



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:54 AM UTC

PDB ID : 4QJ0 / pdb_00004qj0
Title : Crystal structure of catalytic domain of human carbonic anhydrase isozyme XII with inhibitor
Authors : Manakova, E.; Smirnov, A.; Grazulis, S.
Deposited on : 2014-06-03
Resolution : 1.55 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

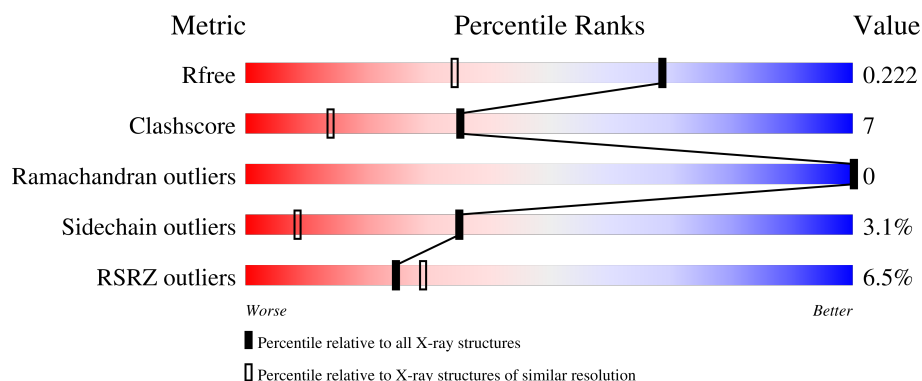
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	263	3% 84% 13% ..
1	B	263	5% 83% 14% ..
1	C	263	17% 70% 24% ..
1	D	263	% 89% 9% ..

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
4	WWX	B	303	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9838 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 Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	6	0
			2133	1354	364	407	8			
1	B	261	Total	C	N	O	S	0	6	0
			2150	1365	368	410	7			
1	C	260	Total	C	N	O	S	0	8	0
			2150	1364	365	413	8			
1	D	260	Total	C	N	O	S	0	9	0
			2160	1368	368	417	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O43570
B	1	MET	-	expression tag	UNP O43570
C	1	MET	-	expression tag	UNP O43570
D	1	MET	-	expression tag	UNP O43570

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

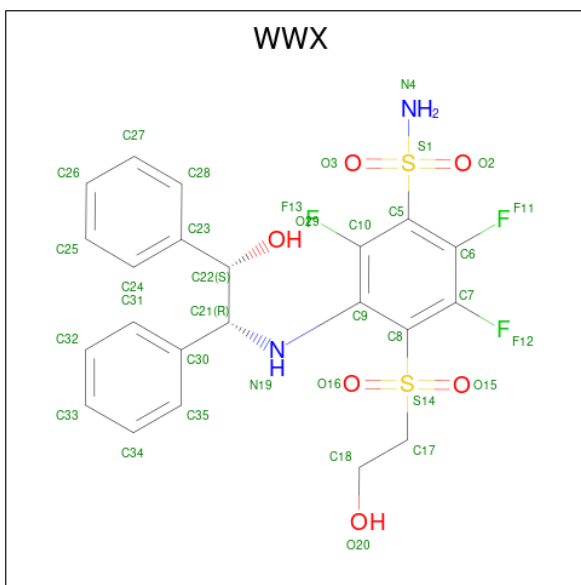
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is 2,3,6-trifluoro-5-[(1R,2S)-2-hydroxy-1,2-diphenylethyl]amino}-4-[(2-hydroxyethyl)sulfonyl]benzenesulfonamide (CCD ID: WWX) (formula: C₂₂H₂₁F₃N₂O₆S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			35	22	3	2	6	2		
4	B	1	Total	C	F	N	O	S	0	0
			35	22	3	2	6	2		
4	C	1	Total	C	F	N	O	S	0	0
			35	22	3	2	6	2		
4	D	1	Total	C	F	N	O	S	0	1
			70	44	6	4	12	4		

