



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2020 – 07:47 AM EST

PDB ID : 6NQT
Title : GalNac-T2 soaked with UDP-sugar
Authors : Fernandez, D.; Bertozzi, C.R.; Schumann, B.; Agbay, A.
Deposited on : 2019-01-21
Resolution : 3.05 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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

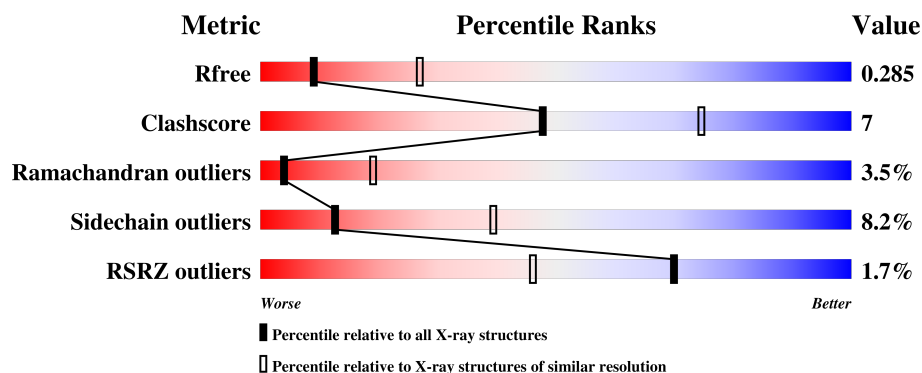
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	111664	1497 (3.10-3.02)
Clashscore	122126	1601 (3.10-3.02)
Ramachandran outliers	120053	1548 (3.10-3.02)
Sidechain outliers	120020	1547 (3.10-3.02)
RSRZ outliers	108989	1462 (3.10-3.02)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	571	<div> <div>66%</div> <div>17%</div> <div>•</div> <div>13%</div> </div>
1	B	571	<div> <div>68%</div> <div>14%</div> <div>• •</div> <div>13%</div> </div>
1	C	571	<div> <div>68%</div> <div>15%</div> <div>•</div> <div>14%</div> </div>
1	D	571	<div> <div>68%</div> <div>15%</div> <div>• •</div> <div>13%</div> </div>
1	E	571	<div> <div>66%</div> <div>15%</div> <div>•</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	571	

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
3	LR7	D	702	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23138 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Polypeptide N-acetylgalactosaminyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3954	2487	719	724	24			
1	B	494	Total	C	N	O	S	0	0	0
			3802	2388	687	704	23			
1	C	491	Total	C	N	O	S	0	0	0
			3796	2394	676	702	24			
1	D	495	Total	C	N	O	S	0	0	0
			3829	2409	689	707	24			
1	E	485	Total	C	N	O	S	0	0	0
			3700	2328	665	684	23			
1	F	483	Total	C	N	O	S	0	0	0
			3604	2264	644	673	23			

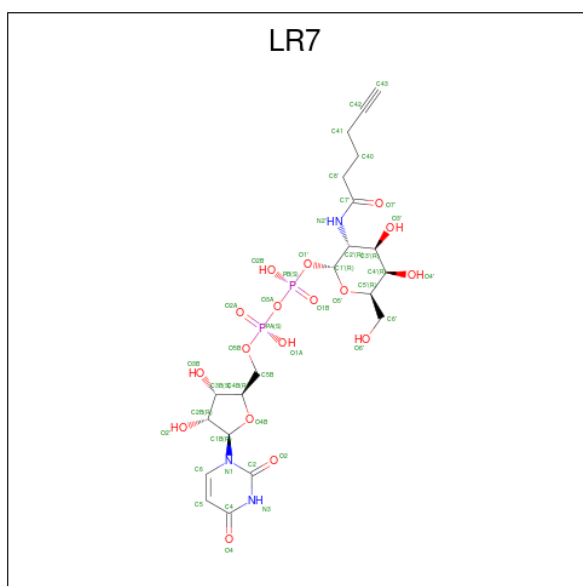
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	ALA	ILE	engineered mutation	UNP Q10471
A	310	ALA	LEU	engineered mutation	UNP Q10471
B	253	ALA	ILE	engineered mutation	UNP Q10471
B	310	ALA	LEU	engineered mutation	UNP Q10471
C	253	ALA	ILE	engineered mutation	UNP Q10471
C	310	ALA	LEU	engineered mutation	UNP Q10471
D	253	ALA	ILE	engineered mutation	UNP Q10471
D	310	ALA	LEU	engineered mutation	UNP Q10471
E	253	ALA	ILE	engineered mutation	UNP Q10471
E	310	ALA	LEU	engineered mutation	UNP Q10471
F	253	ALA	ILE	engineered mutation	UNP Q10471
F	310	ALA	LEU	engineered mutation	UNP Q10471

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is [[(2 {R},3 {S},4 {R},5 {R})-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {R},4 {R},5 {R},6 {R})-3-(hex-5-ynoylamino)-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl] hydrogen phosphate (three-letter code: LR7) (formula: C₂₁H₃₁N₃O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 21	N 3	O 17	P 2	0	0
3	B	1	Total 43	C 21	N 3	O 17	P 2	0	0
3	C	1	Total 43	C 21	N 3	O 17	P 2	0	0
3	D	1	Total 43	C 21	N 3	O 17	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			43	21	3	17	2		
3	F	1	Total	C	N	O	P	0	0
			43	21	3	17	2		

- Molecule 4 is water.

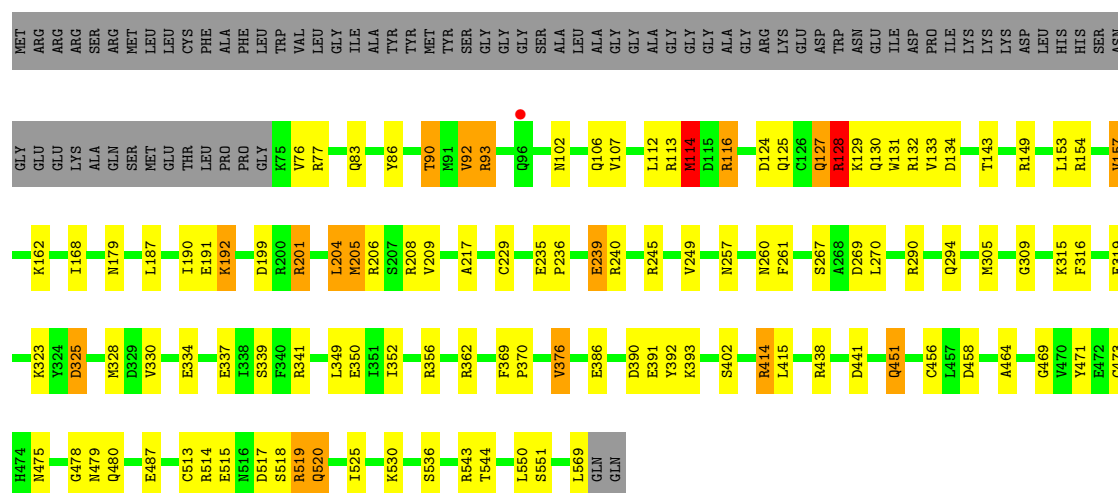
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	33	Total	O	0	0
			33	33		
4	C	27	Total	O	0	0
			27	27		
4	D	30	Total	O	0	0
			30	30		
4	E	17	Total	O	0	0
			17	17		
4	F	11	Total	O	0	0
			11	11		

3 Residue-property plots

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.

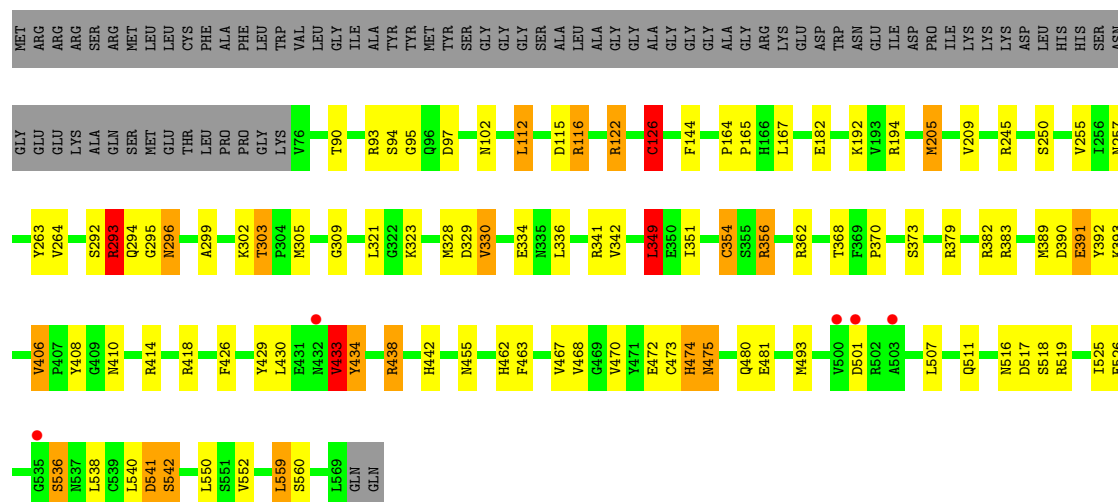
• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

Chain A: 

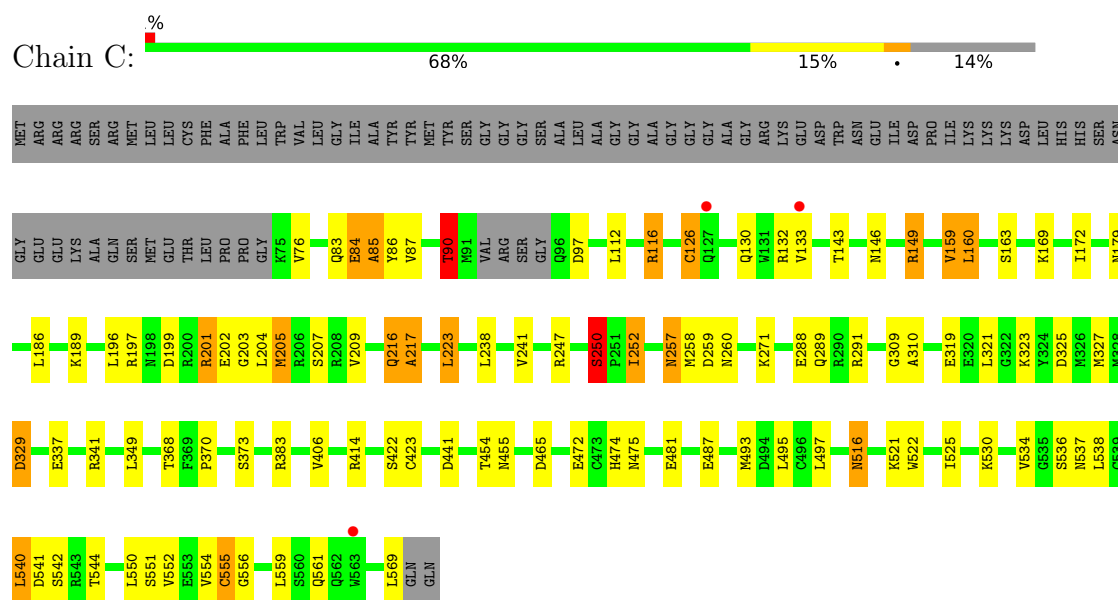


• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

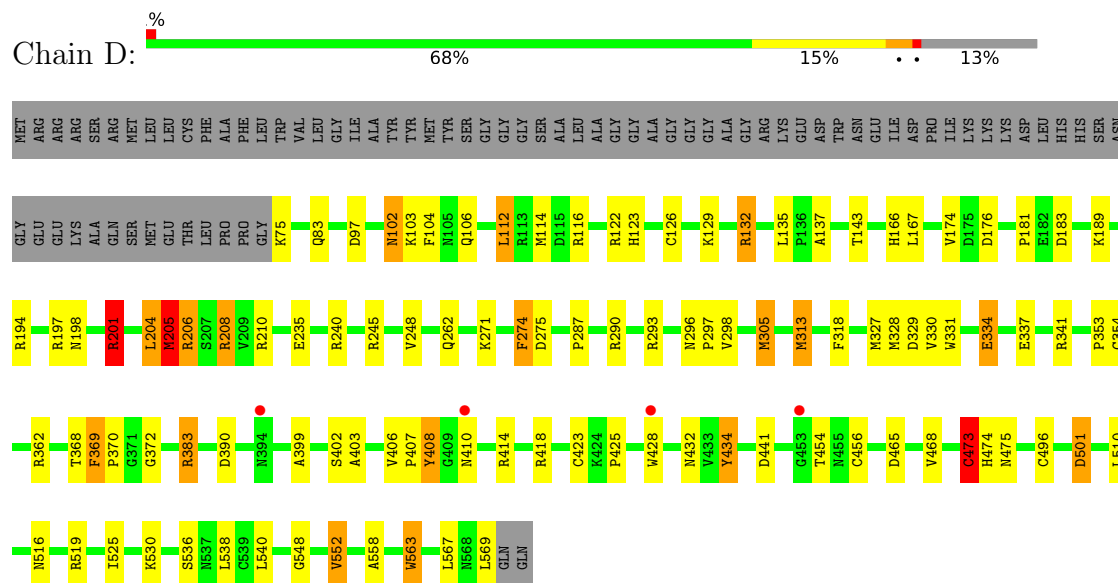
Chain B: 



