



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:41 AM UTC

PDB ID : 5FV9 / pdb_00005fv9
Title : Crystal structure of GalNAc-T2 in complex with compound 16d
Authors : Ghirardello, M.; Rivas, M.; Lacetera, A.; Delso, I.; Lira-Navarrete, E.; Tejero, T.; Martin-Santamaria, S.; Hurtado-Guerrero, R.; Merino, P.
Deposited on : 2016-02-03
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

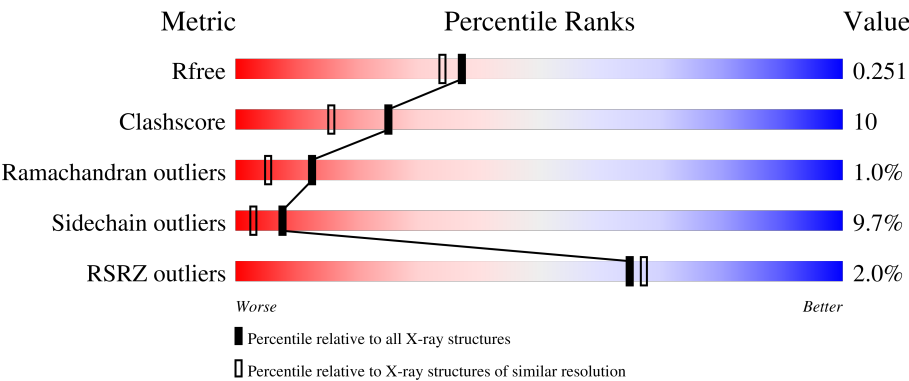
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.07 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	571	% 65% 14% . 15%
1	B	571	% 67% 14% . 15%
1	C	571	2% 63% 18% . 16%
1	D	571	3% 57% 16% . 22%
1	E	571	% 66% 15% . 15%

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Mol	Chain	Length	Quality of chain
1	F	571	2% 62% 18% • • 16%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24993 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.

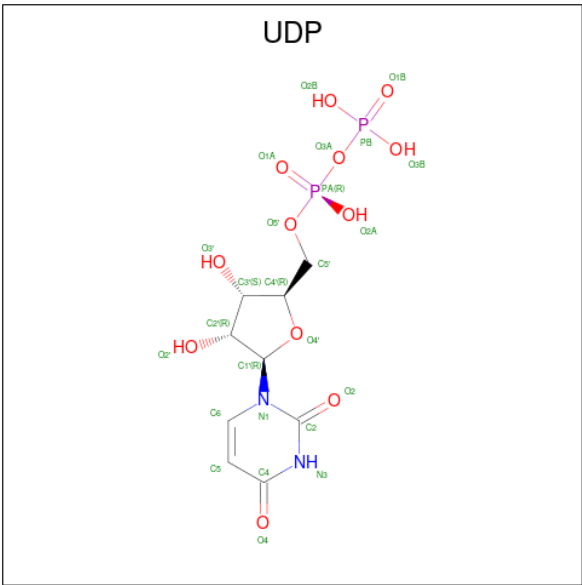
- Molecule 1 is a protein called GALNAC-T2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	20	2	0
			3896	2451	709	712	24			
1	B	484	Total	C	N	O	S	20	1	0
			3894	2450	709	711	24			
1	C	482	Total	C	N	O	S	20	3	0
			3897	2451	712	710	24			
1	D	443	Total	C	N	O	S	20	0	0
			3575	2256	645	652	22			
1	E	483	Total	C	N	O	S	20	1	0
			3885	2445	705	711	24			
1	F	481	Total	C	N	O	S	20	1	0
			3869	2432	706	707	24			

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 URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

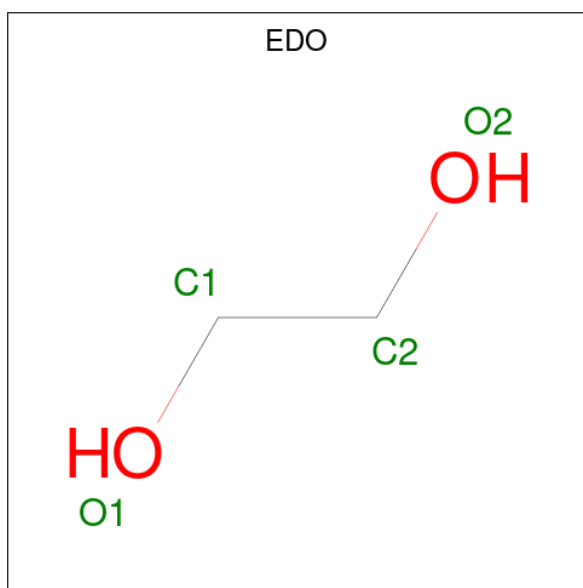


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



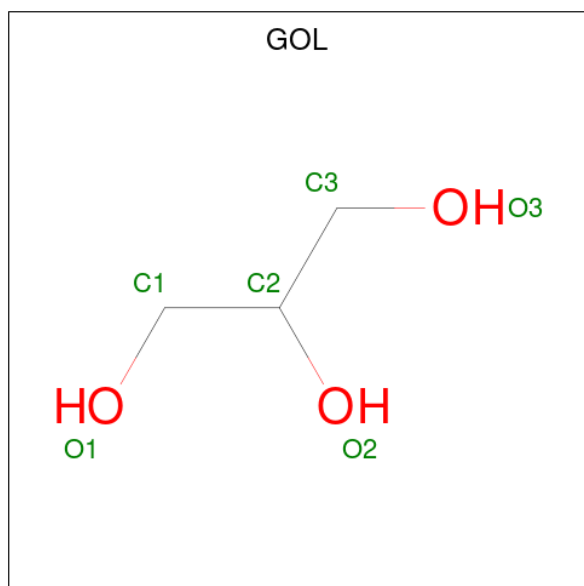
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total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

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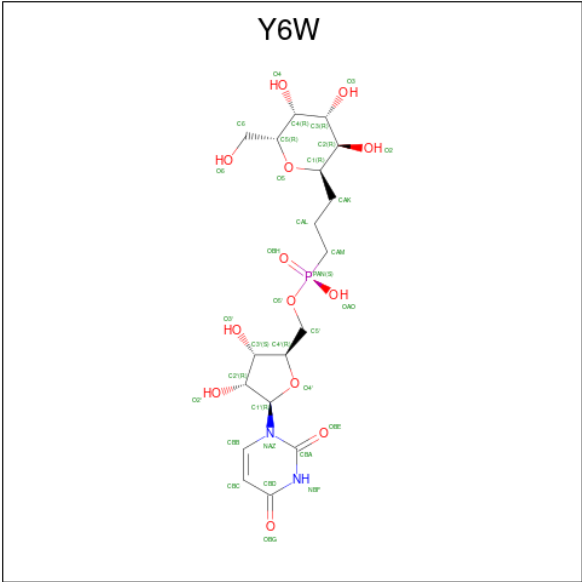
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is [(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl hydrogen (S)-{3-[(2R,3R,4R,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl]propyl}phosphonate (CCD ID: Y6W) (formula: $C_{18}H_{29}N_2O_{13}P$).



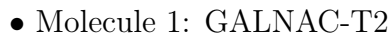
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			34	18	2	13	1		
6	E	1	Total	C	N	O	P	0	0
			34	18	2	13	1		
6	F	1	Total	C	N	O	P	0	0
			34	18	2	13	1		

- Molecule 7 is water.

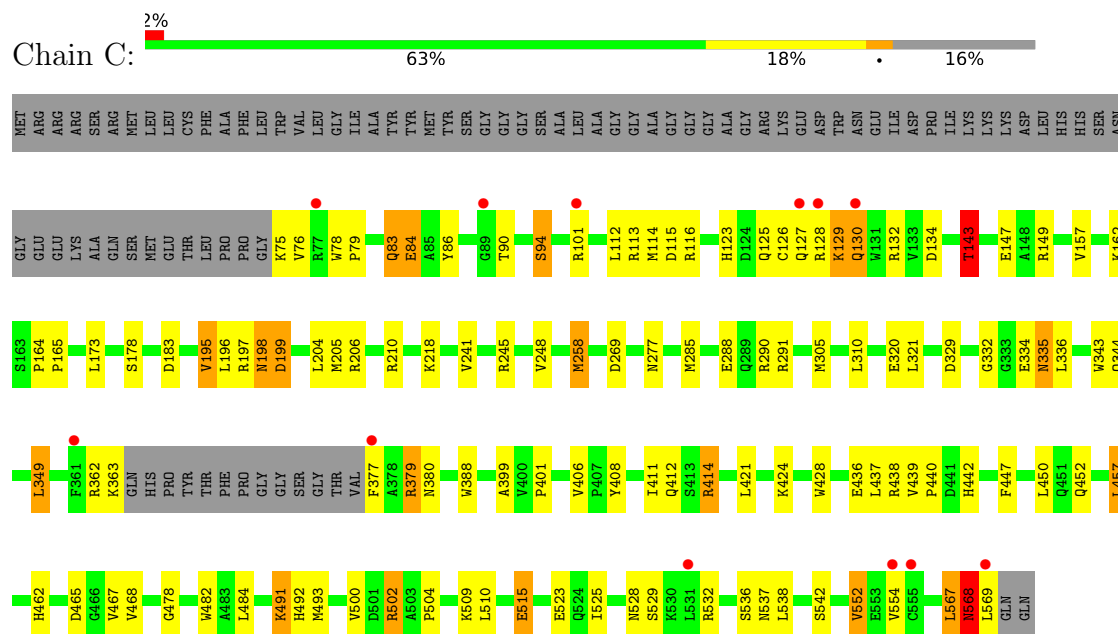
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	346	Total	O	0	0
			346	346		
7	B	299	Total	O	0	0
			299	299		
7	C	306	Total	O	0	0
			306	306		
7	D	184	Total	O	0	0
			184	184		
7	E	290	Total	O	0	0
			290	290		
7	F	208	Total	O	0	0
			208	208		

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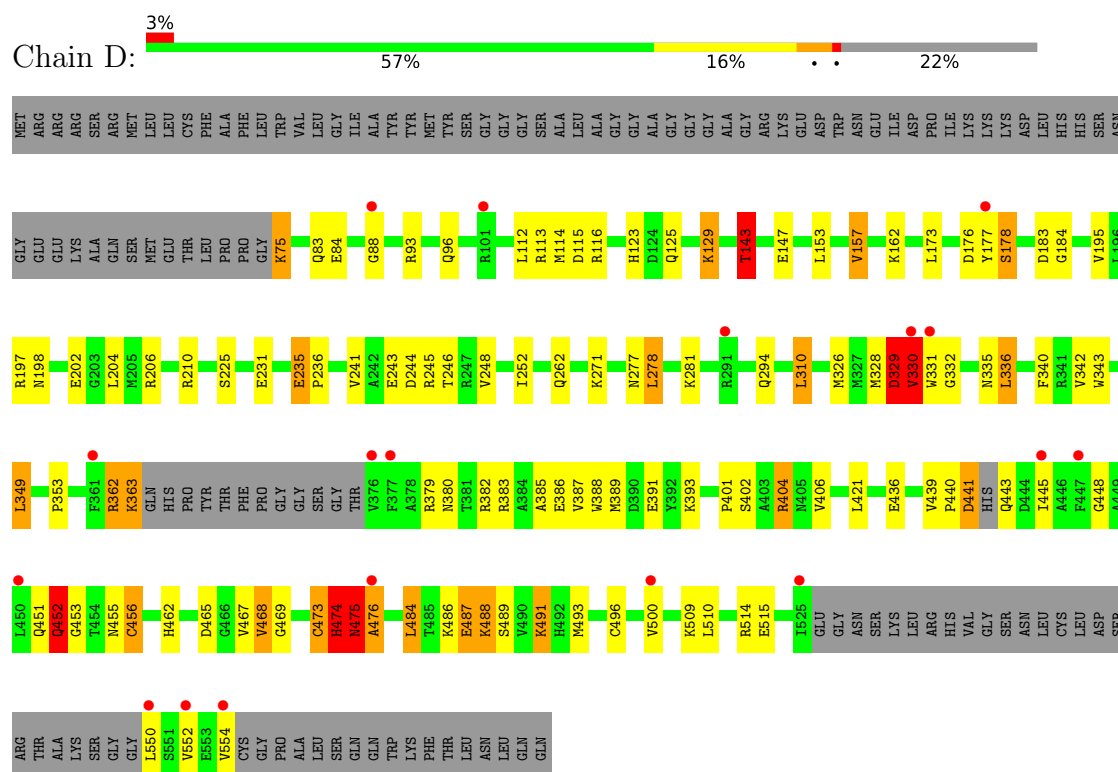
- Molecule 1: GALNAC-T2



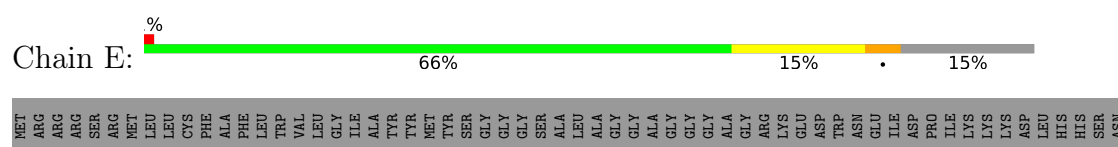
• Molecule 1: GALNAC-T2

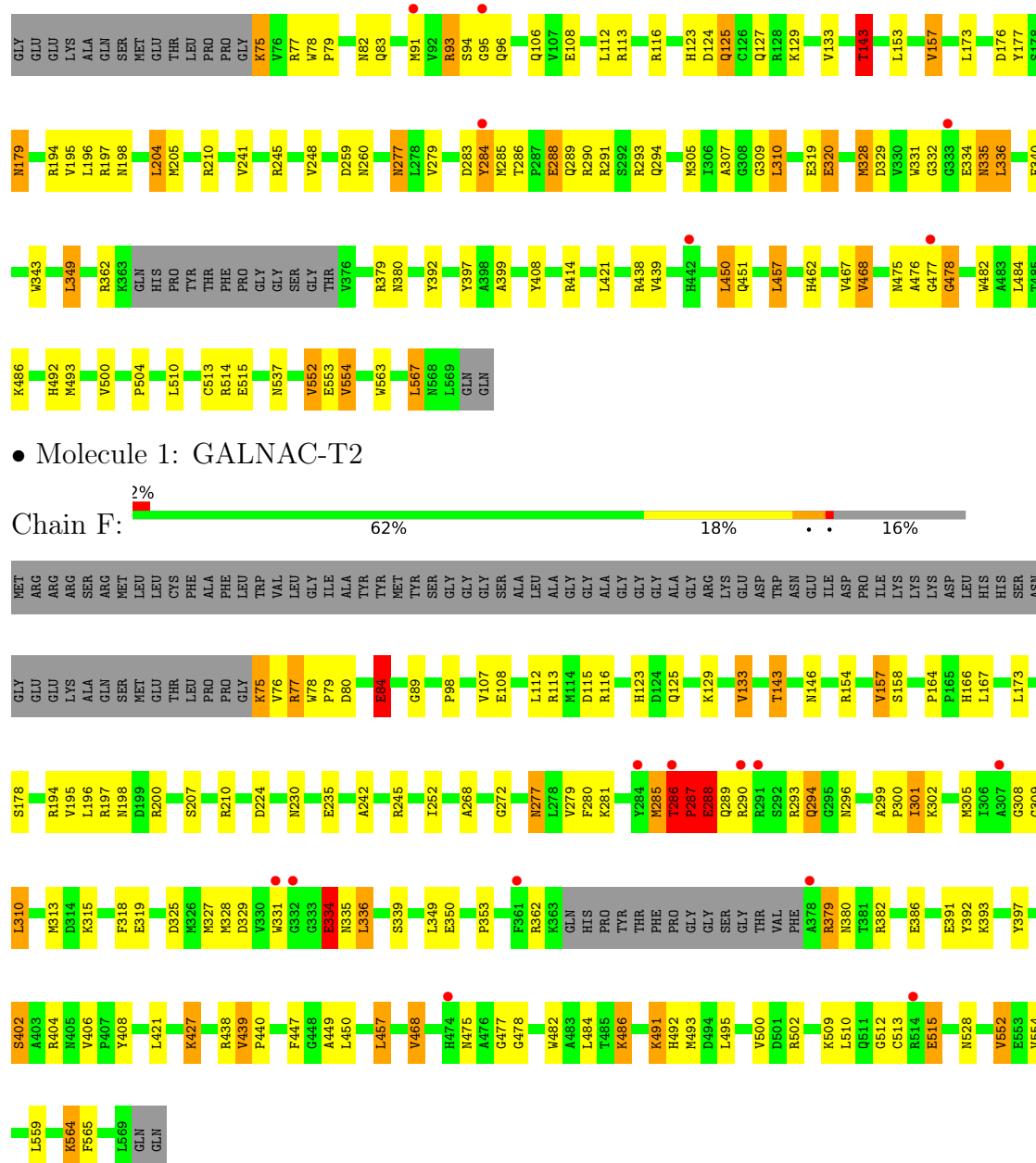


• Molecule 1: GALNAC-T2



• Molecule 1: GALNAC-T2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.49Å 121.75Å 250.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	250.15 – 2.07 125.08 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (250.15-2.07) 99.8 (125.08-2.07)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.190 , 0.247 0.198 , 0.251	Depositor DCC
R_{free} test set	5938 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24993	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, Y6W, GOL, MN, UDP

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	1.24	6/3982 (0.2%)	1.23	17/5380 (0.3%)
1	B	1.22	10/3980 (0.3%)	1.19	9/5378 (0.2%)
1	C	1.14	7/3986 (0.2%)	1.16	15/5384 (0.3%)
1	D	1.11	7/3653 (0.2%)	1.15	13/4935 (0.3%)
1	E	1.35	13/3971 (0.3%)	1.28	31/5366 (0.6%)
1	F	1.20	10/3954 (0.3%)	1.24	21/5342 (0.4%)
All	All	1.21	53/23526 (0.2%)	1.21	106/31785 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	2
1	D	0	4
1	E	0	1
1	F	0	4
All	All	0	14

