Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 11:31 am GMT

PDB ID	:	5NDF
Title	:	Small-molecule inhibition of ppGalNAc-Ts selectively reduces mucin-type O-glycosylation
Authors	:	Hurtado-Guerrero, R.; De las Rivas, M.
Deposited on	:	2017-03-08
Resolution	:	2.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

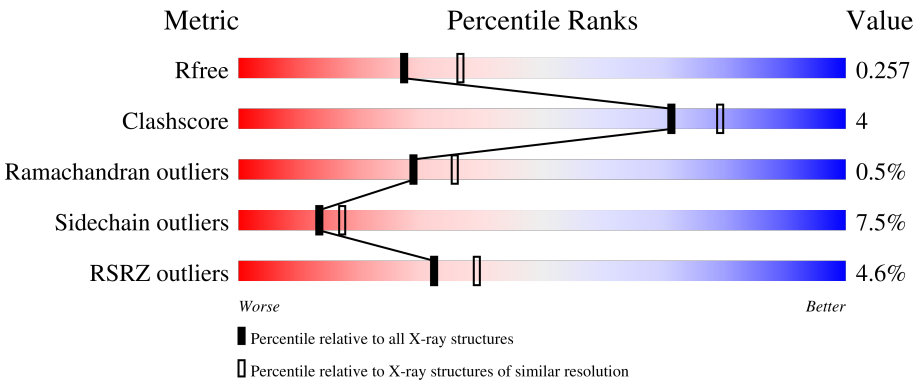
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	571	% 76% 9% • 13%
1	B	571	3% 74% 10% • 13%
1	C	571	4% 75% 9% • 13%
1	D	571	4% 75% 9% • 13%
1	E	571	7% 74% 10% • 14%

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Mol	Chain	Length	Quality of chain
1	F	571	6% 77% 8% • 13%

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	LU2	A	608	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 24971 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
			Total	C	N	O	S			
1	A	495	3976	2503	720	729	24	20	2	0
1	B	495	3983	2507	725	727	24	20	2	0
1	C	495	3987	2510	724	729	24	20	3	0
1	D	495	3983	2507	725	727	24	20	2	0
1	E	492	3962	2493	719	726	24	20	3	0
1	F	495	3973	2501	720	728	24	20	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ASP	ASN	engineered mutation	UNP Q10471
B	516	ASP	ASN	engineered mutation	UNP Q10471
C	516	ASP	ASN	engineered mutation	UNP Q10471
D	516	ASP	ASN	engineered mutation	UNP Q10471
E	516	ASP	ASN	engineered mutation	UNP Q10471
F	516	ASP	ASN	engineered mutation	UNP Q10471

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

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

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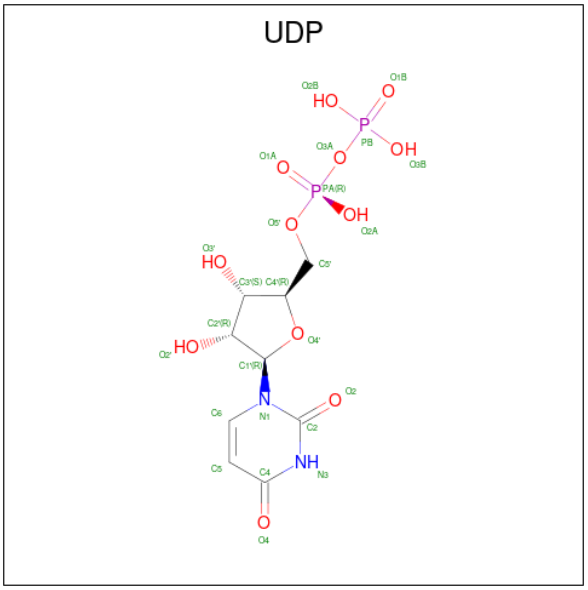
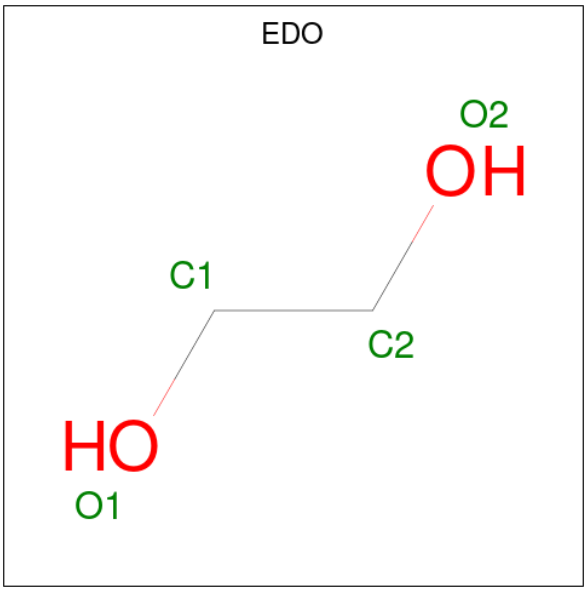
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	D	1	1	1	0	0
			Total	Mn		
2	E	1	1	1	0	0
			Total	Mn		
2	F	1	1	1	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



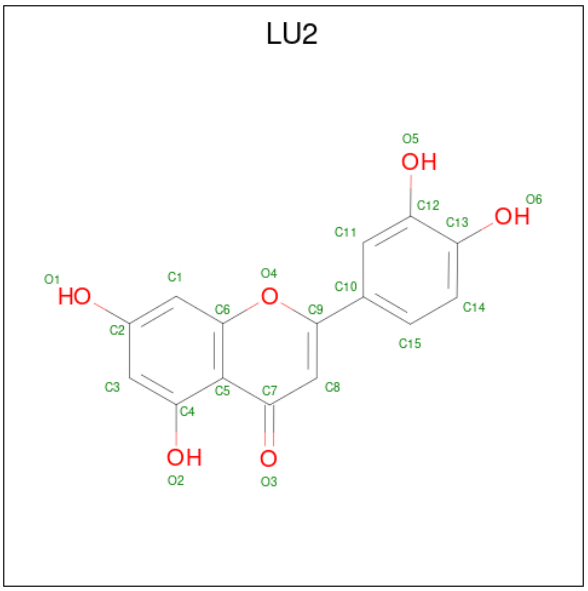
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	25	9	2	12	2	0	0
			Total	C	N	O	P		
3	B	1	25	9	2	12	2	0	0
			Total	C	N	O	P		
3	C	1	25	9	2	12	2	0	0
			Total	C	N	O	P		
3	D	1	25	9	2	12	2	0	0
			Total	C	N	O	P		
3	E	1	25	9	2	12	2	0	0
			Total	C	N	O	P		
3	F	1	25	9	2	12	2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
4	A	1	4	2	2	0	0
4	A	1	4	2	2	0	0
4	A	1	4	2	2	0	0
4	A	1	4	2	2	0	0
4	B	1	4	2	2	0	0
4	C	1	4	2	2	0	0
4	D	1	4	2	2	0	0
4	E	1	4	2	2	0	0
4	F	1	4	2	2	0	0

- Molecule 5 is 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-chromen-4-one (three-letter code: LU2) (formula: $C_{15}H_{10}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 21 15 6	0	0
5	B	1	Total C O 21 15 6	0	0
5	D	1	Total C O 21 15 6	0	0

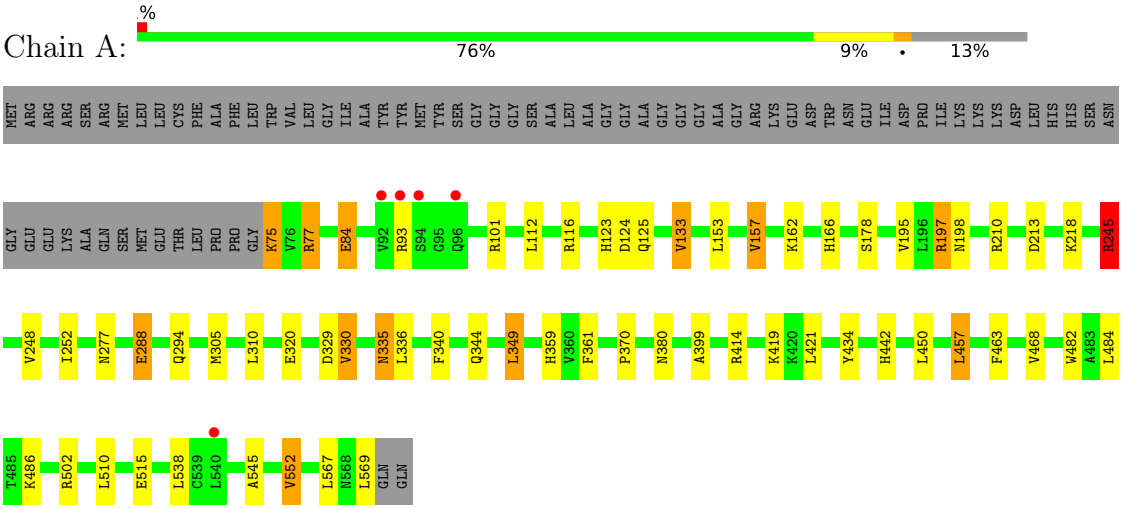
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	194	Total O 194 194	0	0
6	B	147	Total O 147 147	0	0
6	C	138	Total O 138 138	0	0
6	D	163	Total O 163 163	0	0
6	E	117	Total O 117 117	0	0
6	F	89	Total O 89 89	0	0

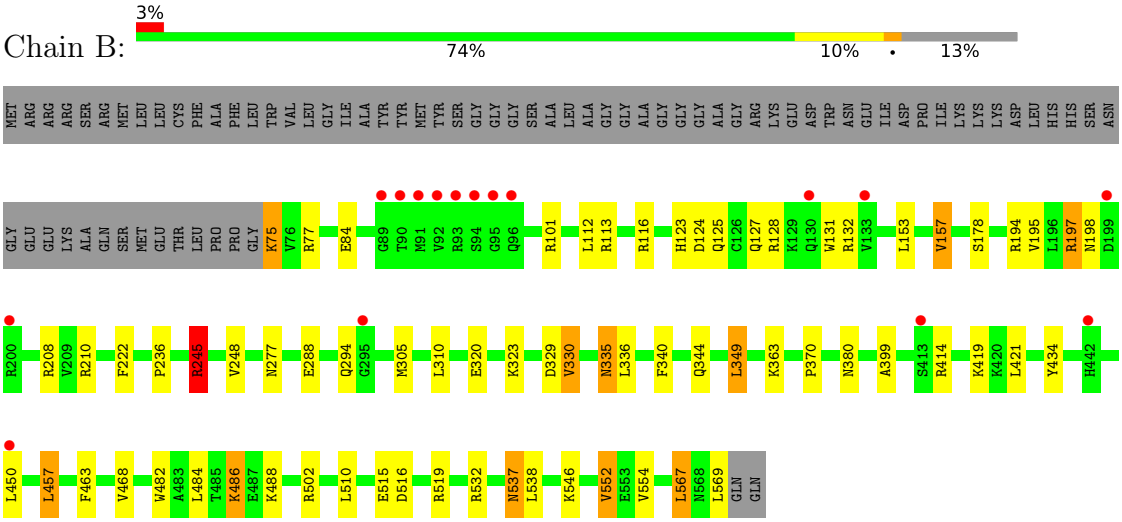
3 Residue-property plots (i)

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

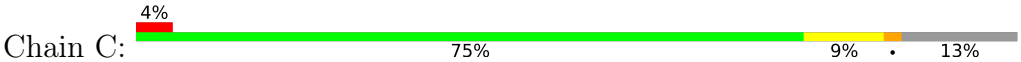
• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

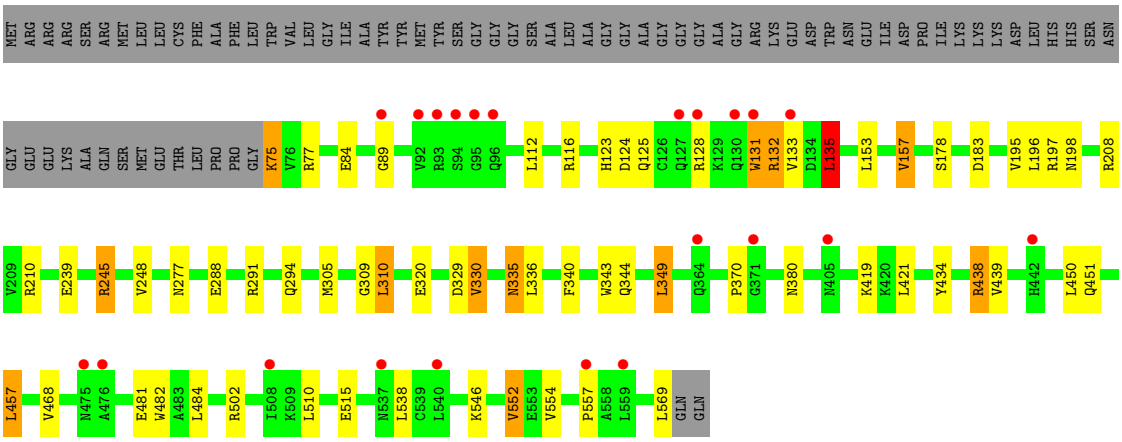


• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2



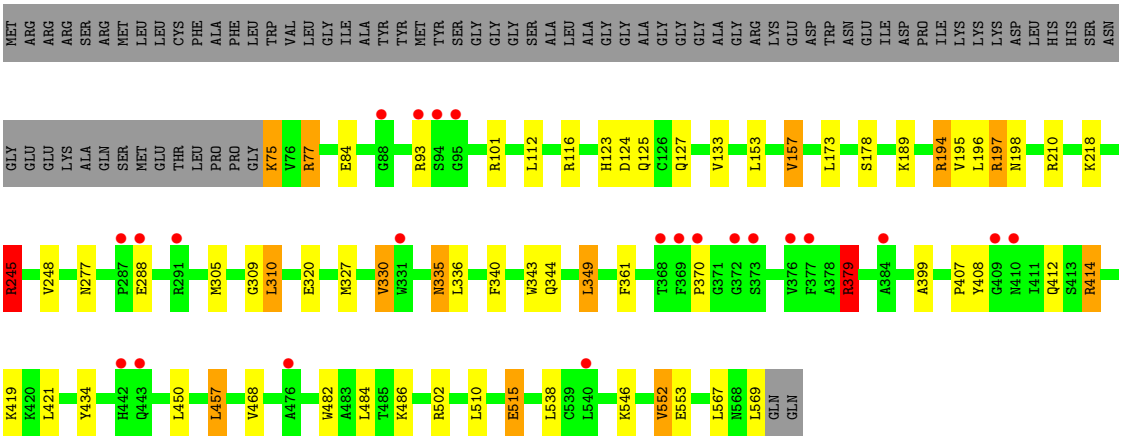
• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2