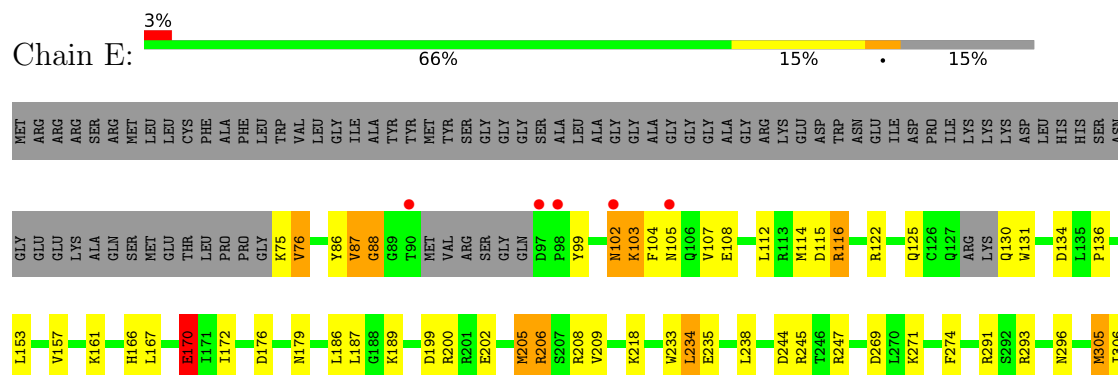
• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

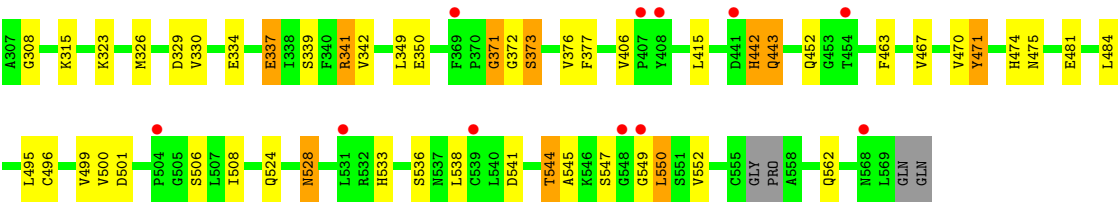


• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

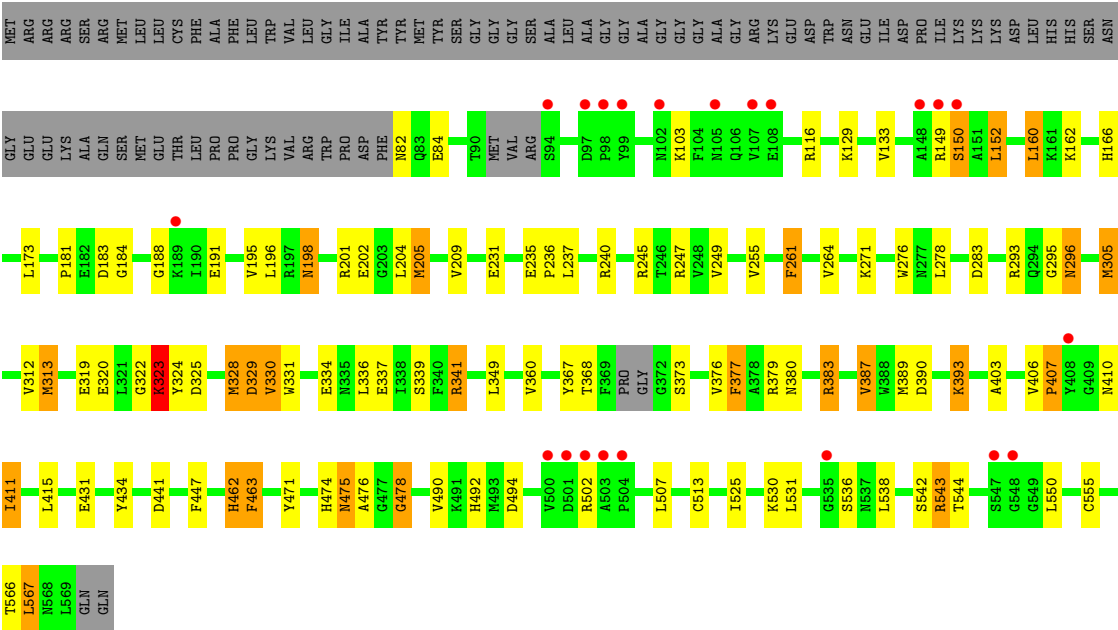


• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2





● Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.58Å 120.13Å 247.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.70 – 3.05 38.87 – 3.05	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.70-3.05) 96.6 (38.87-3.05)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.231 , 0.286 0.234 , 0.285	Depositor DCC
R_{free} test set	3349 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23138	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, LR7

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	0.76	0/4046	1.02	22/5473 (0.4%)
1	B	0.80	1/3890 (0.0%)	1.07	20/5287 (0.4%)
1	C	0.76	1/3885 (0.0%)	1.04	15/5277 (0.3%)
1	D	0.81	2/3920 (0.1%)	1.11	28/5325 (0.5%)
1	E	0.82	0/3784	1.14	25/5141 (0.5%)
1	F	0.86	1/3684 (0.0%)	1.13	27/5015 (0.5%)
All	All	0.80	5/23209 (0.0%)	1.09	137/31518 (0.4%)

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	D	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	235	GLU	CD-OE1	8.13	1.34	1.25
1	B	536	SER	CB-OG	-7.09	1.33	1.42
1	C	250	SER	CB-OG	-5.24	1.35	1.42
1	F	320	GLU	CD-OE2	-5.16	1.20	1.25
1	D	337	GLU	CD-OE1	-5.14	1.20	1.25

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	541	ASP	CB-CG-OD1	-15.16	104.66	118.30
1	E	541	ASP	CB-CG-OD2	14.25	131.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	341	ARG	NE-CZ-NH2	11.95	126.27	120.30
1	E	341	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	F	293	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	F	377	PHE	CB-CG-CD1	9.52	127.46	120.80
1	C	223	LEU	CB-CG-CD1	9.16	126.58	111.00
1	B	418	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	B	517	ASP	CB-CG-OD2	8.95	126.36	118.30
1	A	206	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	349	LEU	CB-CG-CD1	-8.62	96.36	111.00
1	D	176	ASP	CB-CG-OD1	8.53	125.98	118.30
1	F	247	ARG	NE-CZ-NH2	8.53	124.57	120.30
1	B	354	CYS	CA-CB-SG	-8.09	99.43	114.00
1	E	329	ASP	CB-CG-OD2	7.94	125.45	118.30
1	C	540	LEU	CB-CG-CD1	7.92	124.47	111.00
1	D	116	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	B	245	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	A	458	ASP	CB-CG-OD2	7.57	125.11	118.30
1	F	377	PHE	CB-CG-CD2	-7.50	115.55	120.80
1	B	245	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	F	325	ASP	CB-CG-OD2	7.27	124.84	118.30
1	F	494	ASP	CB-CA-C	-7.17	96.06	110.40
1	E	202	GLU	N-CA-C	-7.14	91.72	111.00
1	A	316	PHE	CB-CG-CD1	7.07	125.75	120.80
1	D	116	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	F	201	ARG	NE-CZ-NH2	6.99	123.80	120.30
1	E	170	GLU	CG-CD-OE1	-6.97	104.36	118.30
1	A	319	GLU	CB-CA-C	6.95	124.29	110.40
1	E	326	MET	CG-SD-CE	6.92	111.28	100.20
1	D	473	CYS	CA-CB-SG	6.89	126.41	114.00
1	E	337	GLU	OE1-CD-OE2	-6.81	115.13	123.30
1	B	517	ASP	CB-CG-OD1	-6.77	112.21	118.30
1	D	441	ASP	CB-CG-OD2	6.64	124.27	118.30
1	B	126	CYS	CA-CB-SG	6.60	125.89	114.00
1	D	112	LEU	CA-CB-CG	6.54	130.33	115.30
1	B	97	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	341	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	E	377	PHE	CB-CG-CD2	-6.44	116.29	120.80
1	B	414	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	C	97	ASP	CB-CG-OD1	6.38	124.04	118.30
1	F	323	LYS	CB-CA-C	-6.37	97.66	110.40
1	B	501	ASP	CB-CG-OD1	6.36	124.02	118.30
1	E	234	LEU	CB-CG-CD1	-6.34	100.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ASP	CB-CG-OD1	6.33	123.99	118.30
1	D	510	LEU	CA-CB-CG	6.32	129.84	115.30
1	A	208	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	E	134	ASP	CB-CG-OD1	6.24	123.91	118.30
1	B	329	ASP	CB-CG-OD2	-6.23	112.70	118.30
1	D	240	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	F	543	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	E	170	GLU	CG-CD-OE2	6.11	130.53	118.30
1	E	208	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	C	260	ASN	CB-CA-C	-6.05	98.29	110.40
1	E	377	PHE	CB-CG-CD1	6.04	125.03	120.80
1	A	441	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	F	328	MET	N-CA-C	5.98	127.15	111.00
1	A	441	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	192	LYS	CD-CE-NZ	5.97	125.43	111.70
1	F	202	GLU	N-CA-C	-5.97	94.88	111.00
1	F	247	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	356	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	B	433	VAL	CA-C-O	5.89	132.47	120.10
1	E	484	LEU	CB-CG-CD2	5.86	120.95	111.00
1	A	206	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	127	GLN	N-CA-C	-5.85	95.20	111.00
1	C	383	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	415	LEU	CA-CB-CG	5.79	128.61	115.30
1	D	362	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	239	GLU	OE1-CD-OE2	5.79	130.24	123.30
1	D	274	PHE	CB-CG-CD2	5.78	124.84	120.80
1	F	245	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	A	316	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	D	122	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	F	550	LEU	CA-CB-CG	5.61	128.21	115.30
1	F	271	LYS	CA-CB-CG	5.59	125.70	113.40
1	A	270	LEU	CB-CG-CD1	5.59	120.50	111.00
1	D	434	TYR	CB-CG-CD1	5.58	124.35	121.00
1	D	205	MET	N-CA-C	-5.56	95.99	111.00
1	F	261	PHE	CB-CG-CD1	-5.55	116.92	120.80
1	D	183	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	A	114	MET	CG-SD-CE	5.52	109.03	100.20
1	C	247	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	C	160	LEU	N-CA-CB	5.50	121.40	110.40
1	F	152	LEU	CB-CG-CD2	5.50	120.35	111.00
1	B	122	ARG	NE-CZ-NH2	-5.50	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	206	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	C	247	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	A	204	LEU	CB-CG-CD1	-5.49	101.67	111.00
1	C	252	ILE	CB-CA-C	5.48	122.56	111.60
1	D	208	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	441	ASP	CB-CG-OD1	5.45	123.20	118.30
1	E	176	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	E	234	LEU	CB-CG-CD2	5.41	120.19	111.00
1	F	538	LEU	CB-CG-CD1	5.35	120.10	111.00
1	A	458	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	B	414	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	321	LEU	CB-CG-CD2	5.32	120.05	111.00
1	D	201	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	D	262	GLN	CA-CB-CG	5.32	125.10	113.40
1	C	258	MET	CA-CB-CG	5.30	122.32	113.30
1	E	199	ASP	CB-CG-OD2	5.27	123.05	118.30
1	F	494	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	A	350	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	D	204	LEU	CA-CB-CG	5.27	127.41	115.30
1	E	115	ASP	N-CA-CB	-5.26	101.13	110.60
1	E	481	GLU	CG-CD-OE1	5.25	128.81	118.30
1	F	341	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	507	LEU	CA-CB-CG	5.22	127.30	115.30
1	F	283	ASP	CB-CG-OD2	-5.22	113.61	118.30
1	D	204	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	B	541	ASP	N-CA-C	5.20	125.05	111.00
1	D	414	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	F	462	HIS	CB-CA-C	5.20	120.80	110.40
1	B	115	ASP	N-CA-CB	-5.19	101.26	110.60
1	F	393	LYS	CB-CA-C	-5.17	100.05	110.40
1	F	383	ARG	CA-CB-CG	5.17	124.77	113.40
1	C	204	LEU	CB-CG-CD1	5.17	119.78	111.00
1	C	349	LEU	CB-CG-CD2	5.16	119.78	111.00
1	E	269	ASP	CB-CG-OD1	5.16	122.95	118.30
1	D	501	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	D	519	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	414	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	F	261	PHE	CB-CG-CD2	5.13	124.39	120.80
1	D	418	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	B	559	LEU	CB-CA-C	5.12	119.92	110.20
1	E	329	ASP	CB-CG-OD1	-5.11	113.71	118.30
1	D	97	ASP	CB-CG-OD2	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	114	MET	CA-CB-CG	5.10	121.97	113.30
1	A	392	TYR	CB-CG-CD1	5.07	124.04	121.00
1	E	199	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	F	240	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	F	313	MET	CB-CG-SD	5.02	127.47	112.40
1	E	496	CYS	CA-CB-SG	5.01	123.03	114.00
1	B	303	THR	CA-CB-CG2	5.01	119.41	112.40
1	D	408	TYR	N-CA-C	5.01	124.52	111.00
1	C	541	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
1	D	137	ALA	Mainchain
1	D	407	PRO	Peptide

