYS	2.9
3	C	258	GLY	2.9
3	A	535	ALA	2.9
3	B	903	PHE	2.9
3	C	897	LEU	2.9
3	A	789	ALA	2.9
3	B	252	VAL	2.9
3	D	252	VAL	2.9
3	A	533	LEU	2.8
3	A	808	ILE	2.8
3	A	786	ASN	2.8
3	B	503	LEU	2.8
3	A	841	PHE	2.8
3	A	640	LYS	2.8
3	C	253	ILE	2.8
3	A	509	SER	2.8
3	A	301	GLY	2.8
3	B	520	PHE	2.8
3	A	303	LEU	2.7
3	A	857	LEU	2.7
3	B	1	MET	2.7
3	A	261	GLU	2.7
3	A	801	CYS	2.7
3	D	1	MET	2.6
3	A	800	LYS	2.6
3	A	252	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	805	ILE	2.6
3	D	257	TYR	2.6
3	A	390	PRO	2.6
3	A	862	VAL	2.6
3	A	541	MET	2.5
3	A	496	GLY	2.5
3	D	526	ILE	2.5
3	A	791	TYR	2.5
3	B	516	VAL	2.5
3	A	490	LEU	2.5
3	C	508	LEU	2.5
3	A	505	ASN	2.5
3	B	513	PRO	2.5
3	B	309	ILE	2.4
3	B	526	ILE	2.4
3	D	262	ILE	2.4
3	A	487	GLY	2.4
3	B	518	TYR	2.4
3	B	514	LEU	2.4
3	D	897	LEU	2.4
3	B	490	LEU	2.4
1	E	910	DA	2.4
3	B	505	ASN	2.4
3	D	468	ASP	2.4
3	D	541	MET	2.4
3	C	123	PHE	2.4
3	B	173	GLN	2.3
3	B	310	SER	2.3
1	H	911	DC	2.3
3	A	819	ILE	2.3
3	B	499	ILE	2.3
3	C	1	MET	2.3
3	A	833	LEU	2.3
3	A	804	HIS	2.3
1	E	928	DG	2.3
3	A	257	TYR	2.3
3	A	523	SER	2.3
3	D	899	ASP	2.3
3	B	496	GLY	2.3
3	A	814	ALA	2.2
3	A	531	LYS	2.2
3	A	493	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	391	TYR	2.2
3	A	797	PRO	2.2
3	D	514	LEU	2.2
3	A	552	GLY	2.2
3	B	531	LYS	2.2
3	B	897	LEU	2.2
3	B	550	VAL	2.2
3	A	394	ALA	2.2
3	A	555	ALA	2.2
3	D	41	CYS	2.2
3	A	818	ASN	2.2
3	B	524	ASP	2.2
1	E	920	DA	2.2
2	I	940	DG	2.1
3	D	900	MET	2.1
3	B	262	ILE	2.1
3	D	44	SER	2.1
3	A	172	GLU	2.1
3	B	529	LYS	2.1
3	A	258	GLY	2.1
3	A	902	ASP	2.1
3	B	510	VAL	2.1
3	C	530	ILE	2.1
3	C	639	SER	2.1
3	B	535	ALA	2.1
3	A	254	GLU	2.1
3	D	638	GLU	2.1
3	C	260	ARG	2.1
3	A	788	ILE	2.1
3	B	123	PHE	2.1
3	B	259	SER	2.1
3	B	502	ALA	2.1
3	B	532	LYS	2.1
3	D	539	ASN	2.1
3	A	824	VAL	2.1
3	A	521	ASP	2.0
3	B	541	MET	2.0
3	C	256	MET	2.0
3	C	122	GLY	2.0
3	A	260	ARG	2.0
3	B	160	GLU	2.0
3	A	784	SER	2.0

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Mol	Chain	Res	Type	RSRZ
3	A	548	THR	2.0
3	B	45	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

