Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2023 – 02:01 am GMT

PDB ID	:	4D11
Title	:	GalNAc-T2 crystal soaked with UDP-5SGalNAc, mEA2 peptide and manganese (Lower resolution dataset)
Authors	:	Lira-Navarrete, E.; Iglesias-Fernandez, J.; Zandberg, W.F.; Companon, I.; Kong, Y.; Corzana, F.; Pinto, B.M.; Clausen, H.; Peregrina, J.M.; Vocadlo, D.; Rovira, C.; Hurtado-Guerrero, R.
Deposited on	:	2014-05-01
Resolution	:	2.85 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 (1)) were used in the production of this report:

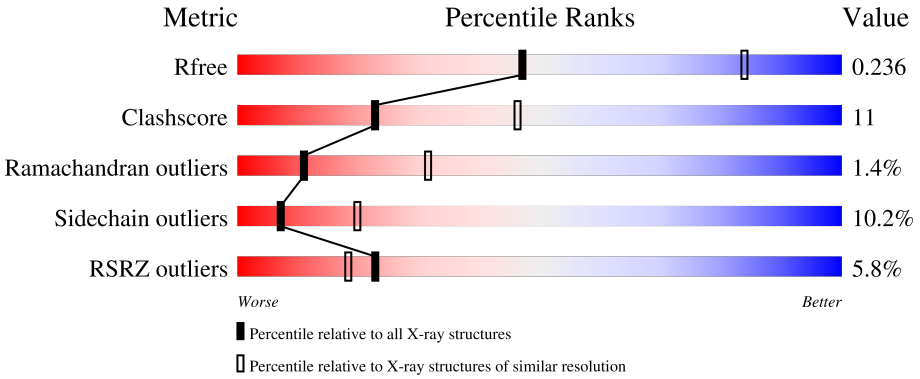
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	2% 71% 11% • 14%
1	B	571	2% 65% 16% • • 16%
1	D	571	3% 65% 15% • • 15%
1	E	571	3% 68% 14% • 15%
1	F	571	7% 36% 10% • 52%

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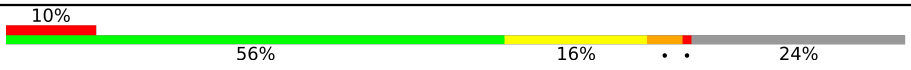
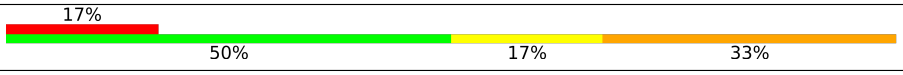
Mol	Chain	Length	Quality of chain
2	C	571	
3	L	6	
3	O	6	
3	P	6	
3	X	6	
3	Z	6	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21829 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 GALNAC-TRANSFERASE T2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	20	0	0
			3938	2477	715	722	24			
1	B	482	Total	C	N	O	S	20	1	0
			3877	2441	703	710	23			
1	D	487	Total	C	N	O	S	20	0	0
			3916	2465	711	716	24			
1	E	487	Total	C	N	O	S	20	0	0
			3917	2465	711	717	24			
1	F	276	Total	C	N	O	S	8	0	0
			2246	1419	406	407	14			

There are 5 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
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 a protein called POLYPEPTIDE GALNAC-TRANSFERASE T2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	436	Total	C	N	O	S	20	0	0
			3560	2249	646	644	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	74	SER	GLY	conflict	UNP Q10471
C	516	ASP	ASN	engineered mutation	UNP Q10471

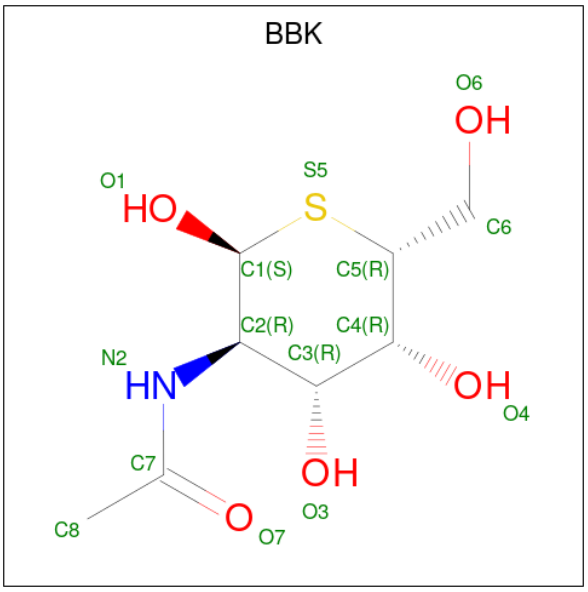
- Molecule 3 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	O	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	P	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	X	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
3	Z	5	Total	C	N	O	S	0	0	0
			31	18	5	7	1			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

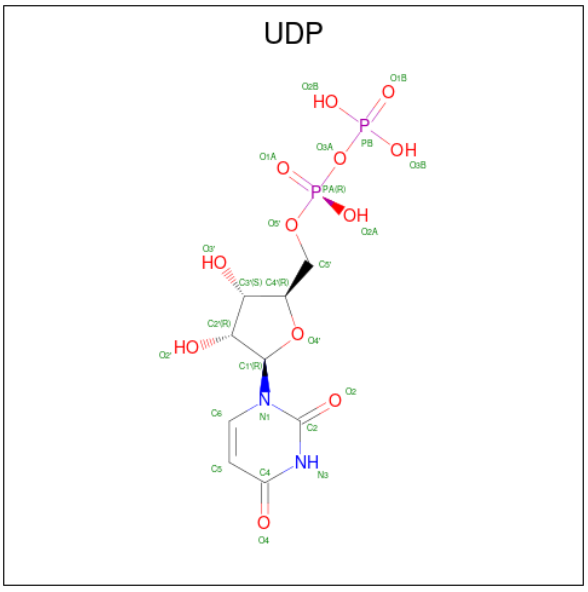
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		
4	E	1	Total	Mn	0	0
			1	1		
4	F	1	Total	Mn	0	0
			1	1		

- Molecule 5 is 2-acetamido-2-deoxy-5-thio-alpha-D-galactopyranose (three-letter code: BBK) (formula: $C_8H_{15}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	E	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



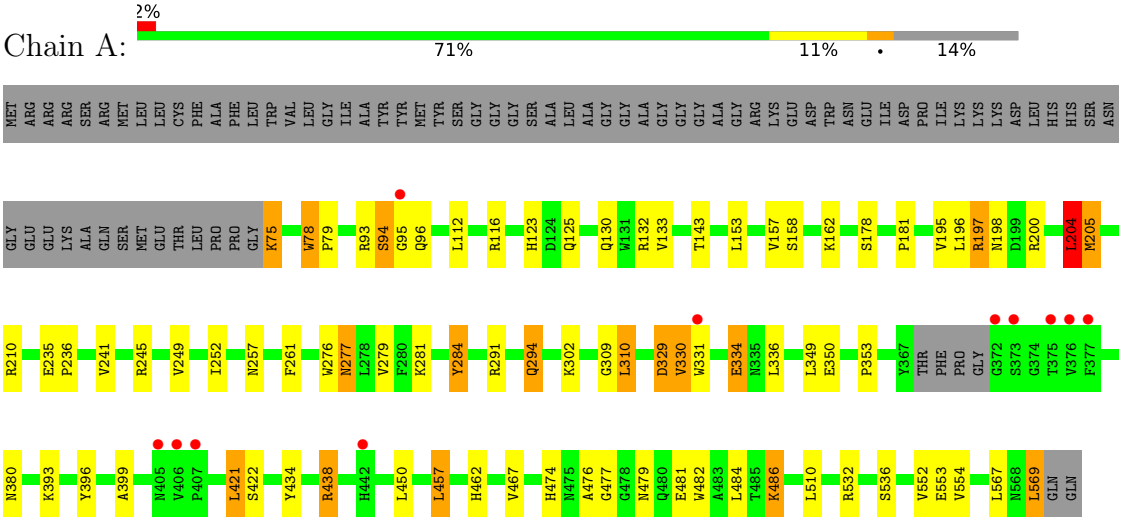
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
6	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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.

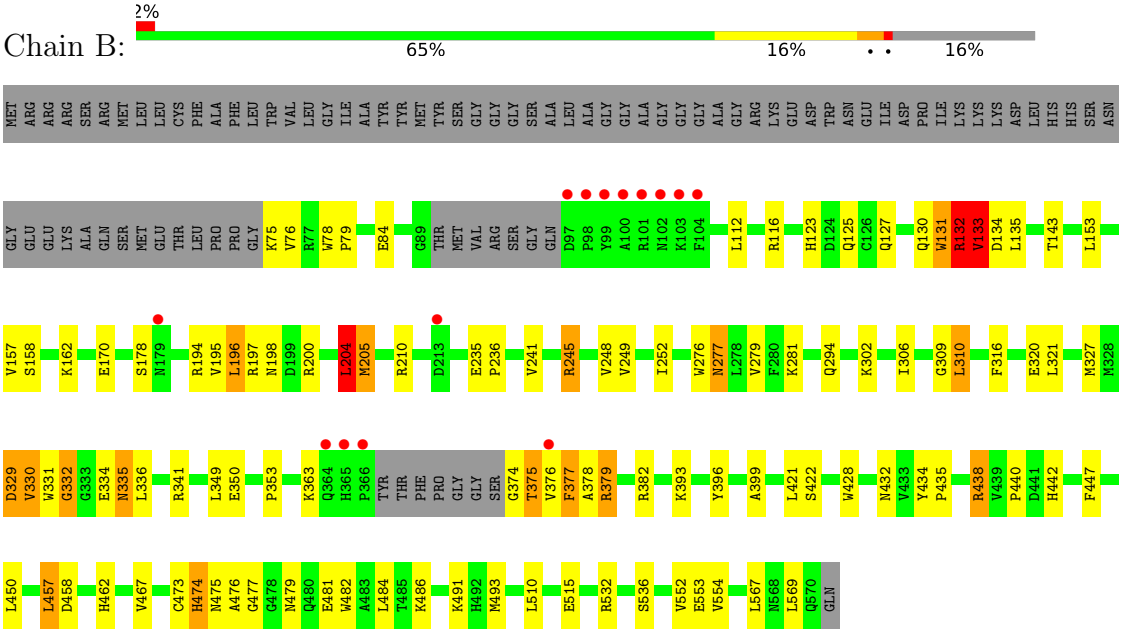
• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2

Chain A:

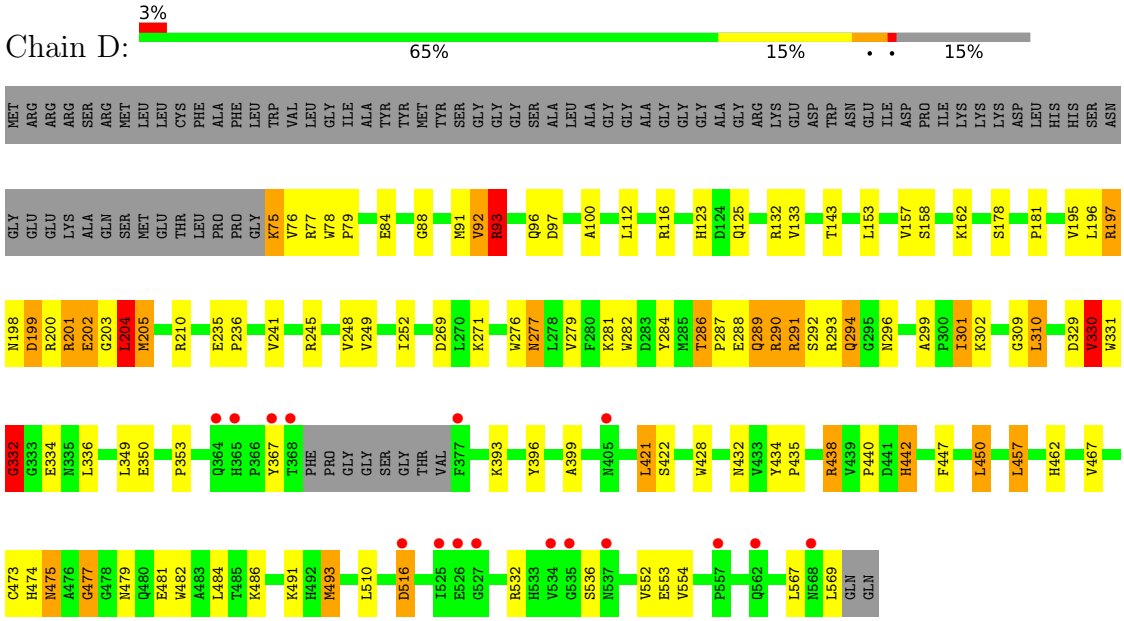


• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2

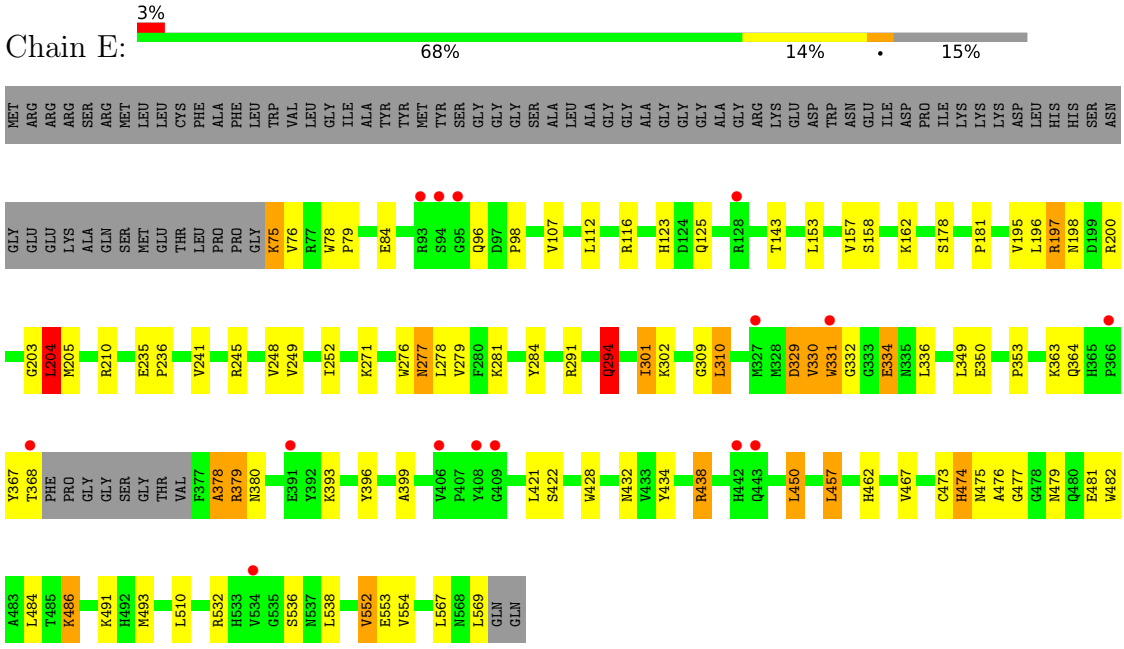
Chain B:



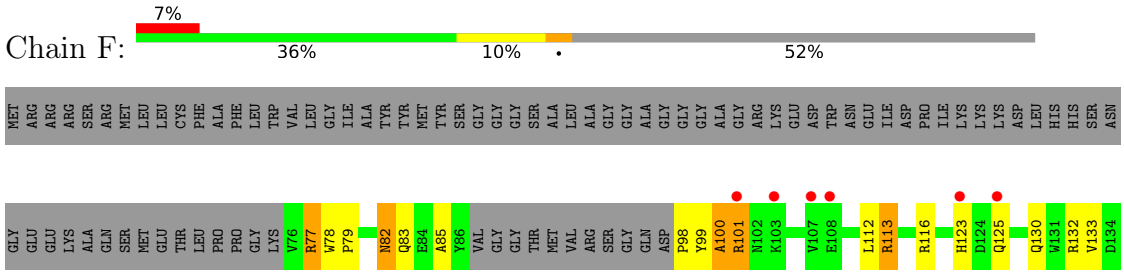
• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2