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	3954	0	3867	58	0
1	B	3802	0	3592	47	0
1	C	3796	0	3604	52	0
1	D	3829	0	3627	48	0
1	E	3700	0	3446	46	0
1	F	3604	0	3310	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	43	0	0	5	0
3	B	43	0	0	4	0
3	C	43	0	0	3	0
3	D	43	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	43	0	0	0	0
3	F	43	0	0	1	0
4	A	71	0	0	4	0
4	B	33	0	0	1	0
4	C	27	0	0	1	0
4	D	30	0	0	1	0
4	E	17	0	0	0	0
4	F	11	0	0	0	0
All	All	23138	0	21446	293	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (293) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:VAL:HG21	1:D:354:CYS:SG	1.88	1.14
1:B:293:ARG:O	1:B:295:GLY:N	1.86	1.06
1:D:456:CYS:SG	1:D:473:CYS:HB2	1.97	1.05
1:E:75:LYS:O	1:E:189:LYS:O	1.77	1.01
1:B:255:VAL:O	1:B:263:TYR:O	1.78	1.01
3:D:702:LR7:C1'	3:D:702:LR7:O7'	2.22	0.88
1:B:429:TYR:O	1:B:433:VAL:O	1.94	0.85
1:D:201:ARG:NH1	1:D:368:THR:OG1	2.10	0.84
3:D:702:LR7:C7'	3:D:702:LR7:O1'	2.16	0.81
1:A:309:GLY:HA2	3:A:702:LR7:O3'	1.81	0.80
1:C:76:VAL:HG12	1:C:189:LYS:O	1.84	0.78
1:C:87:VAL:O	1:C:90:THR:OG1	2.02	0.77
1:F:249:VAL:HG23	1:F:312:VAL:HG12	1.66	0.77
1:D:102:ASN:O	1:D:104:PHE:N	2.19	0.76
1:E:87:VAL:O	1:E:88:GLY:O	2.05	0.74
1:C:497:LEU:O	1:C:522:TRP:CZ3	2.42	0.73
1:D:126:CYS:SG	1:D:298:VAL:HG21	2.29	0.73
1:C:257:ASN:HD22	1:C:259:ASP:H	1.34	0.72
1:F:276:TRP:O	1:F:278:LEU:HD13	1.90	0.72
1:C:309:GLY:HA2	3:C:702:LR7:O3'	1.90	0.72
1:A:83:GLN:O	1:A:86:TYR:O	2.09	0.70
1:C:90:THR:HG21	1:C:149:ARG:HG3	1.73	0.70
1:D:298:VAL:HG23	1:D:353:PRO:HB2	1.74	0.69
1:A:124:ASP:O	1:A:127:GLN:O	2.11	0.68
1:F:255:VAL:HG23	1:F:264:VAL:HB	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:702:LR7:O1'	3:D:702:LR7:O7'	2.12	0.68
1:A:469:GLY:HA2	1:A:550:LEU:HD13	1.74	0.68
1:D:298:VAL:CG2	1:D:354:CYS:SG	2.74	0.68
1:B:473:CYS:O	1:B:475:ASN:N	2.27	0.67
1:F:249:VAL:CG2	1:F:312:VAL:HG12	2.25	0.67
1:D:248:VAL:HG22	1:D:313:MET:HG2	1.75	0.67
1:C:497:LEU:O	1:C:522:TRP:CH2	2.48	0.66
1:A:309:GLY:CA	3:A:702:LR7:O3'	2.42	0.66
1:B:309:GLY:CA	3:B:702:LR7:O3'	2.43	0.66
1:A:451:GLN:HG3	1:A:456:CYS:SG	2.35	0.66
1:C:84:GLU:O	1:C:85:ALA:HB3	1.96	0.66
1:A:217:ALA:O	1:A:315:LYS:HE3	1.96	0.66
1:A:514:ARG:H	1:A:520:GLN:HE22	1.42	0.65
1:A:187:LEU:O	1:A:190:ILE:HG13	1.97	0.65
1:C:309:GLY:CA	3:C:702:LR7:O3'	2.45	0.65
1:F:383:ARG:O	1:F:387:VAL:HG23	1.98	0.64
1:F:474:HIS:ND1	1:F:474:HIS:O	2.30	0.64
1:A:114:MET:HB2	1:A:157:VAL:HG11	1.78	0.64
1:E:99:TYR:O	1:E:103:LYS:HA	1.97	0.64
1:D:248:VAL:HG22	1:D:313:MET:CG	2.28	0.64
1:B:309:GLY:HA2	3:B:702:LR7:O3'	1.98	0.64
1:A:201:ARG:NH1	3:A:702:LR7:O4	2.31	0.64
1:D:456:CYS:SG	1:D:473:CYS:CB	2.81	0.63
1:A:128:ARG:HG3	1:A:128:ARG:O	1.98	0.63
1:F:249:VAL:CG2	1:F:312:VAL:CG1	2.77	0.63
1:E:104:PHE:HD1	1:E:105:ASN:O	1.82	0.63
1:C:84:GLU:O	1:C:85:ALA:CB	2.47	0.62
1:F:149:ARG:O	1:F:150:SER:HB2	1.98	0.62
1:F:183:ASP:OD1	1:F:184:GLY:N	2.32	0.62
1:F:305:MET:HE1	1:F:336:LEU:HD12	1.80	0.62
1:E:234:LEU:HD21	1:E:238:LEU:HD11	1.82	0.61
1:E:166:HIS:CD2	1:E:167:LEU:HD13	2.36	0.61
1:E:274:PHE:CD1	1:E:305:MET:CE	2.84	0.60
1:E:452:GLN:NE2	1:E:562:GLN:O	2.34	0.60
3:D:702:LR7:O7'	3:D:702:LR7:C5'	2.50	0.60
1:D:456:CYS:HG	1:D:473:CYS:HB2	1.64	0.60
1:E:86:TYR:O	1:E:88:GLY:N	2.32	0.60
1:A:90:THR:HG21	1:A:149:ARG:HD2	1.85	0.59
1:A:93:ARG:HA	1:A:93:ARG:HE	1.67	0.59
1:F:478:GLY:O	1:F:492:HIS:CE1	2.55	0.59
1:D:298:VAL:O	1:D:298:VAL:HG22	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:PHE:HD2	1:D:305:MET:CE	2.15	0.59
1:B:164:PRO:HG2	1:B:167:LEU:HD12	1.85	0.58
1:C:112:LEU:HD22	1:C:116:ARG:HD3	1.85	0.58
1:B:323:LYS:O	1:B:341:ARG:NH2	2.37	0.58
1:E:501:ASP:CB	1:E:506:SER:HB3	2.34	0.58
1:C:257:ASN:ND2	1:C:259:ASP:H	2.02	0.58
1:F:383:ARG:O	1:F:387:VAL:CG2	2.53	0.57
1:D:403:ALA:O	1:D:406:VAL:HG22	2.05	0.56
1:A:323:LYS:O	1:A:341:ARG:NH2	2.39	0.56
1:B:389:MET:HA	1:B:426:PHE:CD2	2.40	0.56
1:D:166:HIS:CD2	1:D:167:LEU:CD1	2.89	0.56
1:C:542:SER:HA	1:C:550:LEU:HD23	1.87	0.55
1:E:323:LYS:O	1:E:341:ARG:NH2	2.40	0.55
1:F:162:LYS:HE3	1:F:231:GLU:HA	1.89	0.54
1:C:323:LYS:O	1:C:341:ARG:NH2	2.40	0.54
1:B:296:ASN:HB3	1:B:299:ALA:HB2	1.88	0.54
1:F:337:GLU:OE2	1:F:341:ARG:NH1	2.41	0.54
1:F:237:LEU:HB3	1:F:312:VAL:HG11	1.90	0.54
1:B:303:THR:O	1:B:349:LEU:CD1	2.55	0.54
1:C:555:CYS:HA	1:C:561:GLN:HE22	1.71	0.54
1:F:133:VAL:CG2	1:F:166:HIS:CE1	2.91	0.54
1:F:447:PHE:O	1:F:567:LEU:HB3	2.07	0.54
1:A:290:ARG:HH21	1:C:493:MET:HE1	1.74	0.53
1:A:93:ARG:NE	1:A:93:ARG:HA	2.24	0.53
1:D:368:THR:HG21	4:D:807:HOH:O	2.08	0.53
1:E:166:HIS:CD2	1:E:167:LEU:CD1	2.91	0.53
1:C:497:LEU:O	1:C:522:TRP:HZ3	1.88	0.53
1:C:112:LEU:HD13	1:C:116:ARG:NH2	2.24	0.53
1:F:330:VAL:HG23	1:F:331:TRP:N	2.24	0.52
1:D:274:PHE:CD2	1:D:305:MET:CE	2.93	0.52
1:E:501:ASP:CB	1:E:506:SER:CB	2.88	0.52
1:C:271:LYS:HD3	1:C:289:GLN:HE22	1.74	0.52
1:E:161:LYS:HD3	1:E:161:LYS:O	2.10	0.52
1:B:112:LEU:HG	1:B:116:ARG:HD3	1.92	0.52
1:E:86:TYR:CZ	1:E:187:LEU:HD11	2.45	0.52
1:E:233:TRP:CZ2	1:E:234:LEU:HD12	2.45	0.52
1:C:250:SER:OG	1:C:310:ALA:O	2.28	0.52
1:B:391:GLU:O	1:B:393:LYS:N	2.37	0.52
1:D:166:HIS:CD2	1:D:167:LEU:HD13	2.45	0.52
1:D:540:LEU:O	1:D:563:TRP:HZ3	1.93	0.52
1:E:470:VAL:O	1:E:471:TYR:O	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:VAL:O	1:E:88:GLY:C	2.48	0.51
1:A:543:ARG:NH1	1:D:501:ASP:OD2	2.43	0.51
1:A:179:ASN:O	4:A:801:HOH:O	2.19	0.51
1:D:201:ARG:NH2	3:D:702:LR7:O4	2.43	0.51
1:C:238:LEU:HA	1:C:241:VAL:HG22	1.93	0.51
1:D:205:MET:O	1:D:206:ARG:HB2	2.10	0.51
1:C:516:ASN:OD1	1:C:516:ASN:N	2.43	0.51
1:B:379:ARG:O	1:B:383:ARG:HG3	2.11	0.51
1:D:248:VAL:HG13	1:D:313:MET:HG3	1.92	0.51
1:D:525:ILE:HG13	1:D:530:LYS:HB2	1.91	0.51
1:B:455:ASN:HB3	1:B:470:VAL:CG1	2.40	0.51
1:B:541:ASP:O	1:B:542:SER:OG	2.26	0.50
1:A:153:LEU:O	1:A:157:VAL:HG13	2.12	0.50
1:B:257:ASN:ND2	1:D:465:ASP:OD2	2.45	0.50
1:B:438:ARG:HG2	1:B:481:GLU:OE1	2.12	0.50
1:A:337:GLU:OE2	1:A:341:ARG:NH1	2.44	0.50
1:C:337:GLU:OE2	1:C:341:ARG:NH1	2.44	0.50
1:D:208:ARG:NH2	3:D:702:LR7:O6'	2.45	0.50
1:E:337:GLU:OE2	1:E:341:ARG:NH1	2.45	0.50
1:D:143:THR:HG22	1:D:174:VAL:HB	1.94	0.49
1:B:330:VAL:HG21	1:B:370:PRO:HD2	1.94	0.49
1:B:538:LEU:HB3	1:B:552:VAL:HG22	1.94	0.49
1:F:474:HIS:O	1:F:476:ALA:N	2.45	0.49
1:B:144:PHE:HA	3:B:702:LR7:O2'	2.12	0.49
1:F:249:VAL:HG23	1:F:312:VAL:CG1	2.38	0.49
1:C:90:THR:CG2	1:C:149:ARG:HG3	2.42	0.49
1:F:255:VAL:CG2	1:F:264:VAL:HB	2.42	0.49
1:C:146:ASN:HD21	1:C:179:ASN:H	1.59	0.49
1:C:455:ASN:HD22	1:C:472:GLU:HA	1.77	0.49
1:D:327:MET:HB2	1:D:383:ARG:CZ	2.43	0.49
1:E:170:GLU:HG3	1:E:172:ILE:HG13	1.94	0.49
1:E:470:VAL:O	1:E:471:TYR:C	2.50	0.49
1:A:112:LEU:HB2	1:A:154:ARG:NH1	2.27	0.49
1:B:390:ASP:C	1:B:391:GLU:O	2.50	0.49
1:E:371:GLY:HA3	1:E:376:VAL:HG23	1.95	0.49
1:B:122:ARG:HG2	1:B:356:ARG:HG2	1.94	0.49
1:D:205:MET:HG3	1:D:328:MET:HB2	1.95	0.49
1:E:339:SER:HA	1:E:349:LEU:HD21	1.94	0.49