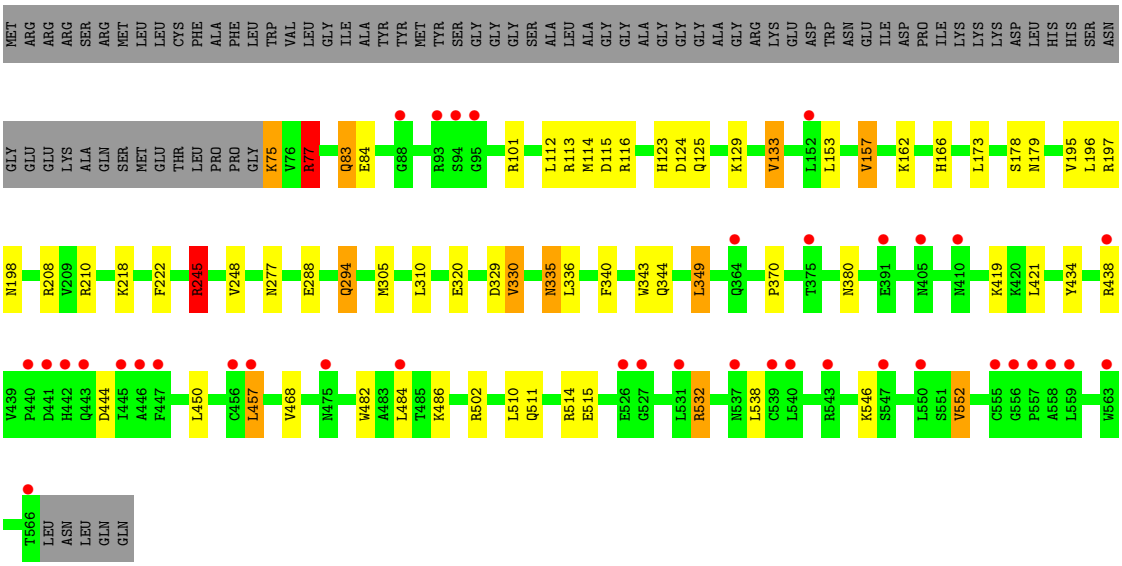
• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

Chain D:



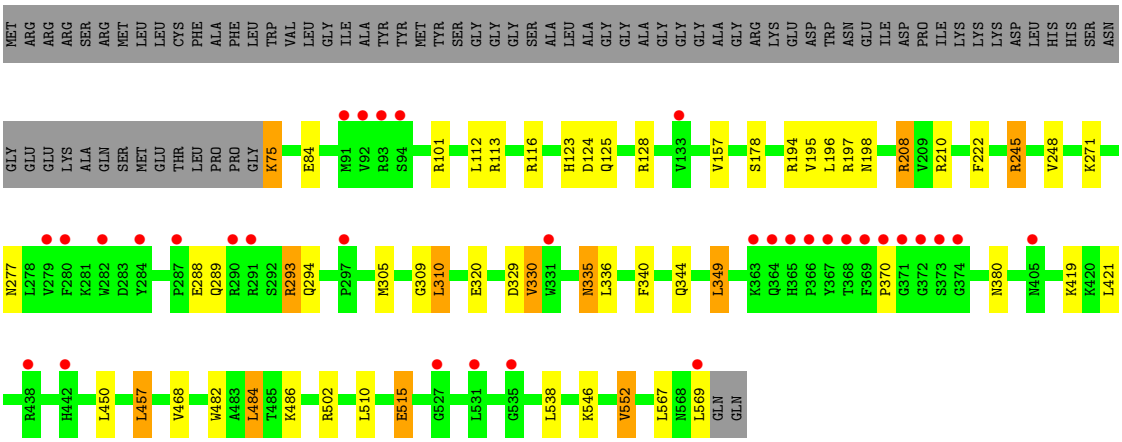
• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

Chain E:



• Molecule 1: Polypeptide N-acetylgalactosaminyltransferase 2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.98Å 123.11Å 248.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.08 – 2.30 19.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (124.08-2.30) 95.5 (19.96-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.251 0.216 , 0.257	Depositor DCC
R_{free} test set	4316 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 27.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24971	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.03% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, LU2, EDO, MN

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	0.74	3/4074 (0.1%)	0.90	9/5510 (0.2%)
1	B	0.82	6/4081 (0.1%)	0.90	9/5517 (0.2%)
1	C	0.87	3/4088 (0.1%)	0.94	11/5527 (0.2%)
1	D	0.91	4/4081 (0.1%)	1.01	17/5517 (0.3%)
1	E	0.79	2/4063 (0.0%)	0.93	8/5493 (0.1%)
1	F	0.92	5/4068 (0.1%)	0.94	13/5501 (0.2%)
All	All	0.84	23/24455 (0.1%)	0.94	67/33065 (0.2%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	515	GLU	CB-CG	-34.57	0.86	1.52
1	D	515	GLU	CB-CG	-28.61	0.97	1.52
1	E	75	LYS	CB-CG	-26.13	0.82	1.52
1	C	75	LYS	CB-CG	-22.73	0.91	1.52
1	C	515	GLU	CB-CG	-21.94	1.10	1.52
1	B	84	GLU	CB-CG	-18.87	1.16	1.52
1	C	294	GLN	CB-CG	-17.96	1.04	1.52
1	F	486	LYS	CB-CG	-16.65	1.07	1.52
1	A	294	GLN	CB-CG	-16.58	1.07	1.52
1	D	75	LYS	CB-CG	-15.97	1.09	1.52
1	D	486	LYS	CB-CG	-14.69	1.12	1.52
1	B	75	LYS	CB-CG	-13.81	1.15	1.52
1	D	84	GLU	CB-CG	-13.19	1.27	1.52
1	B	515	GLU	CB-CG	-12.48	1.28	1.52
1	E	294	GLN	CB-CG	-10.72	1.23	1.52
1	B	486	LYS	CB-CG	-9.91	1.25	1.52
1	F	84	GLU	CB-CG	-9.73	1.33	1.52
1	A	486	LYS	CB-CG	9.05	1.76	1.52
1	F	294	GLN	CB-CG	-7.05	1.33	1.52
1	F	75	LYS	CB-CG	-6.38	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	294	GLN	CB-CG	-5.73	1.37	1.52
1	B	537	ASN	CB-CG	5.20	1.63	1.51
1	A	75	LYS	CB-CG	-5.13	1.38	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	75	LYS	CA-CB-CG	23.81	165.78	113.40
1	D	515	GLU	CA-CB-CG	22.38	162.63	113.40
1	E	75	LYS	CA-CB-CG	19.09	155.40	113.40
1	F	294	GLN	CA-CB-CG	-18.16	73.45	113.40
1	C	84	GLU	CB-CG-CD	16.59	158.99	114.20
1	A	75	LYS	CA-CB-CG	14.99	146.39	113.40
1	B	75	LYS	CA-CB-CG	12.76	141.47	113.40
1	E	77	ARG	NE-CZ-NH2	10.73	125.67	120.30
1	F	75	LYS	CA-CB-CG	9.97	135.33	113.40
1	F	208	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	F	293	ARG	NE-CZ-NH1	-8.72	115.94	120.30
1	C	135	LEU	CA-CB-CG	8.60	135.07	115.30
1	A	486	LYS	CB-CG-CD	-8.30	90.01	111.60
1	F	515	GLU	CA-CB-CG	-8.24	95.27	113.40
1	D	379[A]	ARG	NE-CZ-NH1	-7.85	116.37	120.30
1	D	379[B]	ARG	NE-CZ-NH1	-7.85	116.37	120.30
1	F	113	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	C	75	LYS	CB-CG-CD	7.67	131.54	111.60
1	A	294	GLN	CA-CB-CG	-7.48	96.94	113.40
1	F	208	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	C	515	GLU	CA-CB-CG	7.23	129.30	113.40
1	F	208	ARG	CB-CG-CD	7.06	129.96	111.60
1	D	77	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	D	379[A]	ARG	CG-CD-NE	-6.93	97.25	111.80
1	D	379[B]	ARG	CG-CD-NE	-6.93	97.25	111.80
1	D	379[A]	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	D	379[B]	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	F	486	LYS	CB-CG-CD	-6.72	94.13	111.60
1	A	77	ARG	NE-CZ-NH2	6.61	123.60	120.30
1	F	194	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	E	514	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	B	486	LYS	CB-CG-CD	-5.97	96.08	111.60
1	D	245	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	F	194	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	D	486	LYS	CB-CG-CD	-5.87	96.34	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	B	414	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	C	84	GLU	CA-CB-CG	-5.83	100.56	113.40
1	A	245	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	C	132	ARG	N-CA-C	5.78	126.61	111.00
1	C	77	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	F	208	ARG	CG-CD-NE	5.74	123.86	111.80
1	E	532	ARG	CA-CB-CG	5.72	125.98	113.40
1	C	294	GLN	CA-CB-CG	5.65	125.84	113.40
1	A	84	GLU	CB-CG-CD	5.63	129.40	114.20
1	B	532	ARG	NE-CZ-NH1	-5.63	117.49	120.30
1	E	486	LYS	CA-CB-CG	-5.62	101.03	113.40
1	A	486	LYS	CA-CB-CG	-5.62	101.04	113.40
1	E	129	LYS	CD-CE-NZ	5.54	124.45	111.70
1	B	519	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	197	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	515	GLU	CB-CG-CD	-5.45	99.48	114.20
1	C	131	TRP	CB-CA-C	-5.41	99.58	110.40
1	D	414	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	E	444	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	D	93	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	245	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	E	245	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	D	194[A]	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	D	194[B]	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	B	77	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	B	502	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	A	197	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	F	75	LYS	CB-CG-CD	-5.06	98.43	111.60
1	D	75	LYS	CB-CG-CD	-5.06	98.44	111.60
1	A	93	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	291	ARG	NE-CZ-NH2	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3976	0	3903	28	0
1	B	3983	0	3916	36	0
1	C	3987	0	3919	26	0
1	D	3983	0	3916	32	0
1	E	3962	0	3887	27	0
1	F	3973	0	3898	20	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	25	0	11	0	0
3	B	25	0	11	0	0
3	C	25	0	11	0	0
3	D	25	0	11	0	0
3	E	25	0	11	0	0
3	F	25	0	11	0	0
4	A	20	0	30	3	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	1	0
4	E	4	0	6	0	0
4	F	4	0	6	1	0
5	A	21	0	6	5	0
5	B	21	0	7	4	0
5	D	21	0	7	1	0
6	A	194	0	0	5	0
6	B	147	0	0	2	0
6	C	138	0	0	4	0
6	D	163	0	0	6	0
6	E	117	0	0	4	0
6	F	89	0	0	1	0
All	All	24971	0	23585	166	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 4.

