Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:07 am BST

PDB ID	:	5NC5
Title	:	Crystal structure of AcrBZ in complex with antibiotic puromycin
Authors	:	Du, D.; Luisi, B.
Deposited on	:	2017-03-03
Resolution	:	3.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

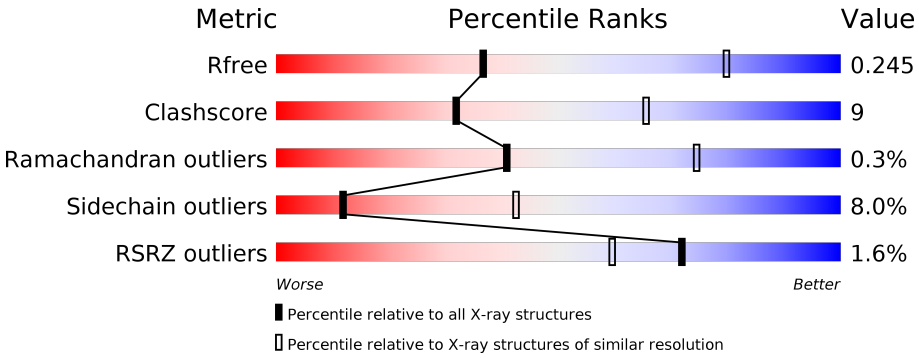
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1049	2% 76% 22% •
1	B	1049	% 72% 23% • •
1	C	1049	% 71% 24% • •
2	D	169	% 73% 17% • 8%
2	E	169	% 68% 20% • 10%
3	F	49	10% 35% 33% 8% 24%

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Mol	Chain	Length	Quality of chain
3	G	49	8% 29% 39% 27%
3	H	49	8% 39% 31% 6% 24%

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
5	D12	B	1104	-	-	-	X
6	D10	A	1105	-	-	-	X
6	D10	A	1109	-	-	-	X
6	D10	B	1114	-	-	-	X
6	D10	B	1122	-	-	-	X
6	D10	C	1111	-	-	-	X
6	D10	C	1114	-	-	-	X
6	D10	C	1115	-	-	-	X
6	D10	C	1116	-	-	-	X
6	D10	C	1117	-	-	-	X
7	DD9	A	1114	-	-	-	X
7	DD9	B	1106	-	-	-	X
7	DD9	B	1109	-	-	-	X
7	DD9	B	1112	-	-	-	X
8	PUY	B	1120	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 55690 atoms, of which 28293 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1044	Total	C	H	N	O	S	0	0	0
			15927	5086	8019	1308	1470	44			
1	B	1033	Total	C	H	N	O	S	0	0	0
			15835	5049	7990	1294	1458	44			
1	C	1033	Total	C	H	N	O	S	0	0	0
			15835	5049	7990	1294	1458	44			

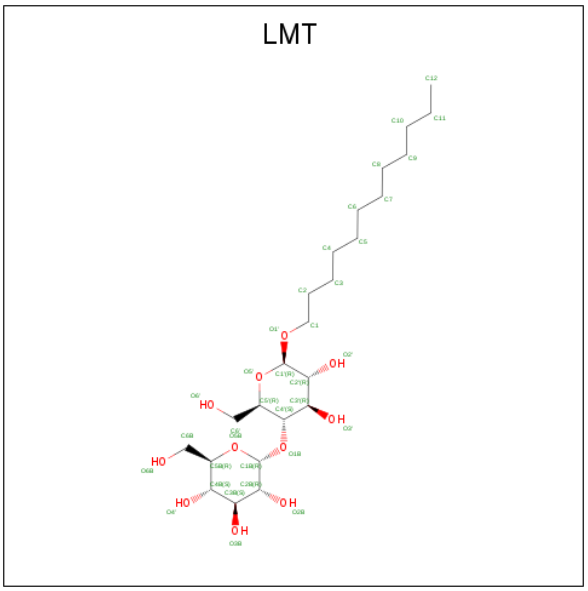
- Molecule 2 is a protein called DARPin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	156	Total	C	H	N	O	S	0	0	0
			2336	741	1159	206	229	1			
2	E	152	Total	C	H	N	O	S	0	0	0
			2287	726	1136	202	222	1			

- Molecule 3 is a protein called Multidrug efflux pump accessory protein AcrZ.

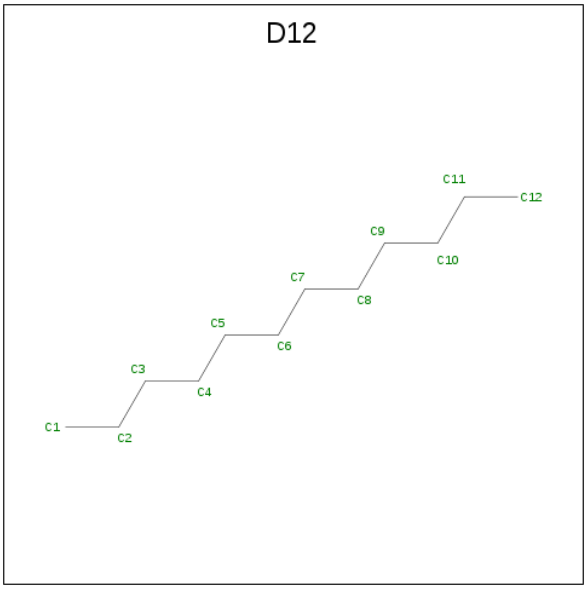
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	37	Total	C	H	N	O	S	0	0	0
			601	196	318	39	45	3			
3	G	36	Total	C	H	N	O	S	0	0	0
			590	193	313	38	43	3			
3	H	37	Total	C	H	N	O	S	0	0	0
			601	196	318	39	45	3			

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 59 18 35 6	0	0
4	A	1	Total C H 35 12 23	0	0
4	A	1	Total C H 35 12 23	0	0

- Molecule 5 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H 38 12 26	0	0

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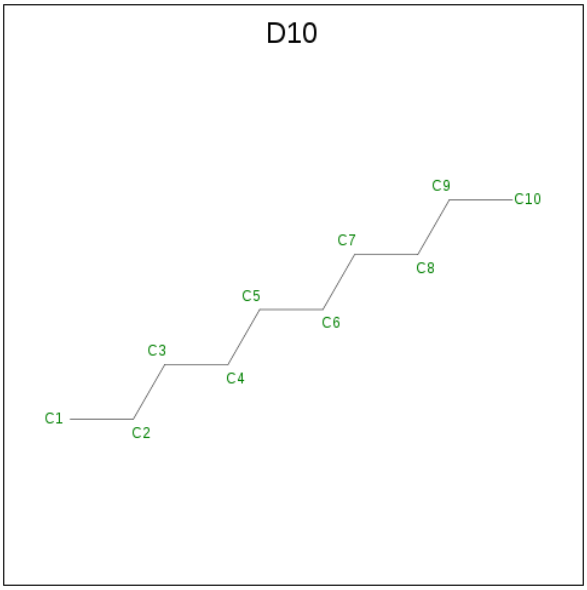
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H 38 12 26	0	0
5	B	1	Total C H 28 9 19	0	0
5	B	1	Total C H 34 11 23	0	0
5	C	1	Total C H 38 12 26	0	0
5	C	1	Total C H 38 12 26	0	0
5	C	1	Total C H 38 12 26	0	0
5	C	1	Total C H 16 5 11	0	0

- Molecule 6 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H 32 10 22	0	0
6	A	1	Total C H 32 10 22	0	0
6	A	1	Total C H 32 10 22	0	0
6	A	1	Total C H 32 10 22	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	B	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0
6	C	1	Total C H 32 10 22	0	0

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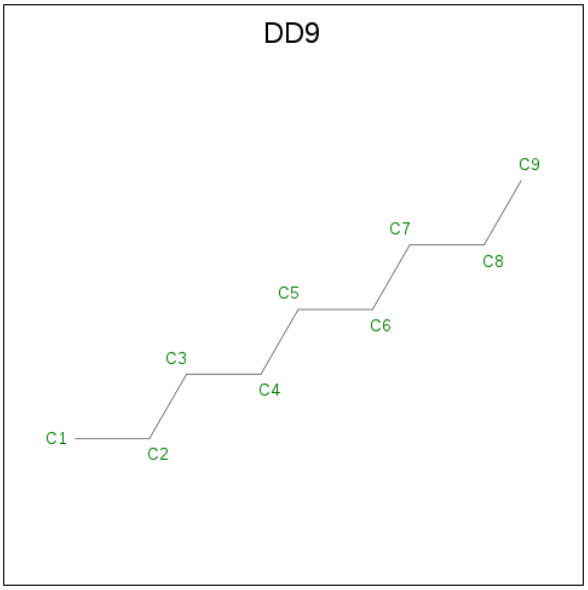
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C H 32 10 22	0	0

- Molecule 7 is nonane (three-letter code: DD9) (formula: C_9H_{20}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H 28 9 19	0	0
7	A	1	Total C H 16 5 11	0	0
7	A	1	Total C H 22 7 15	0	0
7	A	1	Total C H 28 9 19	0	0
7	B	1	Total C H 16 5 11	0	0
7	B	1	Total C H 17 7 10	0	0
7	B	1	Total C H 19 6 13	0	0
7	B	1	Total C H 25 9 16	0	0
7	B	1	Total C H 22 7 15	0	0
7	B	1	Total C H 19 6 13	0	0

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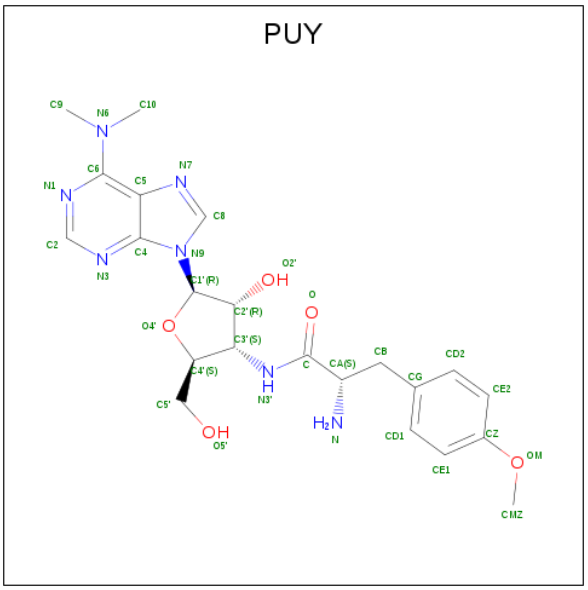
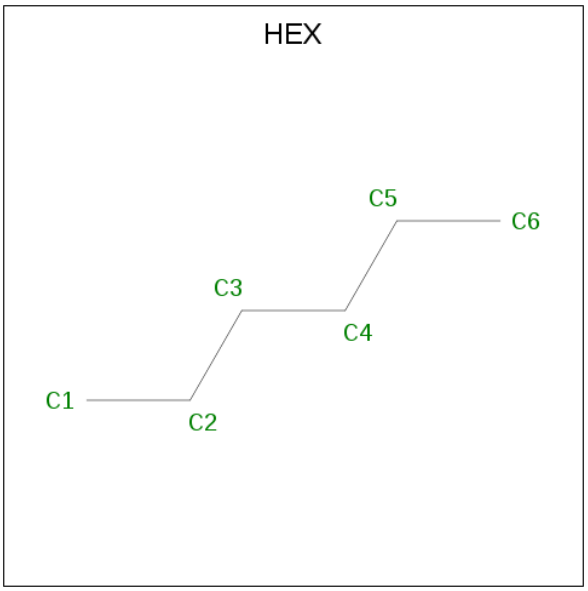
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C H 28 9 19	0	0
7	C	1	Total C H 13 4 9	0	0
7	C	1	Total C H 19 6 13	0	0
7	C	1	Total C H 25 8 17	0	0

- Molecule 8 is PUROMYCIN (three-letter code: PUY) (formula: $C_{22}H_{29}N_7O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O 34 22 7 5	0	0

- Molecule 9 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C H 20 6 14	0	0

- Molecule 10 is water.

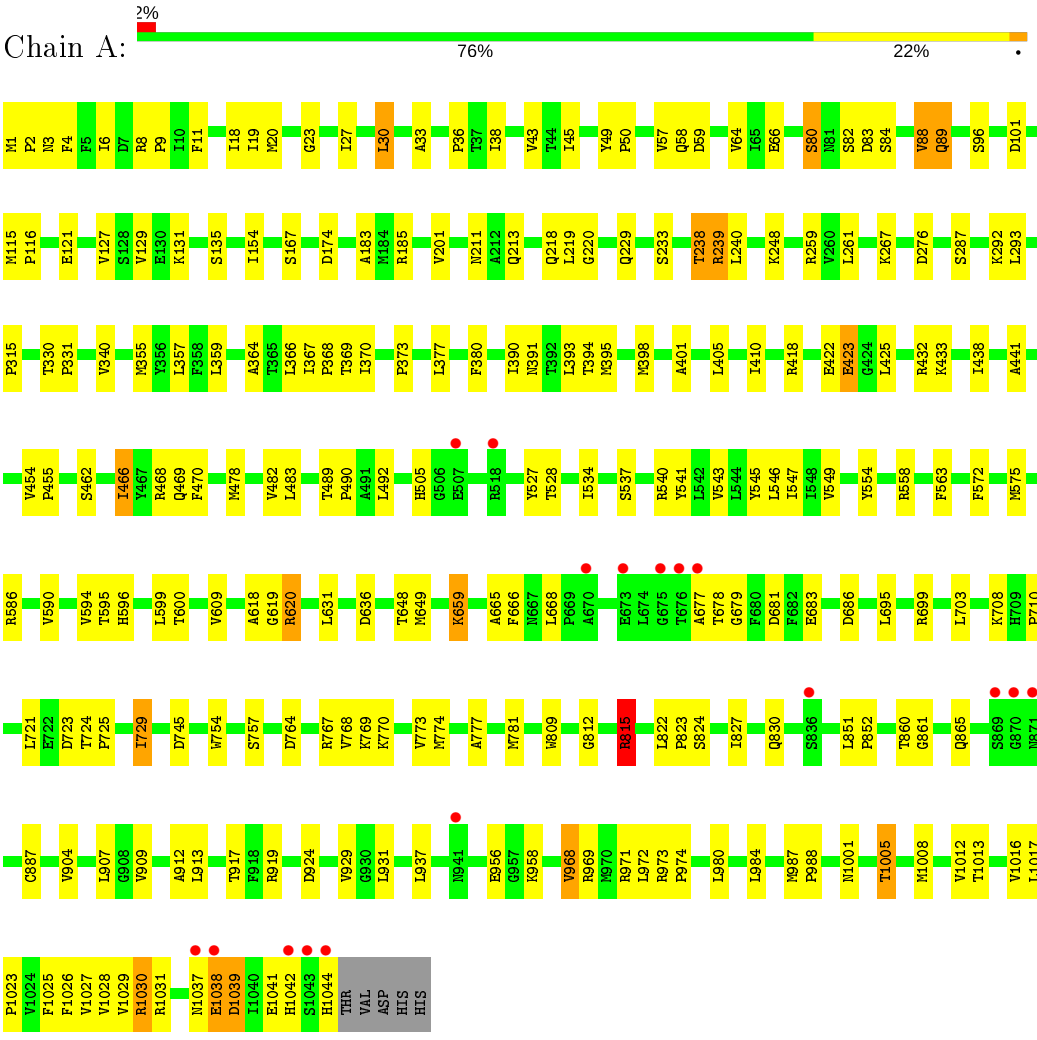
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	50	Total O 50 50	0	0
10	B	26	Total O 26 26	0	0
10	C	21	Total O 21 21	0	0
10	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