1:D:274:PHE:HD2	1:D:305:MET:HE2	1.77	0.48
1:D:313:MET:CE	1:D:318:PHE:HD1	2.25	0.48
1:F:249:VAL:HG22	1:F:312:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ALA:O	1:A:315:LYS:CE	2.61	0.48
1:B:303:THR:O	1:B:349:LEU:HD12	2.13	0.48
1:F:542:SER:O	1:F:544:THR:N	2.46	0.48
1:F:328:MET:O	1:F:380:ASN:OD1	2.31	0.48
1:A:249:VAL:HG13	1:A:352:ILE:HG12	1.96	0.48
1:A:525:ILE:HG13	1:A:530:LYS:HB2	1.95	0.48
1:C:159:VAL:HG22	1:C:159:VAL:O	2.12	0.48
1:D:334:GLU:OE2	3:D:702:LR7:C6'	2.61	0.48
1:D:331:TRP:HB3	1:D:369:PHE:CZ	2.47	0.48
1:E:86:TYR:OH	1:E:187:LEU:HD11	2.14	0.48
1:E:247:ARG:HD3	1:E:350:GLU:OE2	2.14	0.48
1:B:205:MET:HE3	1:B:334:GLU:OE1	2.13	0.48
1:A:162:LYS:HD3	1:A:229:CYS:O	2.15	0.47
1:F:204:LEU:HD13	3:F:702:LR7:O4B	2.13	0.47
1:D:198:ASN:HD22	1:D:210:ARG:NH1	2.12	0.47
1:D:538:LEU:HB3	1:D:552:VAL:HG22	1.97	0.47
1:C:201:ARG:NH2	3:C:702:LR7:O4	2.47	0.47
1:C:525:ILE:HG13	1:C:530:LYS:HB2	1.96	0.47
1:B:303:THR:HG21	1:B:351:ILE:CD1	2.45	0.47
1:C:561:GLN:O	4:C:801:HOH:O	2.20	0.47
1:B:293:ARG:C	1:B:295:GLY:N	2.59	0.47
1:A:116:ARG:NH2	1:A:261:PHE:O	2.47	0.47
1:B:165:PRO:O	1:B:192:LYS:NZ	2.48	0.47
1:A:168:ILE:O	1:A:192:LYS:HE3	2.14	0.46
1:B:390:ASP:O	1:B:391:GLU:O	2.33	0.46
1:B:93:ARG:O	1:B:95:GLY:O	2.34	0.46
1:E:104:PHE:CD1	1:E:105:ASN:O	2.64	0.46
1:A:204:LEU:HD13	3:A:702:LR7:O4B	2.15	0.46
1:E:524:GLN:HG2	1:E:528:ASN:HB2	1.98	0.46
1:A:90:THR:HG21	1:A:149:ARG:CD	2.45	0.46
1:B:525:ILE:HD12	1:B:526:GLU:HG3	1.98	0.45
1:D:327:MET:HB2	1:D:383:ARG:NH2	2.32	0.45
1:B:468:VAL:HG13	1:B:550:LEU:HD13	1.98	0.45
1:A:290:ARG:HE	1:C:493:MET:HE3	1.81	0.45
1:C:497:LEU:C	1:C:522:TRP:HH2	2.19	0.45
1:B:303:THR:CG2	1:B:351:ILE:HG13	2.46	0.45
1:A:132:ARG:HG2	1:A:134:ASP:OD1	2.17	0.45
1:C:90:THR:HG21	1:C:149:ARG:CG	2.45	0.45
1:E:114:MET:O	1:E:157:VAL:HG21	2.16	0.45
1:E:463:PHE:O	1:E:495:LEU:HD21	2.17	0.45
1:F:367:TYR:O	1:F:368:THR:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:O	1:A:131:TRP:N	2.50	0.45
1:B:309:GLY:HA3	3:B:702:LR7:O3'	2.16	0.45
1:E:114:MET:HE2	1:E:153:LEU:HD21	1.99	0.45
1:E:467:VAL:HG23	1:E:508:ILE:O	2.17	0.45
1:F:276:TRP:O	1:F:278:LEU:CD1	2.63	0.45
1:A:334:GLU:OE1	3:A:702:LR7:O6'	2.33	0.45
1:A:544:THR:OG1	1:A:551:SER:HB3	2.17	0.45
1:A:76:VAL:HG12	1:A:77:ARG:O	2.16	0.45
1:D:425:PRO:O	1:D:428:TRP:HB3	2.17	0.45
1:F:160:LEU:HD23	1:F:160:LEU:O	2.17	0.45
1:B:292:SER:O	1:B:293:ARG:O	2.36	0.44
1:C:203:GLY:HA3	1:C:329:ASP:O	2.17	0.44
1:E:205:MET:O	1:E:209:VAL:HG23	2.17	0.44
1:E:234:LEU:CD2	1:E:238:LEU:HD11	2.48	0.44
1:A:339:SER:HA	1:A:349:LEU:HD21	1.98	0.44
1:A:386:GLU:OE2	1:A:393:LYS:NZ	2.49	0.44
1:B:293:ARG:O	1:B:295:GLY:CA	2.65	0.44
1:B:382:ARG:NH1	1:B:406:VAL:O	2.50	0.44
1:A:469:GLY:CA	1:A:550:LEU:HD13	2.44	0.44
1:F:330:VAL:CG2	1:F:331:TRP:N	2.81	0.44
1:A:92:VAL:HG21	1:A:107:VAL:HG22	2.00	0.44
1:E:371:GLY:O	1:E:373:SER:N	2.51	0.44
1:D:123:HIS:CE1	1:D:297:PRO:HG2	2.53	0.43
1:A:114:MET:HE2	1:A:153:LEU:HD11	2.00	0.43
1:A:257:ASN:OD1	1:C:465:ASP:OD2	2.36	0.43
1:C:530:LYS:NZ	1:C:556:GLY:O	2.51	0.43
1:F:383:ARG:NH1	1:F:410:ASN:O	2.51	0.43
1:C:521:LYS:HB2	1:C:534:VAL:HG12	1.99	0.43
1:D:204:LEU:HD11	3:D:702:LR7:C6'	2.48	0.43
1:B:442:HIS:O	4:B:801:HOH:O	2.21	0.43
1:C:554:VAL:O	1:C:555:CYS:HB3	2.18	0.43
1:E:499:VAL:HG21	1:E:533:HIS:CD2	2.53	0.43
1:E:467:VAL:HG21	1:E:549:GLY:O	2.18	0.43
1:E:102:ASN:ND2	1:E:102:ASN:N	2.67	0.43
1:F:339:SER:HA	1:F:349:LEU:HD21	1.99	0.43
1:A:267:SER:HB2	1:C:495:LEU:HD21	2.00	0.43
1:B:321:LEU:HD21	1:B:342:VAL:HA	2.01	0.43
1:C:143:THR:HG21	1:C:207:SER:HB2	2.00	0.43
1:B:205:MET:HE3	1:B:334:GLU:HB3	2.01	0.43
1:A:205:MET:HG2	4:A:812:HOH:O	2.19	0.43
1:B:102:ASN:O	1:B:362:ARG:NH1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ASP:O	1:B:393:LYS:HE2	2.18	0.43
1:B:383:ARG:NH1	1:B:410:ASN:O	2.51	0.43
1:A:205:MET:O	1:A:209:VAL:HG23	2.19	0.42
1:A:90:THR:HG21	1:A:149:ARG:NE	2.34	0.42
1:F:566:THR:O	1:F:567:LEU:HB2	2.19	0.42
1:C:538:LEU:HB3	1:C:552:VAL:HG22	2.02	0.42
1:D:274:PHE:CD2	1:D:305:MET:HE2	2.53	0.42
1:D:313:MET:HE1	1:D:318:PHE:HD1	1.84	0.42
1:C:86:TYR:CE2	1:C:149:ARG:HB3	2.54	0.42
1:F:205:MET:HE3	1:F:329:ASP:O	2.18	0.42
1:A:106:GLN:NE2	4:A:802:HOH:O	2.52	0.42
1:C:497:LEU:C	1:C:522:TRP:CH2	2.91	0.42
1:D:198:ASN:ND2	1:D:210:ARG:HH11	2.17	0.42
1:D:287:PRO:HA	1:D:290:ARG:HG2	2.01	0.42
1:E:136:PRO:O	1:E:238:LEU:HD13	2.20	0.42
1:F:379:ARG:HG3	1:F:407:PRO:O	2.18	0.42
1:E:131:TRP:CG	1:E:235:GLU:HB3	2.55	0.42
1:E:104:PHE:O	1:E:105:ASN:C	2.58	0.42
1:F:278:LEU:HD21	1:F:389:MET:SD	2.60	0.42
1:D:383:ARG:NH2	1:D:410:ASN:O	2.53	0.42
1:C:216:GLN:O	1:C:217:ALA:O	2.38	0.42
1:D:399:ALA:HB2	1:D:567:LEU:HD21	2.02	0.42
1:E:442:HIS:O	1:E:443:GLN:HB2	2.20	0.42
1:A:236:PRO:O	1:A:240:ARG:HG2	2.20	0.42
1:B:205:MET:O	1:B:209:VAL:HG23	2.20	0.42
1:D:205:MET:O	1:D:206:ARG:CB	2.67	0.42
1:E:306:ILE:CD1	1:E:308:GLY:HA2	2.49	0.42
1:F:198:ASN:N	1:F:198:ASN:OD1	2.53	0.42
1:A:133:VAL:HG22	4:A:855:HOH:O	2.20	0.41
1:A:90:THR:CG2	1:A:149:ARG:HD2	2.50	0.41
1:B:426:PHE:CE1	1:B:430:LEU:HG	2.55	0.41
1:C:325:ASP:CG	1:C:414:ARG:HD2	2.40	0.41
1:D:132:ARG:HB3	1:D:135:LEU:HD21	2.02	0.41
1:F:322:GLY:O	1:F:323:LYS:C	2.59	0.41
1:A:369:PHE:HD2	1:A:376:VAL:HG11	1.83	0.41
1:A:390:ASP:O	1:A:393:LYS:HG2	2.21	0.41
1:F:133:VAL:CG2	1:F:166:HIS:HE1	2.32	0.41
1:A:235:GLU:HB2	1:A:236:PRO:HD3	2.02	0.41
1:A:257:ASN:HD22	1:A:260:ASN:H	1.67	0.41
1:E:274:PHE:CD1	1:E:305:MET:HE2	2.55	0.41
1:A:325:ASP:CG	1:A:414:ARG:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ILE:HG23	1:C:196:LEU:HD13	2.02	0.41
1:C:544:THR:OG1	1:C:551:SER:HB3	2.20	0.41
1:D:181:PRO:HB3	1:D:197:ARG:HD3	2.03	0.41
1:E:108:GLU:O	1:E:112:LEU:HD13	2.20	0.41
1:C:205:MET:O	1:C:209:VAL:HG23	2.20	0.41
1:F:295:GLY:O	1:F:296:ASN:HB2	2.20	0.41
1:A:517:ASP:CB	1:A:519:ARG:NH2	2.84	0.41
1:B:540:LEU:HD11	1:B:550:LEU:HD23	2.03	0.41
1:F:205:MET:O	1:F:209:VAL:HG23	2.21	0.41
1:F:525:ILE:HG13	1:F:530:LYS:HB2	2.03	0.41
1:C:325:ASP:HA	1:C:414:ARG:NH2	2.36	0.41
1:C:497:LEU:O	1:C:522:TRP:HH2	2.00	0.41
1:C:537:ASN:O	1:C:555:CYS:HB3	2.21	0.41
1:B:205:MET:HG3	1:B:328:MET:HB2	2.02	0.40
1:E:342:VAL:HB	1:E:349:LEU:HD11	2.02	0.40
1:F:235:GLU:HB2	1:F:236:PRO:HD3	2.03	0.40
1:F:490:VAL:HG21	1:F:531:LEU:HD21	2.03	0.40
1:A:205:MET:HG3	1:A:328:MET:HB2	2.03	0.40
1:A:386:GLU:OE2	1:A:393:LYS:CE	2.69	0.40
1:C:555:CYS:HA	1:C:561:GLN:NE2	2.36	0.40
1:E:538:LEU:CB	1:E:552:VAL:CG1	2.99	0.40
1:F:387:VAL:HG22	1:F:411:ILE:HG21	2.03	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	493/571 (86%)	455 (92%)	28 (6%)	10 (2%)	8	30
1	B	492/571 (86%)	435 (88%)	38 (8%)	19 (4%)	3	17
1	C	487/571 (85%)	439 (90%)	34 (7%)	14 (3%)	5	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	493/571 (86%)	449 (91%)	32 (6%)	12 (2%)	6	26
1	E	477/571 (84%)	417 (87%)	38 (8%)	22 (5%)	2	14
1	F	477/571 (84%)	406 (85%)	45 (9%)	26 (6%)	2	10
All	All	2919/3426 (85%)	2601 (89%)	215 (7%)	103 (4%)	4	19

