WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 08:55 PM EDT

PDB ID	:	2F2H
Title	:	Structure of the YicI thiosugar Michaelis complex
Authors	:	Kim, Y.-W.; Lovering, A.L.; Strynadka, N.C.J.; Withers, S.G.
Deposited on	:	2005-11-16
Resolution	:	1.95 Å(reported)

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

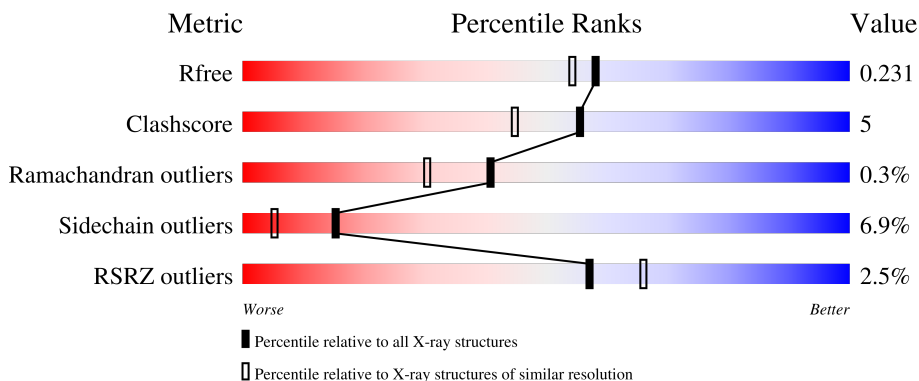|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

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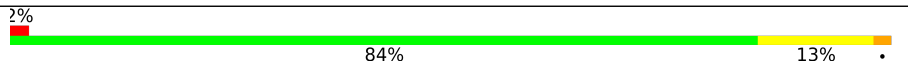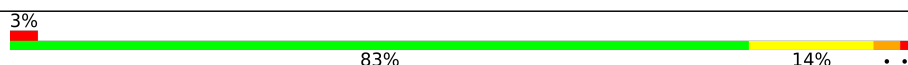
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	Percentile Ranks	Value
Rfree		0.231
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		6.9%
RSRZ outliers		2.5%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	773	2% 85% 12% •
1	B	773	3% 86% 12% •
1	C	773	2% 84% 13% •
1	D	773	3% 85% 12% •
1	E	773	3% 83% 14% • •

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
1	F	773	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	F	3001	-	-	X	-

2 Entity composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 39799 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 Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			
1	B	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			
1	C	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			
1	D	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			
1	E	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			
1	F	773	Total	C	N	O	S	0	0	0
			6232	3981	1071	1148	32			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	773	HIS	-	expression tag	UNP P31434
B	773	HIS	-	expression tag	UNP P31434
C	773	HIS	-	expression tag	UNP P31434
D	773	HIS	-	expression tag	UNP P31434
E	773	HIS	-	expression tag	UNP P31434
F	773	HIS	-	expression tag	UNP P31434

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	E	1	Total 5	O 4	S 1	0	0
2	E	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0

- Molecule 3 is 4-NITROPHENYL 6-THIO-6-S-ALPHA-D-XYLOPYRANOSYL-BETA-D-G LUCOPYRANOSIDE (three-letter code: XTG) (formula: $C_{17}H_{23}NO_{11}S$).
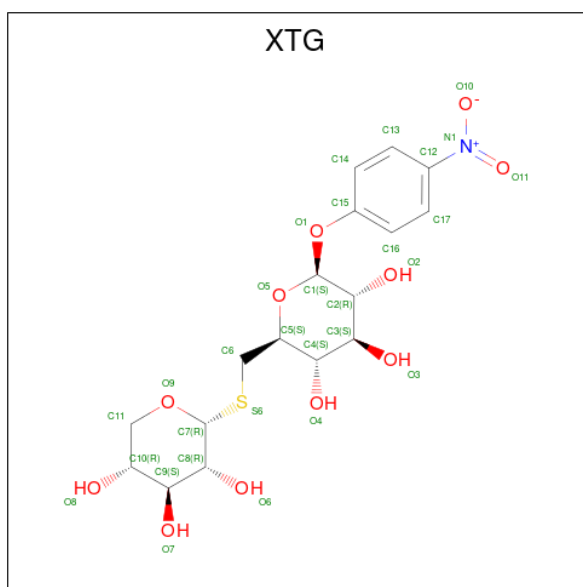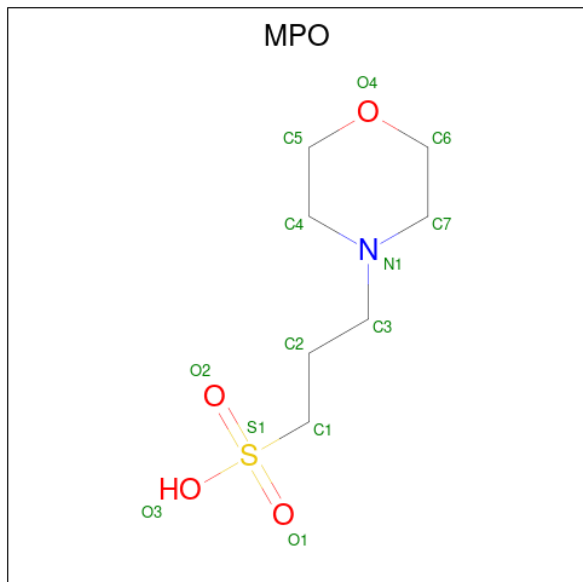
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	B	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	C	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	D	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	E	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	F	1	Total	C	N	O	S	0	0
			30	17	1	11	1		
3	F	1	Total	C	N	O	S	0	0
			30	17	1	11	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	F	1	Total 6	C 3	O 3	0	0
4	F	1	Total 6	C 3	O 3	0	0

- Molecule 5 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
5	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
5	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
5	E	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
5	F	1	Total	C	N	O	S	5	0
			13	7	1	4	1		

- Molecule 6 is water.

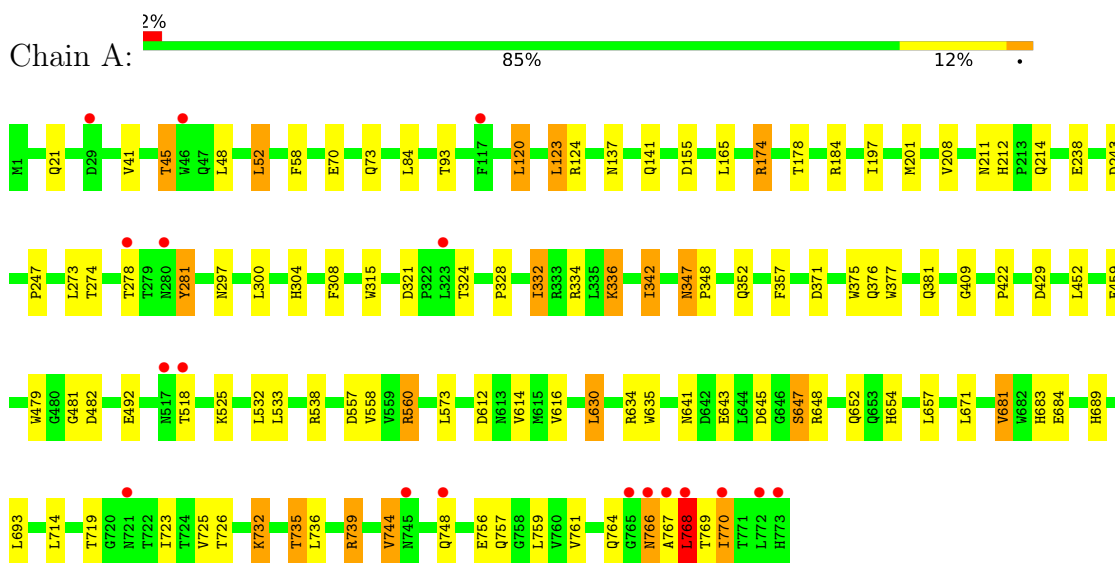| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	373	Total	O	0	0
			373	373		
6	B	290	Total	O	0	0
			290	290		
6	C	344	Total	O	0	0
			344	344		
6	D	370	Total	O	0	0
			370	370		
6	E	300	Total	O	0	0
			300	300		

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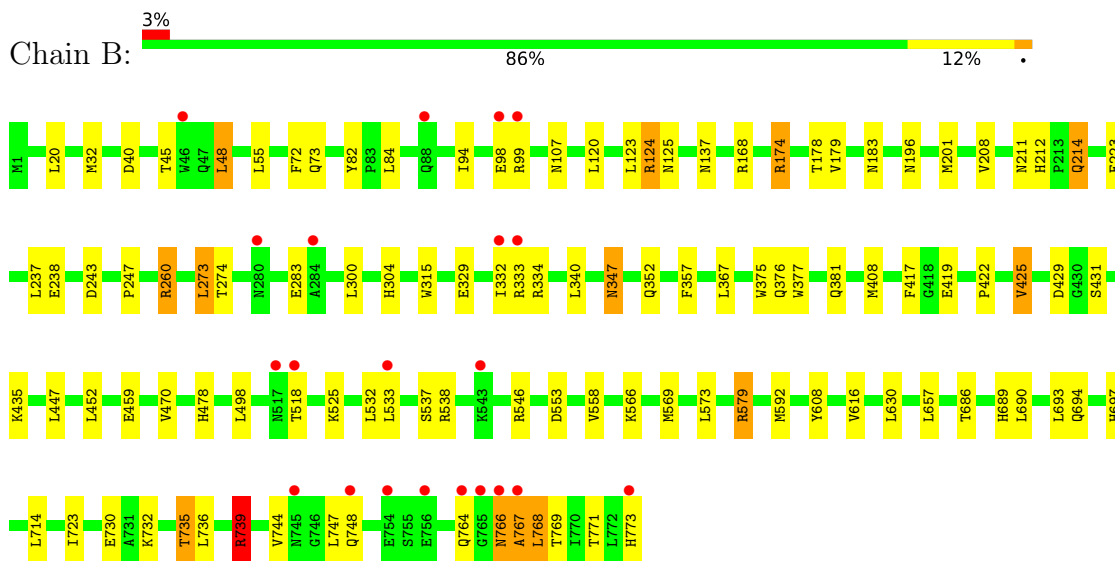| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	326	Total 326	O 326	0	0

3 Residue-property plots ⓘ

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.
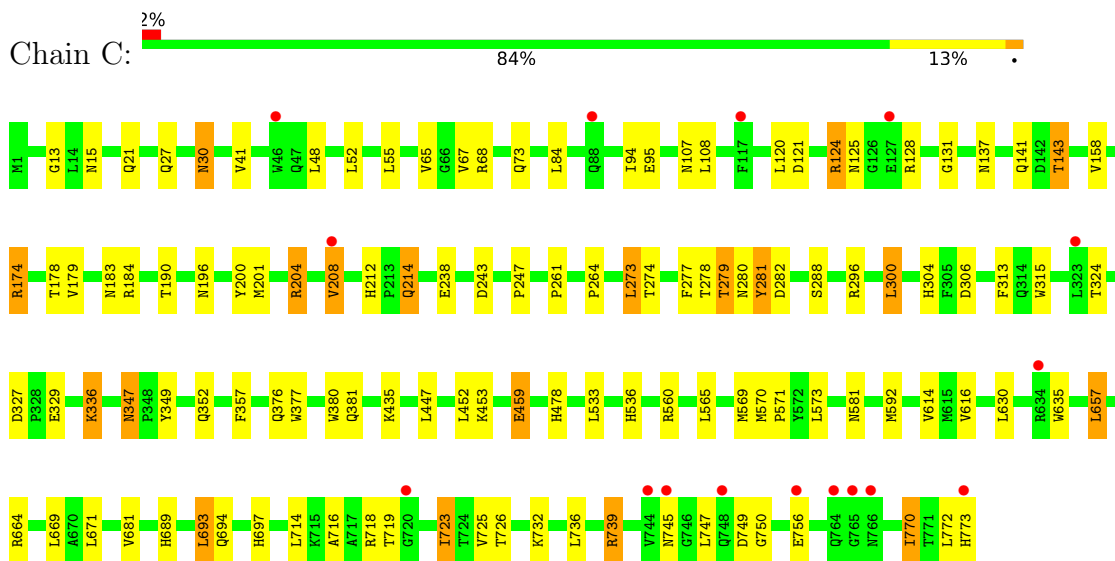
- Molecule 1: Putative family 31 glucosidase yicI

Chain A:
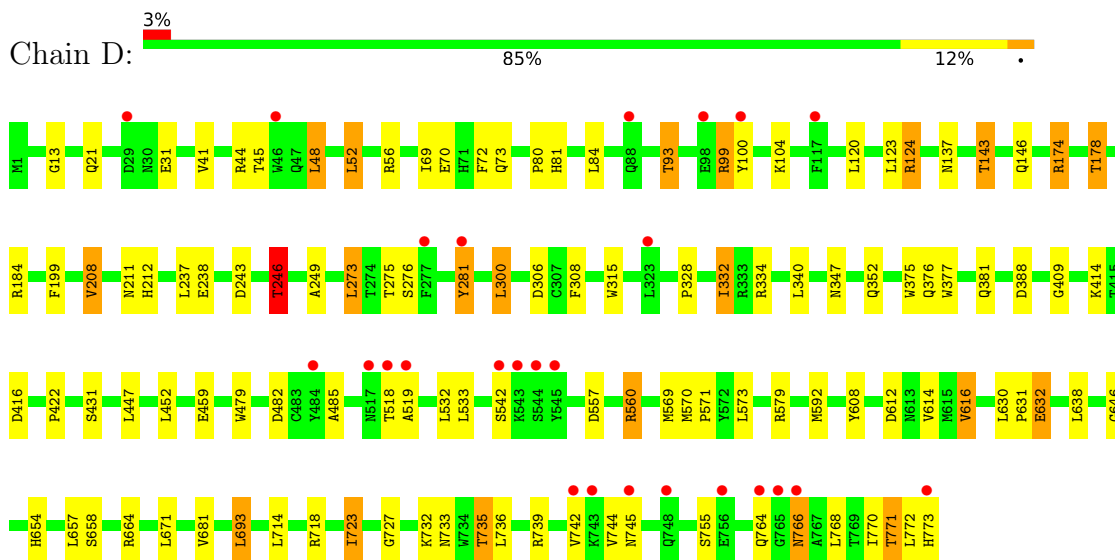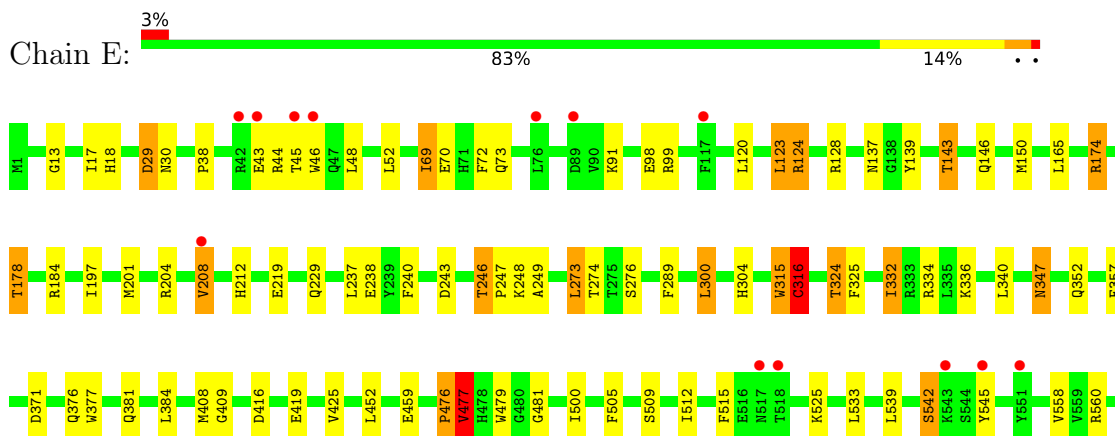
- Molecule 1: Putative family 31 glucosidase yicI