All (166) 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:B:194[B]:ARG:HH21	1:B:194[B]:ARG:CB	1.19	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194[B]:ARG:NH2	1:B:194[B]:ARG:HB3	1.44	1.29
1:B:194[B]:ARG:HH21	1:B:194[B]:ARG:CG	1.53	1.17
1:B:194[B]:ARG:CB	1:B:194[B]:ARG:NH2	2.01	1.15
1:B:194[B]:ARG:HH21	1:B:194[B]:ARG:HB3	0.90	1.00
1:B:194[B]:ARG:NH2	1:B:194[B]:ARG:CG	2.22	0.86
1:D:327:MET:O	1:D:379[A]:ARG:NH1	2.13	0.81
1:D:414:ARG:HD3	6:D:721:HOH:O	1.81	0.81
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.18	0.79
1:E:457:LEU:HD13	1:E:482:TRP:CE2	2.18	0.79
1:C:457:LEU:HD13	1:C:482:TRP:CE2	2.18	0.78
1:D:457:LEU:HD13	1:D:482:TRP:CE2	2.18	0.78
1:F:457:LEU:HD13	1:F:482:TRP:CE2	2.19	0.78
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.18	0.77
1:C:438:ARG:NH1	1:C:481:GLU:HG2	2.00	0.76
1:B:194[B]:ARG:NH2	1:B:194[B]:ARG:HG2	2.02	0.75
5:A:608:LU2:O3	1:B:463:PHE:HB2	1.88	0.74
1:A:361:PHE:CZ	5:A:608:LU2:H1	2.23	0.73
1:D:361:PHE:CZ	5:D:604:LU2:H1	2.26	0.70
5:A:608:LU2:O3	1:B:463:PHE:CD2	2.46	0.69
1:D:194[B]:ARG:HH21	1:D:194[B]:ARG:HG2	1.57	0.68
1:D:194[B]:ARG:HH21	1:D:194[B]:ARG:CG	2.07	0.67
1:D:198:ASN:HD22	1:D:210:ARG:HH11	1.43	0.66
1:C:198:ASN:HD22	1:C:210:ARG:HH11	1.45	0.65
1:B:198:ASN:HD22	1:B:210:ARG:HH11	1.45	0.64
1:A:198:ASN:HD22	1:A:210:ARG:HH11	1.46	0.63
1:B:363:LYS:HG2	5:B:604:LU2:O6	1.99	0.62
1:F:198:ASN:HD22	1:F:210:ARG:HH11	1.45	0.62
1:C:439:VAL:HG12	6:C:761:HOH:O	2.00	0.61
1:C:132:ARG:HD2	1:C:239:GLU:OE1	2.00	0.61
1:C:89:GLY:O	1:D:412:GLN:HG2	2.01	0.60
1:E:198:ASN:HD22	1:E:210:ARG:HH11	1.46	0.60
1:E:115:ASP:OD2	6:E:701:HOH:O	2.16	0.60
1:C:132:ARG:CD	1:C:239:GLU:OE1	2.50	0.60
1:A:463:PHE:CD2	5:B:604:LU2:O3	2.57	0.58
1:C:554:VAL:HG13	6:C:741:HOH:O	2.04	0.57
1:E:77:ARG:HD2	6:E:794:HOH:O	2.03	0.57
1:E:179:ASN:HB3	1:F:128:ARG:HB3	1.88	0.56
1:D:194[B]:ARG:HB3	1:D:194[B]:ARG:NH2	2.21	0.56
5:A:608:LU2:O3	1:B:463:PHE:CB	2.53	0.56
1:A:252:ILE:HG12	4:A:603:EDO:H11	1.88	0.55
1:E:329:ASP:H	1:E:380:ASN:HD21	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:MET:HE1	1:E:336:LEU:HA	1.89	0.55
1:C:538:LEU:HB3	1:C:552:VAL:HG22	1.90	0.54
1:B:329:ASP:H	1:B:380:ASN:HD21	1.55	0.54
1:A:123:HIS:HD2	1:A:125:GLN:H	1.56	0.53
1:C:329:ASP:H	1:C:380:ASN:HD21	1.56	0.53
1:A:538:LEU:HB3	1:A:552:VAL:HG22	1.90	0.53
1:C:305:MET:HE1	1:C:336:LEU:HA	1.91	0.53
1:E:123:HIS:HD2	1:E:125:GLN:H	1.57	0.53
1:F:538:LEU:HB3	1:F:552:VAL:HG22	1.91	0.53
1:A:329:ASP:H	1:A:380:ASN:HD21	1.57	0.52
1:A:305:MET:HE2	1:A:336:LEU:HA	1.91	0.52
1:D:178:SER:O	1:D:197:ARG:NH2	2.43	0.52
1:B:554:VAL:HG13	6:B:725:HOH:O	2.10	0.52
1:E:538:LEU:HB3	1:E:552:VAL:HG22	1.90	0.52
1:F:178:SER:O	1:F:197:ARG:NH2	2.42	0.52
1:E:178:SER:O	1:E:197:ARG:NH2	2.42	0.52
1:A:414:ARG:HD3	6:A:712:HOH:O	2.08	0.51
1:B:305:MET:HE1	1:B:336:LEU:HA	1.92	0.51
1:B:178:SER:O	1:B:197:ARG:NH2	2.43	0.51
1:D:123:HIS:HD2	1:D:125:GLN:H	1.58	0.51
1:A:178:SER:O	1:A:197:ARG:NH2	2.43	0.51
1:B:538:LEU:HB3	1:B:552:VAL:HG22	1.93	0.51
1:A:359:HIS:CE1	4:A:605:EDO:H22	2.46	0.51
1:B:123:HIS:HD2	1:B:125:GLN:H	1.59	0.51
1:D:194[B]:ARG:HH21	1:D:194[B]:ARG:HB3	1.76	0.50
1:F:329:ASP:H	1:F:380:ASN:HD21	1.57	0.50
1:B:516:ASP:HB2	1:E:113:ARG:CZ	2.42	0.50
1:D:538:LEU:HB3	1:D:552:VAL:HG22	1.92	0.50
1:C:178:SER:O	1:C:197:ARG:NH2	2.42	0.50
1:B:516:ASP:HB2	1:E:113:ARG:NH2	2.27	0.50
1:D:399:ALA:HB2	1:D:567:LEU:HD22	1.93	0.50
1:C:123:HIS:HD2	1:C:125:GLN:H	1.60	0.50
1:A:399:ALA:HB2	1:A:567:LEU:HD22	1.94	0.49
1:E:511:GLN:NE2	6:E:704:HOH:O	2.36	0.49
1:A:248:VAL:HB	1:A:349:LEU:HD12	1.95	0.49
1:D:248:VAL:HB	1:D:349:LEU:HD12	1.95	0.49
1:B:399:ALA:HB2	1:B:567:LEU:HD22	1.94	0.49
1:D:407:PRO:HA	6:D:845:HOH:O	2.12	0.48
1:E:248:VAL:HB	1:E:349:LEU:HD12	1.95	0.48
1:F:123:HIS:HD2	1:F:125:GLN:H	1.59	0.48
1:F:305:MET:HE2	1:F:336:LEU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ARG:CD	6:D:721:HOH:O	2.51	0.48
1:B:194[B]:ARG:HB3	1:B:194[B]:ARG:HH22	1.61	0.48
1:C:248:VAL:HB	1:C:349:LEU:HD12	1.95	0.48
1:B:131:TRP:CH2	1:B:236:PRO:HG3	2.49	0.47
1:B:248:VAL:HB	1:B:349:LEU:HD12	1.95	0.47
1:D:553:GLU:CG	6:D:723:HOH:O	2.62	0.47
1:E:133:VAL:HG13	1:E:166:HIS:CE1	2.48	0.47
1:A:252:ILE:HG12	4:A:603:EDO:C1	2.43	0.47
1:E:162:LYS:HE2	6:E:720:HOH:O	2.15	0.47
1:D:194[B]:ARG:HH21	1:D:194[B]:ARG:CB	2.27	0.47
5:A:608:LU2:O3	1:B:463:PHE:CG	2.68	0.47
1:D:127:GLN:HB2	6:D:808:HOH:O	2.13	0.47
1:F:248:VAL:HB	1:F:349:LEU:HD12	1.97	0.47
1:B:245:ARG:NH1	1:B:320:GLU:OE2	2.47	0.47
1:D:245:ARG:NH1	1:D:320:GLU:OE2	2.48	0.47
1:D:553:GLU:HG2	6:D:723:HOH:O	2.15	0.46
1:E:198:ASN:ND2	1:E:210:ARG:HH11	2.13	0.46
1:C:245:ARG:NH1	1:C:320:GLU:OE2	2.48	0.46
1:C:132:ARG:CG	1:C:135:LEU:HD13	2.46	0.46
1:B:340:PHE:HB3	1:B:344:GLN:NE2	2.31	0.46
1:A:162:LYS:HE2	6:A:778:HOH:O	2.16	0.45
1:F:208:ARG:HD2	1:F:222:PHE:CD1	2.51	0.45
1:F:245:ARG:NH1	1:F:320:GLU:OE2	2.49	0.45
1:E:340:PHE:HB3	1:E:344:GLN:NE2	2.32	0.45
1:A:213:ASP:HB3	4:D:603:EDO:H21	1.97	0.45
1:A:545:ALA:O	6:A:701:HOH:O	2.21	0.45
1:A:198:ASN:ND2	1:A:210:ARG:HH11	2.14	0.45
1:A:288:GLU:HG2	6:A:884:HOH:O	2.16	0.45
1:F:198:ASN:ND2	1:F:210:ARG:HH11	2.13	0.45
1:A:457:LEU:HD13	1:A:482:TRP:CD2	2.52	0.44
1:D:305:MET:HE2	1:D:336:LEU:HA	1.99	0.44
1:F:457:LEU:HD13	1:F:482:TRP:CD2	2.52	0.44
1:F:484:LEU:HD11	4:F:603:EDO:H21	2.00	0.44
1:D:335:ASN:HD22	1:D:335:ASN:H	1.66	0.44
1:C:153:LEU:O	1:C:157:VAL:HG13	2.18	0.44
1:B:198:ASN:ND2	1:B:210:ARG:HH11	2.14	0.44
1:C:340:PHE:HB3	1:C:344:GLN:NE2	2.33	0.44
1:C:183:ASP:HB2	6:C:772:HOH:O	2.17	0.43
1:C:457:LEU:HD13	1:C:482:TRP:CD2	2.53	0.43
1:D:198:ASN:ND2	1:D:210:ARG:HH11	2.12	0.43
1:B:323:LYS:O	6:B:701:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83[A]:GLN:HE21	1:E:83[A]:GLN:HB2	1.57	0.43
1:A:340:PHE:HB3	1:A:344:GLN:NE2	2.32	0.43
1:E:335:ASN:H	1:E:335:ASN:HD22	1.67	0.43
1:B:153:LEU:O	1:B:157:VAL:HG13	2.18	0.43
1:B:335:ASN:H	1:B:335:ASN:HD22	1.66	0.43
1:B:457:LEU:HD13	1:B:482:TRP:CD2	2.52	0.43
1:D:340:PHE:HB3	1:D:344:GLN:NE2	2.34	0.43
1:D:457:LEU:HD13	1:D:482:TRP:CD2	2.52	0.43
1:B:363:LYS:CG	5:B:604:LU2:O6	2.66	0.43
1:A:245:ARG:NH1	1:A:320:GLU:OE2	2.51	0.43
1:C:438:ARG:NH1	6:C:707:HOH:O	2.51	0.43
1:E:335:ASN:HD22	1:E:335:ASN:N	2.17	0.43
1:E:457:LEU:HD13	1:E:482:TRP:CD2	2.53	0.43
1:A:153:LEU:O	1:A:157:VAL:HG13	2.18	0.43
1:B:335:ASN:HD22	1:B:335:ASN:N	2.17	0.43
1:F:340:PHE:HB3	1:F:344:GLN:NE2	2.34	0.43
1:E:153:LEU:O	1:E:157:VAL:HG13	2.19	0.43
1:A:133:VAL:HG13	1:A:166:HIS:CE1	2.54	0.42
1:C:335:ASN:HD22	1:C:335:ASN:N	2.17	0.42
1:F:320:GLU:HB2	6:F:781:HOH:O	2.19	0.42
1:A:335:ASN:HD22	1:A:335:ASN:N	2.17	0.42
1:D:335:ASN:HD22	1:D:335:ASN:N	2.17	0.42
1:F:271:LYS:HD3	1:F:289[A]:GLN:HE22	1.85	0.42
1:C:335:ASN:HD22	1:C:335:ASN:H	1.66	0.42
1:F:335:ASN:N	1:F:335:ASN:HD22	2.18	0.42
1:E:245:ARG:NH1	1:E:320:GLU:OE2	2.52	0.42
1:E:83[A]:GLN:OE1	1:E:114:MET:HG2	2.19	0.42
1:A:335:ASN:HD22	1:A:335:ASN:H	1.67	0.41
1:C:198:ASN:ND2	1:C:210:ARG:HH11	2.13	0.41
1:D:379[A]:ARG:HG3	1:D:408:TYR:HA	2.02	0.41
1:D:309:GLY:C	1:D:310:LEU:HD23	2.40	0.41
1:A:442:HIS:HB2	6:A:871:HOH:O	2.21	0.41
5:B:604:LU2:H15	5:B:604:LU2:H8	1.72	0.41
1:C:309:GLY:C	1:C:310:LEU:HD23	2.41	0.41
1:D:153:LEU:O	1:D:157:VAL:HG13	2.20	0.41
1:E:343:TRP:CD1	1:E:349:LEU:HD22	2.56	0.41
1:B:208:ARG:HD3	1:B:222:PHE:CD1	2.56	0.40
1:F:309:GLY:C	1:F:310:LEU:HD23	2.41	0.40
1:C:343:TRP:CD1	1:C:349:LEU:HD22	2.56	0.40
1:D:343:TRP:CD1	1:D:349:LEU:HD22	2.56	0.40
1:E:208:ARG:HD3	1:E:222:PHE:CD1	2.56	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	495/571 (87%)	481 (97%)	12 (2%)	2 (0%)	34	42
1	B	495/571 (87%)	478 (97%)	15 (3%)	2 (0%)	34	42
1	C	496/571 (87%)	479 (97%)	13 (3%)	4 (1%)	19	23
1	D	495/571 (87%)	481 (97%)	12 (2%)	2 (0%)	34	42
1	E	493/571 (86%)	478 (97%)	13 (3%)	2 (0%)	34	42
1	F	494/571 (86%)	479 (97%)	13 (3%)	2 (0%)	34	42
All	All	2968/3426 (87%)	2876 (97%)	78 (3%)	14 (0%)	29	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	B	330	VAL
1	C	133	VAL
1	C	330	VAL
1	D	330	VAL
1	E	330	VAL
1	F	330	VAL
1	A	370	PRO
1	B	370	PRO
1	C	370	PRO
1	D	370	PRO
1	E	370	PRO
1	F	370	PRO
1	C	557	PRO

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	430/485 (89%)	400 (93%)	30 (7%)	15	19
1	B	430/485 (89%)	397 (92%)	33 (8%)	13	16
1	C	431/485 (89%)	400 (93%)	31 (7%)	14	18
1	D	430/485 (89%)	394 (92%)	36 (8%)	11	13
1	E	428/485 (88%)	391 (91%)	37 (9%)	10	12
1	F	429/485 (88%)	401 (94%)	28 (6%)	17	23
All	All	2578/2910 (89%)	2383 (92%)	195 (8%)	13	16

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	77	ARG
1	A	84	GLU
1	A	101	ARG
1	A	112	LEU
1	A	116	ARG
1	A	124	ASP
1	A	133	VAL
1	A	157	VAL
1	A	195	VAL
1	A	218	LYS
1	A	245	ARG
1	A	277	ASN
1	A	288	GLU
1	A	310	LEU
1	A	330	VAL
1	A	335	ASN
1	A	349	LEU
1	A	419	LYS
1	A	421	LEU
1	A	434	TYR
1	A	450	LEU

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Mol	Chain	Res	Type
1	A	457	LEU
1	A	468	VAL
1	A	484	LEU
1	A	502	ARG
1	A	510	LEU
1	A	515	GLU
1	A	552	VAL
1	A	569	LEU
1	B	75	LYS
1	B	101	ARG
1	B	112	LEU
1	B	113	ARG
1	B	116	ARG
1	B	124	ASP
1	B	127	GLN
1	B	128	ARG
1	B	132	ARG
1	B	157	VAL
1	B	195	VAL
1	B	245	ARG
1	B	277	ASN
1	B	288	GLU
1	B	310	LEU
1	B	330	VAL
1	B	335	ASN
1	B	349	LEU
1	B	419	LYS
1	B	421	LEU
1	B	434	TYR
1	B	450	LEU
1	B	457	LEU
1	B	468	VAL
1	B	484	LEU
1	B	486	LYS
1	B	488	LYS
1	B	510	LEU
1	B	537	ASN
1	B	546	LYS
1	B	552	VAL
1	B	567	LEU
1	B	569	LEU
1	C	75	LYS

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Mol	Chain	Res	Type
1	C	112	LEU
1	C	116	ARG
1	C	124	ASP
1	C	128	ARG
1	C	131	TRP
1	C	135	LEU
1	C	157	VAL
1	C	195	VAL
1	C	196	LEU
1	C	245	ARG
1	C	277	ASN
1	C	288	GLU
1	C	310	LEU
1	C	330	VAL
1	C	335	ASN
1	C	349	LEU
1	C	419	LYS
1	C	421	LEU
1	C	434	TYR
1	C	438	ARG
1	C	450	LEU
1	C	451	GLN
1	C	457	LEU
1	C	468	VAL
1	C	484	LEU
1	C	502	ARG
1	C	510	LEU
1	C	546	LYS
1	C	552	VAL
1	C	569	LEU
1	D	75	LYS
1	D	77	ARG
1	D	101	ARG
1	D	112	LEU
1	D	116	ARG
1	D	124	ASP
1	D	133	VAL
1	D	157	VAL
1	D	173	LEU
1	D	189	LYS
1	D	195	VAL
1	D	196	LEU