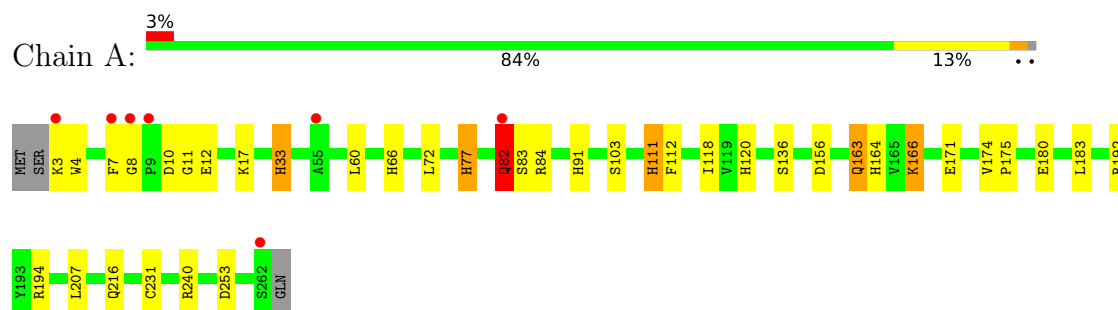
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	243	Total	O	0	0
			243	243		
5	B	290	Total	O	0	0
			290	290		
5	C	212	Total	O	0	0
			212	212		
5	D	297	Total	O	0	0
			297	297		

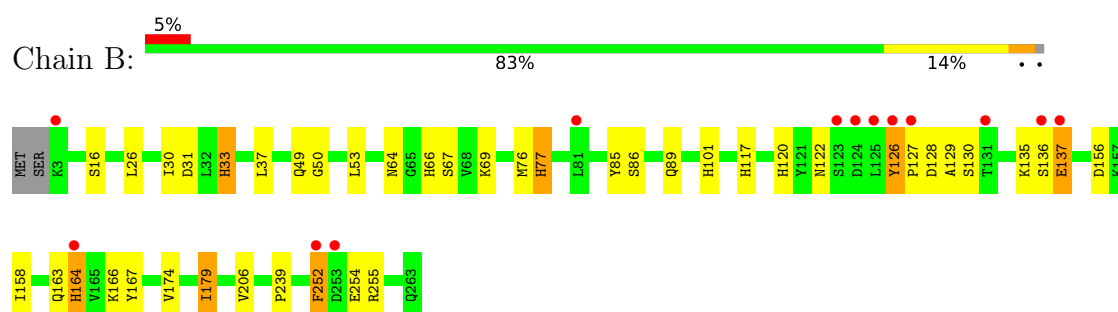
3 Residue-property plots [i](#)