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	THR
1	A	128	ARG
1	A	191	GLU
1	A	475	ASN
1	B	94	SER
1	B	293	ARG
1	B	294	GLN
1	B	391	GLU
1	B	433	VAL
1	B	474	HIS
1	B	475	ASN
1	C	85	ALA
1	C	217	ALA
1	C	406	VAL
1	C	475	ASN
1	D	103	LYS
1	D	206	ARG
1	D	296	ASN
1	D	408	TYR
1	D	475	ASN
1	D	558	ALA
1	E	179	ASN
1	E	244	ASP
1	E	296	ASN
1	E	475	ASN
1	E	545	ALA
1	E	550	LEU
1	F	103	LYS
1	F	188	GLY
1	F	323	LYS
1	F	324	TYR
1	F	463	PHE
1	F	475	ASN

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Mol	Chain	Res	Type
1	F	543	ARG
1	F	567	LEU
1	A	130	GLN
1	A	330	VAL
1	B	90	THR
1	B	126	CYS
1	B	330	VAL
1	B	392	TYR
1	B	462	HIS
1	B	472	GLU
1	C	90	THR
1	C	126	CYS
1	C	160	LEU
1	D	129	LYS
1	D	330	VAL
1	E	87	VAL
1	E	88	GLY
1	E	125	GLN
1	E	372	GLY
1	E	373	SER
1	E	442	HIS
1	E	443	GLN
1	E	471	TYR
1	E	547	SER
1	F	84	GLU
1	F	150	SER
1	F	191	GLU
1	F	329	ASP
1	F	373	SER
1	F	390	ASP
1	F	478	GLY
1	F	502	ARG
1	A	464	ALA
1	B	463	PHE
1	B	542	SER
1	C	373	SER
1	C	559	LEU
1	D	390	ASP
1	E	116	ARG
1	E	330	VAL
1	E	544	THR
1	F	330	VAL

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Mol	Chain	Res	Type
1	F	403	ALA
1	F	462	HIS
1	F	555	CYS
1	A	479	ASN
1	A	518	SER
1	C	216	GLN
1	C	422	SER
1	D	370	PRO
1	E	76	VAL
1	F	296	ASN
1	F	393	LYS
1	F	407	PRO
1	B	264	VAL
1	B	560	SER
1	C	130	GLN
1	C	423	CYS
1	D	372	GLY
1	E	371	GLY
1	E	528	ASN
1	F	129	LYS
1	B	434	TYR
1	F	195	VAL
1	F	196	LEU
1	B	296	ASN
1	E	500	VAL
1	C	370	PRO
1	A	478	GLY
1	D	548	GLY

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	
1	A	424/483 (88%)	389 (92%)	35 (8%)	12	39
1	B	389/483 (80%)	358 (92%)	31 (8%)	13	41
1	C	392/483 (81%)	356 (91%)	36 (9%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	395/483 (82%)	361 (91%)	34 (9%)	11	38
1	E	371/483 (77%)	345 (93%)	26 (7%)	16	46
1	F	353/483 (73%)	324 (92%)	29 (8%)	12	39
All	All	2324/2898 (80%)	2133 (92%)	191 (8%)	12	39

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	93	ARG
1	A	102	ASN
1	A	113	ARG
1	A	114	MET
1	A	116	ARG
1	A	125	GLN
1	A	128	ARG
1	A	143	THR
1	A	157	VAL
1	A	199	ASP
1	A	201	ARG
1	A	205	MET
1	A	239	GLU
1	A	245	ARG
1	A	269	ASP
1	A	294	GLN
1	A	305	MET
1	A	362	ARG
1	A	370	PRO
1	A	376	VAL
1	A	391	GLU
1	A	402	SER
1	A	438	ARG
1	A	451	GLN
1	A	471	TYR
1	A	473	CYS
1	A	480	GLN
1	A	487	GLU
1	A	513	CYS
1	A	515	GLU
1	A	519	ARG
1	A	520	GLN

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Mol	Chain	Res	Type
1	A	536	SER
1	A	569	LEU
1	B	112	LEU
1	B	116	ARG
1	B	126	CYS
1	B	182	GLU
1	B	194	ARG
1	B	205	MET
1	B	250	SER
1	B	293	ARG
1	B	302	LYS
1	B	305	MET
1	B	336	LEU
1	B	349	LEU
1	B	354	CYS
1	B	356	ARG
1	B	368	THR
1	B	373	SER
1	B	406	VAL
1	B	408	TYR
1	B	433	VAL
1	B	434	TYR
1	B	438	ARG
1	B	467	VAL
1	B	474	HIS
1	B	480	GLN
1	B	493	MET
1	B	511	GLN
1	B	516	ASN
1	B	518	SER
1	B	519	ARG
1	B	536	SER
1	B	559	LEU
1	C	83	GLN
1	C	84	GLU
1	C	90	THR
1	C	116	ARG
1	C	126	CYS
1	C	132	ARG
1	C	133	VAL
1	C	149	ARG
1	C	159	VAL

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Mol	Chain	Res	Type
1	C	163	SER
1	C	169	LYS
1	C	186	LEU
1	C	197	ARG
1	C	199	ASP
1	C	201	ARG
1	C	202	GLU
1	C	205	MET
1	C	223	LEU
1	C	250	SER
1	C	252	ILE
1	C	257	ASN
1	C	288	GLU
1	C	291	ARG
1	C	319	GLU
1	C	327	MET
1	C	329	ASP
1	C	368	THR
1	C	454	THR
1	C	474	HIS
1	C	481	GLU
1	C	487	GLU
1	C	516	ASN
1	C	536	SER
1	C	540	LEU
1	C	555	CYS
1	C	569	LEU
1	D	75	LYS
1	D	83	GLN
1	D	102	ASN
1	D	106	GLN
1	D	112	LEU
1	D	132	ARG
1	D	189	LYS
1	D	194	ARG
1	D	201	ARG
1	D	205	MET
1	D	245	ARG
1	D	271	LYS
1	D	275	ASP
1	D	293	ARG
1	D	305	MET

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Mol	Chain	Res	Type
1	D	313	MET
1	D	329	ASP
1	D	334	GLU
1	D	369	PHE
1	D	383	ARG
1	D	402	SER
1	D	423	CYS
1	D	432	ASN
1	D	434	TYR
1	D	454	THR
1	D	468	VAL
1	D	473	CYS
1	D	474	HIS
1	D	496	CYS
1	D	516	ASN
1	D	536	SER
1	D	552	VAL
1	D	563	TRP
1	D	569	LEU
1	E	76	VAL
1	E	102	ASN
1	E	103	LYS
1	E	107	VAL
1	E	116	ARG
1	E	122	ARG
1	E	130	GLN
1	E	170	GLU
1	E	186	LEU
1	E	200	ARG
1	E	205	MET
1	E	206	ARG
1	E	218	LYS
1	E	245	ARG
1	E	271	LYS
1	E	291	ARG
1	E	293	ARG
1	E	305	MET
1	E	315	LYS
1	E	334	GLU
1	E	406	VAL
1	E	415	LEU
1	E	474	HIS

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Mol	Chain	Res	Type
1	E	536	SER
1	E	544	THR
1	E	550	LEU
1	F	82	ASN
1	F	116	ARG
1	F	152	LEU
1	F	160	LEU
1	F	173	LEU
1	F	181	PRO
1	F	198	ASN
1	F	205	MET
1	F	261	PHE
1	F	305	MET
1	F	313	MET
1	F	319	GLU
1	F	334	GLU
1	F	360	VAL
1	F	376	VAL
1	F	377	PHE
1	F	387	VAL
1	F	406	VAL
1	F	411	ILE
1	F	415	LEU
1	F	431	GLU
1	F	434	TYR
1	F	441	ASP
1	F	463	PHE
1	F	471	TYR
1	F	475	ASN
1	F	507	LEU
1	F	513	CYS
1	F	536	SER

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

Mol	Chain	Res	Type
1	A	257	ASN
1	A	294	GLN
1	A	344	GLN
1	A	380	ASN
1	A	452	GLN
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	520	GLN
1	A	533	HIS
1	B	102	ASN
1	B	106	GLN
1	B	452	GLN
1	B	474	HIS
1	B	480	GLN
1	C	146	ASN
1	C	257	ASN
1	C	344	GLN
1	C	452	GLN
1	C	455	ASN
1	C	480	GLN
1	C	533	HIS
1	D	123	HIS
1	D	146	ASN
1	D	198	ASN
1	D	533	HIS
1	D	568	ASN
1	E	146	ASN
1	E	166	HIS
1	E	344	GLN
1	E	462	HIS
1	F	123	HIS
1	F	432	ASN
1	F	452	GLN
1	F	533	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
3	LR7	A	702	2	37,45,45	0.85	1 (2%)	48,66,66	1.64	7 (14%)
3	LR7	B	702	2	37,45,45	0.81	1 (2%)	48,66,66	2.11	12 (25%)
3	LR7	C	702	2	37,45,45	0.80	1 (2%)	48,66,66	1.59	7 (14%)
3	LR7	D	702	2	37,45,45	1.05	2 (5%)	48,66,66	3.95	13 (27%)
3	LR7	E	702	2	37,45,45	0.83	1 (2%)	48,66,66	2.14	13 (27%)
3	LR7	F	702	2	37,45,45	0.80	1 (2%)	48,66,66	1.52	6 (12%)

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
3	LR7	A	702	2	-	8/26/68/68	0/3/3/3
3	LR7	B	702	2	-	12/26/68/68	0/3/3/3
3	LR7	C	702	2	-	6/26/68/68	0/3/3/3
3	LR7	D	702	2	1/1/12/13	8/26/68/68	0/3/3/3
3	LR7	E	702	2	-	9/26/68/68	0/3/3/3
3	LR7	F	702	2	-	7/26/68/68	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	702	LR7	C4-N3	3.36	1.38	1.33
3	B	702	LR7	C4-N3	3.32	1.38	1.33
3	E	702	LR7	C4-N3	3.25	1.38	1.33
3	F	702	LR7	C4-N3	3.18	1.38	1.33
3	D	702	LR7	C4-N3	3.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	LR7	C4-N3	3.11	1.38	1.33
3	D	702	LR7	PB-O1'	2.48	1.67	1.60

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	LR7	O5'-C1'-O1'	16.10	132.41	111.36
3	D	702	LR7	C1'-C2'-N2'	-14.69	85.15	110.96
3	D	702	LR7	C3'-C2'-N2'	-12.02	87.62	110.58
3	E	702	LR7	O5'-C1'-O1'	6.63	120.03	111.36
3	E	702	LR7	O5'-C1'-C2'	-6.50	97.70	110.58
3	B	702	LR7	PB-O1'-C1'	6.07	143.20	119.74
3	A	702	LR7	PB-O1'-C1'	5.88	142.48	119.74
3	B	702	LR7	O5'-C1'-C2'	-5.70	99.28	110.58
3	B	702	LR7	O5'-C1'-O1'	5.62	118.72	111.36
3	A	702	LR7	O5'-C1'-O1'	5.18	118.13	111.36
3	C	702	LR7	O5'-C1'-O1'	5.13	118.06	111.36
3	E	702	LR7	C3'-C2'-N2'	4.58	119.33	110.58
3	C	702	LR7	PB-O1'-C1'	4.53	137.27	119.74
3	F	702	LR7	C3'-C2'-N2'	4.50	119.17	110.58
3	F	702	LR7	PB-O1'-C1'	4.24	136.14	119.74
3	B	702	LR7	O1'-C1'-C2'	-4.22	100.76	108.40
3	D	702	LR7	C6'-C5'-C4'	4.00	122.41	113.00
3	D	702	LR7	C5-C4-N3	-4.00	114.31	123.28
3	B	702	LR7	C3'-C2'-N2'	3.98	118.18	110.58
3	C	702	LR7	C5-C4-N3	-3.94	114.44	123.28
3	E	702	LR7	O5'-C5'-C6'	-3.90	96.69	106.43
3	A	702	LR7	O5'-C1'-C2'	-3.84	102.96	110.58
3	F	702	LR7	O5'-C1'-C2'	-3.83	102.98	110.58
3	F	702	LR7	C5-C4-N3	-3.82	114.71	123.28
3	C	702	LR7	O5'-C1'-C2'	-3.75	103.15	110.58
3	A	702	LR7	C5-C4-N3	-3.73	114.93	123.28
3	E	702	LR7	C5-C4-N3	-3.72	114.94	123.28
3	E	702	LR7	PB-O1'-C1'	3.63	133.78	119.74
3	B	702	LR7	C5-C4-N3	-3.57	115.28	123.28
3	D	702	LR7	O1'-C1'-C2'	3.50	114.74	108.40
3	B	702	LR7	C3'-C4'-C5'	-3.50	103.94	110.23
3	D	702	LR7	C41-C42-C43	-3.46	168.00	177.14
3	E	702	LR7	O3A-PB-O1'	-3.35	95.73	102.48
3	D	702	LR7	O3A-PB-O1'	2.84	108.21	102.48
3	C	702	LR7	O1'-C1'-C2'	-2.75	103.42	108.40
3	F	702	LR7	C1'-C2'-N2'	2.73	115.76	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	LR7	C6'-C5'-C4'	-2.65	106.78	113.00
3	B	702	LR7	O5'-C5'-C6'	-2.56	100.05	106.43
3	D	702	LR7	C1'-O5'-C5'	-2.50	108.78	113.70
3	B	702	LR7	O4'-C4'-C5'	2.48	115.48	109.29
3	E	702	LR7	O1'-C1'-C2'	2.47	112.86	108.40
3	C	702	LR7	C3'-C2'-N2'	2.46	115.28	110.58
3	D	702	LR7	O7'-C7'-C8'	-2.42	117.58	122.02
3	D	702	LR7	O4'-C4'-C5'	-2.34	103.44	109.29
3	D	702	LR7	C2'-N2'-C7'	2.29	126.31	122.98
3	E	702	LR7	C1'-C2'-N2'	2.27	114.95	110.96
3	E	702	LR7	O2B-PB-O1'	2.25	115.65	106.78
3	E	702	LR7	C41-C40-C8'	-2.22	110.43	113.45
3	E	702	LR7	C3'-C4'-C5'	-2.19	106.29	110.23
3	C	702	LR7	C41-C40-C8'	-2.18	110.49	113.45
3	F	702	LR7	C4B-O4B-C1B	-2.15	107.59	109.83
3	E	702	LR7	C4'-C3'-C2'	-2.13	107.19	110.35
3	B	702	LR7	O4'-C4'-C3'	2.08	115.18	110.34
3	D	702	LR7	O5'-C5'-C4'	-2.04	105.95	109.68
3	A	702	LR7	C3'-C2'-N2'	2.04	114.46	110.58
3	A	702	LR7	O3'-C3'-C2'	2.03	113.72	109.65
3	A	702	LR7	C1'-C2'-N2'	-2.02	107.42	110.96
3	B	702	LR7	C1'-C2'-N2'	2.01	114.49	110.96