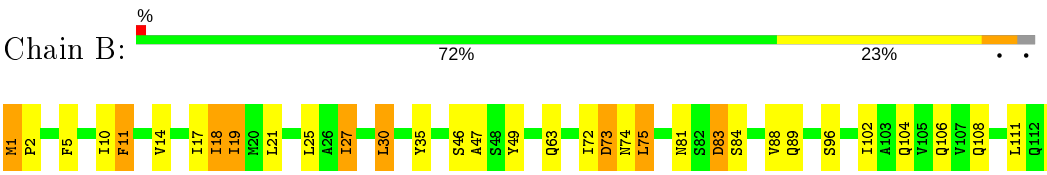
- Molecule 1: Multidrug efflux pump subunit AcrB

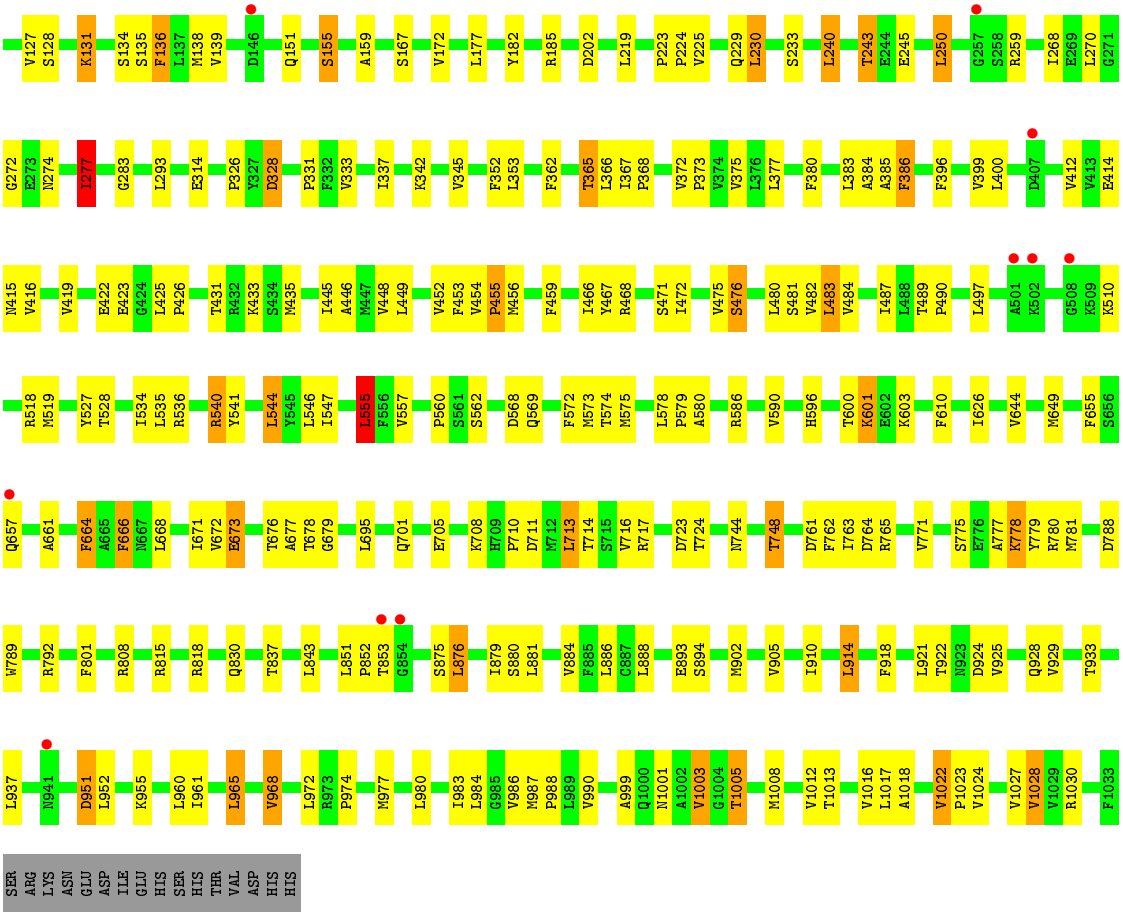
Chain A:



- Molecule 1: Multidrug efflux pump subunit AcrB

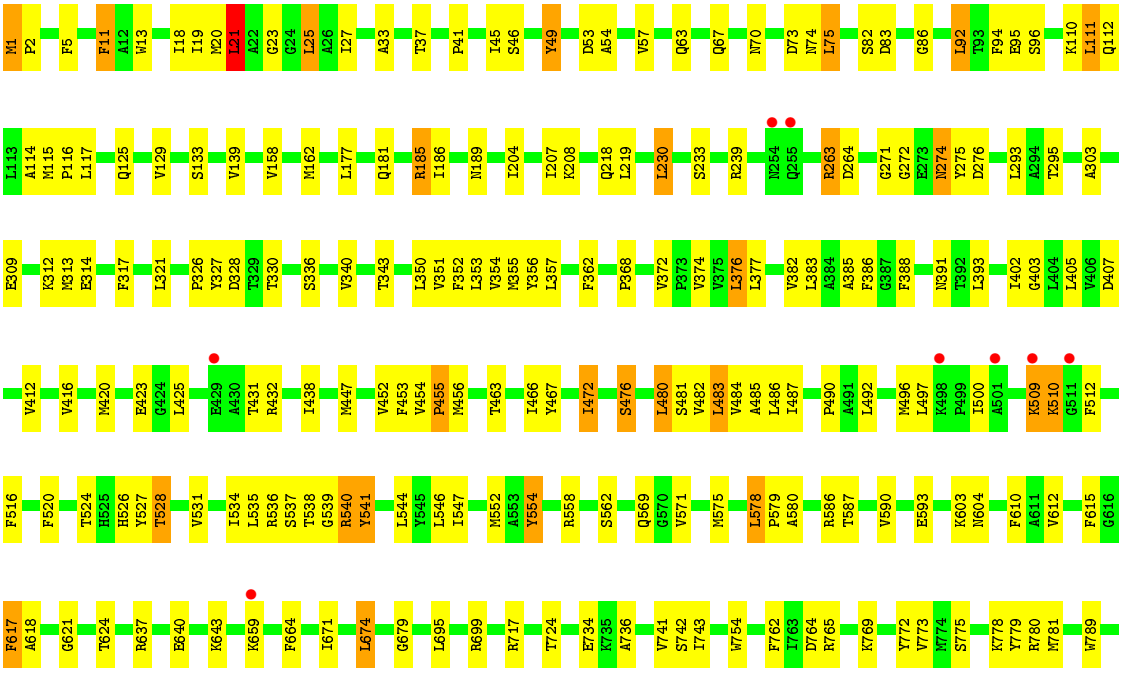
Chain B:

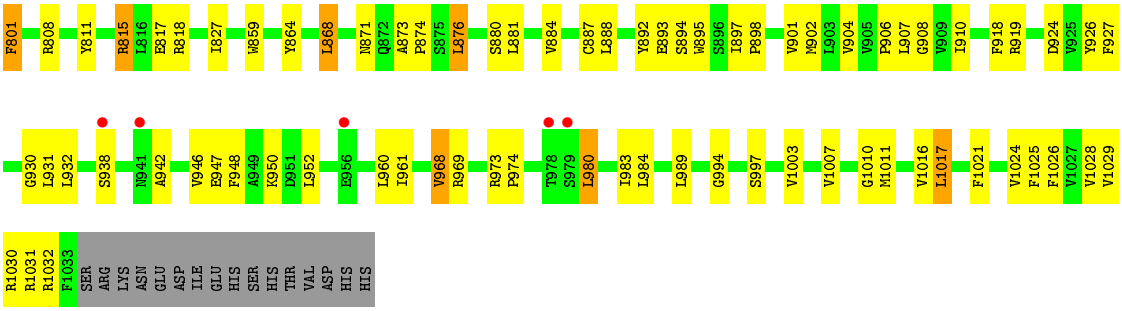




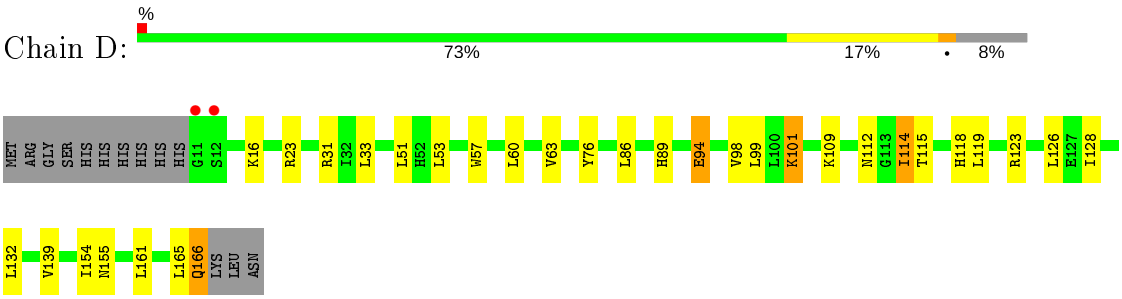
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain C:

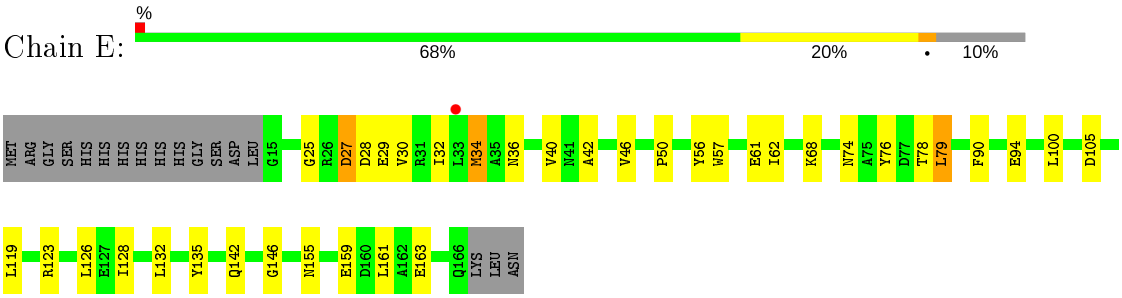




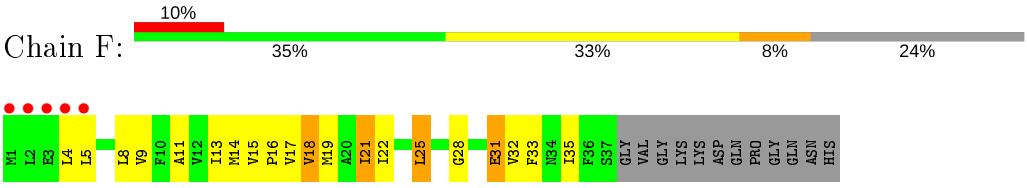
• Molecule 2: DARPin



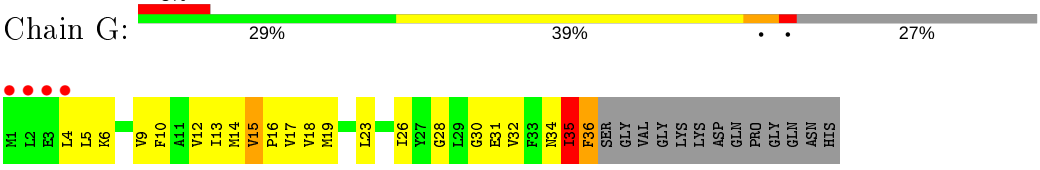
• Molecule 2: DARPin



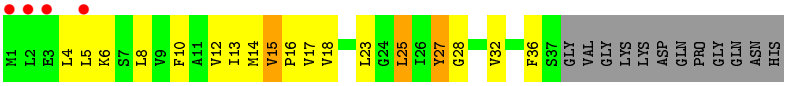
• Molecule 3: Multidrug efflux pump accessory protein AcrZ



• Molecule 3: Multidrug efflux pump accessory protein AcrZ



• Molecule 3: Multidrug efflux pump accessory protein AcrZ


M1
L2
E3
L4
L5
K6
S7
L8
V9
F10
A11
V12
I13
M14
V15
P16
V17
V18
L23
G24
L25
I26
Y27
G28
V32
F36
S37
GLY
VAL
GLY
LYS
LYS
ASP
GLN
PRO
GLY
GLN
ASN
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	147.25Å 167.65Å 249.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.93 – 3.20 34.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.0 (34.93-3.20) 92.0 (34.97-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.183 , 0.245 0.183 , 0.245	Depositor DCC
R_{free} test set	4696 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	55690	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DD9, D10, D12, LMT, HEX, PUY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.89	10/8060 (0.1%)	0.92	17/10947 (0.2%)
1	B	0.91	10/7995 (0.1%)	1.00	20/10859 (0.2%)
1	C	0.94	9/7995 (0.1%)	1.23	76/10859 (0.7%)
2	D	0.83	1/1196 (0.1%)	1.14	7/1626 (0.4%)
2	E	0.78	1/1170 (0.1%)	0.80	0/1591
3	F	0.82	0/287	0.86	0/388
3	G	0.76	0/281	1.28	1/380 (0.3%)
3	H	0.83	0/287	1.38	5/388 (1.3%)
All	All	0.90	31/27271 (0.1%)	1.06	126/37038 (0.3%)

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
1	A	0	1
1	B	0	4
1	C	0	5
All	All	0	10

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	GLY	C-N	-8.34	1.14	1.34
1	A	88	VAL	CB-CG2	-6.89	1.38	1.52
1	A	64	VAL	CB-CG2	-6.77	1.38	1.52
1	C	497	LEU	C-N	6.72	1.49	1.34
1	B	771	VAL	CB-CG2	-6.70	1.38	1.52
1	B	951	ASP	CB-CG	6.63	1.65	1.51
1	C	593	GLU	CG-CD	6.34	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	PHE	C-O	-6.19	1.11	1.23
1	A	683	GLU	CG-CD	6.17	1.61	1.51
1	B	422	GLU	CB-CG	6.16	1.63	1.52
1	A	815	ARG	CG-CD	6.03	1.67	1.51
1	C	859	TRP	CB-CG	-5.99	1.39	1.50
1	A	43	VAL	CB-CG2	-5.83	1.40	1.52
1	A	129	VAL	CB-CG1	-5.78	1.40	1.52
1	C	664	PHE	CB-CG	-5.77	1.41	1.51
1	C	314	GLU	CG-CD	5.66	1.60	1.51
1	B	139	VAL	C-O	-5.57	1.12	1.23
1	A	201	VAL	CB-CG1	-5.53	1.41	1.52
1	C	275	TYR	CE2-CZ	-5.50	1.31	1.38
2	E	57	TRP	CB-CG	5.42	1.60	1.50
1	B	422	GLU	CG-CD	5.39	1.60	1.51
1	A	723	ASP	CB-CG	5.33	1.62	1.51
1	C	817	GLU	CG-CD	5.19	1.59	1.51
1	C	815	ARG	CB-CG	-5.18	1.38	1.52
1	A	812	GLY	C-N	5.11	1.45	1.34
1	C	590	VAL	CB-CG1	-5.07	1.42	1.52
2	D	98	VAL	CB-CG1	-5.06	1.42	1.52
1	B	664	PHE	C-O	-5.04	1.13	1.23
1	B	88	VAL	CB-CG1	-5.04	1.42	1.52
1	B	673	GLU	CG-CD	5.03	1.59	1.51
1	A	66	GLU	CD-OE2	5.01	1.31	1.25

