WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 02:51 PM EDT

PDB ID	:	1Q9X
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:

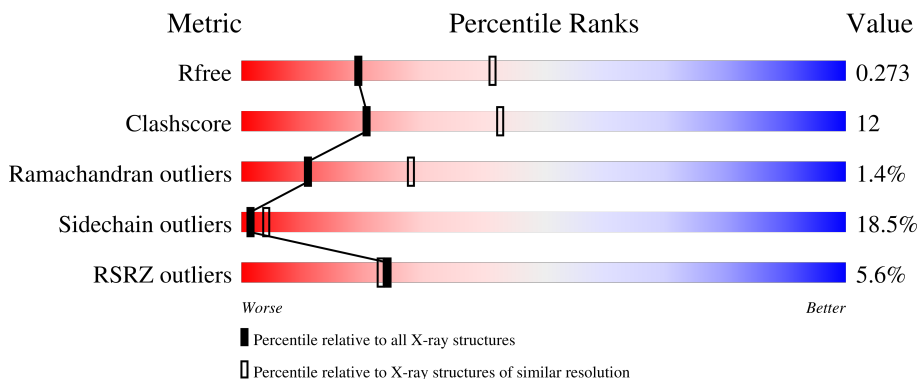|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance ⓘ

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.
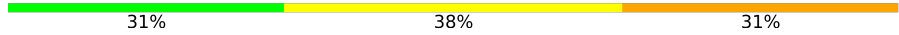
Metric	Percentile Ranks	Value
Rfree		0.273
Clashscore		12
Ramachandran outliers		1.4%
Sidechain outliers		18.5%
RSRZ outliers		5.6%

Worse   *Better*

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

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	28% / 22% 33% 44%
1	F	18	17% / 33% 33% 33%
1	G	18	11% / 28% 33% 39%
1	H	18	6% / 33% 44% 22%
2	I	13	8% 54% 38%

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Mol	Chain	Length	Quality of chain
2	J	13	31% 38% 31%
2	K	13	8% 62% 31%
2	L	13	46% 38% 15%
3	A	903	11% 60% 32% 7%
3	B	903	7% 64% 29% 6%
3	C	903	3% 67% 25% 7%
3	D	903	2% 63% 29% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DGP	F	908	-	-	-	X
6	DGP	G	908	-	-	-	X
6	DGP	K	955	-	-	-	X

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 (three-letter code: 3DR) (formula: $C_5H_{11}O_6P$).
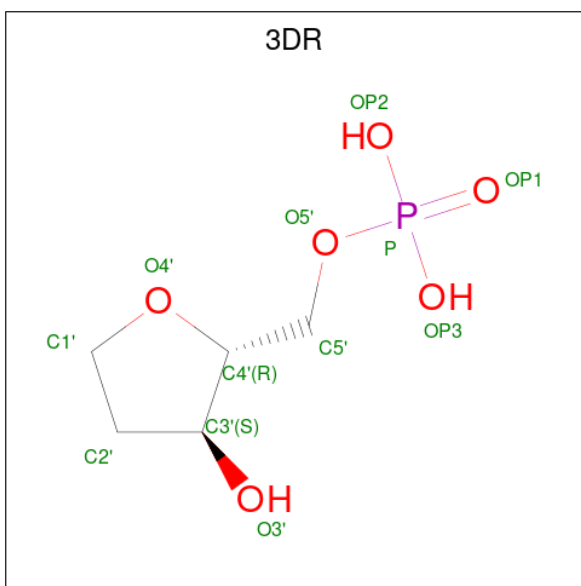
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total 11	C 5	O 5	P 1	0	0
4	F	1	Total 11	C 5	O 5	P 1	0	0
4	G	1	Total 11	C 5	O 5	P 1	0	0
4	H	1	Total 11	C 5	O 5	P 1	0	0

- Molecule 5 is 2',3'-DIDEOXYCYTIDINE-5'-MONOPHOSPHATE (three-letter code: DOC) (formula: $C_9H_{14}N_3O_6P$).
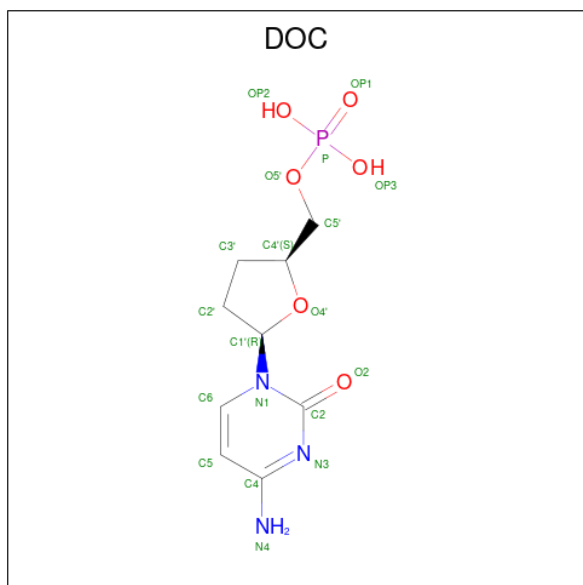
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	I	1	Total	C	N	O	P	0	0
			18	9	3	5	1		
5	J	1	Total	C	N	O	P	0	0
			18	9	3	5	1		
5	K	1	Total	C	N	O	P	0	0
			18	9	3	5	1		
5	L	1	Total	C	N	O	P	0	0
			18	9	3	5	1		

- Molecule 6 is 2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE (three-letter code: DGP) (formula: $C_{10}H_{14}N_5O_7P$).
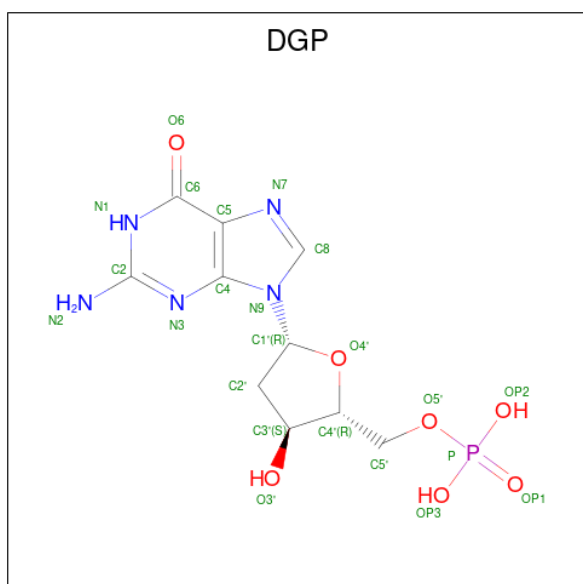
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total 19	C 10	N 5	O 4		0	0
6	G	1	Total 1	O 1				0	0
6	G	1	Total 22	C 10	N 5	O 6	P 1	0	0
6	K	1	Total 22	C 10	N 5	O 6	P 1	0	0
6	H	1	Total 19	C 10	N 5	O 4		0	0
6	L	1	Total 22	C 10	N 5	O 6	P 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is water.

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

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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 ⓘ

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, or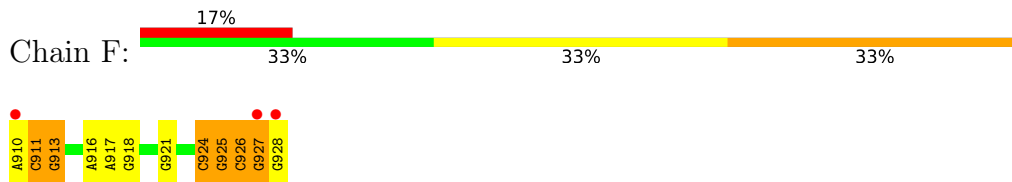ange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 5'-GCGGACTGCTTAC(dideoxycytidine)-3'
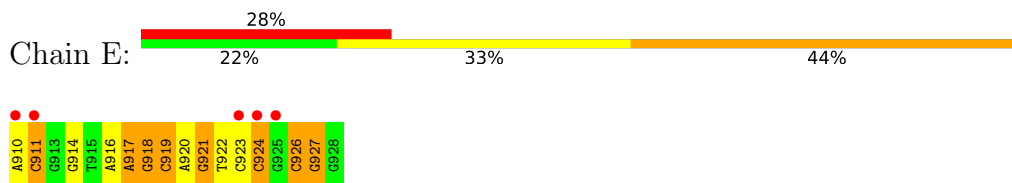
Chain E:

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

Chain F:

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

Chain G:

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

Chain H:

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

Chain I:

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

Chain J:

31%   38%   31%

G940 C941 G942 G943 A944 C945 T946 G947 C948 T949 T950 A951 C952

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

Chain K:

8%   62%   31%

G940 C941 G942 G943 A944 C945 T946 G947 C948 T949 T950 A951 C952

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

Chain L:

46%   38%   15%

G940 C941 G942 C945 T946 G947 T950 A951 C952

• Molecule 3: DNA polymerase

Chain A:

11%

60%   32%   7%   •

• Molecule 3: DNA polymerase

Chain B:

• Molecule 3: DNA polymerase

Chain C:

• Molecule 3: DNA polymerase

Chain D:
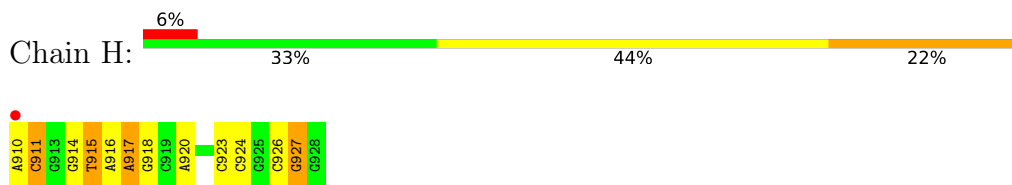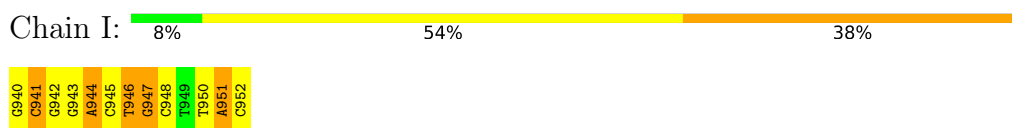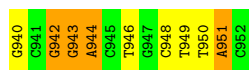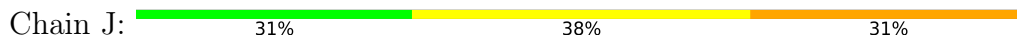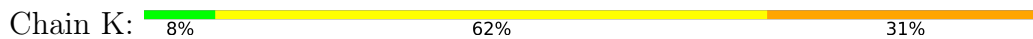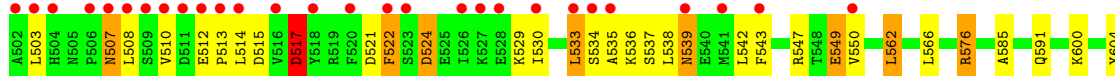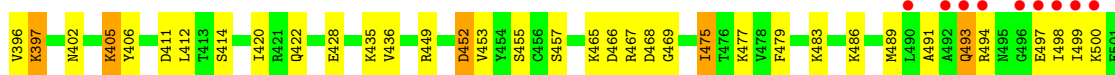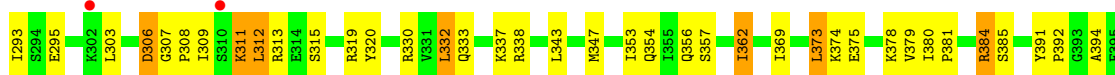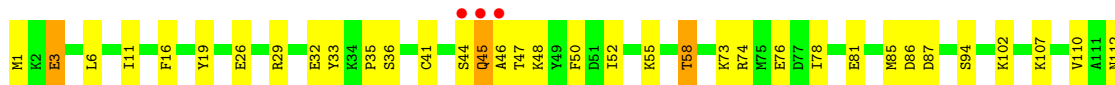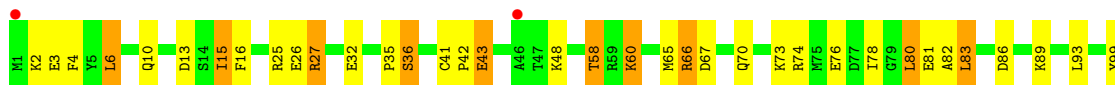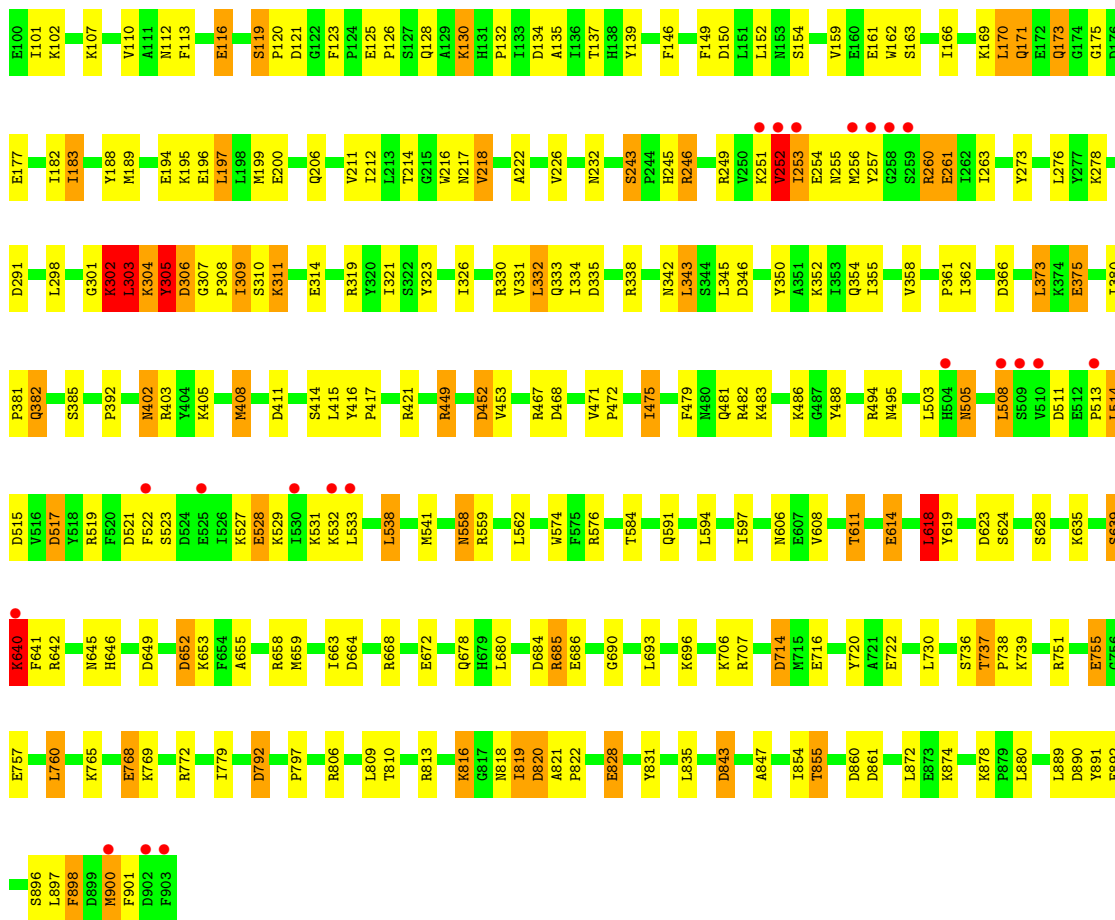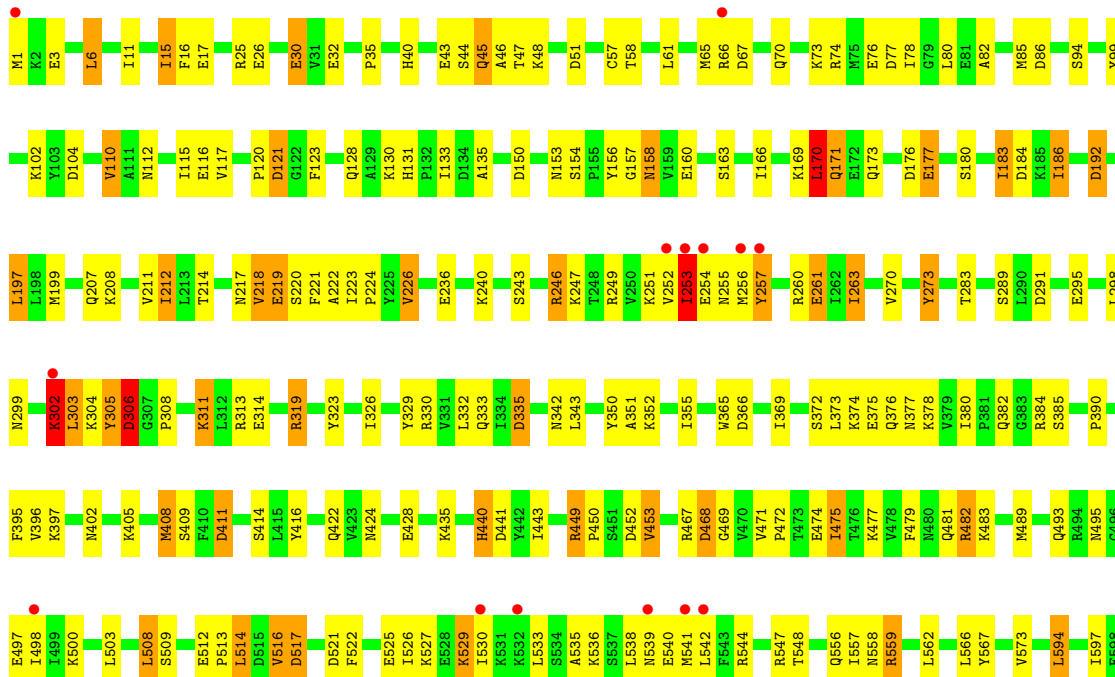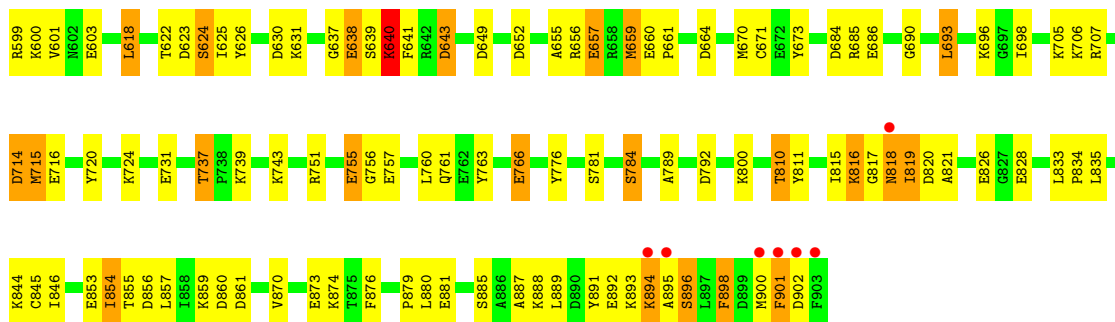
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.95Å 122.24Å 165.36Å 90.00° 96.85° 90.00°	Depositor
Resolution (Å)	47.00 – 2.69 45.07 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.7 (47.00-2.69) 95.1 (45.07-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [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)	0.30 , 45.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, 3DR, DGP, CA

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	1.19	0/415	2.02	23/637 (3.6%)
1	F	1.07	0/415	1.77	8/637 (1.3%)
1	G	1.28	2/415 (0.5%)	2.14	18/637 (2.8%)
1	H	1.43	4/415 (1.0%)	1.90	13/637 (2.0%)
2	I	1.06	0/294	1.78	9/452 (2.0%)
2	J	1.15	0/294	1.90	7/452 (1.5%)
2	K	1.20	0/294	1.89	9/452 (2.0%)
2	L	1.25	1/294 (0.3%)	1.84	6/452 (1.3%)
3	A	0.56	0/7545	0.83	32/10196 (0.3%)
3	B	0.62	0/7545	0.83	28/10196 (0.3%)
3	C	0.65	0/7545	0.87	26/10196 (0.3%)
3	D	0.60	0/7545	0.83	27/10196 (0.3%)
All	All	0.68	7/33016 (0.0%)	0.99	206/45140 (0.5%)

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)
1	H	926	DC	C4-C5	9.24	1.50	1.43
1	G	926	DC	C4-C5	6.59	1.48	1.43
1	H	926	DC	N1-C2	6.51	1.46	1.40
1	H	926	DC	N1-C6	6.47	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	926	DC	N1-C2	5.28	1.45	1.40
1	H	926	DC	N3-C4	5.25	1.37	1.33
2	L	941	DC	N1-C2	5.01	1.45	1.40