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

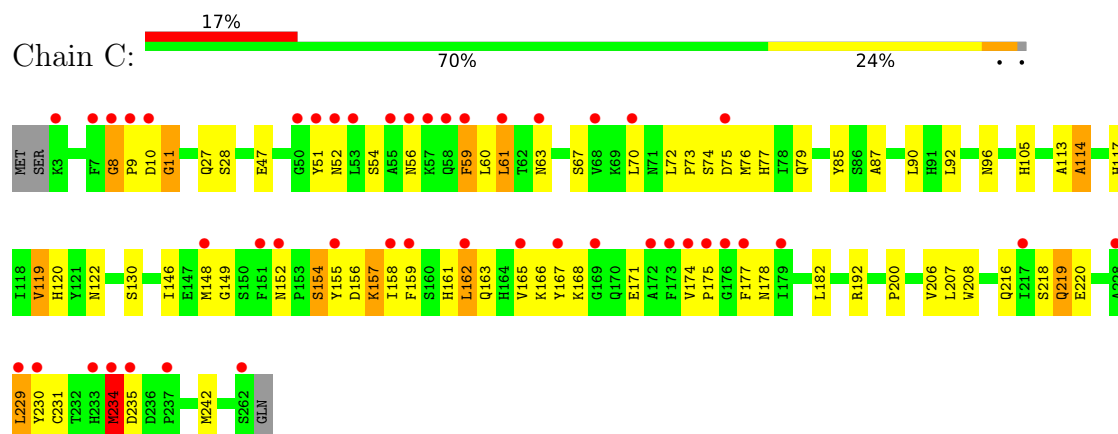
• Molecule 1: Carbonic anhydrase 12



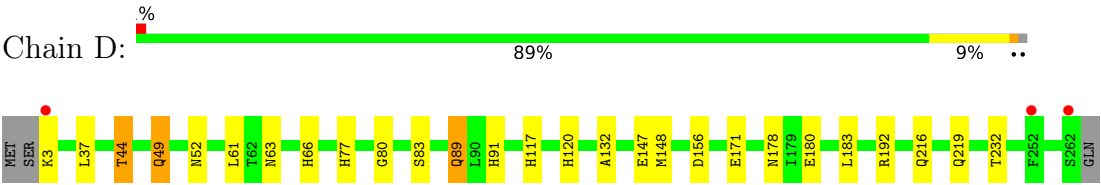
• Molecule 1: Carbonic anhydrase 12



• Molecule 1: Carbonic anhydrase 12



• Molecule 1: Carbonic anhydrase 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.51Å 74.24Å 91.42Å 90.00° 108.87° 90.00°	Depositor
Resolution (Å)	67.80 – 1.55 67.80 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (67.80-1.55) 99.3 (67.80-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.15 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.180 , 0.225 0.179 , 0.222	Depositor DCC
R_{free} test set	13984 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9838	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1208e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: WWX, EDO, ZN

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	1.49	13/2196 (0.6%)	1.25	7/2988 (0.2%)
1	B	1.51	14/2214 (0.6%)	1.30	10/3012 (0.3%)
1	C	1.56	21/2214 (0.9%)	1.37	16/3014 (0.5%)
1	D	1.45	7/2223 (0.3%)	1.23	4/3025 (0.1%)
All	All	1.50	55/8847 (0.6%)	1.29	37/12039 (0.3%)