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	C	610	PHE	CB-CG-CD1	9.36	127.35	120.80
1	C	927	PHE	CB-CG-CD1	-9.27	114.31	120.80
1	C	610	PHE	CB-CG-CD2	-9.22	114.35	120.80
2	D	33	LEU	CB-CG-CD2	-8.71	96.20	111.00
2	D	101	LYS	CD-CE-NZ	8.24	130.66	111.70
1	C	815	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	C	1032	ARG	NE-CZ-NH2	-8.08	116.26	120.30
3	G	15	VAL	CG1-CB-CG2	-7.92	98.22	110.90
2	D	86	LEU	CB-CG-CD2	7.82	124.30	111.00
1	C	541	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	A	185	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	818	ARG	NE-CZ-NH2	7.64	124.12	120.30
2	D	99	LEU	CB-CG-CD2	7.61	123.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	466	ILE	CG1-CB-CG2	-7.58	94.72	111.40
1	C	472	ILE	CG1-CB-CG2	-7.43	95.06	111.40
1	C	1032	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	717	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	B	536	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	204	ILE	CG1-CB-CG2	-7.29	95.37	111.40
1	A	19	ILE	CG1-CB-CG2	-7.24	95.46	111.40
1	C	1032	ARG	CD-NE-CZ	7.21	133.70	123.60
1	C	37	THR	CA-CB-CG2	-7.16	102.38	112.40
1	B	468	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	C	509	LYS	N-CA-C	-7.12	91.78	111.00
1	C	801	PHE	CB-CG-CD1	-7.11	115.83	120.80
3	H	15	VAL	CG1-CB-CG2	-7.09	99.56	110.90
1	B	555	LEU	CA-CB-CG	7.07	131.56	115.30
3	H	14	MET	CA-CB-CG	-7.03	101.36	113.30
2	D	53	LEU	CA-CB-CG	7.00	131.39	115.30
3	H	25	LEU	CB-CG-CD2	-6.99	99.11	111.00
1	B	818	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	C	516	PHE	CB-CG-CD2	-6.95	115.94	120.80
1	C	312	LYS	CA-CB-CG	6.86	128.49	113.40
2	D	31	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	745	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	C	75	LEU	CA-CB-CG	6.59	130.47	115.30
1	C	512	PHE	CB-CG-CD2	-6.59	116.19	120.80
1	C	586	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	815	ARG	CG-CD-NE	-6.55	98.05	111.80
1	C	927	PHE	CB-CG-CD2	6.52	125.36	120.80
1	C	21	LEU	CB-CG-CD1	-6.48	99.99	111.00
1	C	496	MET	CA-CB-CG	6.42	124.22	113.30
1	C	432	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	C	293	LEU	CB-CG-CD1	6.37	121.83	111.00
1	C	818	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	B	723	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	230	LEU	CB-CG-CD1	-6.28	100.33	111.00
1	C	520	PHE	CB-CG-CD2	6.26	125.18	120.80
1	B	139	VAL	CA-C-N	6.21	130.86	117.20
1	A	259	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	C	520	PHE	CB-CG-CD1	-6.18	116.47	120.80
1	C	92	LEU	CB-CG-CD2	6.08	121.33	111.00
1	A	239	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	B	277	ILE	CA-C-N	6.05	130.52	117.20
1	C	932	LEU	CB-CG-CD2	6.05	121.29	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	745	ASP	CB-CG-OD1	6.04	123.74	118.30
1	C	25	LEU	CB-CG-CD1	-6.03	100.75	111.00
1	C	983	ILE	CG1-CB-CG2	-6.03	98.14	111.40
1	C	541	TYR	CB-CG-CD1	6.02	124.61	121.00
1	B	518	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	C	133	SER	N-CA-CB	5.93	119.39	110.50
1	C	376	LEU	CB-CG-CD2	5.92	121.06	111.00
1	B	250	LEU	CA-CB-CG	5.90	128.87	115.30
1	C	801	PHE	CB-CG-CD2	5.90	124.93	120.80
1	C	868	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	B	75	LEU	CA-CB-CG	5.87	128.81	115.30
1	B	788	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	C	637	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	468	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	C	263	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	C	92	LEU	CB-CG-CD1	-5.80	101.15	111.00
1	A	609	VAL	CG1-CB-CG2	5.78	120.14	110.90
1	C	637	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	276	ASP	CB-CG-OD1	5.69	123.42	118.30
3	H	27	TYR	CB-CG-CD2	5.69	124.41	121.00
1	C	11	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	C	509	LYS	CA-C-N	5.61	129.54	117.20
3	H	23	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	C	111	LEU	CB-CG-CD1	5.56	120.45	111.00
1	C	467	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	B	586	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	480	LEU	CB-CG-CD2	5.50	120.35	111.00
1	C	554	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	A	822	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	C	717	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	512	PHE	CB-CG-CD1	5.43	124.60	120.80
1	C	177	LEU	CB-CG-CD2	5.42	120.21	111.00
1	A	1031	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	C	664	PHE	CB-CA-C	-5.41	99.58	110.40
1	C	230	LEU	CA-CB-CG	5.37	127.65	115.30
1	C	295	THR	CA-CB-CG2	-5.36	104.90	112.40
1	C	452	VAL	CB-CA-C	5.35	121.56	111.40
1	C	509	LYS	O-C-N	-5.34	114.15	122.70
1	C	1026	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	C	765	ARG	CG-CD-NE	-5.33	100.60	111.80
1	C	617	PHE	N-CA-C	-5.32	96.63	111.00
1	A	468	ARG	NE-CZ-NH2	-5.31	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	761	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	772	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	C	881	LEU	CB-CG-CD1	-5.27	102.05	111.00
1	C	643	LYS	CD-CE-NZ	5.24	123.75	111.70
1	C	679	GLY	N-CA-C	5.23	126.18	113.10
1	B	277	ILE	CA-C-O	-5.21	109.16	120.10
1	C	263	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	A	681	ASP	CB-CG-OD1	5.19	122.97	118.30
2	D	114	ILE	CG1-CB-CG2	-5.19	99.99	111.40
1	C	516	PHE	CB-CG-CD1	5.16	124.41	120.80
1	C	674	LEU	CA-CB-CG	-5.16	103.44	115.30
1	A	301	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	933	THR	CA-CB-CG2	-5.13	105.21	112.40
1	C	82	SER	N-CA-CB	-5.13	102.80	110.50
1	C	765	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	C	531	VAL	CG1-CB-CG2	5.12	119.09	110.90
1	C	910	ILE	CG1-CB-CG2	-5.10	100.19	111.40
1	B	765	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	578	LEU	CA-CB-CG	5.08	126.99	115.30
1	C	230	LEU	CB-CG-CD2	5.08	119.64	111.00
1	C	274	ASN	N-CA-CB	5.07	119.72	110.60
1	B	139	VAL	CA-C-O	-5.06	109.47	120.10
1	A	18	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	C	968	VAL	CG1-CB-CG2	5.06	118.99	110.90
1	C	95	GLU	OE1-CD-OE2	5.04	129.34	123.30
1	C	185	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	A	586	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	C	779	TYR	CB-CG-CD1	-5.00	118.00	121.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1037	ASN	Peptide
1	B	138	MET	Mainchain
1	B	326	PRO	Mainchain
1	B	328	ASP	Mainchain
1	B	572	PHE	Mainchain
1	C	218	GLN	Sidechain
1	C	264	ASP	Sidechain
1	C	271	GLY	Mainchain
1	C	385	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	C	902	MET	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7908	8019	8019	136	0
1	B	7845	7990	7989	152	0
1	C	7845	7990	7990	144	0
2	D	1177	1159	1159	12	0
2	E	1151	1136	1136	19	0
3	F	283	318	318	15	0
3	G	277	313	313	20	0
3	H	283	318	318	13	0
4	A	48	81	81	3	0
5	A	24	52	52	0	0
5	B	20	42	38	1	0
5	C	41	89	87	0	0
6	A	50	110	110	2	0
6	B	120	264	264	3	0
6	C	90	198	198	1	0
7	A	30	64	62	2	0
7	B	49	97	97	3	0
7	C	18	39	33	2	0
8	B	34	0	28	5	0
9	C	6	14	14	0	0
10	A	50	0	0	3	0
10	B	26	0	0	0	0
10	C	21	0	0	0	0
10	D	1	0	0	0	0
All	All	27397	28293	28306	492	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (492) 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:F:14:MET:O	3:F:18:VAL:HG12	1.78	0.83
1:B:600:THR:HG22	1:B:601:LYS:HD2	1.59	0.83
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.66	0.76
3:F:28:GLY:O	3:F:32:VAL:HG23	1.85	0.76
1:A:618:ALA:H	1:A:619:GLY:HA2	1.52	0.75
1:B:30:LEU:HD13	1:B:384:ALA:HB2	1.68	0.74
1:C:897:ILE:HD11	1:C:950:LYS:HD2	1.70	0.72
1:B:1001:ASN:O	1:B:1005:THR:HG23	1.90	0.71
3:H:6:LYS:HE2	3:H:10:PHE:CE2	2.26	0.70
1:C:961:ILE:HD11	1:C:1031:ARG:NH2	2.09	0.68
1:B:243:THR:HG22	1:B:268:ILE:HG22	1.76	0.68
1:C:524:THR:O	1:C:528:THR:OG1	2.12	0.67
1:C:764:ASP:HB3	1:C:769:LYS:HD2	1.77	0.66
1:C:336:SER:O	1:C:340:VAL:HG23	1.96	0.66
1:B:425:LEU:HD23	1:B:426:PRO:HD2	1.78	0.66
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.78	0.66
3:G:13:ILE:O	3:G:17:VAL:HG23	1.95	0.66
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.27	0.65
1:B:568:ASP:OD2	1:B:644:VAL:HG23	1.97	0.65
3:H:6:LYS:O	3:H:6:LYS:NZ	2.24	0.65
1:B:352:PHE:CE1	1:B:365:THR:HG21	2.31	0.65
3:F:13:ILE:O	3:F:17:VAL:HG23	1.97	0.65
1:A:619:GLY:O	1:A:620:ARG:O	2.15	0.64
1:A:1025:PHE:O	1:A:1029:VAL:HG23	1.97	0.64
1:A:590:VAL:O	1:A:594:VAL:HG23	1.98	0.64
1:A:879:ILE:HD12	1:C:25:LEU:HD11	1.80	0.64
1:B:555:LEU:HD21	1:B:914:LEU:CD1	2.28	0.64
1:C:303:ALA:HB2	1:C:330:THR:HG21	1.80	0.64
1:C:535:LEU:HA	1:C:538:THR:CG2	2.28	0.64
1:A:1001:ASN:O	1:A:1005:THR:HG23	1.98	0.63
8:B:1120:PUY:H2'	8:B:1120:PUY:N3	2.13	0.62
1:B:229:GLN:HG2	1:B:230:LEU:N	2.13	0.62
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.81	0.62
1:B:924:ASP:O	1:B:928:GLN:HG3	1.98	0.62
1:C:892:TYR:CE1	1:C:947:GLU:OE1	2.52	0.62
1:C:357:LEU:HD23	3:F:19:MET:CE	2.29	0.62
1:B:472:ILE:O	1:B:476:SER:OG	2.18	0.62
1:C:92:LEU:HD12	1:C:92:LEU:N	2.16	0.61
1:A:213:GLN:HB2	1:A:239:ARG:HG2	1.83	0.61
1:B:135:SER:OG	1:B:135:SER:O	2.13	0.61
1:A:809:TRP:NE1	2:E:79:LEU:HD23	2.16	0.61
1:A:563:PHE:O	1:A:924:ASP:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:MET:O	1:A:398:MET:HB2	2.02	0.60
1:B:375:VAL:HG21	1:B:481:SER:HA	1.84	0.60
1:A:677:ALA:O	1:A:678:THR:HB	2.00	0.60
2:D:60:LEU:HD22	2:D:94:GLU:HG3	1.82	0.60
1:B:1018:ALA:O	1:B:1022:VAL:HG13	2.02	0.60
1:B:459:PHE:CE1	1:B:876:LEU:HD23	2.36	0.60
3:H:6:LYS:HE2	3:H:10:PHE:CZ	2.36	0.60
1:C:328:ASP:OD1	1:C:330:THR:HG23	2.02	0.60
1:A:618:ALA:HB3	1:A:619:GLY:O	2.02	0.59
1:B:1024:VAL:O	1:B:1028:VAL:HG13	2.02	0.59
1:B:400:LEU:HD21	1:B:1003:VAL:HB	1.84	0.59
1:C:578:LEU:HD21	1:C:587:THR:HA	1.83	0.59
1:A:595:THR:HG22	1:A:599:LEU:HD12	1.84	0.59
1:A:572:PHE:HE1	1:A:631:LEU:HD21	1.67	0.59
1:B:744:ASN:O	1:B:748:THR:HG23	2.03	0.59
1:A:537:SER:HB2	1:A:540:ARG:HD3	1.83	0.59
1:A:956:GLU:OE1	1:A:958:LYS:HE2	2.03	0.59
1:B:352:PHE:HE1	1:B:365:THR:HG21	1.68	0.59
1:C:994:GLY:O	1:C:997:SER:HB3	2.02	0.59
1:A:183:ALA:HB1	1:A:770:LYS:O	2.03	0.58
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.85	0.58
1:A:423:GLU:OE2	1:A:433:LYS:NZ	2.36	0.58
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.86	0.58
1:B:35:TYR:CD1	1:B:671:ILE:HD11	2.38	0.58
1:C:554:TYR:CZ	1:C:558:ARG:HD2	2.38	0.58
1:A:703:LEU:HD23	1:A:716:VAL:HG12	1.86	0.58
1:C:482:VAL:O	1:C:486:LEU:HG	2.04	0.58
1:B:229:GLN:HG2	1:B:230:LEU:H	1.69	0.58
1:A:38:ILE:HG21	1:A:462:SER:HB3	1.86	0.58
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.85	0.58
1:B:30:LEU:CD1	1:B:384:ALA:HB2	2.34	0.57
1:A:860:THR:OG1	1:A:861:GLY:N	2.38	0.57
2:E:34:MET:CE	2:E:40:VAL:HG12	2.34	0.57
2:E:34:MET:HE1	2:E:40:VAL:HG12	1.87	0.57
1:A:545:TYR:O	1:A:549:VAL:HG23	2.05	0.57
1:C:350:LEU:HD21	3:F:11:ALA:HB1	1.85	0.57
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.87	0.57
1:B:562:SER:HA	1:B:677:ALA:CB	2.34	0.57
1:B:151:GLN:O	1:B:155:SER:OG	2.22	0.56
3:G:35:ILE:HG22	3:G:35:ILE:O	2.05	0.56
3:H:6:LYS:HE2	3:H:10:PHE:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HD23	1:A:330:THR:HB	1.87	0.56
1:B:476:SER:HB3	6:B:1113:D10:H103	1.87	0.56
2:D:112:ASN:HB2	2:D:114:ILE:HD12	1.87	0.56
3:G:30:GLY:O	3:G:34:ASN:OD1	2.23	0.56
1:A:240:LEU:HD12	1:A:240:LEU:N	2.21	0.56
1:C:1024:VAL:O	1:C:1028:VAL:HG23	2.05	0.56
1:A:213:GLN:OE1	1:A:238:THR:HG22	2.05	0.55
1:A:369:THR:O	1:A:373:PRO:HD2	2.05	0.55
3:F:9:VAL:O	3:F:13:ILE:HD13	2.06	0.55
1:A:1016:VAL:HG12	3:G:26:ILE:HG23	1.88	0.55
1:A:666:PHE:CE1	1:A:668:LEU:HD21	2.41	0.55
1:B:185:ARG:HD3	1:B:272:GLY:O	2.06	0.55
1:B:544:LEU:O	1:B:544:LEU:HD12	2.07	0.55
1:A:543:VAL:O	1:A:547:ILE:HG12	2.07	0.55
1:C:919:ARG:CG	1:C:919:ARG:O	2.55	0.55
1:C:534:ILE:HG12	1:C:541:TYR:CZ	2.42	0.55
1:C:534:ILE:HD11	3:F:33:PHE:CD2	2.42	0.55
7:B:1112:DD9:C1	7:B:1119:DD9:H1B	2.37	0.55
1:A:777:ALA:O	1:A:781:MET:HG2	2.07	0.55
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.37	0.55
2:E:25:GLY:HA2	2:E:62:ILE:HD12	1.89	0.55
1:A:3:ASN:HA	1:A:6:ILE:HD12	1.89	0.54
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.42	0.54
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.89	0.54
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.90	0.54
1:A:83:ASP:HB3	1:A:815:ARG:HG3	1.89	0.53
1:B:471:SER:O	1:B:475:VAL:HG23	2.07	0.53
1:C:189:ASN:OD1	1:C:189:ASN:C	2.46	0.53
1:A:423:GLU:HB2	1:A:425:LEU:HG	1.89	0.53
1:A:578:LEU:HD23	1:A:582:ALA:HB1	1.90	0.53
1:A:401:ALA:O	1:A:405:LEU:HG	2.09	0.53
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.74	0.53
1:A:101:ASP:OD2	10:A:1201:HOH:O	2.19	0.53
1:C:412:VAL:HG22	1:C:438:ILE:HD11	1.90	0.53
1:C:736:ALA:HB1	1:C:741:VAL:HG23	1.90	0.53
1:B:775:SER:HB3	1:B:780:ARG:HD3	1.89	0.53
1:B:780:ARG:HH21	1:B:780:ARG:HG3	1.74	0.53
1:C:926:TYR:CD1	1:C:1003:VAL:HG23	2.43	0.53
1:C:447:MET:SD	1:C:887:CYS:HB3	2.49	0.52
1:B:47:ALA:HB2	1:B:127:VAL:HG13	1.91	0.52
1:B:875:SER:O	1:B:879:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:HD23	1:A:582:ALA:CB	2.39	0.52
1:B:884:VAL:HG11	6:B:1116:D10:H102	1.91	0.52
8:B:1120:PUY:N3	8:B:1120:PUY:C2'	2.72	0.52
2:D:126:LEU:HD23	2:D:161:LEU:HD13	1.91	0.52
1:C:537:SER:HA	1:C:540:ARG:NH2	2.24	0.52
1:C:762:PHE:CE2	1:C:764:ASP:HB2	2.44	0.52
1:B:182:TYR:CD2	1:B:270:LEU:HD23	2.44	0.52
2:D:165:LEU:O	2:D:166:GLN:HG2	2.11	0.51
1:A:659:LYS:CD	1:A:659:LYS:H	2.23	0.51
1:B:277:ILE:N	1:B:277:ILE:CD1	2.73	0.51
2:E:27:ASP:OD2	2:E:61:GLU:HB3	2.11	0.51
1:B:678:THR:HG23	1:B:830:GLN:CB	2.41	0.51
1:A:357:LEU:CD2	3:G:19:MET:HE2	2.40	0.51
1:A:708:LYS:C	1:A:710:PRO:HD3	2.30	0.51
1:B:668:LEU:N	1:B:668:LEU:HD23	2.24	0.51
1:B:562:SER:HA	1:B:677:ALA:HB2	1.93	0.51
1:B:672:VAL:HG11	8:B:1120:PUY:H4'	1.93	0.51
1:B:527:TYR:CE2	1:B:968:VAL:HG13	2.46	0.51
1:B:225:VAL:HG23	1:C:781:MET:HG3	1.93	0.51
1:A:454:VAL:N	1:A:455:PRO:CD	2.75	0.50
1:B:73:ASP:HB2	1:B:106:GLN:OE1	2.10	0.50
1:B:968:VAL:HG21	1:B:1023:PRO:HG3	1.93	0.50
1:C:423:GLU:HB2	1:C:425:LEU:HD13	1.92	0.50
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	1.92	0.50
1:C:73:ASP:O	1:C:74:ASN:HB2	2.10	0.50
1:A:174:ASP:HB3	1:A:292:LYS:HG3	1.93	0.50
1:B:448:VAL:O	1:B:452:VAL:HG23	2.11	0.50
1:B:677:ALA:O	1:B:837:THR:HG21	2.11	0.50
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.93	0.50
3:G:34:ASN:O	3:G:36:PHE:N	2.40	0.50
1:A:88:VAL:HG12	1:A:89:GLN:N	2.25	0.50
1:C:1017:LEU:N	1:C:1017:LEU:CD1	2.74	0.50
2:E:30:VAL:O	2:E:34:MET:HB2	2.12	0.50
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.93	0.50
4:A:1111:LMT:H122	7:A:1113:DD9:C6	2.42	0.50
1:C:612:VAL:HG11	1:C:615:PHE:HB3	1.94	0.50
1:A:370:ILE:HD11	6:A:1106:D10:H92	1.94	0.49
1:B:676:THR:OG1	1:B:679:GLY:HA3	2.11	0.49
10:A:1201:HOH:O	1:B:73:ASP:OD2	2.20	0.49
7:C:1109:DD9:H1B	7:C:1110:DD9:C2	2.42	0.49
1:C:509:LYS:HA	1:C:510:LYS:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:PHE:CE2	1:B:764:ASP:HB2	2.48	0.49
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.94	0.49