Chain B:

- Molecule 1: Putative family 31 glucosidase yicI

Chain C:

• Molecule 1: Putative family 31 glucosidase yicI

Chain D:

• Molecule 1: Putative family 31 glucosidase yicI

Chain E:

K566 M569 L573 E594 V616 L630 W635 E643 Q652 Q653 H654 L657 R664 L668 L671 L690 L693 Q694 H697 L714 R718 T719 G720 N721 T722 I723 G727 T735 L736 R739 V742 N745 P763 Q764 G765 N766 A767

L768 T769 I770 T771 L772 H773

• Molecule 1: Putative family 31 glucosidase yicI

Chain F:

2%

84%   13%   •

M1 G13 H18 Q21 E26 Q27 Q28 D29 M32 P38 V41 R42 E43 R44 T45 W46 Q47 L48 L52 Q61 Q73 L76 N77 L84 Q88 E95 A101 N107 L120 D121 R124 N125 R128 N137 T143 R174 T178

V179 R184 H212 P213 Q214 E219 E238 D243 T246 A249 R256 F257 W267 L273 N280 Y281 D282 L300 D306 F313 Q314 W315 C316 L323 E329 R334 L335 K336 I342 N347 Q352 F357 K358 E359 K363 Q376 W377

Q381 D416 D429 G430 S431 L452 E459 P476 V477 H478 W479 G480 G481 D482 C483 E488 S489 E492 L498 I512 N517 T518 H522 K525 L532 L533 S537 R538 L539 K543 S544 V558 V559 R560 M569 L573 R579 M592

Y608 D612 V616 E622 L630 P631 L638 G646 Q652 Q653 H654 R664 L671 V681 W682 H683 L693 Q694 H697 L714 T719 E730 A731 K732 T735 L736 R739 V744 L747 E754 S755 E756 Q764 G765 N766 A767 L768 T769 I770

T771 L772 H773

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	162.32Å 175.84Å 210.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.64 – 1.95 28.64 – 1.95	Depositor EDS
% Data completeness (in resolution range)	86.4 (28.64-1.95) 86.4 (28.64-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$<I/\sigma(I)>$ [1]	2.58 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.225 0.188 , 0.231	Depositor DCC
R_{free} test set	18828 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.2	EDS
L-test for twinning[2]	$<|L|> = 0.47$, $<L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	39799	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MPO, XTG, SO4

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	0.90	2/6416 (0.0%)	0.97	28/8719 (0.3%)
1	B	0.83	2/6416 (0.0%)	0.89	15/8719 (0.2%)
1	C	0.85	1/6416 (0.0%)	0.91	13/8719 (0.1%)
1	D	0.88	2/6416 (0.0%)	0.93	16/8719 (0.2%)
1	E	0.85	1/6416 (0.0%)	0.93	17/8719 (0.2%)
1	F	0.90	5/6416 (0.1%)	0.94	21/8719 (0.2%)
All	All	0.87	13/38496 (0.0%)	0.93	110/52314 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	6
1	F	0	4
All	All	0	12

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	483	CYS	CB-SG	-8.95	1.67	1.82
1	F	537	SER	CB-OG	8.53	1.53	1.42
1	F	43	GLU	CG-CD	7.21	1.62	1.51
1	A	214	GLN	CB-CG	-6.47	1.35	1.52
1	C	336	LYS	CD-CE	6.32	1.67	1.51
1	D	632	GLU	CG-CD	6.29	1.61	1.51
1	F	329	GLU	CD-OE2	6.25	1.32	1.25
1	B	730	GLU	CD-OE2	5.68	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	GLU	CB-CG	-5.55	1.41	1.52
1	E	70	GLU	CB-CG	-5.52	1.41	1.52
1	D	664	ARG	CB-CG	-5.52	1.37	1.52
1	F	730	GLU	CG-CD	5.23	1.59	1.51
1	B	98	GLU	CG-CD	5.20	1.59	1.51

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	174	ARG	NE-CZ-NH2	-16.54	112.03	120.30
1	E	174	ARG	NE-CZ-NH1	15.85	128.23	120.30
1	A	174	ARG	NE-CZ-NH2	-14.53	113.04	120.30
1	A	174	ARG	NE-CZ-NH1	14.36	127.48	120.30
1	F	174	ARG	NE-CZ-NH2	-13.02	113.79	120.30
1	D	174	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	D	174	ARG	NE-CZ-NH1	12.67	126.64	120.30
1	F	174	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	B	174	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	F	739	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	B	174	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	C	174	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	E	739	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	184	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	F	739	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	739	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	D	124	ARG	NE-CZ-NH2	8.60	124.60	120.30
1	C	739	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	612	ASP	CB-CG-OD1	8.08	125.57	118.30
1	F	334	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	C	174	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	B	20	LEU	CA-CB-CG	7.88	133.42	115.30
1	D	664	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	F	334	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	C	739	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	A	560	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	E	739	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	F	128	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	F	560	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	F	316	CYS	N-CA-C	7.32	130.77	111.00
1	E	316	CYS	N-CA-C	7.29	130.68	111.00
1	B	579	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	D	334	ARG	NE-CZ-NH2	-7.18	116.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	124	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	D	612	ASP	CB-CG-OD1	7.07	124.67	118.30
1	A	184	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	E	739	ARG	CG-CD-NE	-6.99	97.13	111.80
1	E	124	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	F	579	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	E	560	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	E	184	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	739	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	F	579	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	F	128	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	D	739	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	E	560	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	E	477	VAL	N-CA-C	6.40	128.28	111.00
1	A	334	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	E	124	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	B	124	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	C	124	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	E	476	PRO	C-N-CA	6.18	137.14	121.70
1	A	52	LEU	CA-CB-CG	6.06	129.24	115.30
1	F	477	VAL	N-CA-C	6.05	127.33	111.00
1	A	334	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	C	124	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	A	538	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	647	SER	CB-CA-C	5.96	121.43	110.10
1	A	429	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	155	ASP	CB-CG-OD1	5.90	123.61	118.30
1	F	416	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	184	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	174	ARG	CD-NE-CZ	5.89	131.85	123.60
1	A	214	GLN	CB-CA-C	-5.88	98.65	110.40
1	A	560	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	739	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	C	184	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	664	ARG	N-CA-CB	-5.86	100.05	110.60
1	B	168	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	273	LEU	CA-CB-CG	5.83	128.70	115.30
1	F	184	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	E	371	ASP	CB-CG-OD1	5.80	123.53	118.30
1	E	476	PRO	CA-C-N	-5.78	104.49	117.20
1	F	739	ARG	CG-CD-NE	-5.77	99.68	111.80
1	A	630	LEU	CB-CG-CD1	5.77	120.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	371	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	123	LEU	CA-CB-CG	5.72	128.46	115.30
1	C	204	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	B	260	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	D	579	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	174	ARG	CD-NE-CZ	5.70	131.57	123.60
1	E	371	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	C	306	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	40	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	579	ARG	CG-CD-NE	-5.59	100.06	111.80
1	A	648	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	F	184	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	334	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	F	560	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	273	LEU	CA-CB-CG	5.50	127.95	115.30
1	D	560	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	D	739	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	D	184	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	52	LEU	CB-CG-CD2	5.34	120.08	111.00
1	C	327	ASP	CB-CG-OD1	5.32	123.08	118.30
1	F	273	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	120	LEU	CB-CG-CD2	5.29	119.99	111.00
1	A	174	ARG	CB-CG-CD	5.28	125.33	111.60
1	D	246	THR	N-CA-CB	-5.26	100.31	110.30
1	B	214	GLN	CB-CA-C	-5.24	99.92	110.40
1	C	282	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	123	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	579	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	630	LEU	CA-CB-CG	5.12	127.09	115.30
1	F	664	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	D	52	LEU	CA-CB-CG	5.10	127.03	115.30
1	C	657	LEU	CB-CG-CD1	5.05	119.58	111.00
1	F	612	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	538	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	342	ILE	CG1-CB-CG2	-5.01	100.38	111.40

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	766	ASN	Peptide
1	D	766	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	E	315	TRP	Peptide,Mainchain
1	E	476	PRO	Peptide,Mainchain
1	E	763	PRO	Peptide
1	E	766	ASN	Peptide
1	F	315	TRP	Peptide,Mainchain
1	F	476	PRO	Peptide,Mainchain

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	6232	0	5939	63	0
1	B	6232	0	5939	59	0
1	C	6232	0	5939	65	0
1	D	6232	0	5939	74	0
1	E	6232	0	5939	71	0
1	F	6232	0	5939	67	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	10	0	0	1	0
2	F	15	0	0	3	0
3	A	30	0	23	2	0
3	B	30	0	23	1	0
3	C	30	0	23	0	0
3	D	30	0	23	7	0
3	E	30	0	23	1	0
3	F	60	0	46	1	0
4	A	18	0	24	5	0
4	B	12	0	16	2	0
4	C	18	0	24	1	0
4	D	12	0	16	2	0
4	E	12	0	16	0	0
4	F	12	0	16	1	0
5	B	13	0	15	0	0
5	C	13	0	15	0	0
5	D	13	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	13	0	15	0	0
5	F	13	0	15	0	0
6	A	373	0	0	4	0
6	B	290	0	0	4	0
6	C	344	0	0	6	0
6	D	370	0	0	10	0
6	E	300	0	0	9	0
6	F	326	0	0	6	0
All	All	39799	0	35982	379	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 5.