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	911	DC	C1'-O4'-C4'	-13.14	96.96	110.10
1	G	911	DC	O4'-C1'-N1	12.56	116.80	108.00
1	E	918	DG	O4'-C1'-N9	12.30	116.61	108.00
2	K	943	DG	O4'-C1'-N9	11.64	116.15	108.00
1	E	919	DC	O4'-C1'-N1	10.99	115.69	108.00
2	I	946	DT	O4'-C1'-N1	-10.78	100.46	108.00
1	G	918	DG	O4'-C1'-N9	9.75	114.83	108.00
1	H	911	DC	C1'-O4'-C4'	-9.75	100.35	110.10
1	G	926	DC	P-O3'-C3'	9.55	131.16	119.70
1	E	927	DG	O4'-C4'-C3'	-9.54	100.28	106.00
3	A	899	ASP	CB-CG-OD2	9.19	126.57	118.30
1	H	911	DC	O4'-C1'-N1	9.16	114.41	108.00
1	F	911	DC	O4'-C1'-N1	9.03	114.32	108.00
3	B	411	ASP	CB-CG-OD2	8.96	126.37	118.30
1	E	923	DC	P-O3'-C3'	8.80	130.26	119.70
3	B	466	ASP	CB-CG-OD2	8.60	126.03	118.30
1	F	924	DC	P-O3'-C3'	8.10	129.42	119.70
3	C	197	LEU	CA-CB-CG	8.02	133.76	115.30
1	G	911	DC	O4'-C4'-C3'	-7.98	101.21	106.00
2	I	941	DC	O4'-C1'-N1	7.92	113.54	108.00
2	I	947	DG	P-O3'-C3'	7.65	128.88	119.70
1	G	920	DA	O4'-C1'-N9	7.65	113.36	108.00
2	J	944	DA	P-O3'-C3'	7.58	128.79	119.70
2	J	942	DG	P-O3'-C3'	7.57	128.78	119.70
2	J	951	DA	O5'-P-OP2	-7.47	98.97	105.70
3	B	684	ASP	CB-CG-OD2	7.39	124.95	118.30
1	G	910	DA	C1'-O4'-C4'	-7.37	102.73	110.10
2	J	948	DC	O4'-C1'-N1	7.35	113.15	108.00
3	A	197	LEU	CA-CB-CG	7.29	132.06	115.30
3	A	792	ASP	CB-CG-OD2	7.29	124.86	118.30
3	C	150	ASP	CB-CG-OD2	7.28	124.85	118.30
3	B	150	ASP	CB-CG-OD2	7.20	124.78	118.30
1	G	910	DA	O4'-C1'-N9	7.19	113.03	108.00
1	E	911	DC	O4'-C1'-N1	7.14	113.00	108.00
3	B	623	ASP	CB-CG-OD2	7.08	124.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	618	LEU	CA-CB-CG	7.06	131.53	115.30
3	D	684	ASP	CB-CG-OD2	7.04	124.64	118.30
3	D	335	ASP	CB-CG-OD2	7.04	124.63	118.30
1	E	917	DA	O4'-C1'-N9	6.99	112.89	108.00
3	A	618	LEU	CA-CB-CG	6.96	131.32	115.30
3	C	649	ASP	CB-CG-OD2	6.91	124.52	118.30
2	K	941	DC	P-O3'-C3'	6.91	127.99	119.70
3	C	652	ASP	CB-CG-OD2	6.90	124.51	118.30
2	J	943	DG	P-O3'-C3'	6.89	127.97	119.70
2	I	946	DT	P-O3'-C3'	6.88	127.96	119.70
2	L	945	DC	C1'-O4'-C4'	-6.86	103.24	110.10
3	C	366	ASP	CB-CG-OD2	6.84	124.45	118.30
1	E	927	DG	P-O3'-C3'	6.82	127.88	119.70
2	K	940	DG	O4'-C1'-N9	-6.80	103.24	108.00
3	B	197	LEU	CA-CB-CG	6.76	130.84	115.30
3	C	618	LEU	CA-CB-CG	6.70	130.71	115.30
3	A	150	ASP	CB-CG-OD2	6.64	124.28	118.30
3	B	652	ASP	CB-CG-OD2	6.64	124.28	118.30
1	F	924	DC	O4'-C1'-N1	6.64	112.65	108.00
3	C	861	ASP	CB-CG-OD2	6.62	124.26	118.30
3	B	792	ASP	CB-CG-OD2	6.62	124.25	118.30
3	C	792	ASP	CB-CG-OD2	6.59	124.23	118.30
3	D	77	ASP	CB-CG-OD2	6.55	124.20	118.30
1	G	927	DG	O4'-C1'-N9	6.55	112.58	108.00
3	D	792	ASP	CB-CG-OD2	6.54	124.19	118.30
3	A	714	ASP	CB-CG-OD2	6.54	124.19	118.30
1	E	926	DC	P-O3'-C3'	6.54	127.55	119.70
2	I	941	DC	P-O3'-C3'	6.53	127.54	119.70
3	D	649	ASP	CB-CG-OD2	6.52	124.17	118.30
2	K	946	DT	C6-C5-C7	-6.52	118.99	122.90
3	B	899	ASP	CB-CG-OD2	6.50	124.15	118.30
3	C	515	ASP	CB-CG-OD2	6.49	124.14	118.30
3	C	517	ASP	CB-CG-OD2	6.47	124.12	118.30
1	E	919	DC	C1'-O4'-C4'	-6.46	103.64	110.10
3	D	664	ASP	CB-CG-OD2	6.43	124.09	118.30
3	A	684	ASP	CB-CG-OD2	6.42	124.08	118.30
3	A	184	ASP	CB-CG-OD2	6.42	124.08	118.30
1	H	926	DC	O4'-C1'-N1	6.40	112.48	108.00
3	C	820	ASP	CB-CG-OD2	6.39	124.05	118.30
3	D	861	ASP	CB-CG-OD2	6.36	124.02	118.30
1	H	918	DG	C1'-O4'-C4'	-6.35	103.75	110.10
1	E	922	DT	C4-C5-C7	6.34	122.80	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	466	ASP	CB-CG-OD2	6.32	123.98	118.30
2	I	951	DA	C4'-C3'-C2'	-6.31	97.42	103.10
3	A	623	ASP	CB-CG-OD2	6.31	123.98	118.30
1	G	918	DG	P-O3'-C3'	6.30	127.26	119.70
2	K	946	DT	C4-C5-C7	6.26	122.75	119.00
3	D	150	ASP	CB-CG-OD2	6.23	123.90	118.30
1	E	921	DG	P-O3'-C3'	6.22	127.17	119.70
2	K	952	DC	O5'-P-OP2	-6.22	100.10	105.70
3	D	197	LEU	CA-CB-CG	6.22	129.60	115.30
3	A	291	ASP	CB-CG-OD2	6.19	123.87	118.30
2	K	945	DC	C1'-O4'-C4'	-6.18	103.92	110.10
3	A	835	LEU	CA-CB-CG	6.17	129.50	115.30
3	B	515	ASP	CB-CG-OD2	6.17	123.86	118.30
3	A	144	ASP	CB-CG-OD2	6.17	123.85	118.30
3	B	87	ASP	CB-CG-OD2	6.16	123.84	118.30
3	B	452	ASP	CB-CG-OD2	6.16	123.84	118.30
3	A	411	ASP	CB-CG-OD2	6.14	123.82	118.30
1	E	914	DG	P-O3'-C3'	6.13	127.06	119.70
2	I	948	DC	P-O3'-C3'	6.12	127.05	119.70
1	H	918	DG	P-O3'-C3'	6.11	127.03	119.70
1	E	919	DC	P-O3'-C3'	6.07	126.98	119.70
3	A	861	ASP	CB-CG-OD2	6.04	123.74	118.30
3	C	86	ASP	CB-CG-OD2	6.03	123.73	118.30
2	J	950	DT	O5'-P-OP2	-6.01	100.29	105.70
1	G	913	DG	N1-C6-O6	-6.00	116.30	119.90
1	G	919	DC	P-O3'-C3'	5.98	126.88	119.70
1	F	911	DC	C1'-O4'-C4'	-5.95	104.15	110.10
2	L	945	DC	O4'-C1'-N1	5.95	112.16	108.00
3	D	170	LEU	CA-CB-CG	5.94	128.97	115.30
3	C	134	ASP	CB-CG-OD2	5.93	123.64	118.30
1	F	927	DG	P-O3'-C3'	5.93	126.82	119.70
3	D	521	ASP	CB-CG-OD2	5.90	123.61	118.30
1	E	927	DG	C3'-C2'-C1'	-5.89	95.43	102.50
3	C	714	ASP	CB-CG-OD2	5.89	123.60	118.30
3	A	856	ASP	CB-CG-OD2	5.87	123.59	118.30
1	G	927	DG	C1'-O4'-C4'	-5.87	104.23	110.10
3	B	517	ASP	CB-CG-OD2	5.87	123.58	118.30
3	A	630	ASP	CB-CG-OD2	5.85	123.57	118.30
3	B	192	ASP	CB-CG-OD2	5.83	123.55	118.30
1	E	917	DA	C4'-C3'-C2'	-5.82	97.86	103.10
2	L	951	DA	O5'-P-OP2	-5.79	100.49	105.70
2	I	944	DA	P-O3'-C3'	5.78	126.64	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	306	ASP	CB-CG-OD2	5.78	123.50	118.30
3	D	306	ASP	CB-CG-OD2	5.77	123.49	118.30
3	D	192	ASP	CB-CG-OD2	5.77	123.49	118.30
3	A	77	ASP	CB-CG-OD2	5.76	123.48	118.30
3	B	861	ASP	CB-CG-OD2	5.75	123.47	118.30
1	G	922	DT	O4'-C1'-N1	-5.71	104.00	108.00
2	L	947	DG	O4'-C1'-N9	5.70	111.99	108.00
1	H	926	DC	P-O3'-C3'	5.69	126.53	119.70
3	C	452	ASP	CB-CG-OD2	5.65	123.39	118.30
1	E	921	DG	C5-C6-O6	-5.64	125.21	128.60
3	A	621	ASP	CB-CG-OD2	5.63	123.37	118.30
3	B	86	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	926	DC	C1'-O4'-C4'	-5.60	104.50	110.10
1	F	925	DG	O4'-C1'-N9	5.59	111.92	108.00
1	H	914	DG	N1-C6-O6	-5.59	116.55	119.90
1	G	926	DC	C6-N1-C2	5.59	122.54	120.30
3	D	121	ASP	CB-CG-OD2	5.59	123.33	118.30
2	K	951	DA	O5'-P-OP2	-5.55	100.70	105.70
3	A	441	ASP	CB-CG-OD2	5.55	123.30	118.30
3	A	649	ASP	CB-CG-OD2	5.55	123.30	118.30
1	E	922	DT	P-O3'-C3'	5.50	126.30	119.70
3	A	515	ASP	CB-CG-OD2	5.48	123.23	118.30
3	C	13	ASP	CB-CG-OD2	5.48	123.23	118.30
3	D	714	ASP	CB-CG-OD2	5.47	123.22	118.30
3	D	517	ASP	CB-CG-OD2	5.46	123.21	118.30
3	C	338	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	H	918	DG	O4'-C4'-C3'	-5.45	102.32	104.50
2	L	947	DG	C8-N9-C4	-5.45	104.22	106.40
1	F	913	DG	O4'-C4'-C3'	-5.43	102.33	104.50
2	J	949	DT	C1'-O4'-C4'	-5.43	104.67	110.10
1	E	917	DA	P-O3'-C3'	5.42	126.20	119.70
1	E	921	DG	C1'-O4'-C4'	-5.41	104.69	110.10
1	H	917	DA	P-O3'-C3'	5.41	126.19	119.70
1	E	922	DT	O4'-C1'-C2'	-5.40	101.58	105.90
3	D	856	ASP	CB-CG-OD2	5.40	123.16	118.30
3	B	468	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	924	DC	O4'-C1'-N1	5.38	111.77	108.00
1	H	920	DA	P-O3'-C3'	5.36	126.14	119.70
3	D	291	ASP	CB-CG-OD2	5.36	123.13	118.30
3	A	643	ASP	CB-CG-OD2	5.36	123.12	118.30
3	C	664	ASP	CB-CG-OD2	5.34	123.11	118.30
3	A	140	ASP	CB-CG-OD2	5.34	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	346	ASP	CB-CG-OD2	5.32	123.08	118.30
1	F	926	DC	P-O3'-C3'	5.31	126.07	119.70
3	D	86	ASP	CB-CG-OD2	5.30	123.07	118.30
2	I	946	DT	N1-C1'-C2'	5.30	122.66	112.60
3	D	468	ASP	CB-CG-OD2	5.29	123.06	118.30
3	D	630	ASP	CB-CG-OD2	5.28	123.05	118.30
1	H	917	DA	O4'-C1'-N9	5.28	111.70	108.00
3	A	652	ASP	CB-CG-OD2	5.28	123.05	118.30
3	C	623	ASP	CB-CG-OD2	5.26	123.04	118.30
1	H	915	DT	O4'-C4'-C3'	5.26	109.16	106.00
3	B	524	ASP	CB-CG-OD2	5.25	123.03	118.30
3	A	87	ASP	CB-CG-OD2	5.24	123.02	118.30
3	B	860	ASP	CB-CG-OD2	5.23	123.01	118.30
3	D	67	ASP	CB-CG-OD2	5.23	123.01	118.30
3	A	511	ASP	CB-CG-OD2	5.22	123.00	118.30
1	G	915	DT	C5-C4-O4	-5.21	121.25	124.90
1	G	918	DG	N1-C6-O6	-5.21	116.77	119.90
3	B	843	ASP	CB-CG-OD2	5.20	122.98	118.30
3	B	253	ILE	N-CA-C	5.19	125.01	111.00
3	C	121	ASP	CB-CG-OD2	5.19	122.97	118.30
3	C	67	ASP	CB-CG-OD2	5.18	122.96	118.30
3	D	623	ASP	CB-CG-OD2	5.18	122.96	118.30
3	C	860	ASP	CB-CG-OD2	5.18	122.96	118.30
3	D	104	ASP	CB-CG-OD2	5.17	122.95	118.30
3	C	890	ASP	CB-CG-OD2	5.16	122.94	118.30
3	B	867	ASP	CB-CG-OD2	5.15	122.93	118.30
3	A	524	ASP	CB-CG-OD2	5.14	122.93	118.30
1	G	922	DT	N1-C1'-C2'	5.14	122.36	112.60
3	B	114	ASP	CB-CG-OD2	5.14	122.92	118.30
3	C	684	ASP	CB-CG-OD2	5.13	122.92	118.30
3	D	184	ASP	CB-CG-OD2	5.13	122.92	118.30
3	A	664	ASP	CB-CG-OD2	5.11	122.90	118.30
3	A	86	ASP	CB-CG-OD2	5.10	122.89	118.30
3	B	890	ASP	CB-CG-OD2	5.09	122.88	118.30
2	L	941	DC	P-O3'-C3'	5.07	125.78	119.70
2	K	948	DC	C1'-O4'-C4'	-5.06	105.04	110.10
1	E	927	DG	O4'-C1'-N9	5.04	111.53	108.00
1	H	927	DG	O4'-C1'-N9	5.03	111.52	108.00
3	D	411	ASP	CB-CG-OD2	5.02	122.82	118.30
3	A	890	ASP	CB-CG-OD2	5.02	122.82	118.30
3	B	521	ASP	CB-CG-OD2	5.02	122.82	118.30
3	B	820	ASP	CB-CG-OD2	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	366	ASP	CB-CG-OD2	5.01	122.81	118.30
3	A	121	ASP	CB-CG-OD2	5.01	122.81	118.30
3	C	335	ASP	CB-CG-OD2	5.01	122.81	118.30