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	486	LYS	CB-CG	-25.66	0.75	1.52
1	F	515	GLU	CB-CG	-20.29	0.91	1.52
1	E	513	CYS	C-N	-14.28	1.15	1.33
1	D	486	LYS	CB-CG	11.77	1.87	1.52
1	A	515	GLU	CB-CG	-11.53	1.17	1.52
1	A	332	GLY	N-CA	11.10	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	LYS	CB-CG	-10.83	1.20	1.52
1	B	486	LYS	CB-CG	-10.49	1.21	1.52
1	E	319	GLU	C-N	-10.47	1.19	1.33
1	E	332	GLY	N-CA	10.45	1.56	1.45
1	C	515	GLU	CB-CG	-10.28	1.21	1.52
1	B	75	LYS	CB-CG	-9.74	1.23	1.52
1	A	486	LYS	CB-CG	9.62	1.81	1.52
1	C	84	GLU	CB-CG	-9.43	1.24	1.52
1	D	294	GLN	CB-CG	-8.83	1.25	1.52
1	F	84	GLU	CB-CG	-8.19	1.27	1.52
1	A	75	LYS	CB-CG	-8.08	1.28	1.52
1	B	294	GLN	CB-CG	-8.08	1.28	1.52
1	D	84	GLU	CB-CG	-8.00	1.28	1.52
1	A	469	GLY	C-O	7.71	1.29	1.23
1	C	90	THR	N-CA	7.55	1.53	1.46
1	F	224	ASP	CA-CB	7.17	1.64	1.53
1	B	84	GLU	CB-CG	-6.92	1.31	1.52
1	F	509	LYS	CA-C	-6.91	1.44	1.52
1	E	307	ALA	N-CA	6.62	1.54	1.46
1	E	294	GLN	CB-CG	6.57	1.72	1.52
1	F	154	ARG	CA-C	-6.23	1.44	1.52
1	B	547	SER	N-CA	-6.07	1.39	1.46
1	B	143	THR	CB-CG2	-5.88	1.33	1.52
1	E	328	MET	C-O	5.87	1.31	1.23
1	D	310	LEU	C-O	-5.81	1.17	1.24
1	B	356	ARG	N-CA	-5.75	1.39	1.46
1	C	199	ASP	CA-C	5.70	1.60	1.52
1	F	230	ASN	CA-C	5.70	1.61	1.53
1	F	468	VAL	N-CA	-5.66	1.39	1.46
1	F	294	GLN	CB-CG	5.65	1.69	1.52
1	D	178	SER	CA-C	5.64	1.59	1.52
1	E	514	ARG	C-N	-5.56	1.26	1.34
1	F	235	GLU	N-CA	5.54	1.51	1.46
1	C	195	VAL	C-O	-5.53	1.18	1.24
1	D	475	ASN	N-CA	5.45	1.52	1.46
1	E	478	GLY	N-CA	5.41	1.49	1.45
1	C	183	ASP	N-CA	5.39	1.52	1.46
1	B	356	ARG	CA-C	-5.35	1.46	1.52
1	D	235	GLU	N-CA	5.31	1.51	1.46
1	E	284	TYR	CA-C	-5.28	1.46	1.52
1	A	131	TRP	C-O	-5.27	1.17	1.23
1	B	316	PHE	C-O	-5.23	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	397	TYR	CA-C	5.18	1.59	1.52
1	F	158	SER	N-CA	-5.11	1.40	1.46
1	E	176	ASP	CA-C	-5.06	1.47	1.53
1	E	179	ASN	C-O	-5.01	1.18	1.24
1	B	439	VAL	CA-C	5.01	1.57	1.52

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	75	LYS	CB-CG-CD	14.92	145.61	111.30
1	B	75	LYS	CA-CB-CG	14.79	143.68	114.10
1	A	486	LYS	CB-CG-CD	-14.41	78.16	111.30
1	E	486	LYS	CA-CB-CG	13.08	140.27	114.10
1	C	75	LYS	CA-CB-CG	12.62	139.34	114.10
1	A	486	LYS	CA-CB-CG	-12.32	89.46	114.10
1	E	197	ARG	NE-CZ-NH2	-11.67	108.69	119.20
1	D	84	GLU	CA-CB-CG	11.48	137.06	114.10
1	E	75	LYS	CB-CG-CD	10.99	136.59	111.30
1	F	294	GLN	CA-CB-CG	-10.88	92.34	114.10
1	D	486	LYS	CB-CG-CD	10.29	134.98	111.30
1	E	478	GLY	N-CA-C	-10.07	101.05	110.21
1	D	486	LYS	CA-CB-CG	10.01	134.12	114.10
1	F	75	LYS	CA-CB-CG	-9.77	94.57	114.10
1	D	475	ASN	N-CA-C	9.76	124.80	113.38
1	D	75	LYS	CB-CG-CD	8.70	131.31	111.30
1	A	294	GLN	CA-CB-CG	8.66	131.43	114.10
1	F	515	GLU	CA-CB-CG	8.64	131.39	114.10
1	D	473	CYS	N-CA-C	8.62	123.45	113.19
1	E	294	GLN	CA-CB-CG	-8.49	97.13	114.10
1	E	320	GLU	O-C-N	8.29	131.59	122.15
1	E	514	ARG	CA-C-N	8.17	132.05	120.28
1	E	514	ARG	C-N-CA	8.17	132.05	120.28
1	F	294	GLN	CB-CG-CD	8.14	126.44	112.60
1	E	319	GLU	CA-C-N	7.82	131.39	120.29
1	E	319	GLU	C-N-CA	7.82	131.39	120.29
1	E	197	ARG	NE-CZ-NH1	7.81	129.31	121.50
1	C	406	VAL	N-CA-C	7.51	115.09	108.63
1	E	514	ARG	O-C-N	-7.47	113.72	123.28
1	A	75	LYS	CB-CG-CD	-7.37	94.34	111.30
1	F	468	VAL	N-CA-CB	-7.29	100.20	112.44
1	F	84	GLU	CA-CB-CG	7.27	128.64	114.10
1	F	157	VAL	N-CA-CB	7.07	120.16	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	VAL	N-CA-C	7.02	118.40	108.36
1	D	474	HIS	N-CA-C	6.96	125.62	110.80
1	E	197	ARG	CD-NE-CZ	6.75	133.84	124.40
1	E	468	VAL	N-CA-CB	-6.67	101.24	112.44
1	B	118	ILE	N-CA-C	-6.66	103.73	109.19
1	A	436	GLU	CA-CB-CG	6.57	127.24	114.10
1	A	75	LYS	CA-CB-CG	6.56	127.22	114.10
1	C	75	LYS	CB-CG-CD	-6.48	96.39	111.30
1	C	76	VAL	N-CA-CB	-6.45	103.69	110.72
1	A	197	ARG	CG-CD-NE	-6.43	97.86	112.00
1	A	439	VAL	N-CA-C	6.41	114.87	107.89
1	A	335	ASN	N-CA-C	-6.38	103.84	111.69
1	F	146	ASN	N-CA-C	6.37	120.19	111.39
1	B	486	LYS	CA-CB-CG	6.33	126.76	114.10
1	E	283	ASP	CA-C-N	-6.33	111.89	122.64
1	E	283	ASP	C-N-CA	-6.33	111.89	122.64
1	F	287	PRO	CA-C-N	6.30	133.05	121.70
1	F	287	PRO	C-N-CA	6.30	133.05	121.70
1	B	195	VAL	N-CA-C	6.29	116.98	108.17
1	F	286	THR	CA-C-N	-6.24	112.04	119.84
1	F	286	THR	C-N-CA	-6.24	112.04	119.84
1	D	184	GLY	N-CA-C	6.21	120.00	112.49
1	C	334	GLU	N-CA-C	6.20	120.56	113.19
1	B	468	VAL	N-CA-CB	-6.18	102.06	112.44
1	E	320	GLU	CA-C-N	-6.15	109.64	121.94
1	E	320	GLU	C-N-CA	-6.15	109.64	121.94
1	E	197	ARG	CG-CD-NE	-6.12	98.55	112.00
1	C	195	VAL	N-CA-C	6.11	117.27	108.48
1	E	552	VAL	N-CA-CB	-6.05	103.66	110.92
1	F	493	MET	CB-CA-C	-6.04	109.59	116.54
1	E	552	VAL	CB-CA-C	6.00	119.00	110.84
1	D	84	GLU	CB-CG-CD	5.99	122.78	112.60
1	B	491	LYS	N-CA-C	5.98	118.95	109.50
1	A	515	GLU	CA-CB-CG	5.96	126.02	114.10
1	F	515	GLU	CB-CG-CD	5.96	122.73	112.60
1	B	478	GLY	N-CA-C	-5.84	99.34	113.18
1	B	320	GLU	CB-CA-C	-5.82	101.12	110.79
1	C	437	LEU	CA-C-N	-5.81	114.00	122.19
1	C	437	LEU	C-N-CA	-5.81	114.00	122.19
1	C	143	THR	N-CA-CB	-5.79	100.75	110.83
1	F	334	GLU	N-CA-C	5.77	119.14	111.75
1	C	130	GLN	N-CA-C	5.75	119.03	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	568	ASN	N-CA-CB	-5.73	102.13	110.84
1	F	552	VAL	CB-CA-C	5.71	119.35	110.83
1	E	143	THR	N-CA-CB	-5.69	100.92	110.83
1	A	552	VAL	CB-CA-C	5.69	119.00	110.98
1	F	308	GLY	N-CA-C	-5.56	104.58	112.81
1	F	491	LYS	N-CA-C	5.53	118.57	109.72
1	E	319	GLU	O-C-N	-5.52	115.85	122.15
1	F	77	ARG	N-CA-C	-5.47	102.79	110.50
1	E	331	TRP	N-CA-C	5.41	118.68	112.57
1	C	552	VAL	CB-CA-C	5.39	118.59	110.98
1	A	303	THR	CA-C-N	5.36	125.03	119.56
1	A	303	THR	C-N-CA	5.36	125.03	119.56
1	C	205	MET	CB-CG-SD	5.36	128.77	112.70
1	D	278	LEU	N-CA-C	5.26	118.99	112.58
1	A	500	VAL	N-CA-C	-5.25	105.67	113.39
1	E	486	LYS	CB-CG-CD	5.23	123.33	111.30
1	C	414	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	E	515	GLU	CB-CG-CD	5.17	121.39	112.60
1	B	245	ARG	CG-CD-NE	-5.17	100.63	112.00
1	C	147	GLU	N-CA-C	-5.16	102.11	110.32
1	E	125	GLN	N-CA-C	5.16	117.65	111.71
1	E	513	CYS	CA-C-N	-5.15	114.77	122.39
1	E	513	CYS	C-N-CA	-5.15	114.77	122.39
1	F	486	LYS	CA-CB-CG	5.14	124.37	114.10
1	D	84	GLU	N-CA-C	-5.12	105.59	111.07
1	A	195	VAL	CG1-CB-CG2	5.10	122.01	110.80
1	D	468	VAL	CB-CA-C	5.09	118.29	110.55
1	E	392	TYR	N-CA-C	-5.07	107.04	113.18
1	A	157	VAL	N-CA-CB	5.07	117.43	110.54
1	D	143	THR	N-CA-CB	-5.05	102.04	110.83
1	E	552	VAL	CG1-CB-CG2	5.02	121.84	110.80

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	VAL	Peptide
1	A	476	ALA	Peptide
1	B	332	GLY	Peptide
1	C	129	LYS	Peptide
1	C	198	ASN	Peptide
1	D	329	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	D	330	VAL	Peptide
1	D	452	GLN	Peptide
1	D	475	ASN	Peptide
1	E	476	ALA	Peptide
1	F	285	MET	Peptide
1	F	286	THR	Peptide
1	F	288	GLU	Peptide
1	F	89	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3896	0	3829	86	0
1	B	3894	0	3831	80	0
1	C	3897	0	3835	69	0
1	D	3575	0	3512	82	0
1	E	3885	0	3817	61	1
1	F	3869	0	3806	74	1
2	A	25	0	11	3	0
2	B	25	0	4	3	0
2	C	25	0	11	1	0
2	D	25	0	11	3	0
2	E	25	0	8	2	0
2	F	25	0	4	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	12	0	18	2	0
4	B	8	0	12	0	0
4	C	8	0	12	0	0
4	E	16	0	24	2	0
4	F	12	0	18	0	0
5	A	12	0	16	0	0
5	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	12	0	16	0	0
6	B	34	0	0	10	0
6	E	34	0	0	1	0
6	F	34	0	0	1	0
7	A	346	0	0	17	0
7	B	299	0	0	17	0
7	C	306	0	0	10	0
7	D	184	0	0	6	0
7	E	290	0	0	14	1
7	F	208	0	0	9	1
All	All	24993	0	22803	442	2

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 10.