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.93	0.49
1:A:554:TYR:CZ	1:A:558:ARG:HD2	2.47	0.49
1:B:449:LEU:O	1:B:453:PHE:HD2	1.95	0.49
1:C:901:VAL:O	1:C:904:VAL:HG12	2.12	0.49
7:B:1112:DD9:H1B	7:B:1119:DD9:H1B	1.95	0.49
1:B:851:LEU:HB3	1:B:852:PRO:HD2	1.94	0.49
1:B:999:ALA:O	1:B:1003:VAL:HG13	2.12	0.49
7:C:1109:DD9:H1B	7:C:1110:DD9:H2A	1.93	0.49
1:C:303:ALA:CB	1:C:330:THR:HG21	2.43	0.49
1:C:357:LEU:HD23	3:F:19:MET:HE2	1.93	0.49
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.13	0.49
1:C:20:MET:HG2	1:C:374:VAL:HA	1.95	0.49
1:C:485:ALA:O	1:C:490:PRO:HD3	2.12	0.49
1:B:902:MET:O	1:B:905:VAL:HG23	2.12	0.49
1:B:678:THR:HG23	1:B:830:GLN:HB2	1.94	0.48
1:A:1020:PHE:O	1:A:1023:PRO:HD2	2.13	0.48
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.94	0.48
1:A:907:LEU:HD13	1:A:1017:LEU:HB3	1.94	0.48
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.95	0.48
1:A:980:LEU:HD11	3:G:19:MET:SD	2.54	0.48
1:B:328:ASP:O	1:B:331:PRO:HD2	2.14	0.48
1:C:456:MET:HB3	1:C:876:LEU:HD21	1.94	0.48
1:C:671:ILE:HG22	1:C:671:ILE:O	2.13	0.48
1:A:101:ASP:O	1:A:105:VAL:HG23	2.12	0.48
1:A:3:ASN:OD1	1:A:432:ARG:HG2	2.14	0.48
1:B:104:GLN:OE1	1:B:131:LYS:HD3	2.13	0.48
1:B:5:PHE:CG	1:B:487:ILE:HG23	2.49	0.48
1:B:596:HIS:O	1:B:600:THR:HB	2.13	0.48
1:B:10:ILE:HB	1:C:893:GLU:OE2	2.12	0.48
1:B:664:PHE:CD2	1:B:664:PHE:O	2.67	0.48
1:C:919:ARG:HG2	1:C:919:ARG:O	2.12	0.48
1:C:115:MET:N	1:C:116:PRO:HD2	2.27	0.48
1:C:454:VAL:HB	1:C:455:PRO:CD	2.44	0.48
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.44	0.48
1:A:248:LYS:HA	1:A:261:LEU:HD13	1.95	0.48
1:C:480:LEU:O	1:C:484:VAL:HG23	2.14	0.48
2:D:89:HIS:CD2	2:D:119:LEU:HD22	2.48	0.48
1:A:8:ARG:N	1:A:9:PRO:HD3	2.29	0.48
1:C:1025:PHE:O	1:C:1029:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASN:O	1:C:110:LYS:NZ	2.44	0.48
1:C:617:PHE:O	1:C:618:ALA:HB3	2.14	0.48
3:G:15:VAL:HB	3:G:16:PRO:HD3	1.96	0.48
3:F:31:GLU:O	3:F:35:ILE:HD12	2.12	0.47
1:A:809:TRP:CD1	2:E:79:LEU:HD23	2.50	0.47
1:C:185:ARG:HD3	1:C:272:GLY:O	2.14	0.47
1:B:984:LEU:HG	3:H:18:VAL:HG11	1.95	0.47
1:B:573:MET:HE1	8:B:1120:PUY:H3	1.78	0.47
1:B:815:ARG:HH11	1:B:815:ARG:HG2	1.79	0.47
1:C:186:ILE:HD12	1:C:207:ILE:HD11	1.96	0.47
1:B:716:VAL:HG13	1:B:716:VAL:O	2.14	0.47
1:B:990:VAL:HG13	1:B:1005:THR:HG22	1.95	0.47
3:H:13:ILE:O	3:H:17:VAL:HG23	2.15	0.47
1:A:489:THR:HB	1:A:490:PRO:HD3	1.96	0.47
1:A:648:THR:HG23	1:A:665:ALA:O	2.14	0.47
1:B:666:PHE:N	1:B:666:PHE:CD2	2.83	0.47
1:B:73:ASP:O	1:B:74:ASN:HB2	2.15	0.47
1:C:33:ALA:O	1:C:391:ASN:HA	2.15	0.47
1:C:416:VAL:HG22	1:C:431:THR:HA	1.97	0.47
1:C:535:LEU:HA	1:C:538:THR:HG23	1.95	0.47
2:E:42:ALA:O	2:E:50:PRO:HD3	2.14	0.47
1:C:980:LEU:HD21	3:F:22:ILE:HD11	1.95	0.47
1:B:678:THR:O	1:B:837:THR:HG22	2.14	0.47
1:C:476:SER:O	1:C:480:LEU:HB2	2.14	0.47
1:C:537:SER:CA	1:C:540:ARG:HH21	2.28	0.47
1:A:773:VAL:O	1:A:774:MET:HB2	2.14	0.47
1:B:35:TYR:CE1	1:B:671:ILE:HD11	2.49	0.47
1:B:983:ILE:HG23	1:B:1008:MET:HG3	1.96	0.47
1:A:1008:MET:O	1:A:1012:VAL:HG23	2.15	0.47
1:A:359:LEU:HD13	1:A:364:ALA:HB1	1.95	0.47
1:C:23:GLY:O	1:C:27:ILE:HG13	2.15	0.47
3:H:27:TYR:C	3:H:27:TYR:CD1	2.87	0.47
1:A:240:LEU:CD1	1:A:240:LEU:N	2.78	0.47
1:B:425:LEU:HD23	1:B:426:PRO:CD	2.44	0.47
1:B:777:ALA:O	1:B:781:MET:HG2	2.14	0.47
1:B:555:LEU:HD21	1:B:914:LEU:HD13	1.98	0.46
1:C:263:ARG:NH2	2:E:155:ASN:O	2.49	0.46
1:C:420:MET:HB3	1:C:500:ILE:HB	1.97	0.46
3:G:12:VAL:O	3:G:16:PRO:HD2	2.15	0.46
3:H:28:GLY:O	3:H:32:VAL:HG23	2.15	0.46
1:A:38:ILE:O	1:A:38:ILE:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.45	0.46
1:C:952:LEU:HD23	1:C:952:LEU:HA	1.85	0.46
3:F:35:ILE:O	3:F:35:ILE:HG22	2.14	0.46
1:A:357:LEU:HD23	3:G:19:MET:HE2	1.97	0.46
1:A:38:ILE:CG2	1:A:462:SER:HB3	2.46	0.46
1:B:711:ASP:OD1	1:B:711:ASP:N	2.48	0.46
1:B:416:VAL:HG22	1:B:431:THR:HA	1.98	0.46
1:B:952:LEU:HA	1:B:952:LEU:HD23	1.73	0.46
1:C:901:VAL:HG13	1:C:942:ALA:HB3	1.97	0.46
1:B:225:VAL:CG2	1:C:781:MET:HG3	2.46	0.46
1:C:674:LEU:HA	1:C:674:LEU:HD23	1.68	0.46
1:C:354:VAL:CG2	1:C:984:LEU:HG	2.46	0.46
2:D:154:ILE:HG13	2:D:155:ASN:N	2.31	0.46
2:E:126:LEU:CD1	2:E:161:LEU:HD13	2.44	0.46
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.96	0.46
1:C:185:ARG:NH1	1:C:272:GLY:O	2.46	0.46
1:C:699:ARG:HG3	1:C:827:ILE:HD11	1.98	0.46
1:A:45:ILE:HD11	1:A:107:VAL:CG1	2.45	0.46
1:A:438:ILE:O	1:A:441:ALA:N	2.48	0.46
1:B:412:VAL:HG22	1:B:435:MET:HE1	1.97	0.46
3:G:12:VAL:O	3:G:16:PRO:CD	2.64	0.46
3:H:15:VAL:HB	3:H:16:PRO:HD3	1.97	0.46
4:A:1111:LMT:H122	7:A:1113:DD9:H6	1.98	0.46
1:B:259:ARG:NE	1:C:734:GLU:OE2	2.34	0.46
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.98	0.46
1:A:1026:PHE:O	1:A:1030:ARG:HB2	2.16	0.46
1:A:23:GLY:HA3	1:A:377:LEU:O	2.16	0.46
1:C:1016:VAL:HG12	1:C:1017:LEU:HD12	1.98	0.46
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.98	0.46
3:G:28:GLY:O	3:G:32:VAL:HG13	2.16	0.46
1:C:908:GLY:O	1:C:1010:GLY:HA2	2.16	0.45
1:C:509:LYS:CA	1:C:510:LYS:CB	2.94	0.45
1:C:876:LEU:O	1:C:876:LEU:HD22	2.17	0.45
1:A:211:ASN:HA	1:A:240:LEU:HD13	1.98	0.45
1:B:655:PHE:C	1:B:657:GLN:H	2.19	0.45
1:C:372:VAL:HG13	1:C:376:LEU:HD12	1.99	0.45
1:B:159:ALA:HB2	1:B:177:LEU:HD22	1.99	0.45
1:B:412:VAL:HG13	1:B:435:MET:CE	2.46	0.45
1:B:540:ARG:HB3	3:H:36:PHE:CZ	2.52	0.45
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.17	0.45
1:A:596:HIS:O	1:A:600:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:HD11	1:B:380:PHE:CD2	2.51	0.45
1:B:655:PHE:C	1:B:657:GLN:N	2.70	0.45
1:B:984:LEU:HD23	1:B:984:LEU:HA	1.84	0.45
1:C:453:PHE:O	1:C:456:MET:HG2	2.17	0.45
3:F:15:VAL:HB	3:F:16:PRO:HD3	1.98	0.45
1:A:330:THR:N	1:A:331:PRO:CD	2.80	0.45
1:A:36:PRO:HG3	1:A:469:GLN:CG	2.46	0.45
1:B:664:PHE:CG	1:B:664:PHE:O	2.70	0.45
1:C:780:ARG:HH11	1:C:780:ARG:HG3	1.81	0.45
1:C:811:TYR:CD1	1:C:811:TYR:N	2.85	0.45
1:C:968:VAL:HG12	1:C:969:ARG:N	2.30	0.45
2:E:142:GLN:HB3	2:E:146:GLY:HA2	1.98	0.45
1:B:880:SER:O	1:B:884:VAL:HG23	2.16	0.45
1:C:45:ILE:HD13	1:C:111:LEU:HD22	1.99	0.45
2:E:34:MET:CE	2:E:34:MET:HA	2.47	0.45
1:A:678:THR:HG23	1:A:679:GLY:N	2.31	0.45
2:D:115:THR:O	2:D:118:HIS:HB2	2.17	0.45
3:F:13:ILE:O	3:F:16:PRO:HD2	2.17	0.45
3:G:10:PHE:O	3:G:13:ILE:HG22	2.17	0.45
1:C:377:LEU:HD23	1:C:377:LEU:HA	1.83	0.45
2:E:100:LEU:HB3	2:E:135:TYR:CE2	2.52	0.45
2:E:46:VAL:O	2:E:78:THR:HG23	2.17	0.45
1:B:362:PHE:O	1:B:365:THR:HG22	2.17	0.44
1:A:540:ARG:NH2	3:G:36:PHE:C	2.71	0.44
1:B:527:TYR:OH	1:B:968:VAL:HG13	2.17	0.44
2:D:51:LEU:HD11	2:D:63:VAL:HG13	1.99	0.44
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.98	0.44
2:D:128:ILE:O	2:D:132:LEU:HG	2.17	0.44
3:G:23:LEU:HD23	3:G:26:ILE:HD11	1.98	0.44
1:B:775:SER:HB2	1:B:789:TRP:CZ2	2.53	0.44
1:C:158:VAL:HG22	1:C:162:MET:SD	2.58	0.44
1:C:382:VAL:HG13	1:C:386:PHE:CE2	2.52	0.44
1:C:403:GLY:O	1:C:407:ASP:OD1	2.35	0.44
1:A:4:PHE:CZ	1:A:8:ARG:HD2	2.52	0.44
1:A:931:LEU:HA	1:A:931:LEU:HD23	1.88	0.44
1:B:277:ILE:N	1:B:277:ILE:HD13	2.32	0.44
1:B:375:VAL:HG23	1:B:484:VAL:HG21	1.99	0.44
1:B:534:ILE:HG23	1:B:541:TYR:CD2	2.52	0.44
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.99	0.44
1:C:580:ALA:CB	1:C:724:THR:HG22	2.46	0.44
2:D:23:ARG:HG3	2:D:57:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PHE:CE1	1:A:929:VAL:HG21	2.53	0.44
1:B:372:VAL:HB	1:B:373:PRO:HD3	2.00	0.44
1:C:139:VAL:O	1:C:326:PRO:HD2	2.17	0.44
2:E:74:ASN:HD21	2:E:105:ASP:HB2	1.81	0.44
1:A:528:THR:HG21	1:A:969:ARG:HD3	2.00	0.44
1:A:699:ARG:HG3	1:A:827:ILE:HD11	1.98	0.44
1:B:987:MET:N	1:B:988:PRO:CD	2.80	0.44
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.99	0.44
1:C:483:LEU:HD13	1:C:483:LEU:HA	1.77	0.44
1:B:102:ILE:O	1:B:106:GLN:HG3	2.17	0.44
1:B:414:GLU:OE1	1:B:974:PRO:HD3	2.18	0.44
1:C:897:ILE:HG23	1:C:946:VAL:HG11	2.00	0.44
4:A:1101:LMT:H121	6:A:1106:D10:C1	2.48	0.44
1:A:131:LYS:HG3	1:A:131:LYS:O	2.18	0.44
1:C:5:PHE:CG	1:C:487:ILE:HG23	2.52	0.44
1:C:931:LEU:HA	1:C:931:LEU:HD23	1.79	0.44
1:A:58:GLN:HG2	1:A:59:ASP:OD1	2.18	0.43
1:A:912:ALA:HB3	1:A:931:LEU:HD21	1.98	0.43
1:B:115:MET:N	1:B:116:PRO:CD	2.81	0.43
1:C:352:PHE:CD1	1:C:352:PHE:C	2.91	0.43
1:C:930:GLY:HA2	1:C:1007:VAL:CG1	2.48	0.43
1:C:111:LEU:HD23	1:C:129:VAL:CG2	2.48	0.43
1:C:472:ILE:O	1:C:476:SER:OG	2.34	0.43
1:B:83:ASP:OD1	1:B:83:ASP:C	2.57	0.43
3:H:6:LYS:HZ1	3:H:10:PHE:HB2	1.83	0.43
1:A:904:VAL:CG1	1:A:1022:VAL:HG22	2.48	0.43
1:A:729:ILE:HG21	1:A:729:ILE:HD13	1.63	0.43
5:B:1121:D12:H61	6:C:1112:D10:H13	1.98	0.43
1:C:186:ILE:HB	1:C:773:VAL:HG12	2.00	0.43
1:A:686:ASP:HB3	1:A:823:PRO:HB2	2.00	0.43
1:A:527:TYR:OH	1:A:968:VAL:HG22	2.19	0.43
1:B:1012:VAL:HG12	1:B:1013:THR:N	2.33	0.43
1:B:456:MET:HG3	1:B:471:SER:HB2	1.99	0.43
1:B:961:ILE:HG22	1:B:965:LEU:HD22	2.00	0.43
1:C:775:SER:HB2	1:C:789:TRP:CZ2	2.53	0.43
1:C:871:ASN:O	1:C:874:PRO:HD2	2.19	0.43
1:C:552:MET:SD	1:C:906:PRO:HB3	2.59	0.43
3:F:14:MET:O	3:F:18:VAL:CG1	2.60	0.43
1:B:219:LEU:HD23	1:C:754:TRP:HZ3	1.84	0.43
1:B:815:ARG:NH1	1:B:815:ARG:HG2	2.34	0.43
1:C:743:ILE:N	1:C:743:ILE:HD13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:13:ILE:O	3:G:16:PRO:HD2	2.18	0.43
1:C:621:GLY:O	1:C:624:THR:HG22	2.19	0.43
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.51	0.43
1:B:560:PRO:O	1:B:922:THR:HB	2.18	0.43
1:C:888:LEU:HA	1:C:888:LEU:HD23	1.85	0.43
1:A:267:LYS:HD2	10:A:1240:HOH:O	2.19	0.43
1:B:18:ILE:O	1:B:21:LEU:N	2.51	0.43
1:B:466:ILE:O	1:B:467:TYR:C	2.57	0.43
1:B:72:ILE:HG22	1:B:73:ASP:N	2.33	0.43
2:E:68:LYS:O	2:E:68:LYS:HG2	2.17	0.43
3:G:35:ILE:N	3:G:35:ILE:CD1	2.81	0.43
1:B:10:ILE:HD11	1:C:895:TRP:CD1	2.54	0.43
1:B:25:LEU:HD12	1:B:25:LEU:HA	1.73	0.43
1:C:13:TRP:CZ2	1:C:492:LEU:HD21	2.54	0.43
1:A:721:LEU:HD12	1:A:815:ARG:HB2	2.01	0.42
1:C:973:ARG:HB3	1:C:974:PRO:HD3	2.01	0.42
1:A:33:ALA:O	1:A:391:ASN:HA	2.19	0.42
1:B:11:PHE:O	1:B:11:PHE:HD1	2.03	0.42
1:B:72:ILE:CG2	1:B:73:ASP:N	2.82	0.42
1:C:317:PHE:CD2	1:C:321:LEU:HD23	2.55	0.42
2:E:56:TYR:CE1	2:E:90:PHE:CZ	3.07	0.42
2:E:74:ASN:HD21	2:E:105:ASP:CB	2.32	0.42
1:A:648:THR:CG2	1:A:665:ALA:O	2.67	0.42
1:B:1016:VAL:HG12	1:B:1017:LEU:HD23	2.02	0.42
1:B:454:VAL:HB	1:B:455:PRO:HD3	2.01	0.42
1:B:708:LYS:C	1:B:710:PRO:HD3	2.39	0.42
1:C:53:ASP:O	1:C:54:ALA:C	2.55	0.42
1:C:63:GLN:O	1:C:67:GLN:HG2	2.20	0.42
1:C:907:LEU:HD11	1:C:1021:PHE:HB2	2.01	0.42
1:A:449:LEU:HB3	1:A:478:MET:SD	2.60	0.42
1:A:912:ALA:CB	1:A:931:LEU:HD21	2.49	0.42
1:B:578:LEU:HD21	1:B:590:VAL:HG21	2.00	0.42
1:B:713:LEU:HD22	1:B:843:LEU:HD23	2.01	0.42
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.83	0.42
1:B:573:MET:HE3	8:B:1120:PUY:HB1	2.01	0.42
1:C:5:PHE:CD2	1:C:487:ILE:HG23	2.55	0.42
1:C:864:TYR:O	1:C:868:LEU:HD12	2.19	0.42
3:H:6:LYS:NZ	3:H:10:PHE:CG	2.87	0.42
1:A:20:MET:HE2	1:A:20:MET:HB2	1.91	0.42
1:B:1022:VAL:HG22	1:B:1023:PRO:HD3	2.00	0.42
1:B:414:GLU:HG3	1:B:977:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:MET:SD	1:C:368:PRO:HG2	2.60	0.42
1:A:38:ILE:O	1:A:38:ILE:CG2	2.68	0.42
1:A:391:ASN:H	1:A:394:THR:HG1	1.65	0.42
1:B:352:PHE:CE1	1:B:365:THR:CG2	3.01	0.42
1:C:562:SER:O	1:C:924:ASP:HA	2.20	0.42
2:D:89:HIS:CD2	2:D:123:ARG:HD3	2.54	0.42
3:G:10:PHE:O	3:G:14:MET:HG2	2.20	0.42
1:A:30:LEU:HD23	1:A:390:ILE:HG13	2.02	0.42
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.50	0.42
1:B:127:VAL:O	1:C:112:GLN:NE2	2.53	0.42
1:B:386:PHE:CD1	1:B:386:PHE:N	2.86	0.42
1:A:220:GLY:HA2	1:B:781:MET:CE	2.49	0.42
1:B:415:ASN:O	1:B:419:VAL:HG23	2.19	0.42
1:C:1017:LEU:N	1:C:1017:LEU:HD12	2.35	0.42
1:B:423:GLU:OE2	1:B:433:LYS:HE3	2.19	0.41
1:C:49:TYR:N	1:C:86:GLY:O	2.44	0.41
3:F:21:ILE:O	3:F:25:LEU:HD12	2.19	0.41
1:A:2:PRO:O	1:A:6:ILE:HG13	2.20	0.41
1:C:536:ARG:HH11	1:C:536:ARG:CG	2.33	0.41
2:D:109:LYS:HG2	2:D:115:THR:HG22	2.02	0.41
1:A:1027:VAL:HG23	1:A:1028:VAL:N	2.36	0.41
1:A:314:GLU:N	1:A:315:PRO:CD	2.83	0.41
1:A:679:GLY:HA3	1:A:830:GLN:HA	2.01	0.41
1:B:910:ILE:O	1:B:914:LEU:HD22	2.19	0.41
1:C:114:ALA:HA	1:C:117:LEU:HD12	2.01	0.41
1:C:537:SER:HA	1:C:540:ARG:HH21	1.82	0.41
1:A:418:ARG:HG2	1:A:418:ARG:HH11	1.85	0.41
1:A:618:ALA:N	1:A:619:GLY:HA2	2.22	0.41
1:B:446:ALA:HB2	1:B:482:VAL:HG21	2.03	0.41
1:B:893:GLU:O	1:B:893:GLU:HG3	2.20	0.41
1:A:27:ILE:HD11	1:A:380:PHE:CD2	2.55	0.41
1:A:768:VAL:HG23	1:B:63:GLN:CD	2.40	0.41
1:A:127:VAL:O	1:B:113:LEU:HD13	2.20	0.41
1:B:333:VAL:O	1:B:337:ILE:HG12	2.20	0.41
1:B:445:ILE:O	1:B:449:LEU:HG	2.21	0.41
1:C:356:TYR:HE2	1:C:362:PHE:CD1	2.38	0.41
1:A:909:VAL:HG12	1:A:913:LEU:HD12	2.01	0.41
1:B:385:ALA:O	7:B:1119:DD9:H5	2.20	0.41
1:B:396:PHE:CE2	1:B:999:ALA:HB1	2.56	0.41
1:C:873:ALA:N	1:C:874:PRO:CD	2.84	0.41
1:C:918:PHE:HD1	1:C:918:PHE:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HG12	1:A:541:TYR:CZ	2.56	0.41
1:A:724:THR:HB	1:A:725:PRO:CD	2.49	0.41
1:B:240:LEU:HG	1:B:245:GLU:HB3	2.02	0.41
1:B:578:LEU:HB3	1:B:579:PRO:CD	2.51	0.41
1:B:701:GLN:O	1:B:705:GLU:HG2	2.21	0.41
1:B:778:LYS:HE2	1:B:779:TYR:CZ	2.55	0.41
1:C:181:GLN:HB3	1:C:181:GLN:HE21	1.71	0.41
1:A:115:MET:N	1:A:116:PRO:HD2	2.35	0.41
1:C:536:ARG:HH11	1:C:536:ARG:HG2	1.85	0.41
1:B:414:GLU:HG3	1:B:977:MET:HE1	2.03	0.41
1:B:483:LEU:HA	1:B:483:LEU:HD13	1.95	0.41
1:C:880:SER:O	1:C:884:VAL:HG23	2.20	0.41
1:B:367:ILE:HB	1:B:368:PRO:HD3	2.03	0.41
1:B:400:LEU:HD13	1:B:929:VAL:HG12	2.01	0.41
1:C:351:VAL:HG21	1:C:402:ILE:HG22	2.03	0.41
1:B:578:LEU:HD22	1:B:661:ALA:HB2	2.03	0.41
3:G:6:LYS:O	3:G:9:VAL:HG22	2.21	0.41
3:H:12:VAL:O	3:H:16:PRO:HD2	2.21	0.41
1:A:1038:GLU:OE1	1:A:1039:ASP:CA	2.69	0.40
1:A:1:MET:HB2	1:A:2:PRO:HD3	2.04	0.40
1:C:388:PHE:CE2	1:C:472:ILE:HG21	2.56	0.40
1:C:327:TYR:CE1	1:C:571:VAL:HB	2.56	0.40
1:A:984:LEU:CD1	3:G:15:VAL:HG22	2.51	0.40
1:A:987:MET:N	1:A:988:PRO:CD	2.85	0.40
1:C:456:MET:HB2	1:C:456:MET:HE2	1.99	0.40
2:E:128:ILE:O	2:E:132:LEU:HG	2.21	0.40
1:A:367:ILE:HG12	1:A:492:LEU:HB3	2.04	0.40
1:A:418:ARG:O	1:A:422:GLU:HG3	2.21	0.40
1:C:544:LEU:HD23	1:C:1021:PHE:CZ	2.56	0.40
1:C:309:GLU:HG3	1:C:313:MET:HE3	2.03	0.40
1:A:1038:GLU:OE1	1:A:1039:ASP:HA	2.21	0.40
1:A:355:MET:HE1	1:A:410:ILE:HD11	2.03	0.40
1:A:917:THR:O	1:A:917:THR:HG22	2.21	0.40
1:A:937:LEU:HA	1:A:937:LEU:HD23	1.97	0.40
1:B:14:VAL:HA	1:B:17:ILE:HD12	2.04	0.40
1:B:19:ILE:HG12	6:B:1118:D10:H51	2.03	0.40
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.92	0.40
1:A:879:ILE:HG23	1:C:21:LEU:HD13	2.02	0.40
1:C:544:LEU:HA	1:C:547:ILE:HD12	2.03	0.40
1:A:1:MET:N	1:A:2:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1042/1049 (99%)	1003 (96%)	36 (4%)	3 (0%)	41 74
1	B	1031/1049 (98%)	1005 (98%)	24 (2%)	2 (0%)	47 79
1	C	1031/1049 (98%)	1003 (97%)	24 (2%)	4 (0%)	34 69
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100 100
2	E	150/169 (89%)	148 (99%)	2 (1%)	0	100 100
3	F	35/49 (71%)	34 (97%)	1 (3%)	0	100 100
3	G	34/49 (69%)	33 (97%)	0	1 (3%)	4 28
3	H	35/49 (71%)	35 (100%)	0	0	100 100
All	All	3512/3632 (97%)	3413 (97%)	89 (2%)	10 (0%)	41 74