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	3	0
3	A	7365	0	7257	191	0
3	B	7365	0	7258	158	0
3	C	7365	0	7258	172	0
3	D	7365	0	7258	188	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	1	0
5	L	18	0	12	0	0
6	F	19	0	12	0	0
6	G	23	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	16	0
8	B	129	0	0	18	0
8	C	126	0	0	21	0
8	D	111	0	0	18	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
All	All	32756	0	30567	769	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 12.

All (769) 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:514:LEU:H	3:C:541:MET:HE2	1.11	1.12
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:319:ARG:HG2	3:A:319:ARG:HH11	1.32	0.92
3:C:639:SER:C	3:C:641:PHE:H	1.72	0.92
3:A:251:LYS:HB3	3:A:262:ILE:HD13	1.52	0.91
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
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:C:514:LEU:N	3:C:541:MET:HE2	1.91	0.84
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:A:196:GLU:OE2	8:A:1101:HOH:O	1.96	0.83
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: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:D:533:LEU:HD13	3:D:541:MET:HE3	1.63	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:A:639:SER:C	3:A:641:PHE:H	1.88	0.77
3:B:606:ASN:OD1	3:B:611:THR:HG22	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:513:PRO:HA	3:D:541:MET:HE2	1.68	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: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
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:C:408:MET:HE1	3:C:655:ALA:HB2	1.69	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
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:D:408:MET:CE	3:D:655:ALA:HB2	2.20	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:HE2	3:D:655:ALA:HB2	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:163:SER:HA	8:B:1066:HOH:O	1.91	0.70
3:B:640:LYS:O	3:B:640:LYS:HG2	1.90	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: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:D:304:LYS:O	3:D:305:TYR:HB3	1.93	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
3:B:251:LYS:HB3	3:B:262:ILE:CD1	2.23	0.67
3:C:305:TYR:CD1	3:C:305:TYR:C	2.66	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: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: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
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:347:MET:SD	3:A:562:LEU:HD13	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:639:SER:O	3:B:640:LYS:C	2.38	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: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
3:D:652:ASP:CG	3:D:656:ARG:HH21	2.04	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:A:639:SER:C	3:A:641:PHE:N	2.53	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: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:639:SER:C	3:C:641:PHE:N	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:513:PRO:HA	3:D:541:MET:CE	2.31	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:308:PRO:HG2	3:C:311:LYS:HZ3	1.66	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
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:343:LEU:HD22	3:C:558:ASN:ND2	2.19	0.58
3:A:44:SER:C	3:A:46:ALA:H	2.07	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:A:139:TYR:OH	3:A:144:ASP:OD1	2.17	0.57
3:B:894:LYS:HG3	3:B:897:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:898:PHE:CD1	3:D:898:PHE:C	2.78	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: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
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:C:252:VAL:C	3:C:253:ILE:HG13	2.25	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:C:305:TYR:HD1	3:C:305:TYR:C	2.05	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: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:38:PHE:CE2	3:A:59:ARG:HG3	2.41	0.55
3:B:330:ARG:HD3	3:B:333:GLN:NE2	2.21	0.55
3:A:777:ILE:CD1	3:A:848:TRP:HZ2	2.20	0.55
3:C:896:SER:C	3:C:898:PHE:H	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:166:ILE:O	3:B:166:ILE:HG22	2.09	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: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:642:ARG:H	3:B:646:HIS:HD2	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:686:GLU:OE1	3:D:716:GLU:HG3	2.09	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
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: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:C:514:LEU:HD22	3:C:541:MET:HE1	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: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:C:411:ASP:OD2	3:C:624:SER:OG	2.23	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:A:898:PHE:O	3:A:899:ASP:CG	2.49	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:A:165:GLU:CD	3:A:165:GLU:H	2.15	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:D:253:ILE:HG22	3:D:260:ARG:C	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:G:920:DA:OP2	8:G:443:HOH:O	2.19	0.49
1:E:916:DA:H5"	3:A:705:LYS:CD	2.41	0.49
3:A:408:MET:HE2	3:A:685:ARG:HD2	1.94	0.49
3:B:236:GLU:O	3:B:240:LYS:HG2	2.12	0.49
3:C:99:TYR:O	3:C:352:LYS:NZ	2.43	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: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:740:ALA:HB3	3:A:779:ILE:HG22	1.94	0.49
3:C:304:LYS:O	3:C:323:TYR:OH	2.30	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:308:PRO:O	3:C:310:SER:N	2.45	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:D:639:SER:C	3:D:641:PHE:N	2.66	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:566:LEU:O	3:A:567:TYR:C	2.51	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:199:MET:HA	3:A:199:MET:HE3	1.94	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
3:D:533:LEU:CD1	3:D:541:MET:CE	2.91	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: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: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: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
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:B:165:GLU:H	3:B:165:GLU:CD	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:311:LYS:N	3:D:311:LYS:HZ2	2.12	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:HG22	3:D:263:ILE:O	2.13	0.47
3:A:806:ARG:HB3	3:A:845:CYS:SG	2.55	0.47
3:D:639:SER:C	3:D:641:PHE:H	2.18	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:A:440:HIS:CD2	3:A:440:HIS:C	2.88	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: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
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:518:TYR:HB3	8:A:1065:HOH:O	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:639:SER:O	3:D:641:PHE:N	2.47	0.47
3:D:715:MET:HE3	8:D:1045:HOH:O	2.15	0.47
3:A:468:ASP:HB3	3:A:677:LYS:HZ3	1.80	0.47
3:B:44:SER:C	3:B:46:ALA:H	2.19	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:C:408:MET:HE2	3:C:655:ALA:HB2	1.96	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:C:652:ASP:OD1	3:C:685:ARG:NH1	2.47	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
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: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
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:D:222:ALA:O	3:D:226:VAL:HG13	2.16	0.45
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: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
2:I:946:DT:H1'	2:I:947:DG:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:699:GLY:C	3:A:753:LEU:HD22	2.37	0.45
3:A:121:ASP:HB2	3:A:122:GLY:H	1.59	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:D:16:PHE:CE1	3:D:30:GLU:HG3	2.52	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: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:408:MET:HE3	3:A:688:ILE:HG12	1.99	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:469:GLY:C	3:D:472:PRO:HD2	2.38	0.44
3:D:720:TYR:CZ	3:D:724:LYS:HD2	2.51	0.44
3:B:311:LYS:HZ2	3:B:311:LYS:H	1.64	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:C:686:GLU:OE1	3:C:716:GLU:CD	2.55	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
3:B:171:GLN:OE1	3:B:177:GLU:HG3	2.17	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:926:DC:H2"	1:F:927:DG:OP2	2.17	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
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: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: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
2:I:942:DG:H2"	2:I:943:DG:OP2	2.18	0.43
3:C:513:PRO:HA	3:C:541:MET:HE3	2.00	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: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:C:15:ILE:HD12	3:C:65:MET:CE	2.49	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:A:414:SER:O	3:A:415:LEU:C	2.56	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
2:I:952:DC:OP1	3:A:728:MET:HE3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:171:GLN:CD	3:B:171:GLN:H	2.20	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
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:A:181:GLU:CD	3:A:181:GLU:H	2.22	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: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: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
3:B:457:SER:OG	3:B:585:ALA:O	2.35	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:15:ILE:HD12	3:D:65:MET:CE	2.48	0.42
3:A:90:LEU:O	3:A:94:SER:HB2	2.19	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:D:304:LYS:O	3:D:305:TYR:CB	2.65	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:196:GLU:CD	8:A:1101:HOH:O	2.52	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
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: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:D:898:PHE:C	3:D:898:PHE:HD1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:819:ILE:C	3:A:821:ALA:H	2.23	0.41
3:B:145:ARG:HB3	8:B:1124:HOH:O	2.20	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
3:D:895:ALA:O	3:D:896:SER:C	2.58	0.41
1:F:921:DG:N2	2:J:946:DT:O2	2.53	0.41
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: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:D:15:ILE:HD12	3:D:65:MET:HE1	2.01	0.41
3:A:408:MET:CE	3:A:685:ARG:HD2	2.49	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
1:E:910:DA:H8	1:E:911:DC:O2	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:608:VAL:HG12	3:A:609:CYS:N	2.36	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:169:LYS:C	3:C:175:GLY:HA3	2.40	0.41
3:C:212:ILE:CD1	3:C:345:LEU:HD21	2.51	0.41
3:D:80:LEU:HD23	3:D:80:LEU:HA	1.93	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:C:414:SER:O	3:C:415:LEU:C	2.59	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:D:901:PHE:O	3:D:902:ASP:C	2.58	0.41
3:B:394:ALA:C	3:B:591:GLN:OE1	2.59	0.40
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:C:416:TYR:O	3:C:417:PRO:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:894:LYS:C	3:D:896:SER:H	2.25	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:354:GLN:O	3:A:355:ILE:C	2.59	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: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
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:517:ASP:N	3:B:517:ASP:OD1	2.53	0.40
3:B:730:LEU:HD13	3:B:883:PHE:CE1	2.55	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	9	23
3	B	901/903 (100%)	830 (92%)	62 (7%)	9 (1%)	15	37
3	C	901/903 (100%)	827 (92%)	60 (7%)	14 (2%)	9	24
3	D	901/903 (100%)	823 (91%)	64 (7%)	14 (2%)	9	24
All	All	3604/3612 (100%)	3285 (91%)	267 (7%)	52 (1%)	11	28

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
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

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Mol	Chain	Res	Type
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
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%)	636 (80%)	162 (20%)	1	3
3	B	798/800 (100%)	640 (80%)	158 (20%)	1	3
3	C	798/800 (100%)	669 (84%)	129 (16%)	2	6
3	D	798/800 (100%)	656 (82%)	142 (18%)	2	4
All	All	3192/3200 (100%)	2601 (82%)	591 (18%)	1	4