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	702	LR7	C1'

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	LR7	C5B-O5B-PA-O2A
3	F	702	LR7	C1'-O1'-PB-O2B
3	F	702	LR7	O5'-C1'-O1'-PB
3	D	702	LR7	O4B-C4B-C5B-O5B
3	D	702	LR7	C5B-O5B-PA-O1A
3	D	702	LR7	C1'-C2'-N2'-C7'
3	E	702	LR7	O4B-C4B-C5B-O5B
3	E	702	LR7	C1'-O1'-PB-O2B
3	E	702	LR7	O5'-C1'-O1'-PB
3	A	702	LR7	C41-C40-C8'-C7'
3	E	702	LR7	O5'-C5'-C6'-O6'

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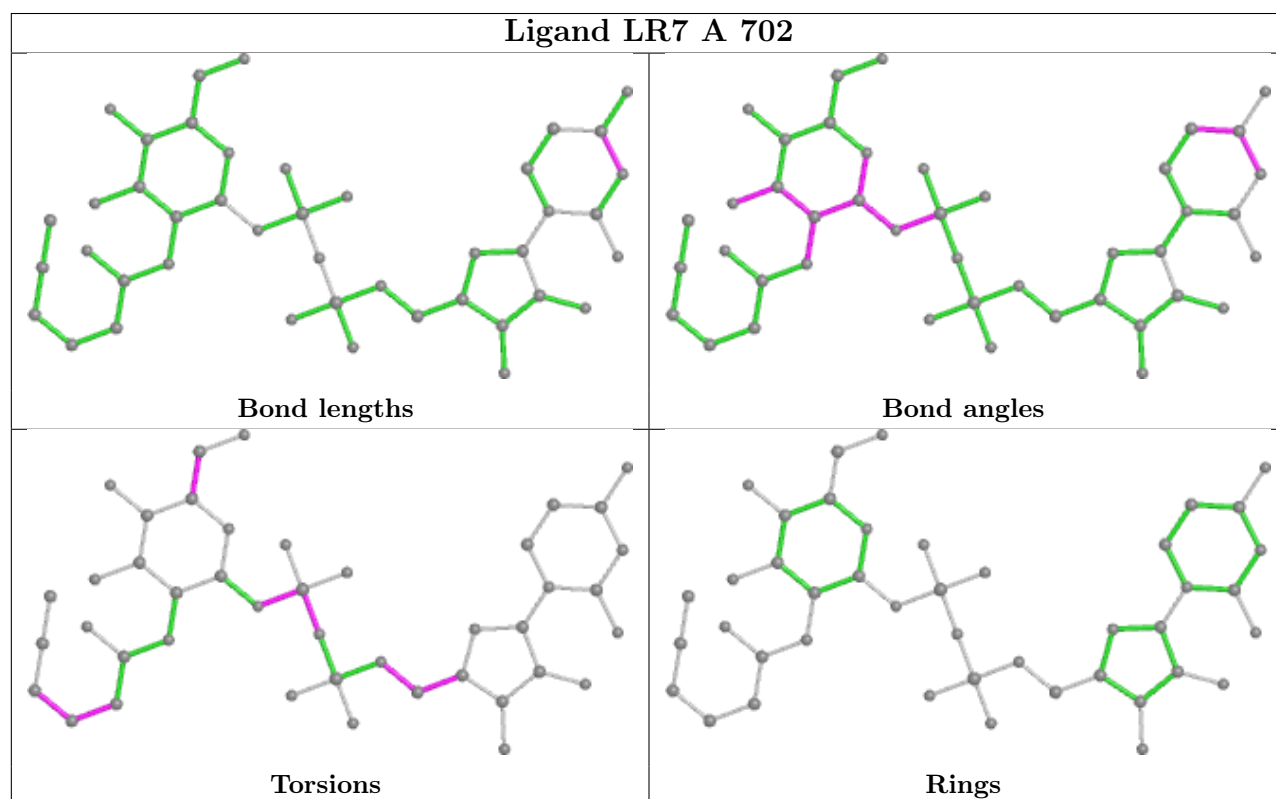
Mol	Chain	Res	Type	Atoms
3	C	702	LR7	C1'-O1'-PB-O3A
3	E	702	LR7	C3B-C4B-C5B-O5B
3	E	702	LR7	C4'-C5'-C6'-O6'
3	F	702	LR7	C1'-O1'-PB-O3A
3	E	702	LR7	C1'-O1'-PB-O3A
3	B	702	LR7	O5'-C5'-C6'-O6'
3	A	702	LR7	O5'-C5'-C6'-O6'
3	F	702	LR7	O5'-C5'-C6'-O6'
3	F	702	LR7	C8'-C40-C41-C42
3	C	702	LR7	O5'-C5'-C6'-O6'
3	B	702	LR7	PB-O3A-PA-O2A
3	C	702	LR7	PA-O3A-PB-O1B
3	C	702	LR7	C1'-O1'-PB-O2B
3	A	702	LR7	C8'-C40-C41-C42
3	A	702	LR7	C1'-O1'-PB-O3A
3	B	702	LR7	C4'-C5'-C6'-O6'
3	B	702	LR7	C5B-O5B-PA-O3A
3	D	702	LR7	C5B-O5B-PA-O3A
3	A	702	LR7	O4B-C4B-C5B-O5B
3	F	702	LR7	C1'-O1'-PB-O1B
3	E	702	LR7	C1'-O1'-PB-O1B
3	B	702	LR7	PA-O3A-PB-O1B
3	A	702	LR7	C4B-C5B-O5B-PA
3	D	702	LR7	C4B-C5B-O5B-PA
3	D	702	LR7	C5B-O5B-PA-O2A
3	B	702	LR7	O4B-C4B-C5B-O5B
3	F	702	LR7	C41-C40-C8'-C7'
3	E	702	LR7	C41-C40-C8'-C7'
3	B	702	LR7	PB-O3A-PA-O1A
3	C	702	LR7	PA-O3A-PB-O2B
3	B	702	LR7	C41-C40-C8'-C7'
3	B	702	LR7	C4B-C5B-O5B-PA
3	A	702	LR7	PA-O3A-PB-O2B
3	D	702	LR7	C3B-C4B-C5B-O5B
3	D	702	LR7	C3'-C2'-N2'-C7'
3	B	702	LR7	C1'-O1'-PB-O3A
3	A	702	LR7	C1'-O1'-PB-O1B
3	C	702	LR7	PB-O3A-PA-O1A
3	B	702	LR7	C1'-O1'-PB-O2B

There are no ring outliers.

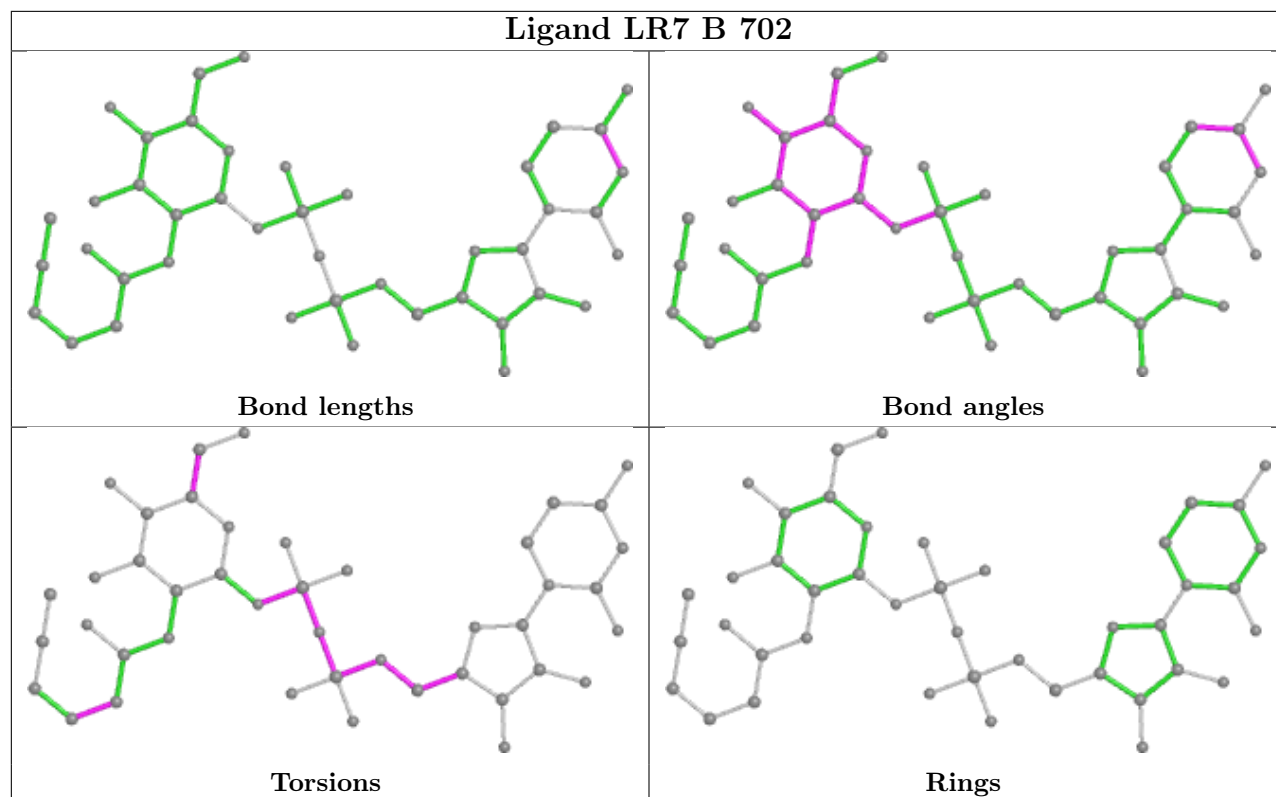
5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	LR7	5	0
3	B	702	LR7	4	0
3	C	702	LR7	3	0
3	D	702	LR7	8	0
3	F	702	LR7	1	0