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	VAL	CA-C	7.57	1.58	1.52
1	B	53	LEU	CA-C	7.29	1.62	1.52
1	D	77	HIS	CA-C	-7.20	1.43	1.52
1	C	11	GLY	N-CA	7.19	1.54	1.45
1	D	117	HIS	ND1-CE1	6.89	1.39	1.32
1	B	37	LEU	N-CA	6.77	1.54	1.46
1	D	120	HIS	ND1-CE1	6.72	1.39	1.32
1	C	72	LEU	CA-C	6.71	1.59	1.52
1	A	120	HIS	CE1-NE2	6.69	1.39	1.32
1	A	111	HIS	CE1-NE2	6.51	1.39	1.32
1	C	117	HIS	C-O	-6.38	1.16	1.24
1	C	117	HIS	CA-CB	-6.36	1.44	1.53
1	C	105	HIS	CE1-NE2	6.34	1.38	1.32
1	B	77	HIS	ND1-CE1	6.31	1.38	1.32
1	C	113	ALA	C-O	-6.22	1.16	1.24
1	A	118	ILE	C-O	6.16	1.30	1.24
1	B	66	HIS	CD2-NE2	-6.08	1.31	1.37
1	B	120	HIS	CE1-NE2	6.02	1.38	1.32
1	C	161	HIS	CA-C	-5.90	1.45	1.52
1	C	59	PHE	C-O	-5.86	1.17	1.24
1	B	117	HIS	CE1-NE2	5.83	1.38	1.32
1	C	177	PHE	N-CA	5.77	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	PRO	C-O	5.75	1.30	1.23
1	B	85	TYR	CA-C	-5.70	1.45	1.52
1	A	91	HIS	CG-ND1	-5.67	1.32	1.38
1	C	200	PRO	CA-C	5.63	1.57	1.52
1	C	120	HIS	N-CA	5.61	1.52	1.45
1	A	72	LEU	CA-CB	5.59	1.61	1.54
1	B	122	ASN	CA-C	5.58	1.60	1.52
1	C	114	ALA	N-CA	-5.58	1.39	1.46
1	A	120	HIS	N-CA	5.54	1.53	1.45
1	C	155	TYR	C-O	5.53	1.30	1.24
1	D	63	ASN	CA-CB	5.46	1.60	1.53
1	A	11	GLY	N-CA	5.45	1.52	1.45
1	A	82	GLN	C-O	5.44	1.30	1.24
1	A	33	HIS	ND1-CE1	5.42	1.38	1.32
1	C	28	SER	N-CA	5.34	1.51	1.45
1	D	37	LEU	N-CA	5.32	1.53	1.46
1	C	229	LEU	CA-C	-5.30	1.46	1.52
1	B	179	ILE	N-CA	5.30	1.53	1.46
1	C	208	TRP	CA-C	-5.27	1.46	1.52
1	C	96	ASN	N-CA	5.18	1.50	1.46
1	D	66	HIS	ND1-CE1	5.17	1.37	1.32
1	C	67	SER	CA-CB	5.17	1.60	1.53
1	A	84	ARG	NE-CZ	5.16	1.38	1.33
1	C	182	LEU	CA-C	5.15	1.59	1.52
1	A	120	HIS	ND1-CE1	5.15	1.37	1.32
1	B	101	HIS	CA-C	-5.15	1.47	1.53
1	C	122	ASN	N-CA	5.15	1.53	1.46
1	A	8	GLY	N-CA	5.14	1.51	1.44
1	D	83	SER	C-O	5.12	1.30	1.23
1	B	69	LYS	N-CA	5.10	1.52	1.45
1	A	112	PHE	C-O	5.10	1.30	1.23
1	B	33	HIS	CB-CG	5.08	1.57	1.50
1	C	85	TYR	C-O	-5.04	1.18	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	ALA	N-CA-C	8.41	120.45	111.28
1	C	234	MET	N-CA-C	8.08	121.11	111.33
1	C	10	ASP	CA-C-N	7.86	132.17	121.01
1	C	10	ASP	C-N-CA	7.86	132.17	121.01
1	C	229	LEU	N-CA-C	7.44	121.39	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	HIS	N-CA-C	7.21	120.04	109.07
1	C	152	ASN	CA-C-N	6.56	126.80	119.32
1	C	152	ASN	C-N-CA	6.56	126.80	119.32
1	A	12	GLU	N-CA-C	6.40	119.07	111.71
1	B	67	SER	CA-C-N	-6.29	114.99	123.10
1	B	67	SER	C-N-CA	-6.29	114.99	123.10
1	D	44	THR	CA-C-N	-6.26	113.22	119.99
1	D	44	THR	C-N-CA	-6.26	113.22	119.99
1	C	8	GLY	N-CA-C	6.14	124.88	112.34
1	B	126	TYR	CA-C-N	6.10	125.80	119.64
1	B	126	TYR	C-N-CA	6.10	125.80	119.64
1	D	77	HIS	N-CA-C	6.09	118.03	108.96
1	A	8	GLY	CA-C-N	6.04	125.66	119.56
1	A	8	GLY	C-N-CA	6.04	125.66	119.56
1	B	50	GLY	N-CA-C	-5.82	107.21	115.30
1	C	119	VAL	N-CA-CB	5.69	116.73	110.53
1	B	158	ILE	N-CA-C	-5.64	106.20	111.45
1	A	77	HIS	N-CA-C	5.64	117.64	109.07
1	D	132	ALA	N-CA-C	5.63	118.19	111.71
1	B	164	HIS	CB-CA-C	5.54	119.54	110.17
1	B	206	VAL	N-CA-C	5.50	115.87	108.17
1	C	216	GLN	N-CA-C	5.50	118.69	109.95
1	C	157	LYS	N-CA-C	-5.40	106.20	112.89
1	A	10	ASP	O-C-N	5.35	128.84	122.26
1	C	27	GLN	N-CA-C	5.18	118.39	110.20
1	B	77	HIS	CA-C-N	-5.18	116.77	123.19
1	B	77	HIS	C-N-CA	-5.18	116.77	123.19
1	C	206	VAL	N-CA-C	5.16	115.28	107.80
1	C	158	ILE	N-CA-C	-5.07	106.20	111.58
1	A	194	ARG	CA-C-N	-5.04	118.28	122.16
1	A	194	ARG	C-N-CA	-5.04	118.28	122.16
1	C	74	SER	N-CA-C	5.01	118.88	112.87