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	620	ARG
1	B	18	ILE
1	C	510	LYS
3	G	35	ILE
1	A	1041	GLU
1	C	18	ILE
1	C	539	GLY
1	C	19	ILE
1	B	19	ILE
1	A	80	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	840/855 (98%)	792 (94%)	48 (6%)	20 56
1	B	838/855 (98%)	742 (88%)	96 (12%)	5 24
1	C	838/855 (98%)	791 (94%)	47 (6%)	21 57
2	D	120/132 (91%)	114 (95%)	6 (5%)	24 60
2	E	117/132 (89%)	104 (89%)	13 (11%)	6 25
3	F	32/41 (78%)	25 (78%)	7 (22%)	1 5
3	G	31/41 (76%)	25 (81%)	6 (19%)	1 7
3	H	32/41 (78%)	28 (88%)	4 (12%)	4 21
All	All	2848/2952 (96%)	2621 (92%)	227 (8%)	12 42

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	30	LEU
1	A	49	TYR
1	A	50	PRO
1	A	80	SER
1	A	82	SER
1	A	84	SER
1	A	89	GLN
1	A	96	SER
1	A	121	GLU
1	A	135	SER
1	A	167	SER
1	A	218	GLN
1	A	219	LEU
1	A	229	GLN
1	A	233	SER
1	A	238	THR
1	A	276	ASP
1	A	293	LEU
1	A	366	LEU
1	A	423	GLU
1	A	483	LEU
1	A	505	HIS
1	A	546	LEU