All (591) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2	LYS
3	A	6	LEU
3	A	15	ILE
3	A	27	ARG
3	A	32	GLU
3	A	34	LYS
3	A	43	GLU
3	A	48	LYS
3	A	55	LYS
3	A	58	THR
3	A	59	ARG
3	A	66	ARG

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Mol	Chain	Res	Type
3	A	73	LYS
3	A	76	GLU
3	A	80	LEU
3	A	94	SER
3	A	98	ASN
3	A	100	GLU
3	A	101	ILE
3	A	105	HIS
3	A	106	THR
3	A	112	ASN
3	A	121	ASP
3	A	128	GLN
3	A	130	LYS
3	A	163	SER
3	A	170	LEU
3	A	171	GLN
3	A	172	GLU
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	237	SER
3	A	246	ARG
3	A	247	LYS
3	A	252	VAL
3	A	254	GLU
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	291	ASP
3	A	295	GLU
3	A	302	LYS
3	A	303	LEU
3	A	304	LYS
3	A	309	ILE

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Mol	Chain	Res	Type
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	357	SER
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	402	ASN
3	A	408	MET
3	A	426	SER
3	A	435	LYS
3	A	440	HIS
3	A	448	GLU
3	A	449	ARG
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	520	PHE
3	A	521	ASP
3	A	524	ASP
3	A	529	LYS

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Mol	Chain	Res	Type
3	A	530	ILE
3	A	531	LYS
3	A	532	LYS
3	A	533	LEU
3	A	536	LYS
3	A	538	LEU
3	A	541	MET
3	A	542	LEU
3	A	543	PHE
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	558	ASN
3	A	562	LEU
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	703	THR
3	A	725	LEU
3	A	735	SER
3	A	737	THR
3	A	743	LYS
3	A	758	GLU
3	A	759	SER
3	A	760	LEU
3	A	773	GLN
3	A	777	ILE
3	A	783	SER

Continued from previous page...

Mol	Chain	Res	Type
3	A	784	SER
3	A	806	ARG
3	A	810	THR
3	A	813	ARG
3	A	819	ILE
3	A	825	VAL
3	A	826	GLU
3	A	829	LYS
3	A	831	TYR
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	870	VAL
3	A	874	LYS
3	A	878	LYS
3	A	880	LEU
3	A	881	GLU
3	A	885	SER
3	A	899	ASP
3	A	900	MET
3	B	1	MET
3	B	3	GLU
3	B	6	LEU
3	B	26	GLU
3	B	32	GLU
3	B	36	SER
3	B	45	GLN
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	102	LYS
3	B	107	LYS
3	B	110	VAL

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Mol	Chain	Res	Type
3	B	112	ASN
3	B	113	PHE
3	B	123	PHE
3	B	128	GLN
3	B	130	LYS
3	B	141	SER
3	B	154	SER
3	B	158	ASN
3	B	169	LYS
3	B	170	LEU
3	B	171	GLN
3	B	173	GLN
3	B	177	GLU
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
3	B	261	GLU
3	B	262	ILE
3	B	263	ILE
3	B	279	LYS
3	B	281	SER
3	B	283	THR
3	B	291	ASP
3	B	295	GLU
3	B	303	LEU
3	B	306	ASP

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Mol	Chain	Res	Type
3	B	309	ILE
3	B	311	LYS
3	B	312	LEU
3	B	315	SER
3	B	319	ARG
3	B	332	LEU
3	B	337	LYS
3	B	338	ARG
3	B	343	LEU
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	384	ARG
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	467	ARG
3	B	475	ILE
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	517	ASP
3	B	522	PHE

Continued from previous page...

Mol	Chain	Res	Type
3	B	524	ASP
3	B	530	ILE
3	B	533	LEU
3	B	536	LYS
3	B	538	LEU
3	B	539	ASN
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	611	THR
3	B	614	GLU
3	B	618	LEU
3	B	628	SER
3	B	640	LYS
3	B	642	ARG
3	B	646	HIS
3	B	653	LYS
3	B	656	ARG
3	B	664	ASP
3	B	693	LEU
3	B	715	MET
3	B	716	GLU
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	781	SER
3	B	800	LYS
3	B	810	THR
3	B	816	LYS
3	B	819	ILE
3	B	820	ASP
3	B	826	GLU
3	B	828	GLU

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Mol	Chain	Res	Type
3	B	829	LYS
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	880	LEU
3	B	885	SER
3	B	890	ASP
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
3	C	43	GLU
3	C	48	LYS
3	C	58	THR
3	C	60	LYS
3	C	66	ARG
3	C	73	LYS
3	C	74	ARG
3	C	76	GLU
3	C	80	LEU
3	C	83	LEU
3	C	102	LYS
3	C	107	LYS
3	C	110	VAL
3	C	116	GLU
3	C	119	SER
3	C	123	PHE
3	C	130	LYS
3	C	154	SER

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Mol	Chain	Res	Type
3	C	163	SER
3	C	170	LEU
3	C	171	GLN
3	C	173	GLN
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	218	VAL
3	C	243	SER
3	C	246	ARG
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	273	TYR
3	C	278	LYS
3	C	291	ASP
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	342	ASN
3	C	343	LEU
3	C	373	LEU
3	C	375	GLU
3	C	382	GLN
3	C	402	ASN
3	C	408	MET
3	C	449	ARG

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Mol	Chain	Res	Type
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	503	LEU
3	C	505	ASN
3	C	508	LEU
3	C	511	ASP
3	C	514	LEU
3	C	523	SER
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	558	ASN
3	C	562	LEU
3	C	594	LEU
3	C	597	ILE
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	737	THR
3	C	739	LYS
3	C	755	GLU
3	C	760	LEU
3	C	765	LYS
3	C	768	GLU

Continued from previous page...

Mol	Chain	Res	Type
3	C	769	LYS
3	C	772	ARG
3	C	810	THR
3	C	816	LYS
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	25	ARG
3	D	26	GLU
3	D	30	GLU
3	D	32	GLU
3	D	43	GLU
3	D	45	GLN
3	D	48	LYS
3	D	58	THR
3	D	61	LEU
3	D	66	ARG
3	D	70	GLN
3	D	73	LYS
3	D	74	ARG
3	D	76	GLU
3	D	102	LYS
3	D	110	VAL
3	D	123	PHE
3	D	128	GLN
3	D	130	LYS
3	D	154	SER

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Mol	Chain	Res	Type
3	D	158	ASN
3	D	160	GLU
3	D	163	SER
3	D	170	LEU
3	D	171	GLN
3	D	177	GLU
3	D	180	SER
3	D	183	ILE
3	D	186	ILE
3	D	192	ASP
3	D	197	LEU
3	D	199	MET
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	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	273	TYR
3	D	283	THR
3	D	289	SER
3	D	295	GLU
3	D	299	ASN
3	D	302	LYS
3	D	306	ASP
3	D	311	LYS
3	D	314	GLU
3	D	319	ARG
3	D	332	LEU
3	D	342	ASN
3	D	372	SER
3	D	373	LEU

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Mol	Chain	Res	Type
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	422	GLN
3	D	435	LYS
3	D	440	HIS
3	D	441	ASP
3	D	449	ARG
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	536	LYS
3	D	538	LEU
3	D	544	ARG
3	D	547	ARG
3	D	548	THR
3	D	559	ARG
3	D	562	LEU
3	D	594	LEU
3	D	600	LYS
3	D	618	LEU
3	D	624	SER

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Mol	Chain	Res	Type
3	D	631	LYS
3	D	640	LYS
3	D	643	ASP
3	D	657	GLU
3	D	659	MET
3	D	693	LEU
3	D	715	MET
3	D	737	THR
3	D	739	LYS
3	D	743	LYS
3	D	755	GLU
3	D	760	LEU
3	D	766	GLU
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	826	GLU
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
3	D	873	GLU
3	D	880	LEU
3	D	888	LYS
3	D	894	LYS
3	D	898	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	23	ASN
3	A	105	HIS
3	A	131	HIS
3	A	153	ASN
3	A	158	ASN

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Mol	Chain	Res	Type
3	A	171	GLN
3	A	173	GLN
3	A	333	GLN
3	A	376	GLN
3	A	402	ASN
3	A	440	HIS
3	A	481	GLN
3	A	485	HIS
3	A	495	ASN
3	A	558	ASN
3	A	595	GLN
3	A	646	HIS
3	A	761	GLN
3	A	839	ASN
3	A	864	HIS
3	B	45	GLN
3	B	153	ASN
3	B	158	ASN
3	B	171	GLN
3	B	173	GLN
3	B	255	ASN
3	B	333	GLN
3	B	376	GLN
3	B	382	GLN
3	B	402	ASN
3	B	440	HIS
3	B	480	ASN
3	B	481	GLN
3	B	507	ASN
3	B	546	GLN
3	B	646	HIS
3	B	761	GLN
3	B	818	ASN
3	C	40	HIS
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	255	ASN

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Mol	Chain	Res	Type
3	C	333	GLN
3	C	354	GLN
3	C	376	GLN
3	C	402	ASN
3	C	480	ASN
3	C	481	GLN
3	C	495	ASN
3	C	505	ASN
3	C	507	ASN
3	C	546	GLN
3	C	558	ASN
3	C	761	GLN
3	C	818	ASN
3	D	40	HIS
3	D	70	GLN
3	D	112	ASN
3	D	131	HIS
3	D	255	ASN
3	D	333	GLN
3	D	354	GLN
3	D	376	GLN
3	D	402	ASN
3	D	440	HIS
3	D	481	GLN
3	D	495	ASN
3	D	546	GLN
3	D	556	GLN
3	D	646	HIS
3	D	679	HIS
3	D	761	GLN
3	D	786	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 monosaccharides 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	G	912	1	8,11,12	0.88	0	9,14,17	1.31	2 (22%)
5	DOC	L	953	2	16,19,20	0.52	0	20,26,29	1.07	1 (5%)
5	DOC	J	953	2	16,19,20	0.69	0	20,26,29	1.22	2 (10%)
4	3DR	F	912	1	8,11,12	0.48	0	9,14,17	0.96	0
6	DGP	K	955	-	18,24,25	1.19	3 (16%)	19,35,38	1.39	4 (21%)
5	DOC	K	953	2	16,19,20	0.49	0	20,26,29	1.95	3 (15%)
6	DGP	G	908	6,7	18,24,25	1.19	2 (11%)	19,35,38	0.86	0
4	3DR	E	912	1	8,11,12	0.64	0	9,14,17	0.98	0
6	DGP	F	908	-	18,21,25	1.03	1 (5%)	19,31,38	1.35	3 (15%)
6	DGP	L	955	-	18,24,25	1.20	2 (11%)	19,35,38	0.69	0
6	DGP	H	908	-	18,21,25	1.24	2 (11%)	19,31,38	1.14	1 (5%)
5	DOC	I	953	2	16,19,20	0.50	0	20,26,29	0.86	1 (5%)
4	3DR	H	912	1	8,11,12	0.62	0	9,14,17	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3DR	G	912	1	-	1/3/15/16	0/1/1/1
5	DOC	L	953	2	-	0/7/18/19	0/2/2/2
5	DOC	J	953	2	-	0/7/18/19	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3DR	F	912	1	-	0/3/15/16	0/1/1/1
6	DGP	K	955	-	-	1/3/21/22	0/3/3/3
5	DOC	K	953	2	-	2/7/18/19	0/2/2/2
6	DGP	G	908	6,7	-	2/3/21/22	0/3/3/3
4	3DR	E	912	1	-	2/3/15/16	0/1/1/1
6	DGP	F	908	-	-	2/2/18/22	0/3/3/3
6	DGP	L	955	-	-	1/3/21/22	0/3/3/3
6	DGP	H	908	-	-	0/2/18/22	0/3/3/3
5	DOC	I	953	2	-	2/7/18/19	0/2/2/2
4	3DR	H	912	1	-	2/3/15/16	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	955	DGP	C5-C6	-2.99	1.41	1.47
6	G	908	DGP	C8-N7	-2.90	1.30	1.35
6	H	908	DGP	C8-N7	-2.78	1.30	1.35
6	L	955	DGP	C8-N7	-2.76	1.30	1.35
6	G	908	DGP	C5-C6	-2.61	1.42	1.47
6	K	955	DGP	C5-C6	-2.51	1.42	1.47
6	F	908	DGP	C8-N7	-2.38	1.31	1.35
6	K	955	DGP	C5-C4	-2.33	1.37	1.43
6	K	955	DGP	C8-N7	-2.30	1.31	1.35
6	H	908	DGP	C5-C6	-2.19	1.43	1.47