There are no chirality outliers.

There are no planarity outliers.

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	2133	0	2023	29	0
1	B	2150	0	2035	30	0
1	C	2150	0	2026	52	0
1	D	2160	0	2034	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	12	0	18	3	0
4	A	35	0	21	0	0
4	B	35	0	21	5	0
4	C	35	0	21	1	0
4	D	70	0	42	0	0
5	A	243	0	0	8	0
5	B	290	0	0	0	0
5	C	212	0	0	1	0
5	D	297	0	0	1	0
All	All	9838	0	8259	127	0

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

All (127) 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:C:61:LEU:HD21	1:C:174:VAL:CG2	1.53	1.36
1:C:61:LEU:CD2	1:C:174:VAL:HG23	1.77	1.15
1:C:61:LEU:CD2	1:C:174:VAL:CG2	2.25	1.13
1:C:61:LEU:HD21	1:C:174:VAL:HG21	1.06	1.03
1:A:82:GLN:HG2	1:A:83:SER:H	1.20	1.01
1:D:178:ASN:OD1	1:D:180[B]:GLU:HG2	1.63	0.98
1:C:175:PRO:HB2	5:C:509:HOH:O	1.66	0.95
1:B:31:ASP:O	1:B:252[B]:PHE:HZ	1.50	0.94
1:C:61:LEU:HD22	1:C:174:VAL:HG23	1.48	0.93
1:C:61:LEU:CD2	1:C:174:VAL:HG21	1.97	0.91
1:A:82:GLN:HG3	5:A:621:HOH:O	1.70	0.89
1:B:129:ALA:HB1	4:B:303:WWX:H12	1.54	0.89
1:A:7:PHE:CD2	5:A:638:HOH:O	2.27	0.87
1:A:7:PHE:HD2	5:A:638:HOH:O	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:HIS:CE1	1:B:86:SER:OG	2.33	0.82
1:A:216:GLN:HG3	5:A:623:HOH:O	1.78	0.82
1:A:82:GLN:HG2	1:A:83:SER:N	1.93	0.81
1:C:61:LEU:HD12	1:C:61:LEU:N	1.96	0.81
1:C:159:PHE:O	1:C:162:LEU:HG	1.83	0.78
1:C:231[A]:CYS:SG	1:C:242:MET:HA	2.23	0.78
1:C:168:LYS:HB2	1:C:231[A]:CYS:O	1.83	0.78
1:B:31:ASP:O	1:B:252[B]:PHE:CZ	2.36	0.76
1:B:252[A]:PHE:CD2	1:B:255[A]:ARG:O	2.40	0.74
1:B:77:HIS:CE1	1:B:86:SER:HG	2.06	0.74
1:B:252[A]:PHE:CE2	1:B:255[A]:ARG:O	2.41	0.74
1:C:149:GLY:O	1:C:218:SER:HA	1.88	0.73
1:B:30:ILE:HD12	1:B:252[B]:PHE:HE1	1.55	0.70
1:C:59:PHE:O	1:C:61:LEU:CD1	2.41	0.68
1:C:63[B]:ASN:OD1	1:C:165:VAL:HB	1.93	0.68