All (379) 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:124:ARG:NH2	1:A:243:ASP:OD1	1.88	1.04
1:D:569:MET:HE2	1:D:638:LEU:HD21	1.51	0.91
1:B:32:MET:CE	1:B:94:ILE:HG23	2.03	0.89
1:C:30:ASN:HD22	1:C:30:ASN:H	1.19	0.88
1:C:352:GLN:NE2	1:D:73:GLN:H	1.72	0.86
1:D:352:GLN:HE21	1:D:376:GLN:HE22	1.24	0.85
1:B:32:MET:HE2	1:B:94:ILE:HG23	1.57	0.85
1:C:352:GLN:HE22	1:D:73:GLN:H	1.23	0.84
1:C:352:GLN:HE21	1:C:376:GLN:HE22	1.28	0.81
1:C:158:VAL:O	1:C:204:ARG:NH2	2.13	0.81
1:C:13:GLY:O	1:C:143:THR:HB	1.81	0.80
1:D:70:GLU:OE1	6:D:3123:HOH:O	1.99	0.79
1:F:212:HIS:HE1	1:F:238:GLU:H	1.28	0.79
1:E:204:ARG:NH2	6:E:3297:HOH:O	2.15	0.78
1:F:246:THR:HG21	2:F:3001:SO4:O3	1.86	0.75
3:B:3016:XTG:H14	1:F:48:LEU:HD11	1.66	0.75
1:D:727:GLY:H	1:D:766:ASN:HD21	1.35	0.74
1:A:352:GLN:NE2	1:B:73:GLN:H	1.85	0.74
1:A:352:GLN:HE22	1:B:73:GLN:H	1.35	0.74
1:A:201:MET:HE1	1:A:247:PRO:HB3	1.71	0.73
1:D:569:MET:CE	1:D:638:LEU:CD2	2.66	0.73
1:D:569:MET:CE	1:D:638:LEU:HD21	2.18	0.72
1:B:352:GLN:HE21	1:B:376:GLN:HE22	1.37	0.72
1:A:352:GLN:HE21	1:A:376:GLN:HE22	1.36	0.72
1:B:566:LYS:HA	1:B:569:MET:HE2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLN:CD	6:A:3289:HOH:O	2.27	0.71
1:A:641:ASN:HD21	1:A:739:ARG:HH21	1.36	0.71
1:B:332:ILE:CD1	1:B:408:MET:O	2.39	0.71
1:B:211:ASN:ND2	4:B:3026:GOL:H32	2.07	0.69
1:D:485:ALA:HB1	1:D:519:ALA:HB2	1.73	0.69
1:F:306:ASP:OD1	6:F:3038:HOH:O	2.10	0.69
1:A:212:HIS:HE1	1:A:238:GLU:H	1.40	0.68
1:F:13:GLY:O	1:F:143:THR:HB	1.93	0.68
1:F:719:THR:HG22	6:F:3241:HOH:O	1.93	0.68
1:D:352:GLN:NE2	1:E:73:GLN:H	1.92	0.67
1:B:332:ILE:HD12	1:B:333:ARG:N	2.10	0.66
1:D:306:ASP:OD2	3:D:3018:XTG:H112	1.96	0.66
1:B:211:ASN:HD21	4:B:3026:GOL:H32	1.61	0.66
1:C:30:ASN:H	1:C:30:ASN:ND2	1.93	0.65
1:E:347:ASN:C	1:E:347:ASN:HD22	2.00	0.65
1:E:723:ILE:HG12	1:E:770:ILE:HB	1.79	0.65
1:A:73:GLN:H	1:F:352:GLN:HE22	1.45	0.65
1:B:212:HIS:HE1	1:B:238:GLU:H	1.44	0.65
1:F:694:GLN:HB2	1:F:697:HIS:CD2	2.32	0.65
1:D:681:VAL:O	1:D:681:VAL:HG13	1.96	0.65
1:B:32:MET:HE3	1:B:94:ILE:HG23	1.77	0.65
1:E:300:LEU:HD13	1:E:340:LEU:HD21	1.77	0.64
1:A:45:THR:HB	1:F:543:LYS:HZ1	1.62	0.64
1:D:93:THR:HG22	1:D:104:LYS:HB3	1.78	0.64
1:C:296:ARG:O	1:C:560:ARG:NH1	2.30	0.64
1:E:336:LYS:HE2	1:E:409:GLY:O	1.98	0.63
1:F:280:ASN:HD22	1:F:282:ASP:H	1.43	0.63
1:A:73:GLN:H	1:F:352:GLN:NE2	1.95	0.63
1:A:211:ASN:ND2	4:A:3029:GOL:H32	2.12	0.63
1:F:212:HIS:CE1	1:F:238:GLU:H	2.14	0.63
1:A:525:LYS:HG2	1:A:558:VAL:HG21	1.81	0.63
1:D:744:VAL:HG21	1:D:770:ILE:HG23	1.81	0.63
1:E:212:HIS:HE1	1:E:238:GLU:H	1.47	0.62
1:D:246:THR:HG22	1:D:249:ALA:CB	2.29	0.62
1:E:566:LYS:HA	1:E:569:MET:HE2	1.81	0.62
1:E:143:THR:HG22	6:E:3181:HOH:O	1.99	0.62
1:C:770:ILE:HD11	1:C:772:LEU:HD13	1.81	0.62
1:D:273:LEU:HB2	1:D:300:LEU:HD21	1.82	0.62
1:F:178:THR:CG2	6:F:3256:HOH:O	2.48	0.62
1:D:212:HIS:HE1	1:D:238:GLU:H	1.48	0.61
1:E:315:TRP:H	1:E:381:GLN:HE21	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TYR:O	1:A:324:THR:HG23	2.00	0.61
1:E:13:GLY:O	1:E:143:THR:HB	2.01	0.61
1:C:212:HIS:HE1	1:C:238:GLU:H	1.46	0.61
1:F:767:ALA:O	1:F:768:LEU:C	2.38	0.60
1:A:641:ASN:ND2	1:A:739:ARG:HH21	1.98	0.60
1:E:246:THR:HG23	1:E:249:ALA:H	1.67	0.60
1:F:336:LYS:HD2	1:F:342:ILE:HD12	1.83	0.60
1:A:744:VAL:HG21	1:A:770:ILE:HD13	1.83	0.60
1:B:283:GLU:OE1	1:B:334:ARG:HD2	2.01	0.60
1:B:525:LYS:HG2	1:B:558:VAL:HG21	1.83	0.60
1:D:352:GLN:NE2	1:D:376:GLN:HE22	1.96	0.59
1:E:352:GLN:HE21	1:E:376:GLN:HE22	1.49	0.59
1:E:332:ILE:HD11	1:E:409:GLY:HA3	1.83	0.59
1:F:280:ASN:ND2	1:F:282:ASP:H	1.99	0.59
1:C:716:ALA:HB1	1:C:723:ILE:HD13	1.85	0.59
1:A:93:THR:HA	4:A:3024:GOL:H12	1.84	0.58
1:F:735:THR:CG2	6:F:3193:HOH:O	2.50	0.58
1:A:681:VAL:HG23	1:A:683:HIS:CE1	2.39	0.58
1:B:124:ARG:HD3	1:B:243:ASP:OD1	2.04	0.58
1:F:347:ASN:C	1:F:347:ASN:HD22	2.07	0.58
1:C:214:GLN:HG3	1:C:435:LYS:HG2	1.86	0.58
1:B:352:GLN:NE2	1:B:376:GLN:HE22	2.01	0.57
1:D:211:ASN:ND2	4:D:3032:GOL:H32	2.20	0.57
1:F:489:SER:HA	1:F:492:GLU:HG3	1.86	0.57
1:C:124:ARG:HD3	1:C:243:ASP:OD1	2.03	0.57
1:C:73:GLN:H	1:E:352:GLN:NE2	2.01	0.57
1:B:735:THR:HG23	6:B:3294:HOH:O	2.04	0.57
1:C:121:ASP:OD1	1:C:128:ARG:NH2	2.37	0.57
1:C:274:THR:HG22	1:C:304:HIS:HB3	1.87	0.57
1:D:13:GLY:O	1:D:143:THR:HB	2.04	0.57
1:F:61:GLN:NE2	1:F:257:PHE:HA	2.20	0.57
1:E:124:ARG:HD3	1:E:243:ASP:OD1	2.05	0.57
1:E:727:GLY:H	1:E:766:ASN:HD21	1.50	0.57
1:B:690:LEU:O	1:B:739:ARG:HB2	2.05	0.56
1:D:735:THR:CG2	6:D:3161:HOH:O	2.54	0.56
1:B:352:GLN:NE2	1:F:73:GLN:H	2.04	0.56
1:D:485:ALA:CB	1:D:519:ALA:HB2	2.34	0.56
1:A:725:VAL:HB	1:A:768:LEU:HB3	1.88	0.56
1:E:315:TRP:H	1:E:381:GLN:NE2	2.04	0.55
1:A:352:GLN:NE2	1:A:376:GLN:HE22	2.03	0.55
1:C:347:ASN:C	1:C:347:ASN:HD22	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:GLN:HE22	1:F:256:ARG:C	2.09	0.55
1:C:723:ILE:HD11	1:C:725:VAL:HG22	1.88	0.55
1:E:18:HIS:O	1:E:38:PRO:HA	2.07	0.55
1:E:246:THR:HG21	2:E:3004:SO4:O4	2.06	0.55
1:E:352:GLN:NE2	1:E:376:GLN:HE22	2.05	0.55
1:E:525:LYS:HG2	1:E:558:VAL:HG21	1.87	0.55
1:A:744:VAL:CG2	1:A:770:ILE:HD13	2.37	0.55
1:F:478:HIS:HD2	6:F:3069:HOH:O	1.89	0.55
1:A:347:ASN:C	1:A:347:ASN:HD22	2.10	0.54
1:C:128:ARG:HH22	1:C:131:GLY:HA3	1.72	0.54
1:A:328:PRO:O	1:A:332:ILE:HG23	2.08	0.54
1:D:352:GLN:HE22	1:E:73:GLN:H	1.55	0.54
1:F:488:GLU:O	1:F:492:GLU:HG2	2.08	0.54
1:D:124:ARG:HD3	1:D:243:ASP:OD1	2.07	0.54
1:C:352:GLN:NE2	1:C:376:GLN:HE22	2.02	0.54
1:B:429:ASP:OD1	1:B:431:SER:OG	2.23	0.54
1:D:21:GLN:HE22	1:D:41:VAL:H	1.55	0.54
1:D:178:THR:CG2	6:D:3276:HOH:O	2.54	0.54
1:A:641:ASN:HD21	1:A:739:ARG:NH2	2.05	0.54
1:D:212:HIS:CE1	1:D:238:GLU:H	2.26	0.53
1:C:347:ASN:ND2	1:C:349:TYR:H	2.06	0.53
1:F:352:GLN:HE21	1:F:376:GLN:HE22	1.54	0.53
1:F:681:VAL:HG23	1:F:683:HIS:CE1	2.44	0.53
1:D:275:THR:O	1:D:276:SER:HB2	2.08	0.53
1:C:201:MET:HE1	1:C:247:PRO:HB3	1.91	0.53
1:C:107:ASN:ND2	1:C:125:ASN:HD21	2.07	0.53
1:C:73:GLN:H	1:E:352:GLN:HE22	1.57	0.52
1:C:273:LEU:HB2	1:C:300:LEU:HD21	1.90	0.52
1:C:719:THR:HG22	6:C:3086:HOH:O	2.08	0.52
1:E:512:ILE:HB	1:E:539:LEU:HD23	1.91	0.52
1:D:246:THR:HG22	1:D:249:ALA:HB2	1.90	0.52
1:B:212:HIS:CE1	1:B:238:GLU:H	2.27	0.52
1:D:300:LEU:HD13	1:D:340:LEU:HD21	1.90	0.52
1:E:347:ASN:C	1:E:347:ASN:ND2	2.62	0.52
4:A:3029:GOL:H31	6:A:3127:HOH:O	2.09	0.52
1:B:767:ALA:O	1:B:768:LEU:O	2.28	0.52
1:C:329:GLU:HB2	6:C:3243:HOH:O	2.09	0.52
1:C:459:GLU:CD	1:C:459:GLU:H	2.13	0.52
1:F:124:ARG:HD3	1:F:243:ASP:OD1	2.10	0.52
1:E:212:HIS:CE1	1:E:238:GLU:H	2.26	0.52
1:D:482:ASP:OD2	3:D:3018:XTG:H62	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:GLN:HA	1:B:357:PHE:CD2	2.45	0.51
1:F:48:LEU:HD12	1:F:48:LEU:O	2.10	0.51
1:F:429:ASP:OD1	1:F:431:SER:OG	2.25	0.51
1:A:315:TRP:H	1:A:381:GLN:HE21	1.57	0.51
1:B:352:GLN:HE22	1:F:73:GLN:H	1.57	0.51
1:B:367:LEU:HD11	1:B:425:VAL:HG13	1.92	0.51
1:D:447:LEU:C	1:D:447:LEU:HD23	2.30	0.51
1:F:246:THR:HG23	1:F:249:ALA:H	1.76	0.51
1:E:212:HIS:HD2	6:E:3148:HOH:O	1.94	0.51
1:B:447:LEU:HD23	1:B:447:LEU:C	2.31	0.51
1:D:93:THR:CG2	6:D:3217:HOH:O	2.58	0.51
1:E:45:THR:HG23	1:E:46:TRP:CD1	2.46	0.51
1:B:329:GLU:HA	1:B:332:ILE:HG13	1.92	0.50
1:B:375:TRP:CE2	1:B:422:PRO:HG3	2.46	0.50
1:D:352:GLN:HE22	1:E:72:PHE:HA	1.76	0.50
1:B:332:ILE:HD13	1:B:408:MET:O	2.11	0.50
1:B:735:THR:CG2	6:B:3294:HOH:O	2.60	0.50
1:B:55:LEU:HD12	1:B:55:LEU:N	2.27	0.50
1:F:482:ASP:OD2	3:F:3020:XTG:H62	2.11	0.50
1:C:478:HIS:HE1	6:C:3149:HOH:O	1.95	0.50
1:B:478:HIS:HD2	6:B:3236:HOH:O	1.93	0.50
1:D:723:ILE:HG12	1:D:770:ILE:HB	1.93	0.50
1:E:123:LEU:HD12	1:E:128:ARG:HA	1.92	0.50
1:E:324:THR:HG23	1:E:325:PHE:CD2	2.47	0.50
1:C:723:ILE:HD11	1:C:725:VAL:CG2	2.42	0.49
1:F:61:GLN:HE22	1:F:257:PHE:N	2.09	0.49
1:A:278:THR:HG21	1:B:45:THR:HA	1.94	0.49
1:C:279:THR:O	1:D:44:ARG:NH2	2.44	0.49
1:B:201:MET:CE	1:B:247:PRO:HB3	2.42	0.49
1:E:416:ASP:OD2	3:E:3019:XTG:H8	2.13	0.49
1:C:447:LEU:C	1:C:447:LEU:HD23	2.33	0.49
1:F:638:LEU:O	1:F:739:ARG:NH2	2.44	0.49
1:A:352:GLN:HA	1:A:357:PHE:CD2	2.47	0.49
1:A:641:ASN:HD21	1:A:739:ARG:HE	1.60	0.49
1:B:32:MET:HE2	1:B:94:ILE:CG2	2.36	0.49
1:D:306:ASP:OD1	3:D:3018:XTG:O8	2.13	0.49
1:D:332:ILE:HD11	1:D:409:GLY:HA3	1.95	0.49
1:C:212:HIS:CE1	1:C:238:GLU:H	2.29	0.48
1:E:43:GLU:H	1:E:43:GLU:CD	2.16	0.48
1:E:300:LEU:HD13	1:E:340:LEU:CD2	2.43	0.48
1:A:238:GLU:OE1	4:A:3029:GOL:H32	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:HIS:CE1	1:A:238:GLU:H	2.26	0.48
1:B:417:PHE:HA	1:B:419:GLU:OE2	2.13	0.48
1:C:15:ASN:HD22	1:C:141:GLN:NE2	2.12	0.48
1:F:178:THR:HB	1:F:219:GLU:OE1	2.14	0.48
1:A:332:ILE:HD11	1:A:409:GLY:HA3	1.95	0.48
1:D:306:ASP:OD2	3:D:3018:XTG:C11	2.61	0.48
1:A:281:TYR:CZ	1:A:308:PHE:HB2	2.49	0.48
1:C:478:HIS:HD2	6:C:3063:HOH:O	1.96	0.48
1:D:81:HIS:HB2	6:D:3206:HOH:O	2.14	0.48
1:F:246:THR:HG21	2:F:3001:SO4:S	2.54	0.48
1:A:315:TRP:H	1:A:381:GLN:NE2	2.11	0.48
1:A:684:GLU:HG2	1:A:732:LYS:HB2	1.96	0.48
1:F:681:VAL:HG12	2:F:3003:SO4:O3	2.14	0.47
1:B:332:ILE:HG12	1:B:408:MET:O	2.14	0.47
1:E:693:LEU:HD13	1:E:718:ARG:HB2	1.95	0.47
1:A:58:PHE:CZ	4:A:3028:GOL:H12	2.49	0.47
1:A:482:ASP:OD2	3:A:3015:XTG:H62	2.12	0.47
1:B:201:MET:HE1	1:B:247:PRO:HB3	1.96	0.47
1:A:770:ILE:HD12	1:A:770:ILE:C	2.34	0.47
1:C:30:ASN:HD22	1:C:30:ASN:N	1.93	0.47
1:D:557:ASP:OD1	1:D:560:ARG:NH2	2.47	0.47
1:E:332:ILE:CD1	1:E:409:GLY:HA3	2.44	0.47
1:E:332:ILE:C	1:E:332:ILE:HD12	2.35	0.47
1:E:212:HIS:CE1	1:E:237:LEU:HD12	2.50	0.47
1:B:329:GLU:O	1:B:332:ILE:HG13	2.15	0.47
1:F:315:TRP:H	1:F:381:GLN:NE2	2.12	0.47
1:F:347:ASN:C	1:F:347:ASN:ND2	2.68	0.47
1:B:766:ASN:ND2	6:B:3171:HOH:O	2.47	0.47
1:D:485:ALA:HB1	1:D:519:ALA:CB	2.44	0.47
1:F:32:MET:HE2	1:F:101:ALA:HB1	1.97	0.47
1:D:199:PHE:HA	1:D:208:VAL:O	2.15	0.46
1:D:735:THR:HG22	6:D:3161:HOH:O	2.16	0.46
1:E:17:ILE:CG1	1:E:139:TYR:HB3	2.45	0.46
1:F:352:GLN:NE2	1:F:376:GLN:HE22	2.13	0.46
1:C:352:GLN:HE22	1:D:73:GLN:N	2.01	0.46
1:A:274:THR:HG22	1:A:304:HIS:HB3	1.97	0.46
1:C:27:GLN:HG3	1:C:94:ILE:HD13	1.97	0.46
1:F:273:LEU:HB2	1:F:300:LEU:HD21	1.97	0.46
1:E:735:THR:HG22	6:E:3178:HOH:O	2.15	0.46
1:A:761:VAL:CG1	1:A:768:LEU:HD21	2.46	0.46
1:E:143:THR:CG2	6:E:3181:HOH:O	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:GLU:CD	1:F:28:GLN:HE21	2.19	0.46
1:A:45:THR:HB	1:F:543:LYS:NZ	2.29	0.46
1:A:70:GLU:HG3	6:A:3251:HOH:O	2.15	0.46
1:B:766:ASN:O	1:B:767:ALA:HB2	2.16	0.46
1:E:248:LYS:NZ	1:E:594:GLU:OE1	2.49	0.46
1:A:21:GLN:NE2	1:A:41:VAL:H	2.13	0.46
1:E:477:VAL:HG11	1:E:509:SER:HB2	1.97	0.46
3:A:3015:XTG:C14	1:B:48:LEU:HD11	2.46	0.46
1:E:500:ILE:HG12	1:E:505:PHE:HB2	1.98	0.46
1:F:359:GLU:OE2	1:F:363:LYS:NZ	2.40	0.46
1:E:274:THR:HG22	1:E:304:HIS:HB3	1.98	0.45
1:F:267:TRP:HD1	4:F:3022:GOL:HO3	1.63	0.45
1:A:767:ALA:O	1:A:769:THR:N	2.49	0.45
1:B:498:LEU:HD21	1:B:608:TYR:HB3	1.97	0.45
1:D:479:TRP:HH2	3:D:3018:XTG:HO7	1.64	0.45
1:A:336:LYS:HE2	1:A:409:GLY:O	2.17	0.45
1:B:767:ALA:O	1:B:768:LEU:C	2.54	0.45
1:F:512:ILE:HB	1:F:539:LEU:HD23	1.99	0.45
1:E:204:ARG:HG3	6:E:3297:HOH:O	2.15	0.45
1:F:107:ASN:HD22	1:F:125:ASN:HD21	1.64	0.45
1:C:380:TRP:CZ3	1:D:48:LEU:HD13	2.51	0.45
1:E:91:LYS:CE	6:E:3177:HOH:O	2.64	0.45
1:D:93:THR:HG23	6:D:3217:HOH:O	2.15	0.45
1:A:297:ASN:O	1:A:560:ARG:HD3	2.17	0.45
1:C:65:VAL:HG12	1:C:108:LEU:CD2	2.46	0.45
1:F:479:TRP:CZ3	1:F:481:GLY:HA2	2.52	0.45
1:A:21:GLN:HE22	1:A:41:VAL:H	1.64	0.45
1:C:67:VAL:O	1:C:238:GLU:HA	2.17	0.45
1:A:767:ALA:C	1:A:769:THR:N	2.71	0.45
1:B:214:GLN:HG3	1:B:435:LYS:HG2	1.98	0.45
1:B:315:TRP:H	1:B:381:GLN:HE21	1.62	0.45
1:D:238:GLU:OE1	4:D:3032:GOL:H32	2.17	0.45
1:A:652:GLN:NE2	1:A:654:HIS:NE2	2.64	0.44
1:B:300:LEU:HD12	1:B:340:LEU:HD21	1.99	0.44
1:D:693:LEU:HD13	1:D:718:ARG:HB2	1.98	0.44
1:F:315:TRP:H	1:F:381:GLN:HE21	1.64	0.44
1:C:281:TYR:O	1:C:324:THR:CG2	2.66	0.44
1:D:654:HIS:ND1	1:D:658:SER:OG	2.36	0.44
1:E:289:PHE:HZ	1:E:545:TYR:CD1	2.34	0.44
1:A:352:GLN:HE22	1:B:72:PHE:HA	1.82	0.44
1:B:107:ASN:ND2	1:B:125:ASN:HD21	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:VAL:CG1	1:E:509:SER:HB2	2.48	0.44
1:E:515:PHE:O	1:E:542:SER:HB2	2.17	0.44
1:E:635:TRP:O	1:E:643:GLU:HA	2.18	0.44
1:F:336:LYS:HD2	1:F:342:ILE:CD1	2.46	0.44
1:B:274:THR:HG22	1:B:304:HIS:HB3	1.99	0.44
1:C:30:ASN:ND2	1:C:30:ASN:N	2.61	0.44
1:E:668:LEU:HD21	1:E:714:LEU:HD13	1.99	0.44
1:B:183:ASN:HA	1:B:196:ASN:ND2	2.32	0.44
1:D:328:PRO:O	1:D:332:ILE:HG23	2.18	0.44
1:C:570:MET:N	1:C:571:PRO:CD	2.81	0.44
1:E:352:GLN:HA	1:E:357:PHE:CD2	2.53	0.44
1:E:479:TRP:CZ3	1:E:481:GLY:HA2	2.53	0.44
1:A:748:GLN:HG2	1:A:769:THR:CG2	2.47	0.43
1:C:565:LEU:O	1:C:569:MET:HG3	2.18	0.43
1:C:689:HIS:ND1	1:C:739:ARG:HD3	2.33	0.43
1:E:178:THR:CG2	6:E:3308:HOH:O	2.66	0.43
1:B:212:HIS:CE1	1:B:237:LEU:HD12	2.53	0.43
1:F:313:PHE:HA	1:F:381:GLN:NE2	2.33	0.43
1:C:261:PRO:O	1:C:581:ASN:HA	2.18	0.43
1:E:165:LEU:HA	1:E:197:ILE:O	2.18	0.43
1:D:414:LYS:HZ3	3:D:3018:XTG:H10	1.84	0.43
1:D:123:LEU:N	1:D:123:LEU:HD22	2.34	0.43
1:D:570:MET:N	1:D:571:PRO:CD	2.82	0.43
1:D:744:VAL:HG22	1:D:771:THR:O	2.18	0.43
1:E:767:ALA:O	1:E:768:LEU:C	2.57	0.43
1:C:315:TRP:H	1:C:381:GLN:NE2	2.17	0.43
1:D:300:LEU:HD13	1:D:340:LEU:CD2	2.49	0.43
1:A:635:TRP:O	1:A:643:GLU:HA	2.18	0.43
1:C:693:LEU:HD13	1:C:718:ARG:HB2	2.01	0.43
1:D:246:THR:HG21	2:D:3002:SO4:O2	2.19	0.43
1:C:352:GLN:HE22	1:D:72:PHE:HA	1.84	0.42
1:C:635:TRP:CH2	1:C:664:ARG:HG2	2.54	0.42
1:D:31:GLU:OE1	1:D:56:ARG:HD3	2.19	0.42
1:A:557:ASP:OD1	1:A:560:ARG:NH2	2.52	0.42
1:D:375:TRP:CE2	1:D:422:PRO:HG3	2.54	0.42
1:E:69:ILE:HG12	1:E:150:MET:CE	2.49	0.42
1:F:61:GLN:NE2	1:F:257:PHE:CA	2.82	0.42
1:A:321:ASP:OD1	1:A:321:ASP:C	2.58	0.42
1:C:277:PHE:CD2	1:C:278:THR:HG23	2.55	0.42
1:A:165:LEU:HA	1:A:197:ILE:O	2.20	0.42
1:A:281:TYR:O	1:A:324:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:681:VAL:O	1:D:681:VAL:CG1	2.66	0.42
4:C:3023:GOL:H12	6:C:3365:HOH:O	2.19	0.42
1:D:212:HIS:CE1	1:D:237:LEU:HD12	2.55	0.42
1:A:634:ARG:NH2	1:A:645:ASP:OD1	2.53	0.42
1:C:536:HIS:HA	6:C:3099:HOH:O	2.19	0.42
1:F:18:HIS:O	1:F:38:PRO:HA	2.19	0.42
1:F:498:LEU:HD21	1:F:608:TYR:HB3	2.00	0.42
1:F:631:PRO:O	1:F:646:GLY:HA3	2.19	0.42
1:F:735:THR:HG23	6:F:3193:HOH:O	2.17	0.42
1:C:200:TYR:CZ	1:C:208:VAL:HG13	2.54	0.42
1:F:652:GLN:NE2	1:F:654:HIS:NE2	2.68	0.42
1:D:178:THR:HG23	6:D:3276:HOH:O	2.19	0.42
1:C:352:GLN:HA	1:C:357:PHE:CD2	2.55	0.41
1:D:143:THR:CG2	6:D:3311:HOH:O	2.68	0.41
1:D:416:ASP:OD2	3:D:3018:XTG:H8	2.20	0.41
1:E:219:GLU:HB2	1:E:229:GLN:HB3	2.02	0.41
1:F:121:ASP:OD1	1:F:128:ARG:HD2	2.20	0.41
1:B:748:GLN:O	1:B:768:LEU:HA	2.20	0.41
1:C:313:PHE:CA	1:C:381:GLN:HE22	2.33	0.41
1:E:201:MET:HE1	1:E:247:PRO:HB3	2.02	0.41
1:E:273:LEU:HB2	1:E:300:LEU:HD21	2.02	0.41
1:E:690:LEU:O	1:E:739:ARG:HB2	2.19	0.41
1:D:99:ARG:NH2	1:D:100:TYR:OH	2.53	0.41
1:E:48:LEU:HD23	1:E:48:LEU:N	2.36	0.41
1:F:352:GLN:HA	1:F:357:PHE:CD2	2.55	0.41
1:F:525:LYS:HG2	1:F:558:VAL:HG21	2.03	0.41
1:C:183:ASN:HA	1:C:196:ASN:ND2	2.36	0.41
1:E:29:ASP:HB3	1:E:30:ASN:H	1.73	0.41
1:B:82:TYR:CD1	1:B:470:VAL:HB	2.55	0.41
1:B:347:ASN:C	1:B:347:ASN:HD22	2.24	0.41
1:D:281:TYR:CZ	1:D:308:PHE:HB2	2.56	0.41
1:F:522:HIS:CB	1:F:622:GLU:HG3	2.50	0.41
1:F:768:LEU:HD12	1:F:768:LEU:HA	1.82	0.41
1:C:747:LEU:HD22	1:C:750:GLY:O	2.20	0.41
1:F:569:MET:HB2	1:F:573:LEU:HD22	2.03	0.41
1:A:375:TRP:CE2	1:A:422:PRO:HG3	2.56	0.41
1:A:748:GLN:HB2	1:A:769:THR:HG22	2.03	0.41
1:B:223:GLU:O	1:C:190:THR:HA	2.20	0.41
1:B:748:GLN:HB2	1:B:769:THR:HB	2.03	0.41
1:F:21:GLN:NE2	1:F:41:VAL:H	2.19	0.41
1:A:342:ILE:N	1:A:342:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:GLN:HB2	1:B:697:HIS:CD2	2.55	0.41
1:C:21:GLN:NE2	1:C:41:VAL:H	2.19	0.41
1:C:55:LEU:HA	1:C:68:ARG:O	2.21	0.41
1:C:128:ARG:NH2	1:C:131:GLY:HA3	2.34	0.41
1:C:347:ASN:C	1:C:347:ASN:ND2	2.73	0.41
1:C:694:GLN:HB2	1:C:697:HIS:CD2	2.56	0.41
1:D:388:ASP:OD1	1:D:388:ASP:C	2.59	0.41
1:D:631:PRO:O	1:D:646:GLY:HA3	2.21	0.41
1:A:479:TRP:CZ3	1:A:481:GLY:HA2	2.56	0.41
1:E:208:VAL:HA	1:E:240:PHE:O	2.22	0.41
1:E:694:GLN:HB2	1:E:697:HIS:CD2	2.56	0.41
1:A:735:THR:HG23	6:A:3229:HOH:O	2.22	0.40
1:A:689:HIS:ND1	1:A:739:ARG:HD3	2.36	0.40
1:D:608:TYR:CZ	1:D:616:VAL:HG22	2.56	0.40
1:E:376:GLN:HA	1:E:384:LEU:O	2.21	0.40
1:F:744:VAL:HG22	1:F:771:THR:O	2.21	0.40
1:D:735:THR:HG23	6:D:3161:HOH:O	2.21	0.40
1:C:21:GLN:HE22	1:C:41:VAL:H	1.68	0.40
1:D:315:TRP:H	1:D:381:GLN:NE2	2.19	0.40
1:F:107:ASN:ND2	1:F:125:ASN:HD21	2.20	0.40
1:A:726:THR:HA	1:A:766:ASN:HD21	1.87	0.40
1:B:689:HIS:HB3	1:B:739:ARG:HH11	1.86	0.40
1:D:80:PRO:HD3	1:D:431:SER:HB3	2.03	0.40
1:E:91:LYS:HE2	6:E:3177:HOH:O	2.22	0.40
1:E:315:TRP:N	1:E:381:GLN:HE21	2.17	0.40
1:E:652:GLN:NE2	1:E:654:HIS:NE2	2.70	0.40