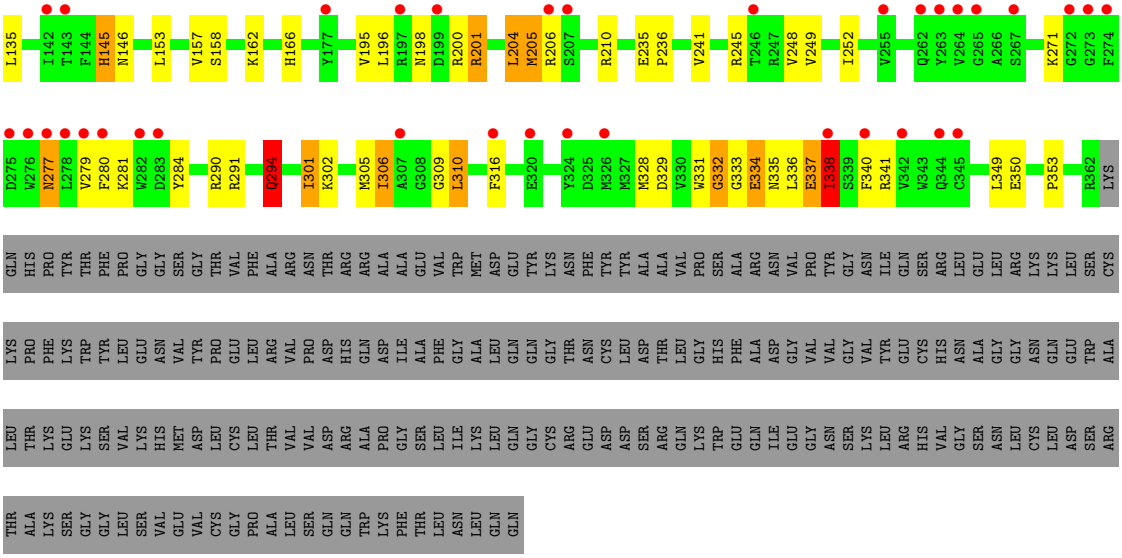


• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2

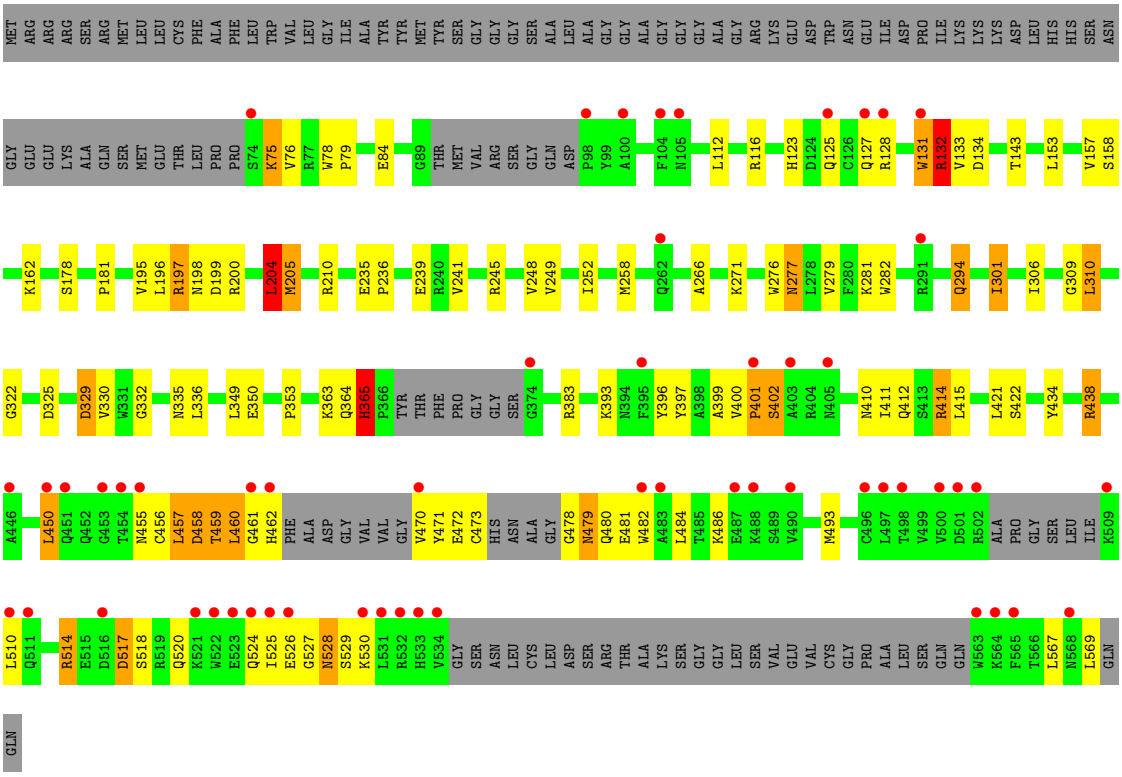


• Molecule 1: POLYPEPTIDE GALNAC-TRANSFERASE T2





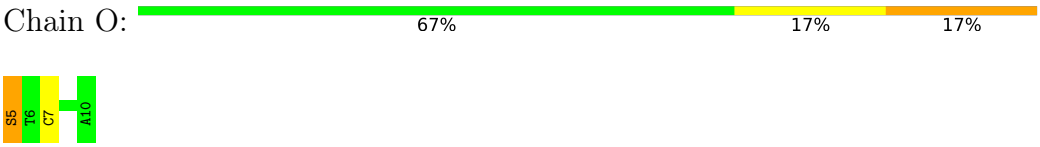
• Molecule 2: POLYPEPTIDE GALNAC-TRANSFERASE T2



• Molecule 3: PEPTIDE

• Molecule 3: PEPTIDE

Chain O:

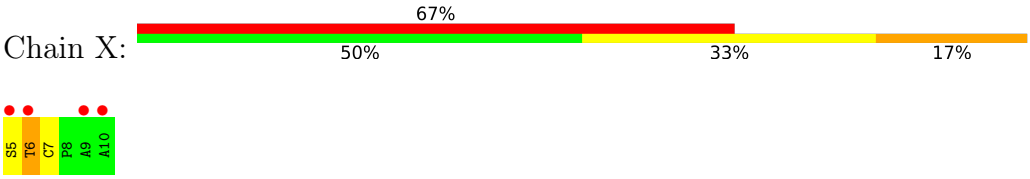


• Molecule 3: PEPTIDE

Chain P:

• Molecule 3: PEPTIDE

Chain X:



• Molecule 3: PEPTIDE

Chain Z:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.77Å 120.90Å 249.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	249.61 – 2.85 46.14 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (249.61-2.85) 100.0 (46.14-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.216 , 0.235 0.219 , 0.236	Depositor DCC
R_{free} test set	2285 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å^2)	64.9	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21829	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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, BBK, 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	0.95	4/4027 (0.1%)	1.03	4/5443 (0.1%)
1	B	1.19	5/3967 (0.1%)	1.05	6/5361 (0.1%)
1	D	1.18	4/4005 (0.1%)	1.05	8/5413 (0.1%)
1	E	1.12	3/4006 (0.1%)	1.05	7/5415 (0.1%)
1	F	0.84	1/2297 (0.0%)	1.03	2/3104 (0.1%)
2	C	0.90	2/3639 (0.1%)	1.03	3/4909 (0.1%)
3	L	0.64	0/32	0.65	0/44
3	O	0.87	0/32	1.25	0/44
3	P	0.94	0/32	1.33	0/44
3	X	0.68	0/32	0.89	0/44
3	Z	0.90	0/31	0.93	0/42
All	All	1.05	19/22100 (0.1%)	1.04	30/29863 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	C	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	LYS	CB-CG	-34.06	0.60	1.52
1	D	202	GLU	C-N	-33.06	0.73	1.33
1	B	84	GLU	CB-CG	-32.47	0.90	1.52
1	E	84	GLU	CB-CG	-30.61	0.94	1.52
1	D	486	LYS	CB-CG	-25.67	0.83	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	75	LYS	CB-CG	-25.50	0.83	1.52
2	C	75	LYS	CB-CG	-25.45	0.83	1.52
1	D	75	LYS	CB-CG	-23.67	0.88	1.52
1	E	486	LYS	CB-CG	-21.82	0.93	1.52
1	A	294	GLN	CB-CG	-19.74	0.99	1.52
1	D	84	GLU	CB-CG	-19.63	1.14	1.52
1	B	486	LYS	CB-CG	-19.11	1.00	1.52
1	B	294	GLN	CB-CG	-14.55	1.13	1.52
1	F	294	GLN	CB-CG	-14.29	1.14	1.52
1	A	75	LYS	CB-CG	-12.67	1.18	1.52
1	B	515	GLU	CB-CG	9.37	1.70	1.52
1	A	486	LYS	CB-CG	-7.99	1.30	1.52
1	A	78	TRP	CB-CG	-6.17	1.39	1.50
2	C	84	GLU	CB-CG	-5.95	1.40	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	75	LYS	CB-CG-CD	18.38	159.39	111.60
1	B	84	GLU	CA-CB-CG	13.47	143.04	113.40
1	A	294	GLN	CA-CB-CG	11.16	137.95	113.40
1	B	75	LYS	CA-CB-CG	11.01	137.63	113.40
2	C	75	LYS	CB-CG-CD	10.64	139.28	111.60
1	F	294	GLN	CA-CB-CG	10.56	136.64	113.40
1	E	75	LYS	CA-CB-CG	9.63	134.59	113.40
1	B	294	GLN	CA-CB-CG	8.86	132.90	113.40
1	A	486	LYS	CB-CG-CD	-7.42	92.30	111.60
1	B	84	GLU	CB-CG-CD	7.17	133.57	114.20
1	B	473	CYS	CA-CB-SG	6.85	126.33	114.00
1	A	75	LYS	CA-CB-CG	6.65	128.04	113.40
2	C	294	GLN	CA-CB-CG	-6.62	98.85	113.40
1	E	84	GLU	CA-CB-CG	6.49	127.68	113.40
1	E	75	LYS	CB-CG-CD	6.33	128.06	111.60
1	E	473	CYS	CA-CB-SG	6.21	125.17	114.00
1	D	75	LYS	CA-CB-CG	-6.07	100.05	113.40
1	D	516	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	D	493	MET	CG-SD-CE	5.51	109.02	100.20
1	D	286	THR	C-N-CD	5.42	139.77	128.40
1	E	204	LEU	CA-CB-CG	5.42	127.76	115.30
1	E	294	GLN	CA-CB-CG	5.41	125.30	113.40
1	D	77	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	D	204	LEU	CA-CB-CG	5.33	127.55	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	204	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	204	LEU	CA-CB-CG	5.29	127.46	115.30
1	B	204	LEU	CA-CB-CG	5.23	127.33	115.30
1	E	486	LYS	CA-CB-CG	5.23	124.90	113.40
1	F	204	LEU	CA-CB-CG	5.14	127.12	115.30
1	D	473	CYS	CA-CB-SG	5.04	123.08	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	127	GLN	Peptide
1	D	332	GLY	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	3938	0	3863	41	0
1	B	3877	0	3804	99	0
1	D	3916	0	3842	83	0
1	E	3917	0	3843	76	0
1	F	2246	0	2214	88	0
2	C	3560	0	3495	106	0
3	L	32	0	28	3	0
3	O	32	0	28	1	0
3	P	32	0	28	0	0
3	X	32	0	28	7	0
3	Z	31	0	28	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	15	0	14	4	0
5	B	15	0	15	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	15	0	15	1	0
5	E	15	0	15	1	0
6	A	25	0	11	0	0
6	B	25	0	11	0	0
6	C	25	0	11	0	0
6	D	25	0	11	0	0
6	E	25	0	11	1	0
6	F	25	0	11	0	0
All	All	21829	0	21326	492	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (492) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:328:MET:SD	1:F:334:GLU:CB	2.07	1.42
1:D:202:GLU:C	1:D:203:GLY:CA	1.92	1.36
1:D:202:GLU:CA	1:D:203:GLY:N	1.92	1.30
1:F:328:MET:SD	1:F:334:GLU:HB2	1.68	1.29
1:B:329:ASP:HB2	1:B:379:ARG:NH2	1.47	1.28
1:D:202:GLU:O	1:D:203:GLY:N	1.73	1.19
2:C:258:MET:HE3	2:C:363:LYS:HE3	1.22	1.16
1:F:328:MET:SD	1:F:334:GLU:HB3	1.79	1.14
1:B:332:GLY:HA2	1:B:334:GLU:OE1	1.48	1.11
2:C:258:MET:CE	2:C:363:LYS:CE	2.35	1.03
1:B:330:VAL:HG23	1:B:331:TRP:N	1.76	1.01
2:C:457:LEU:HD12	2:C:458:ASP:N	1.76	1.00
2:C:258:MET:CE	2:C:363:LYS:HE2	1.91	1.00
1:F:145:HIS:HE1	1:F:146:ASN:ND2	1.61	0.99
2:C:258:MET:HE3	2:C:363:LYS:CE	1.92	0.98
1:E:205:MET:SD	1:E:330:VAL:HG22	2.05	0.96
2:C:525:ILE:CG1	2:C:530:LYS:HB2	1.94	0.96
1:F:145:HIS:HE1	1:F:146:ASN:HD22	1.13	0.96
1:F:331:TRP:HD1	1:F:332:GLY:H	1.10	0.95
2:C:258:MET:HE1	2:C:363:LYS:HE2	1.46	0.95
2:C:514:ARG:HG3	2:C:514:ARG:HH11	1.31	0.94
1:B:329:ASP:CB	1:B:379:ARG:HH21	1.81	0.93
1:B:329:ASP:CB	1:B:379:ARG:NH2	2.31	0.93
1:F:145:HIS:CE1	1:F:146:ASN:ND2	2.35	0.93
1:B:329:ASP:HB2	1:B:379:ARG:HH21	1.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:PRO:HG2	1:F:99:TYR:HA	1.51	0.92
2:C:258:MET:CE	2:C:363:LYS:HE3	1.97	0.92
1:D:329:ASP:O	1:D:330:VAL:HG23	1.70	0.90
1:B:132:ARG:HG2	1:B:134:ASP:OD1	1.71	0.90
2:C:459:THR:HG23	2:C:460:LEU:HB3	1.54	0.89
1:D:202:GLU:O	1:D:203:GLY:CA	2.13	0.88
2:C:525:ILE:HD11	2:C:530:LYS:HB2	1.54	0.88
1:B:330:VAL:HG23	1:B:331:TRP:H	1.33	0.86
1:F:133:VAL:CG1	1:F:166:HIS:CE1	2.57	0.86
2:C:517:ASP:OD1	2:C:518:SER:N	2.08	0.86
2:C:525:ILE:CD1	2:C:530:LYS:HB2	2.05	0.86
2:C:131:TRP:HB3	2:C:239:GLU:OE1	1.76	0.85
1:B:379:ARG:HG3	1:B:379:ARG:HH11	1.42	0.85
1:E:277:ASN:CG	1:E:279:VAL:HG12	1.97	0.85
2:C:411:ILE:HD12	2:C:415:LEU:HD12	1.56	0.85
1:B:330:VAL:HG21	1:B:331:TRP:CE3	2.12	0.85
2:C:411:ILE:HD12	2:C:415:LEU:CD1	2.07	0.85
1:B:329:ASP:O	1:B:376:VAL:HG11	1.78	0.83
1:D:286:THR:OG1	1:D:289:GLN:HB2	1.78	0.83
1:F:82:ASN:ND2	1:F:85:ALA:H	1.76	0.82
1:B:330:VAL:CG2	1:B:331:TRP:H	1.91	0.82
2:C:411:ILE:CD1	2:C:415:LEU:CD1	2.56	0.82
1:F:98:PRO:CG	1:F:99:TYR:HA	2.09	0.82
1:B:329:ASP:HB2	1:B:379:ARG:HH22	1.40	0.81
2:C:459:THR:HA	2:C:460:LEU:HB2	1.60	0.81
2:C:410:ASN:OD1	2:C:411:ILE:N	2.13	0.81
1:E:204:LEU:N	1:E:330:VAL:HG21	1.96	0.81
1:E:204:LEU:H	1:E:330:VAL:HG21	1.44	0.81
2:C:478:GLY:O	2:C:479:ASN:HB2	1.80	0.80
1:F:98:PRO:HB2	1:F:100:ALA:N	1.96	0.80
1:B:331:TRP:CE3	1:B:376:VAL:HG21	2.17	0.79
1:E:205:MET:SD	1:E:330:VAL:CG2	2.70	0.79
2:C:525:ILE:HD11	2:C:530:LYS:HE3	1.64	0.79
1:F:133:VAL:CG1	1:F:166:HIS:HE1	1.93	0.79
1:B:331:TRP:CE3	1:B:376:VAL:CG2	2.65	0.79
1:F:334:GLU:O	1:F:337:GLU:N	2.16	0.78
1:B:331:TRP:HE3	1:B:376:VAL:CG2	1.97	0.78
1:D:202:GLU:C	1:D:203:GLY:N	0.73	0.78
2:C:401:PRO:HD2	2:C:402:SER:H	1.49	0.78
2:C:459:THR:CA	2:C:460:LEU:HB2	2.14	0.78
1:D:200:ARG:O	1:D:202:GLU:HG2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:258:MET:HE1	2:C:363:LYS:CE	2.08	0.77
3:X:5:SER:O	3:X:6:THR:O	2.03	0.76
2:C:525:ILE:HD11	2:C:530:LYS:CB	2.15	0.76
1:A:479:ASN:HB2	5:A:1571:BBK:H4	1.68	0.76
1:B:245:ARG:HH12	1:B:316:PHE:HD2	1.29	0.76
3:X:6:THR:HG22	3:X:7:CYS:N	2.01	0.75
1:B:245:ARG:NH1	1:B:316:PHE:HD2	1.84	0.75
1:E:329:ASP:CG	1:E:379:ARG:NE	2.40	0.75
2:C:411:ILE:CD1	2:C:415:LEU:HD12	2.17	0.75
1:D:252:ILE:HD12	1:D:353:PRO:HA	1.68	0.74
3:X:6:THR:HG22	3:X:7:CYS:H	1.53	0.73
1:E:277:ASN:OD1	1:E:279:VAL:CG1	2.36	0.73
1:E:329:ASP:OD2	1:E:379:ARG:NE	2.22	0.73
1:B:331:TRP:HE3	1:B:376:VAL:CB	2.01	0.73
1:B:332:GLY:CA	1:B:334:GLU:OE1	2.33	0.72
2:C:411:ILE:HD11	2:C:415:LEU:HD11	1.69	0.72
1:E:329:ASP:OD2	1:E:379:ARG:NH2	2.22	0.72
1:F:334:GLU:OE1	1:F:335:ASN:N	2.22	0.72
2:C:252:ILE:HD12	2:C:353:PRO:HA	1.70	0.72
2:C:514:ARG:HG3	2:C:514:ARG:NH1	2.05	0.71
1:F:145:HIS:ND1	1:F:145:HIS:C	2.44	0.71
1:D:198:ASN:HD22	1:D:210:ARG:HH11	1.36	0.71
1:F:98:PRO:HG2	1:F:100:ALA:H	1.55	0.71
2:C:131:TRP:HD1	2:C:132:ARG:O	1.72	0.71
2:C:411:ILE:CD1	2:C:415:LEU:HD11	2.20	0.70
1:F:145:HIS:HD2	1:F:201:ARG:NE	1.89	0.70
2:C:459:THR:HG23	2:C:460:LEU:CB	2.21	0.70
1:F:133:VAL:HG13	1:F:166:HIS:CE1	2.23	0.70
1:E:329:ASP:OD1	1:E:379:ARG:CD	2.39	0.70
1:F:331:TRP:CD1	1:F:332:GLY:N	2.56	0.70
1:D:198:ASN:ND2	1:D:210:ARG:HH11	1.88	0.70
1:E:329:ASP:OD1	1:E:379:ARG:HD3	1.92	0.70
1:F:252:ILE:HD12	1:F:353:PRO:HA	1.74	0.69
1:D:329:ASP:C	1:D:330:VAL:CG2	2.61	0.69
1:E:277:ASN:ND2	1:E:279:VAL:HG12	2.06	0.69
2:C:325:ASP:HB2	2:C:414:ARG:NH1	2.07	0.69
1:B:334:GLU:HG2	1:B:335:ASN:H	1.56	0.69
1:F:145:HIS:CD2	1:F:201:ARG:CZ	2.76	0.69
1:E:123:HIS:HD2	1:E:125:GLN:H	1.40	0.69
1:F:98:PRO:HD2	1:F:99:TYR:CD1	2.28	0.69
1:E:329:ASP:OD1	1:E:379:ARG:NE	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:123:HIS:HD2	2:C:125:GLN:H	1.42	0.68
1:F:328:MET:SD	1:F:334:GLU:CG	2.81	0.68
1:B:131:TRP:O	1:B:132:ARG:O	2.11	0.68
1:B:330:VAL:CG2	1:B:331:TRP:CE3	2.76	0.68
1:D:479:ASN:HB2	5:D:1572:BBK:H4	1.76	0.68
1:B:331:TRP:HE3	1:B:376:VAL:HB	1.57	0.68
1:D:202:GLU:O	1:D:203:GLY:HA3	1.92	0.68
1:A:252:ILE:HD12	1:A:353:PRO:HA	1.75	0.68
1:E:329:ASP:OD2	1:E:379:ARG:CZ	2.42	0.68
1:E:252:ILE:HD12	1:E:353:PRO:HA	1.74	0.67
1:B:252:ILE:HD12	1:B:353:PRO:HA	1.76	0.67
1:F:337:GLU:OE2	1:F:341:ARG:NH2	2.27	0.67
2:C:178:SER:O	2:C:197:ARG:NH2	2.28	0.67
2:C:459:THR:CB	2:C:460:LEU:HB2	2.25	0.66
2:C:456:CYS:N	2:C:473:CYS:SG	2.69	0.66
2:C:478:GLY:N	2:C:481:GLU:HB2	2.10	0.66
1:F:123:HIS:HD2	1:F:125:GLN:H	1.43	0.66
2:C:461:GLY:O	2:C:462:HIS:CD2	2.49	0.66
1:D:92:VAL:HG12	1:D:93:ARG:N	2.11	0.66
1:D:290:ARG:HH11	1:D:290:ARG:CG	2.09	0.65
1:D:123:HIS:HD2	1:D:125:GLN:H	1.44	0.65
1:E:331:TRP:CH2	3:O:5:SER:HA	2.31	0.65
1:A:123:HIS:HD2	1:A:125:GLN:H	1.42	0.65
1:B:331:TRP:CE3	1:B:376:VAL:HB	2.31	0.65
1:D:329:ASP:C	1:D:330:VAL:HG23	2.16	0.65
1:B:123:HIS:HD2	1:B:125:GLN:H	1.45	0.65
2:C:411:ILE:HD11	2:C:415:LEU:CD1	2.25	0.65
1:F:328:MET:CE	1:F:334:GLU:HB2	2.27	0.65
1:F:145:HIS:CD2	1:F:201:ARG:NE	2.64	0.65
1:A:569:LEU:HD12	1:A:569:LEU:N	2.11	0.64
5:A:1571:BBK:S5	5:B:1572:BBK:H6	2.36	0.64
1:E:205:MET:HE1	1:E:332:GLY:H	1.62	0.64
2:C:525:ILE:HG13	2:C:530:LYS:HB2	1.78	0.64
1:E:178:SER:O	1:E:197:ARG:NH2	2.31	0.64
1:D:202:GLU:N	1:D:203:GLY:N	2.46	0.64
1:F:337:GLU:OE2	1:F:341:ARG:NE	2.31	0.64
1:F:334:GLU:O	1:F:337:GLU:HB3	1.98	0.63
2:C:401:PRO:CD	2:C:402:SER:H	2.10	0.63
1:E:277:ASN:CG	1:E:279:VAL:CG1	2.65	0.63
1:D:475:ASN:C	1:D:477:GLY:H	2.00	0.63
2:C:457:LEU:HD12	2:C:457:LEU:C	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:MET:CE	1:E:332:GLY:H	2.11	0.63
1:E:378:ALA:O	1:E:380:ASN:N	2.32	0.63
1:E:203:GLY:HA3	1:E:330:VAL:HG21	1.80	0.62
2:C:410:ASN:OD1	2:C:412:GLN:N	2.31	0.62
1:F:82:ASN:C	1:F:82:ASN:HD22	2.02	0.62
1:A:329:ASP:N	1:A:329:ASP:OD1	2.31	0.62
1:D:199:ASP:OD1	1:D:199:ASP:N	2.33	0.62
1:D:290:ARG:HH11	1:D:290:ARG:HG3	1.65	0.62
1:F:305:MET:HG2	1:F:306:ILE:N	2.14	0.62
1:F:335:ASN:O	1:F:338:ILE:HG23	2.00	0.62
1:F:336:LEU:O	1:F:336:LEU:HD23	1.99	0.61
1:B:330:VAL:CG2	1:B:331:TRP:N	2.45	0.61
1:B:374:GLY:C	1:B:377:PHE:HB2	2.21	0.61
1:B:379:ARG:HH11	1:B:379:ARG:CG	2.12	0.61
1:F:98:PRO:CD	1:F:99:TYR:HD1	2.13	0.61
1:A:178:SER:O	1:A:197:ARG:NH2	2.34	0.61
1:E:329:ASP:OD1	1:E:329:ASP:N	2.34	0.61
1:D:291:ARG:O	1:D:293:ARG:N	2.28	0.61
1:F:145:HIS:CD2	1:F:201:ARG:NH2	2.69	0.61
1:B:331:TRP:HE3	1:B:376:VAL:HG21	1.58	0.61
2:C:271:LYS:HG2	2:C:301:ILE:HD11	1.83	0.61
1:B:329:ASP:O	1:B:330:VAL:HG22	2.01	0.60
1:E:205:MET:HG3	1:E:334:GLU:HG3	1.83	0.60
1:E:205:MET:HE1	1:E:332:GLY:N	2.15	0.60
1:D:178:SER:O	1:D:197:ARG:NH2	2.35	0.60
1:F:98:PRO:CG	1:F:100:ALA:H	2.14	0.60
1:E:457:LEU:HD13	1:E:482:TRP:CE2	2.36	0.60
1:F:309:GLY:C	1:F:310:LEU:HD23	2.22	0.60
1:E:271:LYS:HG2	1:E:301:ILE:HD11	1.83	0.59
2:C:459:THR:OG1	2:C:460:LEU:HB2	2.01	0.59
1:D:291:ARG:O	1:D:292:SER:HB3	2.01	0.59
1:D:435:PRO:HB2	1:E:291:ARG:HE	1.67	0.59
1:F:331:TRP:HD1	1:F:332:GLY:N	1.92	0.59
1:D:198:ASN:HD22	1:D:210:ARG:NH1	2.01	0.59
1:F:271:LYS:HG2	1:F:301:ILE:HD11	1.85	0.59
1:B:329:ASP:O	1:B:376:VAL:CG1	2.48	0.59
1:E:329:ASP:O	1:E:330:VAL:HB	2.03	0.58
2:C:458:ASP:CG	2:C:459:THR:N	2.57	0.58
2:C:518:SER:C	2:C:520:GLN:H	2.07	0.58
1:D:271:LYS:HG2	1:D:301:ILE:HD11	1.85	0.58
2:C:525:ILE:CD1	2:C:530:LYS:HE3	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:309:GLY:C	2:C:310:LEU:HD23	2.25	0.57
1:D:201:ARG:HH22	1:D:367:TYR:HB2	1.68	0.57
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.40	0.57
1:B:335:ASN:N	1:B:335:ASN:HD22	2.02	0.57
1:E:309:GLY:C	1:E:310:LEU:HD23	2.25	0.57
1:E:399:ALA:HB2	1:E:567:LEU:HD22	1.86	0.57
1:A:330:VAL:HG22	1:A:331:TRP:N	2.19	0.56
1:E:198:ASN:HD22	1:E:210:ARG:HH11	1.52	0.56
1:E:205:MET:CG	1:E:334:GLU:HG3	2.35	0.56
1:E:277:ASN:OD1	1:E:279:VAL:HG11	2.05	0.56
1:A:329:ASP:OD1	1:A:380:ASN:ND2	2.29	0.56
1:B:131:TRP:C	1:B:132:ARG:O	2.42	0.56
1:E:249:VAL:HG12	1:E:350:GLU:HB2	1.88	0.56
1:E:205:MET:HE2	1:E:334:GLU:OE1	2.06	0.56
1:A:474:HIS:CE1	1:A:476:ALA:HB3	2.41	0.56
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.40	0.56