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Mol	Chain	Res	Type
1	A	575	MET
1	A	578	LEU
1	A	636	ASP
1	A	649	MET
1	A	659	LYS
1	A	695	LEU
1	A	713	LEU
1	A	729	ILE
1	A	757	SER
1	A	767	ARG
1	A	815	ARG
1	A	824	SER
1	A	865	GLN
1	A	881	LEU
1	A	919	ARG
1	A	968	VAL
1	A	971	ARG
1	A	972	LEU
1	A	1005	THR
1	A	1030	ARG
1	A	1038	GLU
1	A	1039	ASP
1	A	1042	HIS
1	A	1044	HIS
1	B	1	MET
1	B	11	PHE
1	B	27	ILE
1	B	30	LEU
1	B	46	SER
1	B	49	TYR
1	B	73	ASP
1	B	75	LEU
1	B	81	ASN
1	B	83	ASP
1	B	84	SER
1	B	89	GLN
1	B	96	SER
1	B	108	GLN
1	B	111	LEU
1	B	128	SER
1	B	131	LYS
1	B	134	SER

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Mol	Chain	Res	Type
1	B	136	PHE
1	B	155	SER
1	B	167	SER
1	B	172	VAL
1	B	230	LEU
1	B	233	SER
1	B	240	LEU
1	B	243	THR
1	B	250	LEU
1	B	274	ASN
1	B	277	ILE
1	B	293	LEU
1	B	314	GLU
1	B	342	LYS
1	B	345	VAL
1	B	353	LEU
1	B	365	THR
1	B	366	LEU
1	B	377	LEU
1	B	383	LEU
1	B	386	PHE
1	B	399	VAL
1	B	455	PRO
1	B	476	SER
1	B	480	LEU
1	B	483	LEU
1	B	497	LEU
1	B	510	LYS
1	B	519	MET
1	B	528	THR
1	B	540	ARG
1	B	544	LEU
1	B	546	LEU
1	B	547	ILE
1	B	555	LEU
1	B	557	VAL
1	B	569	GLN
1	B	574	THR
1	B	575	MET
1	B	601	LYS
1	B	603	LYS
1	B	610	PHE

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Mol	Chain	Res	Type
1	B	626	ILE
1	B	649	MET
1	B	666	PHE
1	B	673	GLU
1	B	695	LEU
1	B	713	LEU
1	B	714	THR
1	B	748	THR
1	B	763	ILE
1	B	778	LYS
1	B	801	PHE
1	B	808	ARG
1	B	853	THR
1	B	876	LEU
1	B	881	LEU
1	B	886	LEU
1	B	888	LEU
1	B	894	SER
1	B	914	LEU
1	B	918	PHE
1	B	921	LEU
1	B	925	VAL
1	B	937	LEU
1	B	951	ASP
1	B	955	LYS
1	B	960	LEU
1	B	965	LEU
1	B	968	VAL
1	B	972	LEU
1	B	980	LEU
1	B	986	VAL
1	B	1003	VAL
1	B	1005	THR
1	B	1022	VAL
1	B	1028	VAL
1	B	1030	ARG
1	C	1	MET
1	C	11	PHE
1	C	21	LEU
1	C	46	SER
1	C	49	TYR
1	C	75	LEU

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Mol	Chain	Res	Type
1	C	83	ASP
1	C	96	SER
1	C	125	GLN
1	C	208	LYS
1	C	230	LEU
1	C	233	SER
1	C	239	ARG
1	C	274	ASN
1	C	353	LEU
1	C	383	LEU
1	C	405	LEU
1	C	455	PRO
1	C	463	THR
1	C	476	SER
1	C	481	SER
1	C	483	LEU
1	C	526	HIS
1	C	528	THR
1	C	540	ARG
1	C	546	LEU
1	C	569	GLN
1	C	575	MET
1	C	578	LEU
1	C	603	LYS
1	C	604	ASN
1	C	640	GLU
1	C	659	LYS
1	C	695	LEU
1	C	742	SER
1	C	778	LYS
1	C	801	PHE
1	C	808	ARG
1	C	815	ARG
1	C	876	LEU
1	C	894	SER
1	C	948	PHE
1	C	960	LEU
1	C	980	LEU
1	C	1011	MET
1	C	1017	LEU
1	C	1030	ARG
2	D	16	LYS

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Mol	Chain	Res	Type
2	D	76	TYR
2	D	94	GLU
2	D	101	LYS
2	D	139	VAL
2	D	166	GLN
2	E	27	ASP
2	E	28	ASP
2	E	29	GLU
2	E	32	ILE
2	E	34	MET
2	E	36	ASN
2	E	76	TYR
2	E	79	LEU
2	E	94	GLU
2	E	119	LEU
2	E	123	ARG
2	E	159	GLU
2	E	163	GLU
3	F	4	LEU
3	F	5	LEU
3	F	8	LEU
3	F	18	VAL
3	F	21	ILE
3	F	25	LEU
3	F	31	GLU
3	G	4	LEU
3	G	5	LEU
3	G	18	VAL
3	G	31	GLU
3	G	35	ILE
3	G	36	PHE
3	H	4	LEU
3	H	5	LEU
3	H	8	LEU
3	H	25	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

53 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	D10	B	1111	-	9,9,9	0.71	0	8,8,8	0.33	0
7	DD9	B	1112	-	6,6,8	0.41	0	5,5,7	0.56	0
7	DD9	B	1119	-	8,8,8	0.60	0	7,7,7	0.27	0
7	DD9	B	1115	-	5,5,8	0.47	0	4,4,7	0.29	0
6	D10	C	1115	-	9,9,9	0.48	0	8,8,8	0.62	0
7	DD9	A	1114	-	8,8,8	0.56	0	7,7,7	0.37	0
7	DD9	B	1106	-	6,6,8	0.70	0	5,5,7	0.14	0
6	D10	B	1101	-	9,9,9	0.65	0	8,8,8	0.39	0
5	D12	B	1104	-	8,8,11	0.50	0	7,7,10	0.43	0
5	D12	B	1121	-	10,10,11	0.69	0	9,9,10	0.33	0
7	DD9	C	1110	-	7,7,8	0.55	0	6,6,7	0.41	0
7	DD9	B	1107	-	5,5,8	0.55	0	4,4,7	0.19	0
7	DD9	C	1101	-	3,3,8	0.54	0	2,2,7	0.65	0
6	D10	B	1103	-	9,9,9	0.65	0	8,8,8	0.40	0
6	D10	A	1106	-	9,9,9	0.64	0	8,8,8	0.42	0
6	D10	B	1113	-	9,9,9	0.45	0	8,8,8	0.52	0
7	DD9	A	1113	-	6,6,8	0.60	0	5,5,7	0.38	0
6	D10	B	1117	-	9,9,9	0.56	0	8,8,8	0.57	0
4	LMT	A	1111	-	11,11,36	0.46	0	10,10,47	0.36	0
7	DD9	A	1110	-	4,4,8	0.49	0	3,3,7	0.32	0
4	LMT	A	1102	-	11,11,36	0.46	0	10,10,47	0.40	0
5	D12	C	1108	-	4,4,11	0.51	0	3,3,10	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LMT	A	1101	-	24,24,36	1.18	3 (12%)	29,29,47	1.30	3 (10%)
5	D12	C	1106	-	11,11,11	0.39	0	10,10,10	0.70	0
6	D10	A	1104	-	9,9,9	0.56	0	8,8,8	0.52	0
5	D12	C	1107	-	11,11,11	0.79	0	10,10,10	0.29	0
6	D10	C	1114	-	9,9,9	0.55	0	8,8,8	0.55	0
6	D10	B	1110	-	9,9,9	0.63	0	8,8,8	0.31	0
6	D10	B	1108	-	9,9,9	0.60	0	8,8,8	0.37	0
7	DD9	C	1109	-	5,5,8	0.58	0	4,4,7	0.20	0
6	D10	C	1111	-	9,9,9	0.56	0	8,8,8	0.28	0
6	D10	C	1113	-	9,9,9	0.65	0	8,8,8	0.32	0
7	DD9	B	1102	-	4,4,8	0.44	0	3,3,7	0.44	0
6	D10	C	1102	-	9,9,9	0.74	0	8,8,8	0.35	0
6	D10	B	1105	-	9,9,9	0.61	0	8,8,8	0.47	0
5	D12	C	1103	-	11,11,11	0.61	0	10,10,10	0.66	0
5	D12	A	1103	-	11,11,11	0.50	0	10,10,10	0.65	0
6	D10	B	1116	-	9,9,9	0.61	0	8,8,8	0.50	0
6	D10	C	1116	-	9,9,9	0.55	0	8,8,8	0.34	0
6	D10	A	1109	-	9,9,9	0.66	0	8,8,8	0.26	0
7	DD9	B	1109	-	8,8,8	0.60	0	7,7,7	0.42	0
6	D10	A	1105	-	9,9,9	0.56	0	8,8,8	0.39	0
6	D10	C	1117	-	9,9,9	0.53	0	8,8,8	0.41	0
6	D10	A	1108	-	9,9,9	0.65	0	8,8,8	0.29	0
6	D10	C	1112	-	9,9,9	0.42	0	8,8,8	0.67	0
8	PUY	B	1120	-	32,37,37	3.58	12 (37%)	33,53,53	6.44	12 (36%)
6	D10	B	1114	-	9,9,9	0.51	0	8,8,8	0.53	0
5	D12	A	1112	-	11,11,11	0.62	0	10,10,10	0.43	0
6	D10	B	1122	-	9,9,9	0.60	0	8,8,8	0.35	0
7	DD9	A	1107	-	8,8,8	0.72	0	7,7,7	0.32	0
6	D10	C	1104	-	9,9,9	0.53	0	8,8,8	0.58	0
9	HEX	C	1105	-	5,5,5	0.62	0	4,4,4	0.19	0
6	D10	B	1118	-	9,9,9	0.67	0	8,8,8	0.41	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
6	D10	B	1111	-	-	3/7/7/7	-
7	DD9	B	1112	-	-	1/4/4/6	-
7	DD9	B	1119	-	-	3/6/6/6	-
7	DD9	B	1115	-	-	2/3/3/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	D10	C	1115	-	-	2/7/7/7	-
7	DD9	A	1114	-	-	4/6/6/6	-
7	DD9	B	1106	-	-	2/4/4/6	-
6	D10	B	1101	-	-	2/7/7/7	-
5	D12	B	1104	-	-	4/6/6/9	-
5	D12	B	1121	-	-	4/8/8/9	-
7	DD9	C	1110	-	-	3/5/5/6	-
7	DD9	B	1107	-	-	2/3/3/6	-
7	DD9	C	1101	-	-	0/1/1/6	-
6	D10	B	1103	-	-	3/7/7/7	-
6	D10	A	1106	-	-	2/7/7/7	-
6	D10	B	1113	-	-	4/7/7/7	-
7	DD9	A	1113	-	-	3/4/4/6	-
6	D10	B	1117	-	-	3/7/7/7	-
4	LMT	A	1111	-	-	6/9/9/61	-
7	DD9	A	1110	-	-	1/2/2/6	-
4	LMT	A	1102	-	-	1/9/9/61	-
5	D12	C	1108	-	-	0/2/2/9	-
4	LMT	A	1101	-	-	5/15/35/61	0/1/1/2
5	D12	C	1106	-	-	4/9/9/9	-
6	D10	A	1104	-	-	1/7/7/7	-
5	D12	C	1107	-	-	5/9/9/9	-
6	D10	C	1114	-	-	1/7/7/7	-
6	D10	B	1110	-	-	4/7/7/7	-
6	D10	B	1108	-	-	3/7/7/7	-
7	DD9	C	1109	-	-	2/3/3/6	-
6	D10	C	1111	-	-	4/7/7/7	-
6	D10	C	1113	-	-	0/7/7/7	-
7	DD9	B	1102	-	-	1/2/2/6	-
6	D10	C	1102	-	-	4/7/7/7	-
6	D10	B	1105	-	-	5/7/7/7	-
5	D12	C	1103	-	-	4/9/9/9	-
5	D12	A	1103	-	-	6/9/9/9	-
6	D10	B	1116	-	-	2/7/7/7	-
6	D10	C	1116	-	-	6/7/7/7	-
6	D10	A	1109	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DD9	B	1109	-	-	0/6/6/6	-
6	D10	A	1105	-	-	2/7/7/7	-
6	D10	C	1117	-	-	4/7/7/7	-
6	D10	A	1108	-	-	4/7/7/7	-
6	D10	C	1112	-	-	2/7/7/7	-
8	PUY	B	1120	-	-	13/20/40/40	0/4/4/4
6	D10	B	1114	-	-	3/7/7/7	-
5	D12	A	1112	-	-	5/9/9/9	-
6	D10	B	1122	-	-	1/7/7/7	-
7	DD9	A	1107	-	-	4/6/6/6	-
6	D10	C	1104	-	-	4/7/7/7	-
9	HEX	C	1105	-	-	3/3/3/3	-
6	D10	B	1118	-	-	6/7/7/7	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1120	PUY	O4'-C1'	11.81	1.57	1.41
8	B	1120	PUY	C2'-C1'	-11.08	1.37	1.53
8	B	1120	PUY	C-N3'	6.72	1.48	1.34
8	B	1120	PUY	O4'-C4'	-4.63	1.34	1.45
8	B	1120	PUY	O-C	-4.22	1.15	1.23
4	A	1101	LMT	C3'-C2'	3.35	1.60	1.52
4	A	1101	LMT	C4'-C3'	3.25	1.60	1.52
8	B	1120	PUY	C6-N1	-3.11	1.28	1.33
8	B	1120	PUY	C5-C4	-3.07	1.32	1.40
8	B	1120	PUY	C4'-C3'	2.75	1.57	1.52
8	B	1120	PUY	C5-N7	-2.34	1.31	1.39
8	B	1120	PUY	CB-CG	2.28	1.56	1.51
8	B	1120	PUY	C2-N3	2.10	1.35	1.32
4	A	1101	LMT	C1'-C2'	2.06	1.58	1.52
8	B	1120	PUY	OM-CZ	2.03	1.41	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1120	PUY	N1-C6-N6	-30.24	85.23	117.06
8	B	1120	PUY	CA-C-N3'	11.63	132.28	116.15
8	B	1120	PUY	CG-CB-CA	7.77	130.28	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1120	PUY	C4-C5-N7	-7.40	101.69	109.40
8	B	1120	PUY	CB-CA-C	6.88	125.07	108.97
8	B	1120	PUY	O-C-N3'	-6.68	110.55	122.93
8	B	1120	PUY	N3-C2-N1	-6.32	118.80	128.68
4	A	1101	LMT	C4'-C3'-C2'	3.99	117.78	110.82
8	B	1120	PUY	O4'-C4'-C5'	3.59	116.97	109.21
8	B	1120	PUY	CE2-CD2-CG	3.52	125.86	121.03
8	B	1120	PUY	CD2-CG-CD1	-3.11	113.28	118.17
4	A	1101	LMT	O1'-C1'-C2'	2.38	112.02	108.30
8	B	1120	PUY	O2'-C2'-C3'	-2.35	105.41	111.16
4	A	1101	LMT	C1'-C2'-C3'	2.33	114.84	110.00
8	B	1120	PUY	O4'-C4'-C3'	2.23	107.27	104.06

There are no chirality outliers.