There are no symmetry-related clashes.

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	771/773 (100%)	744 (96%)	25 (3%)	2 (0%)	41	30
1	B	771/773 (100%)	736 (96%)	33 (4%)	2 (0%)	41	30
1	C	771/773 (100%)	740 (96%)	30 (4%)	1 (0%)	51	43
1	D	771/773 (100%)	743 (96%)	28 (4%)	0	100	100
1	E	771/773 (100%)	740 (96%)	27 (4%)	4 (0%)	29	17
1	F	771/773 (100%)	737 (96%)	28 (4%)	6 (1%)	19	9
All	All	4626/4638 (100%)	4440 (96%)	171 (4%)	15 (0%)	41	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	LEU
1	B	768	LEU
1	E	316	CYS
1	E	477	VAL
1	F	316	CYS
1	B	767	ALA
1	E	766	ASN
1	F	768	LEU
1	C	279	THR
1	E	768	LEU
1	F	77	ASN
1	F	477	VAL
1	F	767	ALA
1	A	348	PRO
1	F	476	PRO

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	660/660 (100%)	617 (94%)	43 (6%)	17	6
1	B	660/660 (100%)	618 (94%)	42 (6%)	17	6
1	C	660/660 (100%)	614 (93%)	46 (7%)	15	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	660/660 (100%)	610 (92%)	50 (8%)	13	4
1	E	660/660 (100%)	609 (92%)	51 (8%)	13	4
1	F	660/660 (100%)	617 (94%)	43 (6%)	17	6
All	All	3960/3960 (100%)	3685 (93%)	275 (7%)	15	5

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	48	LEU
1	A	52	LEU
1	A	84	LEU
1	A	120	LEU
1	A	123	LEU
1	A	137	ASN
1	A	174	ARG
1	A	178	THR
1	A	208	VAL
1	A	281	TYR
1	A	300	LEU
1	A	332	ILE
1	A	336	LYS
1	A	347	ASN
1	A	377	TRP
1	A	452	LEU
1	A	459	GLU
1	A	518	THR
1	A	532	LEU
1	A	533	LEU
1	A	573	LEU
1	A	614	VAL
1	A	616	VAL
1	A	630	LEU
1	A	647	SER
1	A	657	LEU
1	A	671	LEU
1	A	681	VAL
1	A	693	LEU
1	A	714	LEU
1	A	719	THR
1	A	723	ILE

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Mol	Chain	Res	Type
1	A	732	LYS
1	A	735	THR
1	A	736	LEU
1	A	744	VAL
1	A	756	GLU
1	A	757	GLN
1	A	759	LEU
1	A	764	GLN
1	A	768	LEU
1	A	770	ILE
1	B	48	LEU
1	B	84	LEU
1	B	99	ARG
1	B	120	LEU
1	B	137	ASN
1	B	174	ARG
1	B	178	THR
1	B	179	VAL
1	B	208	VAL
1	B	260	ARG
1	B	273	LEU
1	B	347	ASN
1	B	377	TRP
1	B	425	VAL
1	B	452	LEU
1	B	459	GLU
1	B	518	THR
1	B	532	LEU
1	B	533	LEU
1	B	537	SER
1	B	546	ARG
1	B	553	ASP
1	B	573	LEU
1	B	579	ARG
1	B	592	MET
1	B	616	VAL
1	B	630	LEU
1	B	657	LEU
1	B	686	THR
1	B	693	LEU
1	B	714	LEU
1	B	723	ILE

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Mol	Chain	Res	Type
1	B	732	LYS
1	B	735	THR
1	B	736	LEU
1	B	739	ARG
1	B	744	VAL
1	B	747	LEU
1	B	764	GLN
1	B	766	ASN
1	B	771	THR
1	B	773	HIS
1	C	30	ASN
1	C	48	LEU
1	C	52	LEU
1	C	84	LEU
1	C	95	GLU
1	C	120	LEU
1	C	137	ASN
1	C	143	THR
1	C	174	ARG
1	C	178	THR
1	C	179	VAL
1	C	208	VAL
1	C	214	GLN
1	C	264	PRO
1	C	273	LEU
1	C	280	ASN
1	C	281	TYR
1	C	288	SER
1	C	300	LEU
1	C	336	LYS
1	C	347	ASN
1	C	377	TRP
1	C	452	LEU
1	C	453	LYS
1	C	459	GLU
1	C	533	LEU
1	C	573	LEU
1	C	592	MET
1	C	614	VAL
1	C	616	VAL
1	C	630	LEU
1	C	657	LEU

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Mol	Chain	Res	Type
1	C	669	LEU
1	C	671	LEU
1	C	681	VAL
1	C	693	LEU
1	C	714	LEU
1	C	723	ILE
1	C	726	THR
1	C	732	LYS
1	C	736	LEU
1	C	745	ASN
1	C	749	ASP
1	C	756	GLU
1	C	770	ILE
1	C	773	HIS
1	D	45	THR
1	D	48	LEU
1	D	52	LEU
1	D	69	ILE
1	D	84	LEU
1	D	93	THR
1	D	99	ARG
1	D	120	LEU
1	D	137	ASN
1	D	143	THR
1	D	146	GLN
1	D	174	ARG
1	D	178	THR
1	D	208	VAL
1	D	246	THR
1	D	273	LEU
1	D	281	TYR
1	D	300	LEU
1	D	332	ILE
1	D	347	ASN
1	D	377	TRP
1	D	452	LEU
1	D	459	GLU
1	D	518	THR
1	D	532	LEU
1	D	533	LEU
1	D	542	SER
1	D	573	LEU

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Mol	Chain	Res	Type
1	D	592	MET
1	D	614	VAL
1	D	616	VAL
1	D	630	LEU
1	D	632	GLU
1	D	657	LEU
1	D	671	LEU
1	D	693	LEU
1	D	714	LEU
1	D	723	ILE
1	D	732	LYS
1	D	733	ASN
1	D	735	THR
1	D	736	LEU
1	D	742	VAL
1	D	745	ASN
1	D	755	SER
1	D	764	GLN
1	D	768	LEU
1	D	771	THR
1	D	772	LEU
1	D	773	HIS
1	E	29	ASP
1	E	44	ARG
1	E	52	LEU
1	E	69	ILE
1	E	98	GLU
1	E	99	ARG
1	E	120	LEU
1	E	123	LEU
1	E	137	ASN
1	E	143	THR
1	E	146	GLN
1	E	174	ARG
1	E	178	THR
1	E	208	VAL
1	E	246	THR
1	E	273	LEU
1	E	276	SER
1	E	300	LEU
1	E	316	CYS
1	E	324	THR