1:B:134:ASP:OD1	1:B:134:ASP:N	2.36	0.55
1:D:289:GLN:O	1:D:293:ARG:HG3	2.07	0.55
1:F:98:PRO:HB2	1:F:99:TYR:C	2.26	0.55
1:D:92:VAL:O	1:D:93:ARG:HB2	2.06	0.55
1:B:331:TRP:CZ3	1:B:376:VAL:CG2	2.89	0.55
2:C:198:ASN:HD22	2:C:210:ARG:HH11	1.55	0.55
1:F:133:VAL:HG12	1:F:166:HIS:CE1	2.38	0.55
1:F:82:ASN:HD21	1:F:85:ALA:H	1.53	0.55
1:E:203:GLY:CA	1:E:330:VAL:HG21	2.37	0.55
1:D:293:ARG:NH1	1:D:299:ALA:O	2.40	0.55
2:C:383:ARG:NH1	2:C:410:ASN:O	2.36	0.54
1:F:98:PRO:N	1:F:99:TYR:HD1	2.05	0.54
1:F:198:ASN:HD22	1:F:210:ARG:HH11	1.55	0.54
1:B:329:ASP:CG	1:B:379:ARG:HH21	2.11	0.54
1:A:198:ASN:HD22	1:A:210:ARG:HH11	1.53	0.54
1:B:198:ASN:HD22	1:B:210:ARG:HH11	1.56	0.54
1:B:399:ALA:HB2	1:B:567:LEU:HD22	1.89	0.54
2:C:325:ASP:CB	2:C:414:ARG:NH1	2.70	0.54
1:F:98:PRO:CD	1:F:99:TYR:CD1	2.90	0.54
1:B:330:VAL:HG22	1:B:376:VAL:HG11	1.89	0.54
1:F:98:PRO:CB	1:F:100:ALA:N	2.68	0.54
1:D:92:VAL:HG12	1:D:93:ARG:H	1.72	0.53
1:F:98:PRO:HG2	1:F:100:ALA:N	2.22	0.53
2:C:329:ASP:N	2:C:329:ASP:OD1	2.41	0.53
1:D:249:VAL:HG12	1:D:350:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLY:C	1:A:310:LEU:HD23	2.28	0.53
1:B:249:VAL:HG12	1:B:350:GLU:HB2	1.90	0.53
1:B:309:GLY:C	1:B:310:LEU:HD23	2.29	0.53
2:C:131:TRP:CD1	2:C:132:ARG:O	2.58	0.53
1:F:249:VAL:HG12	1:F:350:GLU:HB2	1.90	0.53
1:B:316:PHE:CE2	1:B:320:GLU:OE2	2.62	0.53
1:A:249:VAL:HG12	1:A:350:GLU:HB2	1.91	0.52
2:C:131:TRP:C	2:C:132:ARG:O	2.44	0.52
1:D:442:HIS:C	1:D:442:HIS:HD1	2.13	0.52
1:E:277:ASN:ND2	1:E:279:VAL:CG1	2.70	0.52
1:B:458:ASP:OD1	5:B:1572:BBK:O3	2.25	0.52
1:D:457:LEU:HD13	1:D:482:TRP:CE2	2.44	0.52
3:L:6:THR:HG22	3:L:7:CYS:N	2.24	0.52
2:C:249:VAL:HG12	2:C:350:GLU:HB2	1.90	0.52
2:C:524:GLN:OE1	2:C:528:ASN:HB3	2.10	0.52
2:C:158:SER:O	2:C:162:LYS:HB2	2.10	0.52
2:C:282:TRP:NE1	3:L:7:CYS:O	2.38	0.52
1:A:330:VAL:CG2	1:A:331:TRP:N	2.72	0.52
1:E:205:MET:HE1	1:E:330:VAL:HA	1.92	0.52
3:X:6:THR:CG2	3:X:7:CYS:N	2.70	0.52
1:B:170:GLU:OE1	1:B:194:ARG:NH1	2.38	0.51
1:B:327:MET:O	1:B:329:ASP:OD1	2.27	0.51
1:F:98:PRO:CB	1:F:99:TYR:HA	2.40	0.51
1:B:375:THR:C	1:B:377:PHE:N	2.62	0.51
2:C:181:PRO:HB3	2:C:197:ARG:NE	2.25	0.51
1:A:158:SER:O	1:A:162:LYS:HB2	2.11	0.51
2:C:364:GLN:O	2:C:365:HIS:ND1	2.44	0.51
1:D:158:SER:O	1:D:162:LYS:HB2	2.10	0.51
1:E:204:LEU:H	1:E:330:VAL:CG2	2.18	0.51
1:F:98:PRO:CG	1:F:100:ALA:N	2.74	0.51
1:A:399:ALA:HB2	1:A:567:LEU:HD22	1.93	0.51
1:D:329:ASP:O	1:D:330:VAL:CG2	2.50	0.51
1:D:288:GLU:O	1:D:288:GLU:HG3	2.11	0.50
1:B:316:PHE:HE2	1:B:320:GLU:OE2	1.94	0.50
1:B:334:GLU:HG2	1:B:335:ASN:N	2.23	0.50
1:D:309:GLY:C	1:D:310:LEU:HD23	2.32	0.50
2:C:458:ASP:O	2:C:459:THR:HB	2.11	0.50
1:E:158:SER:O	1:E:162:LYS:HB2	2.12	0.50
2:C:459:THR:CG2	2:C:460:LEU:HB3	2.34	0.50
1:D:331:TRP:O	1:D:332:GLY:O	2.30	0.50
1:F:336:LEU:HD21	1:F:340:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:6:THR:C	3:X:7:CYS:SG	2.89	0.50
1:B:331:TRP:CZ3	1:B:376:VAL:HG21	2.47	0.50
1:F:158:SER:O	1:F:162:LYS:HB2	2.12	0.50
2:C:271:LYS:HG2	2:C:301:ILE:CD1	2.42	0.50
2:C:461:GLY:O	2:C:462:HIS:CG	2.64	0.49
1:D:287:PRO:O	1:D:290:ARG:N	2.45	0.49
1:B:158:SER:O	1:B:162:LYS:HB2	2.12	0.49
1:B:194:ARG:NH2	1:D:97:ASP:OD2	2.40	0.49
2:C:401:PRO:CD	2:C:402:SER:N	2.74	0.49
1:B:379:ARG:CG	1:B:379:ARG:NH1	2.73	0.49
1:A:277:ASN:HD21	1:A:279:VAL:HG12	1.77	0.49
1:A:205:MET:HG3	1:A:334:GLU:HG2	1.95	0.49
1:F:334:GLU:OE1	1:F:334:GLU:N	2.46	0.49
1:A:181:PRO:HB3	1:A:197:ARG:NE	2.26	0.49
1:D:93:ARG:HB3	1:D:96:GLN:HG3	1.95	0.49
1:D:435:PRO:HB2	1:E:291:ARG:NE	2.27	0.49
2:C:459:THR:CB	2:C:460:LEU:CB	2.91	0.48
1:F:328:MET:SD	1:F:334:GLU:HG3	2.53	0.48
1:B:329:ASP:O	1:B:331:TRP:N	2.45	0.48
2:C:438:ARG:HG2	2:C:481:GLU:OE2	2.13	0.48
1:D:181:PRO:HB3	1:D:197:ARG:NE	2.28	0.48
1:D:462:HIS:HD2	1:D:467:VAL:O	1.96	0.48
1:E:331:TRP:HZ2	6:E:1572:UDP:O1B	1.95	0.48
1:B:462:HIS:HD2	1:B:467:VAL:O	1.97	0.48
1:D:293:ARG:O	1:D:296:ASN:N	2.47	0.48
1:F:98:PRO:CB	1:F:99:TYR:CA	2.90	0.48
1:F:331:TRP:O	1:F:332:GLY:O	2.32	0.48
1:F:337:GLU:O	1:F:340:PHE:N	2.46	0.48
2:C:414:ARG:HD2	2:C:414:ARG:N	2.28	0.48
1:F:77:ARG:HG2	1:F:79:PRO:HD2	1.96	0.48
1:E:78:TRP:CG	1:E:79:PRO:HD3	2.49	0.48
1:E:277:ASN:OD1	1:E:279:VAL:HG12	2.08	0.48
1:F:98:PRO:HG2	1:F:99:TYR:CA	2.34	0.48
1:D:438:ARG:HG2	1:D:481:GLU:OE2	2.14	0.48
1:B:479:ASN:HB2	5:B:1572:BBK:H4	1.95	0.48
1:E:479:ASN:HB2	5:E:1571:BBK:H4	1.95	0.48
1:D:532:ARG:HD3	1:D:536:SER:O	2.13	0.48
2:C:459:THR:CG2	2:C:460:LEU:CB	2.92	0.47
2:C:493:MET:SD	1:F:290:ARG:NH1	2.87	0.47
1:D:276:TRP:O	1:D:396:TYR:HA	2.14	0.47
1:A:329:ASP:O	1:A:331:TRP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:MET:H	1:B:205:MET:HE2	1.80	0.47
2:C:364:GLN:O	2:C:365:HIS:CB	2.62	0.47
2:C:457:LEU:HD12	2:C:458:ASP:H	1.70	0.47
2:C:525:ILE:HG12	2:C:530:LYS:HB2	1.86	0.47
1:D:284:TYR:CE1	1:E:493:MET:HG3	2.48	0.47
1:A:438:ARG:HG2	1:A:481:GLU:OE2	2.15	0.47
2:C:266:ALA:HB1	3:L:9:ALA:O	2.15	0.47
3:X:6:THR:O	3:X:7:CYS:SG	2.70	0.47
1:A:78:TRP:CG	1:A:79:PRO:HD3	2.50	0.47
1:B:178:SER:O	1:B:197:ARG:NH2	2.47	0.47
2:C:518:SER:C	2:C:520:GLN:N	2.68	0.47
1:D:277:ASN:HD21	1:D:279:VAL:HG12	1.78	0.47
1:D:291:ARG:C	1:D:293:ARG:H	2.15	0.47
1:F:133:VAL:HG13	1:F:166:HIS:HE1	1.66	0.47
1:A:393:LYS:O	1:A:396:TYR:HB3	2.15	0.47
1:E:271:LYS:HG2	1:E:301:ILE:CD1	2.44	0.47
1:F:277:ASN:HD21	1:F:279:VAL:HG12	1.80	0.47
1:A:198:ASN:ND2	1:A:210:ARG:HH11	2.13	0.47
1:F:337:GLU:OE2	1:F:341:ARG:CZ	2.63	0.47
1:B:474:HIS:NE2	5:B:1572:BBK:H6A	2.30	0.46
2:C:277:ASN:HD21	2:C:279:VAL:HG12	1.80	0.46
1:D:271:LYS:HG2	1:D:301:ILE:CD1	2.44	0.46
1:E:98:PRO:HB3	1:E:107:VAL:HG23	1.98	0.46
1:E:532:ARG:HD3	1:E:536:SER:O	2.14	0.46
2:C:460:LEU:HD22	2:C:471:TYR:HE2	1.80	0.46
1:B:532:ARG:HD3	1:B:536:SER:O	2.15	0.46
1:D:399:ALA:HB2	1:D:567:LEU:HD22	1.98	0.46
1:E:181:PRO:HB3	1:E:197:ARG:NE	2.30	0.46
1:F:271:LYS:HG2	1:F:301:ILE:CD1	2.45	0.46
1:D:393:LYS:O	1:D:396:TYR:HB3	2.16	0.46
1:E:367:TYR:HD1	1:E:368:THR:HG23	1.81	0.46
1:E:428:TRP:CD1	1:E:432:ASN:ND2	2.84	0.46
1:F:83:GLN:HE22	1:F:113:ARG:HG3	1.80	0.46
1:F:145:HIS:CE1	1:F:146:ASN:HD22	2.04	0.46
2:C:133:VAL:CG1	2:C:134:ASP:N	2.78	0.46
2:C:276:TRP:O	2:C:396:TYR:HA	2.16	0.46
2:C:514:ARG:NH1	2:C:514:ARG:CG	2.76	0.46
1:A:532:ARG:HD3	1:A:536:SER:O	2.15	0.46
2:C:457:LEU:HD11	2:C:482:TRP:CZ2	2.51	0.46
1:B:277:ASN:HD21	1:B:279:VAL:HG12	1.81	0.46
2:C:364:GLN:O	2:C:365:HIS:CG	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:GLY:HA2	1:D:91:MET:HG3	1.97	0.46
1:B:329:ASP:C	1:B:330:VAL:HG22	2.35	0.45
1:E:393:LYS:O	1:E:396:TYR:HB3	2.16	0.45
1:B:330:VAL:HG23	1:B:331:TRP:CB	2.46	0.45
1:A:462:HIS:HD2	1:A:467:VAL:O	1.99	0.45
1:D:235:GLU:HB2	1:D:236:PRO:HD3	1.98	0.45
1:A:277:ASN:ND2	1:A:279:VAL:HG12	2.32	0.45
1:D:277:ASN:ND2	1:D:279:VAL:HG12	2.32	0.45
1:F:305:MET:HG2	1:F:306:ILE:H	1.81	0.45
1:B:235:GLU:HB2	1:B:236:PRO:HD3	1.99	0.45
1:B:379:ARG:HG3	1:B:379:ARG:NH1	2.20	0.45
2:C:399:ALA:HB2	2:C:567:LEU:HD22	1.98	0.45
2:C:527:GLY:C	2:C:529:SER:N	2.69	0.45
1:F:332:GLY:HA2	1:F:333:GLY:HA2	1.60	0.45
2:C:78:TRP:CG	2:C:79:PRO:HD3	2.52	0.45
1:D:205:MET:HE2	1:D:205:MET:H	1.82	0.45
1:F:78:TRP:CG	1:F:79:PRO:HD3	2.52	0.45
1:F:235:GLU:HB2	1:F:236:PRO:HD3	1.98	0.45
2:C:397:TYR:O	2:C:400:VAL:O	2.35	0.45
1:E:203:GLY:C	1:E:330:VAL:HG21	2.37	0.45
1:E:205:MET:SD	1:E:330:VAL:HG23	2.55	0.45
1:E:277:ASN:N	1:E:277:ASN:HD22	2.15	0.45
1:F:291:ARG:O	1:F:294:GLN:HB2	2.16	0.45
1:B:78:TRP:CG	1:B:79:PRO:HD3	2.52	0.44
1:B:331:TRP:CZ3	1:B:376:VAL:HG23	2.52	0.44
1:D:143:THR:HG21	1:D:204:LEU:HD23	1.99	0.44
1:B:276:TRP:O	1:B:396:TYR:HA	2.16	0.44
2:C:393:LYS:O	2:C:396:TYR:HB3	2.17	0.44
1:D:290:ARG:C	1:D:291:ARG:O	2.53	0.44
1:E:329:ASP:CG	1:E:379:ARG:HE	2.16	0.44
1:E:438:ARG:HG2	1:E:481:GLU:OE2	2.17	0.44
1:E:474:HIS:O	1:E:476:ALA:N	2.51	0.44
1:B:143:THR:HG21	1:B:204:LEU:HD23	1.99	0.44
1:B:363:LYS:HD2	1:B:363:LYS:HA	1.61	0.44
1:E:291:ARG:O	1:E:294:GLN:HB2	2.17	0.44
1:B:133:VAL:C	1:B:135:LEU:H	2.21	0.44
1:B:375:THR:O	1:B:376:VAL:C	2.55	0.44
1:B:438:ARG:HG2	1:B:481:GLU:OE2	2.18	0.44
1:B:474:HIS:C	1:B:476:ALA:H	2.21	0.44
1:A:276:TRP:O	1:A:396:TYR:HA	2.18	0.44
1:B:329:ASP:CG	1:B:379:ARG:NH2	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:HIS:O	1:B:476:ALA:N	2.50	0.44
1:D:450:LEU:HD23	1:D:450:LEU:HA	1.93	0.44
1:F:100:ALA:HB1	1:F:101:ARG:HE	1.83	0.44
1:A:479:ASN:HD22	5:A:1571:BBK:H3	1.83	0.43
2:C:457:LEU:C	2:C:457:LEU:CD1	2.82	0.43
1:A:291:ARG:NH1	1:B:435:PRO:HB2	2.33	0.43
1:A:235:GLU:HB2	1:A:236:PRO:HD3	2.01	0.43
1:D:282:TRP:NE1	3:X:7:CYS:O	2.41	0.43
1:D:421:LEU:HD12	1:D:421:LEU:HA	1.93	0.43
1:F:153:LEU:O	1:F:157:VAL:HG13	2.18	0.43
2:C:205:MET:HB2	2:C:205:MET:HE2	1.84	0.43
1:F:133:VAL:HG12	1:F:166:HIS:NE2	2.33	0.43
1:B:379:ARG:O	1:B:382:ARG:HB2	2.18	0.43
1:D:442:HIS:C	1:D:442:HIS:ND1	2.72	0.43
1:D:78:TRP:CG	1:D:79:PRO:HD3	2.54	0.43
1:B:491:LYS:HD3	1:B:493:MET:O	2.19	0.43
1:D:153:LEU:O	1:D:157:VAL:HG13	2.18	0.43
1:A:474:HIS:ND1	1:A:476:ALA:HB3	2.34	0.43
1:E:462:HIS:HD2	1:E:467:VAL:O	2.02	0.43
1:B:334:GLU:CG	1:B:335:ASN:H	2.26	0.43
1:B:393:LYS:O	1:B:396:TYR:HB3	2.19	0.42
2:C:277:ASN:ND2	2:C:279:VAL:HG12	2.34	0.42
1:D:248:VAL:HB	1:D:349:LEU:HD12	2.01	0.42
1:E:143:THR:HG21	1:E:204:LEU:HD23	2.01	0.42
2:C:131:TRP:CB	2:C:239:GLU:OE1	2.57	0.42
2:C:143:THR:HG21	2:C:204:LEU:HD23	2.00	0.42
2:C:198:ASN:ND2	2:C:210:ARG:HH11	2.15	0.42
1:D:92:VAL:O	1:D:93:ARG:CB	2.67	0.42
1:E:276:TRP:O	1:E:396:TYR:HA	2.19	0.42
2:C:414:ARG:CG	2:C:414:ARG:HH11	2.32	0.42
1:E:198:ASN:ND2	1:E:210:ARG:HH11	2.14	0.42
1:E:276:TRP:C	1:E:278:LEU:H	2.23	0.42
1:A:284:TYR:CZ	1:B:493:MET:HG3	2.54	0.42
2:C:153:LEU:O	2:C:157:VAL:HG13	2.18	0.42
2:C:235:GLU:HB2	2:C:236:PRO:HD3	2.00	0.42
1:E:205:MET:CE	1:E:334:GLU:OE1	2.68	0.42
1:A:153:LEU:O	1:A:157:VAL:HG13	2.19	0.42
2:C:322:GLY:O	2:C:414:ARG:NH2	2.52	0.42
1:D:331:TRP:C	1:D:332:GLY:O	2.56	0.42
1:E:235:GLU:HB2	1:E:236:PRO:HD3	2.01	0.42
1:F:336:LEU:CD2	1:F:340:PHE:CZ	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASN:O	1:A:261:PHE:HA	2.20	0.42
1:B:248:VAL:HB	1:B:349:LEU:HD12	2.02	0.42
1:D:290:ARG:CG	1:D:290:ARG:NH1	2.73	0.42
1:E:491:LYS:HD3	1:E:493:MET:O	2.19	0.42
1:F:336:LEU:HD22	1:F:340:PHE:CE2	2.55	0.42
1:B:196:LEU:HD11	1:D:100:ALA:HB2	2.01	0.42
2:C:450:LEU:HD23	2:C:450:LEU:HA	1.96	0.42
2:C:455:ASN:C	2:C:473:CYS:SG	2.99	0.42
1:E:153:LEU:O	1:E:157:VAL:HG13	2.20	0.42
1:E:248:VAL:HB	1:E:349:LEU:HD12	2.02	0.42
1:A:143:THR:HG21	1:A:204:LEU:HD23	2.01	0.42
1:D:440:PRO:HG3	1:D:447:PHE:CD2	2.54	0.42
1:B:330:VAL:CG2	1:B:376:VAL:HG11	2.50	0.41
1:D:200:ARG:O	1:D:201:ARG:C	2.58	0.41
1:D:428:TRP:CD1	1:D:432:ASN:ND2	2.87	0.41
1:E:329:ASP:O	1:E:330:VAL:CB	2.68	0.41
2:C:325:ASP:CA	2:C:414:ARG:NH1	2.83	0.41
2:C:461:GLY:C	2:C:462:HIS:CD2	2.93	0.41
1:B:277:ASN:N	1:B:277:ASN:HD22	2.17	0.41
1:B:377:PHE:HD1	1:B:377:PHE:HA	1.70	0.41
1:F:334:GLU:C	1:F:336:LEU:N	2.73	0.41
1:B:198:ASN:ND2	1:B:210:ARG:HH11	2.17	0.41
1:E:538:LEU:HB3	1:E:552:VAL:HG22	2.03	0.41
1:F:145:HIS:ND1	1:F:146:ASN:N	2.69	0.41
1:F:277:ASN:ND2	1:F:279:VAL:HG12	2.35	0.41
1:F:280:PHE:HD1	1:F:305:MET:SD	2.43	0.41
1:F:333:GLY:C	1:F:335:ASN:N	2.73	0.41
1:B:440:PRO:HG3	1:B:447:PHE:CD2	2.55	0.41
1:B:153:LEU:O	1:B:157:VAL:HG13	2.20	0.41
2:C:248:VAL:HB	2:C:349:LEU:HD12	2.02	0.41
1:D:200:ARG:HE	1:D:200:ARG:HB3	1.70	0.41
1:F:248:VAL:HB	1:F:349:LEU:HD12	2.03	0.41
1:D:252:ILE:CD1	1:D:353:PRO:HA	2.43	0.41
1:D:277:ASN:N	1:D:277:ASN:HD22	2.18	0.41
1:F:277:ASN:N	1:F:277:ASN:HD22	2.19	0.41
1:A:93:ARG:HG3	1:A:94:SER:N	2.35	0.41
1:B:375:THR:O	1:B:378:ALA:N	2.54	0.41
1:D:269:ASP:OD2	1:E:493:MET:HB3	2.21	0.41
1:D:491:LYS:HD3	1:D:493:MET:O	2.21	0.41
1:F:198:ASN:ND2	1:F:210:ARG:HH11	2.16	0.41
1:B:131:TRP:CZ2	1:B:236:PRO:HG3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:LEU:O	1:B:341:ARG:HD2	2.21	0.40
1:B:428:TRP:CD1	1:B:432:ASN:ND2	2.89	0.40
2:C:411:ILE:HD12	2:C:411:ILE:O	2.21	0.40
1:D:200:ARG:O	1:D:202:GLU:CG	2.62	0.40
1:A:479:ASN:ND2	5:A:1571:BBK:H3	2.36	0.40
1:B:479:ASN:HD22	5:B:1572:BBK:H3	1.86	0.40
1:F:205:MET:O	1:F:206:ARG:C	2.60	0.40
1:A:94:SER:HB3	1:A:95:GLY:H	1.50	0.40
2:C:457:LEU:HA	2:C:470:VAL:HG12	2.02	0.40
1:F:133:VAL:CG1	1:F:166:HIS:NE2	2.83	0.40
1:E:450:LEU:HD23	1:E:450:LEU:HA	2.00	0.40
1:F:98:PRO:HB2	1:F:99:TYR:CA	2.51	0.40
1:A:93:ARG:HG3	1:A:94:SER:H	1.86	0.40
1:A:421:LEU:HD12	1:A:421:LEU:HA	1.92	0.40
1:B:277:ASN:ND2	1:B:279:VAL:HG12	2.36	0.40
1:B:442:HIS:CD2	1:B:442:HIS:O	2.74	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	487/571 (85%)	461 (95%)	24 (5%)	2 (0%)	34 62
1	B	477/571 (84%)	445 (93%)	26 (6%)	6 (1%)	12 33
1	D	483/571 (85%)	449 (93%)	28 (6%)	6 (1%)	13 35
1	E	483/571 (85%)	457 (95%)	21 (4%)	5 (1%)	15 40
1	F	272/571 (48%)	252 (93%)	15 (6%)	5 (2%)	8 25
2	C	422/571 (74%)	387 (92%)	27 (6%)	8 (2%)	8 24
3	L	4/6 (67%)	1 (25%)	1 (25%)	2 (50%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	O	4/6 (67%)	2 (50%)	2 (50%)	0	100 100
3	P	4/6 (67%)	3 (75%)	0	1 (25%)	0 0
3	X	4/6 (67%)	1 (25%)	2 (50%)	1 (25%)	0 0
3	Z	3/6 (50%)	3 (100%)	0	0	100 100
All	All	2643/3456 (76%)	2461 (93%)	146 (6%)	36 (1%)	11 31