All (167) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1120	PUY	O-C-CA-CB
8	B	1120	PUY	N3'-C-CA-CB
8	B	1120	PUY	C3'-C4'-C5'-O5'
8	B	1120	PUY	N1-C6-N6-C9
8	B	1120	PUY	N1-C6-N6-C10
8	B	1120	PUY	C5-C6-N6-C9
8	B	1120	PUY	C5-C6-N6-C10
8	B	1120	PUY	C4'-C3'-N3'-C
8	B	1120	PUY	O4'-C4'-C5'-O5'
4	A	1101	LMT	C7-C8-C9-C10
6	A	1109	D10	C3-C4-C5-C6
7	A	1107	DD9	C4-C5-C6-C7
4	A	1111	LMT	C11-C10-C9-C8
5	C	1106	D12	C11-C10-C9-C8
6	B	1108	D10	C3-C4-C5-C6
5	A	1112	D12	C5-C6-C7-C8
6	B	1113	D10	C3-C4-C5-C6
5	A	1112	D12	C2-C3-C4-C5
6	B	1105	D10	C6-C7-C8-C9
6	C	1104	D10	C4-C5-C6-C7
6	B	1117	D10	C3-C4-C5-C6
6	B	1118	D10	C4-C5-C6-C7
7	A	1113	DD9	C3-C4-C5-C6
7	B	1112	DD9	C3-C4-C5-C6
6	B	1110	D10	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
6	C	1111	D10	C6-C7-C8-C9
6	C	1116	D10	C2-C3-C4-C5
6	C	1116	D10	C3-C4-C5-C6
5	B	1121	D12	C2-C3-C4-C5
5	A	1112	D12	C11-C10-C9-C8
6	A	1104	D10	C2-C3-C4-C5
6	C	1116	D10	C5-C6-C7-C8
6	B	1118	D10	C2-C3-C4-C5
5	C	1106	D12	C2-C3-C4-C5
7	C	1109	DD9	C2-C3-C4-C5
6	C	1116	D10	C6-C7-C8-C9
6	C	1112	D10	C5-C6-C7-C8
4	A	1111	LMT	C3-C4-C5-C6
7	B	1119	DD9	C5-C6-C7-C8
6	A	1109	D10	C5-C6-C7-C8
7	A	1107	DD9	C2-C3-C4-C5
6	B	1111	D10	C4-C5-C6-C7
6	B	1118	D10	C3-C4-C5-C6
7	B	1107	DD9	C3-C4-C5-C6
6	B	1116	D10	C6-C7-C8-C9
7	B	1106	DD9	C4-C5-C6-C7
6	C	1111	D10	C4-C5-C6-C7
5	A	1103	D12	C11-C10-C9-C8
6	B	1111	D10	C6-C7-C8-C9
5	B	1121	D12	C5-C6-C7-C8
7	B	1115	DD9	C3-C4-C5-C6
6	B	1105	D10	C2-C3-C4-C5
5	C	1103	D12	C4-C5-C6-C7
6	A	1109	D10	C1-C2-C3-C4
6	B	1101	D10	C6-C7-C8-C9
6	B	1117	D10	C1-C2-C3-C4
5	C	1106	D12	C9-C10-C11-C12
7	C	1109	DD9	C1-C2-C3-C4
6	C	1111	D10	C1-C2-C3-C4
6	B	1110	D10	C7-C8-C9-C10
6	B	1110	D10	C1-C2-C3-C4
6	C	1116	D10	C1-C2-C3-C4
6	C	1117	D10	C6-C7-C8-C9
6	C	1112	D10	C2-C3-C4-C5
7	A	1107	DD9	C5-C6-C7-C8
5	B	1104	D12	C1-C2-C3-C4
5	B	1121	D12	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
5	C	1107	D12	C6-C7-C8-C9
6	B	1118	D10	C5-C6-C7-C8
6	B	1108	D10	C5-C6-C7-C8
6	B	1105	D10	C5-C6-C7-C8
5	A	1103	D12	C6-C7-C8-C9
6	C	1116	D10	C7-C8-C9-C10
4	A	1101	LMT	C9-C10-C11-C12
5	C	1106	D12	C7-C8-C9-C10
9	C	1105	HEX	C1-C2-C3-C4
6	A	1108	D10	C6-C7-C8-C9
7	A	1107	DD9	C1-C2-C3-C4
7	A	1114	DD9	C1-C2-C3-C4
6	B	1103	D10	C6-C7-C8-C9
5	C	1107	D12	C7-C8-C9-C10
7	B	1119	DD9	C3-C4-C5-C6
5	B	1104	D12	C4-C5-C6-C7
5	A	1103	D12	C2-C3-C4-C5
6	C	1114	D10	C6-C7-C8-C9
6	B	1111	D10	C5-C6-C7-C8
4	A	1101	LMT	O1'-C1-C2-C3
6	C	1104	D10	C6-C7-C8-C9
7	B	1106	DD9	C5-C6-C7-C8
6	A	1106	D10	C2-C3-C4-C5
6	B	1113	D10	C4-C5-C6-C7
6	B	1114	D10	C5-C6-C7-C8
6	C	1104	D10	C1-C2-C3-C4
7	C	1110	DD9	C3-C4-C5-C6
8	B	1120	PUY	C-CA-CB-CG
4	A	1101	LMT	C5-C6-C7-C8
6	A	1108	D10	C7-C8-C9-C10
6	B	1118	D10	C6-C7-C8-C9
6	B	1105	D10	C7-C8-C9-C10
6	C	1115	D10	C7-C8-C9-C10
7	A	1114	DD9	C6-C7-C8-C9
5	A	1112	D12	C9-C10-C11-C12
6	C	1117	D10	C3-C4-C5-C6
6	A	1106	D10	C6-C7-C8-C9
4	A	1111	LMT	C6-C7-C8-C9
7	A	1113	DD9	C4-C5-C6-C7
4	A	1101	LMT	C11-C10-C9-C8
7	C	1110	DD9	C2-C3-C4-C5
6	C	1102	D10	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
7	B	1102	DD9	C2-C3-C4-C5
6	B	1117	D10	C7-C8-C9-C10
5	C	1107	D12	C1-C2-C3-C4
6	A	1108	D10	C4-C5-C6-C7
5	A	1103	D12	C9-C10-C11-C12
6	C	1117	D10	C1-C2-C3-C4
7	C	1110	DD9	C5-C6-C7-C8
6	B	1122	D10	C6-C7-C8-C9
6	B	1113	D10	C6-C7-C8-C9
6	B	1108	D10	C1-C2-C3-C4
7	B	1119	DD9	C6-C7-C8-C9
6	B	1103	D10	C7-C8-C9-C10
6	A	1109	D10	C7-C8-C9-C10
7	A	1114	DD9	C4-C5-C6-C7
4	A	1102	LMT	C6-C7-C8-C9
5	A	1112	D12	C4-C5-C6-C7
6	C	1111	D10	C7-C8-C9-C10
4	A	1111	LMT	C9-C10-C11-C12
6	A	1105	D10	C3-C4-C5-C6
6	C	1104	D10	C3-C4-C5-C6
7	A	1113	DD9	C1-C2-C3-C4
6	C	1102	D10	C1-C2-C3-C4
8	B	1120	PUY	N-CA-CB-CG
8	B	1120	PUY	CA-CB-CG-CD2
6	B	1113	D10	C1-C2-C3-C4
5	C	1103	D12	C9-C10-C11-C12
9	C	1105	HEX	C2-C3-C4-C5
5	C	1103	D12	C11-C10-C9-C8
6	C	1102	D10	C3-C4-C5-C6
6	B	1114	D10	C4-C5-C6-C7
6	A	1105	D10	C7-C8-C9-C10
6	B	1101	D10	C3-C4-C5-C6
8	B	1120	PUY	C2'-C3'-N3'-C
6	B	1105	D10	C3-C4-C5-C6
5	C	1107	D12	C4-C5-C6-C7
5	A	1103	D12	C3-C4-C5-C6
7	A	1114	DD9	C5-C6-C7-C8
5	B	1121	D12	C6-C7-C8-C9
6	C	1102	D10	C5-C6-C7-C8
5	B	1104	D12	C6-C7-C8-C9
5	C	1107	D12	C9-C10-C11-C12
6	C	1115	D10	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	B	1116	D10	C4-C5-C6-C7
6	B	1118	D10	C7-C8-C9-C10
6	A	1108	D10	C3-C4-C5-C6
6	B	1114	D10	C3-C4-C5-C6
6	B	1110	D10	C3-C4-C5-C6
4	A	1111	LMT	C2-C3-C4-C5
7	B	1115	DD9	C2-C3-C4-C5
7	B	1107	DD9	C2-C3-C4-C5
4	A	1111	LMT	C4-C5-C6-C7
5	B	1104	D12	C3-C4-C5-C6
5	A	1103	D12	C7-C8-C9-C10
5	C	1103	D12	C1-C2-C3-C4
6	B	1103	D10	C1-C2-C3-C4
9	C	1105	HEX	C3-C4-C5-C6
6	C	1117	D10	C7-C8-C9-C10
7	A	1110	DD9	C2-C3-C4-C5

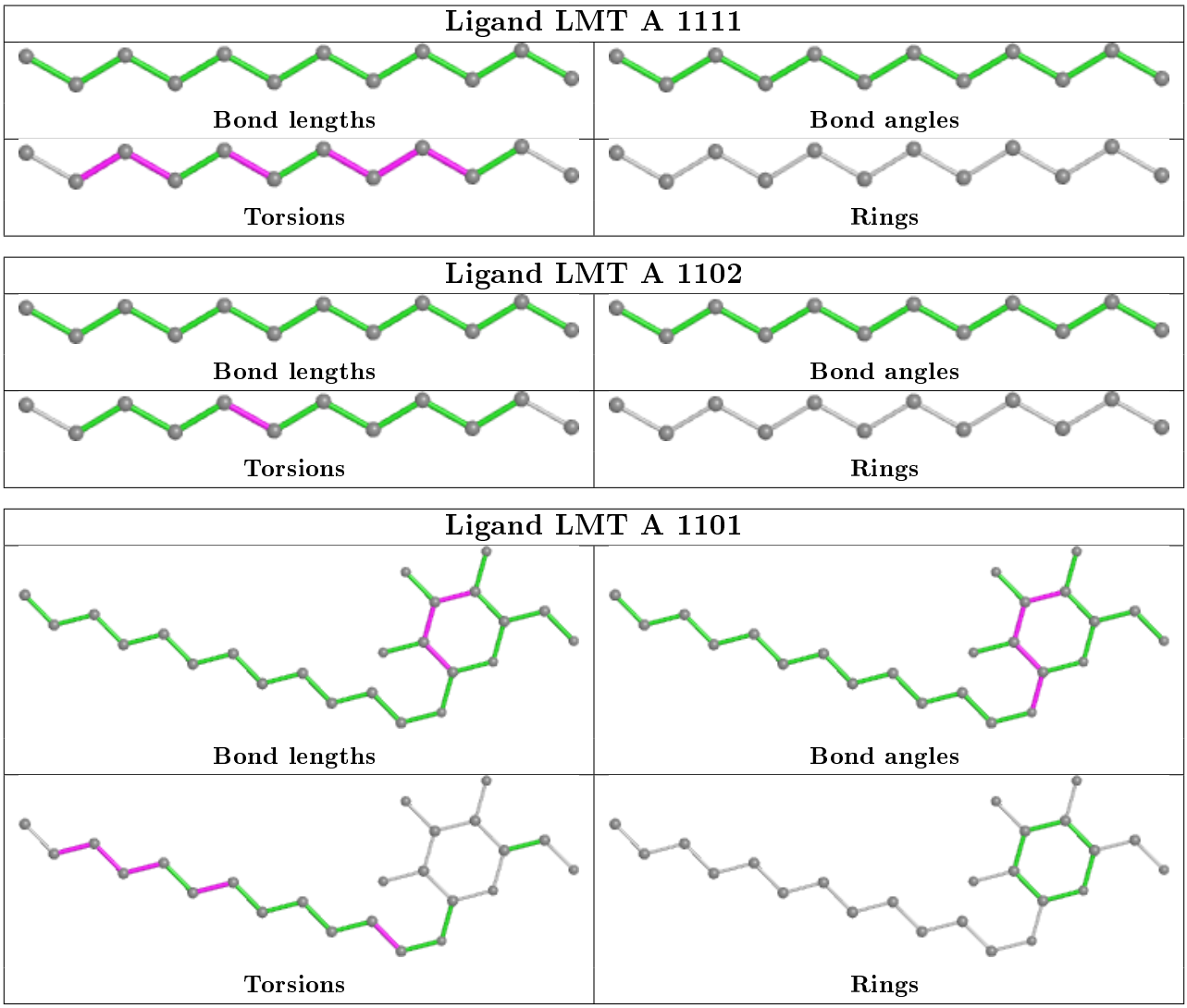
There are no ring outliers.