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Mol	Chain	Res	Type
1	E	332	ILE
1	E	334	ARG
1	E	347	ASN
1	E	377	TRP
1	E	408	MET
1	E	419	GLU
1	E	425	VAL
1	E	452	LEU
1	E	459	GLU
1	E	477	VAL
1	E	533	LEU
1	E	542	SER
1	E	573	LEU
1	E	616	VAL
1	E	630	LEU
1	E	653	GLN
1	E	657	LEU
1	E	664	ARG
1	E	671	LEU
1	E	693	LEU
1	E	714	LEU
1	E	719	THR
1	E	723	ILE
1	E	736	LEU
1	E	739	ARG
1	E	742	VAL
1	E	764	GLN
1	E	769	THR
1	E	771	THR
1	E	772	LEU
1	E	773	HIS
1	F	44	ARG
1	F	45	THR
1	F	52	LEU
1	F	84	LEU
1	F	95	GLU
1	F	120	LEU
1	F	137	ASN
1	F	143	THR
1	F	174	ARG
1	F	178	THR
1	F	179	VAL

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Mol	Chain	Res	Type
1	F	214	GLN
1	F	273	LEU
1	F	280	ASN
1	F	300	LEU
1	F	316	CYS
1	F	336	LYS
1	F	347	ASN
1	F	377	TRP
1	F	452	LEU
1	F	459	GLU
1	F	492	GLU
1	F	532	LEU
1	F	533	LEU
1	F	537	SER
1	F	544	SER
1	F	573	LEU
1	F	579	ARG
1	F	592	MET
1	F	616	VAL
1	F	630	LEU
1	F	671	LEU
1	F	681	VAL
1	F	693	LEU
1	F	714	LEU
1	F	732	LYS
1	F	735	THR
1	F	736	LEU
1	F	739	ARG
1	F	747	LEU
1	F	764	GLN
1	F	770	ILE
1	F	771	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	27	GLN
1	A	73	GLN
1	A	107	ASN
1	A	125	ASN
1	A	133	GLN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	141	GLN
1	A	212	HIS
1	A	347	ASN
1	A	352	GLN
1	A	381	GLN
1	A	564	GLN
1	A	641	ASN
1	A	652	GLN
1	A	692	ASN
1	A	766	ASN
1	B	21	GLN
1	B	27	GLN
1	B	73	GLN
1	B	107	ASN
1	B	133	GLN
1	B	137	ASN
1	B	177	GLN
1	B	212	HIS
1	B	347	ASN
1	B	352	GLN
1	B	381	GLN
1	B	478	HIS
1	B	652	GLN
1	B	692	ASN
1	B	697	HIS
1	B	733	ASN
1	B	766	ASN
1	C	21	GLN
1	C	27	GLN
1	C	30	ASN
1	C	73	GLN
1	C	107	ASN
1	C	133	GLN
1	C	137	ASN
1	C	141	GLN
1	C	177	GLN
1	C	212	HIS
1	C	347	ASN
1	C	352	GLN
1	C	381	GLN
1	C	478	HIS

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Mol	Chain	Res	Type
1	C	517	ASN
1	C	652	GLN
1	C	692	ASN
1	C	733	ASN
1	D	21	GLN
1	D	27	GLN
1	D	73	GLN
1	D	107	ASN
1	D	125	ASN
1	D	133	GLN
1	D	137	ASN
1	D	141	GLN
1	D	146	GLN
1	D	177	GLN
1	D	212	HIS
1	D	347	ASN
1	D	352	GLN
1	D	381	GLN
1	D	564	GLN
1	D	652	GLN
1	D	692	ASN
1	D	766	ASN
1	E	27	GLN
1	E	73	GLN
1	E	107	ASN
1	E	133	GLN
1	E	137	ASN
1	E	212	HIS
1	E	347	ASN
1	E	352	GLN
1	E	381	GLN
1	E	564	GLN
1	E	652	GLN
1	E	653	GLN
1	E	692	ASN
1	E	697	HIS
1	E	745	ASN
1	E	766	ASN
1	F	21	GLN
1	F	27	GLN
1	F	61	GLN
1	F	73	GLN

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Mol	Chain	Res	Type
1	F	107	ASN
1	F	133	GLN
1	F	137	ASN
1	F	177	GLN
1	F	212	HIS
1	F	280	ASN
1	F	347	ASN
1	F	352	GLN
1	F	381	GLN
1	F	478	HIS
1	F	564	GLN
1	F	652	GLN
1	F	697	HIS
1	F	733	ASN
1	F	748	GLN

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 ⓘ

35 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	GOL	D	3032	-	5,5,5	0.45	0	5,5,5	0.93	0
2	SO4	A	3008	-	4,4,4	0.27	0	6,6,6	0.55	0
2	SO4	F	3003	-	4,4,4	0.30	0	6,6,6	0.40	0
2	SO4	F	3001	-	4,4,4	0.20	0	6,6,6	0.75	0
2	SO4	E	3004	-	4,4,4	0.26	0	6,6,6	0.53	0
3	XTG	F	3020	-	31,32,32	2.72	10 (32%)	42,46,46	2.68	13 (30%)
2	SO4	F	3007	-	4,4,4	0.12	0	6,6,6	0.29	0
3	XTG	E	3019	-	31,32,32	2.54	7 (22%)	42,46,46	2.19	11 (26%)
5	MPO	E	3013	-	13,13,13	1.97	1 (7%)	17,17,17	1.72	3 (17%)
4	GOL	A	3029	-	5,5,5	0.53	0	5,5,5	1.16	1 (20%)
5	MPO	C	3011	-	13,13,13	1.93	1 (7%)	17,17,17	1.50	4 (23%)
2	SO4	E	3009	-	4,4,4	0.16	0	6,6,6	0.52	0
4	GOL	A	3024	-	5,5,5	0.42	0	5,5,5	0.84	0
3	XTG	D	3018	-	31,32,32	3.97	10 (32%)	42,46,46	2.97	15 (35%)
4	GOL	D	3031	-	5,5,5	0.43	0	5,5,5	0.58	0
2	SO4	B	3006	-	4,4,4	0.18	0	6,6,6	0.34	0
4	GOL	C	3030	-	5,5,5	0.47	0	5,5,5	0.52	0
5	MPO	F	3014	-	13,13,13	8.04	2 (15%)	17,17,17	8.56	6 (35%)
4	GOL	B	3026	-	5,5,5	0.31	0	5,5,5	0.79	0
4	GOL	B	3025	-	5,5,5	0.40	0	5,5,5	1.06	0
4	GOL	F	3034	-	5,5,5	0.43	0	5,5,5	0.47	0
5	MPO	B	3010	-	13,13,13	2.04	1 (7%)	17,17,17	1.24	2 (11%)
4	GOL	E	3033	-	5,5,5	0.43	0	5,5,5	0.62	0
3	XTG	C	3017	-	31,32,32	2.99	4 (12%)	42,46,46	1.97	6 (14%)
3	XTG	F	3021	-	31,32,32	2.86	6 (19%)	42,46,46	2.21	8 (19%)
5	MPO	D	3012	-	13,13,13	2.07	1 (7%)	17,17,17	1.47	3 (17%)
3	XTG	A	3015	-	31,32,32	2.98	5 (16%)	42,46,46	2.63	17 (40%)
2	SO4	C	3005	-	4,4,4	0.07	0	6,6,6	0.73	0
2	SO4	D	3002	-	4,4,4	0.22	0	6,6,6	0.47	0
4	GOL	C	3023	-	5,5,5	0.56	0	5,5,5	1.43	1 (20%)
4	GOL	F	3022	-	5,5,5	0.60	0	5,5,5	0.81	0
4	GOL	C	3027	-	5,5,5	0.57	0	5,5,5	0.76	0
4	GOL	A	3028	-	5,5,5	0.36	0	5,5,5	0.66	0
4	GOL	E	3035	-	5,5,5	0.64	0	5,5,5	0.79	0
3	XTG	B	3016	-	31,32,32	3.15	7 (22%)	42,46,46	2.77	13 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	3032	-	-	0/4/4/4	-
3	XTG	F	3020	-	-	7/11/50/50	0/3/3/3
3	XTG	E	3019	-	-	5/11/50/50	0/3/3/3
5	MPO	E	3013	-	-	5/7/15/15	0/1/1/1
4	GOL	A	3029	-	-	0/4/4/4	-
5	MPO	C	3011	-	-	0/7/15/15	0/1/1/1
4	GOL	A	3024	-	-	4/4/4/4	-
3	XTG	D	3018	-	-	6/11/50/50	0/3/3/3
4	GOL	D	3031	-	-	4/4/4/4	-
4	GOL	C	3030	-	-	2/4/4/4	-
5	MPO	F	3014	-	-	3/7/15/15	0/1/1/1
4	GOL	B	3026	-	-	2/4/4/4	-
4	GOL	B	3025	-	-	4/4/4/4	-
4	GOL	F	3034	-	-	4/4/4/4	-
5	MPO	B	3010	-	-	0/7/15/15	0/1/1/1
4	GOL	E	3033	-	-	3/4/4/4	-
3	XTG	C	3017	-	-	7/11/50/50	0/3/3/3
3	XTG	F	3021	-	-	2/11/50/50	0/3/3/3
5	MPO	D	3012	-	-	2/7/15/15	0/1/1/1
3	XTG	A	3015	-	-	5/11/50/50	0/3/3/3
4	GOL	C	3023	-	-	0/4/4/4	-
4	GOL	F	3022	-	-	4/4/4/4	-
4	GOL	C	3027	-	-	2/4/4/4	-
4	GOL	A	3028	-	-	4/4/4/4	-
4	GOL	E	3035	-	-	1/4/4/4	-
3	XTG	B	3016	-	-	7/11/50/50	0/3/3/3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3014	MPO	C4-N1	28.04	2.24	1.46
3	D	3018	XTG	O11-N1	15.42	1.48	1.22
3	C	3017	XTG	O11-N1	14.87	1.48	1.22
3	A	3015	XTG	O11-N1	13.74	1.46	1.22
3	B	3016	XTG	O11-N1	13.20	1.45	1.22
3	F	3021	XTG	O11-N1	12.47	1.44	1.22
3	F	3020	XTG	O11-N1	11.43	1.42	1.22
3	E	3019	XTG	O11-N1	10.65	1.40	1.22
3	D	3018	XTG	O9-C11	7.48	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3012	MPO	C1-S1	-6.86	1.67	1.77
5	F	3014	MPO	C1-S1	-6.79	1.67	1.77
5	B	3010	MPO	C1-S1	-6.78	1.67	1.77
5	E	3013	MPO	C1-S1	-6.74	1.67	1.77
5	C	3011	MPO	C1-S1	-6.32	1.68	1.77
3	B	3016	XTG	O1-C1	6.28	1.50	1.41
3	D	3018	XTG	C7-S6	6.21	1.90	1.80
3	D	3018	XTG	O8-C10	5.80	1.55	1.43
3	D	3018	XTG	O9-C7	5.78	1.54	1.41
3	F	3020	XTG	C7-S6	5.36	1.89	1.80
3	F	3021	XTG	O9-C11	5.08	1.51	1.43
3	D	3018	XTG	C7-C8	4.94	1.61	1.53
3	D	3018	XTG	C12-N1	-4.80	1.33	1.45
3	E	3019	XTG	C7-S6	4.74	1.88	1.80
3	A	3015	XTG	O1-C1	4.64	1.48	1.41
3	C	3017	XTG	C12-N1	-4.51	1.34	1.45
3	A	3015	XTG	C7-S6	4.44	1.87	1.80
3	F	3021	XTG	O9-C7	4.30	1.51	1.41
3	B	3016	XTG	C10-C9	4.21	1.58	1.52
3	B	3016	XTG	C7-S6	4.20	1.87	1.80
3	B	3016	XTG	C12-N1	-4.05	1.35	1.45
3	D	3018	XTG	C8-C9	3.99	1.62	1.52
3	F	3021	XTG	C12-N1	-3.85	1.35	1.45
3	A	3015	XTG	C12-N1	-3.77	1.36	1.45
3	F	3020	XTG	C10-C9	3.59	1.57	1.52
3	E	3019	XTG	C12-N1	-3.50	1.36	1.45
3	E	3019	XTG	O1-C1	3.43	1.46	1.41
3	F	3020	XTG	C12-N1	-3.32	1.37	1.45
3	B	3016	XTG	C8-C9	3.20	1.60	1.52
3	E	3019	XTG	C10-C9	3.16	1.57	1.52
3	F	3021	XTG	C11-C10	3.08	1.59	1.52
3	C	3017	XTG	C7-S6	2.98	1.85	1.80
3	F	3020	XTG	O6-C8	2.94	1.49	1.43
3	F	3021	XTG	C7-S6	2.84	1.85	1.80
3	F	3020	XTG	C8-C9	2.60	1.59	1.52
3	F	3020	XTG	O5-C1	2.48	1.48	1.41
3	B	3016	XTG	O9-C11	2.46	1.47	1.43
3	D	3018	XTG	O6-C8	2.30	1.48	1.43
3	F	3020	XTG	O7-C9	2.26	1.48	1.43
3	F	3020	XTG	O9-C7	2.24	1.46	1.41
3	C	3017	XTG	C8-C9	2.24	1.58	1.52
3	E	3019	XTG	C7-C8	2.18	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3018	XTG	C10-C9	2.15	1.55	1.52
3	F	3020	XTG	C7-C8	2.08	1.57	1.53
3	E	3019	XTG	O5-C1	2.01	1.47	1.41
3	A	3015	XTG	C10-C9	2.01	1.55	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3014	MPO	C6-C7-N1	28.67	153.57	110.10
5	F	3014	MPO	C7-N1-C4	-13.89	77.56	108.83
5	F	3014	MPO	C5-C4-N1	11.46	127.48	110.10
3	B	3016	XTG	O5-C5-C6	10.59	124.33	106.48
3	A	3015	XTG	O5-C5-C6	8.96	121.59	106.48
3	D	3018	XTG	O5-C5-C6	8.89	121.47	106.48
3	C	3017	XTG	C6-S6-C7	8.16	115.45	100.13
3	D	3018	XTG	C6-S6-C7	8.02	115.19	100.13
3	F	3020	XTG	O5-C5-C6	8.00	119.97	106.48
3	E	3019	XTG	C6-S6-C7	7.69	114.58	100.13
3	B	3016	XTG	C6-S6-C7	7.64	114.49	100.13
3	A	3015	XTG	C6-S6-C7	7.46	114.15	100.13
3	F	3021	XTG	C6-S6-C7	7.44	114.11	100.13
3	F	3020	XTG	C1-O5-C5	-7.09	99.77	113.69
3	F	3021	XTG	O9-C11-C10	6.95	121.50	110.77
5	F	3014	MPO	O2-S1-C1	6.86	115.18	106.92
3	D	3018	XTG	C11-C10-C9	-6.77	101.35	109.67
3	D	3018	XTG	O8-C10-C11	6.51	122.47	109.15
3	F	3020	XTG	C6-S6-C7	6.48	112.31	100.13
3	E	3019	XTG	O9-C7-C8	-6.42	102.04	110.25
3	B	3016	XTG	C15-O1-C1	-5.97	109.04	117.79
5	F	3014	MPO	C3-N1-C7	5.96	126.46	111.23
3	F	3020	XTG	C6-C5-C4	-5.89	98.07	112.84
3	A	3015	XTG	C1-O5-C5	-5.31	103.27	113.69
3	C	3017	XTG	O5-C5-C6	4.90	114.75	106.48
3	D	3018	XTG	O9-C11-C10	4.86	118.28	110.77
3	F	3021	XTG	O9-C7-C8	4.74	116.29	110.25
3	B	3016	XTG	O5-C1-O1	4.57	119.92	108.29
3	B	3016	XTG	O1-C1-C2	4.49	113.65	107.14
5	E	3013	MPO	O1-S1-C1	4.47	112.29	106.92
3	F	3021	XTG	O5-C5-C6	-4.25	99.32	106.48
3	D	3018	XTG	O8-C10-C9	4.03	118.21	110.14
3	D	3018	XTG	C6-C5-C4	-3.99	102.83	112.84
3	C	3017	XTG	O9-C11-C10	3.71	116.50	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	3013	MPO	O2-S1-C1	3.69	111.36	106.92
3	A	3015	XTG	O11-N1-C12	3.67	123.99	118.80
3	F	3021	XTG	C6-C5-C4	3.53	121.69	112.84
3	D	3018	XTG	O6-C8-C9	3.52	118.49	110.35
3	A	3015	XTG	O6-C8-C9	3.49	118.41	110.35
3	F	3020	XTG	O9-C7-C8	3.45	114.65	110.25
3	A	3015	XTG	O5-C1-O1	3.44	117.03	108.29
3	A	3015	XTG	O9-C11-C10	3.44	116.07	110.77
3	D	3018	XTG	O9-C7-C8	-3.43	105.86	110.25
3	C	3017	XTG	C3-C4-C5	-3.40	104.17	110.24
3	F	3020	XTG	C15-O1-C1	-3.40	112.81	117.79
3	C	3017	XTG	C1-O5-C5	-3.38	107.05	113.69
3	F	3020	XTG	O1-C1-C2	3.38	112.05	107.14
3	E	3019	XTG	C17-C12-N1	3.37	121.91	119.38
3	E	3019	XTG	C1-O5-C5	-3.34	107.14	113.69
3	F	3020	XTG	O6-C8-C9	3.32	118.03	110.35
3	E	3019	XTG	O5-C5-C6	3.30	112.04	106.48
5	D	3012	MPO	O1-S1-C1	3.26	110.84	106.92
3	B	3016	XTG	O9-C7-C8	-3.26	106.08	110.25
5	D	3012	MPO	O3-S1-C1	3.24	111.01	105.77
5	C	3011	MPO	O1-S1-C1	3.11	110.66	106.92
3	B	3016	XTG	O6-C8-C9	3.10	117.52	110.35
3	B	3016	XTG	C3-C4-C5	-3.02	104.85	110.24
3	F	3021	XTG	O9-C7-S6	2.93	116.74	109.82
3	A	3015	XTG	C13-C12-N1	2.91	121.57	119.38
3	B	3016	XTG	C1-O5-C5	-2.88	108.04	113.69
3	D	3018	XTG	O6-C8-C7	2.83	115.46	110.27
3	E	3019	XTG	O1-C1-C2	2.82	111.23	107.14
5	B	3010	MPO	O3-S1-C1	2.82	110.33	105.77
3	D	3018	XTG	O7-C9-C8	2.82	116.86	110.35
3	D	3018	XTG	O9-C7-S6	2.71	116.21	109.82
3	A	3015	XTG	O9-C7-C8	-2.69	106.81	110.25
3	E	3019	XTG	C11-C10-C9	2.68	112.96	109.67
5	C	3011	MPO	O3-S1-C1	2.68	110.10	105.77
3	A	3015	XTG	C3-C4-C5	-2.66	105.49	110.24
3	B	3016	XTG	C13-C12-N1	2.64	121.36	119.38
3	F	3020	XTG	O7-C9-C8	2.64	116.45	110.35
3	A	3015	XTG	O5-C5-C4	-2.60	104.97	109.69
3	D	3018	XTG	O5-C1-O1	2.59	114.87	108.29
3	A	3015	XTG	C6-C5-C4	-2.55	106.44	112.84
3	F	3020	XTG	C17-C12-N1	2.54	121.29	119.38
3	A	3015	XTG	O1-C1-C2	2.53	110.81	107.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3015	XTG	O7-C9-C8	2.50	116.14	110.35
3	A	3015	XTG	C4-C3-C2	-2.49	106.47	110.82
5	F	3014	MPO	O2-S1-O1	-2.42	105.58	113.95
3	D	3018	XTG	C10-C9-C8	-2.37	106.79	110.89
3	E	3019	XTG	O5-C1-O1	2.31	114.16	108.29
3	F	3020	XTG	C3-C4-C5	-2.30	106.14	110.24
3	F	3020	XTG	O3-C3-C2	-2.29	105.07	110.35
3	A	3015	XTG	O6-C8-C7	-2.27	106.10	110.27
5	C	3011	MPO	O2-S1-O1	-2.26	106.14	113.95
3	B	3016	XTG	O8-C10-C9	2.23	114.60	110.14
5	D	3012	MPO	O3-S1-O2	-2.22	105.85	111.27
3	E	3019	XTG	C15-O1-C1	2.22	121.05	117.79
5	C	3011	MPO	O3-S1-O2	-2.20	105.89	111.27
3	F	3020	XTG	C4-C3-C2	-2.20	106.98	110.82
3	F	3021	XTG	O8-C10-C11	2.17	113.59	109.15
5	B	3010	MPO	O1-S1-C1	2.17	109.53	106.92
5	E	3013	MPO	O2-S1-O1	-2.16	106.48	113.95
3	E	3019	XTG	O6-C8-C7	2.16	114.23	110.27
4	C	3023	GOL	O2-C2-C3	2.14	118.56	109.12
3	E	3019	XTG	C3-C4-C5	-2.14	106.42	110.24
3	C	3017	XTG	O2-C2-C1	-2.12	104.89	110.05
3	B	3016	XTG	C11-C10-C9	2.12	112.27	109.67
3	A	3015	XTG	O5-C1-C2	-2.09	105.93	110.35
3	B	3016	XTG	O5-C1-C2	-2.05	106.02	110.35
3	D	3018	XTG	O11-N1-C12	-2.03	115.92	118.80
3	F	3021	XTG	C1-O5-C5	-2.01	109.74	113.69
4	A	3029	GOL	O2-C2-C1	2.01	117.97	109.12