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	A	477	GLY
1	B	132	ARG
1	B	477	GLY
2	C	365	HIS
2	C	460	LEU
1	D	92	VAL
1	D	93	ARG
1	D	477	GLY
1	E	378	ALA
1	E	477	GLY
1	F	329	ASP
1	F	332	GLY
3	L	7	CYS
3	X	6	THR
1	B	330	VAL
1	B	332	GLY
2	C	132	ARG
1	D	332	GLY
1	E	379	ARG
1	F	100	ALA
2	C	330	VAL
2	C	332	GLY
2	C	479	ASN
1	B	133	VAL
2	C	401	PRO
2	C	517	ASP
1	E	330	VAL
1	F	337	GLU
3	L	6	THR
3	P	9	ALA
1	D	294	GLN

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Mol	Chain	Res	Type
1	D	330	VAL
1	E	475	ASN
1	B	475	ASN
1	F	338	ILE

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	425/485 (88%)	386 (91%)	39 (9%)	9 24
1	B	418/485 (86%)	379 (91%)	39 (9%)	9 24
1	D	423/485 (87%)	379 (90%)	44 (10%)	7 19
1	E	423/485 (87%)	384 (91%)	39 (9%)	9 24
1	F	244/485 (50%)	215 (88%)	29 (12%)	5 13
2	C	385/486 (79%)	340 (88%)	45 (12%)	5 14
3	L	4/4 (100%)	4 (100%)	0	100 100
3	O	4/4 (100%)	2 (50%)	2 (50%)	0 0
3	P	4/4 (100%)	3 (75%)	1 (25%)	0 1
3	X	4/4 (100%)	4 (100%)	0	100 100
3	Z	4/4 (100%)	3 (75%)	1 (25%)	0 1
All	All	2338/2931 (80%)	2099 (90%)	239 (10%)	7 20

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	94	SER
1	A	96	GLN
1	A	112	LEU
1	A	116	ARG
1	A	130	GLN
1	A	132	ARG

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Mol	Chain	Res	Type
1	A	133	VAL
1	A	195	VAL
1	A	196	LEU
1	A	197	ARG
1	A	200	ARG
1	A	204	LEU
1	A	205	MET
1	A	241	VAL
1	A	245	ARG
1	A	277	ASN
1	A	281	LYS
1	A	284	TYR
1	A	294	GLN
1	A	302	LYS
1	A	310	LEU
1	A	329	ASP
1	A	334	GLU
1	A	336	LEU
1	A	349	LEU
1	A	421	LEU
1	A	422	SER
1	A	434	TYR
1	A	438	ARG
1	A	450	LEU
1	A	457	LEU
1	A	484	LEU
1	A	486	LYS
1	A	510	LEU
1	A	552	VAL
1	A	553	GLU
1	A	554	VAL
1	A	569	LEU
1	B	76	VAL
1	B	112	LEU
1	B	116	ARG
1	B	127	GLN
1	B	130	GLN
1	B	131	TRP
1	B	132	ARG
1	B	133	VAL
1	B	195	VAL
1	B	196	LEU

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Mol	Chain	Res	Type
1	B	200	ARG
1	B	204	LEU
1	B	205	MET
1	B	241	VAL
1	B	245	ARG
1	B	277	ASN
1	B	281	LYS
1	B	302	LYS
1	B	306	ILE
1	B	310	LEU
1	B	329	ASP
1	B	335	ASN
1	B	336	LEU
1	B	375	THR
1	B	377	PHE
1	B	379	ARG
1	B	421	LEU
1	B	422	SER
1	B	434	TYR
1	B	438	ARG
1	B	450	LEU
1	B	457	LEU
1	B	474	HIS
1	B	484	LEU
1	B	510	LEU
1	B	552	VAL
1	B	553	GLU
1	B	554	VAL
1	B	569	LEU
2	C	75	LYS
2	C	76	VAL
2	C	112	LEU
2	C	116	ARG
2	C	128	ARG
2	C	131	TRP
2	C	132	ARG
2	C	195	VAL
2	C	196	LEU
2	C	197	ARG
2	C	199	ASP
2	C	200	ARG
2	C	204	LEU

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Mol	Chain	Res	Type
2	C	205	MET
2	C	241	VAL
2	C	245	ARG
2	C	277	ASN
2	C	281	LYS
2	C	294	GLN
2	C	301	ILE
2	C	306	ILE
2	C	310	LEU
2	C	329	ASP
2	C	335	ASN
2	C	336	LEU
2	C	365	HIS
2	C	402	SER
2	C	414	ARG
2	C	421	LEU
2	C	422	SER
2	C	434	TYR
2	C	438	ARG
2	C	450	LEU
2	C	457	LEU
2	C	458	ASP
2	C	459	THR
2	C	472	GLU
2	C	480	GLN
2	C	484	LEU
2	C	486	LYS
2	C	510	LEU
2	C	514	ARG
2	C	526	GLU
2	C	528	ASN
2	C	569	LEU
1	D	75	LYS
1	D	76	VAL
1	D	93	ARG
1	D	112	LEU
1	D	116	ARG
1	D	132	ARG
1	D	133	VAL
1	D	195	VAL
1	D	196	LEU
1	D	197	ARG

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Mol	Chain	Res	Type
1	D	199	ASP
1	D	201	ARG
1	D	204	LEU
1	D	205	MET
1	D	241	VAL
1	D	245	ARG
1	D	277	ASN
1	D	281	LYS
1	D	289	GLN
1	D	290	ARG
1	D	291	ARG
1	D	294	GLN
1	D	301	ILE
1	D	302	LYS
1	D	310	LEU
1	D	330	VAL
1	D	334	GLU
1	D	336	LEU
1	D	421	LEU
1	D	422	SER
1	D	434	TYR
1	D	438	ARG
1	D	442	HIS
1	D	450	LEU
1	D	457	LEU
1	D	474	HIS
1	D	475	ASN
1	D	484	LEU
1	D	510	LEU
1	D	516	ASP
1	D	552	VAL
1	D	553	GLU
1	D	554	VAL
1	D	569	LEU
1	E	75	LYS
1	E	76	VAL
1	E	96	GLN
1	E	112	LEU
1	E	116	ARG
1	E	195	VAL
1	E	196	LEU
1	E	197	ARG

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Mol	Chain	Res	Type
1	E	200	ARG
1	E	204	LEU
1	E	241	VAL
1	E	245	ARG
1	E	277	ASN
1	E	281	LYS
1	E	284	TYR
1	E	294	GLN
1	E	301	ILE
1	E	302	LYS
1	E	310	LEU
1	E	329	ASP
1	E	331	TRP
1	E	334	GLU
1	E	336	LEU
1	E	363	LYS
1	E	364	GLN
1	E	421	LEU
1	E	422	SER
1	E	434	TYR
1	E	438	ARG
1	E	450	LEU
1	E	457	LEU
1	E	474	HIS
1	E	484	LEU
1	E	486	LYS
1	E	510	LEU
1	E	552	VAL
1	E	553	GLU
1	E	554	VAL
1	E	569	LEU
1	F	77	ARG
1	F	82	ASN
1	F	101	ARG
1	F	112	LEU
1	F	113	ARG
1	F	116	ARG
1	F	130	GLN
1	F	132	ARG
1	F	135	LEU
1	F	145	HIS
1	F	195	VAL

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Mol	Chain	Res	Type
1	F	196	LEU
1	F	200	ARG
1	F	201	ARG
1	F	204	LEU
1	F	205	MET
1	F	241	VAL
1	F	245	ARG
1	F	277	ASN
1	F	281	LYS
1	F	284	TYR
1	F	294	GLN
1	F	301	ILE
1	F	302	LYS
1	F	306	ILE
1	F	310	LEU
1	F	316	PHE
1	F	334	GLU
1	F	338	ILE
3	O	5	SER
3	O	7	CYS
3	P	7	CYS
3	Z	7	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	198	ASN
1	A	277	ASN
1	A	296	ASN
1	A	344	GLN
1	A	405	ASN
1	A	432	ASN
1	A	452	GLN
1	A	462	HIS
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

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Mol	Chain	Res	Type
1	B	405	ASN
1	B	432	ASN
1	B	442	HIS
1	B	452	GLN
1	B	462	HIS
2	C	123	HIS
2	C	198	ASN
2	C	277	ASN
2	C	296	ASN
2	C	335	ASN
2	C	344	GLN
2	C	380	ASN
2	C	405	ASN
2	C	432	ASN
2	C	462	HIS
2	C	528	ASN
1	D	123	HIS
1	D	198	ASN
1	D	277	ASN
1	D	296	ASN
1	D	344	GLN
1	D	380	ASN
1	D	405	ASN
1	D	432	ASN
1	D	452	GLN
1	D	462	HIS
1	E	123	HIS
1	E	198	ASN
1	E	277	ASN
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	364	GLN
1	E	405	ASN
1	E	432	ASN
1	E	452	GLN
1	E	462	HIS
1	E	537	ASN
1	F	82	ASN
1	F	123	HIS
1	F	145	HIS
1	F	146	ASN

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Mol	Chain	Res	Type
1	F	198	ASN
1	F	277	ASN
1	F	296	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
6	UDP	A	1572	4	24,26,26	1.29	3 (12%)	37,40,40	1.88	9 (24%)
5	BBK	B	1572	-	13,15,15	8.91	4 (30%)	15,21,21	1.65	2 (13%)
6	UDP	F	1364	4	24,26,26	1.22	2 (8%)	37,40,40	1.74	6 (16%)
6	UDP	B	1573	4	24,26,26	1.24	2 (8%)	37,40,40	1.86	7 (18%)
5	BBK	E	1571	-	13,15,15	9.33	4 (30%)	15,21,21	1.50	1 (6%)
6	UDP	D	1571	4	24,26,26	1.30	1 (4%)	37,40,40	1.83	7 (18%)
5	BBK	D	1572	-	13,15,15	9.07	4 (30%)	15,21,21	1.67	4 (26%)
6	UDP	E	1572	4	24,26,26	1.33	2 (8%)	37,40,40	1.89	6 (16%)
6	UDP	C	1571	4	24,26,26	1.23	2 (8%)	37,40,40	1.82	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BBK	A	1571	-	13,15,15	9.04	2 (15%)	15,21,21	1.42	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	UDP	A	1572	4	-	9/16/32/32	0/2/2/2
5	BBK	B	1572	-	-	5/6/26/26	0/1/1/1
6	UDP	F	1364	4	-	10/16/32/32	0/2/2/2
6	UDP	B	1573	4	-	9/16/32/32	0/2/2/2
5	BBK	E	1571	-	-	0/6/26/26	0/1/1/1
6	UDP	D	1571	4	-	9/16/32/32	0/2/2/2
5	BBK	D	1572	-	-	2/6/26/26	0/1/1/1
6	UDP	E	1572	4	-	12/16/32/32	0/2/2/2
6	UDP	C	1571	4	-	10/16/32/32	0/2/2/2
5	BBK	A	1571	-	-	2/6/26/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1571	BBK	C5-S5	-26.28	1.43	1.82
5	A	1571	BBK	C5-S5	-25.58	1.44	1.82
5	D	1572	BBK	C5-S5	-25.45	1.44	1.82
5	B	1572	BBK	C5-S5	-24.98	1.45	1.82
5	E	1571	BBK	C1-S5	-20.58	1.43	1.83
5	A	1571	BBK	C1-S5	-19.99	1.44	1.83
5	D	1572	BBK	C1-S5	-19.84	1.44	1.83
5	B	1572	BBK	C1-S5	-19.59	1.44	1.83
5	D	1572	BBK	C6-C5	4.29	1.56	1.52
6	D	1571	UDP	PB-O1B	4.13	1.63	1.50
6	E	1572	UDP	PB-O1B	4.12	1.63	1.50
6	C	1571	UDP	PB-O1B	3.92	1.63	1.50
5	B	1572	BBK	C6-C5	3.83	1.55	1.52
6	B	1573	UDP	PB-O1B	3.61	1.62	1.50
6	A	1572	UDP	PB-O1B	3.35	1.61	1.50
6	F	1364	UDP	PB-O1B	3.31	1.61	1.50
5	D	1572	BBK	C4-C5	2.92	1.56	1.53
5	E	1571	BBK	C6-C5	2.68	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1572	BBK	C4-C5	2.63	1.55	1.53
6	B	1573	UDP	C2-N1	-2.57	1.34	1.38
5	E	1571	BBK	C4-C5	2.30	1.55	1.53
6	F	1364	UDP	C5-C4	-2.26	1.38	1.43
6	E	1572	UDP	O3'-C3'	2.22	1.48	1.43
6	A	1572	UDP	C5-C4	-2.14	1.38	1.43
6	A	1572	UDP	C4-N3	-2.13	1.34	1.38
6	C	1571	UDP	C5-C4	-2.03	1.39	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1572	UDP	C4-N3-C2	-5.58	119.22	126.58
6	D	1571	UDP	C4-N3-C2	-5.31	119.57	126.58
6	C	1571	UDP	C4-N3-C2	-5.24	119.66	126.58
6	A	1572	UDP	C4-N3-C2	-5.08	119.88	126.58
6	B	1573	UDP	C4-N3-C2	-4.95	120.05	126.58
6	D	1571	UDP	N3-C2-N1	4.94	121.45	114.89
6	B	1573	UDP	N3-C2-N1	4.72	121.15	114.89
6	A	1572	UDP	N3-C2-N1	4.68	121.11	114.89
6	E	1572	UDP	N3-C2-N1	4.57	120.95	114.89
6	C	1571	UDP	C5-C4-N3	4.43	121.47	114.84
6	E	1572	UDP	C5-C4-N3	4.41	121.44	114.84
5	E	1571	BBK	C4-C3-C2	4.35	116.72	110.34
6	F	1364	UDP	C4-N3-C2	-4.25	120.97	126.58
6	C	1571	UDP	N3-C2-N1	4.25	120.53	114.89
6	F	1364	UDP	N3-C2-N1	4.20	120.47	114.89
6	F	1364	UDP	PA-O3A-PB	-4.19	118.44	132.83
6	B	1573	UDP	O2-C2-N1	-4.12	117.31	122.79
6	B	1573	UDP	O3B-PB-O2B	3.95	122.72	107.64
6	E	1572	UDP	PA-O3A-PB	-3.91	119.39	132.83
6	C	1571	UDP	O4-C4-C5	-3.83	118.42	125.16
6	D	1571	UDP	C5-C4-N3	3.80	120.53	114.84
6	A	1572	UDP	C5-C4-N3	3.77	120.48	114.84
5	D	1572	BBK	O4-C4-C5	3.62	116.68	108.82
6	F	1364	UDP	O3B-PB-O2B	3.59	121.35	107.64
6	A	1572	UDP	O3B-PB-O3A	3.53	116.49	104.64
5	B	1572	BBK	O4-C4-C5	3.33	116.04	108.82
6	D	1571	UDP	PA-O3A-PB	-3.30	121.51	132.83
6	A	1572	UDP	O4-C4-C5	-3.27	119.42	125.16
6	C	1571	UDP	O3B-PB-O2B	3.25	120.07	107.64
6	F	1364	UDP	O4-C4-C5	-3.25	119.44	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	1364	UDP	C5-C4-N3	3.13	119.53	114.84
6	B	1573	UDP	C5-C4-N3	3.12	119.51	114.84
6	D	1571	UDP	O4-C4-C5	-3.07	119.77	125.16
6	A	1572	UDP	PA-O3A-PB	-2.97	122.63	132.83
5	D	1572	BBK	C1-C2-C3	2.91	114.88	110.27
5	B	1572	BBK	O6-C6-C5	2.90	117.36	110.73
6	B	1573	UDP	O4-C4-C5	-2.89	120.07	125.16
5	D	1572	BBK	C3-C2-N2	-2.87	105.19	110.62
6	E	1572	UDP	O3B-PB-O2B	2.81	118.37	107.64
5	A	1571	BBK	O1-C1-C2	-2.78	103.57	109.25
6	D	1571	UDP	O2-C2-N1	-2.75	119.13	122.79
6	A	1572	UDP	O3B-PB-O2B	2.71	117.98	107.64
6	D	1571	UDP	O3B-PB-O2B	2.58	117.51	107.64
6	A	1572	UDP	C2'-C1'-N1	2.54	120.41	113.22
6	E	1572	UDP	O4-C4-C5	-2.53	120.70	125.16
6	B	1573	UDP	C2'-C3'-C4'	2.41	107.33	102.64
5	D	1572	BBK	O6-C6-C5	2.38	116.17	110.73
6	A	1572	UDP	O3A-PB-O1B	-2.21	98.93	111.19
5	A	1571	BBK	C3-C2-N2	-2.20	106.46	110.62
5	A	1571	BBK	O4-C4-C5	2.13	113.44	108.82
6	C	1571	UDP	PA-O3A-PB	-2.12	125.55	132.83
6	C	1571	UDP	O2-C2-N3	-2.07	117.65	121.50
5	A	1571	BBK	C1-C2-N2	-2.04	107.55	111.36