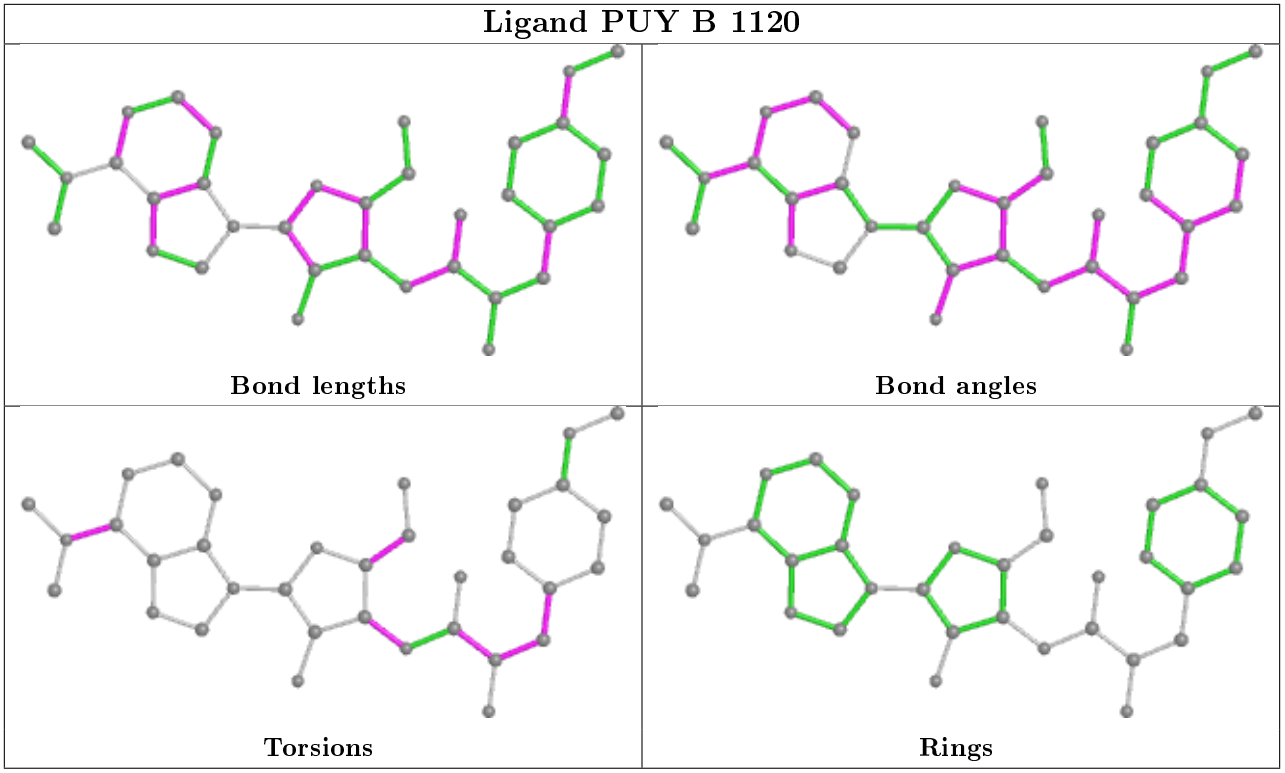
14 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1112	DD9	2	0
7	B	1119	DD9	3	0
5	B	1121	D12	1	0
7	C	1110	DD9	2	0
6	A	1106	D10	2	0
6	B	1113	D10	1	0
7	A	1113	DD9	2	0
4	A	1111	LMT	2	0
4	A	1101	LMT	1	0
7	C	1109	DD9	2	0
6	B	1116	D10	1	0
6	C	1112	D10	1	0
8	B	1120	PUY	5	0
6	B	1118	D10	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	283:GLY	C	284:GLN	N	1.14

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1044/1049 (99%)	-0.33	17 (1%) 72 59	23, 58, 112, 164	0
1	B	1033/1049 (98%)	-0.36	10 (0%) 82 72	26, 56, 83, 110	0
1	C	1033/1049 (98%)	-0.27	13 (1%) 77 65	27, 52, 94, 134	0
2	D	156/169 (92%)	-0.21	2 (1%) 77 65	40, 56, 84, 124	0
2	E	152/169 (89%)	-0.03	1 (0%) 87 81	40, 65, 92, 112	0
3	F	37/49 (75%)	0.21	5 (13%) 3 2	62, 85, 165, 178	0
3	G	36/49 (73%)	0.16	4 (11%) 5 3	86, 106, 138, 164	0
3	H	37/49 (75%)	0.34	4 (10%) 5 3	68, 89, 149, 167	0
All	All	3528/3632 (97%)	-0.29	56 (1%) 72 59	23, 57, 101, 178	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1	MET	7.0
2	D	11	GLY	5.8
2	D	12	SER	5.3
1	A	676	THR	5.2
3	H	2	LEU	5.0
3	G	1	MET	4.7
3	G	2	LEU	4.4
1	A	871	ASN	4.3
1	A	869	SER	3.8
1	B	941	ASN	3.7
3	H	1	MET	3.6
3	F	3	GLU	3.2
1	C	956	GLU	3.1
1	A	675	GLY	3.1
1	C	979	SER	3.0
1	A	1037	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	4	LEU	2.9
1	A	1043	SER	2.9
1	C	938	SER	2.8
1	A	870	GLY	2.8
1	A	670	ALA	2.7
1	A	1044	HIS	2.7
1	C	501	ALA	2.7
3	H	3	GLU	2.7
3	F	2	LEU	2.7
1	A	507	GLU	2.6
1	A	1042	HIS	2.6
1	B	146	ASP	2.5
1	C	509	LYS	2.4
1	A	1038	GLU	2.3
1	C	498	LYS	2.3
1	C	429	GLU	2.3
1	B	854	GLY	2.3
3	G	4	LEU	2.3
1	C	941	ASN	2.3
1	B	257	GLY	2.3
3	G	3	GLU	2.3
1	A	677	ALA	2.3
1	B	657	GLN	2.3
1	A	941	ASN	2.3
1	A	518	ARG	2.3
1	C	978	THR	2.2
1	B	853	THR	2.2
3	H	5	LEU	2.2
1	C	659	LYS	2.2
3	F	5	LEU	2.1
1	B	407	ASP	2.1
1	B	501	ALA	2.1
1	B	508	GLY	2.1
1	C	511	GLY	2.1
1	A	673	GLU	2.1
1	A	836	SER	2.1
2	E	33	LEU	2.1
1	C	255	GLN	2.0
1	C	254	ASN	2.0
1	B	502	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	D10	C	1116	10/10	0.43	0.63	76,109,133,139	0
8	PUY	B	1120	34/34	0.50	0.57	96,159,207,234	0
6	D10	A	1105	10/10	0.60	0.85	68,99,129,130	0
6	D10	C	1115	10/10	0.70	0.70	82,104,124,125	0
7	DD9	B	1109	9/9	0.70	0.61	86,113,126,126	0
6	D10	B	1122	10/10	0.71	0.58	73,110,128,130	0
6	D10	C	1111	10/10	0.74	0.54	75,108,132,134	0
6	D10	C	1117	10/10	0.74	0.95	75,96,113,113	0
7	DD9	B	1106	7/9	0.75	0.41	65,90,110,110	0
6	D10	C	1114	10/10	0.77	0.54	68,97,112,116	0
5	D12	C	1103	12/12	0.77	0.33	51,81,98,104	0
6	D10	A	1109	10/10	0.78	0.54	66,91,103,105	0
7	DD9	B	1112	7/9	0.78	0.55	81,97,108,113	0
6	D10	B	1114	10/10	0.79	0.46	69,92,106,111	0
5	D12	B	1104	9/12	0.79	0.44	79,98,109,111	0
7	DD9	A	1114	9/9	0.80	0.63	72,95,113,116	0
9	HEX	C	1105	6/6	0.81	0.22	61,77,99,99	0
6	D10	B	1118	10/10	0.81	0.37	63,91,108,112	0
7	DD9	B	1119	9/9	0.83	0.51	68,86,103,104	0
7	DD9	A	1107	9/9	0.83	0.34	54,74,88,90	0
6	D10	B	1110	10/10	0.84	0.54	69,90,104,105	0
6	D10	C	1113	10/10	0.84	0.61	58,82,102,111	0
6	D10	A	1104	10/10	0.85	0.47	66,93,111,111	0
6	D10	C	1112	10/10	0.85	0.30	81,106,121,126	0
6	D10	A	1106	10/10	0.86	0.35	60,84,100,105	0
6	D10	C	1102	10/10	0.86	0.43	52,71,88,91	0
7	DD9	A	1113	7/9	0.86	0.28	65,83,96,100	0

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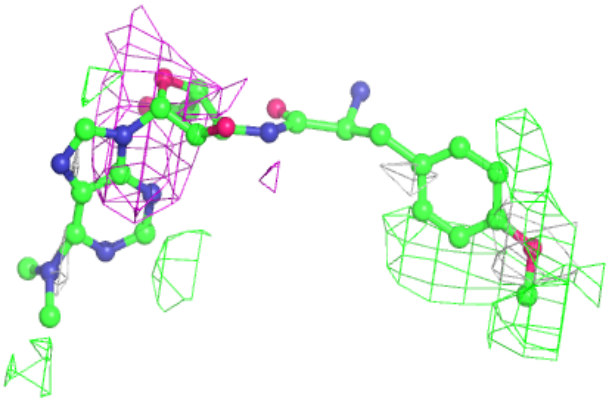
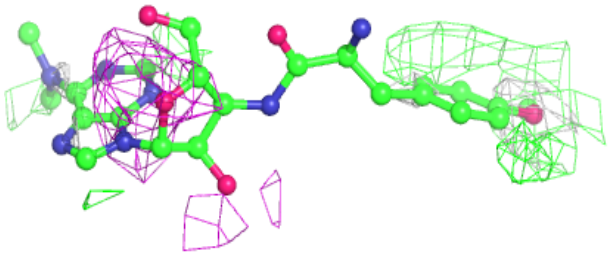
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LMT	A	1102	12/35	0.86	0.37	59,84,101,103	0
5	D12	C	1106	12/12	0.86	0.47	80,97,107,110	0
4	LMT	A	1111	12/35	0.87	0.24	63,85,101,102	0
6	D10	B	1113	10/10	0.87	0.57	73,100,113,115	0
5	D12	C	1108	5/12	0.87	0.43	77,97,105,105	0
7	DD9	C	1109	6/9	0.87	0.49	73,88,108,108	0
7	DD9	B	1115	6/9	0.87	0.55	60,74,87,87	0
5	D12	B	1121	11/12	0.88	0.45	57,88,105,110	0
6	D10	B	1103	10/10	0.89	0.31	63,86,91,92	0
6	D10	B	1116	10/10	0.89	0.30	46,71,86,90	0
6	D10	B	1105	10/10	0.90	0.48	52,72,79,80	0
6	D10	B	1111	10/10	0.90	0.27	44,75,103,105	0
5	D12	A	1103	12/12	0.90	0.38	58,80,90,90	0
5	D12	C	1107	12/12	0.90	0.34	43,56,68,72	0
6	D10	B	1108	10/10	0.91	0.42	64,85,103,103	0
5	D12	A	1112	12/12	0.91	0.28	46,75,99,104	0
4	LMT	A	1101	24/35	0.91	0.24	53,80,116,124	0
6	D10	A	1108	10/10	0.91	0.61	52,67,76,77	0
7	DD9	C	1110	8/9	0.91	0.45	64,91,103,110	0
7	DD9	A	1110	5/9	0.91	0.60	56,67,80,80	0
6	D10	B	1101	10/10	0.93	0.44	52,81,91,95	0
7	DD9	B	1107	6/9	0.93	0.56	66,79,94,94	0
6	D10	B	1117	10/10	0.93	0.27	49,68,100,105	0
6	D10	C	1104	10/10	0.94	0.17	50,70,83,87	0
7	DD9	C	1101	4/9	0.95	0.34	62,75,83,83	0
7	DD9	B	1102	5/9	0.96	0.52	48,65,83,83	0

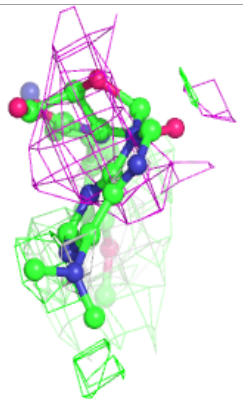
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PUY B 1120:

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

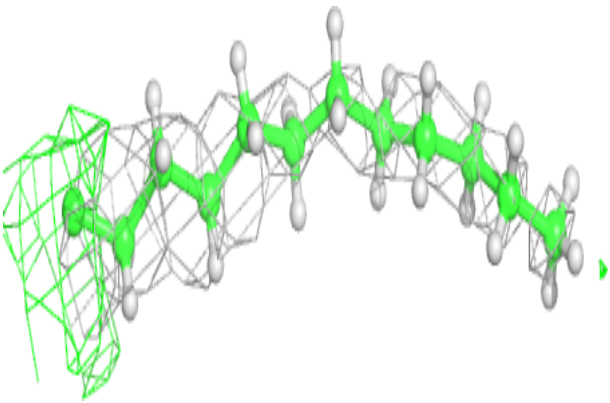


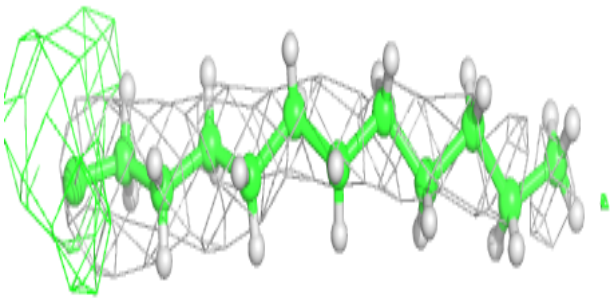


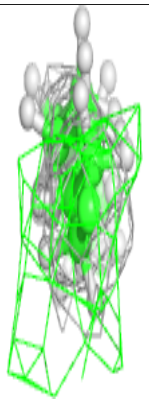


Electron density around LMT A 1102:

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

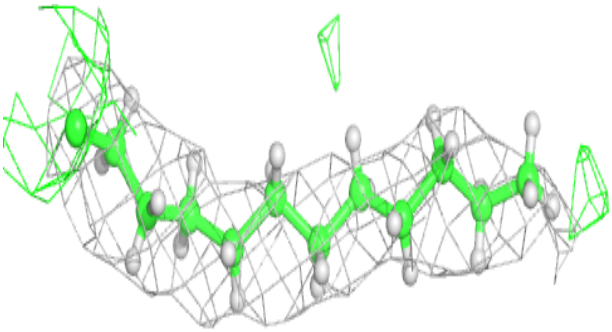


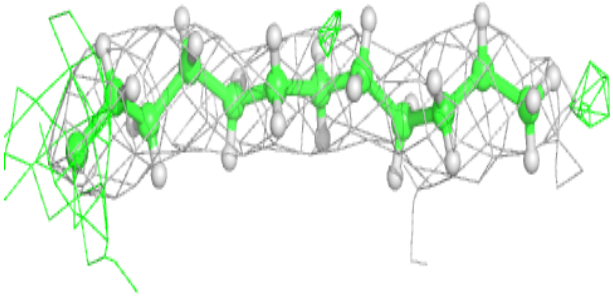


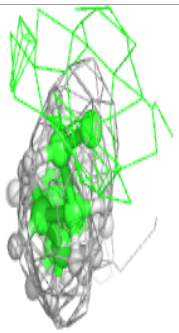


Electron density around LMT A 1111:

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

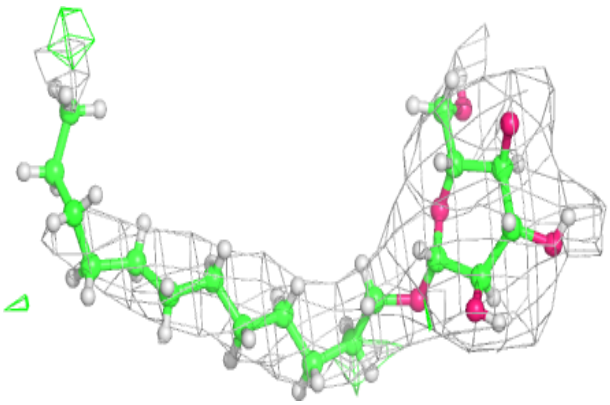


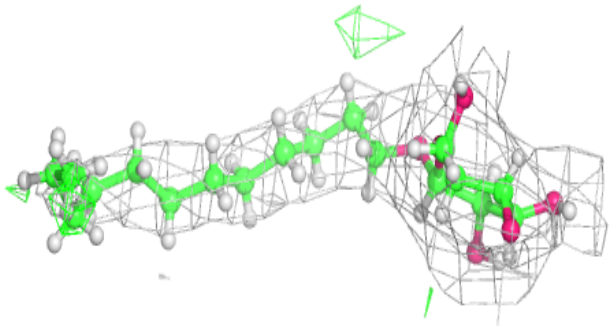


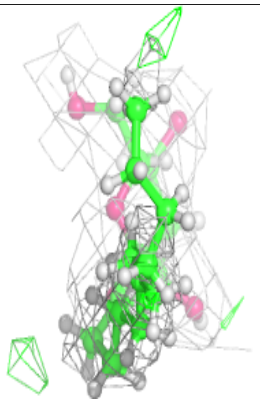


Electron density around LMT A 1101:

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







6.5 Other polymers (i)

There are no such residues in this entry.