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3015	XTG	O5-C5-C6-S6
3	A	3015	XTG	C4-C5-C6-S6
3	A	3015	XTG	O9-C7-S6-C6
3	A	3015	XTG	C8-C7-S6-C6
3	B	3016	XTG	C17-C12-N1-O11
3	B	3016	XTG	O5-C5-C6-S6
3	B	3016	XTG	C4-C5-C6-S6
3	B	3016	XTG	O9-C7-S6-C6
3	B	3016	XTG	C8-C7-S6-C6
3	C	3017	XTG	C13-C12-N1-O11

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Mol	Chain	Res	Type	Atoms
3	C	3017	XTG	C17-C12-N1-O11
3	C	3017	XTG	C4-C5-C6-S6
3	C	3017	XTG	O9-C7-S6-C6
3	D	3018	XTG	C13-C12-N1-O11
3	D	3018	XTG	C17-C12-N1-O11
3	D	3018	XTG	O5-C5-C6-S6
3	D	3018	XTG	C4-C5-C6-S6
3	D	3018	XTG	O9-C7-S6-C6
3	E	3019	XTG	C13-C12-N1-O11
3	E	3019	XTG	C17-C12-N1-O11
3	E	3019	XTG	O5-C1-O1-C15
3	E	3019	XTG	O9-C7-S6-C6
3	F	3020	XTG	C13-C12-N1-O11
3	F	3020	XTG	C17-C12-N1-O11
3	F	3020	XTG	O5-C5-C6-S6
3	F	3020	XTG	C4-C5-C6-S6
3	F	3020	XTG	O9-C7-S6-C6
3	F	3020	XTG	C8-C7-S6-C6
3	F	3021	XTG	O9-C7-S6-C6
3	F	3021	XTG	C8-C7-S6-C6
4	A	3024	GOL	O1-C1-C2-C3
4	A	3024	GOL	C1-C2-C3-O3
4	A	3028	GOL	O1-C1-C2-C3
4	B	3025	GOL	O1-C1-C2-C3
4	C	3030	GOL	O1-C1-C2-C3
4	D	3031	GOL	O1-C1-C2-C3
4	E	3033	GOL	O1-C1-C2-C3
4	F	3022	GOL	O1-C1-C2-C3
4	F	3022	GOL	C1-C2-C3-O3
4	F	3034	GOL	O1-C1-C2-C3
4	F	3034	GOL	C1-C2-C3-O3
5	E	3013	MPO	C2-C1-S1-O2
5	F	3014	MPO	C1-C2-C3-N1
5	F	3014	MPO	C2-C3-N1-C4
3	A	3015	XTG	O5-C1-O1-C15
5	F	3014	MPO	C2-C3-N1-C7
4	A	3024	GOL	O1-C1-C2-O2
4	F	3022	GOL	O1-C1-C2-O2
4	F	3022	GOL	O2-C2-C3-O3
3	B	3016	XTG	C13-C12-N1-O11
5	D	3012	MPO	C2-C3-N1-C7
4	B	3025	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	3030	GOL	O1-C1-C2-O2
4	D	3031	GOL	O1-C1-C2-O2
4	D	3031	GOL	O2-C2-C3-O3
4	E	3033	GOL	O1-C1-C2-O2
4	F	3034	GOL	O1-C1-C2-O2
4	F	3034	GOL	O2-C2-C3-O3
3	B	3016	XTG	O5-C1-O1-C15
3	C	3017	XTG	O5-C1-O1-C15
4	A	3028	GOL	O1-C1-C2-O2
4	C	3027	GOL	O2-C2-C3-O3
4	E	3035	GOL	O2-C2-C3-O3
5	E	3013	MPO	C2-C1-S1-O3
4	A	3028	GOL	O2-C2-C3-O3
4	B	3025	GOL	O2-C2-C3-O3
4	E	3033	GOL	O2-C2-C3-O3
4	D	3031	GOL	C1-C2-C3-O3
3	C	3017	XTG	C8-C7-S6-C6
5	E	3013	MPO	C2-C1-S1-O1
5	D	3012	MPO	C2-C3-N1-C4
3	C	3017	XTG	O5-C5-C6-S6
3	E	3019	XTG	C4-C5-C6-S6
4	A	3024	GOL	O2-C2-C3-O3
4	B	3026	GOL	C1-C2-C3-O3
4	C	3027	GOL	C1-C2-C3-O3
5	E	3013	MPO	C2-C3-N1-C7
4	B	3026	GOL	O2-C2-C3-O3
5	E	3013	MPO	C2-C3-N1-C4
4	A	3028	GOL	C1-C2-C3-O3
4	B	3025	GOL	C1-C2-C3-O3
3	D	3018	XTG	C5-C6-S6-C7
3	F	3020	XTG	C5-C6-S6-C7

There are no ring outliers.

16 monomers are involved in 28 short contacts:

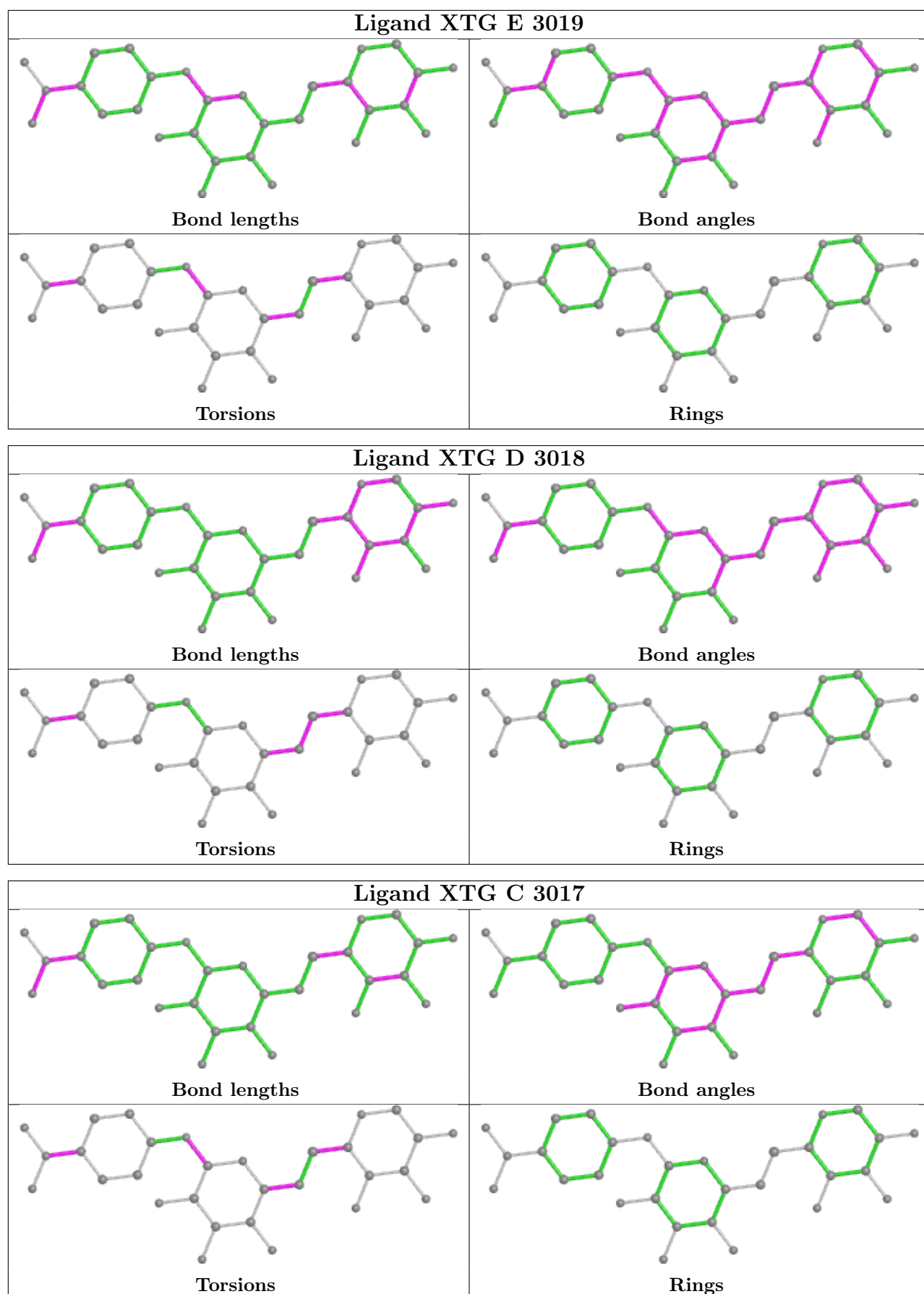| Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3032	GOL	2	0
2	F	3003	SO4	1	0
2	F	3001	SO4	2	0
2	E	3004	SO4	1	0
3	F	3020	XTG	1	0
3	E	3019	XTG	1	0