All (442) 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:A:205:MET:SD	1:A:334:GLU:HB3	1.50	1.50
1:A:205:MET:SD	1:A:334:GLU:CB	2.24	1.23
1:C:291[B]:ARG:HG3	1:C:291[B]:ARG:HH11	1.10	1.13
1:A:438:ARG:HG2	1:A:481:GLU:OE1	1.52	1.08
1:B:362:ARG:HH21	6:B:1570:Y6W:CAL	1.66	1.08
1:D:329:ASP:O	1:D:330:VAL:HG12	1.51	1.08
1:D:475:ASN:N	1:D:476:ALA:HB2	1.69	1.05
1:A:334:GLU:OE1	7:A:2249:HOH:O	1.76	1.03
1:B:226:HIS:CE1	6:B:1570:Y6W:CAM	2.41	1.02
1:C:538:LEU:HB3	1:C:552:VAL:HG22	1.43	1.00
1:E:537:ASN:HB3	7:E:2277:HOH:O	1.57	1.00
1:C:291[B]:ARG:HH11	1:C:291[B]:ARG:CG	1.75	0.99
1:B:362:ARG:NH2	6:B:1570:Y6W:CAM	2.28	0.97
1:F:287:PRO:HB3	1:F:288:GLU:HB2	1.45	0.95
1:C:291[B]:ARG:HG3	1:C:291[B]:ARG:NH1	1.68	0.93
1:E:493:MET:HG2	7:E:2246:HOH:O	1.71	0.90
1:E:277:ASN:ND2	1:E:279:VAL:HG12	1.87	0.89
1:F:293:ARG:NH1	1:F:299:ALA:O	2.06	0.89
1:E:143:THR:HG23	2:E:1570:UDP:O4	1.71	0.89
1:D:455:ASN:O	1:D:473:CYS:SG	2.32	0.88
1:C:123:HIS:HD2	1:C:125:GLN:H	1.20	0.87
1:B:226:HIS:HE1	6:B:1570:Y6W:CAM	1.80	0.87
1:B:277:ASN:ND2	1:B:279:VAL:HG12	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:THR:HG22	7:A:2083:HOH:O	1.75	0.87
1:D:143:THR:HG23	2:D:1555:UDP:O4	1.73	0.86
1:A:290:ARG:HD2	1:B:493:MET:HE1	1.56	0.85
1:D:475:ASN:CA	1:D:476:ALA:HB2	2.07	0.84
1:B:277:ASN:HD21	1:B:279:VAL:HG12	1.42	0.84
1:B:206:ARG:HG3	1:B:206:ARG:HH11	1.41	0.84
1:C:143:THR:HG23	2:C:1570:UDP:O4	1.76	0.84
1:B:143:THR:HG23	6:B:1570:Y6W:OBG	1.77	0.83
1:D:123:HIS:HD2	1:D:125:GLN:H	1.23	0.83
1:B:362:ARG:HH21	6:B:1570:Y6W:CAM	1.91	0.82
7:A:2052:HOH:O	1:B:514[B]:ARG:NH1	2.04	0.81
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.15	0.81
1:A:553[A]:GLU:OE2	1:A:554:VAL:HG12	1.80	0.81
1:A:329:ASP:O	1:A:330:VAL:HG12	1.81	0.81
1:C:128:ARG:HB3	1:C:129:LYS:HA	1.62	0.81
1:B:329:ASP:H	1:B:380:ASN:HD21	1.24	0.80
1:A:205:MET:SD	1:A:334:GLU:HB2	2.21	0.80
1:A:123:HIS:HD2	1:A:125:GLN:H	1.27	0.79
1:B:206:ARG:HG2	7:B:2089:HOH:O	1.81	0.78
1:F:178:SER:O	1:F:197:ARG:NH2	2.16	0.78
1:B:569:LEU:C	7:B:2296:HOH:O	2.25	0.78
1:C:329:ASP:H	1:C:380:ASN:HD21	1.32	0.78
1:F:457:LEU:HD13	1:F:482:TRP:CE2	2.18	0.78
1:E:329:ASP:H	1:E:380:ASN:HD21	1.30	0.77
1:D:329:ASP:O	1:D:330:VAL:CG1	2.32	0.77
1:C:457:LEU:HD13	1:C:482:TRP:CE2	2.19	0.77
1:D:162:LYS:NZ	7:D:2066:HOH:O	2.12	0.77
1:D:231:GLU:OE1	7:D:2091:HOH:O	2.02	0.76
1:B:362:ARG:NH2	6:B:1570:Y6W:CAL	2.46	0.76
1:F:287:PRO:HB2	1:F:289:GLN:N	2.00	0.76
1:A:290:ARG:CD	1:B:493:MET:HE1	2.15	0.76
1:C:291[B]:ARG:NH2	7:C:2180:HOH:O	2.18	0.76
1:F:287:PRO:CB	1:F:288:GLU:HB2	2.16	0.75
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.21	0.75
1:D:206:ARG:HD3	1:D:326:MET:O	1.87	0.75
1:F:287:PRO:HB2	1:F:289:GLN:H	1.51	0.74
1:F:123:HIS:HD2	1:F:125:GLN:H	1.35	0.74
1:E:399:ALA:HB2	1:E:567:LEU:HD22	1.70	0.74
1:C:178:SER:O	1:C:197:ARG:NH2	2.20	0.73
1:F:329:ASP:H	1:F:380:ASN:HD21	1.36	0.73
1:E:277:ASN:HD21	1:E:279:VAL:HG12	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LYS:HD3	7:A:2130:HOH:O	1.89	0.72
1:E:143:THR:HG23	6:E:1572:Y6W:OBG	1.88	0.72
1:E:457:LEU:HD13	1:E:482:TRP:CE2	2.25	0.71
1:B:279:VAL:HG13	7:B:2143:HOH:O	1.91	0.71
1:A:537:ASN:ND2	7:A:2327:HOH:O	2.24	0.70
1:E:328:MET:HB2	7:E:2110:HOH:O	1.90	0.70
1:B:186:LEU:O	1:B:189:LYS:HE3	1.92	0.70
1:C:523:GLU:OE2	1:C:532:ARG:NH1	2.23	0.70
1:B:414:ARG:HD3	7:B:2183:HOH:O	1.91	0.70
1:B:178:SER:O	1:B:197:ARG:NH2	2.25	0.69
1:F:327:MET:O	1:F:379:ARG:NH2	2.25	0.69
1:E:198:ASN:HD22	1:E:210:ARG:HH11	1.38	0.69
1:B:213:ASP:HB3	7:B:2101:HOH:O	1.93	0.68
1:C:442:HIS:HB2	7:C:2248:HOH:O	1.92	0.68
1:F:319:GLU:OE1	7:F:2146:HOH:O	2.09	0.68
1:C:123:HIS:CD2	1:C:125:GLN:H	2.08	0.68
1:B:439:VAL:HG12	7:B:2212:HOH:O	1.93	0.68
1:A:205:MET:CE	1:A:334:GLU:HB3	2.23	0.68
1:E:286:THR:OG1	1:E:288:GLU:HG3	1.93	0.68
1:B:309:GLY:C	1:B:310:LEU:HD23	2.18	0.68
1:E:205:MET:HB3	7:E:2110:HOH:O	1.92	0.67
1:D:473:CYS:O	1:D:475:ASN:N	2.24	0.67
1:B:143:THR:HG23	2:B:1572:UDP:O4	1.94	0.67
1:D:202:GLU:OE1	1:D:206:ARG:NH2	2.28	0.67
1:D:475:ASN:CA	1:D:476:ALA:CB	2.73	0.67
1:F:285:MET:C	1:F:287:PRO:CD	2.68	0.67
1:F:113:ARG:CD	1:F:115:ASP:OD1	2.43	0.67
1:F:287:PRO:HB3	1:F:288:GLU:CB	2.23	0.66
1:D:476:ALA:HB3	7:D:2170:HOH:O	1.96	0.66
1:B:123:HIS:HD2	1:B:125:GLN:H	1.42	0.66
1:F:334:GLU:OE2	6:F:1572:Y6W:O3	2.11	0.66
1:B:186:LEU:O	1:B:189:LYS:CE	2.44	0.65
1:C:83:GLN:HE22	1:C:114:MET:H	1.44	0.65
1:B:206:ARG:HD3	1:B:326:MET:O	1.95	0.65
1:A:75:LYS:HA	1:A:189:LYS:O	1.96	0.65
1:B:113:ARG:NH1	1:B:115:ASP:OD1	2.29	0.65
1:A:285:MET:O	1:A:290:ARG:NH1	2.29	0.65
1:B:335:ASN:HD22	1:B:335:ASN:H	1.44	0.65
1:D:278:LEU:HD11	1:D:389:MET:HE1	1.78	0.64
1:F:382:ARG:NE	1:F:397:TYR:OH	2.29	0.64
1:C:128:ARG:HB3	1:C:129:LYS:CA	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:362:ARG:HB2	7:F:2025:HOH:O	1.96	0.64
1:A:291[B]:ARG:NH2	7:A:2227:HOH:O	2.30	0.64
1:E:414:ARG:HD3	7:E:2196:HOH:O	1.97	0.64
1:A:343:TRP:CD1	1:A:349:LEU:HD22	2.33	0.63
1:C:335:ASN:H	1:C:335:ASN:HD22	1.46	0.63
1:F:285:MET:O	1:F:287:PRO:HD3	1.98	0.63
1:B:399:ALA:HB2	1:B:567:LEU:HD22	1.79	0.63
1:C:290:ARG:HD3	1:D:493:MET:HE1	1.80	0.63
1:D:386:GLU:OE1	1:D:393:LYS:NZ	2.18	0.63
1:C:78:TRP:CG	1:C:79:PRO:HD3	2.35	0.62
1:A:245:ARG:HG2	7:A:2180:HOH:O	1.98	0.62
1:E:143:THR:CG2	2:E:1570:UDP:O4	2.46	0.62
1:F:113:ARG:HD3	1:F:115:ASP:OD1	1.99	0.62
1:C:305:MET:HE1	1:C:336:LEU:HD23	1.82	0.62
1:C:568:ASN:C	1:C:568:ASN:HD22	2.08	0.62
1:C:113:ARG:HD2	1:C:115:ASP:OD1	2.00	0.61
1:E:108:GLU:HG2	1:E:260:ASN:HA	1.82	0.61
1:B:143:THR:CG2	2:B:1572:UDP:O4	2.49	0.61
1:A:177:TYR:CE2	4:A:1573:EDO:H21	2.35	0.61
1:A:283:ASP:HB3	7:A:2214:HOH:O	1.99	0.61
1:C:538:LEU:HB3	1:C:552:VAL:CG2	2.23	0.61
1:F:335:ASN:H	1:F:335:ASN:HD22	1.49	0.60
1:B:462:HIS:HD2	1:B:467:VAL:O	1.83	0.60
1:C:245:ARG:NH2	1:C:320:GLU:OE1	2.28	0.60
1:B:83:GLN:HE22	1:B:114:MET:H	1.49	0.60
1:D:147:GLU:HG2	1:D:225:SER:HB2	1.84	0.60
1:F:113:ARG:HD2	1:F:115:ASP:OD1	2.03	0.59
1:A:198:ASN:HD22	1:A:210:ARG:HH11	1.51	0.59
1:D:206:ARG:NE	7:D:2086:HOH:O	2.13	0.59
1:F:286:THR:C	1:F:287:PRO:O	2.46	0.59
1:A:525:ILE:HG13	1:A:530:LYS:HB2	1.84	0.59
1:D:153:LEU:O	1:D:157:VAL:HG13	2.03	0.58
1:A:277:ASN:ND2	1:A:279:VAL:H	2.01	0.58
1:D:475:ASN:HA	1:D:476:ALA:HB2	1.84	0.58
1:F:78:TRP:CG	1:F:79:PRO:HD3	2.38	0.58
1:C:258:MET:HE1	7:C:2214:HOH:O	2.01	0.58
1:D:383:ARG:O	1:D:387:VAL:HG23	2.02	0.58
1:A:329:ASP:H	1:A:380:ASN:HD21	1.52	0.58
1:C:335:ASN:H	1:C:335:ASN:ND2	2.02	0.58
1:B:245:ARG:HH22	1:B:320:GLU:CD	2.12	0.57
1:F:313:MET:HE2	1:F:318:PHE:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ARG:CD	1:B:493:MET:CE	2.81	0.57
1:B:143:THR:CG2	6:B:1570:Y6W:OBG	2.50	0.57
1:B:78:TRP:CG	1:B:79:PRO:HD3	2.40	0.57
1:B:206:ARG:HG3	1:B:206:ARG:NH1	2.15	0.57
1:F:290:ARG:HA	1:F:290:ARG:NH1	2.20	0.57
1:D:441:ASP:OD1	1:D:443:GLN:N	2.37	0.57
1:C:414:ARG:HD3	7:C:2207:HOH:O	2.04	0.56
1:D:469:GLY:HA2	1:D:550:LEU:HD23	1.87	0.56
1:F:76:VAL:CG2	1:F:80:ASP:HB2	2.36	0.56
1:F:305:MET:HE1	1:F:336:LEU:HD13	1.87	0.56
1:C:128:ARG:CB	1:C:129:LYS:HA	2.31	0.56
1:C:218:LYS:HD2	1:E:82:ASN:HA	1.87	0.56
1:D:385:ALA:CB	1:D:389:MET:HE3	2.36	0.56
1:E:93:ARG:HB2	1:E:96:GLN:CD	2.31	0.56
1:F:277:ASN:O	7:F:2138:HOH:O	2.18	0.56
1:D:475:ASN:H	1:D:476:ALA:HB2	1.64	0.55
1:B:362:ARG:HH22	6:B:1570:Y6W:CAM	2.16	0.55
1:C:414:ARG:CD	7:C:2207:HOH:O	2.55	0.55
1:F:143:THR:HG23	2:F:1570:UDP:O4	2.05	0.55
1:A:438:ARG:CG	1:A:481:GLU:OE1	2.42	0.55
1:A:474:HIS:CD2	1:A:476:ALA:HB3	2.42	0.55
1:A:541:ASP:CB	1:A:553[B]:GLU:HG3	2.37	0.55
1:F:252:ILE:HD12	1:F:353:PRO:HA	1.89	0.55
1:E:414:ARG:CD	7:E:2196:HOH:O	2.54	0.55
1:C:126:CYS:O	1:C:129:LYS:HB2	2.07	0.54
1:E:309:GLY:C	1:E:310:LEU:HD23	2.32	0.54
1:D:336:LEU:CD1	1:D:340:PHE:CE2	2.90	0.54
1:F:528:ASN:O	1:F:564:LYS:HD2	2.06	0.54
1:A:481:GLU:HG2	1:A:482:TRP:N	2.23	0.54
1:F:335:ASN:H	1:F:335:ASN:ND2	2.05	0.54
1:A:325:ASP:HB2	1:A:414:ARG:HD2	1.88	0.54
1:B:478:GLY:O	1:B:492:HIS:HE1	1.91	0.54
1:F:302:LYS:NZ	1:F:350:GLU:OE2	2.38	0.54
1:B:198:ASN:HD22	1:B:210:ARG:HH11	1.55	0.54
1:C:198:ASN:HD22	1:C:210:ARG:HH11	1.54	0.54
1:D:452:GLN:C	1:D:452:GLN:HE21	2.16	0.54
1:A:414:ARG:HD3	7:A:2251:HOH:O	2.07	0.53
1:D:252:ILE:HD12	1:D:353:PRO:HA	1.89	0.53
1:A:444:ASP:OD2	7:A:2277:HOH:O	2.19	0.53
1:E:177:TYR:O	4:E:1575:EDO:H11	2.08	0.53
1:F:143:THR:HG22	7:F:2062:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:ILE:HB	1:D:484:LEU:HD13	1.90	0.53
1:A:277:ASN:C	1:A:277:ASN:HD22	2.16	0.53
1:A:305:MET:HE2	1:A:339:SER:HB2	1.91	0.53
1:C:452:GLN:NE2	1:C:542:SER:OG	2.35	0.53
1:D:475:ASN:HA	1:D:476:ALA:CB	2.38	0.53
1:B:142:ILE:HB	1:B:173:LEU:HD12	1.92	0.52
1:A:177:TYR:CZ	4:A:1573:EDO:H21	2.44	0.52
1:A:378:ALA:HB3	1:A:406:VAL:HG21	1.89	0.52
1:D:183:ASP:HB2	7:D:2076:HOH:O	2.10	0.52
1:B:146:ASN:HD21	1:B:179:ASN:ND2	2.08	0.52
1:B:334:GLU:OE2	6:B:1570:Y6W:O3	2.27	0.52
1:D:441:ASP:CG	1:D:443:GLN:N	2.68	0.52
1:F:194[B]:ARG:NH1	7:F:2093:HOH:O	2.42	0.52
1:F:198:ASN:HD22	1:F:210:ARG:HH11	1.58	0.52
1:C:290:ARG:CZ	1:D:493:MET:HE1	2.40	0.52
1:E:279:VAL:HG13	7:E:2158:HOH:O	2.10	0.52
1:A:143:THR:CG2	1:A:204:LEU:HD22	2.40	0.52
1:A:414:ARG:CD	7:A:2251:HOH:O	2.58	0.52
1:F:309:GLY:C	1:F:310:LEU:HD23	2.35	0.52
1:D:330:VAL:HA	1:D:332:GLY:N	2.24	0.52
1:E:77:ARG:HD3	7:E:2003:HOH:O	2.10	0.51
1:B:391:GLU:H	1:B:391:GLU:CD	2.18	0.51
1:D:382:ARG:NH1	1:D:406:VAL:O	2.31	0.51
1:F:285:MET:HE1	1:F:293:ARG:NH2	2.25	0.51
1:D:474:HIS:CE1	1:D:476:ALA:HB1	2.46	0.51
1:F:491:LYS:HE2	1:F:513:CYS:SG	2.51	0.51
1:E:123:HIS:CD2	1:E:125:GLN:H	2.29	0.51
1:A:450:LEU:HD13	1:A:563:TRP:CE3	2.46	0.50
1:D:462:HIS:HD2	1:D:467:VAL:O	1.94	0.50
1:F:285:MET:C	1:F:287:PRO:HD2	2.35	0.50
1:A:143:THR:HG23	2:A:1570:UDP:C5	2.47	0.50
1:A:329:ASP:O	1:A:330:VAL:CG1	2.57	0.50
1:C:462:HIS:HD2	1:C:467:VAL:O	1.94	0.50
1:D:331:TRP:CD1	1:D:331:TRP:N	2.80	0.50
1:E:205:MET:CB	7:E:2110:HOH:O	2.54	0.50
1:E:285:MET:O	1:E:290:ARG:NH1	2.44	0.50
1:F:287:PRO:CB	1:F:288:GLU:CB	2.86	0.50
1:B:414:ARG:CD	7:B:2183:HOH:O	2.55	0.50
1:B:376:VAL:O	1:B:377:PHE:CB	2.60	0.50
1:B:530:LYS:NZ	7:B:2271:HOH:O	2.42	0.49
1:B:276:TRP:O	1:B:396:TYR:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ARG:NH1	1:D:115:ASP:OD1	2.45	0.49
1:A:123:HIS:CD2	1:A:125:GLN:H	2.19	0.49
1:B:530:LYS:NZ	1:B:556:GLY:O	2.44	0.49
1:F:457:LEU:HD13	1:F:482:TRP:CD2	2.48	0.49
1:A:333:GLY:HA3	1:A:380:ASN:HB3	1.94	0.49
1:A:309:GLY:C	1:A:310:LEU:HD23	2.37	0.49
1:A:325:ASP:OD1	1:A:325:ASP:C	2.54	0.49
1:F:272:GLY:HA2	1:F:280:PHE:CZ	2.48	0.49
1:C:162:LYS:HE2	7:C:2076:HOH:O	2.12	0.49
1:F:252:ILE:CD1	1:F:353:PRO:HA	2.42	0.49
1:B:310:LEU:HD23	1:B:310:LEU:N	2.27	0.49
1:E:335:ASN:H	1:E:335:ASN:HD22	1.61	0.49
1:E:379:ARG:HG3	1:E:408:TYR:HA	1.95	0.48
1:D:143:THR:CG2	2:D:1555:UDP:O4	2.56	0.48
1:D:235:GLU:HB2	1:D:236:PRO:HD3	1.94	0.48
1:F:242:ALA:HA	7:F:2112:HOH:O	2.14	0.48
1:A:343:TRP:NE1	1:A:349:LEU:HD22	2.28	0.48
1:D:83:GLN:HE22	1:D:114:MET:H	1.60	0.48
1:D:491:LYS:HB3	1:D:496:CYS:SG	2.54	0.48
1:E:277:ASN:CG	1:E:279:VAL:HG12	2.36	0.48
1:A:557:PRO:HB2	1:E:259:ASP:HB3	1.95	0.48
1:C:440:PRO:HG3	1:C:447:PHE:CG	2.49	0.48
1:E:179:ASN:HA	4:E:1575:EDO:H12	1.94	0.48
1:C:465:ASP:O	1:C:509:LYS:HE2	2.14	0.48
1:E:362:ARG:HB2	7:E:2009:HOH:O	2.13	0.48
1:A:452:GLN:NE2	1:A:542:SER:OG	2.38	0.48
1:E:343:TRP:CD1	1:E:349:LEU:HD22	2.49	0.48
1:A:462:HIS:HD2	1:A:467:VAL:O	1.96	0.48
1:A:86:TYR:CE2	1:A:149:ARG:HB3	2.49	0.48
1:C:248:VAL:HB	1:C:349:LEU:HD12	1.96	0.48
1:B:376:VAL:O	1:B:377:PHE:HB2	2.13	0.47
2:D:1555:UDP:O1A	2:D:1555:UDP:O3B	2.32	0.47
1:E:194:ARG:HG3	7:E:2091:HOH:O	2.13	0.47
1:F:382:ARG:NH1	1:F:406:VAL:O	2.46	0.47
1:D:281:LYS:NZ	7:D:2118:HOH:O	2.47	0.47
1:C:525:ILE:O	1:C:528:ASN:N	2.45	0.47
1:D:198:ASN:HD22	1:D:210:ARG:HH11	1.63	0.47
1:E:143:THR:HG21	1:E:204:LEU:HD22	1.96	0.47
1:F:286:THR:O	1:F:287:PRO:O	2.32	0.47
1:C:290:ARG:CD	1:D:493:MET:HE1	2.45	0.47
1:B:132:ARG:HG2	7:B:2037:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:LYS:CE	7:F:2102:HOH:O	2.62	0.47
1:D:252:ILE:CD1	1:D:353:PRO:HA	2.45	0.47
1:E:336:LEU:HD13	1:E:340:PHE:CE2	2.50	0.46
1:F:478:GLY:O	1:F:492:HIS:HE1	1.97	0.46
1:A:183:ASP:HB2	7:A:2120:HOH:O	2.15	0.46
1:B:283:ASP:HA	7:B:2150:HOH:O	2.15	0.46
1:B:231:GLU:HG3	7:B:2107:HOH:O	2.15	0.46
1:E:277:ASN:HD21	1:E:279:VAL:CG1	2.23	0.46
1:E:478:GLY:O	1:E:492:HIS:HE1	1.98	0.46
7:A:2320:HOH:O	1:E:95:GLY:HA2	2.15	0.46
1:F:325:ASP:HB3	1:F:328:MET:HG3	1.97	0.46
1:D:362:ARG:C	1:D:363:LYS:HD3	2.40	0.46
1:D:455:ASN:HD22	1:D:455:ASN:HA	1.65	0.46
1:A:378:ALA:O	1:A:382:ARG:HG3	2.16	0.46
1:C:94:SER:HB3	7:C:2016:HOH:O	2.15	0.46
1:D:342:VAL:HG11	1:D:349:LEU:HD13	1.98	0.46
1:E:94:SER:C	1:E:96:GLN:H	2.24	0.46
1:A:91:MET:CE	7:A:2010:HOH:O	2.63	0.46
1:B:330:VAL:HG22	1:B:330:VAL:O	2.14	0.46
1:D:198:ASN:HD22	1:D:210:ARG:NH1	2.14	0.46
1:E:83:GLN:NE2	7:E:2005:HOH:O	2.48	0.46
1:F:500:VAL:O	1:F:500:VAL:CG1	2.64	0.46
1:E:198:ASN:ND2	1:E:210:ARG:HH11	2.10	0.45
1:C:344:GLN:HE22	1:C:388:TRP:HB3	1.81	0.45
1:D:465:ASP:O	1:D:509:LYS:HE2	2.15	0.45
1:A:143:THR:HG21	1:A:204:LEU:HD22	1.97	0.45
1:A:198:ASN:ND2	1:A:210:ARG:HH11	2.12	0.45
1:B:532:ARG:HG2	1:B:533:HIS:N	2.31	0.45
1:C:94:SER:CB	7:C:2016:HOH:O	2.64	0.45
1:D:343:TRP:CD1	1:D:349:LEU:HD22	2.52	0.45
1:D:455:ASN:O	1:D:456:CYS:HB2	2.17	0.45
1:A:330:VAL:HG13	1:A:330:VAL:O	2.16	0.45
1:A:530:LYS:NZ	7:A:2322:HOH:O	2.50	0.45
1:D:329:ASP:H	1:D:380:ASN:HD21	1.63	0.45
1:D:330:VAL:CG2	1:D:331:TRP:HA	2.47	0.45
1:F:164:PRO:HG2	1:F:167:LEU:HD12	1.98	0.45
1:F:439:VAL:HG13	7:F:2167:HOH:O	2.17	0.45
1:A:276:TRP:C	1:A:278:LEU:H	2.24	0.45
1:C:500:VAL:HG13	1:D:262:GLN:HE22	1.82	0.45
1:D:336:LEU:HD11	1:D:340:PHE:CE2	2.52	0.45
1:C:363:LYS:HG2	7:C:2214:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ARG:CD	7:E:2003:HOH:O	2.64	0.44
1:E:124:ASP:HB2	7:E:2033:HOH:O	2.17	0.44
1:E:153:LEU:O	1:E:157:VAL:HG13	2.16	0.44
1:F:280:PHE:CD1	1:F:281:LYS:N	2.85	0.44
1:B:546:LYS:HA	7:B:2281:HOH:O	2.17	0.44
1:C:206:ARG:HG3	7:C:2111:HOH:O	2.17	0.44
1:F:98:PRO:HB3	1:F:107:VAL:HG23	1.99	0.44
1:A:178:SER:O	1:A:197:ARG:NH2	2.43	0.44
1:B:362:ARG:NH2	2:B:1572:UDP:O1B	2.35	0.44
1:D:484:LEU:HA	1:D:489:SER:O	2.18	0.44
1:A:332:GLY:HA2	1:A:380:ASN:HB2	2.00	0.44
1:D:335:ASN:HD22	1:D:335:ASN:H	1.66	0.44
1:B:114:MET:O	1:B:157:VAL:HG22	2.18	0.44
1:B:186:LEU:O	1:B:189:LYS:HE2	2.17	0.44
1:B:257:ASN:OD1	1:B:259:ASP:N	2.47	0.44
1:D:278:LEU:CD1	1:D:389:MET:HE1	2.46	0.44
1:D:328:MET:HA	1:D:380:ASN:ND2	2.33	0.44
1:D:401:PRO:O	1:D:404:ARG:HG3	2.17	0.44
1:D:328:MET:HA	1:D:380:ASN:HD21	1.83	0.44
1:E:462:HIS:HD2	1:E:467:VAL:O	1.99	0.44
1:C:537:ASN:O	1:C:537:ASN:CG	2.61	0.44
1:D:474:HIS:ND1	1:D:476:ALA:CB	2.80	0.44
1:F:564:LYS:HE3	1:F:565:PHE:N	2.33	0.44
1:B:404:ARG:HD2	7:B:2192:HOH:O	2.18	0.43
1:D:487:GLU:O	1:D:488:LYS:HB2	2.18	0.43
1:D:248:VAL:HB	1:D:349:LEU:HD12	1.99	0.43
1:F:76:VAL:HG23	1:F:80:ASP:HB2	1.99	0.43
1:F:379:ARG:HD3	1:F:408:TYR:HA	2.00	0.43
1:A:143:THR:HG23	2:A:1570:UDP:H5	1.82	0.43
1:D:178:SER:O	1:D:197:ARG:NH2	2.37	0.43
1:E:305:MET:HE1	1:E:336:LEU:HD22	2.00	0.43
1:E:457:LEU:HD13	1:E:482:TRP:CD2	2.53	0.43
1:B:131:TRP:HZ2	7:B:2031:HOH:O	2.01	0.43
1:F:386:GLU:OE1	1:F:393:LYS:HD2	2.18	0.43
1:F:495:LEU:HD23	1:F:512:GLY:HA2	2.00	0.43
1:B:462:HIS:HE1	7:B:2105:HOH:O	2.01	0.43
1:C:424:LYS:HD2	1:C:428:TRP:CE2	2.53	0.43
1:A:97:ASP:OD1	1:A:97:ASP:C	2.62	0.43
1:B:198:ASN:ND2	1:B:210:ARG:HH11	2.17	0.43
1:D:206:ARG:CD	1:D:326:MET:O	2.63	0.43
1:A:334:GLU:HG2	1:A:335:ASN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:ARG:HG2	1:C:408:TYR:HA	2.01	0.43
1:A:277:ASN:ND2	1:A:277:ASN:C	2.77	0.43
1:C:258:MET:HE3	1:C:362:ARG:HB2	1.99	0.43
1:C:343:TRP:CD1	1:C:349:LEU:HD22	2.54	0.43
1:C:567:LEU:HD23	1:C:568:ASN:H	1.84	0.43
1:F:198:ASN:ND2	1:F:210:ARG:HH11	2.16	0.43
1:A:276:TRP:O	1:A:396:TYR:HA	2.19	0.43
1:B:342:VAL:CG1	1:B:349:LEU:HD13	2.49	0.43
1:C:198:ASN:ND2	1:C:210:ARG:HH11	2.17	0.43
1:C:399:ALA:C	1:C:401:PRO:HD3	2.44	0.43
1:C:440:PRO:HG3	1:C:447:PHE:CD2	2.54	0.43
1:F:76:VAL:HG22	1:F:77:ARG:O	2.19	0.43
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.88	0.42
1:C:86:TYR:CE2	1:C:149:ARG:HB3	2.54	0.42
1:E:204:LEU:C	1:E:204:LEU:HD13	2.44	0.42
1:E:289:GLN:O	1:E:293:ARG:HG3	2.18	0.42
1:A:197:ARG:HD3	7:A:2142:HOH:O	2.19	0.42
1:B:206:ARG:CD	1:B:326:MET:O	2.65	0.42
1:B:478:GLY:O	1:B:492:HIS:CE1	2.71	0.42
1:E:450:LEU:HD13	1:E:563:TRP:CE3	2.54	0.42
1:A:296:ASN:C	1:A:296:ASN:HD22	2.26	0.42
1:C:502:ARG:O	1:C:538:LEU:HD11	2.20	0.42
1:C:537:ASN:OD1	1:C:554:VAL:HG23	2.18	0.42
1:D:385:ALA:HB2	1:D:389:MET:HE3	2.00	0.42
1:E:123:HIS:HD2	1:E:125:GLN:HB2	1.84	0.42
1:A:277:ASN:HD22	1:A:278:LEU:N	2.17	0.42
1:D:451:GLN:HG2	1:D:453:GLY:HA2	2.01	0.42
1:F:143:THR:OG1	1:F:207:SER:HB3	2.20	0.42
1:F:305:MET:HE2	1:F:339:SER:HB2	2.00	0.42
1:A:76:VAL:HG12	1:A:77:ARG:O	2.18	0.42
1:A:324:TYR:CE1	1:A:334:GLU:HG3	2.55	0.42
1:E:205:MET:HE2	1:E:334:GLU:HB2	2.01	0.42
1:E:248:VAL:HB	1:E:349:LEU:HD12	2.02	0.42
1:E:291:ARG:CZ	1:E:291:ARG:HB3	2.50	0.42
1:C:377:PHE:O	1:C:377:PHE:CG	2.72	0.42
1:C:478:GLY:O	1:C:492:HIS:HE1	2.01	0.42
1:C:491:LYS:HD2	1:C:493:MET:O	2.19	0.42
1:E:78:TRP:N	1:E:79:PRO:CD	2.82	0.42
1:F:268:ALA:O	1:F:293:ARG:NH2	2.53	0.42
1:A:451:GLN:OE1	1:A:566:THR:CG2	2.67	0.42
1:D:244:ASP:OD1	1:D:246:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:VAL:HA	1:D:332:GLY:H	1.85	0.42
1:F:528:ASN:O	1:F:564:LYS:CD	2.68	0.42
1:F:296:ASN:C	1:F:296:ASN:ND2	2.78	0.42
1:A:248:VAL:HB	1:A:349:LEU:HD12	2.02	0.41
1:B:93:ARG:O	1:B:96:GLN:HG2	2.20	0.41
1:C:258:MET:HE3	1:C:362:ARG:CB	2.50	0.41
1:D:330:VAL:HG22	1:D:331:TRP:HA	2.02	0.41
1:E:78:TRP:CG	1:E:79:PRO:HD3	2.55	0.41
1:A:277:ASN:CG	1:A:279:VAL:HG13	2.45	0.41
1:A:290:ARG:HD3	1:B:493:MET:CE	2.50	0.41
1:A:296:ASN:C	1:A:296:ASN:ND2	2.77	0.41
1:D:387:VAL:HB	1:D:388:TRP:CD1	2.55	0.41
1:E:277:ASN:C	1:E:277:ASN:HD22	2.28	0.41
1:E:335:ASN:H	1:E:335:ASN:ND2	2.18	0.41
1:B:169:LYS:NZ	7:B:2074:HOH:O	2.51	0.41
1:D:385:ALA:HA	1:D:389:MET:HG3	2.00	0.41
1:A:457:LEU:HD13	1:A:482:TRP:CD2	2.55	0.41
1:B:335:ASN:H	1:B:335:ASN:ND2	2.14	0.41
1:D:129:LYS:HE2	1:D:129:LYS:HB3	1.96	0.41
1:E:553[A]:GLU:O	1:E:554:VAL:C	2.63	0.41
1:F:133:VAL:HG22	1:F:166:HIS:CE1	2.56	0.41
1:F:449:ALA:O	1:F:565:PHE:HA	2.20	0.41
1:A:283:ASP:OD1	1:A:283:ASP:N	2.53	0.41
1:B:183:ASP:HB2	7:B:2077:HOH:O	2.21	0.41
1:C:568:ASN:C	1:C:568:ASN:ND2	2.73	0.41
1:A:290:ARG:HD3	1:B:493:MET:HE2	2.02	0.41
1:E:106:GLN:O	1:E:106:GLN:HG2	2.19	0.41
1:B:173:LEU:HD22	1:B:193:VAL:HG13	2.02	0.41
1:C:134:ASP:OD1	1:C:134:ASP:N	2.48	0.41
1:F:392:TYR:OH	1:F:427:LYS:HD2	2.21	0.41
1:A:378:ALA:CB	1:A:406:VAL:HG21	2.51	0.41
1:A:399:ALA:HB2	1:A:567:LEU:HD22	2.03	0.41
1:D:380:ASN:HD22	1:D:380:ASN:HA	1.62	0.41
1:A:327:MET:HB2	1:A:383:ARG:CZ	2.51	0.40
1:B:296:ASN:C	1:B:296:ASN:HD22	2.28	0.40
1:D:244:ASP:OD1	1:D:244:ASP:C	2.63	0.40
7:A:2225:HOH:O	1:B:493:MET:HE1	2.21	0.40
1:C:532:ARG:HD3	1:C:536:SER:O	2.21	0.40
1:F:108:GLU:HG3	7:F:2028:HOH:O	2.20	0.40
1:F:285:MET:HE2	1:F:301:ILE:HG21	2.02	0.40
1:F:299:ALA:HA	1:F:300:PRO:HD2	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:THR:HG23	2:A:1570:UDP:O4	2.21	0.40
1:D:176:ASP:OD1	1:D:198:ASN:OD1	2.37	0.40
1:F:440:PRO:HG3	1:F:447:PHE:CD2	2.56	0.40
1:A:153:LEU:O	1:A:157:VAL:HG13	2.21	0.40
1:B:342:VAL:HG11	1:B:349:LEU:CD1	2.52	0.40
1:C:164:PRO:HA	1:C:165:PRO:HD3	1.95	0.40
1:C:269:ASP:HA	1:C:285:MET:HE3	2.03	0.40
1:D:474:HIS:ND1	1:D:476:ALA:HA	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:2235:HOH:O	7:F:2129:HOH:O[1_655]	1.89	0.31
1:E:320:GLU:OE2	1:F:84:GLU:OE2[3_554]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/571 (84%)	462 (96%)	15 (3%)	4 (1%)	16	8
1	B	481/571 (84%)	459 (95%)	19 (4%)	3 (1%)	21	13
1	C	481/571 (84%)	453 (94%)	25 (5%)	3 (1%)	21	13
1	D	435/571 (76%)	402 (92%)	26 (6%)	7 (2%)	7	2
1	E	480/571 (84%)	460 (96%)	17 (4%)	3 (1%)	21	13
1	F	478/571 (84%)	447 (94%)	24 (5%)	7 (2%)	8	2
All	All	2836/3426 (83%)	2683 (95%)	126 (4%)	27 (1%)	12	5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	B	332	GLY
1	B	477	GLY
1	C	199	ASP
1	D	440	PRO
1	D	456	CYS
1	D	474	HIS
1	D	476	ALA
1	F	286	THR
1	F	287	PRO
1	F	288	GLU
1	A	477	GLY
1	B	377	PHE
1	C	332	GLY
1	D	88	GLY
1	E	93	ARG
1	C	94	SER
1	E	477	GLY
1	F	331	TRP
1	F	475	ASN
1	F	477	GLY
1	A	94	SER
1	D	330	VAL
1	E	475	ASN
1	F	402	SER
1	A	479	ASN
1	D	448	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/485 (87%)	382 (91%)	38 (9%)	9	3
1	B	420/485 (87%)	383 (91%)	37 (9%)	9	4
1	C	420/485 (87%)	379 (90%)	41 (10%)	7	3
1	D	385/485 (79%)	341 (89%)	44 (11%)	5	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	419/485 (86%)	382 (91%)	37 (9%)	9	4
1	F	417/485 (86%)	375 (90%)	42 (10%)	7	2
All	All	2481/2910 (85%)	2242 (90%)	239 (10%)	8	3