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1571	BBK	C4-C5-C6-O6
5	A	1571	BBK	S5-C5-C6-O6
5	B	1572	BBK	C4-C5-C6-O6
5	B	1572	BBK	S5-C5-C6-O6
5	D	1572	BBK	C4-C5-C6-O6
5	D	1572	BBK	S5-C5-C6-O6
6	A	1572	UDP	C5'-O5'-PA-O1A
6	A	1572	UDP	C5'-O5'-PA-O2A
6	A	1572	UDP	C5'-O5'-PA-O3A
6	B	1573	UDP	C5'-O5'-PA-O1A
6	C	1571	UDP	C5'-O5'-PA-O1A
6	C	1571	UDP	C5'-O5'-PA-O2A
6	C	1571	UDP	C5'-O5'-PA-O3A
6	C	1571	UDP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
6	D	1571	UDP	C5'-O5'-PA-O1A
6	E	1572	UDP	C5'-O5'-PA-O1A
6	E	1572	UDP	PA-O3A-PB-O3B
6	F	1364	UDP	C5'-O5'-PA-O1A
6	F	1364	UDP	C5'-O5'-PA-O2A
6	B	1573	UDP	O4'-C4'-C5'-O5'
6	B	1573	UDP	C3'-C4'-C5'-O5'
6	D	1571	UDP	PA-O3A-PB-O1B
6	A	1572	UDP	C4'-C5'-O5'-PA
6	C	1571	UDP	C2'-C1'-N1-C6
6	D	1571	UDP	C2'-C1'-N1-C6
6	C	1571	UDP	C4'-C5'-O5'-PA
6	F	1364	UDP	C4'-C5'-O5'-PA
6	E	1572	UDP	PA-O3A-PB-O2B
6	B	1573	UDP	C5'-O5'-PA-O3A
6	D	1571	UDP	C5'-O5'-PA-O3A
6	D	1571	UDP	O4'-C1'-N1-C6
6	B	1573	UDP	C4'-C5'-O5'-PA
6	B	1573	UDP	C5'-O5'-PA-O2A
6	D	1571	UDP	C5'-O5'-PA-O2A
6	E	1572	UDP	C5'-O5'-PA-O2A
6	C	1571	UDP	O4'-C1'-N1-C6
6	D	1571	UDP	O4'-C1'-N1-C2
6	E	1572	UDP	C4'-C5'-O5'-PA
5	B	1572	BBK	C3-C2-N2-C7
6	F	1364	UDP	PB-O3A-PA-O1A
6	F	1364	UDP	O4'-C4'-C5'-O5'
6	C	1571	UDP	O4'-C1'-N1-C2
6	B	1573	UDP	O4'-C1'-N1-C6
6	F	1364	UDP	O4'-C1'-N1-C6
6	A	1572	UDP	C2'-C1'-N1-C6
6	E	1572	UDP	C2'-C1'-N1-C6
6	F	1364	UDP	C2'-C1'-N1-C6
6	A	1572	UDP	O4'-C1'-N1-C2
6	A	1572	UDP	O4'-C1'-N1-C6
6	E	1572	UDP	O4'-C1'-N1-C6
6	F	1364	UDP	PB-O3A-PA-O2A
6	D	1571	UDP	C2'-C1'-N1-C2
6	E	1572	UDP	O4'-C1'-N1-C2
6	E	1572	UDP	PA-O3A-PB-O1B
5	B	1572	BBK	C1-C2-N2-C7
5	B	1572	BBK	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	C	1571	UDP	O4'-C4'-C5'-O5'
6	B	1573	UDP	C2'-C1'-N1-C6
6	E	1572	UDP	C5'-O5'-PA-O3A
6	F	1364	UDP	C5'-O5'-PA-O3A
6	C	1571	UDP	C2'-C1'-N1-C2
6	F	1364	UDP	O4'-C1'-N1-C2
6	A	1572	UDP	O4'-C4'-C5'-O5'
6	D	1571	UDP	O4'-C4'-C5'-O5'
6	E	1572	UDP	O4'-C4'-C5'-O5'
6	B	1573	UDP	O4'-C1'-N1-C2
6	A	1572	UDP	PA-O3A-PB-O1B
6	E	1572	UDP	C2'-C1'-N1-C2

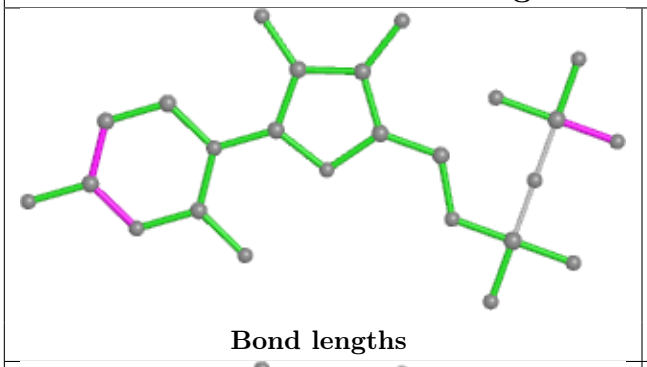
There are no ring outliers.

5 monomers are involved in 11 short contacts:

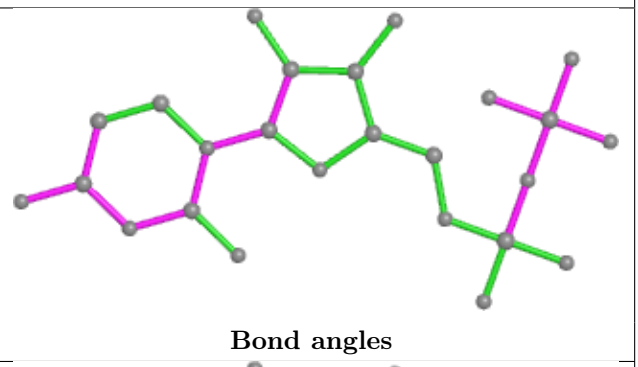
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1572	BBK	5	0
5	E	1571	BBK	1	0
5	D	1572	BBK	1	0
6	E	1572	UDP	1	0
5	A	1571	BBK	4	0

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.