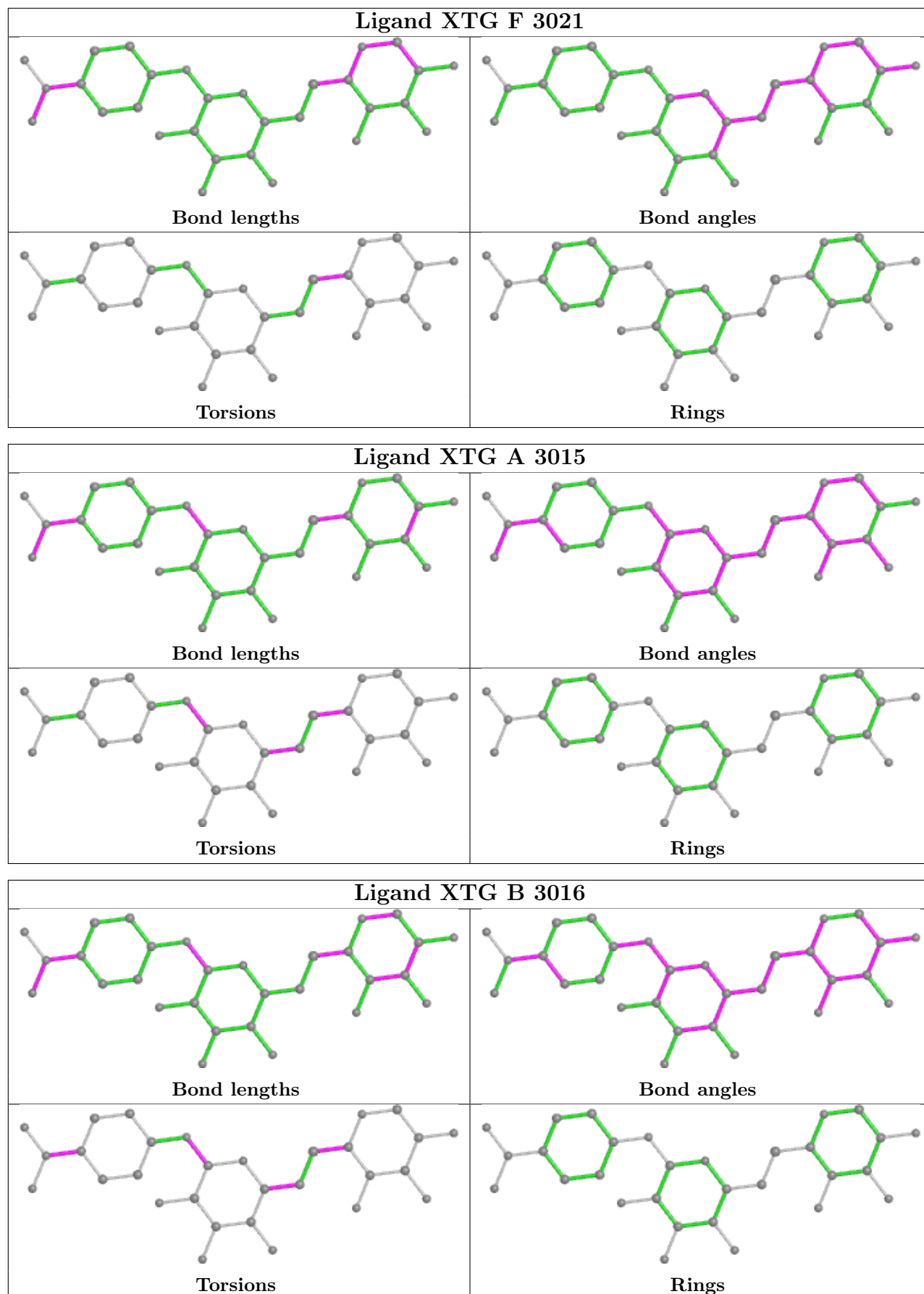*Continued on next page...*

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3029	GOL	3	0
4	A	3024	GOL	1	0
3	D	3018	XTG	7	0
4	B	3026	GOL	2	0
3	A	3015	XTG	2	0
2	D	3002	SO4	1	0
4	C	3023	GOL	1	0
4	F	3022	GOL	1	0
4	A	3028	GOL	1	0
3	B	3016	XTG	1	0

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

Ligand XTG F 3020

Bond lengths

Bond angles

Torsions

Rings

Ligand XTG E 3019

Bond lengths

Bond angles

Torsions

Rings

Ligand XTG D 3018

Bond lengths

Bond angles

Torsions

Rings

Ligand XTG C 3017

Bond lengths

Bond angles

Torsions

Rings

Ligand XTG F 3021

Bond lengths

Bond angles

Torsions

Rings

Ligand XTG A 3015

Bond lengths

Bond angles

Torsions

Rings

Ligand XTG B 3016

Bond lengths

Bond angles

Torsions

Rings
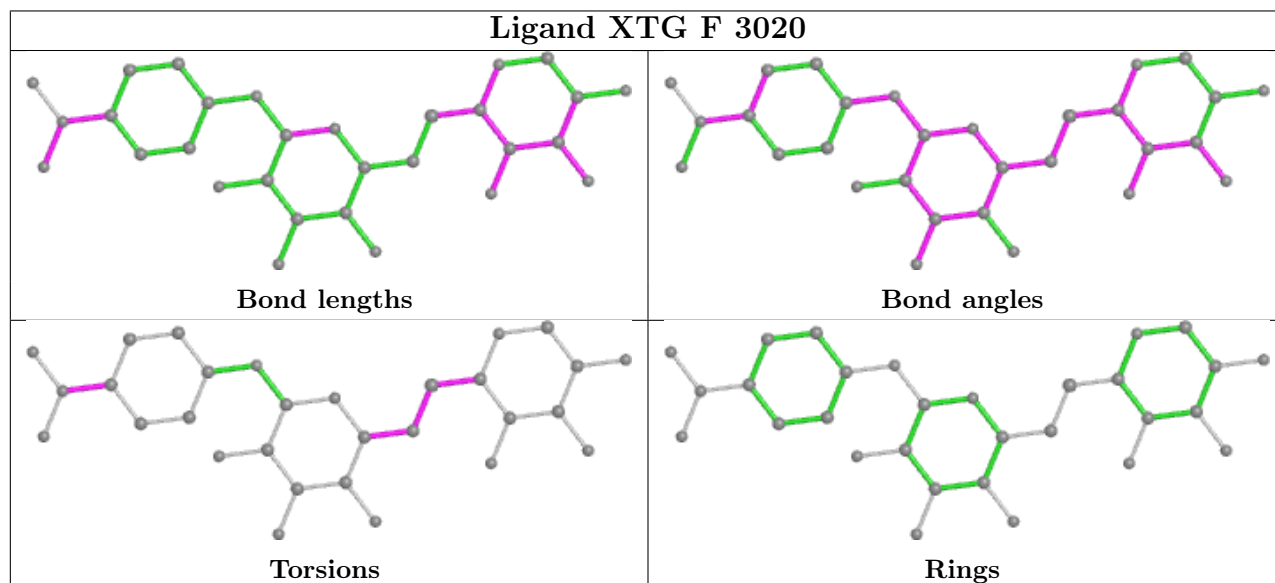
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	773/773 (100%)	-0.20	18 (2%)	60	69	8, 14, 35, 53	0
1	B	773/773 (100%)	-0.03	21 (2%)	54	63	11, 20, 38, 58	0
1	C	773/773 (100%)	-0.11	16 (2%)	63	72	9, 18, 35, 50	0
1	D	773/773 (100%)	-0.07	26 (3%)	45	55	8, 17, 41, 55	0
1	E	773/773 (100%)	-0.04	20 (2%)	56	65	10, 20, 39, 55	0
1	F	773/773 (100%)	-0.13	15 (1%)	66	74	9, 17, 37, 54	0
All	All	4638/4638 (100%)	-0.10	116 (2%)	57	66	8, 18, 38, 58	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	545	TYR	7.5
1	D	773	HIS	5.9
1	B	765	GLY	5.9
1	B	767	ALA	5.7
1	C	773	HIS	5.3
1	E	766	ASN	5.1
1	E	46	TRP	4.8
1	B	766	ASN	4.7
1	D	517	ASN	4.5
1	B	517	ASN	4.5
1	D	765	GLY	4.3
1	A	768	LEU	4.2
1	F	773	HIS	4.2
1	F	767	ALA	4.0
1	E	767	ALA	3.9
1	B	773	HIS	3.8
1	E	765	GLY	3.8
1	E	773	HIS	3.8
1	E	517	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	773	HIS	3.7
1	F	46	TRP	3.7
1	B	518	THR	3.6
1	E	518	THR	3.5
1	B	764	GLN	3.5
1	F	766	ASN	3.5
1	A	117	PHE	3.4
1	A	766	ASN	3.4
1	A	765	GLY	3.4
1	D	742	VAL	3.3
1	F	765	GLY	3.2
1	A	278	THR	3.2
1	B	543	LYS	3.2
1	C	765	GLY	3.1
1	B	46	TRP	3.1
1	A	517	ASN	3.1
1	D	519	ALA	3.0
1	B	748	GLN	3.0
1	A	745	ASN	3.0
1	B	754	GLU	2.9
1	D	518	THR	2.9
1	D	766	ASN	2.9
1	C	720	GLY	2.8
1	F	768	LEU	2.8
1	A	767	ALA	2.8
1	D	756	GLU	2.8
1	D	117	PHE	2.8
1	D	764	GLN	2.8
1	C	744	VAL	2.8
1	D	542	SER	2.8
1	A	518	THR	2.7
1	E	43	GLU	2.7
1	D	29	ASP	2.7
1	E	545	TYR	2.7
1	F	76	LEU	2.7
1	D	323	LEU	2.7
1	E	117	PHE	2.6
1	C	127	GLU	2.6
1	D	544	SER	2.6
1	A	748	GLN	2.6
1	D	88	GLN	2.6
1	F	518	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	754	GLU	2.6
1	D	281	TYR	2.5
1	C	745	ASN	2.5
1	D	484	TYR	2.5
1	B	756	GLU	2.5
1	D	543	LYS	2.5
1	D	745	ASN	2.5
1	D	46	TRP	2.4
1	B	745	ASN	2.4
1	D	743	LYS	2.4
1	E	42	ARG	2.4
1	C	764	GLN	2.4
1	A	46	TRP	2.4
1	E	721	ASN	2.4
1	C	117	PHE	2.3
1	F	517	ASN	2.3
1	C	748	GLN	2.3
1	B	98	GLU	2.3
1	C	766	ASN	2.3
1	D	748	GLN	2.3
1	E	45	THR	2.3
1	C	323	LEU	2.3
1	A	280	ASN	2.2
1	B	284	ALA	2.2
1	F	29	ASP	2.2
1	F	323	LEU	2.2
1	B	280	ASN	2.2
1	F	756	GLU	2.2
1	B	332	ILE	2.2
1	B	333	ARG	2.2
1	E	89	ASP	2.2
1	D	98	GLU	2.2
1	A	772	LEU	2.2
1	A	721	ASN	2.2
1	B	88	GLN	2.2
1	C	208	VAL	2.2
1	F	771	THR	2.1
1	E	543	LYS	2.1
1	E	208	VAL	2.1
1	A	770	ILE	2.1
1	D	100	TYR	2.1
1	C	756	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	533	LEU	2.1
1	E	745	ASN	2.1
1	C	88	GLN	2.1
1	E	551	TYR	2.1
1	E	764	GLN	2.1
1	C	634	ARG	2.1
1	C	46	TRP	2.1
1	A	29	ASP	2.1
1	F	88	GLN	2.1
1	B	99	ARG	2.0
1	A	323	LEU	2.0
1	D	277	PHE	2.0
1	E	76	LEU	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 monosaccharides in this entry.