All (17) 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	C4'-O4'-C1'	-3.21	101.71	109.45
5	K	953	DOC	O4'-C1'-C2'	-3.07	103.34	106.67
5	J	953	DOC	C4'-O4'-C1'	-3.07	106.91	109.81
6	F	908	DGP	O6-C6-N1	-2.95	117.17	120.65
5	I	953	DOC	O4'-C1'-N1	2.86	112.97	107.86
5	L	953	DOC	O4'-C1'-N1	2.67	112.63	107.86
5	J	953	DOC	C3'-C2'-C1'	2.57	105.75	102.78
6	K	955	DGP	O6-C6-N1	-2.55	117.64	120.65
4	G	912	3DR	O4'-C4'-C3'	2.45	107.33	103.73
6	F	908	DGP	O6-C6-C5	2.42	129.10	124.37
5	K	953	DOC	O4'-C4'-C3'	-2.27	101.03	104.80
6	F	908	DGP	O4'-C1'-C2'	-2.20	102.10	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	908	DGP	C2'-C1'-N9	-2.19	109.22	114.27
4	G	912	3DR	C1'-O4'-C4'	-2.15	105.01	108.48
6	K	955	DGP	O6-C6-C5	2.06	128.40	124.37
6	K	955	DGP	O4'-C1'-C2'	-2.06	102.36	106.25

There are no chirality outliers.

All (15) 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'
5	K	953	DOC	O4'-C4'-C5'-O5'
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	L	955	DGP	C4'-C5'-O5'-P
6	G	908	DGP	C3'-C4'-C5'-O5'
6	K	955	DGP	C4'-C5'-O5'-P
4	H	912	3DR	C4'-C5'-O5'-P
4	E	912	3DR	O4'-C4'-C5'-O5'
5	K	953	DOC	C3'-C4'-C5'-O5'
4	E	912	3DR	C3'-C4'-C5'-O5'
4	G	912	3DR	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	912	3DR	3	0
5	J	953	DOC	1	0
4	F	912	3DR	3	0
6	K	955	DGP	1	0
5	K	953	DOC	1	0
6	G	908	DGP	1	0
4	E	912	3DR	1	0
6	L	955	DGP	1	0
6	H	908	DGP	3	0
5	I	953	DOC	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DOC L 953

Ligand DOC J 953

Ligand DGP K 955

Bond lengths

Bond angles

Torsions

Rings

Ligand DOC K 953

Bond lengths

Bond angles

Torsions

Rings

Ligand DGP G 908

Bond lengths

Bond angles

Torsions

Rings

Ligand DGP F 908

Bond lengths

Bond angles

Torsions

Rings

Ligand DGP L 955

Bond lengths

Bond angles

Torsions

Rings

Ligand DGP H 908

Bond lengths

Bond angles

Torsions

Rings

Ligand DOC I 953

Bond lengths

Bond angles

Torsions

Rings

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

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%)	1.33	5 (27%)	0	0	76, 92, 130, 152	0
1	F	18/18 (100%)	0.68	3 (16%)	1	1	39, 75, 149, 176	0
1	G	18/18 (100%)	0.23	2 (11%)	5	4	36, 54, 90, 102	0
1	H	18/18 (100%)	0.25	1 (5%)	24	23	44, 67, 128, 131	0
2	I	13/13 (100%)	0.47	0	100	100	77, 95, 100, 102	0
2	J	13/13 (100%)	-0.05	0	100	100	41, 68, 121, 135	0
2	K	13/13 (100%)	-0.31	0	100	100	36, 55, 77, 83	0
2	L	13/13 (100%)	-0.19	0	100	100	43, 65, 95, 102	0
3	A	903/903 (100%)	0.45	97 (10%)	6	4	30, 64, 147, 260	0
3	B	903/903 (100%)	0.15	59 (6%)	18	17	30, 53, 121, 222	0
3	C	903/903 (100%)	-0.05	23 (2%)	57	59	28, 47, 88, 138	0
3	D	903/903 (100%)	0.01	21 (2%)	60	62	30, 57, 93, 170	0
All	All	3736/3736 (100%)	0.15	211 (5%)	24	23	28, 56, 113, 260	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	510	VAL	14.7
3	B	508	LEU	12.9
3	A	509	SER	12.0
3	D	903	PHE	10.5
3	A	543	PHE	10.4
3	A	508	LEU	10.3
3	A	503	LEU	9.9
3	A	516	VAL	9.7
3	A	514	LEU	9.5
3	A	257	TYR	9.2
3	A	536	LYS	8.8

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Mol	Chain	Res	Type	RSRZ
3	A	504	HIS	8.4
3	B	256	MET	7.6
3	A	253	ILE	7.2
1	E	910	DA	7.1
3	B	507	ASN	7.1
3	A	515	ASP	7.0
3	A	512	GLU	7.0
3	B	539	ASN	6.9
3	D	257	TYR	6.8
3	A	522	PHE	6.8
3	B	257	TYR	6.6
3	B	504	HIS	6.6
3	A	259	SER	6.6
3	B	506	PRO	6.6
3	A	507	ASN	6.6
3	B	500	LYS	6.4
3	B	530	ILE	6.4
3	C	257	TYR	6.1
3	A	550	VAL	6.1
3	B	516	VAL	6.1
3	A	798	GLY	6.0
3	A	506	PRO	5.9
3	B	535	ALA	5.8
3	A	502	ALA	5.7
3	B	258	GLY	5.6
3	B	253	ILE	5.5
3	A	838	GLY	5.4
3	A	500	LYS	5.4
3	A	497	GLU	5.4
3	A	493	GLN	5.2
3	C	530	ILE	5.2
1	F	910	DA	5.1
3	B	173	GLN	5.1
3	A	542	LEU	5.0
3	B	513	PRO	5.0
3	A	256	MET	5.0
3	B	541	MET	5.0
3	B	503	LEU	4.9
3	B	255	ASN	4.8
3	A	530	ILE	4.8
3	C	258	GLY	4.8
3	A	538	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
3	C	903	PHE	4.8
3	A	799	PRO	4.8
3	D	895	ALA	4.8
3	A	529	LYS	4.6
3	C	252	VAL	4.6
3	A	517	ASP	4.5
3	C	900	MET	4.5
1	E	911	DC	4.5
1	G	910	DA	4.4
3	A	518	TYR	4.4
3	A	541	MET	4.4
3	B	512	GLU	4.3
3	A	496	GLY	4.3
3	B	523	SER	4.3
3	A	554	THR	4.2
1	H	910	DA	4.2
3	A	490	LEU	4.1
3	B	794	GLY	4.1
3	D	252	VAL	4.1
3	C	508	LEU	4.1
3	A	540	GLU	4.0
3	A	513	PRO	4.0
3	A	301	GLY	3.9
3	A	858	ILE	3.9
3	D	530	ILE	3.9
3	A	523	SER	3.9
3	B	526	ILE	3.9
3	A	260	ARG	3.9
3	A	1	MET	3.9
3	A	255	ASN	3.8
3	A	535	ALA	3.8
3	A	537	SER	3.8
3	A	803	PHE	3.8
3	D	902	ASP	3.7
3	A	539	ASN	3.7
3	B	527	LYS	3.6
3	A	857	LEU	3.6
3	D	253	ILE	3.6
3	B	514	LEU	3.6
1	F	928	DG	3.6
3	A	47	THR	3.5
3	A	258	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	253	ILE	3.5
3	A	801	CYS	3.5
3	D	539	ASN	3.5
3	A	640	LYS	3.4
3	A	786	ASN	3.4
3	B	502	ALA	3.4
3	A	494	ARG	3.4
3	B	45	GLN	3.4
3	D	541	MET	3.4
3	B	511	ASP	3.4
3	B	509	SER	3.4
3	B	496	GLY	3.4
3	B	499	ILE	3.3
3	B	259	SER	3.3
3	C	509	SER	3.3
3	D	532	LYS	3.3
3	A	795	GLY	3.3
3	A	499	ILE	3.2
3	D	894	LYS	3.2
3	A	252	VAL	3.2
3	A	847	ALA	3.2
3	A	495	ASN	3.2
3	A	547	ARG	3.1
3	D	1	MET	3.1
3	B	498	ILE	3.1
3	D	901	PHE	3.1
3	D	498	ILE	3.1
3	B	799	PRO	3.1
3	C	1	MET	3.0
3	A	528	GLU	3.0
3	A	488	TYR	3.0
3	B	497	GLU	3.0
3	A	527	LYS	3.0
3	B	640	LYS	3.0
3	B	520	PHE	3.0
3	B	310	SER	2.9
3	A	832	VAL	2.9
3	A	498	ILE	2.9
3	C	256	MET	2.9
3	B	518	TYR	2.9
3	B	494	ARG	2.9
3	A	815	ILE	2.9