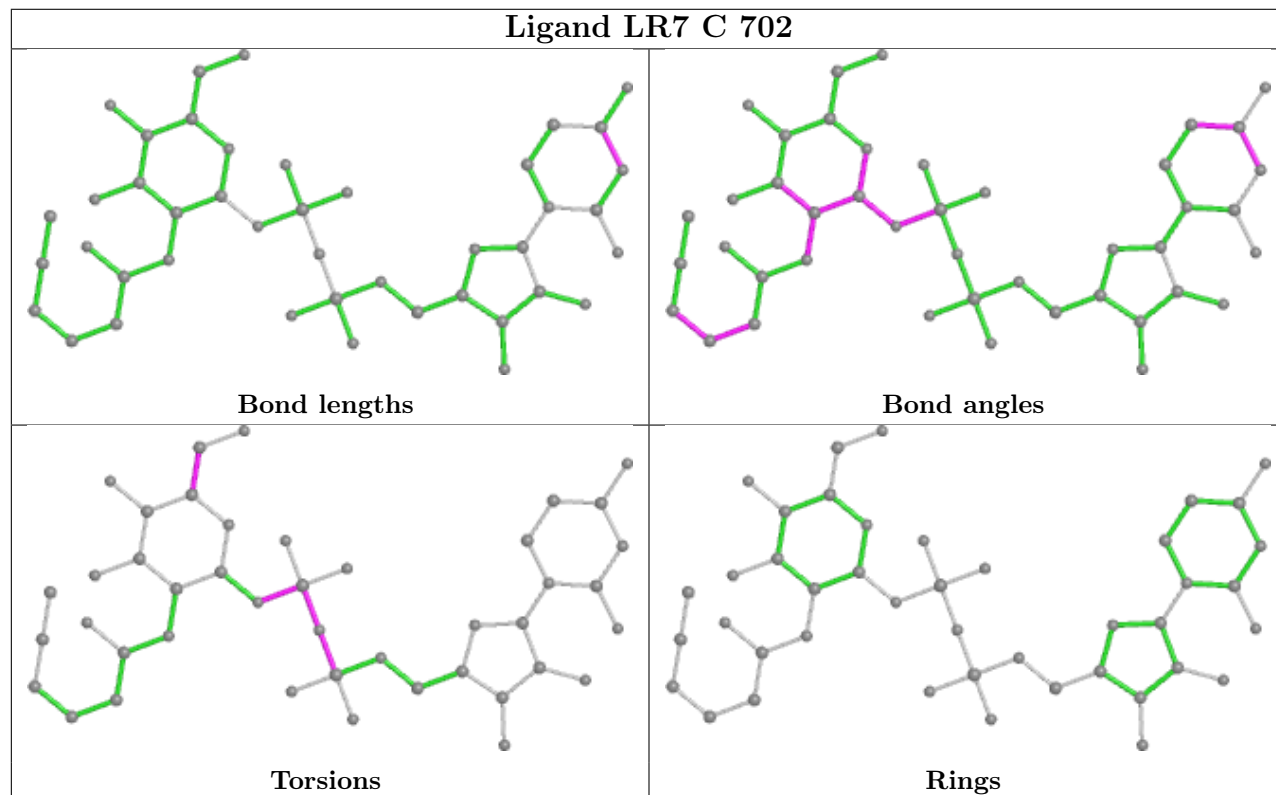
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



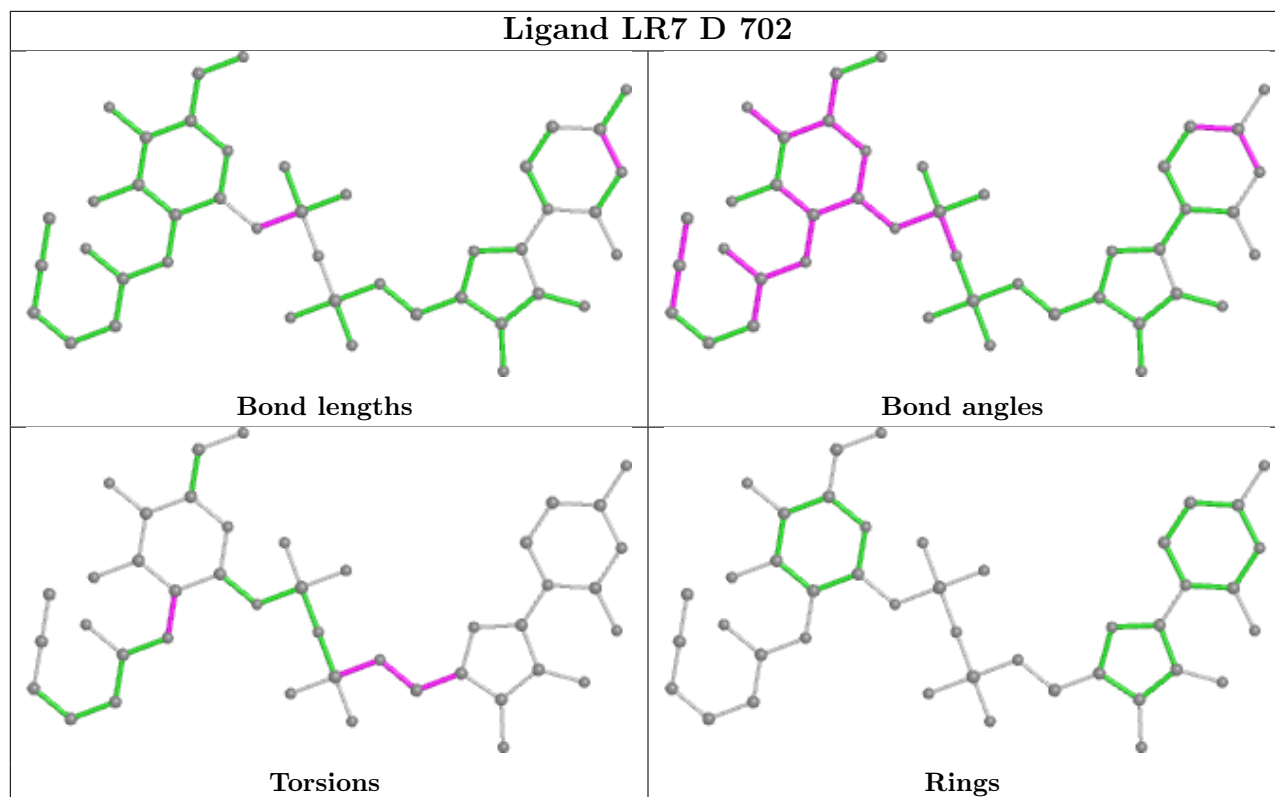
Ligand LR7 B 702



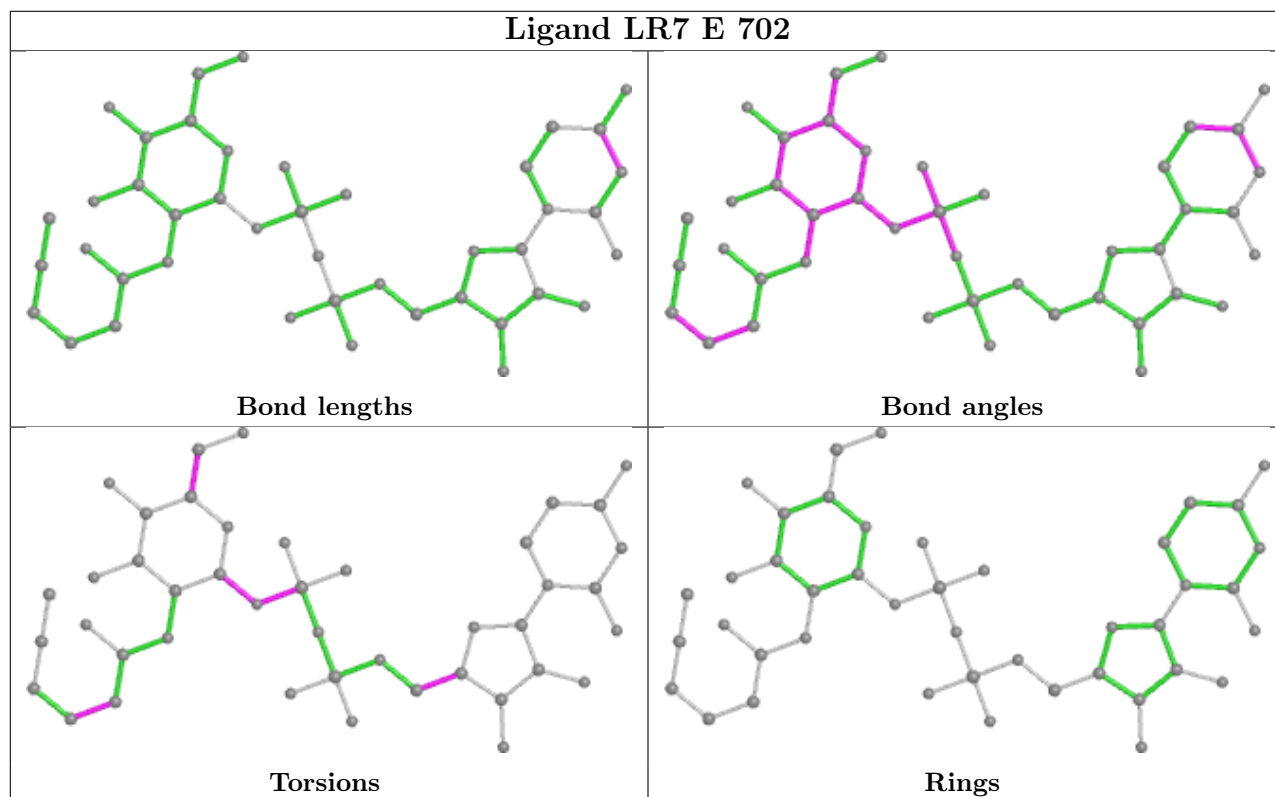
Ligand LR7 C 702

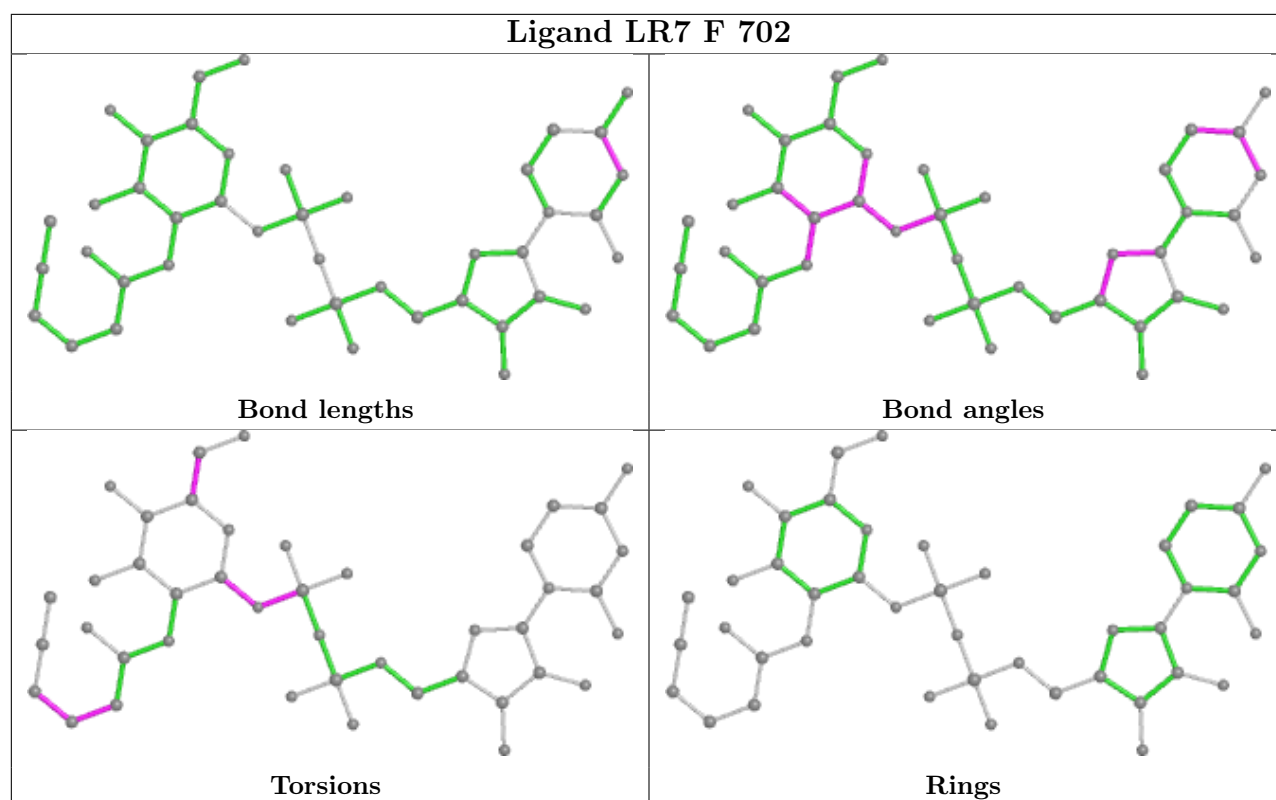


Ligand LR7 D 702



Ligand LR7 E 702





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	A	495/571 (86%)	-0.24	1 (0%) 94 88	30, 52, 73, 89	0
1	B	494/571 (86%)	-0.02	5 (1%) 82 64	32, 63, 95, 117	0
1	C	491/571 (85%)	-0.05	3 (0%) 89 76	34, 60, 88, 118	0
1	D	495/571 (86%)	-0.10	4 (0%) 86 69	33, 62, 85, 124	0
1	E	485/571 (84%)	0.11	16 (3%) 46 23	42, 73, 108, 131	0
1	F	483/571 (84%)	0.25	21 (4%) 35 17	40, 82, 111, 133	0
All	All	2943/3426 (85%)	-0.01	50 (1%) 70 46	30, 64, 101, 133	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	98	PRO	4.3
1	F	547	SER	3.9
1	E	407	PRO	3.7
1	B	500	VAL	3.6
1	E	504	PRO	3.6
1	F	97	ASP	3.4
1	E	98	PRO	3.4
1	E	548	GLY	3.3
1	E	105	ASN	3.1
1	E	568	ASN	3.1
1	F	504	PRO	3.0
1	F	107	VAL	2.9
1	E	102	ASN	2.8
1	B	501	ASP	2.7
1	F	501	ASP	2.6
1	C	133	VAL	2.6
1	F	102	ASN	2.6
1	E	531	LEU	2.6
1	F	503	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	549	GLY	2.6
1	C	563	TRP	2.6
1	D	428	TRP	2.5
1	D	453	GLY	2.5
1	F	105	ASN	2.5
1	E	97	ASP	2.5
1	F	94	SER	2.4
1	C	127	GLN	2.4
1	D	410	ASN	2.3
1	E	441	ASP	2.3
1	B	535	GLY	2.3
1	F	548	GLY	2.3
1	F	408	TYR	2.3
1	E	90	THR	2.3
1	F	148	ALA	2.3
1	E	539	CYS	2.2
1	F	150	SER	2.2
1	B	432	ASN	2.2
1	F	99	TYR	2.2
1	D	394	ASN	2.1
1	E	408	TYR	2.1
1	F	500	VAL	2.1
1	F	149	ARG	2.1
1	F	108	GLU	2.1
1	F	502	ARG	2.1
1	A	96	GLN	2.1
1	E	369	PHE	2.0
1	F	535	GLY	2.0
1	F	189	LYS	2.0
1	B	503	ALA	2.0
1	E	454	THR	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