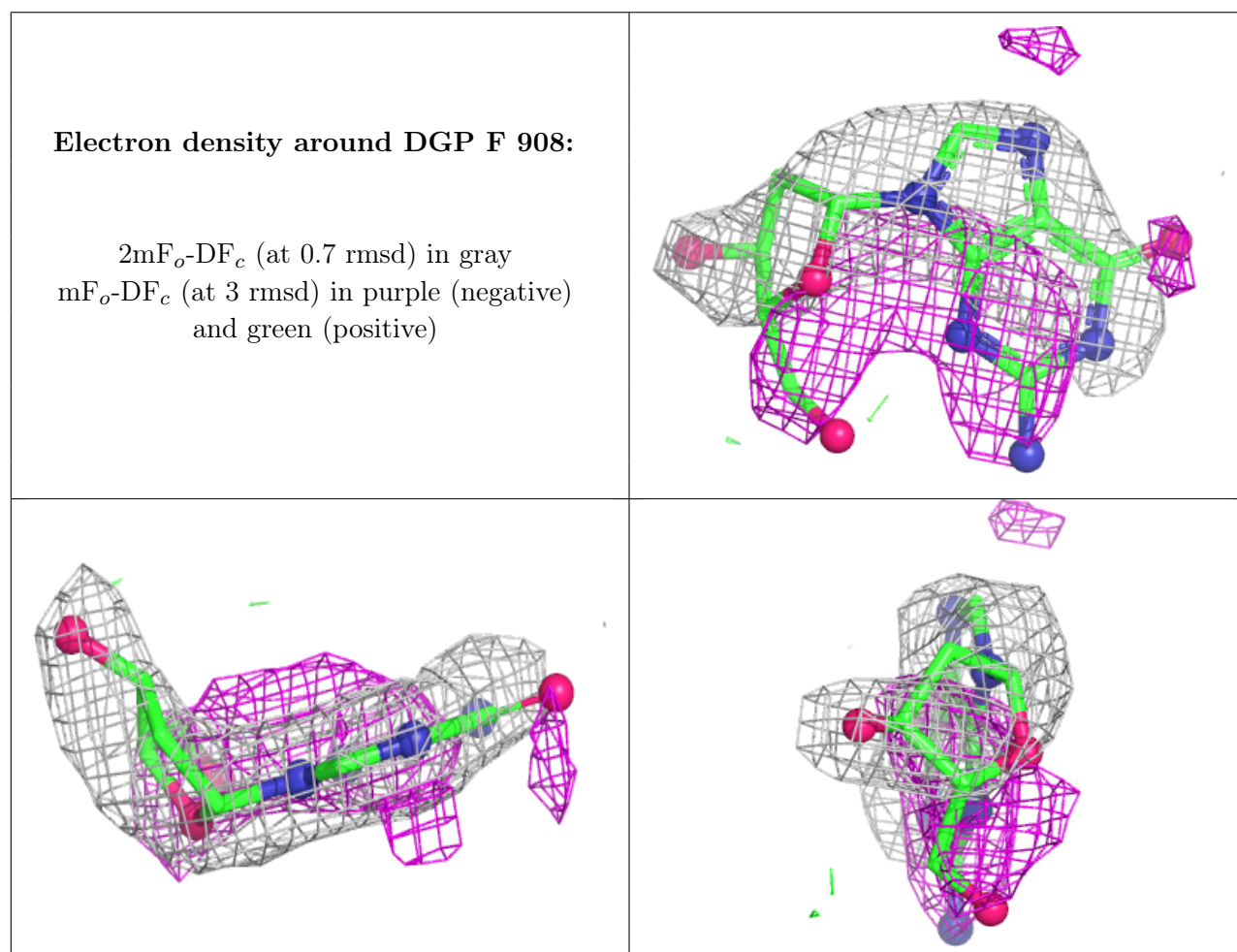
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	DGP	F	908	19/23	0.66	0.18	72,75,81,81	0
6	DGP	G	908	22/23	0.70	0.18	70,72,83,85	0
6	DGP	K	955	22/23	0.71	0.27	51,60,71,72	15
4	3DR	E	912	11/12	0.73	0.16	92,98,109,109	0
6	DGP	H	908	19/23	0.74	0.17	69,71,75,75	0
7	CA	B	1004	1/1	0.74	0.19	96,96,96,96	0
6	DGP	L	955	22/23	0.76	0.25	58,66,76,76	15
7	CA	C	1005	1/1	0.85	0.13	75,75,75,75	0
7	CA	D	1008	1/1	0.86	0.12	79,79,79,79	0
4	3DR	H	912	11/12	0.87	0.12	61,66,81,82	0
4	3DR	G	912	11/12	0.87	0.12	51,55,68,71	0
7	CA	A	1001	1/1	0.87	0.09	91,91,91,91	0
7	CA	D	1007	1/1	0.88	0.09	55,55,55,55	0
5	DOC	I	953	18/19	0.90	0.10	74,81,85,89	0
7	CA	B	1003	1/1	0.90	0.07	54,54,54,54	0
6	DGP	G	907	1/23	0.91	0.54	84,84,84,84	0
7	CA	C	1006	1/1	0.93	0.07	57,57,57,57	0
5	DOC	J	953	18/19	0.94	0.08	39,42,46,46	0
4	3DR	F	912	11/12	0.95	0.09	57,59,74,77	0
7	CA	A	1002	1/1	0.95	0.06	67,67,67,67	0
5	DOC	K	953	18/19	0.96	0.07	32,36,40,40	0