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	RSRZ
3	B	528	GLU	2.9
1	E	924	DC	2.8
3	B	522	PHE	2.8
3	B	490	LEU	2.8
3	B	510	VAL	2.8
3	A	501	GLU	2.8
3	A	489	MET	2.8
3	B	895	ALA	2.8
3	C	259	SER	2.8
3	A	800	LYS	2.8
3	B	493	GLN	2.7
3	A	789	ALA	2.7
3	A	391	TYR	2.7
3	B	543	PHE	2.7
3	B	550	VAL	2.7
3	C	510	VAL	2.7
1	G	911	DC	2.7
3	B	817	GLY	2.7
3	B	533	LEU	2.6
3	A	846	ILE	2.6
3	C	46	ALA	2.6
3	A	817	GLY	2.6
1	E	925	DG	2.6
3	A	505	ASN	2.5
3	C	251	LYS	2.5
3	A	519	ARG	2.5
3	A	544	ARG	2.5
3	C	640	LYS	2.5
3	A	48	LYS	2.5
3	C	525	GLU	2.5
3	B	46	ALA	2.5
3	A	521	ASP	2.5
3	D	66	ARG	2.5
3	A	302	LYS	2.4
3	A	46	ALA	2.4
3	A	819	ILE	2.4
3	A	866	MET	2.4
3	A	45	GLN	2.4
1	F	927	DG	2.3
3	D	256	MET	2.3
3	B	123	PHE	2.3
3	B	793	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	522	PHE	2.3
3	B	820	ASP	2.3
3	A	261	GLU	2.3
1	E	923	DC	2.3
3	A	172	GLU	2.3
3	A	170	LEU	2.2
3	D	900	MET	2.2
3	B	492	ALA	2.2
3	A	808	ILE	2.2
3	A	863	LEU	2.2
3	A	551	ALA	2.2
3	A	390	PRO	2.2
3	B	534	SER	2.2
3	B	302	LYS	2.2
3	D	254	GLU	2.2
3	A	511	ASP	2.2
3	C	902	ASP	2.2
3	A	526	ILE	2.2
3	D	818	ASN	2.2
3	B	169	LYS	2.2
3	D	302	LYS	2.1
3	B	44	SER	2.1
3	C	513	PRO	2.1
3	A	534	SER	2.1
3	A	174	GLY	2.1
3	C	532	LYS	2.1
3	B	899	ASP	2.0
3	D	542	LEU	2.0
3	C	533	LEU	2.0
3	C	504	HIS	2.0
3	A	42	PRO	2.0
3	A	862	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	K	955	22/23	0.61	0.56	51,60,71,72	15
7	CA	B	1004	1/1	0.68	0.23	96,96,96,96	0
6	DGP	L	955	22/23	0.69	0.35	58,66,76,76	15
7	CA	D	1008	1/1	0.69	0.26	79,79,79,79	0
6	DGP	G	908	22/23	0.77	0.41	70,72,83,85	0
6	DGP	F	908	19/23	0.78	0.44	72,75,81,81	0
6	DGP	H	908	19/23	0.81	0.39	69,71,75,75	0
7	CA	A	1001	1/1	0.82	0.14	91,91,91,91	0
7	CA	C	1005	1/1	0.83	0.14	75,75,75,75	0
7	CA	B	1003	1/1	0.84	0.08	54,54,54,54	0
4	3DR	E	912	11/12	0.85	0.21	92,98,109,109	0
7	CA	C	1006	1/1	0.87	0.10	57,57,57,57	0
7	CA	D	1007	1/1	0.89	0.10	55,55,55,55	0
4	3DR	H	912	11/12	0.93	0.21	61,66,81,82	0
5	DOC	I	953	18/19	0.93	0.14	74,81,85,89	0
6	DGP	G	907	1/23	0.94	0.61	84,84,84,84	0
4	3DR	G	912	11/12	0.94	0.17	51,55,68,71	0
4	3DR	F	912	11/12	0.96	0.17	57,59,74,77	0
5	DOC	K	953	18/19	0.97	0.16	32,36,40,40	0
5	DOC	L	953	18/19	0.97	0.15	39,43,51,52	0
5	DOC	J	953	18/19	0.97	0.15	39,42,46,46	0
7	CA	A	1002	1/1	0.99	0.14	67,67,67,67	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.

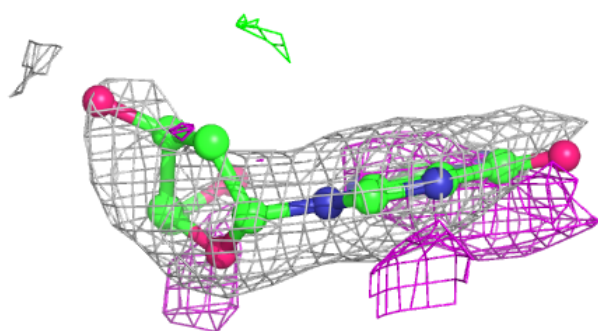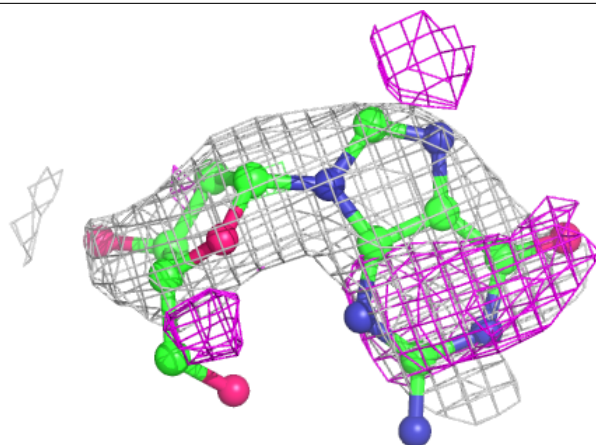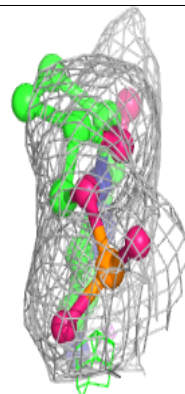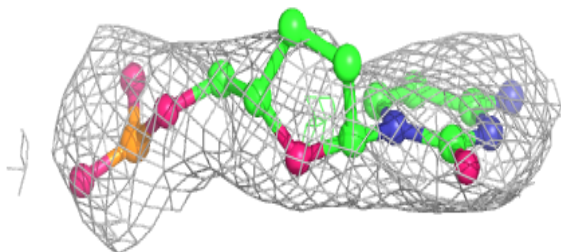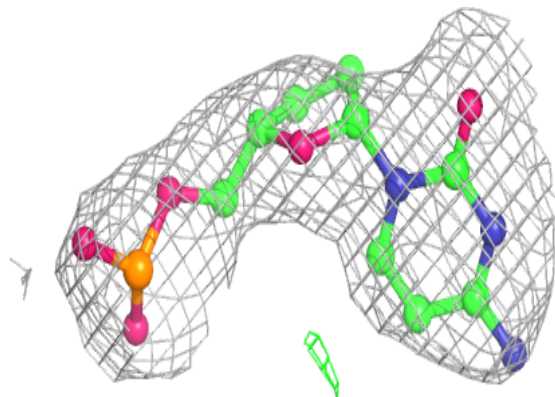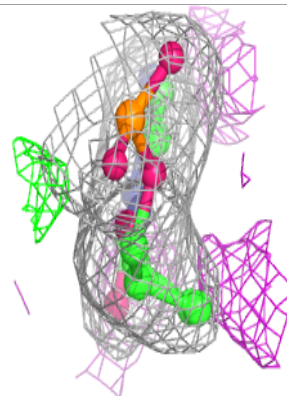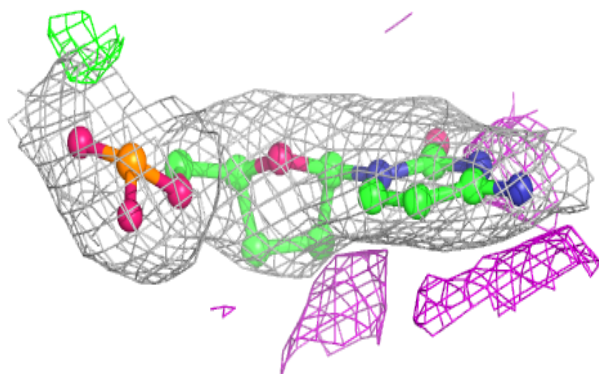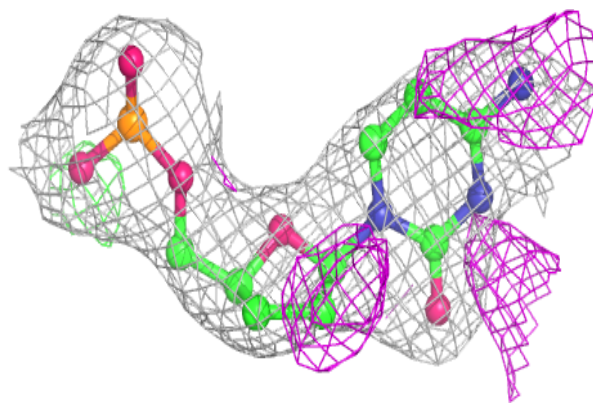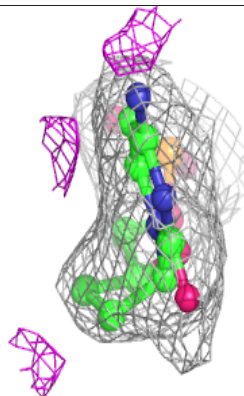**Electron density around DGP K 955:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
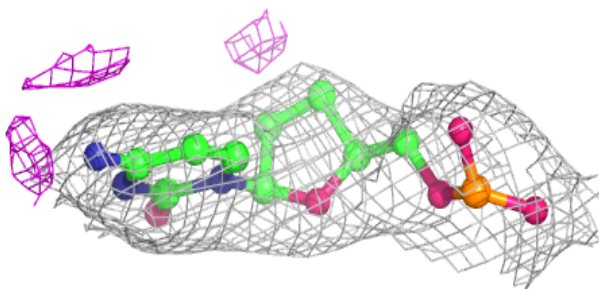and green (positive)
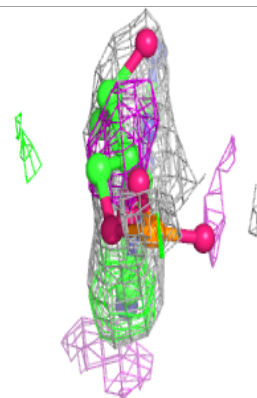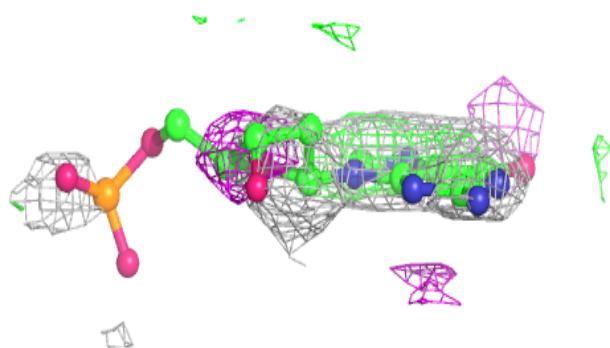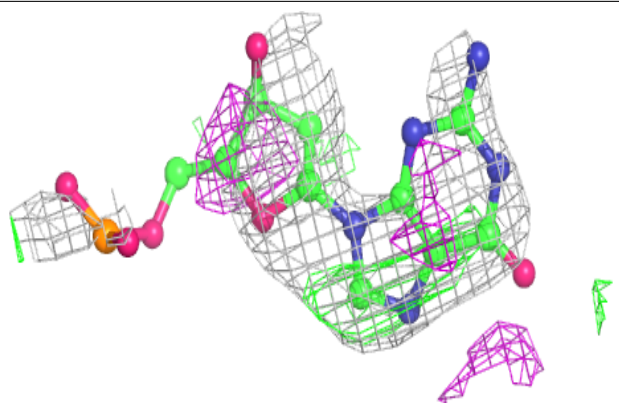
Electron density around DGP L 955:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
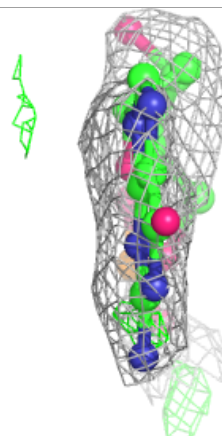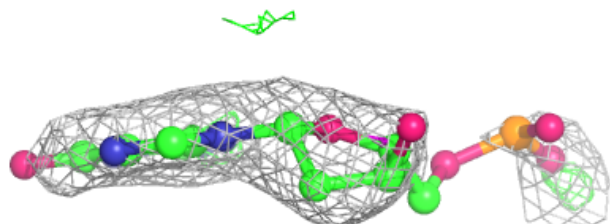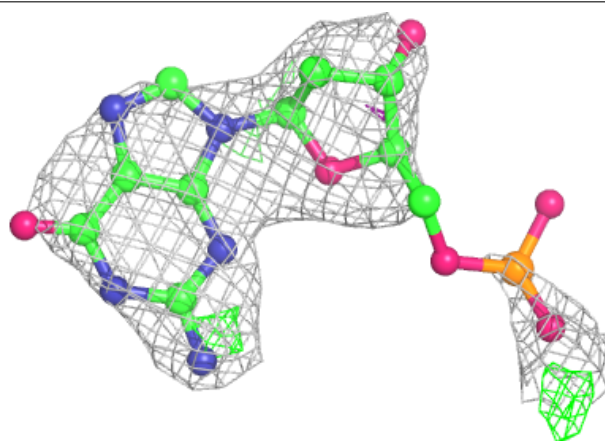
Electron density around DGP G 908:

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

Electron density around DGP F 908:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
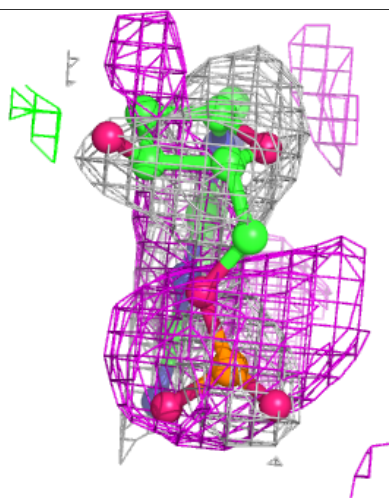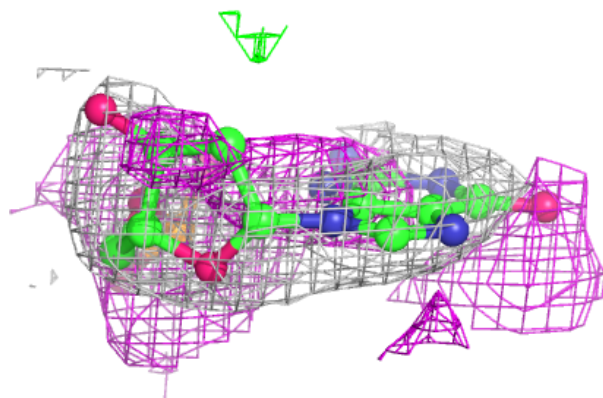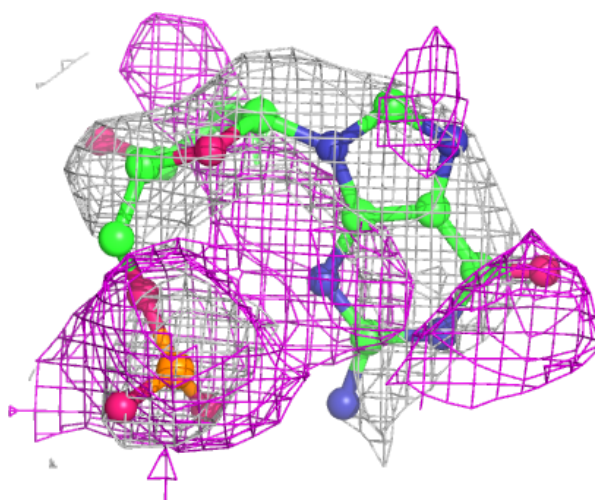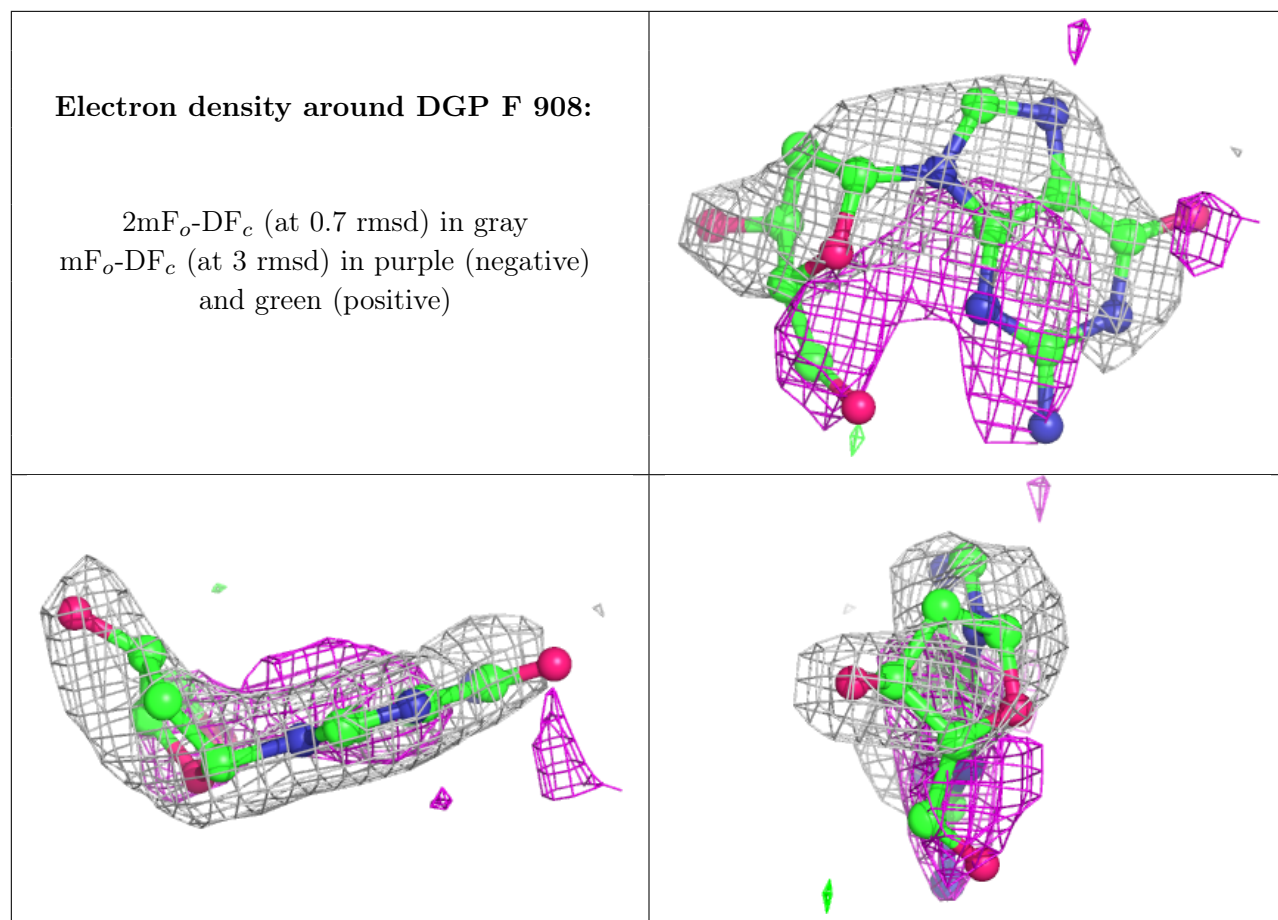
Electron density around DGP H 908:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
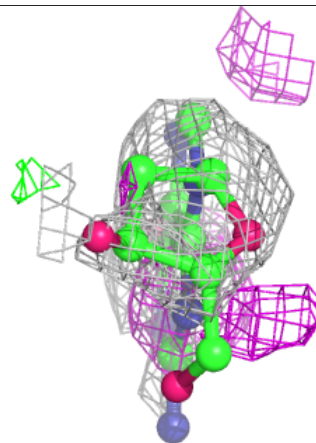
Electron density around DOC I 953:

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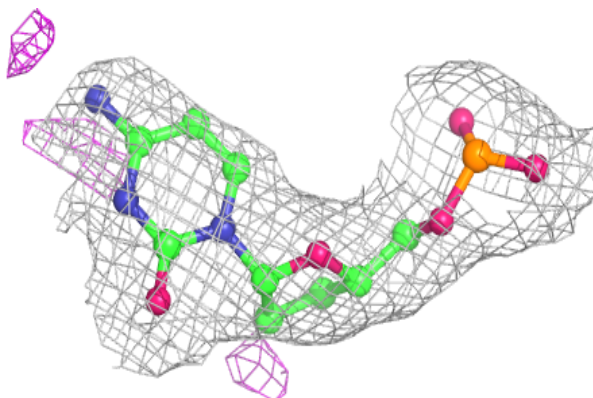mF_o-DF_c (at 3 rmsd) in purple (negative)
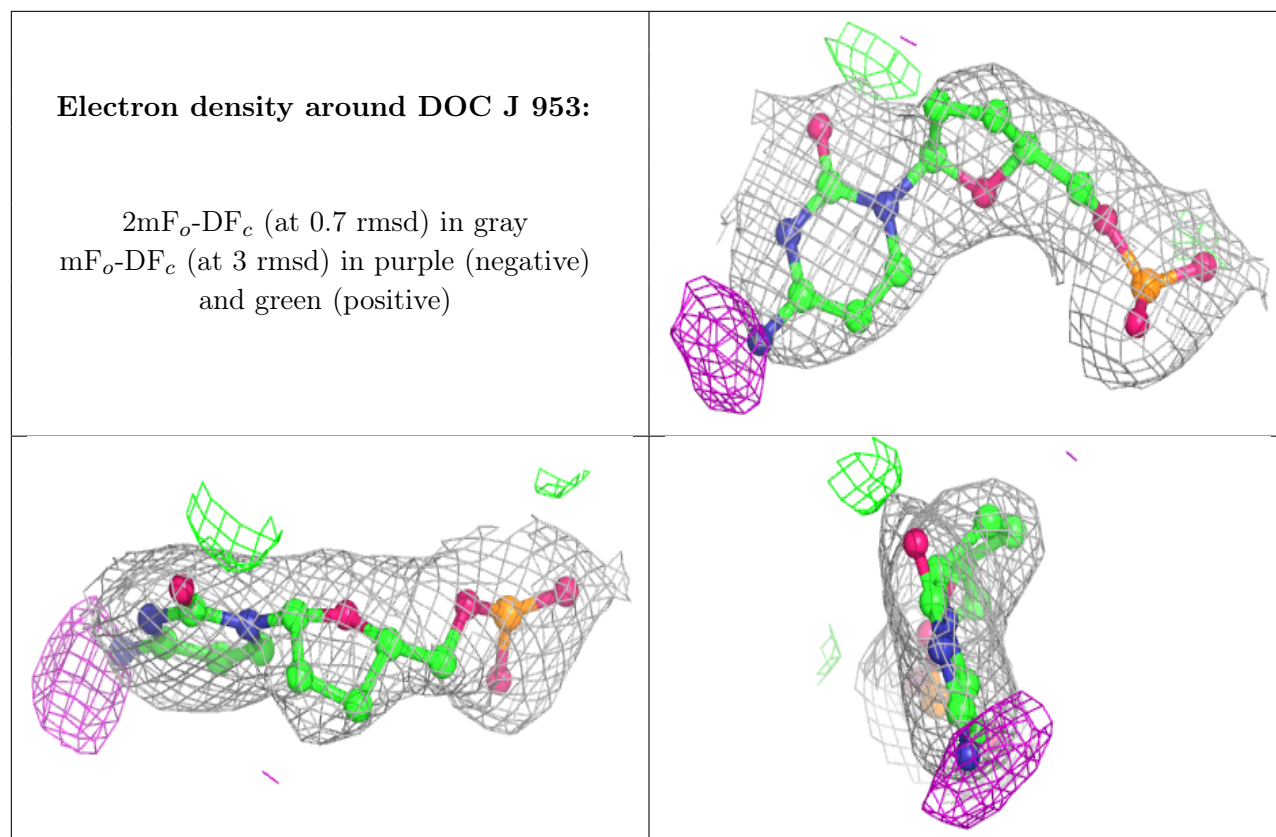and green (positive)

Electron density around DOC 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)

Electron density around DOC L 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:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.