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

Mol	Chain	Res	Type
1	A	84	GLU
1	A	94	SER
1	A	112	LEU
1	A	116	ARG
1	A	157	VAL
1	A	173	LEU
1	A	195	VAL
1	A	196	LEU
1	A	204	LEU
1	A	241	VAL
1	A	245	ARG
1	A	277	ASN
1	A	279	VAL
1	A	283	ASP
1	A	288	GLU
1	A	294	GLN
1	A	310	LEU
1	A	325	ASP
1	A	327	MET
1	A	330	VAL
1	A	335	ASN
1	A	336	LEU
1	A	349	LEU
1	A	379	ARG
1	A	421	LEU
1	A	436	GLU
1	A	438	ARG
1	A	439	VAL
1	A	443	GLN
1	A	450	LEU
1	A	457	LEU
1	A	468	VAL
1	A	484	LEU
1	A	500	VAL

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Mol	Chain	Res	Type
1	A	510	LEU
1	A	515	GLU
1	A	531	LEU
1	A	552	VAL
1	B	76	VAL
1	B	83	GLN
1	B	84	GLU
1	B	96	GLN
1	B	102	ASN
1	B	103	LYS
1	B	107	VAL
1	B	112	LEU
1	B	113	ARG
1	B	143	THR
1	B	157	VAL
1	B	173	LEU
1	B	195	VAL
1	B	204	LEU
1	B	206	ARG
1	B	241	VAL
1	B	277	ASN
1	B	283	ASP
1	B	291	ARG
1	B	310	LEU
1	B	321	LEU
1	B	335	ASN
1	B	336	LEU
1	B	349	LEU
1	B	362	ARG
1	B	376	VAL
1	B	421	LEU
1	B	450	LEU
1	B	457	LEU
1	B	468	VAL
1	B	484	LEU
1	B	488	LYS
1	B	508	ILE
1	B	510	LEU
1	B	515	GLU
1	B	546	LYS
1	B	567	LEU
1	C	83	GLN