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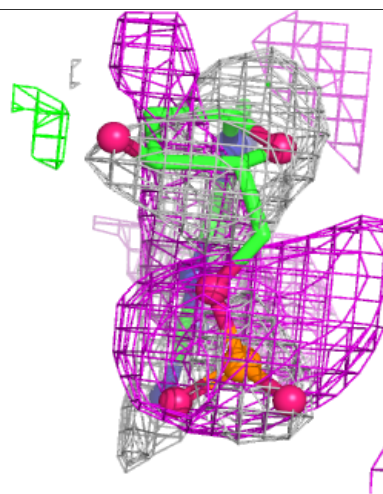
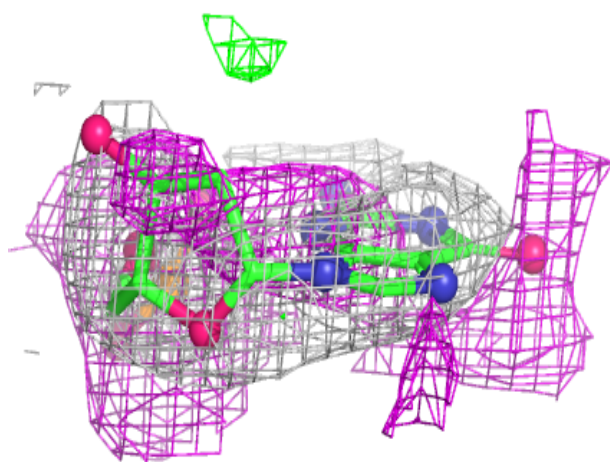
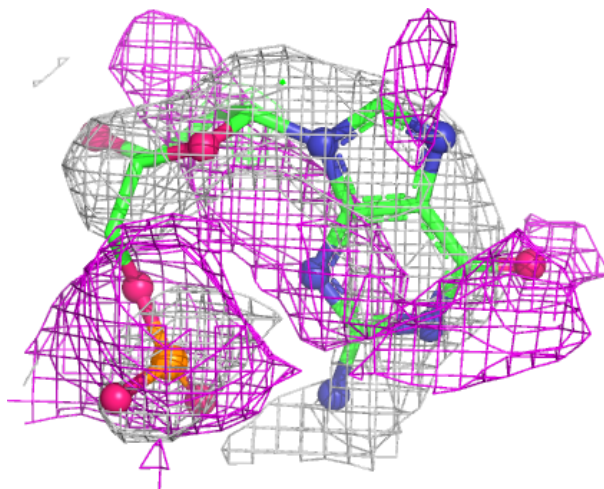
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DOC	L	953	18/19	0.96	0.07	39,43,51,52	0

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.



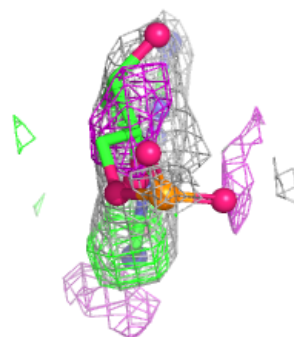
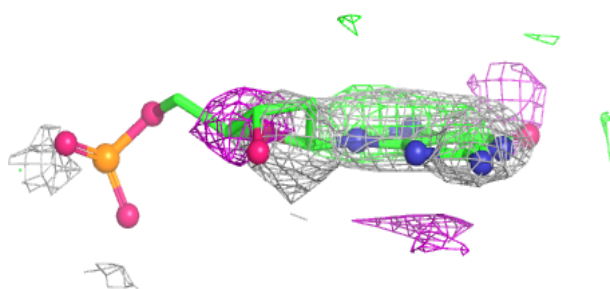
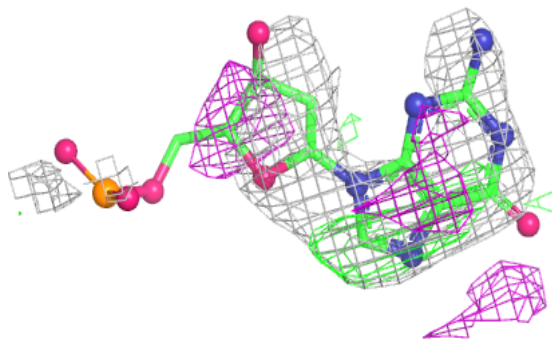
Electron density around DGP G 908:

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

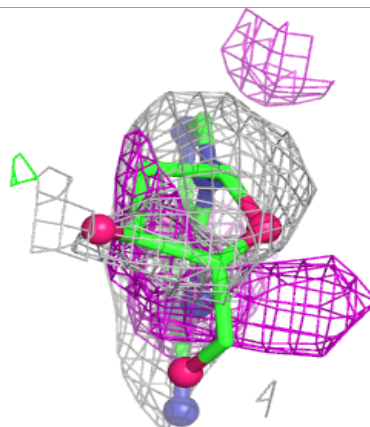
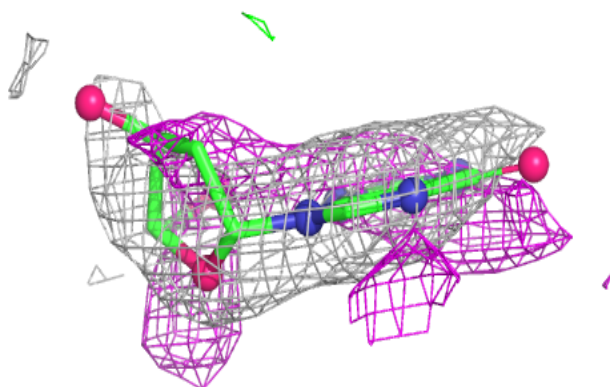
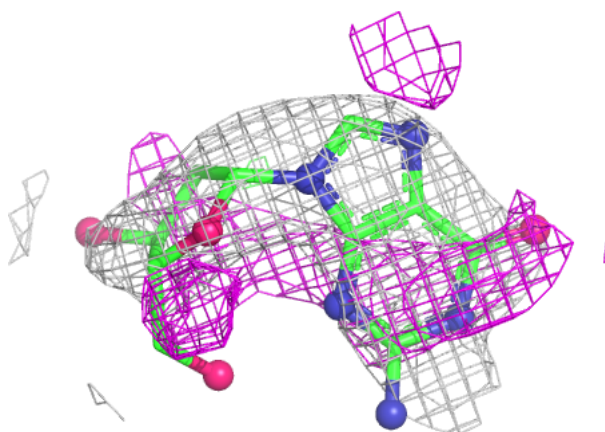


Electron density around DGP K 955:

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

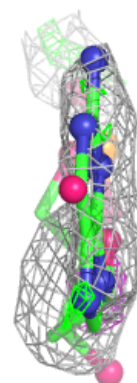
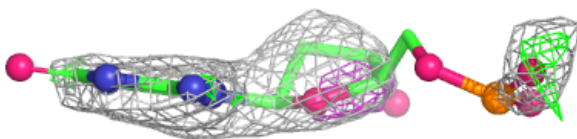
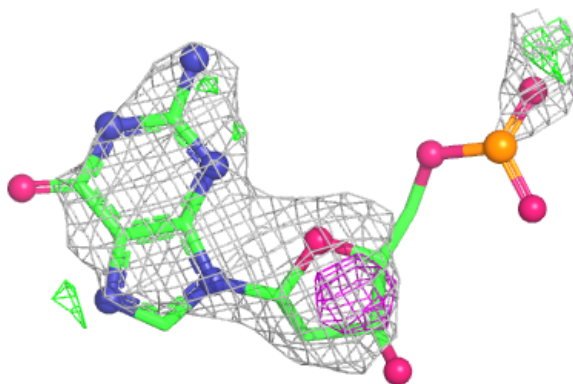
**Electron density around DGP H 908:**