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Mol	Chain	Res	Type
1	D	197	ARG
1	D	218	LYS
1	D	245	ARG
1	D	277	ASN
1	D	288	GLU
1	D	310	LEU
1	D	330	VAL
1	D	335	ASN
1	D	349	LEU
1	D	379[A]	ARG
1	D	379[B]	ARG
1	D	419	LYS
1	D	421	LEU
1	D	434	TYR
1	D	450	LEU
1	D	457	LEU
1	D	468	VAL
1	D	484	LEU
1	D	502	ARG
1	D	510	LEU
1	D	515	GLU
1	D	546	LYS
1	D	552	VAL
1	D	569	LEU
1	E	75	LYS
1	E	77	ARG
1	E	83[A]	GLN
1	E	83[B]	GLN
1	E	84	GLU
1	E	101	ARG
1	E	112	LEU
1	E	116	ARG
1	E	124	ASP
1	E	133	VAL
1	E	157	VAL
1	E	173	LEU
1	E	195	VAL
1	E	196	LEU
1	E	218	LYS
1	E	245	ARG
1	E	277	ASN
1	E	288	GLU

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Mol	Chain	Res	Type
1	E	294	GLN
1	E	310	LEU
1	E	330	VAL
1	E	335	ASN
1	E	349	LEU
1	E	419	LYS
1	E	421	LEU
1	E	434	TYR
1	E	438	ARG
1	E	450	LEU
1	E	457	LEU
1	E	468	VAL
1	E	484	LEU
1	E	502	ARG
1	E	510	LEU
1	E	515	GLU
1	E	532	ARG
1	E	546	LYS
1	E	552	VAL
1	F	75	LYS
1	F	101	ARG
1	F	112	LEU
1	F	116	ARG
1	F	124	ASP
1	F	157	VAL
1	F	195	VAL
1	F	196	LEU
1	F	245	ARG
1	F	277	ASN
1	F	288	GLU
1	F	310	LEU
1	F	330	VAL
1	F	335	ASN
1	F	349	LEU
1	F	419	LYS
1	F	421	LEU
1	F	450	LEU
1	F	457	LEU
1	F	468	VAL
1	F	484	LEU
1	F	502	ARG
1	F	510	LEU

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Mol	Chain	Res	Type
1	F	515	GLU
1	F	546	LYS
1	F	552	VAL
1	F	567	LEU
1	F	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	123	HIS
1	A	125	GLN
1	A	127	GLN
1	A	198	ASN
1	A	277	ASN
1	A	296	ASN
1	A	335	ASN
1	A	344	GLN
1	A	380	ASN
1	A	462	HIS
1	B	96	GLN
1	B	123	HIS
1	B	198	ASN
1	B	277	ASN
1	B	296	ASN
1	B	335	ASN
1	B	344	GLN
1	B	380	ASN
1	B	452	GLN
1	B	462	HIS
1	C	96	GLN
1	C	123	HIS
1	C	127	GLN
1	C	198	ASN
1	C	277	ASN
1	C	296	ASN
1	C	335	ASN
1	C	344	GLN
1	C	380	ASN
1	C	452	GLN
1	C	462	HIS
1	D	96	GLN

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Mol	Chain	Res	Type
1	D	123	HIS
1	D	127	GLN
1	D	198	ASN
1	D	277	ASN
1	D	296	ASN
1	D	335	ASN
1	D	344	GLN
1	D	462	HIS
1	E	96	GLN
1	E	123	HIS
1	E	125	GLN
1	E	127	GLN
1	E	198	ASN
1	E	277	ASN
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	380	ASN
1	E	452	GLN
1	E	462	HIS
1	F	96	GLN
1	F	123	HIS
1	F	125	GLN
1	F	127	GLN
1	F	198	ASN
1	F	277	ASN
1	F	296	ASN
1	F	335	ASN
1	F	344	GLN
1	F	380	ASN
1	F	452	GLN
1	F	462	HIS

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	C	603	-	3,3,3	0.57	0	2,2,2	0.19	0
4	EDO	F	603	-	3,3,3	0.53	0	2,2,2	0.26	0
4	EDO	A	605	-	3,3,3	0.81	0	2,2,2	0.30	0
3	UDP	F	602	2	24,26,26	1.25	4 (16%)	37,40,40	1.89	9 (24%)
5	LU2	A	608	-	23,23,23	2.25	10 (43%)	34,34,34	3.69	18 (52%)
5	LU2	B	604	-	23,23,23	1.89	9 (39%)	34,34,34	2.92	16 (47%)
3	UDP	B	602	2	24,26,26	1.06	1 (4%)	37,40,40	1.48	7 (18%)
3	UDP	E	602	2	24,26,26	1.35	6 (25%)	37,40,40	1.47	5 (13%)
4	EDO	B	603	-	3,3,3	0.24	0	2,2,2	0.50	0
4	EDO	E	603	-	3,3,3	0.76	0	2,2,2	0.08	0
4	EDO	A	603	-	3,3,3	1.39	0	2,2,2	1.43	0
5	LU2	D	604	-	23,23,23	1.67	4 (17%)	34,34,34	3.01	13 (38%)
4	EDO	A	604	-	3,3,3	1.05	0	2,2,2	0.34	0
4	EDO	A	606	-	3,3,3	0.69	0	2,2,2	0.24	0
3	UDP	C	602	2	24,26,26	1.14	2 (8%)	37,40,40	1.96	8 (21%)
3	UDP	D	602	2	24,26,26	1.28	3 (12%)	37,40,40	1.80	8 (21%)
3	UDP	A	602	2	24,26,26	1.07	1 (4%)	37,40,40	1.58	7 (18%)
4	EDO	D	603	-	3,3,3	1.12	0	2,2,2	0.10	0
4	EDO	A	607	-	3,3,3	0.47	0	2,2,2	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	603	-	-	1/1/1/1	-
4	EDO	F	603	-	-	1/1/1/1	-
4	EDO	A	605	-	-	1/1/1/1	-
3	UDP	F	602	2	-	2/16/32/32	0/2/2/2
5	LU2	A	608	-	-	3/4/4/4	0/3/3/3
5	LU2	B	604	-	-	0/4/4/4	0/3/3/3
3	UDP	B	602	2	-	1/16/32/32	0/2/2/2
3	UDP	E	602	2	-	1/16/32/32	0/2/2/2
4	EDO	B	603	-	-	1/1/1/1	-
4	EDO	E	603	-	-	1/1/1/1	-
4	EDO	A	603	-	-	1/1/1/1	-
5	LU2	D	604	-	-	4/4/4/4	0/3/3/3
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	A	606	-	-	1/1/1/1	-
3	UDP	C	602	2	-	1/16/32/32	0/2/2/2
3	UDP	D	602	2	-	1/16/32/32	0/2/2/2
3	UDP	A	602	2	-	2/16/32/32	0/2/2/2
4	EDO	D	603	-	-	1/1/1/1	-
4	EDO	A	607	-	-	1/1/1/1	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	LU2	C8-C7	-4.59	1.34	1.44
5	A	608	LU2	C8-C7	-4.40	1.35	1.44
5	D	604	LU2	C10-C9	-4.27	1.38	1.48
5	D	604	LU2	C8-C7	-4.15	1.35	1.44
5	A	608	LU2	C5-C7	-4.01	1.36	1.46
5	A	608	LU2	O4-C6	3.55	1.44	1.38
5	A	608	LU2	C3-C2	-3.31	1.34	1.39
5	A	608	LU2	C10-C9	-3.19	1.40	1.48
5	B	604	LU2	C1-C2	3.10	1.43	1.39
5	A	608	LU2	O4-C9	3.09	1.41	1.36
3	F	602	UDP	C5-C4	-2.96	1.37	1.43
3	E	602	UDP	O2-C2	2.94	1.28	1.23
5	B	604	LU2	C5-C7	-2.92	1.39	1.46
3	D	602	UDP	C2-N3	-2.82	1.32	1.38
5	B	604	LU2	C10-C9	-2.71	1.41	1.48
5	B	604	LU2	O4-C6	2.62	1.42	1.38
5	A	608	LU2	C3-C4	-2.61	1.35	1.38
5	A	608	LU2	C15-C10	2.60	1.43	1.39
5	D	604	LU2	C5-C7	-2.59	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	UDP	C4-N3	-2.57	1.34	1.38
3	E	602	UDP	C2-N1	2.56	1.42	1.38
5	B	604	LU2	C3-C2	-2.45	1.35	1.39
5	B	604	LU2	O4-C9	2.43	1.40	1.36
5	B	604	LU2	C15-C10	2.42	1.43	1.39
3	C	602	UDP	C2-N3	-2.36	1.33	1.38
3	C	602	UDP	C5-C4	-2.36	1.38	1.43
5	D	604	LU2	C3-C2	-2.28	1.35	1.39
5	B	604	LU2	C1-C6	2.28	1.42	1.38
3	D	602	UDP	C4-N3	-2.25	1.34	1.38
5	A	608	LU2	O3-C7	-2.23	1.19	1.24
5	A	608	LU2	O5-C12	-2.21	1.31	1.36
3	F	602	UDP	C2-N3	-2.20	1.34	1.38
3	E	602	UDP	C6-C5	2.17	1.40	1.35
3	E	602	UDP	C2-N3	-2.17	1.34	1.38
3	D	602	UDP	O4'-C1'	2.09	1.47	1.42
3	A	602	UDP	C2-N1	2.08	1.41	1.38
3	B	602	UDP	C5-C4	-2.05	1.39	1.43
3	F	602	UDP	C2-N1	2.03	1.41	1.38
3	F	602	UDP	C4-N3	-2.02	1.34	1.38
3	E	602	UDP	C5-C4	-2.01	1.39	1.43

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	608	LU2	O4-C9-C10	10.00	127.01	111.92
5	A	608	LU2	O4-C6-C1	9.24	129.66	115.79
5	D	604	LU2	O4-C9-C10	9.08	125.63	111.92
5	B	604	LU2	O4-C9-C10	8.01	124.01	111.92
5	B	604	LU2	O4-C6-C1	7.57	127.15	115.79
5	B	604	LU2	O3-C7-C8	-6.13	111.54	121.79
5	D	604	LU2	C11-C10-C9	-5.98	110.20	120.20
5	D	604	LU2	O4-C6-C1	5.98	124.76	115.79
3	C	602	UDP	O4-C4-C5	-5.93	114.73	125.16
5	A	608	LU2	C1-C6-C5	-5.88	111.51	121.86
5	A	608	LU2	C4-C3-C2	-5.53	114.70	119.70
5	A	608	LU2	O3-C7-C8	-5.44	112.69	121.79
3	C	602	UDP	C5-C4-N3	5.27	122.72	114.84
5	A	608	LU2	C4-C5-C6	5.19	122.62	117.35
5	D	604	LU2	O3-C7-C8	-5.01	113.41	121.79
3	F	602	UDP	O4-C4-C5	-4.97	116.42	125.16
3	C	602	UDP	C4-N3-C2	-4.76	120.30	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	608	LU2	C5-C7-C8	4.62	125.74	116.43
5	D	604	LU2	C15-C10-C9	4.42	128.01	120.78
5	A	608	LU2	C9-C8-C7	-4.41	117.50	122.25
3	F	602	UDP	C5-C4-N3	4.38	121.39	114.84
5	A	608	LU2	C11-C12-C13	4.37	123.73	119.86
3	F	602	UDP	PA-O3A-PB	-4.23	118.32	132.83
3	F	602	UDP	C4-N3-C2	-4.11	121.16	126.58
3	A	602	UDP	PA-O3A-PB	-4.10	118.75	132.83
3	D	602	UDP	C4-N3-C2	-4.05	121.24	126.58
3	E	602	UDP	C5-C4-N3	4.01	120.83	114.84
5	D	604	LU2	C10-C9-C8	-3.92	109.89	122.78
5	B	604	LU2	C1-C6-C5	-3.84	115.10	121.86
3	D	602	UDP	C5-C4-N3	3.78	120.49	114.84
3	B	602	UDP	O4-C4-C5	-3.74	118.59	125.16
5	D	604	LU2	C6-C1-C2	3.62	124.93	119.05
3	E	602	UDP	C4-N3-C2	-3.60	121.83	126.58
5	D	604	LU2	C3-C4-C5	3.58	125.09	120.93
5	B	604	LU2	O1-C2-C1	3.55	129.07	119.84
3	D	602	UDP	O4-C4-C5	-3.49	119.02	125.16
5	B	604	LU2	O4-C6-C5	-3.39	117.75	121.18
5	A	608	LU2	C6-C1-C2	3.39	124.55	119.05
3	A	602	UDP	O4-C4-C5	-3.38	119.21	125.16
5	D	604	LU2	C1-C6-C5	-3.32	116.01	121.86
5	A	608	LU2	C15-C14-C13	-3.29	117.12	120.50
5	B	604	LU2	C15-C14-C13	-3.28	117.13	120.50
5	D	604	LU2	C9-C8-C7	-3.25	118.75	122.25
5	A	608	LU2	C3-C4-C5	3.23	124.69	120.93
3	D	602	UDP	PA-O3A-PB	-3.22	121.77	132.83
5	A	608	LU2	O1-C2-C3	-3.17	111.59	119.84
5	B	604	LU2	O1-C2-C3	-3.16	111.62	119.84
3	B	602	UDP	PA-O3A-PB	-3.15	122.02	132.83
5	A	608	LU2	C10-C9-C8	-3.12	112.53	122.78
5	B	604	LU2	O4-C9-C8	-3.12	118.63	121.68
3	A	602	UDP	C5-C4-N3	3.03	119.38	114.84
3	D	602	UDP	N3-C2-N1	3.02	118.89	114.89
3	C	602	UDP	PA-O3A-PB	-3.00	122.53	132.83
5	B	604	LU2	C3-C4-C5	2.97	124.39	120.93
3	B	602	UDP	C4-N3-C2	-2.96	122.68	126.58
5	B	604	LU2	C5-C7-C8	2.95	122.36	116.43
5	A	608	LU2	C10-C11-C12	-2.88	117.65	120.09
3	F	602	UDP	O2'-C2'-C1'	2.82	119.45	110.02
3	E	602	UDP	N3-C2-N1	2.81	118.62	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	604	LU2	C6-C1-C2	2.78	123.56	119.05
3	E	602	UDP	O4-C4-C5	-2.73	120.35	125.16
3	A	602	UDP	C4-N3-C2	-2.68	123.05	126.58
3	B	602	UDP	C5-C4-N3	2.67	118.83	114.84
5	D	604	LU2	C5-C7-C8	2.66	121.79	116.43
3	B	602	UDP	N3-C2-N1	2.65	118.41	114.89
3	D	602	UDP	O2-C2-N3	-2.60	116.65	121.50
5	A	608	LU2	O1-C2-C1	2.55	126.48	119.84
5	B	604	LU2	C14-C13-C12	2.55	122.47	119.67
3	F	602	UDP	N3-C2-N1	2.50	118.21	114.89
3	F	602	UDP	O3B-PB-O1B	2.39	120.04	110.68
5	A	608	LU2	O4-C6-C5	-2.34	118.81	121.18
3	A	602	UDP	O3B-PB-O2B	2.34	116.58	107.64
3	F	602	UDP	O3A-PB-O1B	-2.32	98.35	111.19
3	B	602	UDP	O3B-PB-O2B	2.30	116.42	107.64
5	B	604	LU2	C10-C9-C8	-2.28	115.28	122.78
3	F	602	UDP	O2A-PA-O1A	2.27	123.45	112.24
3	B	602	UDP	O4-C4-N3	2.23	122.58	119.31
3	D	602	UDP	O2B-PB-O1B	2.22	119.38	110.68
5	B	604	LU2	C4-C5-C6	2.22	119.60	117.35
3	C	602	UDP	O2A-PA-O1A	2.21	123.19	112.24
3	C	602	UDP	O4-C4-N3	2.21	122.56	119.31
5	A	608	LU2	C6-C5-C7	-2.20	117.40	119.59
5	B	604	LU2	C14-C15-C10	2.18	123.32	120.78
3	D	602	UDP	O2'-C2'-C1'	2.17	117.26	110.02
3	A	602	UDP	O2B-PB-O3A	-2.16	97.39	104.64
3	C	602	UDP	O2'-C2'-C3'	2.16	118.79	111.82
3	A	602	UDP	O3A-PB-O1B	-2.14	99.33	111.19
5	D	604	LU2	C14-C15-C10	-2.13	118.30	120.78
3	E	602	UDP	O3A-PB-O1B	-2.12	99.42	111.19
5	D	604	LU2	O1-C2-C1	2.09	125.29	119.84
3	C	602	UDP	N3-C2-N1	2.01	117.56	114.89