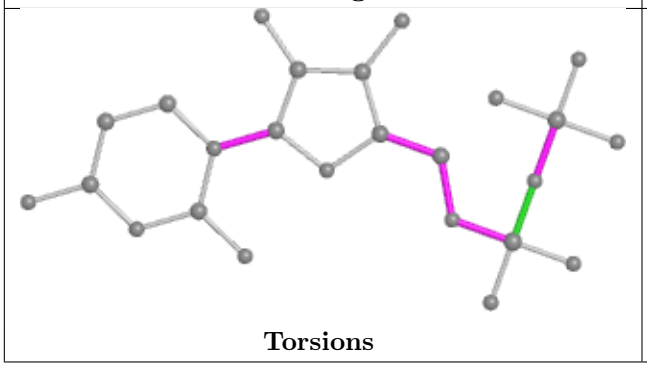
Ligand UDP A 1572



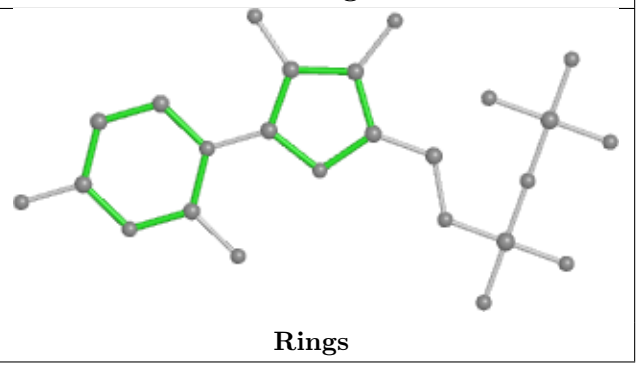
Bond lengths



Bond angles

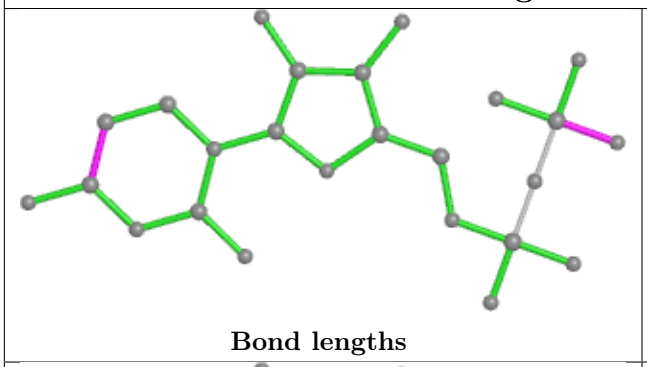


Torsions

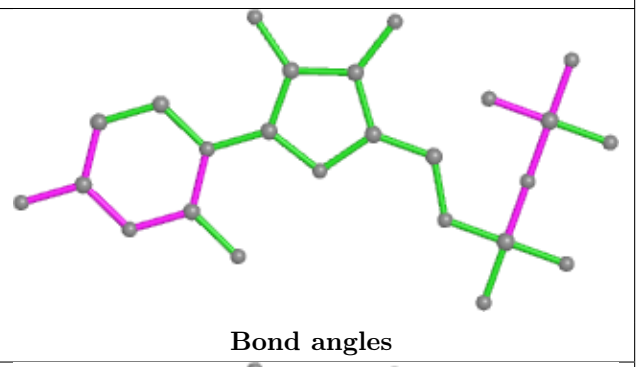


Rings

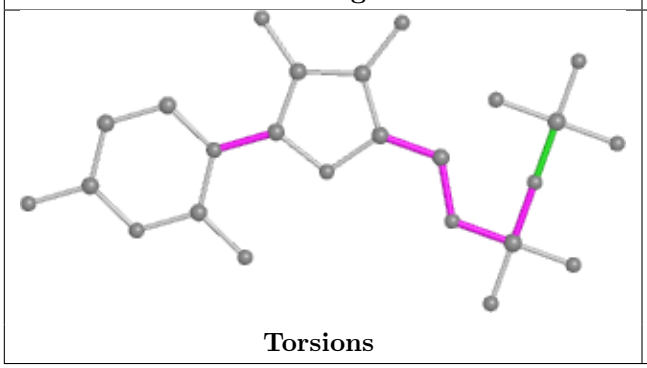
Ligand UDP F 1364



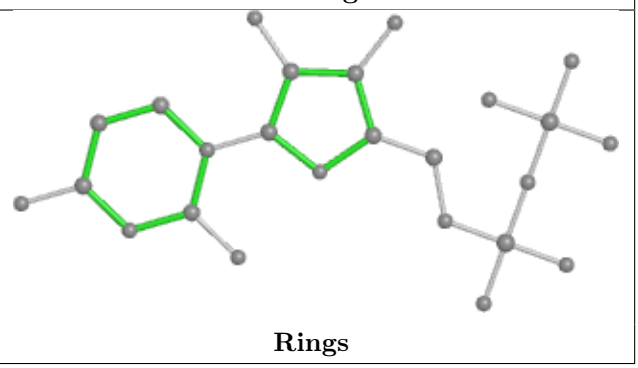
Bond lengths



Bond angles

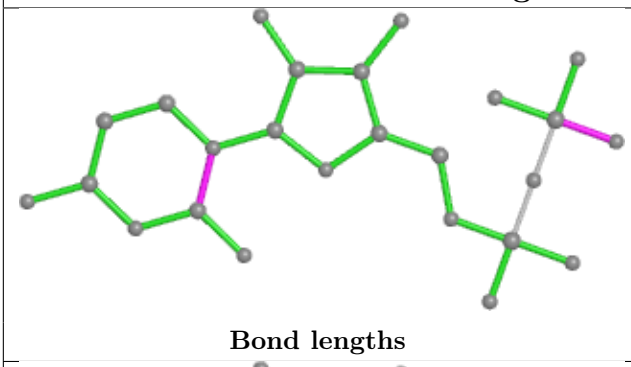


Torsions

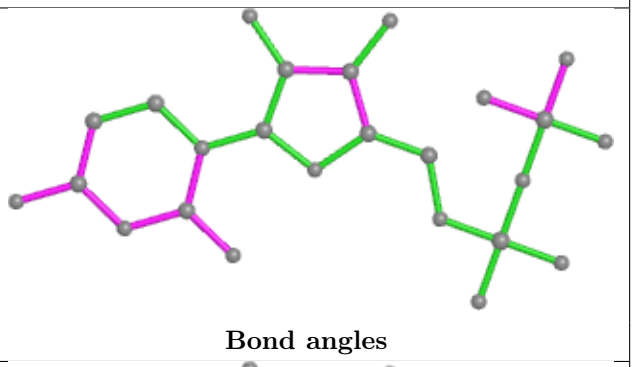


Rings

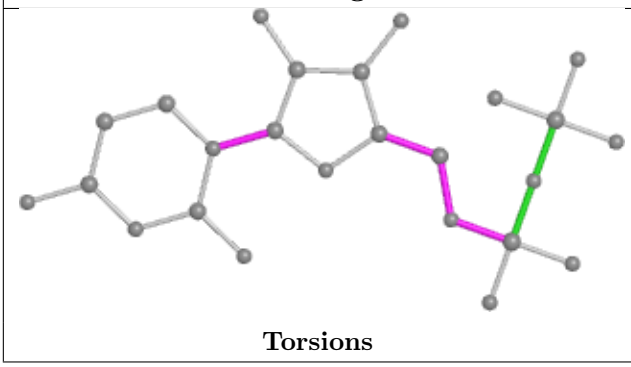
Ligand UDP B 1573



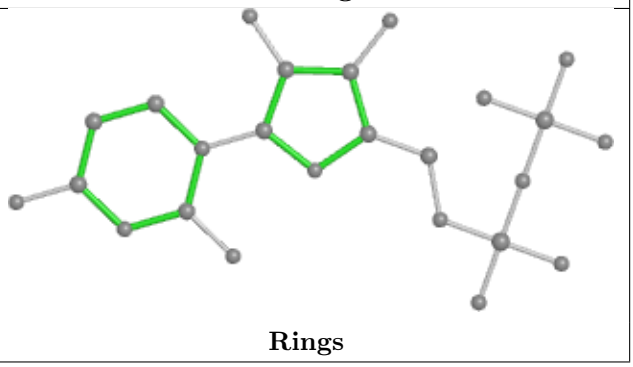
Bond lengths



Bond angles

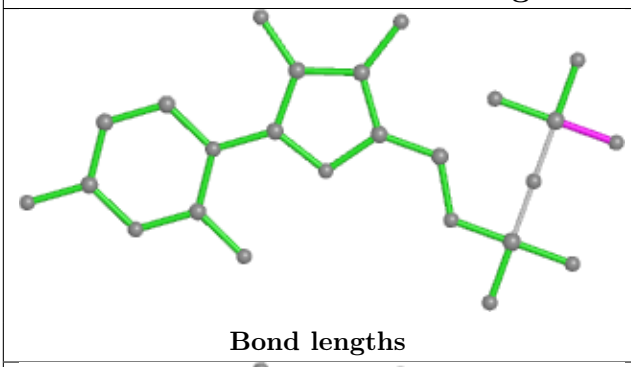


Torsions

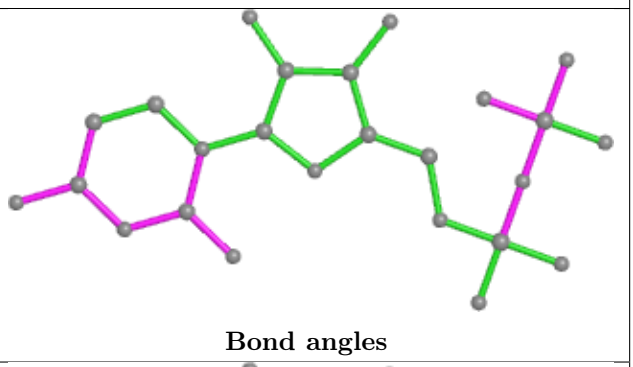


Rings

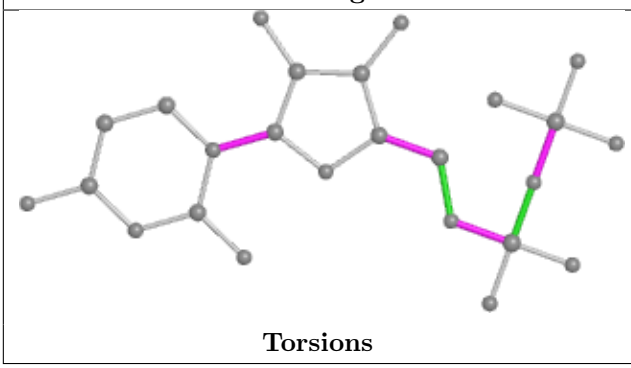
Ligand UDP D 1571



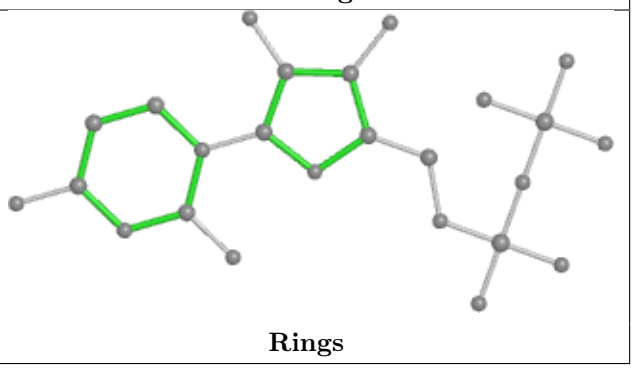
Bond lengths



Bond angles

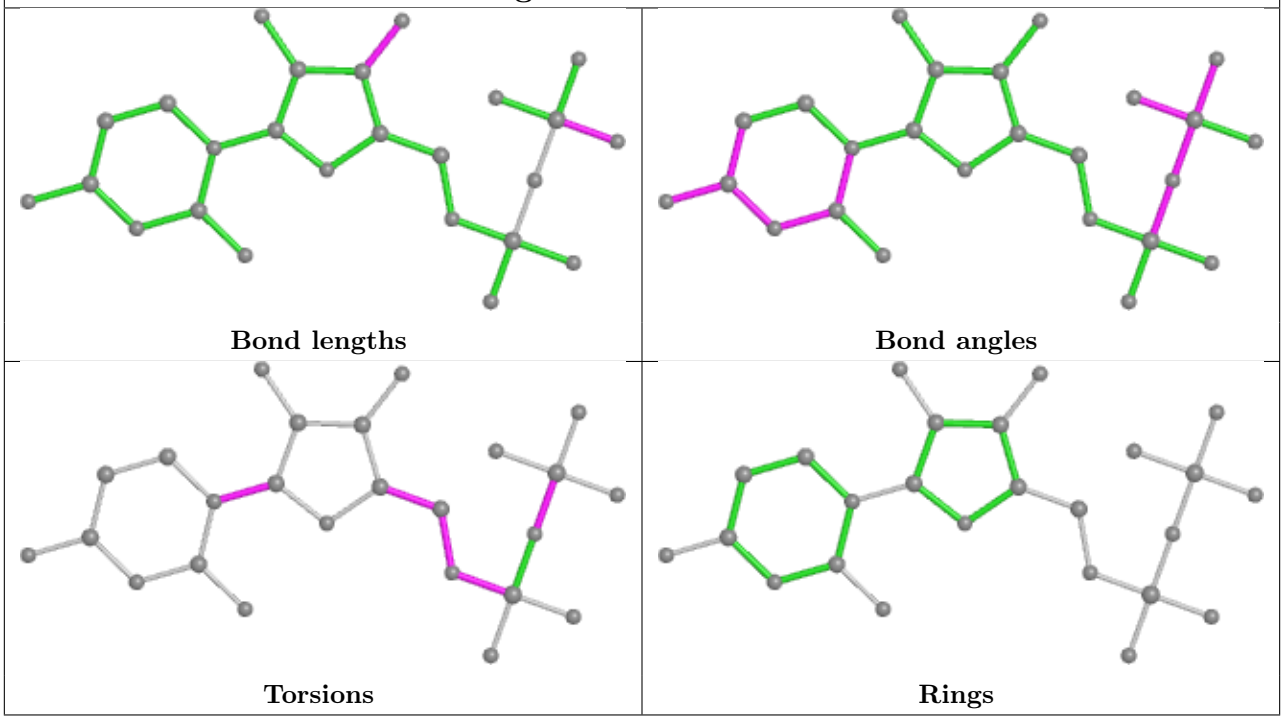


Torsions

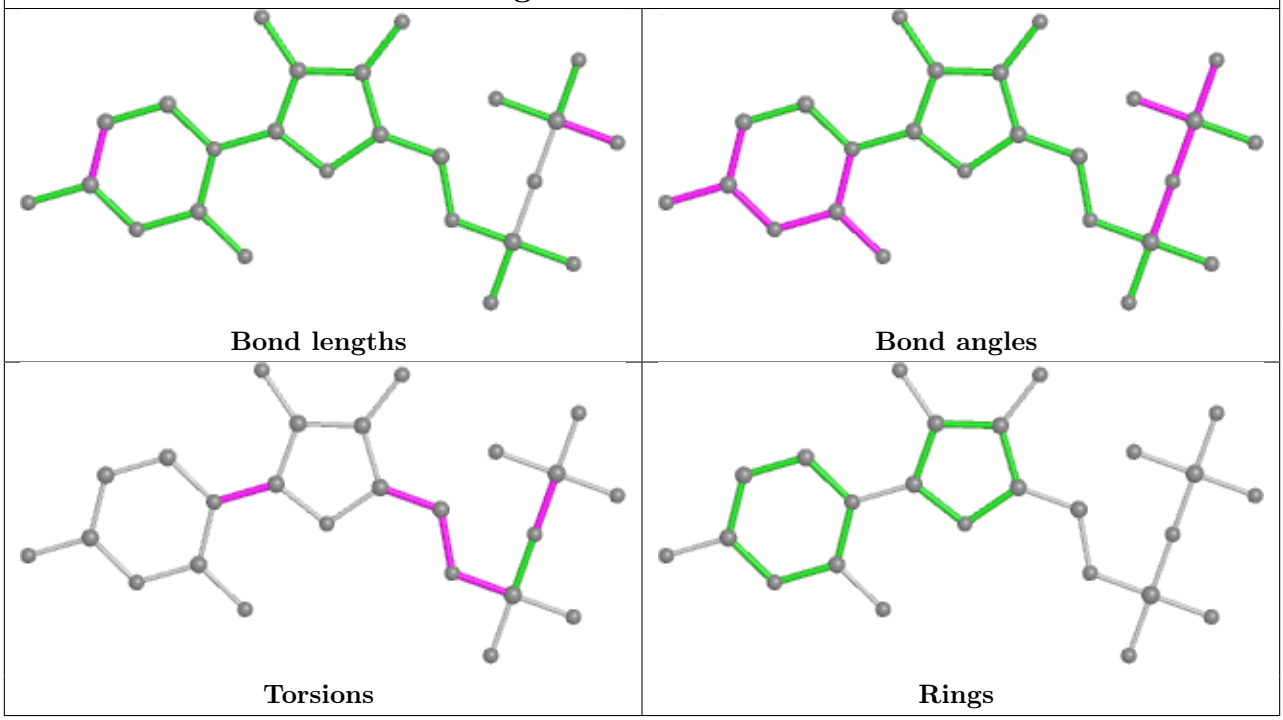


Rings

Ligand UDP E 1572



Ligand UDP C 1571



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	202:GLU	C	203:GLY	N	0.73

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	491/571 (85%)	-0.03	11 (2%) 62 59	28, 56, 96, 129	5 (1%)
1	B	482/571 (84%)	0.08	14 (2%) 51 47	32, 65, 115, 151	5 (1%)
1	D	487/571 (85%)	0.11	16 (3%) 46 41	29, 64, 110, 144	5 (1%)
1	E	487/571 (85%)	0.09	15 (3%) 49 44	31, 58, 105, 159	5 (1%)
1	F	276/571 (48%)	0.87	41 (14%) 2 1	59, 112, 167, 187	2 (0%)
2	C	436/571 (76%)	0.53	55 (12%) 3 2	35, 89, 149, 182	5 (1%)
3	L	6/6 (100%)	1.47	1 (16%) 1 1	86, 109, 116, 126	0
3	O	6/6 (100%)	0.74	0 100 100	72, 94, 105, 110	0
3	P	6/6 (100%)	0.35	0 100 100	44, 72, 78, 90	0
3	X	6/6 (100%)	2.86	4 (66%) 0 0	91, 106, 118, 123	0
3	Z	5/6 (83%)	0.48	0 100 100	72, 73, 88, 92	0
All	All	2688/3456 (77%)	0.23	157 (5%) 23 18	28, 67, 136, 187	27 (1%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	10	ALA	7.5
1	F	264	VAL	7.1
2	C	500	VAL	6.2
1	F	276	TRP	6.1
2	C	511	GLN	5.7
1	F	274	PHE	5.5
2	C	454	THR	5.1
1	E	442	HIS	4.4
2	C	531	LEU	4.4
2	C	533	HIS	4.3
1	B	101	ARG	4.3
2	C	128	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	364	GLN	4.3
2	C	403	ALA	4.2
1	A	372	GLY	4.2
1	F	340	PHE	4.1
1	F	272	GLY	4.1
2	C	497	LEU	4.1
2	C	501	ASP	4.0
1	E	391	GLU	3.9
2	C	524	GLN	3.9
1	A	375	THR	3.9
2	C	563	TRP	3.8
1	B	97	ASP	3.8
1	A	373	SER	3.8
2	C	523	GLU	3.7
2	C	509	LYS	3.7
1	F	273	GLY	3.6
2	C	525	ILE	3.6
1	F	278	LEU	3.6
1	B	102	ASN	3.6
1	A	377	PHE	3.5
1	F	197	ARG	3.5
2	C	526	GLU	3.5
1	B	103	LYS	3.5
2	C	565	PHE	3.4
1	B	99	TYR	3.4
2	C	496	CYS	3.4
1	F	342	VAL	3.4
1	E	94	SER	3.4
1	E	366	PRO	3.3
2	C	446	ALA	3.3
3	L	10	ALA	3.3
2	C	510	LEU	3.3
1	D	368	THR	3.3
2	C	104	PHE	3.3
1	F	277	ASN	3.2
1	D	364	GLN	3.2
1	E	95	GLY	3.2
2	C	488	LYS	3.2
1	F	316	PHE	3.2
1	F	324	TYR	3.1
2	C	568	ASN	3.1
1	F	279	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	442	HIS	3.1
2	C	462	HIS	3.0
2	C	127	GLN	3.0
2	C	483	ALA	3.0
2	C	100	ALA	2.9
1	B	98	PRO	2.9
1	F	206	ARG	2.9
1	D	365	HIS	2.9
2	C	502	ARG	2.9
2	C	532	ARG	2.9
1	F	125	GLN	2.8
2	C	534	VAL	2.8
1	F	280	PHE	2.8
1	F	262	GLN	2.8
2	C	451	GLN	2.8
2	C	490	VAL	2.8
1	D	525	ILE	2.7
1	E	327	MET	2.7
2	C	131	TRP	2.7
2	C	450	LEU	2.7
1	D	526	GLU	2.7
2	C	498	THR	2.7
1	F	344	GLN	2.7
1	F	282	TRP	2.7
1	D	405	ASN	2.7
1	E	443	GLN	2.7
1	F	283	ASP	2.6
1	E	368	THR	2.6
1	F	108	GLU	2.6
1	D	377	PHE	2.6
1	D	557	PRO	2.5
1	E	409	GLY	2.5
2	C	522	TRP	2.5
1	D	516	ASP	2.5
1	F	263	TYR	2.5
1	A	405	ASN	2.5
1	D	537	ASN	2.5
2	C	105	ASN	2.5
2	C	395	PHE	2.5
2	C	125	GLN	2.5
1	F	103	LYS	2.5
2	C	530	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	93	ARG	2.4
1	D	535	GLY	2.4
2	C	374	GLY	2.4
1	F	267	SER	2.4
2	C	461	GLY	2.4
1	F	123	HIS	2.4
1	B	366	PRO	2.4
1	B	376	VAL	2.4
1	B	365	HIS	2.4
1	F	246	THR	2.4
2	C	291	ARG	2.4
1	F	199	ASP	2.4
1	F	177	TYR	2.4
3	X	5	SER	2.4
1	F	338	ILE	2.4
1	B	100	ALA	2.3
1	F	207	SER	2.3
1	F	142	ILE	2.3
2	C	455	ASN	2.3
1	D	527	GLY	2.3
1	F	345	CYS	2.3
2	C	262	GLN	2.3
2	C	401	PRO	2.3
2	C	521	LYS	2.3
2	C	564	LYS	2.3
1	E	128	ARG	2.3
1	B	213	ASP	2.3
1	A	406	VAL	2.2
1	E	406	VAL	2.2
1	D	568	ASN	2.2
2	C	482	TRP	2.2
1	F	143	THR	2.2
1	F	265	GLY	2.2
1	E	408	TYR	2.2
1	A	376	VAL	2.2
2	C	74	SER	2.2
2	C	98	PRO	2.2
1	F	320	GLU	2.2
2	C	516	ASP	2.2
3	X	9	ALA	2.2
1	D	562	GLN	2.2
1	F	107	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	470	VAL	2.1
1	A	407	PRO	2.1
1	F	255	VAL	2.1
1	A	95	GLY	2.1
1	F	307	ALA	2.1
1	E	331	TRP	2.1
1	D	367	TYR	2.1
1	B	179	ASN	2.1
2	C	453	GLY	2.1
2	C	487	GLU	2.1
1	A	331	TRP	2.0
1	F	101	ARG	2.0
1	D	534	VAL	2.0
1	F	326	MET	2.0
1	B	104	PHE	2.0
2	C	405	ASN	2.0
1	E	534	VAL	2.0
1	F	275	ASP	2.0
3	X	6	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 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BBK	D	1572	15/15	0.81	0.27	97,106,117,122	0
5	BBK	B	1572	15/15	0.82	0.26	66,81,110,110	0
5	BBK	E	1571	15/15	0.82	0.30	67,86,120,144	0
5	BBK	A	1571	15/15	0.87	0.22	52,76,82,88	0

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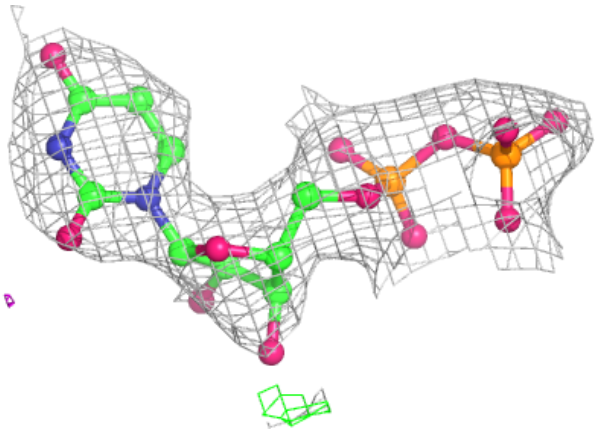
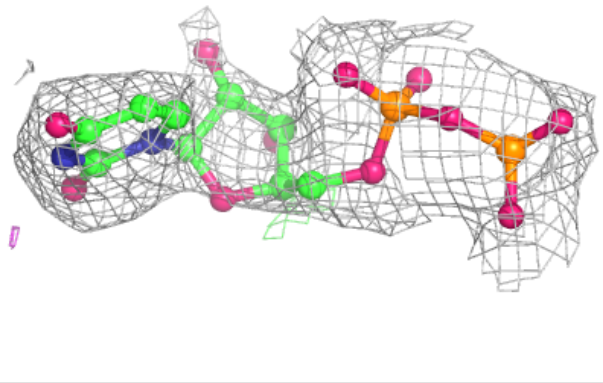
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	UDP	C	1571	25/25	0.92	0.18	83,96,111,114	0
6	UDP	D	1571	25/25	0.92	0.21	64,98,118,128	0
6	UDP	B	1573	25/25	0.94	0.16	77,89,97,106	0
6	UDP	F	1364	25/25	0.94	0.16	107,134,151,177	0
6	UDP	E	1572	25/25	0.96	0.17	69,78,89,97	0
6	UDP	A	1572	25/25	0.97	0.16	54,74,89,97	0
4	MN	E	1570	1/1	0.97	0.13	46,46,46,46	0
4	MN	B	1571	1/1	0.98	0.15	63,63,63,63	0
4	MN	F	1363	1/1	0.98	0.10	93,93,93,93	0
4	MN	D	1570	1/1	0.98	0.13	58,58,58,58	0
4	MN	C	1570	1/1	0.99	0.13	67,67,67,67	0
4	MN	A	1570	1/1	0.99	0.10	46,46,46,46	0