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

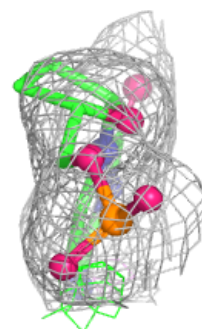
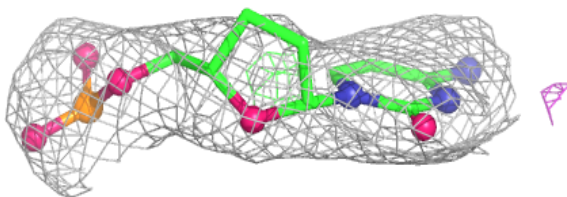
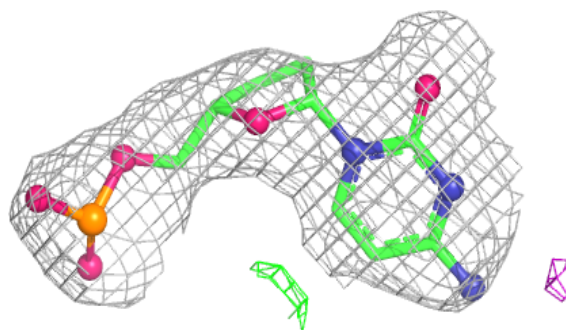


Electron density around DGP L 955:

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

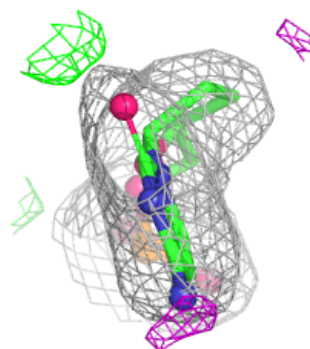
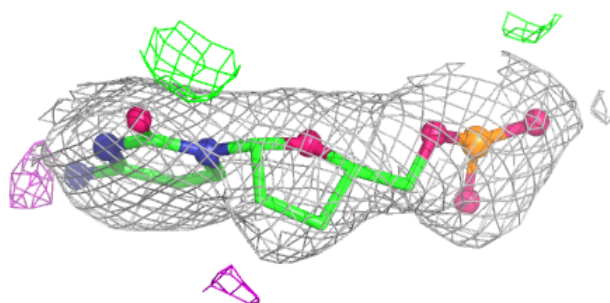
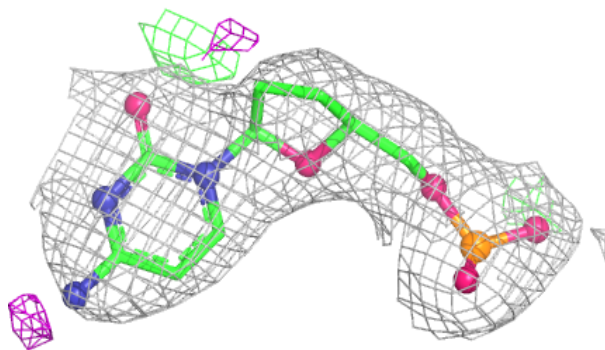
**Electron density around DOC I 953:**

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

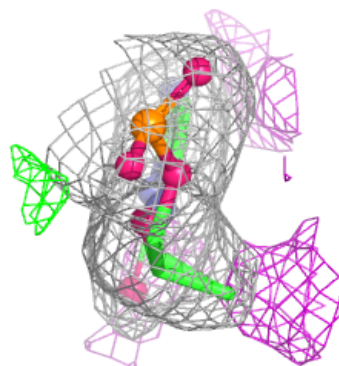
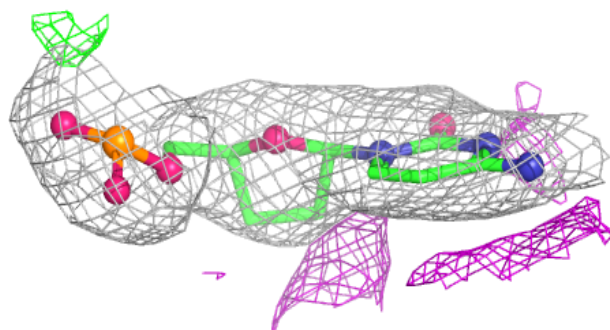
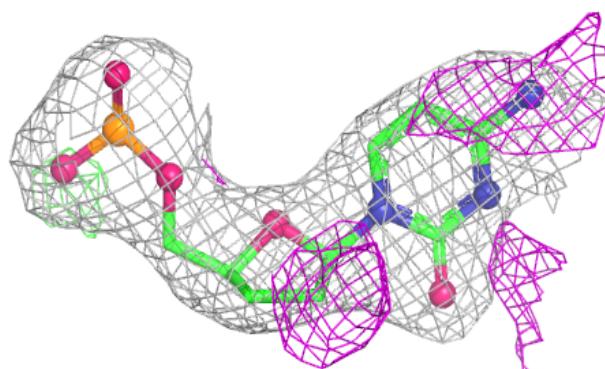