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Mol	Chain	Res	Type
1	C	84	GLU
1	C	101	ARG
1	C	112	LEU
1	C	116	ARG
1	C	130	GLN
1	C	132	ARG
1	C	143	THR
1	C	157	VAL
1	C	173	LEU
1	C	195	VAL
1	C	196	LEU
1	C	204	LEU
1	C	241	VAL
1	C	258	MET
1	C	277	ASN
1	C	288	GLU
1	C	310	LEU
1	C	321	LEU
1	C	335	ASN
1	C	349	LEU
1	C	379	ARG
1	C	411	ILE
1	C	412	GLN
1	C	421	LEU
1	C	436	GLU
1	C	438	ARG
1	C	439	VAL
1	C	450	LEU
1	C	457	LEU
1	C	468	VAL
1	C	484	LEU
1	C	491	LYS
1	C	502	ARG
1	C	504	PRO
1	C	510	LEU
1	C	515	GLU
1	C	529	SER
1	C	567	LEU
1	C	568	ASN
1	C	569	LEU
1	D	75	LYS
1	D	93	ARG

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Mol	Chain	Res	Type
1	D	96	GLN
1	D	112	LEU
1	D	116	ARG
1	D	129	LYS
1	D	143	THR
1	D	157	VAL
1	D	173	LEU
1	D	177	TYR
1	D	195	VAL
1	D	204	LEU
1	D	241	VAL
1	D	243	GLU
1	D	245	ARG
1	D	271	LYS
1	D	277	ASN
1	D	310	LEU
1	D	329	ASP
1	D	336	LEU
1	D	349	LEU
1	D	362	ARG
1	D	363	LYS
1	D	379	ARG
1	D	391	GLU
1	D	402	SER
1	D	404	ARG
1	D	421	LEU
1	D	436	GLU
1	D	439	VAL
1	D	441	ASP
1	D	452	GLN
1	D	468	VAL
1	D	475	ASN
1	D	484	LEU
1	D	487	GLU
1	D	488	LYS
1	D	491	LYS
1	D	500	VAL
1	D	510	LEU
1	D	514	ARG
1	D	515	GLU
1	D	552	VAL
1	D	554	VAL

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Mol	Chain	Res	Type
1	E	75	LYS
1	E	91	MET
1	E	112	LEU
1	E	113	ARG
1	E	116	ARG
1	E	127	GLN
1	E	129	LYS
1	E	133	VAL
1	E	143	THR
1	E	157	VAL
1	E	173	LEU
1	E	195	VAL
1	E	196	LEU
1	E	204	LEU
1	E	241	VAL
1	E	245	ARG
1	E	277	ASN
1	E	284	TYR
1	E	288	GLU
1	E	310	LEU
1	E	335	ASN
1	E	336	LEU
1	E	349	LEU
1	E	421	LEU
1	E	438	ARG
1	E	439	VAL
1	E	450	LEU
1	E	451	GLN
1	E	457	LEU
1	E	468	VAL
1	E	484	LEU
1	E	500	VAL
1	E	504	PRO
1	E	510	LEU
1	E	552	VAL
1	E	554	VAL
1	E	567	LEU
1	F	75	LYS
1	F	84	GLU
1	F	112	LEU
1	F	116	ARG
1	F	129	LYS

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Mol	Chain	Res	Type
1	F	133	VAL
1	F	143	THR
1	F	157	VAL
1	F	173	LEU
1	F	195	VAL
1	F	196	LEU
1	F	200	ARG
1	F	245	ARG
1	F	277	ASN
1	F	279	VAL
1	F	287	PRO
1	F	294	GLN
1	F	301	ILE
1	F	310	LEU
1	F	334	GLU
1	F	336	LEU
1	F	349	LEU
1	F	379	ARG
1	F	391	GLU
1	F	402	SER
1	F	404	ARG
1	F	421	LEU
1	F	427	LYS
1	F	438	ARG
1	F	439	VAL
1	F	450	LEU
1	F	457	LEU
1	F	468	VAL
1	F	484	LEU
1	F	486	LYS
1	F	502	ARG
1	F	510	LEU
1	F	515	GLU
1	F	552	VAL
1	F	554	VAL
1	F	559	LEU
1	F	564	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN

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Mol	Chain	Res	Type
1	A	106	GLN
1	A	123	HIS
1	A	125	GLN
1	A	127	GLN
1	A	198	ASN
1	A	216	GLN
1	A	277	ASN
1	A	296	ASN
1	A	344	GLN
1	A	394	ASN
1	A	405	ASN
1	A	442	HIS
1	A	443	GLN
1	A	452	GLN
1	A	462	HIS
1	A	474	HIS
1	A	524	GLN
1	A	537	ASN
1	A	562	GLN
1	A	568	ASN
1	B	83	GLN
1	B	96	GLN
1	B	106	GLN
1	B	123	HIS
1	B	125	GLN
1	B	179	ASN
1	B	198	ASN
1	B	262	GLN
1	B	277	ASN
1	B	296	ASN
1	B	335	ASN
1	B	344	GLN
1	B	380	ASN
1	B	451	GLN
1	B	452	GLN
1	B	462	HIS
1	B	474	HIS
1	B	475	ASN
1	B	524	GLN
1	B	537	ASN
1	B	562	GLN
1	B	568	ASN

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Mol	Chain	Res	Type
1	C	83	GLN
1	C	123	HIS
1	C	125	GLN
1	C	198	ASN
1	C	262	GLN
1	C	277	ASN
1	C	296	ASN
1	C	335	ASN
1	C	344	GLN
1	C	380	ASN
1	C	451	GLN
1	C	452	GLN
1	C	462	HIS
1	C	474	HIS
1	C	528	ASN
1	C	568	ASN
1	D	83	GLN
1	D	102	ASN
1	D	123	HIS
1	D	198	ASN
1	D	216	GLN
1	D	262	GLN
1	D	277	ASN
1	D	296	ASN
1	D	335	ASN
1	D	344	GLN
1	D	380	ASN
1	D	452	GLN
1	D	455	ASN
1	D	462	HIS
1	E	83	GLN
1	E	102	ASN
1	E	106	GLN
1	E	123	HIS
1	E	127	GLN
1	E	179	ASN
1	E	198	ASN
1	E	277	ASN
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	380	ASN

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Mol	Chain	Res	Type
1	E	443	GLN
1	E	451	GLN
1	E	462	HIS
1	E	474	HIS
1	E	475	ASN
1	E	537	ASN
1	E	562	GLN
1	F	83	GLN
1	F	102	ASN
1	F	106	GLN
1	F	123	HIS
1	F	127	GLN
1	F	130	GLN
1	F	198	ASN
1	F	216	GLN
1	F	262	GLN
1	F	277	ASN
1	F	296	ASN
1	F	335	ASN
1	F	344	GLN
1	F	380	ASN
1	F	462	HIS
1	F	562	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 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$
2	UDP	A	1570	3	25,26,26	1.61	5 (20%)	38,40,40	1.95	11 (28%)
4	EDO	F	1573	-	3,3,3	0.41	0	2,2,2	0.23	0
5	GOL	F	1577	-	5,5,5	0.58	0	5,5,5	0.84	0
5	GOL	F	1576	-	5,5,5	0.42	0	5,5,5	0.80	0
2	UDP	B	1572	3	25,26,26	1.40	4 (16%)	38,40,40	1.73	5 (13%)
4	EDO	E	1576	-	3,3,3	0.21	0	2,2,2	0.68	0
6	Y6W	B	1570	3	35,36,36	1.96	6 (17%)	49,53,53	1.59	8 (16%)
4	EDO	E	1573	-	3,3,3	0.85	0	2,2,2	0.62	0
4	EDO	E	1575	-	3,3,3	0.60	0	2,2,2	0.96	0
5	GOL	C	1574	-	5,5,5	0.58	0	5,5,5	0.50	0
4	EDO	C	1572	-	3,3,3	0.48	0	2,2,2	0.32	0
5	GOL	A	1576	-	5,5,5	0.43	0	5,5,5	0.32	0
4	EDO	A	1572	-	3,3,3	0.38	0	2,2,2	0.33	0
4	EDO	B	1574	-	3,3,3	0.39	0	2,2,2	0.43	0
4	EDO	F	1575	-	3,3,3	0.50	0	2,2,2	0.30	0
4	EDO	F	1574	-	3,3,3	0.58	0	2,2,2	0.13	0
6	Y6W	F	1572	-	35,36,36	2.09	10 (28%)	49,53,53	1.94	14 (28%)
4	EDO	C	1573	-	3,3,3	0.49	0	2,2,2	0.37	0
6	Y6W	E	1572	-	35,36,36	2.12	7 (20%)	49,53,53	2.15	17 (34%)
2	UDP	F	1570	3	25,26,26	2.02	5 (20%)	38,40,40	1.88	9 (23%)
2	UDP	E	1570	3	25,26,26	1.77	4 (16%)	38,40,40	1.71	6 (15%)
5	GOL	A	1575	-	5,5,5	0.34	0	5,5,5	1.27	1 (20%)
4	EDO	E	1574	-	3,3,3	0.50	0	2,2,2	0.11	0
4	EDO	B	1573	-	3,3,3	0.45	0	2,2,2	0.39	0
4	EDO	A	1573	-	3,3,3	0.57	0	2,2,2	0.48	0
2	UDP	D	1555	3	25,26,26	1.20	3 (12%)	38,40,40	1.84	7 (18%)
4	EDO	A	1574	-	3,3,3	0.41	0	2,2,2	0.61	0
2	UDP	C	1570	3	25,26,26	1.67	6 (24%)	38,40,40	1.74	7 (18%)

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
2	UDP	A	1570	3	-	0/16/32/32	0/2/2/2
4	EDO	F	1573	-	-	0/1/1/1	-
5	GOL	F	1577	-	-	2/4/4/4	-
5	GOL	F	1576	-	-	0/4/4/4	-
2	UDP	B	1572	3	-	2/16/32/32	0/2/2/2
4	EDO	E	1576	-	-	0/1/1/1	-
6	Y6W	B	1570	3	-	6/19/55/55	0/3/3/3
4	EDO	E	1573	-	-	1/1/1/1	-
4	EDO	E	1575	-	-	1/1/1/1	-
5	GOL	C	1574	-	-	2/4/4/4	-
4	EDO	C	1572	-	-	0/1/1/1	-
5	GOL	A	1576	-	-	2/4/4/4	-
4	EDO	A	1572	-	-	1/1/1/1	-
4	EDO	B	1574	-	-	0/1/1/1	-
4	EDO	F	1575	-	-	0/1/1/1	-
4	EDO	F	1574	-	-	1/1/1/1	-
6	Y6W	F	1572	-	-	10/19/55/55	0/3/3/3
4	EDO	C	1573	-	-	1/1/1/1	-
6	Y6W	E	1572	-	-	8/19/55/55	0/3/3/3
2	UDP	F	1570	3	-	3/16/32/32	0/2/2/2
2	UDP	E	1570	3	-	2/16/32/32	0/2/2/2
5	GOL	A	1575	-	-	2/4/4/4	-
4	EDO	E	1574	-	-	0/1/1/1	-
4	EDO	B	1573	-	-	1/1/1/1	-
4	EDO	A	1573	-	-	0/1/1/1	-
2	UDP	D	1555	3	-	2/16/32/32	0/2/2/2
4	EDO	A	1574	-	-	1/1/1/1	-
2	UDP	C	1570	3	-	2/16/32/32	0/2/2/2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1572	Y6W	OBE-CBA	7.71	1.36	1.23
6	B	1570	Y6W	OBE-CBA	7.57	1.36	1.23
6	F	1572	Y6W	OBE-CBA	7.35	1.36	1.23
2	F	1570	UDP	PA-O3A	6.36	1.66	1.59
6	B	1570	Y6W	OBG-CBD	6.16	1.36	1.24
2	E	1570	UDP	PA-O3A	6.11	1.66	1.59
6	E	1572	Y6W	OBG-CBD	5.90	1.36	1.24
6	F	1572	Y6W	OBG-CBD	5.25	1.34	1.24
2	C	1570	UDP	PA-O3A	4.77	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1570	UDP	C4-N3	-4.46	1.31	1.38
2	A	1570	UDP	O2-C2	4.19	1.30	1.23
2	A	1570	UDP	C2-N1	3.54	1.44	1.38
2	C	1570	UDP	C2-N1	3.42	1.43	1.38
6	F	1572	Y6W	PAN-OAO	-3.34	1.48	1.56
6	B	1570	Y6W	PAN-OAO	-3.28	1.48	1.56
2	F	1570	UDP	C2-N3	-3.19	1.32	1.38
2	B	1572	UDP	PA-O3A	3.10	1.62	1.59
6	E	1572	Y6W	PAN-OAO	-3.06	1.48	1.56
6	F	1572	Y6W	CBD-NBF	-3.06	1.33	1.38
2	F	1570	UDP	C2-N1	3.05	1.43	1.38
6	E	1572	Y6W	CBD-NBF	-2.98	1.33	1.38
2	B	1572	UDP	C4-N3	-2.91	1.33	1.38
2	C	1570	UDP	C4-N3	-2.85	1.33	1.38
2	E	1570	UDP	C2-N3	-2.85	1.33	1.38
6	E	1572	Y6W	O4'-C1'	2.74	1.48	1.42
2	D	1555	UDP	C2-N3	-2.71	1.33	1.38
2	E	1570	UDP	C2-N1	2.70	1.42	1.38
2	A	1570	UDP	PA-O3A	2.61	1.62	1.59
2	A	1570	UDP	C2-N3	-2.59	1.33	1.38
2	D	1555	UDP	C2-N1	2.58	1.42	1.38
2	D	1555	UDP	PA-O3A	2.55	1.62	1.59
6	B	1570	Y6W	CBA-NAZ	-2.54	1.34	1.38
2	E	1570	UDP	C4-N3	-2.52	1.34	1.38
6	E	1572	Y6W	CBA-NBF	-2.47	1.33	1.38
6	B	1570	Y6W	CBD-NBF	-2.37	1.34	1.38
2	B	1572	UDP	C2-N1	2.36	1.42	1.38
6	F	1572	Y6W	CBA-NBF	-2.28	1.34	1.38
2	C	1570	UDP	O4'-C1'	2.28	1.47	1.42
6	F	1572	Y6W	CAK-C1	2.26	1.57	1.52
6	E	1572	Y6W	O4'-C4'	2.25	1.50	1.45
6	F	1572	Y6W	CBC-CBD	-2.23	1.38	1.43
6	F	1572	Y6W	C4-C5	-2.23	1.48	1.53
6	F	1572	Y6W	CBA-NAZ	-2.17	1.35	1.38
2	C	1570	UDP	C2-N3	-2.17	1.34	1.38
6	F	1572	Y6W	O4'-C1'	2.15	1.47	1.42
2	A	1570	UDP	C5-C4	-2.10	1.39	1.43
2	B	1572	UDP	C2-N3	-2.10	1.34	1.38
2	F	1570	UDP	C5-C4	-2.08	1.39	1.43
2	C	1570	UDP	O2-C2	2.07	1.26	1.23
6	B	1570	Y6W	CBC-CBD	-2.01	1.39	1.43