1:C:163:GLN:OE1	1:C:166:LYS:HD2	1.94	0.68
1:C:61:LEU:N	1:C:61:LEU:CD1	2.58	0.67
1:C:219:GLN:HG3	1:C:220:GLU:OE1	1.95	0.67
1:B:30:ILE:HD12	1:B:252[B]:PHE:CE1	2.29	0.66
1:B:252[A]:PHE:CE1	1:B:255[A]:ARG:HB2	2.30	0.66
1:D:148:MET:HE2	1:D:219[A]:GLN:OE1	1.95	0.66
1:C:63[B]:ASN:CG	1:C:165:VAL:O	2.39	0.66
1:B:129:ALA:HB1	4:B:303:WWX:C33	2.25	0.64
1:C:60:LEU:C	1:C:61:LEU:HD12	2.22	0.64
1:B:252[A]:PHE:CE2	1:B:255[A]:ARG:C	2.78	0.62
1:A:7:PHE:CZ	1:A:240:ARG:NH1	2.68	0.61
1:C:148:MET:SD	1:C:219:GLN:HB3	2.39	0.61
1:C:63[B]:ASN:HD21	1:C:229:LEU:HD22	1.64	0.61
1:D:49:GLN:HE21	1:D:49:GLN:HA	1.65	0.61
1:D:80:GLY:O	3:D:302:EDO:H12	2.01	0.60
1:A:77:HIS:ND1	5:A:606:HOH:O	2.32	0.60
1:C:63[B]:ASN:ND2	1:C:165:VAL:O	2.35	0.60
1:D:180[B]:GLU:HG3	5:D:599:HOH:O	2.01	0.59
1:A:82:GLN:H	1:A:82:GLN:HE21	1.51	0.59
1:C:76:MET:HB3	1:C:87:ALA:HB3	1.83	0.59
1:D:89[B]:GLN:HE21	1:D:91:HIS:HD1	1.49	0.59
1:C:61:LEU:HG	1:C:70:LEU:HD13	1.83	0.59
1:B:252[A]:PHE:CZ	1:B:255[A]:ARG:HB2	2.38	0.58
1:A:7:PHE:CZ	1:A:240:ARG:HD2	2.39	0.57
1:C:47:GLU:HB2	1:C:79:GLN:HB3	1.87	0.57
1:C:159:PHE:O	1:C:162:LEU:CD1	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:PHE:O	1:C:162:LEU:CG	2.52	0.57
1:C:167:TYR:CG	1:C:234:MET:HA	2.40	0.56
1:A:4:TRP:O	1:A:66:HIS:HE1	1.88	0.56
1:C:51:TYR:CD2	1:C:76:MET:HG2	2.41	0.56
1:D:89[B]:GLN:NE2	1:D:91:HIS:HD1	2.03	0.55
1:C:9:PRO:C	1:C:11:GLY:H	2.14	0.55
1:D:44:THR:H	3:D:302:EDO:H21	1.71	0.55
1:A:231[B]:CYS:SG	1:A:240:ARG:HB2	2.47	0.55
1:C:61:LEU:CD1	1:C:70:LEU:CD1	2.85	0.54
1:B:163:GLN:CG	1:B:164:HIS:CE1	2.91	0.54
1:B:163:GLN:HG3	1:B:164:HIS:CE1	2.43	0.54
1:C:61:LEU:HD11	1:C:174:VAL:HB	1.89	0.53
1:D:147[B]:GLU:CG	1:D:216:GLN:HG2	2.39	0.53
1:C:229:LEU:C	1:C:230[B]:TYR:CD2	2.87	0.53
1:C:54:SER:HB3	1:C:56:ASN:OD1	2.09	0.53
1:A:164:HIS:HD2	5:A:581:HOH:O	1.90	0.52