6.4 Ligands ⓘ

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

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MPO	F	3014	13/13	0.76	0.27	41,62,71,72	5
4	GOL	E	3035	6/6	0.77	0.19	54,55,56,56	0
3	XTG	D	3018	30/30	0.79	0.20	24,45,53,56	0
4	GOL	A	3029	6/6	0.82	0.24	30,39,39,39	0
4	GOL	A	3028	6/6	0.85	0.20	29,35,37,39	0
4	GOL	E	3033	6/6	0.86	0.14	29,34,35,37	0
4	GOL	A	3024	6/6	0.87	0.25	37,40,40,40	0
4	GOL	C	3027	6/6	0.88	0.16	41,44,45,45	0
4	GOL	D	3031	6/6	0.89	0.13	23,28,30,32	0
2	SO4	E	3009	5/5	0.90	0.26	68,68,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	3026	6/6	0.90	0.21	34,39,40,41	0
4	GOL	F	3034	6/6	0.90	0.16	32,37,38,38	0
4	GOL	D	3032	6/6	0.90	0.16	31,37,40,41	0
4	GOL	C	3030	6/6	0.91	0.14	25,28,30,30	0
3	XTG	E	3019	30/30	0.92	0.13	17,28,42,47	0
4	GOL	C	3023	6/6	0.92	0.12	25,29,29,30	0
3	XTG	F	3020	30/30	0.92	0.14	12,38,41,44	0
3	XTG	F	3021	30/30	0.92	0.16	12,18,54,56	0
4	GOL	B	3025	6/6	0.92	0.15	26,31,31,32	0
3	XTG	B	3016	30/30	0.93	0.11	12,32,41,44	0
2	SO4	E	3004	5/5	0.94	0.26	45,47,48,49	0
3	XTG	C	3017	30/30	0.94	0.13	12,26,39,43	0
2	SO4	A	3008	5/5	0.94	0.24	45,46,48,49	0
3	XTG	A	3015	30/30	0.94	0.12	12,28,37,40	0
2	SO4	F	3001	5/5	0.95	0.20	37,39,41,44	0
5	MPO	C	3011	13/13	0.95	0.16	29,34,37,38	0
5	MPO	E	3013	13/13	0.95	0.16	43,49,55,56	0
2	SO4	B	3006	5/5	0.95	0.24	45,47,49,50	0
5	MPO	D	3012	13/13	0.96	0.15	20,34,40,40	0
2	SO4	C	3005	5/5	0.96	0.21	46,48,49,50	0
2	SO4	D	3002	5/5	0.96	0.23	51,52,53,54	0
2	SO4	F	3007	5/5	0.97	0.19	48,49,50,50	0
5	MPO	B	3010	13/13	0.97	0.14	29,36,43,43	0
4	GOL	F	3022	6/6	0.97	0.08	16,18,20,22	0
2	SO4	F	3003	5/5	0.99	0.08	14,16,20,20	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.
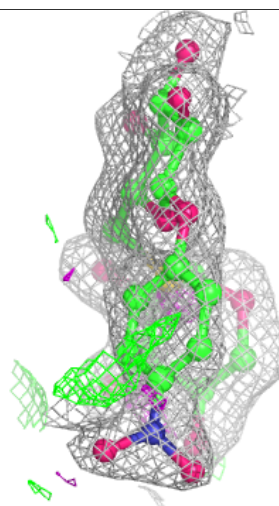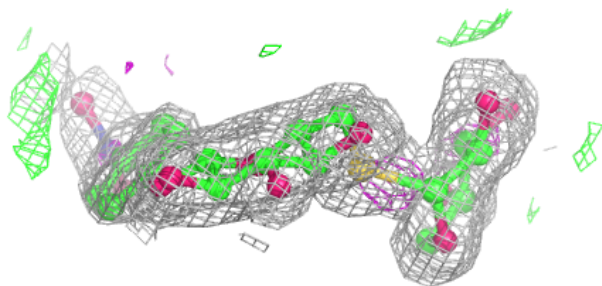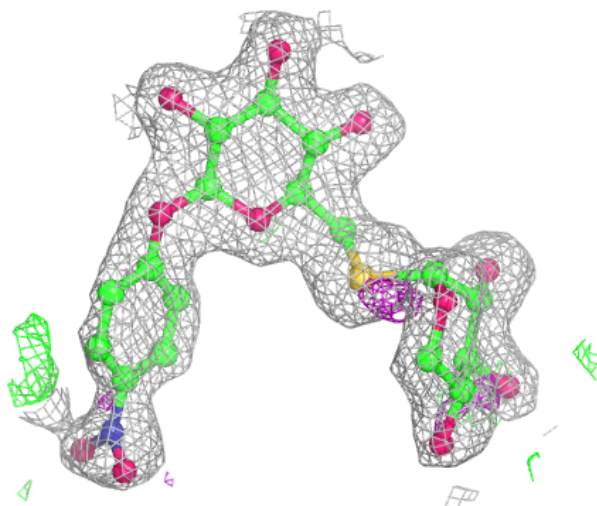
Electron density around XTG D 3018:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
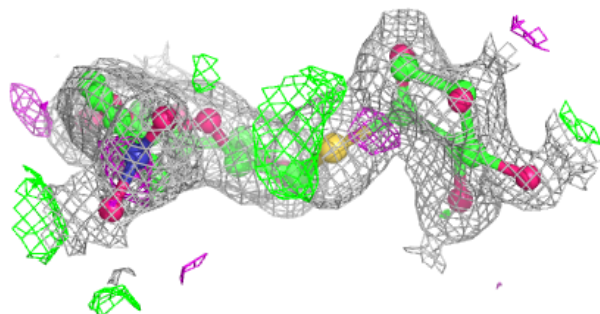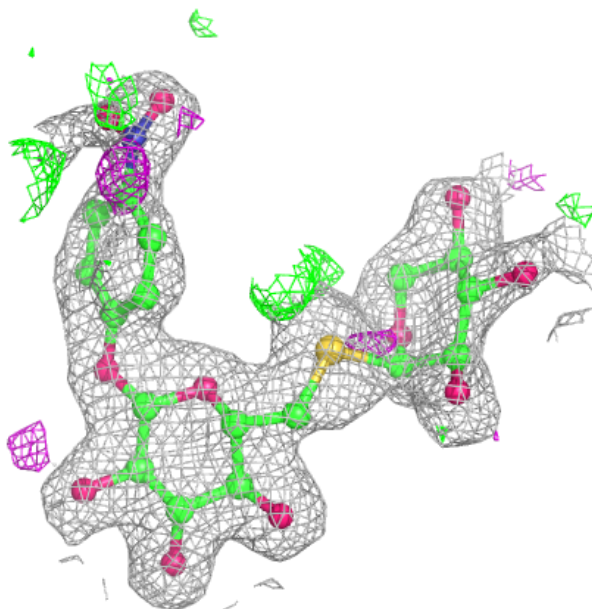and green (positive)
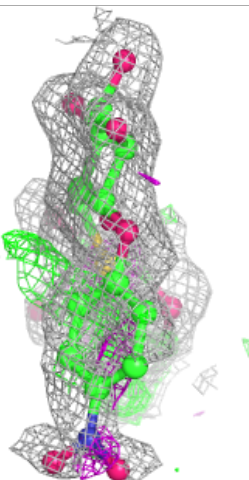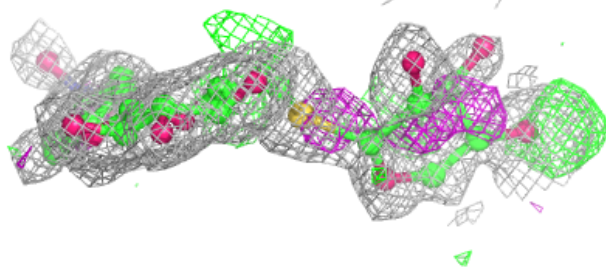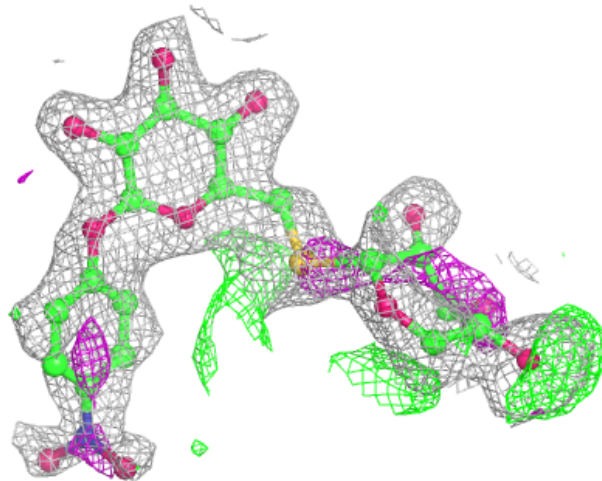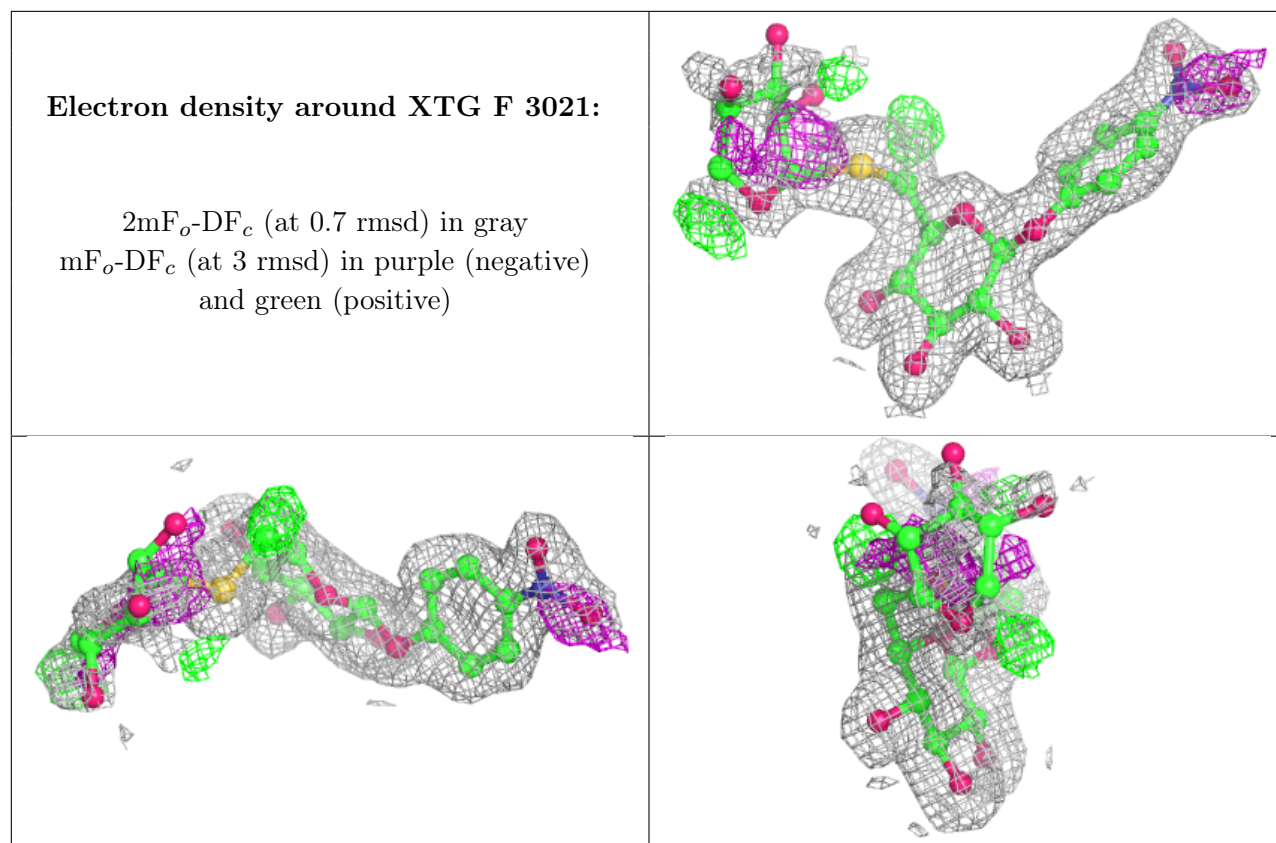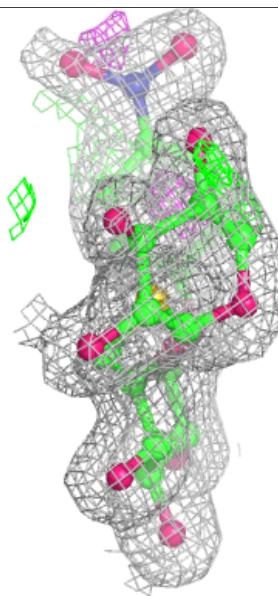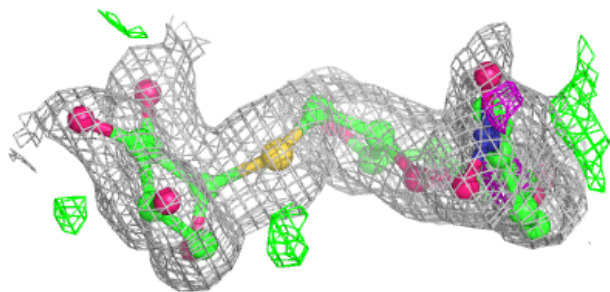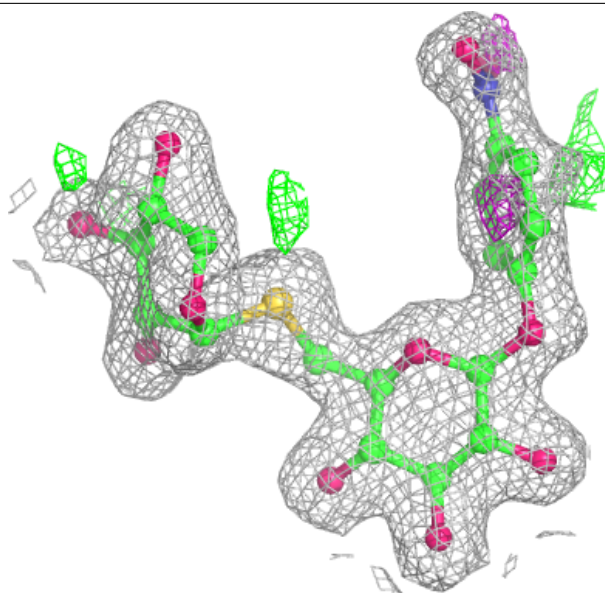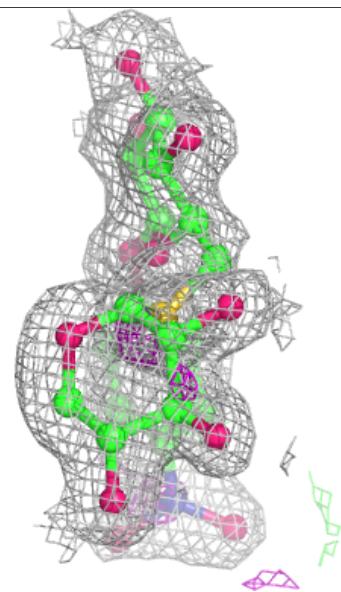
Electron density around XTG E 3019:

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

Electron density around XTG F 3020:

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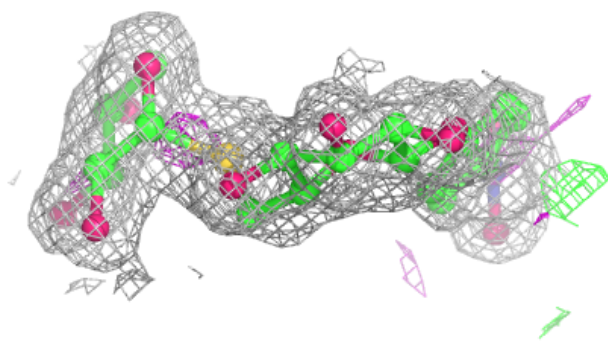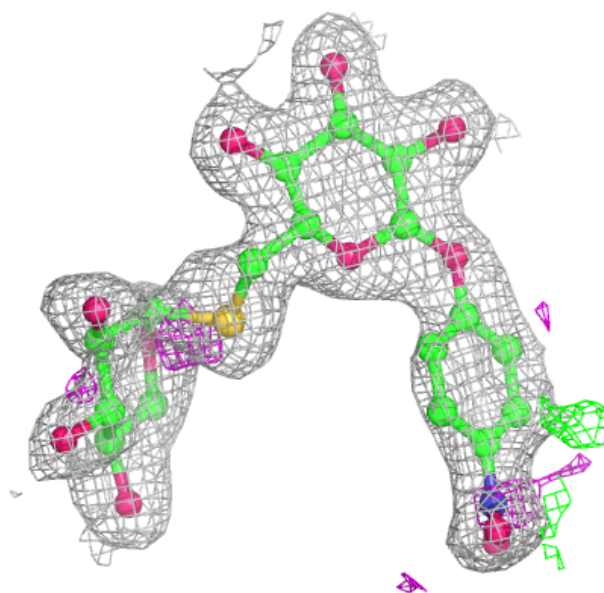and green (positive)

Electron density around XTG F 3021:

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

Electron density around XTG B 3016:

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

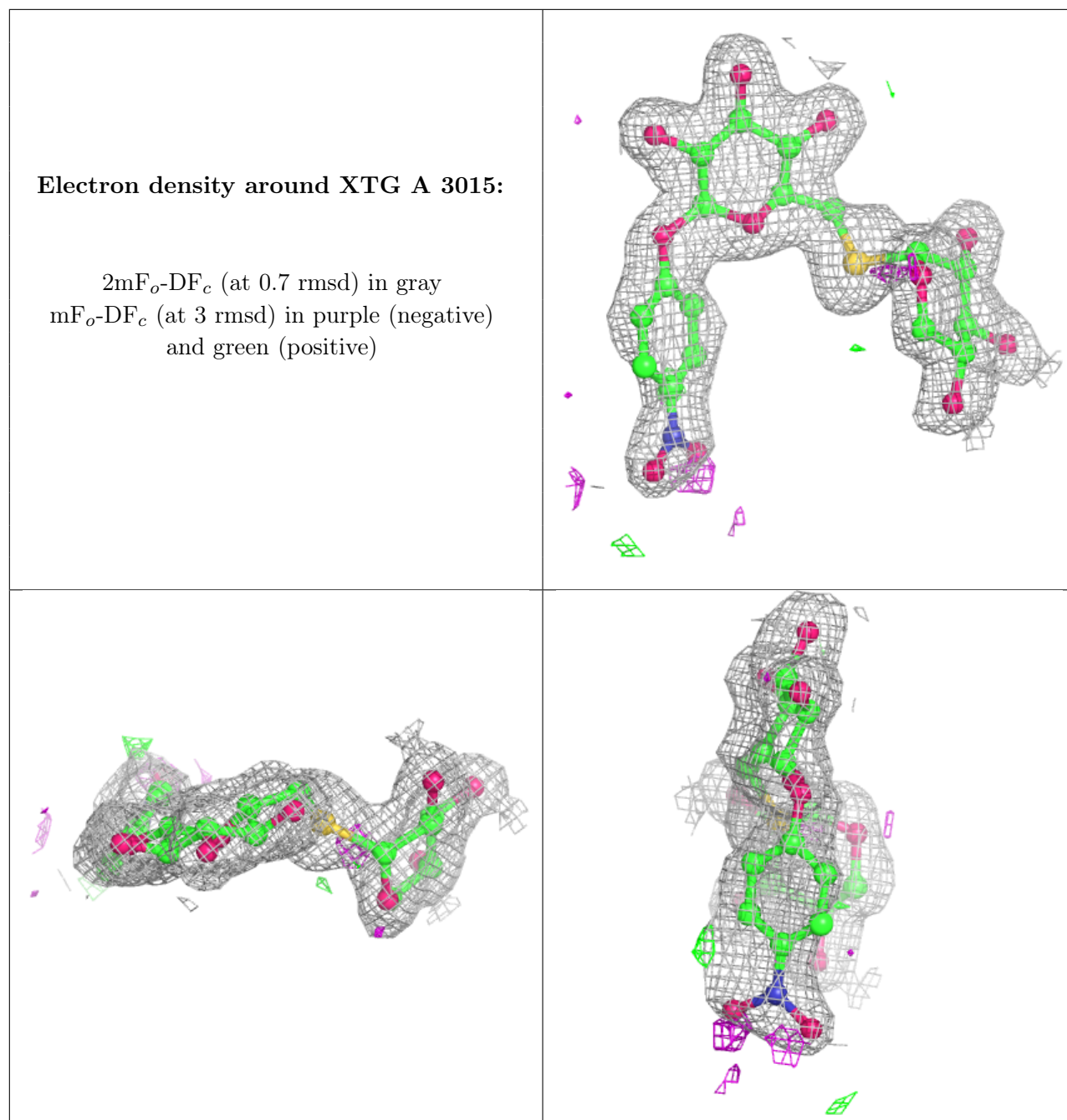**Electron density around XTG C 3017:**

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

Electron density around XTG A 3015:

$2mF_o$-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 ⓘ

There are no such residues in this entry.