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1570	UDP	C5-C4-N3	6.20	123.49	114.80
2	B	1572	UDP	C4-N3-C2	-5.15	120.22	126.61
6	F	1572	Y6W	NBF-CBA-NAZ	5.11	121.54	114.89
2	D	1555	UDP	C4-N3-C2	-5.10	120.28	126.61
2	E	1570	UDP	C5-C4-N3	4.93	121.71	114.80
2	E	1570	UDP	C4-N3-C2	-4.92	120.51	126.61
2	D	1555	UDP	C5-C4-N3	4.90	121.66	114.80
2	C	1570	UDP	C5-C4-N3	4.81	121.54	114.80
2	B	1572	UDP	C5-C4-N3	4.74	121.44	114.80
6	E	1572	Y6W	O5'-PAN-CAM	-4.72	91.88	104.25
6	B	1570	Y6W	NBF-CBA-NAZ	4.60	120.88	114.89
2	F	1570	UDP	C4-N3-C2	-4.60	120.90	126.61
6	E	1572	Y6W	C5-O5-C1	-4.60	105.14	113.19
2	F	1570	UDP	N3-C2-N1	4.57	120.84	114.89
2	F	1570	UDP	C5-C4-N3	4.56	121.19	114.80
2	B	1572	UDP	N3-C2-N1	4.46	120.69	114.89
6	E	1572	Y6W	CBC-CBD-NBF	4.40	120.97	114.80
2	A	1570	UDP	O3B-PB-O3A	4.30	119.04	104.64
2	C	1570	UDP	C4-N3-C2	-4.29	121.29	126.61
6	F	1572	Y6W	CBD-NBF-CBA	-4.26	121.33	126.61
6	B	1570	Y6W	CBD-NBF-CBA	-4.26	121.33	126.61
6	F	1572	Y6W	CBC-CBD-NBF	4.07	120.50	114.80
6	E	1572	Y6W	NBF-CBA-NAZ	3.95	120.03	114.89
2	D	1555	UDP	O3B-PB-O1B	3.84	125.82	110.83
6	E	1572	Y6W	CBD-NBF-CBA	-3.84	121.85	126.61
6	B	1570	Y6W	CBC-CBD-NBF	3.83	120.17	114.80
2	A	1570	UDP	O3A-PB-O1B	-3.73	91.39	111.04
2	A	1570	UDP	C4-N3-C2	-3.57	122.18	126.61
6	E	1572	Y6W	CAK-C1-C2	-3.55	108.17	114.10
2	F	1570	UDP	O2-C2-N3	-3.53	114.99	121.49
6	F	1572	Y6W	O5-C1-C2	-3.45	103.47	109.70
2	D	1555	UDP	N3-C2-N1	3.39	119.31	114.89
6	E	1572	Y6W	C4-C3-C2	3.27	116.56	110.83
6	E	1572	Y6W	O6-C6-C5	-3.12	100.72	111.33
2	E	1570	UDP	N3-C2-N1	3.11	118.94	114.89
2	D	1555	UDP	O2A-PA-O1A	3.11	126.89	112.44
6	B	1570	Y6W	OBG-CBD-CBC	-3.03	119.94	125.16
6	F	1572	Y6W	O6-C6-C5	-3.02	101.04	111.33
6	F	1572	Y6W	O4'-C1'-NAZ	3.01	115.19	108.36
6	F	1572	Y6W	OAO-PAN-OBH	3.01	119.74	109.95
2	A	1570	UDP	C6-C5-C4	-3.00	115.70	119.53
6	B	1570	Y6W	OAO-PAN-OBH	2.98	119.67	109.95
6	E	1572	Y6W	CAK-CAL-CAM	-2.94	106.46	112.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1572	Y6W	OA0-PAN-OBH	2.94	119.53	109.95
6	F	1572	Y6W	O5-C1-CAK	2.92	116.04	108.34
2	E	1570	UDP	O5'-C5'-C4'	2.86	118.72	108.99
2	D	1555	UDP	O4'-C1'-N1	2.85	114.82	108.36
6	F	1572	Y6W	O5'-PAN-CAM	-2.83	96.83	104.25
2	F	1570	UDP	O4-C4-N3	-2.81	115.20	119.27
6	E	1572	Y6W	O4'-C1'-NAZ	2.81	114.73	108.36
2	C	1570	UDP	C2'-C3'-C4'	2.74	107.90	102.61
6	E	1572	Y6W	OBE-CBA-NBF	-2.73	116.45	121.49
6	E	1572	Y6W	OA0-PAN-CAM	2.69	111.88	105.54
6	B	1570	Y6W	CAK-C1-C2	-2.69	109.61	114.10
2	C	1570	UDP	N3-C2-N1	2.67	118.37	114.89
6	E	1572	Y6W	C1'-NAZ-CBA	2.66	122.38	117.59
2	E	1570	UDP	O4-C4-C5	-2.57	120.73	125.16
2	C	1570	UDP	O3B-PB-O1B	2.56	120.82	110.83
2	F	1570	UDP	O3B-PB-O2B	2.55	117.36	107.80
2	A	1570	UDP	O2A-PA-O1A	2.54	124.25	112.44
2	A	1570	UDP	O4-C4-N3	-2.53	115.60	119.27
2	F	1570	UDP	C1'-N1-C2	2.52	122.12	117.59
6	E	1572	Y6W	O3-C3-C2	-2.51	104.46	110.38
2	F	1570	UDP	O4'-C1'-N1	2.49	114.01	108.36
6	B	1570	Y6W	C4'-O4'-C1'	-2.49	103.97	109.47
6	B	1570	Y6W	OBE-CBA-NAZ	-2.47	119.58	122.80
2	A	1570	UDP	O4-C4-C5	-2.47	120.91	125.16
6	F	1572	Y6W	OBG-CBD-CBC	-2.40	121.02	125.16
6	F	1572	Y6W	O4'-C1'-C2'	-2.40	101.48	106.62
2	B	1572	UDP	O4-C4-C5	-2.39	121.04	125.16
6	F	1572	Y6W	CAK-C1-C2	-2.34	110.19	114.10
2	C	1570	UDP	O4'-C1'-N1	2.30	113.58	108.36
2	D	1555	UDP	O4-C4-C5	-2.30	121.20	125.16
2	A	1570	UDP	O3A-PA-O1A	-2.29	103.81	110.70
2	C	1570	UDP	O4-C4-C5	-2.29	121.21	125.16
2	F	1570	UDP	C6-N1-C2	-2.23	118.29	121.00
6	F	1572	Y6W	C5-O5-C1	-2.23	109.29	113.19
2	E	1570	UDP	O3A-PB-O1B	-2.15	99.75	111.04
6	E	1572	Y6W	OBG-CBD-CBC	-2.14	121.47	125.16
2	A	1570	UDP	O3B-PB-O1B	2.10	119.02	110.83
6	F	1572	Y6W	CAK-CAL-CAM	-2.08	108.27	112.61
5	A	1575	GOL	O3-C3-C2	-2.07	101.05	110.38
6	E	1572	Y6W	O4'-C1'-C2'	-2.06	102.20	106.62
2	B	1572	UDP	O5'-C5'-C4'	2.06	116.00	108.99
2	A	1570	UDP	O2-C2-N1	2.00	125.40	122.80

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1572	UDP	PA-O3A-PB-O2B
2	B	1572	UDP	PA-O3A-PB-O3B
2	C	1570	UDP	PA-O3A-PB-O3B
2	D	1555	UDP	PA-O3A-PB-O3B
2	F	1570	UDP	PA-O3A-PB-O3B
5	A	1575	GOL	O1-C1-C2-C3
5	A	1576	GOL	C1-C2-C3-O3
5	C	1574	GOL	O1-C1-C2-C3
6	B	1570	Y6W	O5-C1-CAK-CAL
6	E	1572	Y6W	O5-C1-CAK-CAL
6	F	1572	Y6W	O5-C1-CAK-CAL
6	F	1572	Y6W	C1-CAK-CAL-CAM
6	E	1572	Y6W	O5-C5-C6-O6
6	E	1572	Y6W	C4-C5-C6-O6
6	F	1572	Y6W	C5'-O5'-PAN-CAM
6	E	1572	Y6W	CAK-CAL-CAM-PAN
6	F	1572	Y6W	CAK-CAL-CAM-PAN
6	F	1572	Y6W	O5-C5-C6-O6
5	F	1577	GOL	O1-C1-C2-C3
5	A	1575	GOL	O1-C1-C2-O2
5	A	1576	GOL	O2-C2-C3-O3
4	B	1573	EDO	O1-C1-C2-O2
4	E	1575	EDO	O1-C1-C2-O2
5	C	1574	GOL	O1-C1-C2-O2
5	F	1577	GOL	O1-C1-C2-O2
6	F	1572	Y6W	C4-C5-C6-O6
4	A	1572	EDO	O1-C1-C2-O2
2	E	1570	UDP	PA-O3A-PB-O1B
6	B	1570	Y6W	CAK-CAL-CAM-PAN
6	B	1570	Y6W	C4-C5-C6-O6
6	F	1572	Y6W	CAL-CAM-PAN-OBH
6	B	1570	Y6W	O5-C5-C6-O6
6	E	1572	Y6W	C2-C1-CAK-CAL
6	F	1572	Y6W	C2-C1-CAK-CAL
2	C	1570	UDP	PA-O3A-PB-O1B
2	E	1570	UDP	PA-O3A-PB-O3B
6	F	1572	Y6W	C4'-C5'-O5'-PAN
6	B	1570	Y6W	C4'-C5'-O5'-PAN
4	A	1574	EDO	O1-C1-C2-O2
4	C	1573	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	E	1573	EDO	O1-C1-C2-O2
4	F	1574	EDO	O1-C1-C2-O2
2	F	1570	UDP	PA-O3A-PB-O1B
2	D	1555	UDP	PA-O3A-PB-O2B
2	F	1570	UDP	PA-O3A-PB-O2B
6	B	1570	Y6W	C1-CAK-CAL-CAM
6	E	1572	Y6W	C1-CAK-CAL-CAM
6	E	1572	Y6W	C5'-O5'-PAN-CAM
6	E	1572	Y6W	C4'-C5'-O5'-PAN
6	F	1572	Y6W	CAL-CAM-PAN-O5'

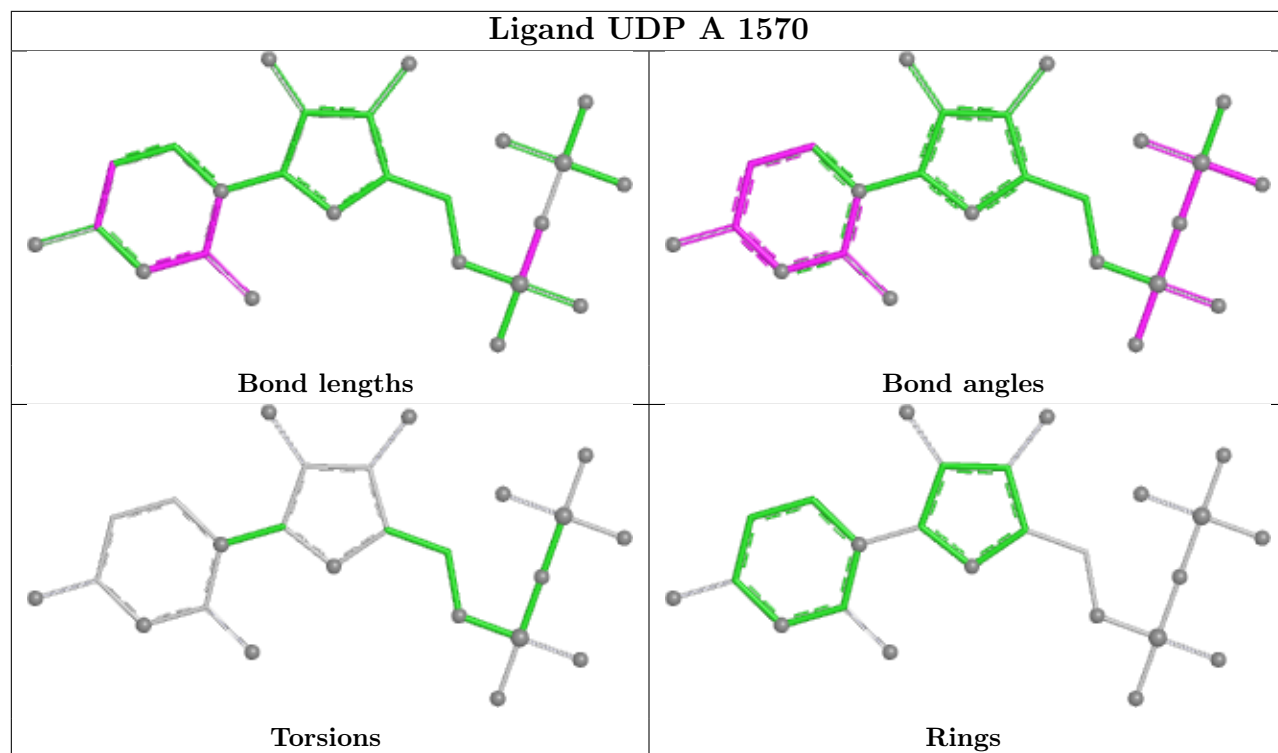
There are no ring outliers.

11 monomers are involved in 29 short contacts:

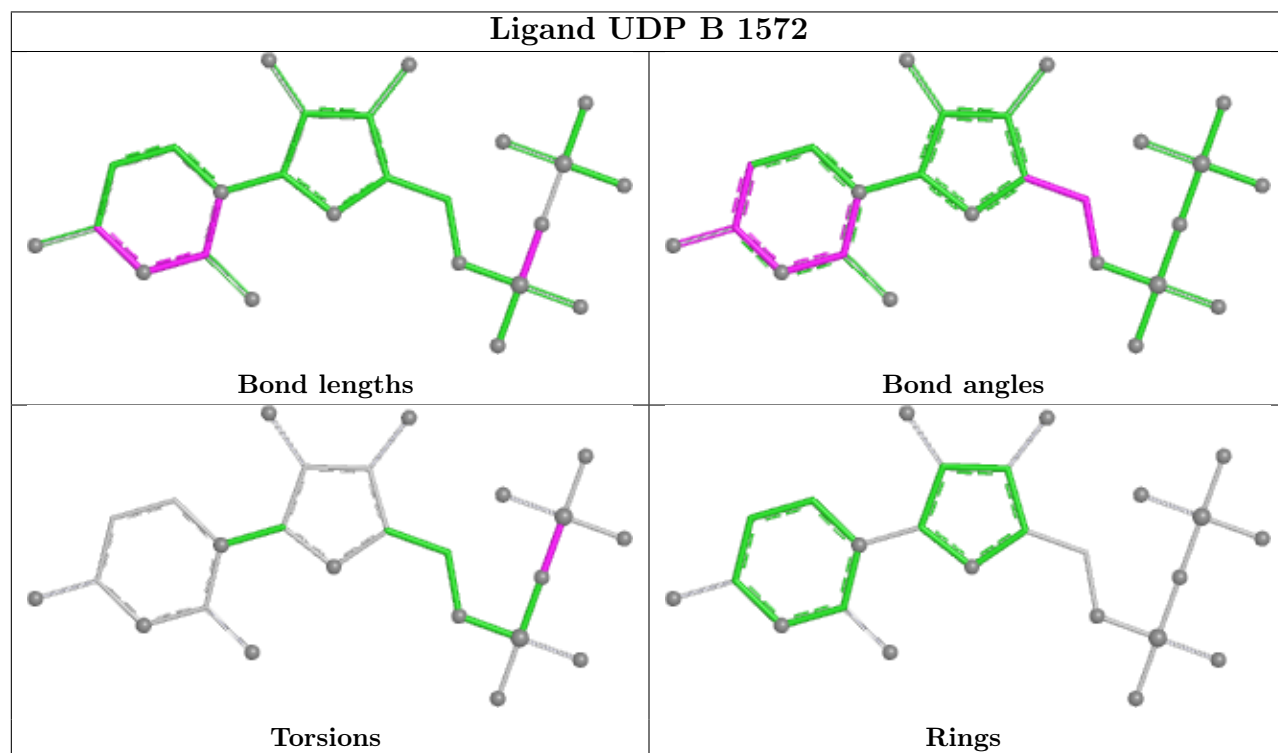
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1570	UDP	3	0
2	B	1572	UDP	3	0
6	B	1570	Y6W	10	0
4	E	1575	EDO	2	0
6	F	1572	Y6W	1	0
6	E	1572	Y6W	1	0
2	F	1570	UDP	1	0
2	E	1570	UDP	2	0
4	A	1573	EDO	2	0
2	D	1555	UDP	3	0
2	C	1570	UDP	1	0