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	604	LU2	C11-C10-C9-O4
5	D	604	LU2	C15-C10-C9-O4
5	D	604	LU2	C11-C10-C9-C8
5	D	604	LU2	C15-C10-C9-C8
5	A	608	LU2	C11-C10-C9-O4

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Mol	Chain	Res	Type	Atoms
5	A	608	LU2	C15-C10-C9-O4
4	C	603	EDO	O1-C1-C2-O2
4	D	603	EDO	O1-C1-C2-O2
4	A	603	EDO	O1-C1-C2-O2
4	F	603	EDO	O1-C1-C2-O2
4	A	605	EDO	O1-C1-C2-O2
4	A	606	EDO	O1-C1-C2-O2
4	A	607	EDO	O1-C1-C2-O2
3	A	602	UDP	PB-O3A-PA-O2A
3	F	602	UDP	O4'-C1'-N1-C6
4	B	603	EDO	O1-C1-C2-O2
4	E	603	EDO	O1-C1-C2-O2
3	D	602	UDP	O4'-C1'-N1-C6
5	A	608	LU2	C11-C10-C9-C8
3	B	602	UDP	C4'-C5'-O5'-PA
3	A	602	UDP	PB-O3A-PA-O1A
3	E	602	UDP	PB-O3A-PA-O1A
3	C	602	UDP	O4'-C1'-N1-C6
3	F	602	UDP	C2'-C1'-N1-C6

There are no ring outliers.

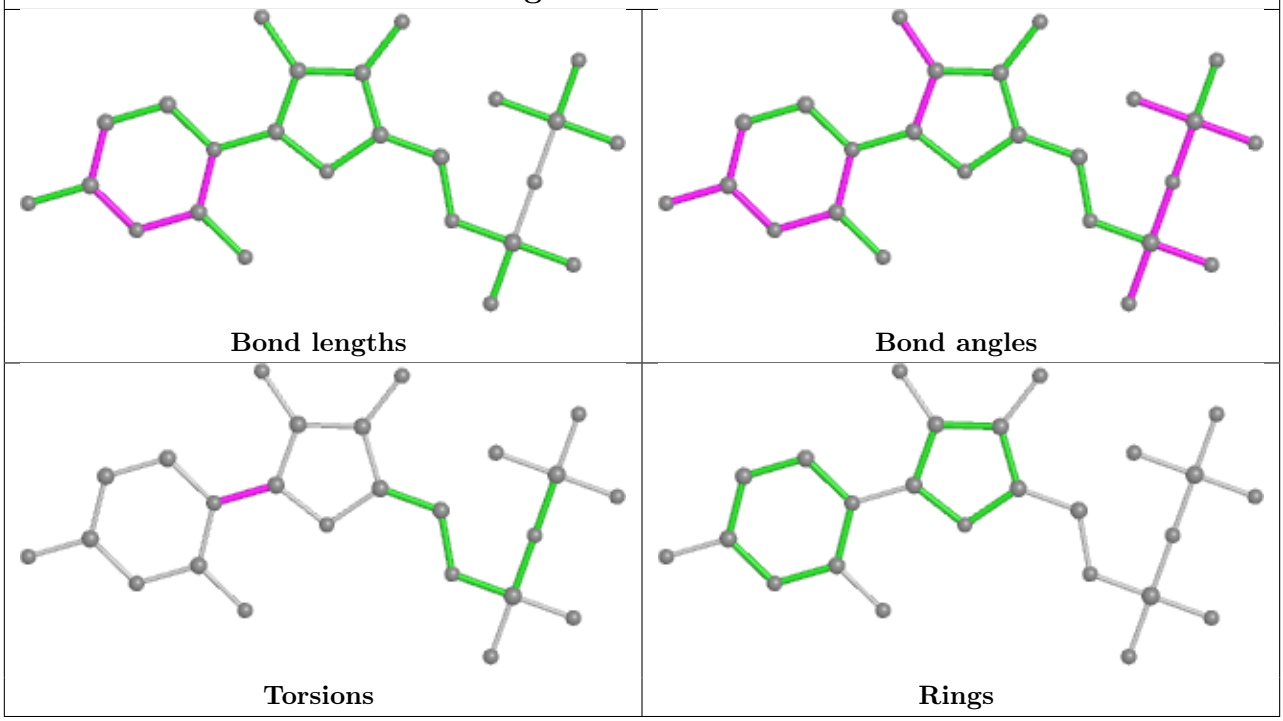
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	603	EDO	1	0
4	A	605	EDO	1	0
5	A	608	LU2	5	0
5	B	604	LU2	4	0
4	A	603	EDO	2	0
5	D	604	LU2	1	0
4	D	603	EDO	1	0

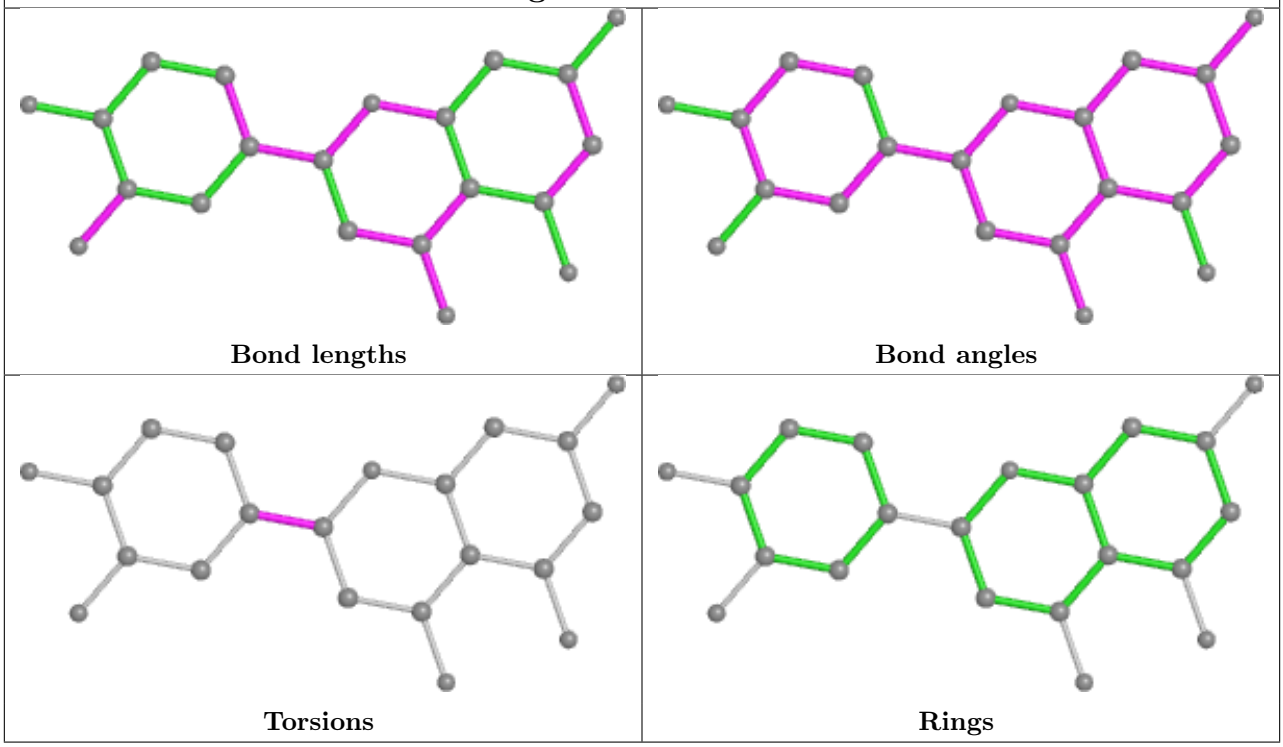
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