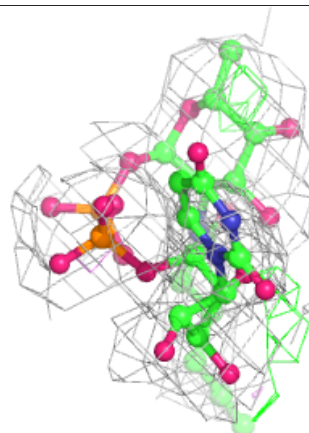
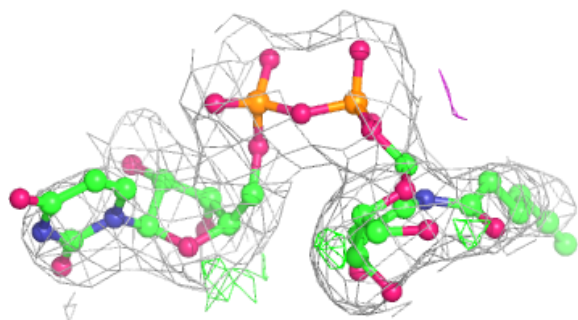
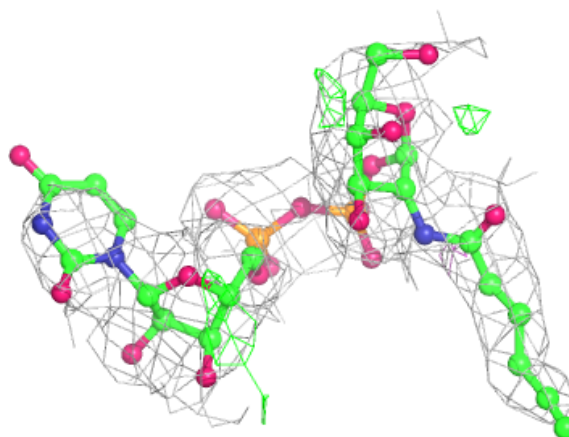
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LR7	E	702	43/43	0.91	0.27	52,69,97,108	0
3	LR7	F	702	43/43	0.92	0.21	64,76,94,96	0
3	LR7	D	702	43/43	0.93	0.25	41,54,78,82	0
3	LR7	A	702	43/43	0.94	0.21	41,48,61,72	0
3	LR7	B	702	43/43	0.95	0.21	41,57,85,97	0
3	LR7	C	702	43/43	0.95	0.23	47,54,67,72	0
2	MN	D	701	1/1	0.97	0.14	50,50,50,50	0
2	MN	F	701	1/1	0.98	0.15	73,73,73,73	0
2	MN	A	701	1/1	0.98	0.19	49,49,49,49	0
2	MN	C	701	1/1	0.99	0.20	48,48,48,48	0
2	MN	E	701	1/1	0.99	0.19	47,47,47,47	0
2	MN	B	701	1/1	1.00	0.14	30,30,30,30	0

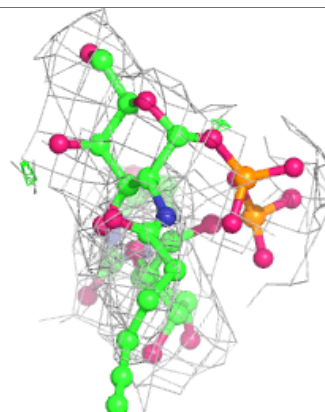
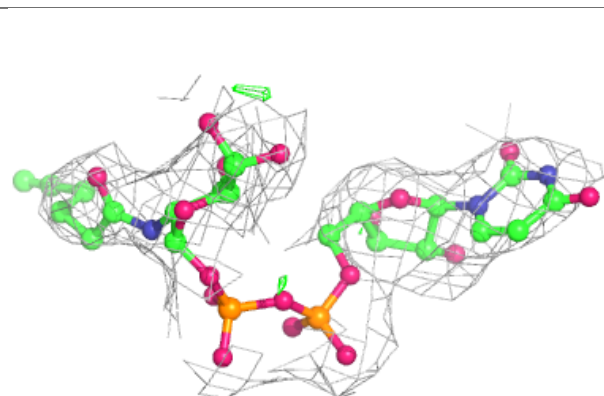
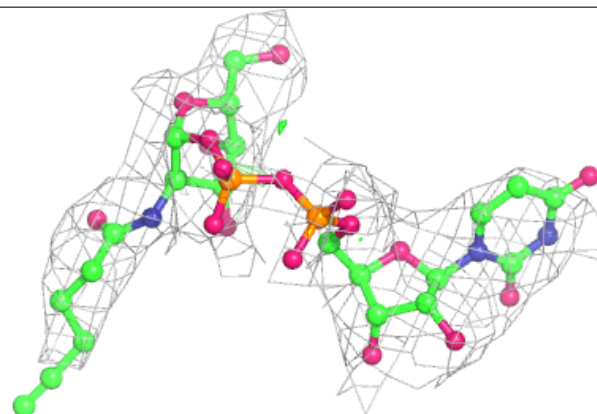
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LR7 E 702:

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

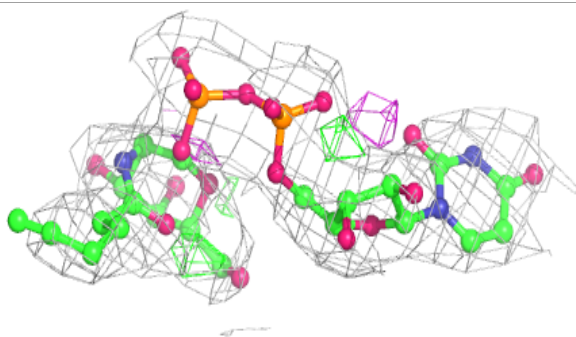
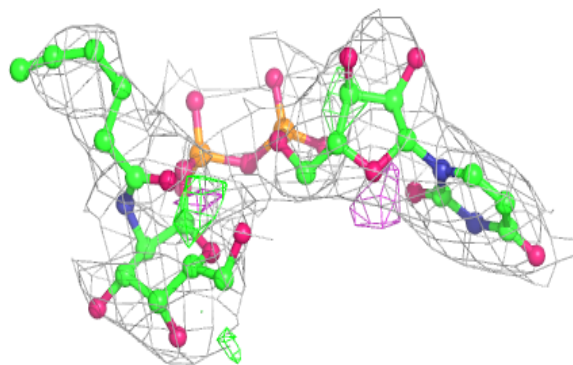
**Electron density around LR7 F 702:**

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

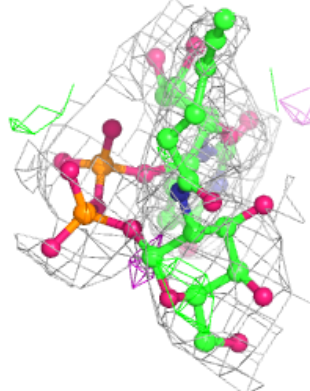
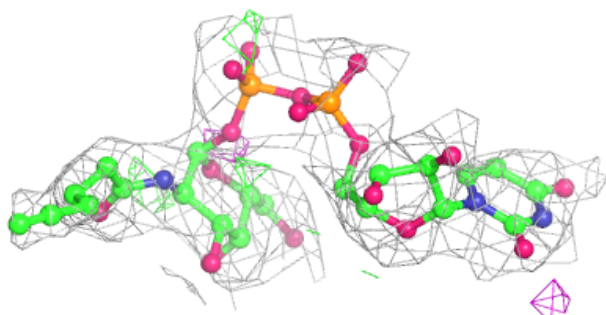
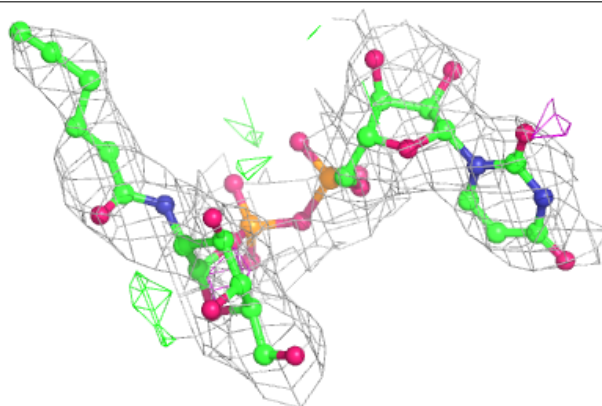


Electron density around LR7 D 702:

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

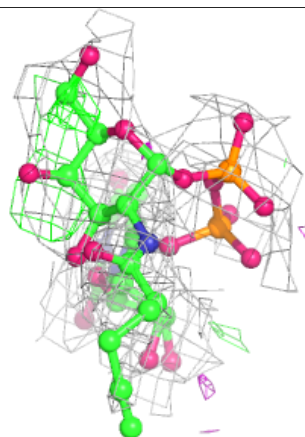
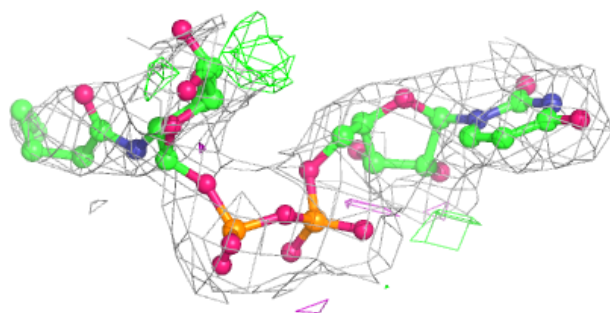
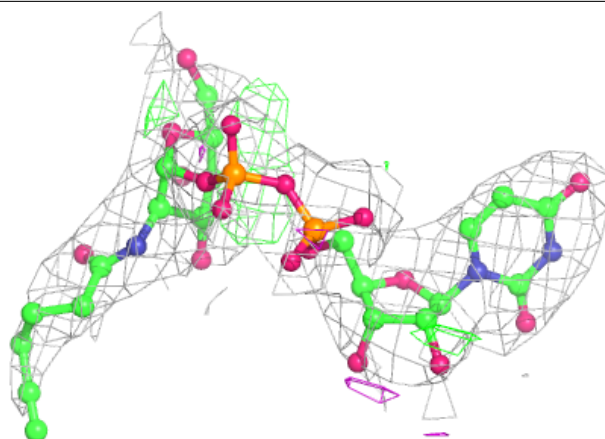
**Electron density around LR7 A 702:**

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

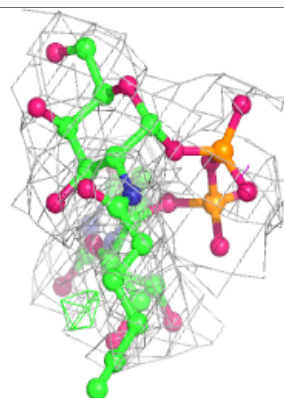
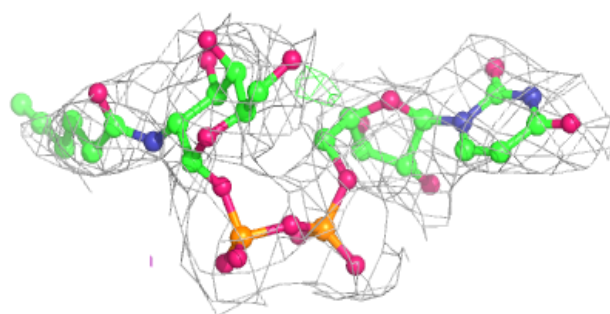
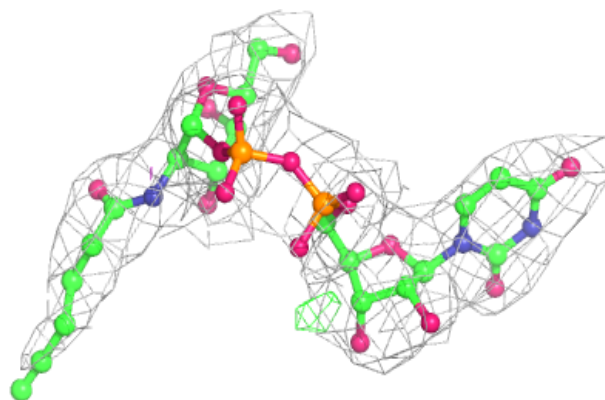


Electron density around LR7 B 702:

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

**Electron density around LR7 C 702:**

$2mF_o-DF_c$ (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.