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

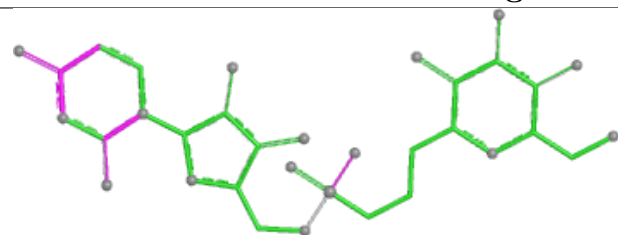
Ligand UDP A 1570



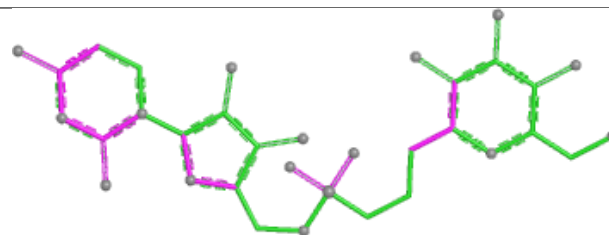
Ligand UDP B 1572



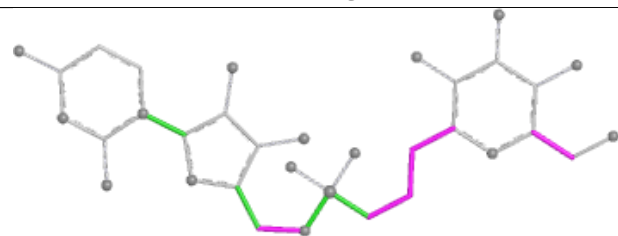
Ligand Y6W B 1570



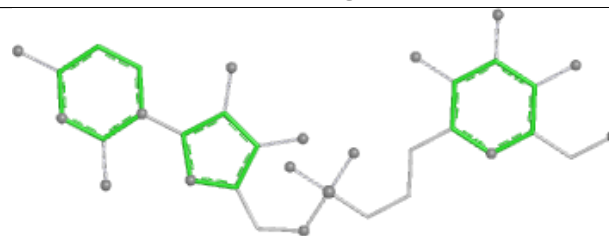
Bond lengths



Bond angles

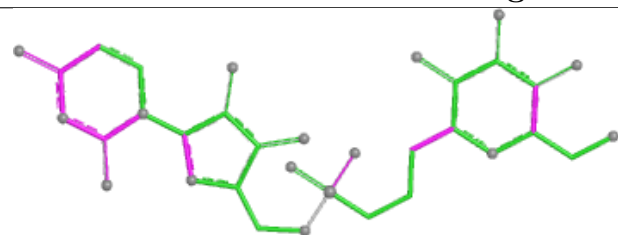


Torsions

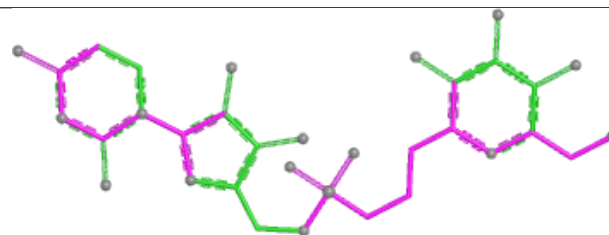


Rings

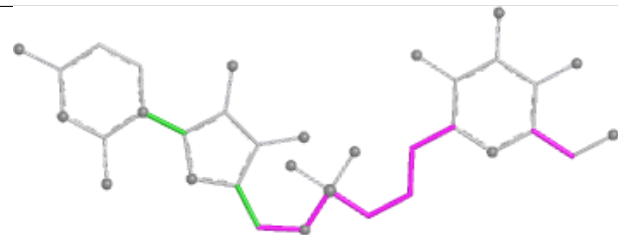
Ligand Y6W F 1572



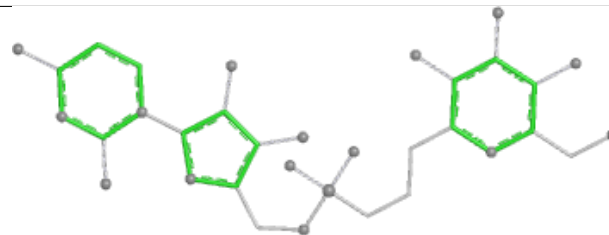
Bond lengths



Bond angles

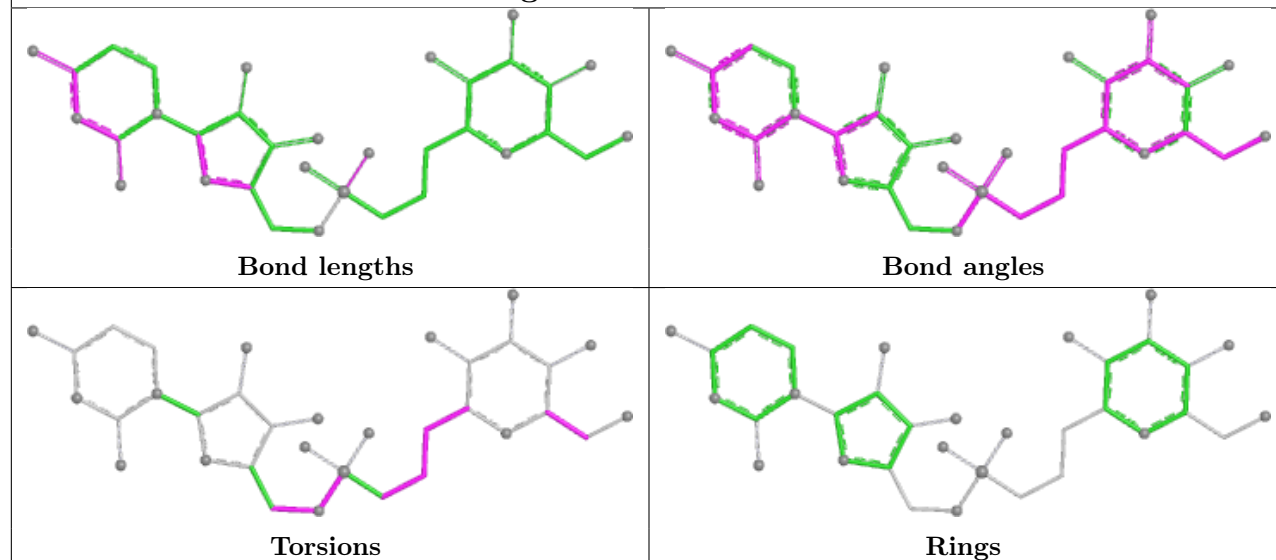


Torsions

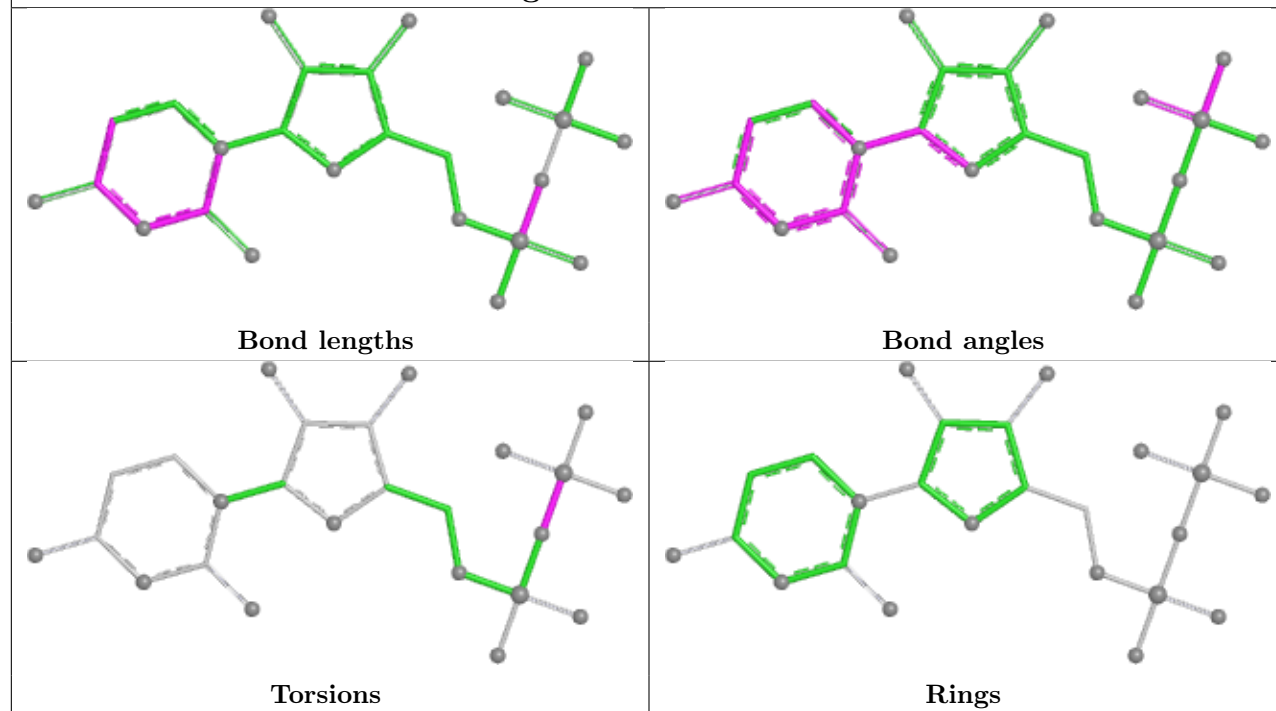


Rings

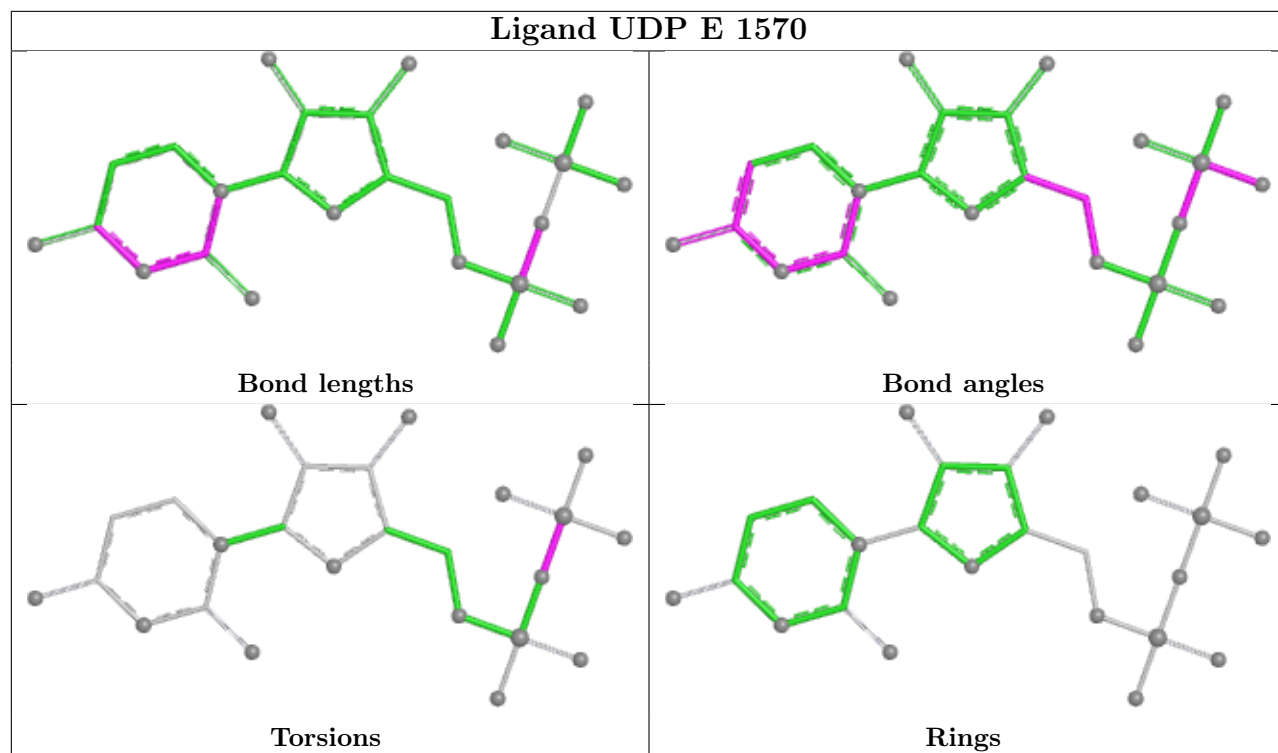
Ligand Y6W E 1572



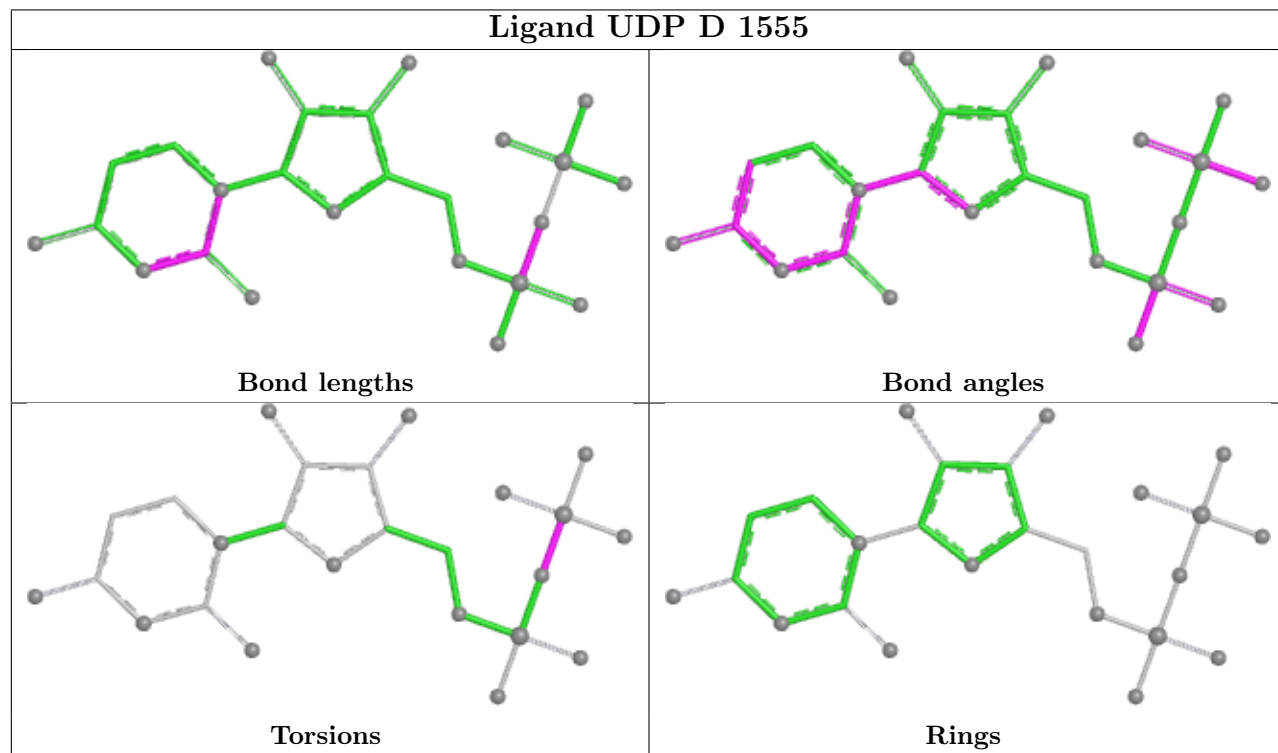
Ligand UDP F 1570

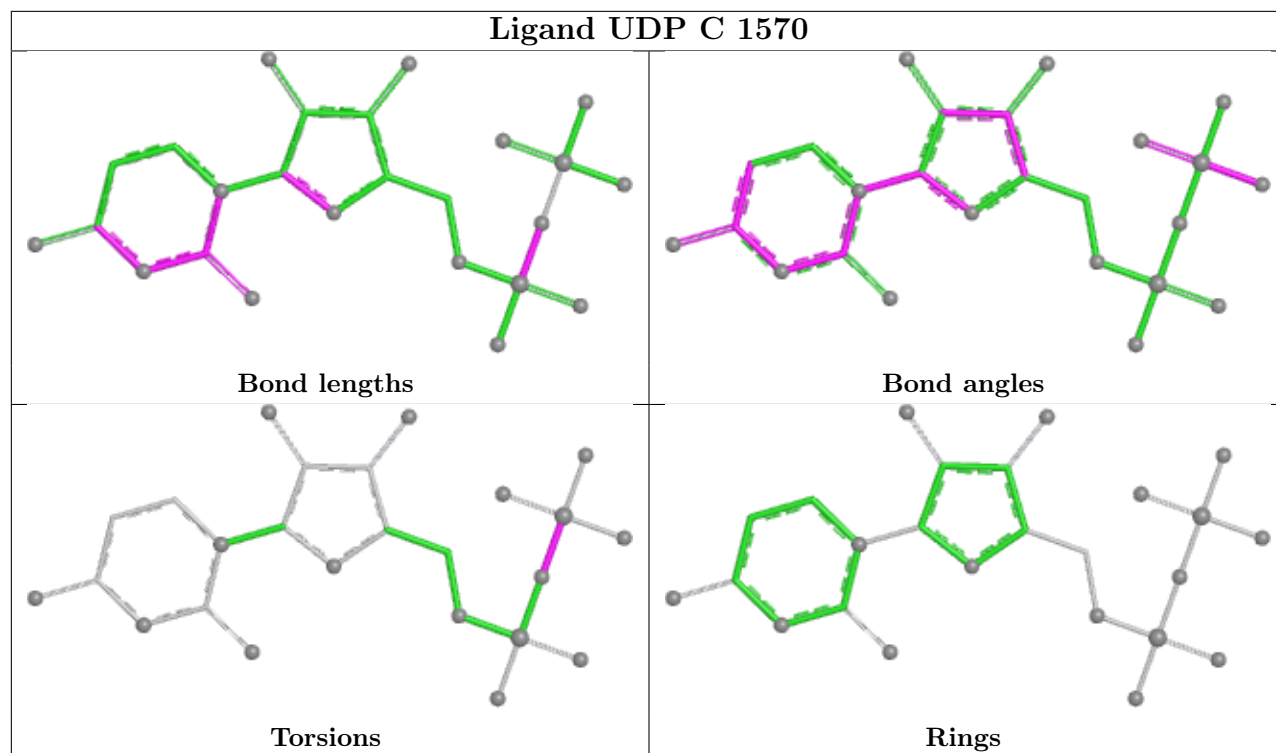


Ligand UDP E 1570



Ligand UDP D 1555





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	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	319:GLU	C	320:GLU	N	1.19
1	E	513:CYS	C	514:ARG	N	1.15

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	483/571 (84%)	-0.18	5 (1%) 79 82	20, 41, 67, 107	7 (1%)
1	B	484/571 (84%)	-0.19	6 (1%) 76 78	19, 40, 73, 147	6 (1%)
1	C	482/571 (84%)	-0.11	12 (2%) 58 60	16, 44, 70, 110	8 (1%)
1	D	443/571 (77%)	0.20	18 (4%) 41 42	27, 51, 87, 107	5 (1%)
1	E	483/571 (84%)	-0.17	6 (1%) 76 78	15, 39, 65, 105	6 (1%)
1	F	481/571 (84%)	0.29	11 (2%) 61 63	26, 54, 82, 96	6 (1%)
All	All	2856/3426 (83%)	-0.03	58 (2%) 65 67	15, 44, 79, 147	38 (1%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	VAL	5.1
1	A	377	PHE	4.9
1	F	378	ALA	4.3
1	C	377	PHE	4.1
1	E	284	TYR	4.0
1	C	569	LEU	3.9
1	D	377	PHE	3.6
1	F	307	ALA	3.5
1	E	333	GLY	3.5
1	D	525	ILE	3.5
1	D	330	VAL	3.4
1	D	554	VAL	3.4
1	B	92	VAL	3.1
1	C	89	GLY	3.1
1	D	331	TRP	3.0
1	D	476	ALA	2.9
1	F	332	GLY	2.9
1	E	95	GLY	2.8
1	F	286	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	361	PHE	2.8
1	B	405	ASN	2.8
1	A	376	VAL	2.8
1	D	447	PHE	2.7
1	C	128	ARG	2.7
1	C	555	CYS	2.6
1	F	361	PHE	2.5
1	D	88	GLY	2.5
1	B	90	THR	2.5
1	E	442	HIS	2.5
1	D	291	ARG	2.4
1	F	474	HIS	2.4
1	A	332	GLY	2.4
1	C	127[A]	GLN	2.4
1	D	376	VAL	2.4
1	B	377	PHE	2.4
1	E	477	GLY	2.3
1	D	552	VAL	2.3
1	B	361	PHE	2.3
1	C	130	GLN	2.3
1	C	77[A]	ARG	2.3
1	C	361	PHE	2.2
1	D	500	VAL	2.2
1	F	284	TYR	2.2
1	F	331	TRP	2.2
1	D	101	ARG	2.2
1	F	514	ARG	2.2
1	C	554	VAL	2.2
1	A	333	GLY	2.1
1	B	100	ALA	2.1
1	C	531	LEU	2.1
1	D	450	LEU	2.1
1	E	91	MET	2.1
1	C	101	ARG	2.1
1	D	177	TYR	2.1
1	D	445	ILE	2.1
1	D	550	LEU	2.0
1	F	291	ARG	2.0
1	F	290	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	1576	6/6	0.72	0.13	74,80,86,89	0
4	EDO	A	1574	4/4	0.75	0.12	72,75,80,80	0
6	Y6W	B	1570	34/34	0.75	0.17	40,53,57,58	34
4	EDO	F	1575	4/4	0.76	0.13	66,69,69,71	0
4	EDO	F	1574	4/4	0.78	0.13	72,73,76,78	0
5	GOL	F	1577	6/6	0.78	0.13	66,67,69,72	0
4	EDO	C	1573	4/4	0.78	0.12	65,72,73,77	0
4	EDO	F	1573	4/4	0.80	0.12	72,74,76,79	0
4	EDO	A	1573	4/4	0.80	0.16	64,65,66,67	0
6	Y6W	F	1572	34/34	0.80	0.18	61,78,100,105	34
4	EDO	A	1572	4/4	0.81	0.11	78,80,81,84	0
4	EDO	E	1575	4/4	0.81	0.13	44,47,51,62	0
5	GOL	C	1574	6/6	0.81	0.11	50,60,63,65	0
6	Y6W	E	1572	34/34	0.83	0.16	48,56,73,74	34
4	EDO	B	1573	4/4	0.83	0.13	55,64,67,70	0
4	EDO	E	1574	4/4	0.85	0.14	63,65,72,73	0
5	GOL	F	1576	6/6	0.85	0.14	68,73,81,87	0
2	UDP	B	1572	25/25	0.86	0.14	35,53,57,58	25
5	GOL	A	1575	6/6	0.87	0.11	56,65,73,78	0
4	EDO	B	1574	4/4	0.91	0.10	50,54,55,56	0
4	EDO	C	1572	4/4	0.91	0.12	52,55,56,60	0
2	UDP	D	1555	25/25	0.93	0.09	51,60,70,76	0
2	UDP	F	1570	25/25	0.93	0.10	37,44,46,49	25
4	EDO	E	1576	4/4	0.95	0.09	44,50,51,60	0
2	UDP	E	1570	25/25	0.95	0.09	29,35,42,42	25
4	EDO	E	1573	4/4	0.95	0.10	30,31,37,40	0
2	UDP	C	1570	25/25	0.96	0.07	40,49,55,59	0