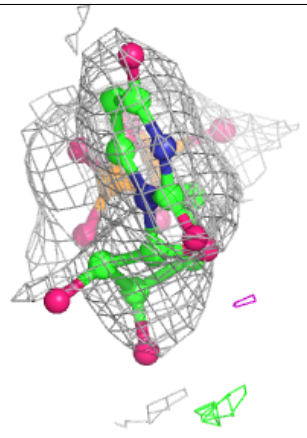
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP C 1571:

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

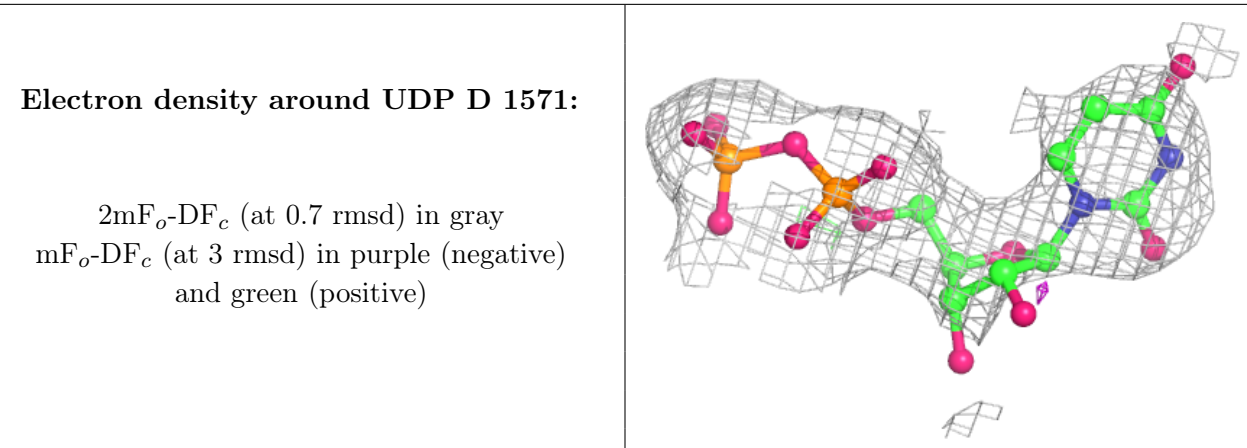






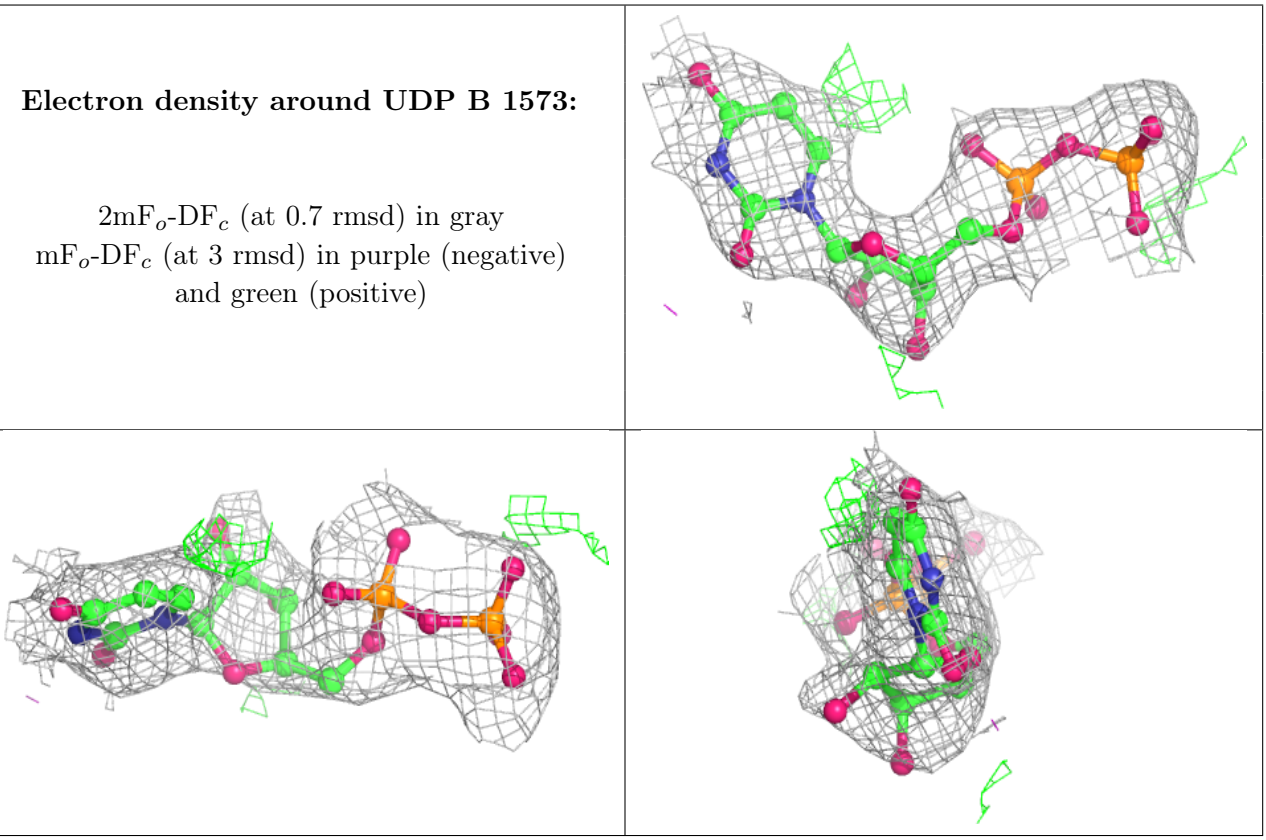
Electron density around UDP D 1571:

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



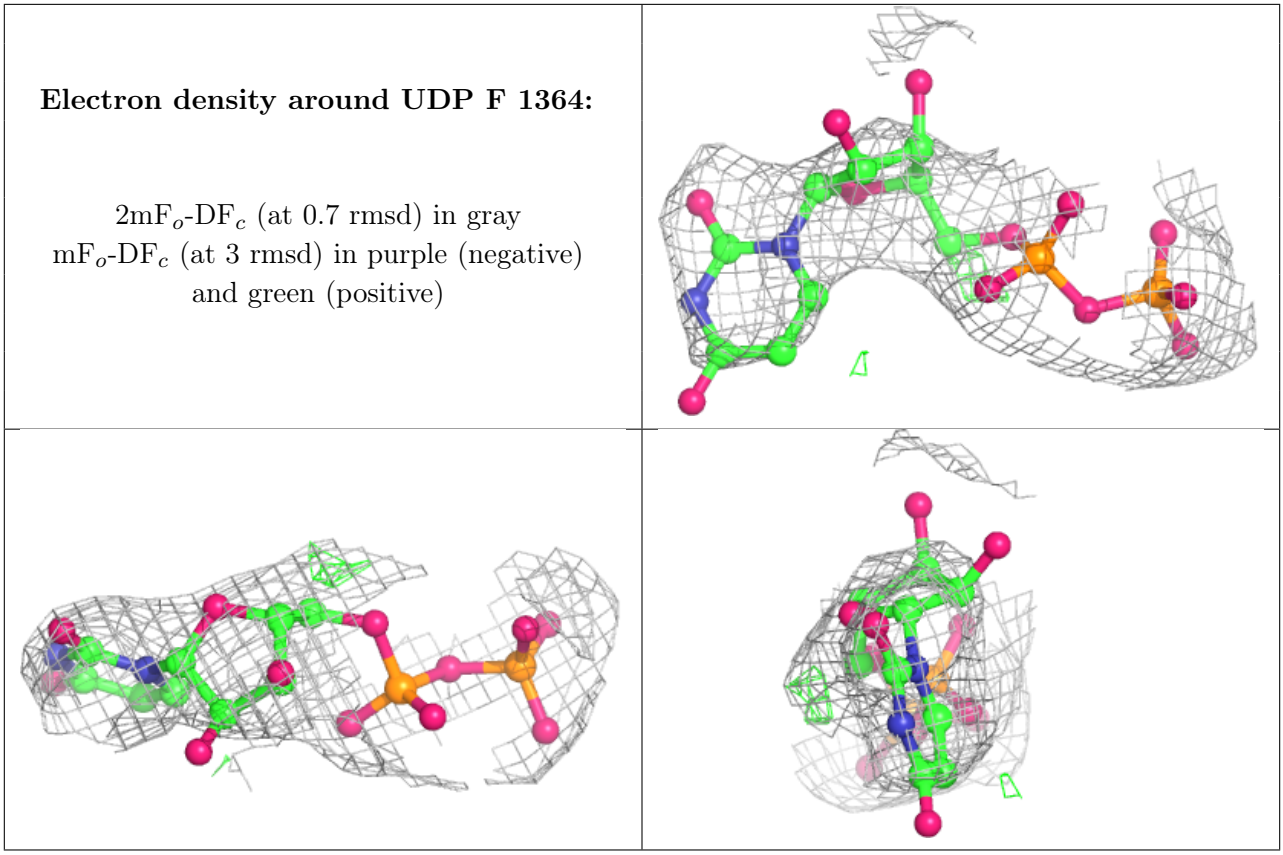
Electron density around UDP B 1573:

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



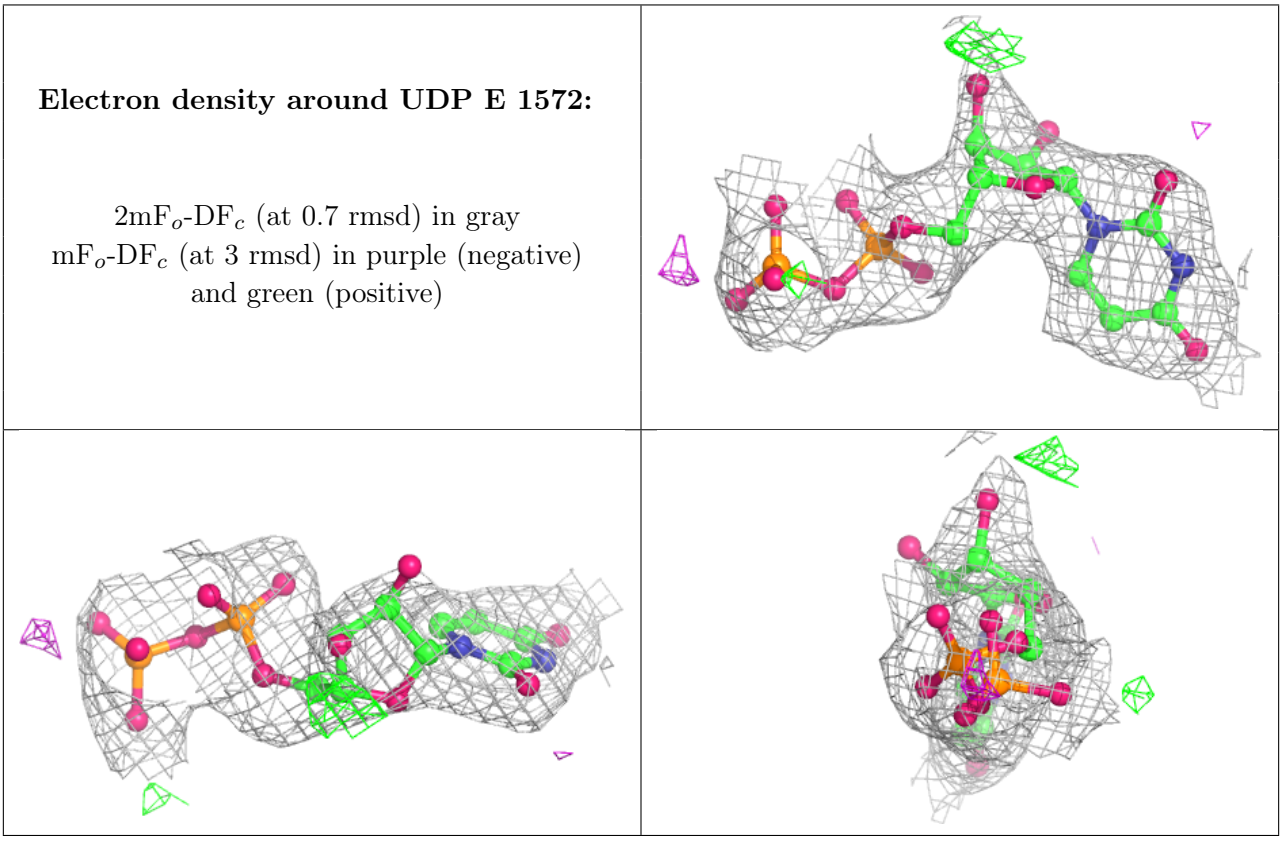
Electron density around UDP F 1364:

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



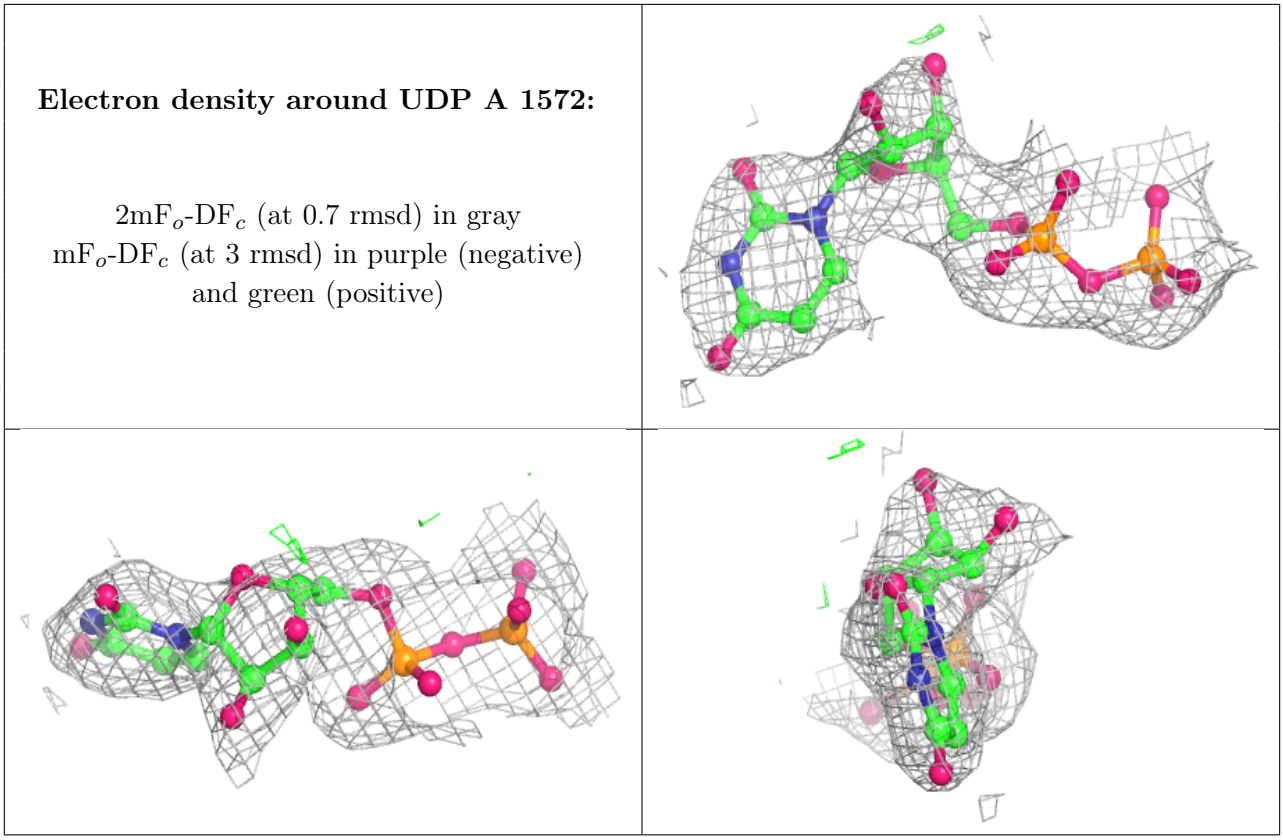
Electron density around UDP E 1572:

$2mF_o$-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 1572:

$2mF_o$-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.