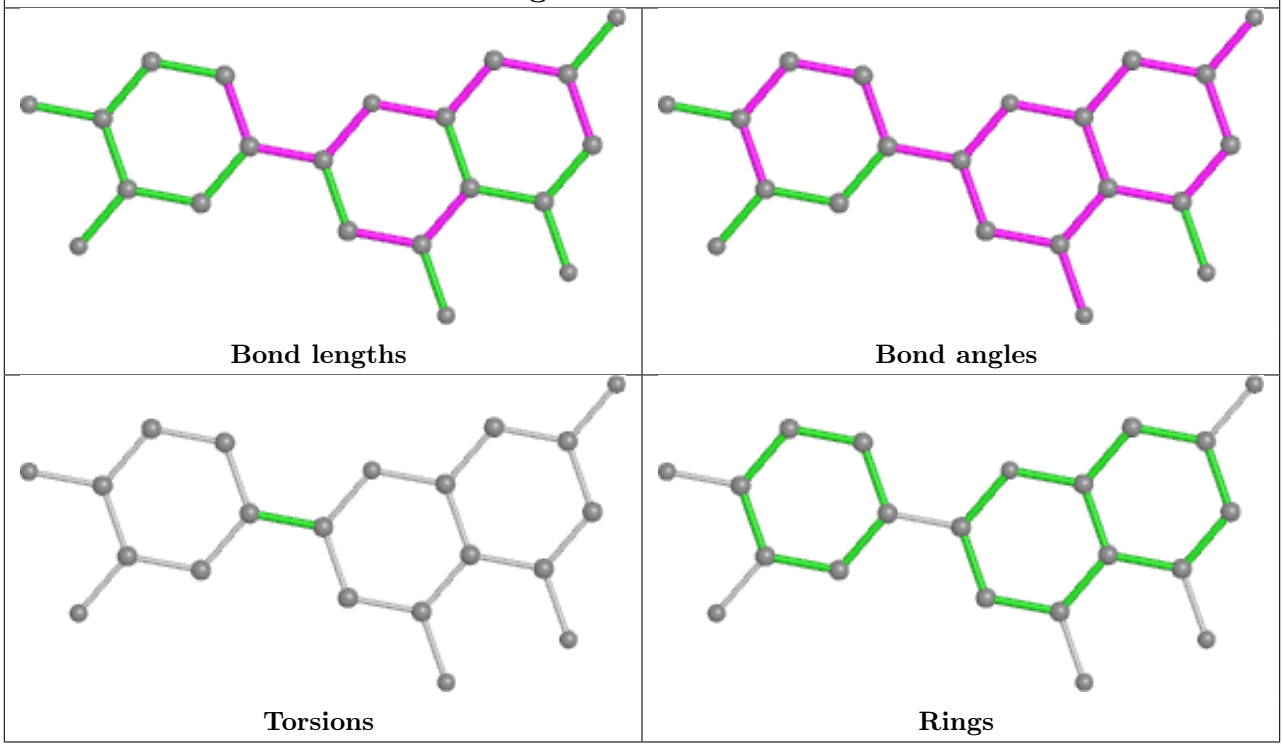
Ligand UDP F 602



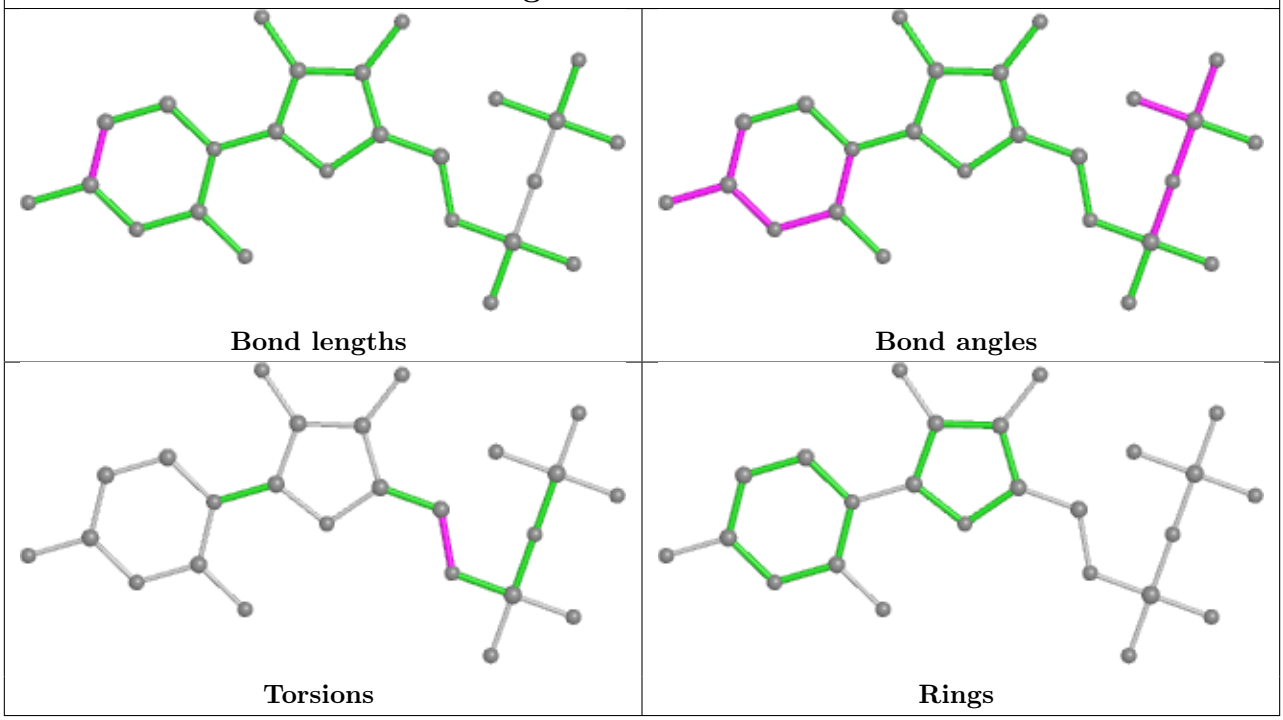
Ligand LU2 A 608



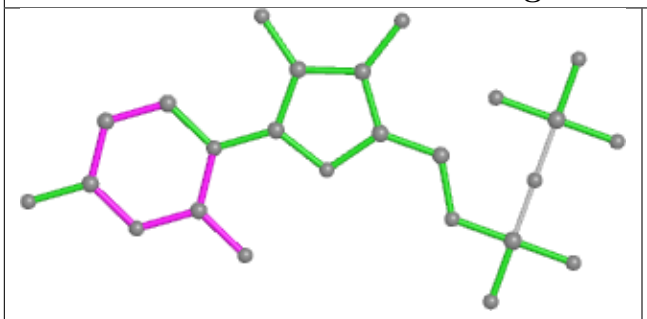
Ligand LU2 B 604



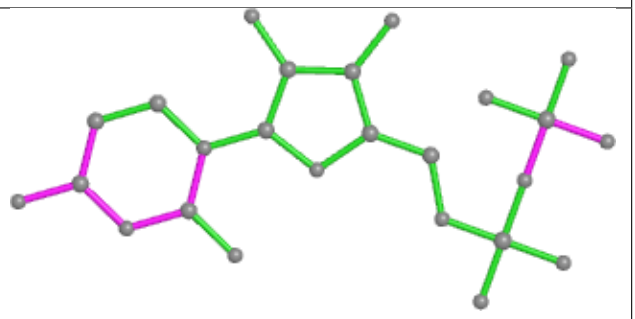
Ligand UDP B 602



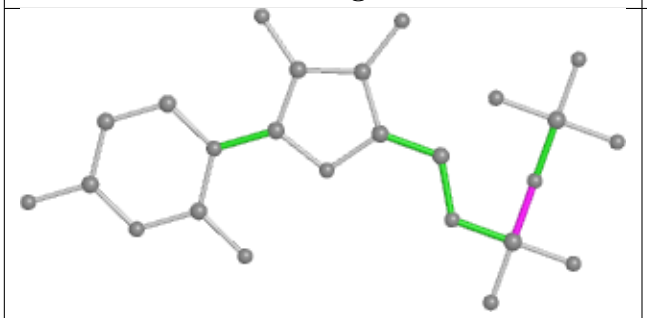
Ligand UDP E 602



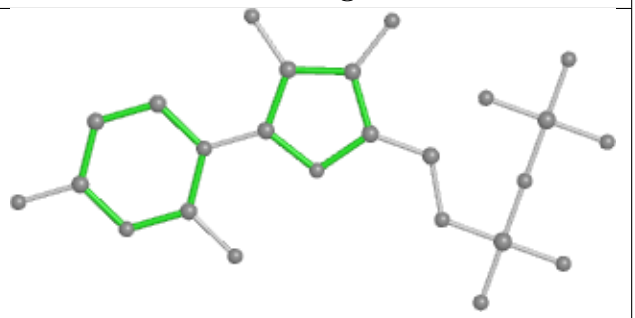
Bond lengths



Bond angles

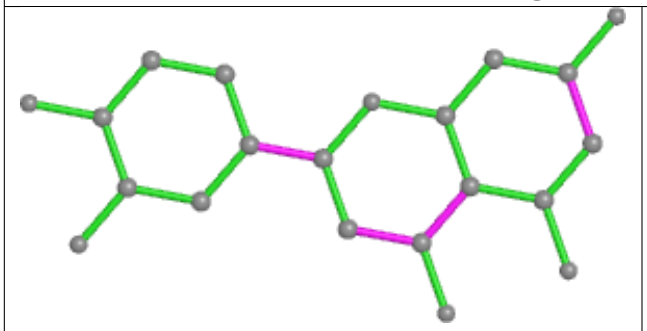


Torsions

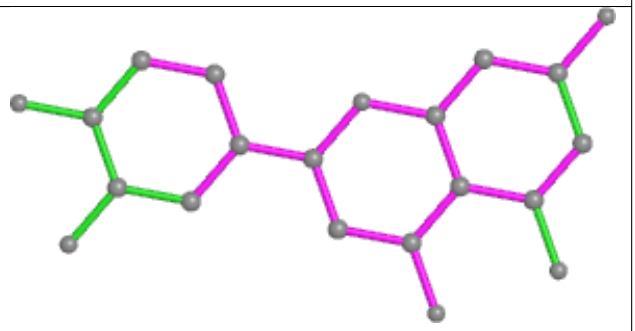


Rings

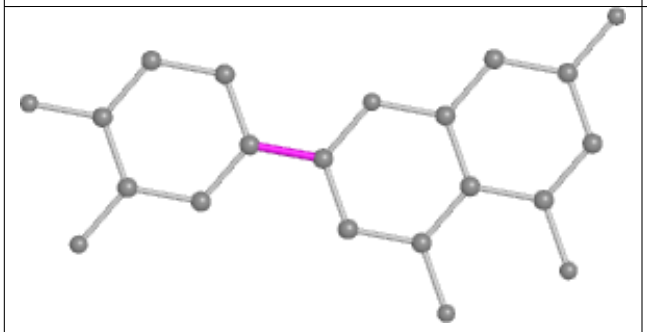
Ligand LU2 D 604



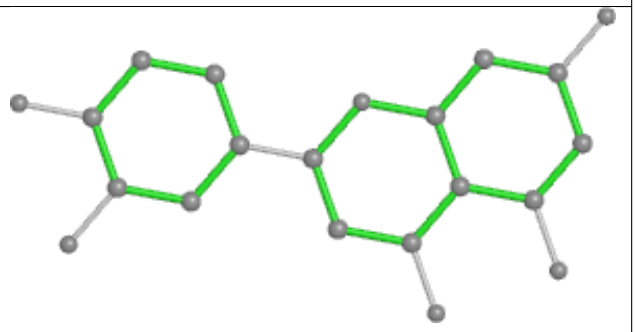
Bond lengths



Bond angles

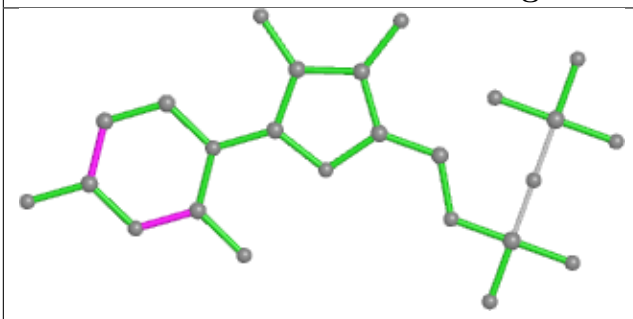


Torsions

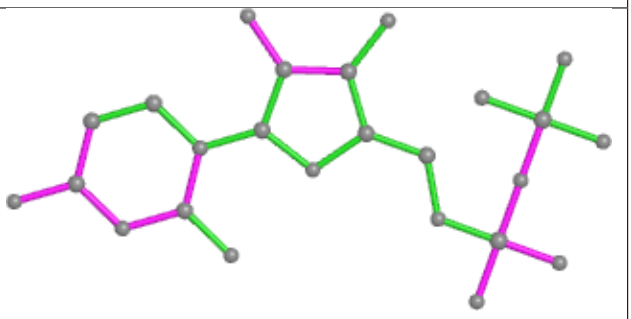


Rings

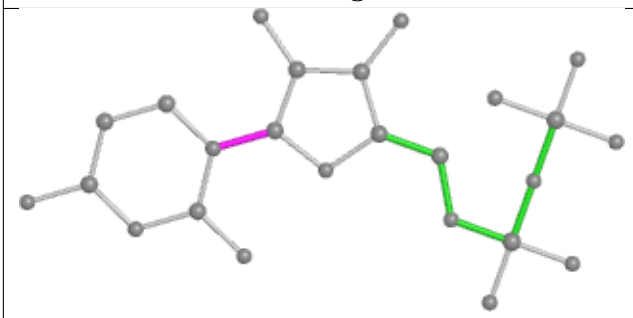
Ligand UDP C 602



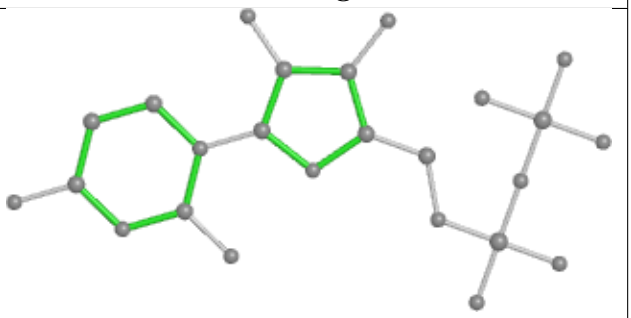
Bond lengths



Bond angles

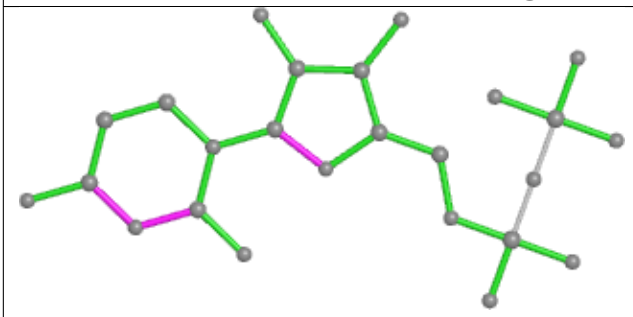


Torsions

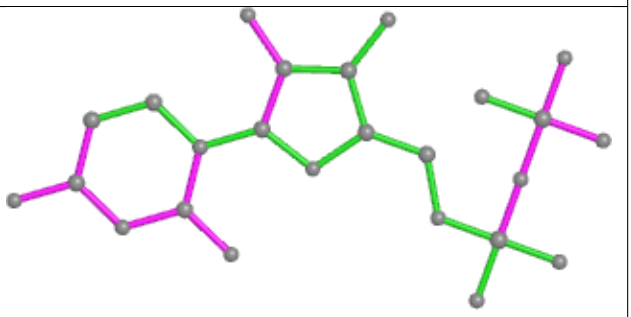


Rings

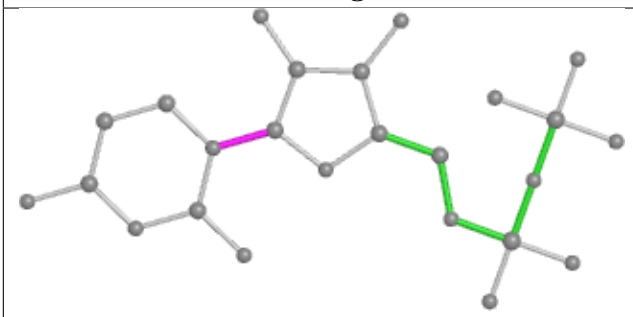
Ligand UDP D 602



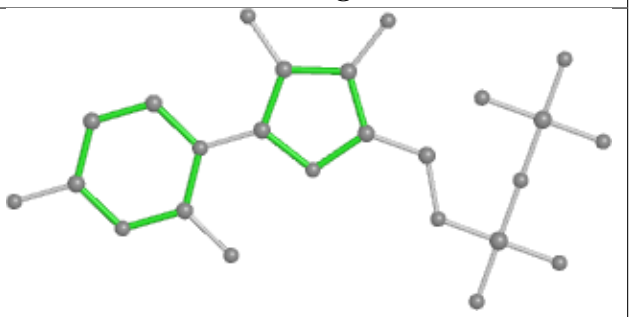
Bond lengths



Bond angles

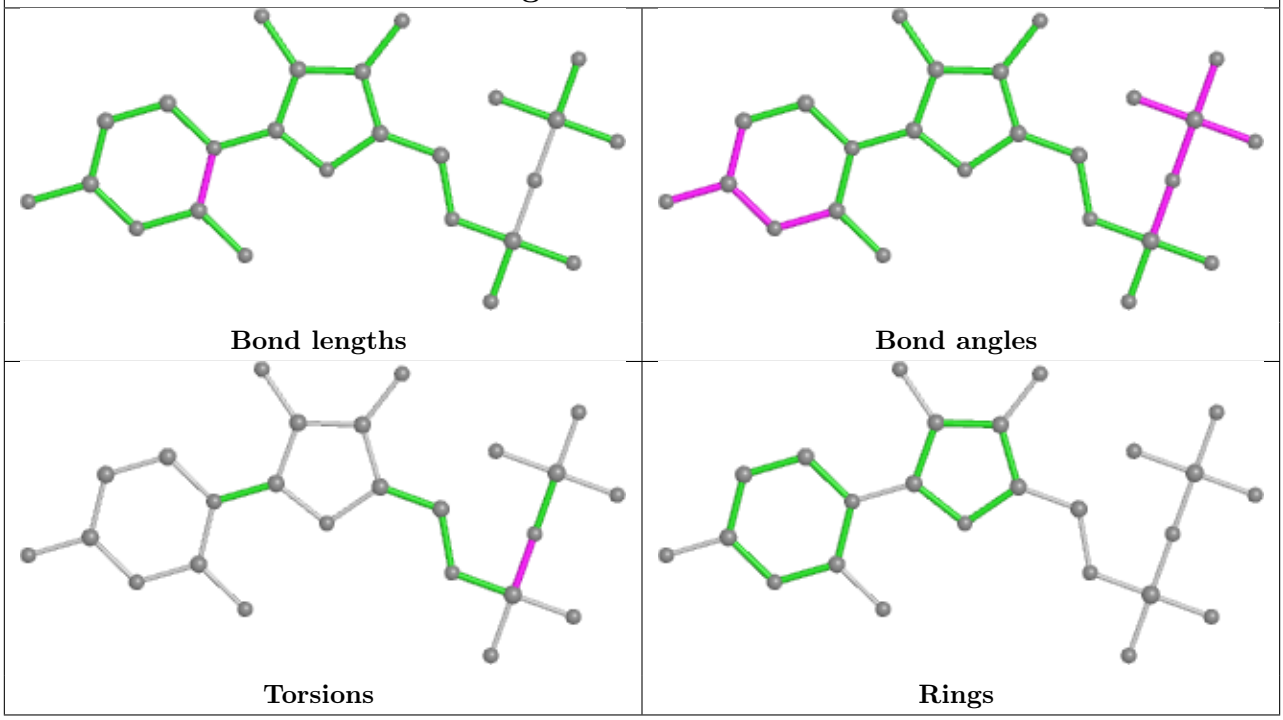


Torsions



Rings

Ligand UDP A 602



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.15	5 (1%)	82	86	27, 43, 72, 116	5 (1%)
1	B	495/571 (86%)	0.00	16 (3%)	47	54	28, 48, 82, 142	5 (1%)
1	C	495/571 (86%)	0.13	22 (4%)	34	41	28, 52, 87, 172	5 (1%)
1	D	495/571 (86%)	0.01	22 (4%)	34	41	28, 45, 79, 120	5 (1%)
1	E	492/571 (86%)	0.37	38 (7%)	13	17	27, 62, 106, 176	5 (1%)
1	F	495/571 (86%)	0.30	33 (6%)	17	23	33, 58, 96, 138	5 (1%)
All	All	2967/3426 (86%)	0.11	136 (4%)	32	39	27, 50, 91, 176	30 (1%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	442	HIS	8.4
1	B	92	VAL	6.1
1	C	128	ARG	6.0
1	F	284	TYR	5.6
1	E	443	GLN	5.6
1	C	95	GLY	5.5
1	F	373	SER	5.3
1	B	91	MET	4.8
1	E	557	PRO	4.7
1	F	287	PRO	4.6
1	B	93	ARG	4.5
1	D	442	HIS	4.5
1	F	371	GLY	4.4
1	F	365	HIS	4.3
1	C	475	ASN	4.1
1	C	133	VAL	4.1
1	E	441	ASP	4.0
1	F	442	HIS	4.0
1	E	540	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	94	SER	3.9
1	D	370	PRO	3.9
1	E	457	LEU	3.9
1	F	367	TYR	3.8
1	C	94	SER	3.7
1	E	94	SER	3.7
1	F	366	PRO	3.7
1	B	89	GLY	3.6
1	C	92	VAL	3.6
1	E	445	ILE	3.6
1	C	127	GLN	3.5
1	E	440	PRO	3.5
1	E	531	LEU	3.5
1	B	95	GLY	3.4
1	F	91	MET	3.4
1	C	89	GLY	3.4
1	F	370	PRO	3.4
1	C	96	GLN	3.4
1	C	557	PRO	3.4
1	F	291	ARG	3.4
1	D	372	GLY	3.3
1	F	535	GLY	3.3
1	E	555	CYS	3.2
1	F	331	TRP	3.2
1	C	93	ARG	3.2
1	F	93	ARG	3.1
1	C	540	LEU	3.1
1	D	410	ASN	3.1
1	E	93	ARG	3.1
1	E	405	ASN	3.0
1	D	291	ARG	3.0
1	F	363	LYS	3.0
1	C	130	GLN	3.0
1	E	563	TRP	3.0
1	A	93	ARG	3.0
1	D	409	GLY	2.9
1	B	96	GLN	2.9
1	F	372	GLY	2.9
1	B	442	HIS	2.9
1	C	442	HIS	2.9
1	F	290	ARG	2.9
1	B	94	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	566	THR	2.8
1	F	531	LEU	2.8
1	E	539	CYS	2.8