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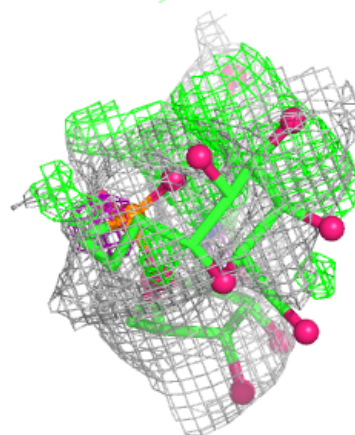
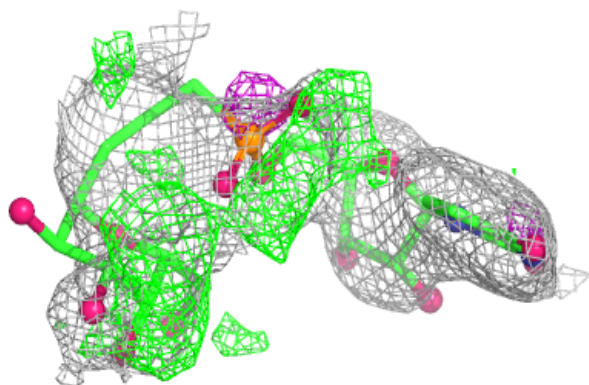
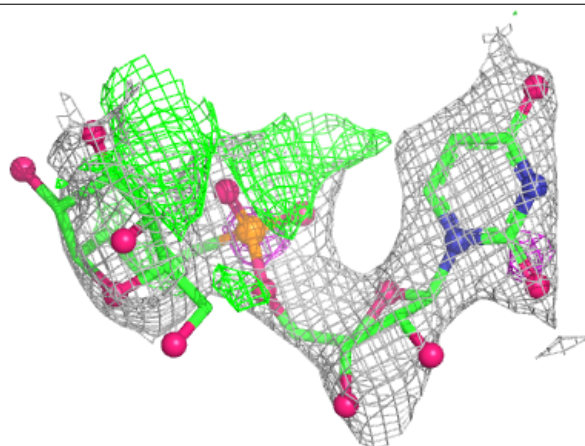
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UDP	A	1570	25/25	0.96	0.07	37,44,50,51	0
3	MN	B	1571	1/1	0.99	0.04	35,35,35,35	0
3	MN	F	1571	1/1	0.99	0.03	34,34,34,34	0
3	MN	E	1571	1/1	1.00	0.03	29,29,29,29	0
3	MN	A	1571	1/1	1.00	0.02	27,27,27,27	0
3	MN	C	1571	1/1	1.00	0.02	30,30,30,30	0
3	MN	D	1556	1/1	1.00	0.03	41,41,41,41	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.

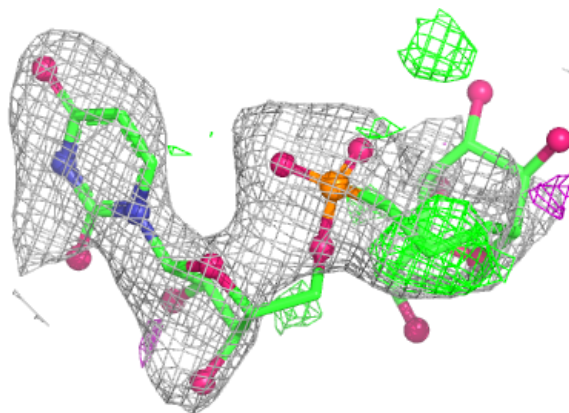
Electron density around Y6W B 1570:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

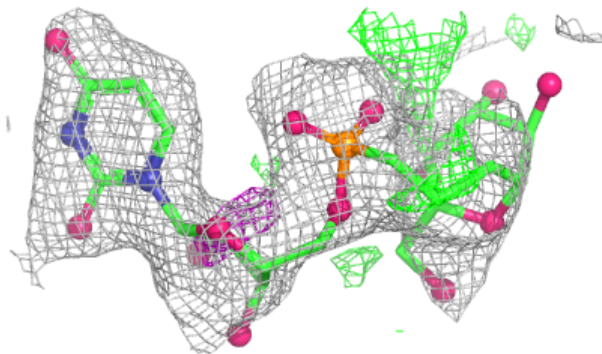


Electron density around Y6W F 1572:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

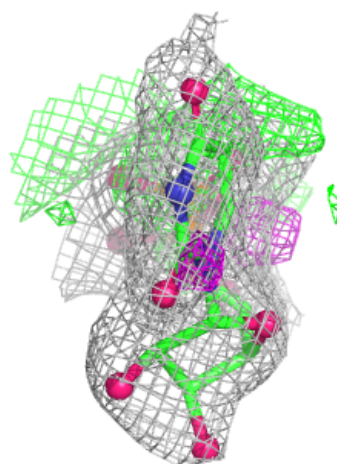
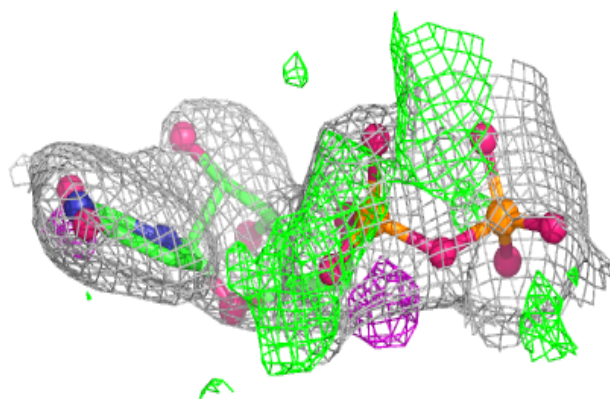
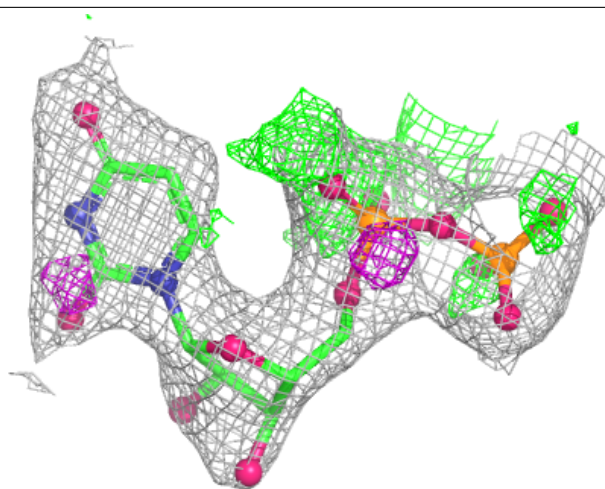
**Electron density around Y6W E 1572:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



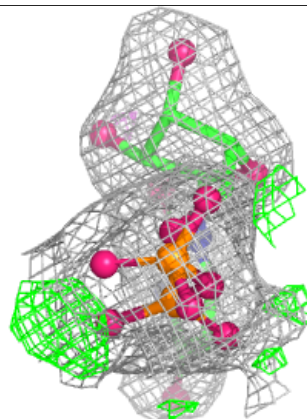
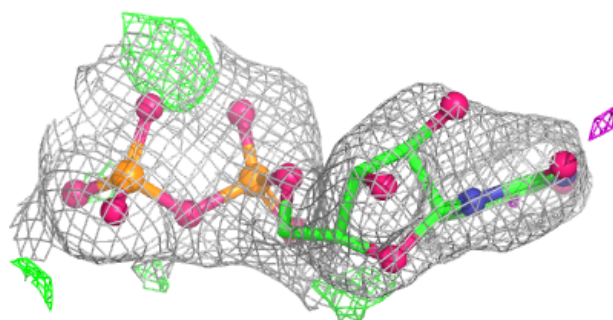
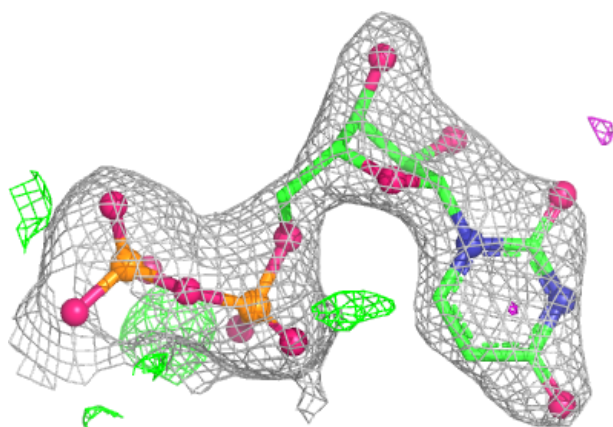
Electron density around UDP B 1572:

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and green (positive)

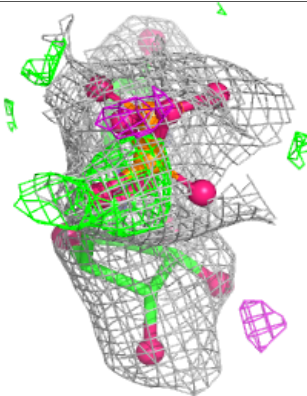
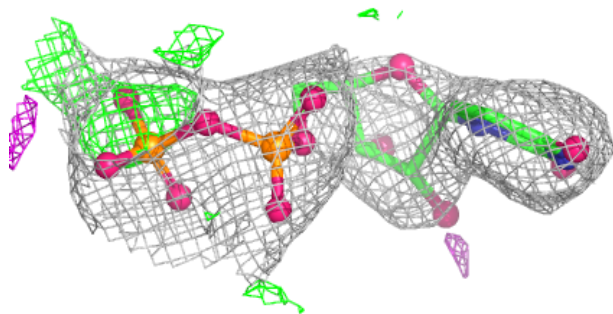
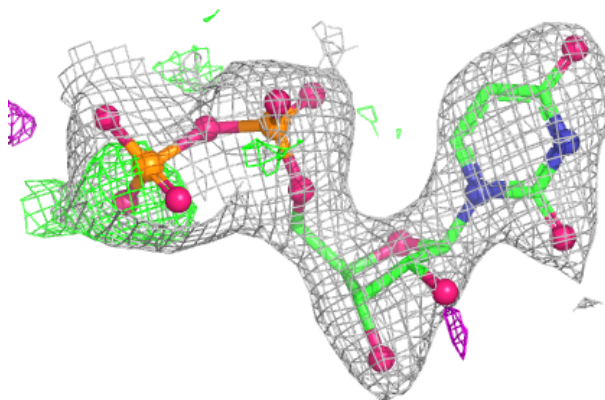


Electron density around UDP D 1555:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

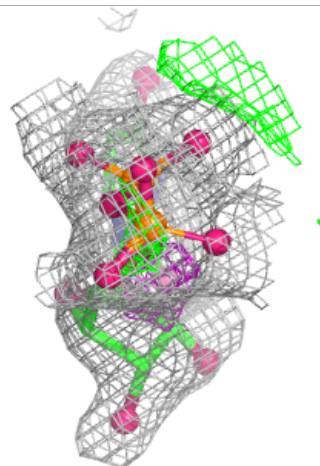
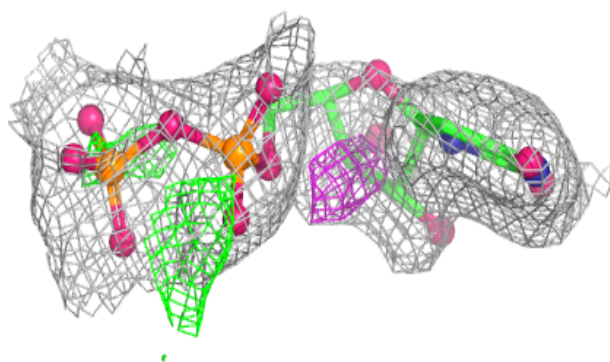
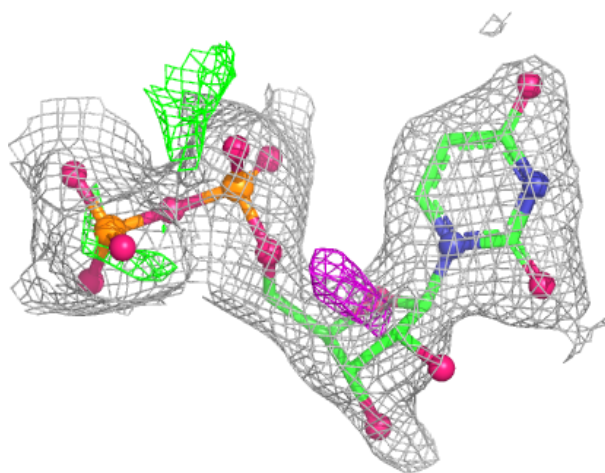
**Electron density around UDP F 1570:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



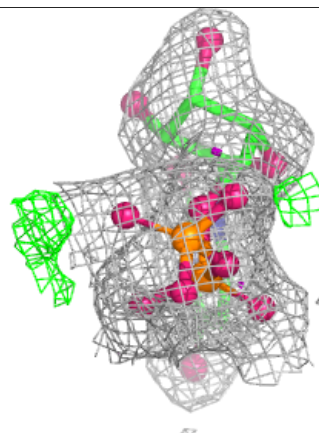
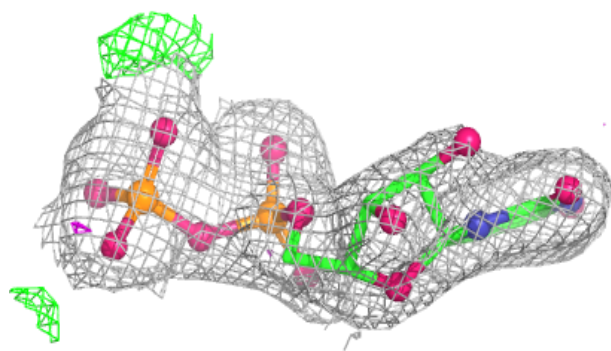
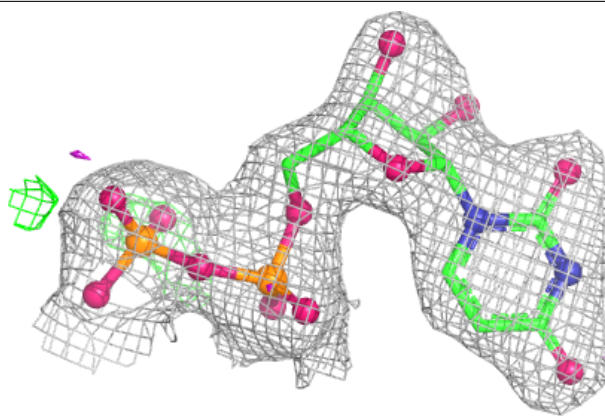
Electron density around UDP E 1570:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



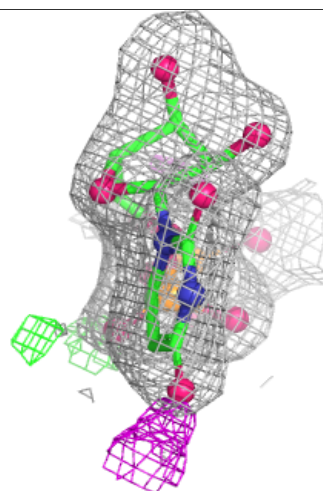
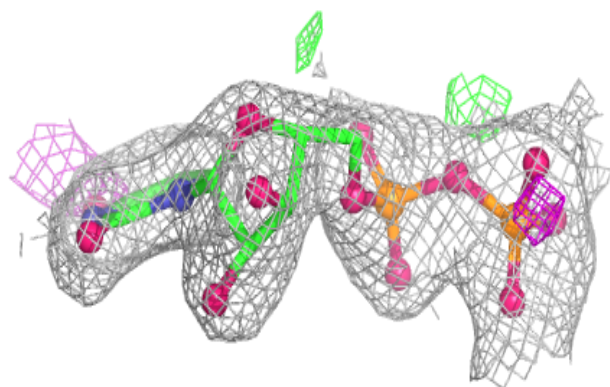
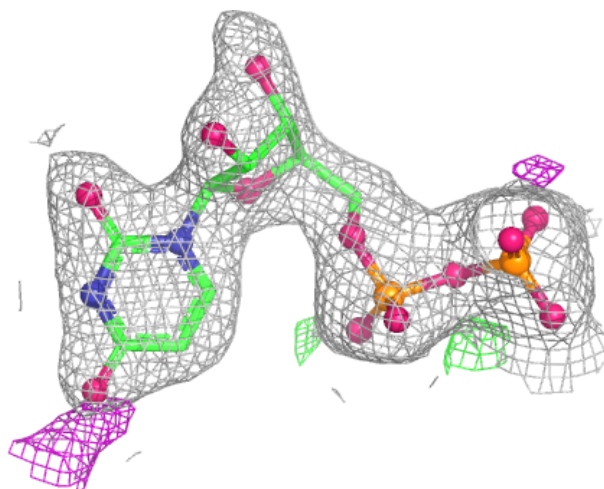
Electron density around UDP C 1570:

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



Electron density around UDP A 1570:

$2mF_o-DF_c$ (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.