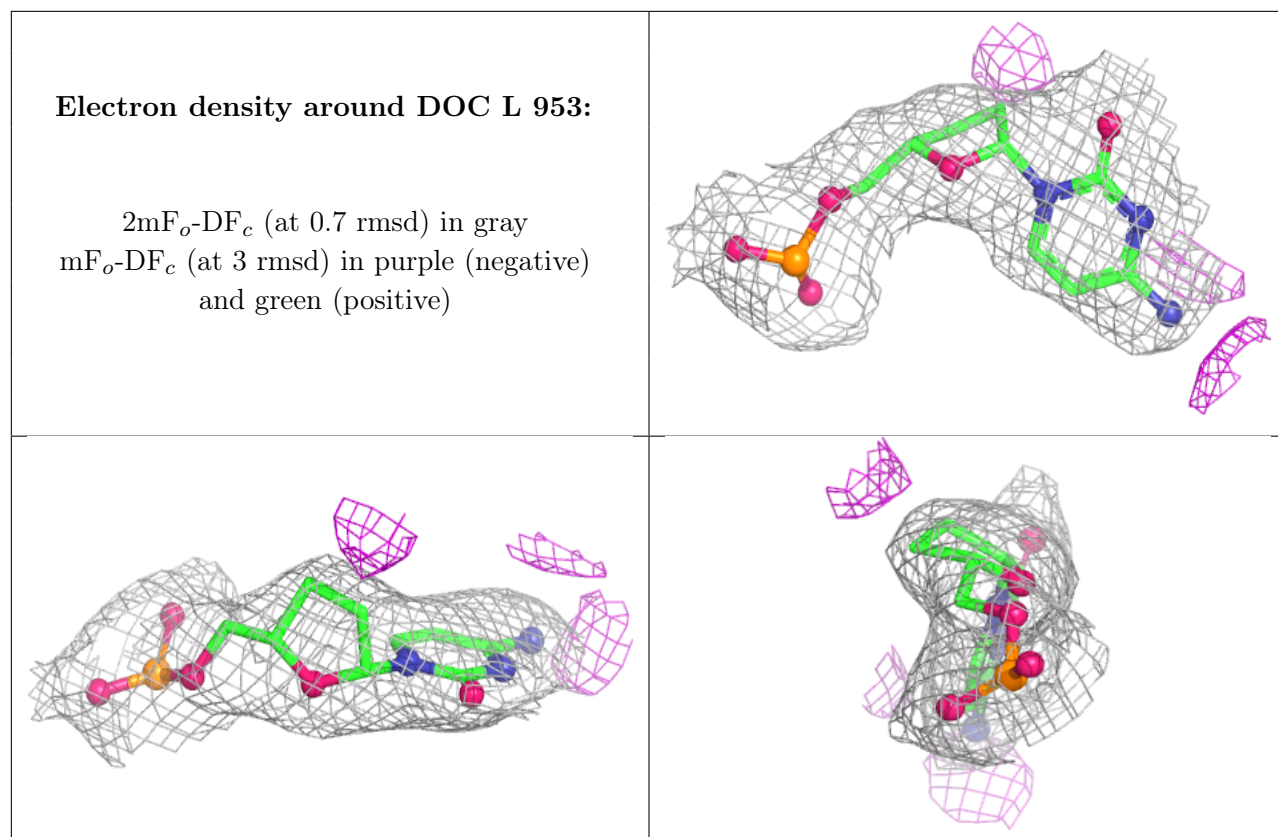
Electron density around DOC J 953:

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

**Electron density around DOC K 953:**

$2mF_o-DF_c$ (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.