1	E	475	ASN	2.8
1	D	443	GLN	2.8
1	F	297	PRO	2.8
1	D	373	SER	2.8
1	F	405	ASN	2.8
1	D	331	TRP	2.8
1	E	410	ASN	2.8
1	D	368	THR	2.7
1	E	543	ARG	2.7
1	E	95	GLY	2.7
1	B	90	THR	2.7
1	A	94	SER	2.6
1	E	447	PHE	2.6
1	E	446	ALA	2.6
1	F	438	ARG	2.6
1	F	368	THR	2.6
1	F	364	GLN	2.6
1	E	527	GLY	2.6
1	F	369	PHE	2.6
1	A	92	VAL	2.5
1	E	558	ALA	2.5
1	B	199	ASP	2.5
1	D	288	GLU	2.5
1	E	375	THR	2.5
1	E	537	ASN	2.5
1	B	450	LEU	2.5
1	D	377	PHE	2.5
1	D	376	VAL	2.4
1	E	438	ARG	2.4
1	F	569	LEU	2.4
1	C	371	GLY	2.4
1	B	130	GLN	2.4
1	C	131	TRP	2.3
1	D	369	PHE	2.3
1	E	456	CYS	2.3
1	C	537	ASN	2.3
1	B	200	ARG	2.3
1	A	96	GLN	2.3
1	C	364	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	364	GLN	2.3
1	F	374	GLY	2.2
1	D	93	ARG	2.2
1	E	152	LEU	2.2
1	F	282	TRP	2.2
1	A	540	LEU	2.2
1	B	133	VAL	2.2
1	C	405	ASN	2.2
1	D	94	SER	2.2
1	E	547	SER	2.2
1	F	280	PHE	2.2
1	D	384	ALA	2.2
1	E	556	GLY	2.2
1	F	279	VAL	2.1
1	C	476	ALA	2.1
1	E	526	GLU	2.1
1	D	540	LEU	2.1
1	D	88	GLY	2.1
1	C	559	LEU	2.1
1	E	550	LEU	2.1
1	E	391	GLU	2.1
1	D	476	ALA	2.1
1	E	484	LEU	2.1
1	D	95	GLY	2.1
1	F	527	GLY	2.1
1	D	287	PRO	2.1
1	C	508	ILE	2.1
1	B	295	GLY	2.1
1	B	413	SER	2.0
1	E	88	GLY	2.0
1	F	92	VAL	2.0
1	F	133	VAL	2.0
1	E	559	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

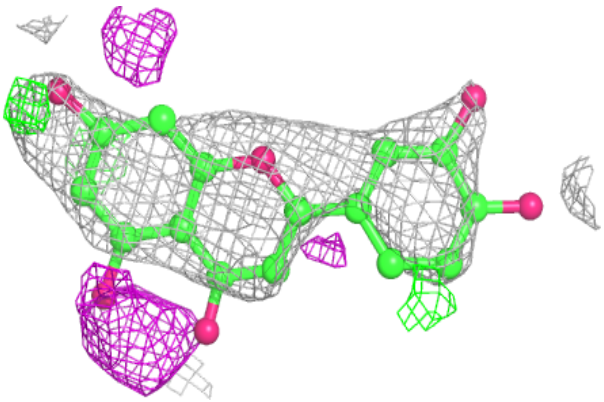
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

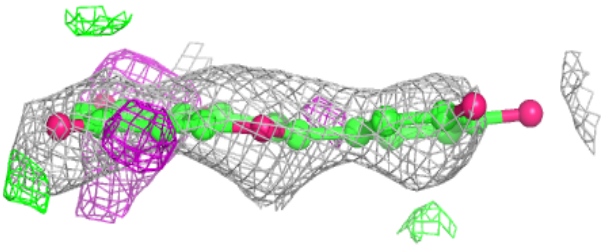
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	C	603	4/4	0.45	0.37	71,79,83,90	0
4	EDO	A	607	4/4	0.65	0.22	79,88,92,96	0
5	LU2	B	604	21/21	0.72	0.37	84,109,128,163	0
4	EDO	F	603	4/4	0.73	0.28	73,73,73,74	0
4	EDO	A	605	4/4	0.78	0.21	46,49,53,59	0
4	EDO	B	603	4/4	0.79	0.16	54,63,64,65	0
4	EDO	A	603	4/4	0.83	0.31	51,52,53,53	0
5	LU2	D	604	21/21	0.83	0.32	60,107,129,161	0
4	EDO	A	606	4/4	0.85	0.23	64,71,74,77	0
4	EDO	A	604	4/4	0.86	0.18	44,56,56,57	0
5	LU2	A	608	21/21	0.87	0.30	53,83,117,166	0
4	EDO	E	603	4/4	0.88	0.18	64,68,72,72	0
4	EDO	D	603	4/4	0.93	0.14	31,33,37,38	0
3	UDP	F	602	25/25	0.93	0.14	53,61,68,71	0
3	UDP	C	602	25/25	0.96	0.10	38,45,52,55	0
3	UDP	D	602	25/25	0.96	0.10	37,42,49,50	0
3	UDP	B	602	25/25	0.97	0.09	39,49,64,70	0
3	UDP	E	602	25/25	0.98	0.07	41,49,60,64	0
3	UDP	A	602	25/25	0.98	0.07	30,39,47,51	0
2	MN	F	601	1/1	0.98	0.04	50,50,50,50	0
2	MN	A	601	1/1	0.99	0.05	33,33,33,33	0
2	MN	B	601	1/1	0.99	0.08	43,43,43,43	0
2	MN	C	601	1/1	0.99	0.05	36,36,36,36	0
2	MN	D	601	1/1	0.99	0.05	36,36,36,36	0
2	MN	E	601	1/1	0.99	0.06	40,40,40,40	0

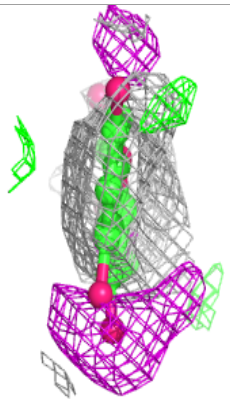
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LU2 B 604:

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

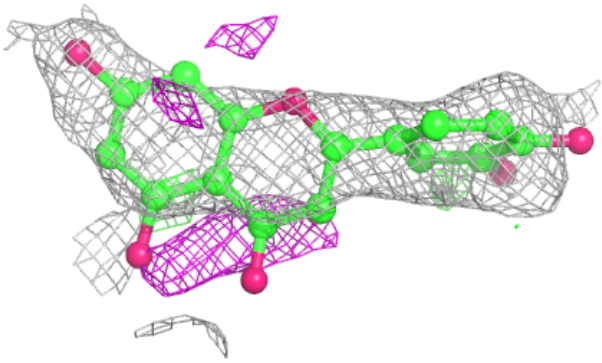


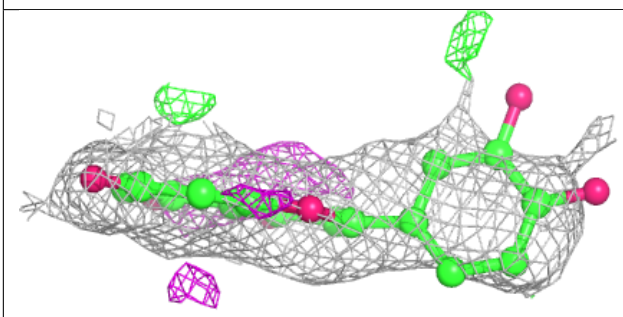


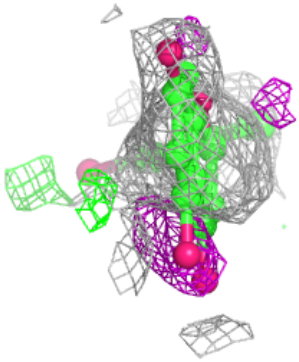


Electron density around LU2 D 604:

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

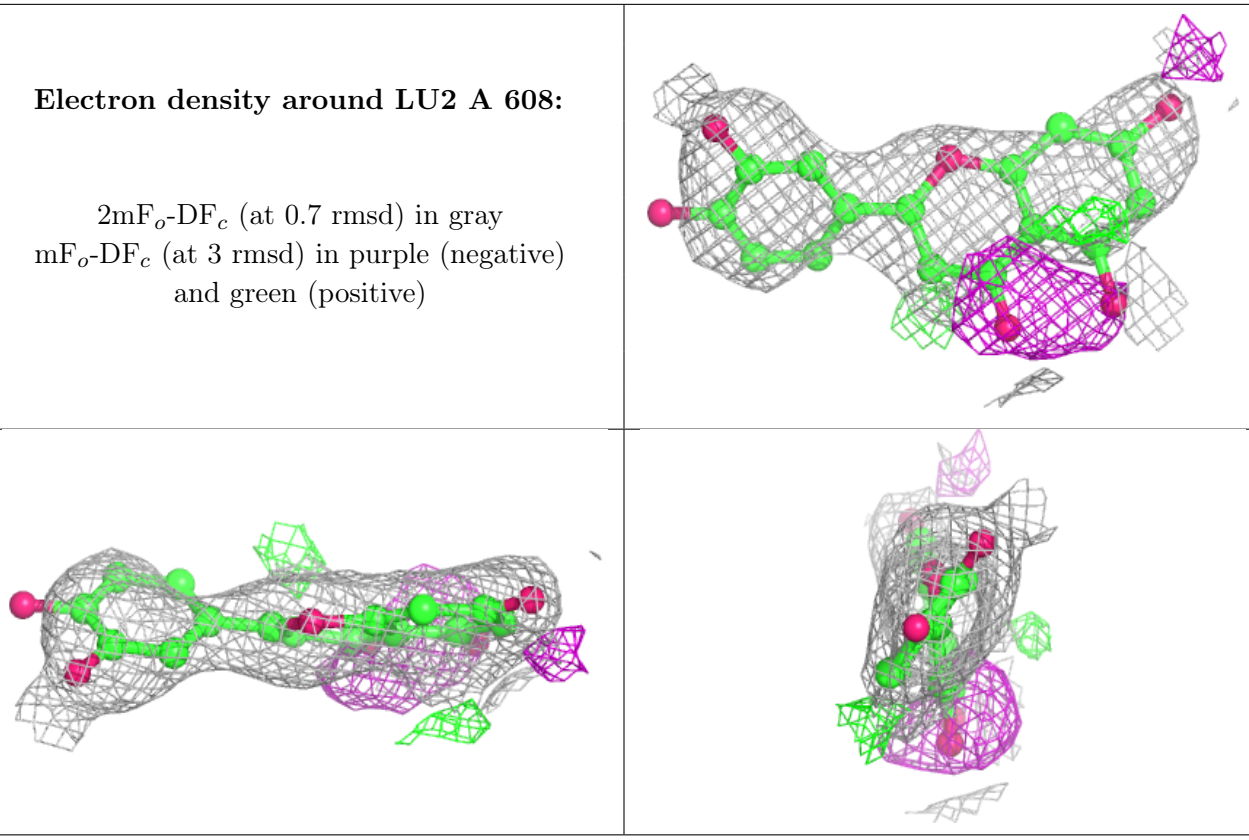






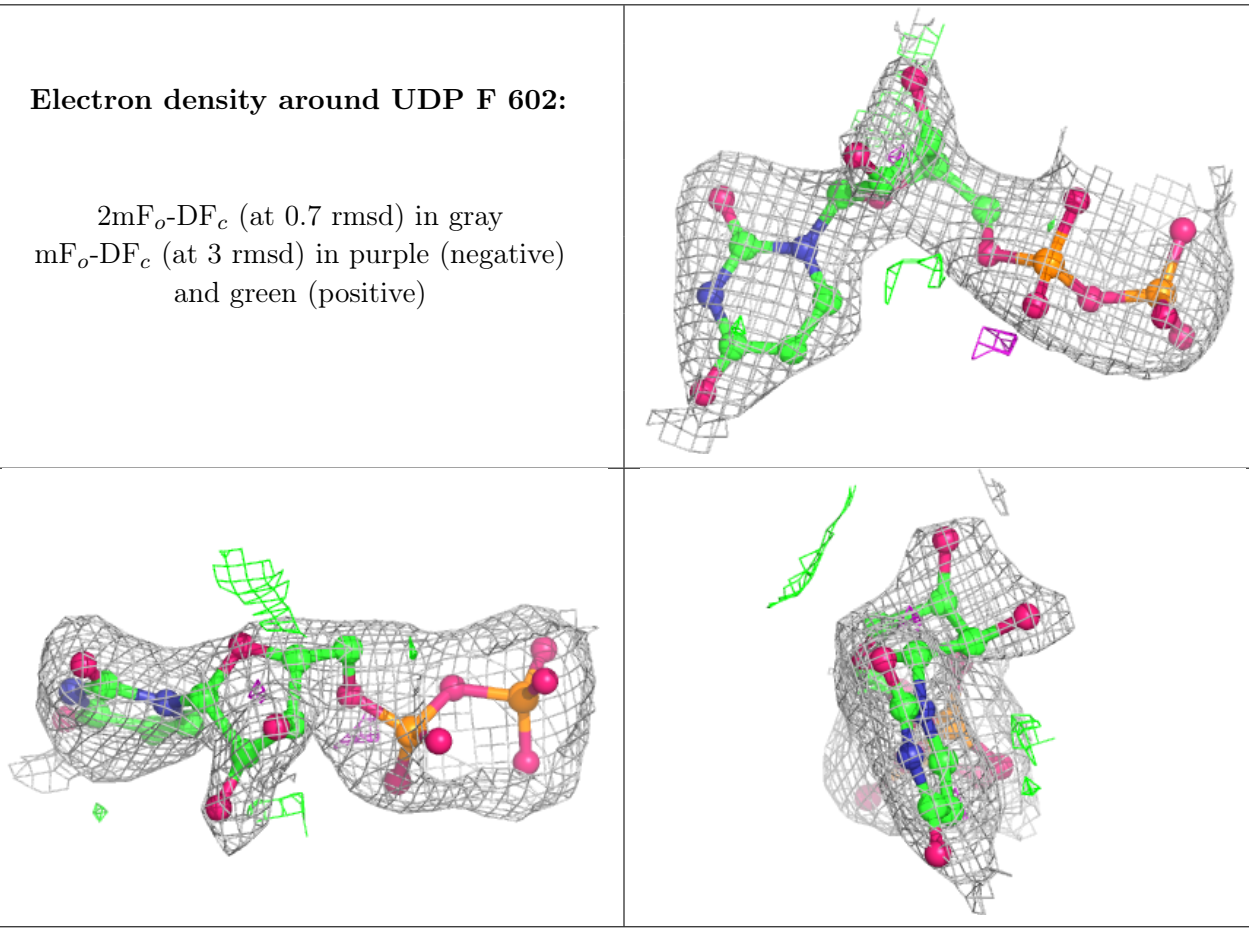
Electron density around LU2 A 608:

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



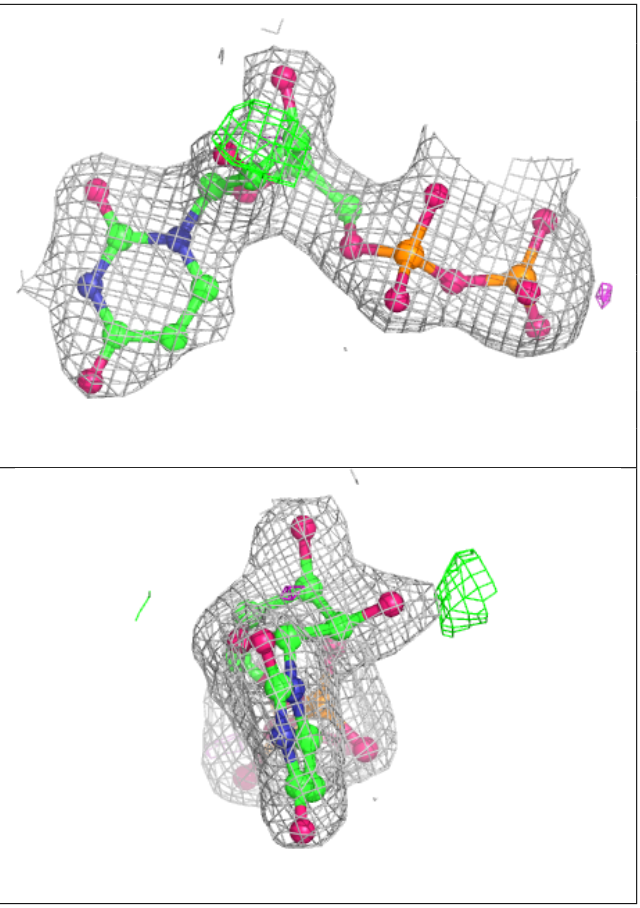
Electron density around UDP F 602:

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



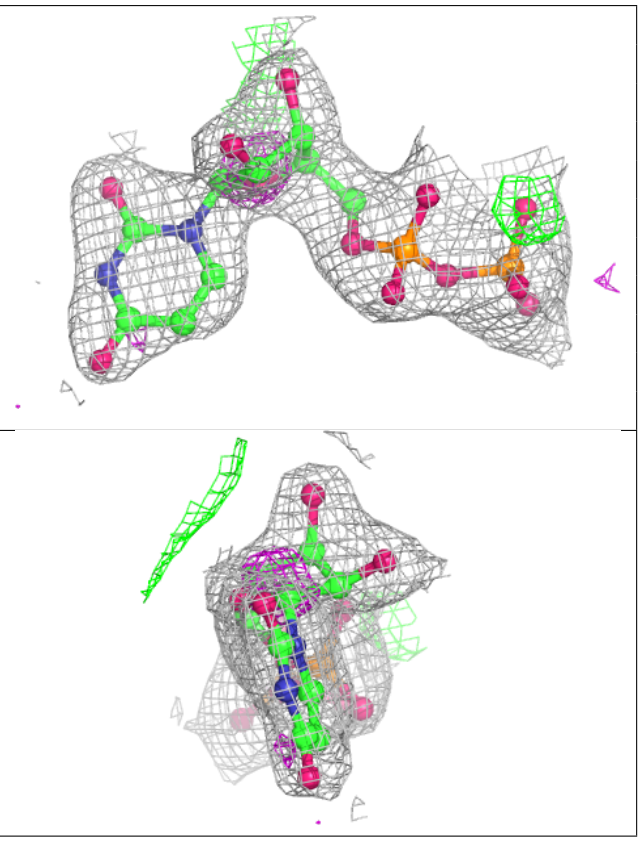
Electron density around UDP C 602:

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



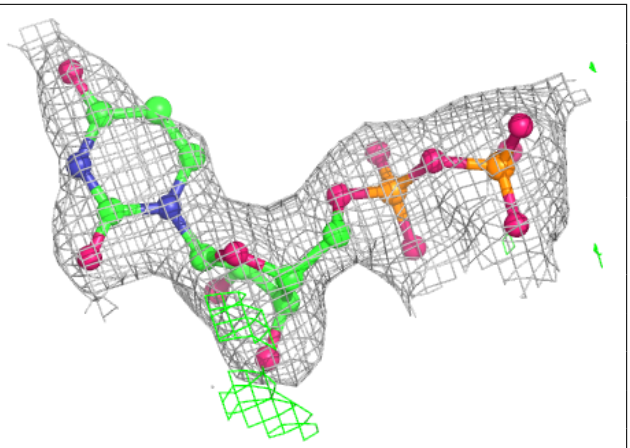
Electron density around UDP D 602:

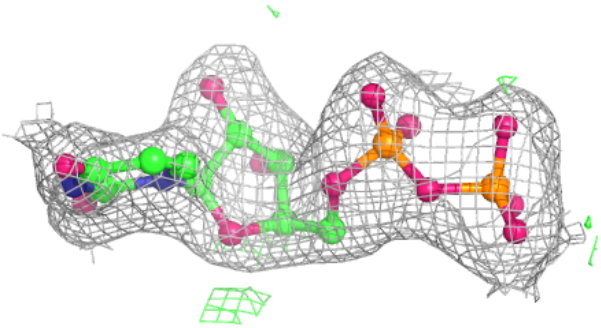
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

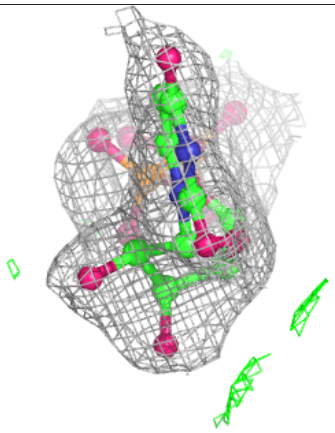


Electron density around UDP B 602:

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

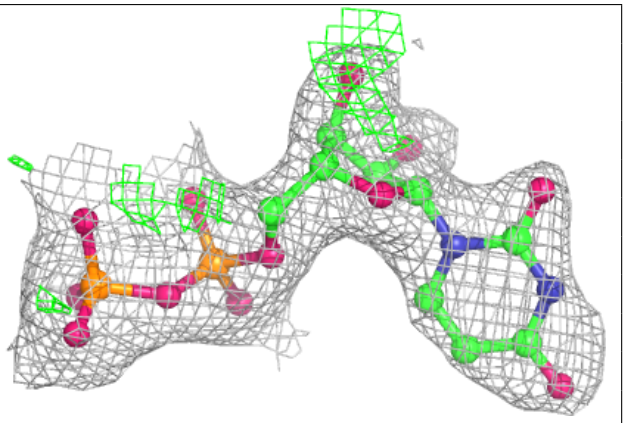


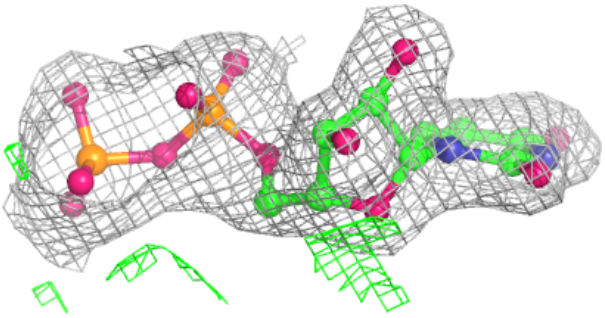


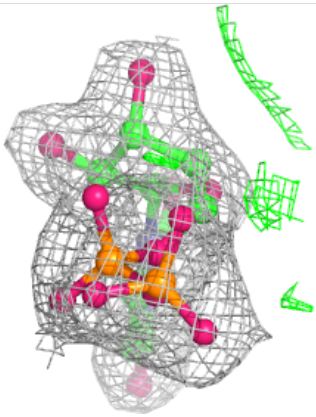


Electron density around UDP E 602:

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

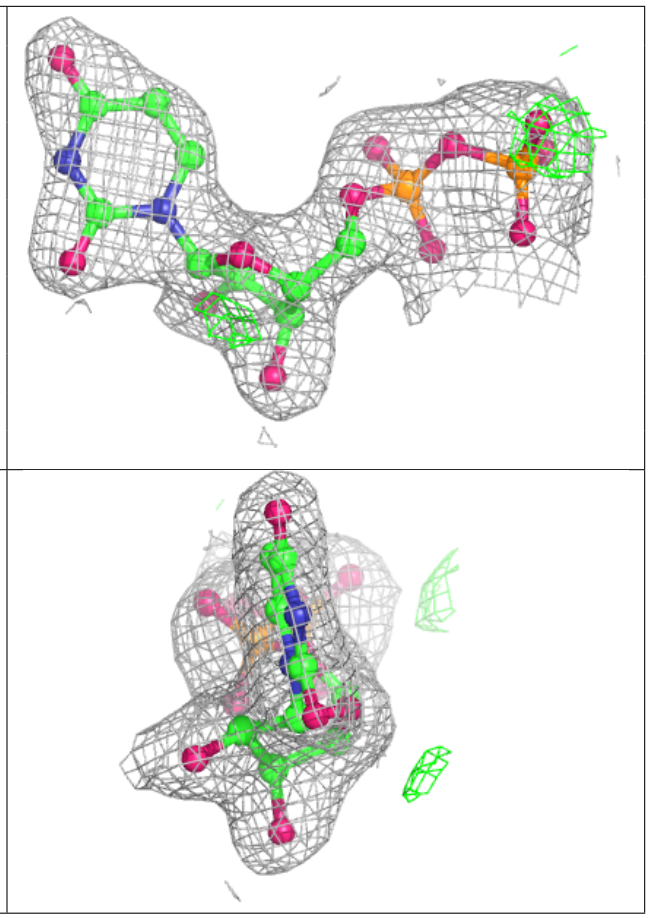






Electron density around UDP A 602:

$2mF_o$-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.