1:D:180[A]:GLU:HG3	1:D:183:LEU:HD12	1.90	0.52
1:A:7:PHE:CE2	1:A:240:ARG:NH1	2.77	0.52
1:C:59:PHE:O	1:C:61:LEU:HD12	2.07	0.52
1:B:26:LEU:HA	1:B:255[A]:ARG:CZ	2.39	0.52
1:A:103:SER:O	1:A:111:HIS:HD2	1.92	0.52
1:B:166[B]:LYS:HD3	1:B:167:TYR:CZ	2.45	0.51
1:C:230[B]:TYR:CD2	1:C:230[B]:TYR:N	2.78	0.51
1:A:82:GLN:CG	1:A:83:SER:N	2.66	0.51
1:A:33:HIS:HE1	5:A:490:HOH:O	1.94	0.51
1:A:60:LEU:HD11	1:A:171:GLU:HB3	1.94	0.50
1:C:192:ARG:HD2	1:C:207:LEU:HD11	1.94	0.50
1:C:154:SER:O	1:C:157:LYS:HG3	2.11	0.50
1:B:33:HIS:HE1	1:B:252[B]:PHE:CE2	2.31	0.49
1:D:44:THR:O	3:D:302:EDO:H11	2.12	0.49
1:C:52:ASN:HA	1:C:178:ASN:HA	1.95	0.49
1:A:180:GLU:HG3	1:A:183:LEU:HD12	1.95	0.48
1:A:7:PHE:HZ	1:A:240:ARG:NH1	2.08	0.48
1:C:174:VAL:HG12	1:C:175:PRO:O	2.14	0.48
1:B:252[B]:PHE:O	1:B:254:GLU:N	2.43	0.48
1:B:163:GLN:HG2	1:B:164:HIS:CE1	2.49	0.48
1:D:89[A]:GLN:OE1	1:D:91:HIS:ND1	2.39	0.47
1:D:147[B]:GLU:HG2	1:D:216:GLN:HG2	1.95	0.47
1:A:166:LYS:HB3	1:A:166:LYS:HE3	1.47	0.46
1:C:231[A]:CYS:SG	1:C:242:MET:CA	3.01	0.45
1:C:60:LEU:HD11	1:C:171:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:TYR:CD2	1:C:234:MET:HG3	2.52	0.45
1:A:17[A]:LYS:HE3	1:B:16:SER:OG	2.16	0.45
1:C:61:LEU:HD11	1:C:70:LEU:CD1	2.47	0.45
1:D:178:ASN:CG	1:D:180[B]:GLU:HG2	2.37	0.44
1:B:64:ASN:ND2	4:B:303:WWX:H4	2.32	0.44
1:B:126:TYR:CE1	1:B:135:LYS:HD2	2.53	0.43
1:B:252[A]:PHE:O	1:B:254:GLU:N	2.51	0.43
1:A:82:GLN:H	1:A:82:GLN:NE2	2.17	0.43
1:A:163:GLN:O	1:A:166:LYS:HG3	2.17	0.43
1:B:76:MET:HE1	1:B:179:ILE:HG21	1.99	0.43
1:B:129:ALA:CB	4:B:303:WWX:H12	2.38	0.43
1:B:64:ASN:HD21	4:B:303:WWX:C17	2.32	0.43
1:C:8:GLY:O	1:C:11:GLY:HA3	2.19	0.42
1:C:167:TYR:CD1	1:C:234:MET:HA	2.54	0.42
1:B:127:PRO:HG2	1:B:128:ASP:OD1	2.19	0.42
1:C:167:TYR:CD2	1:C:234:MET:CG	3.03	0.42
1:B:252[A]:PHE:CZ	1:B:255[A]:ARG:CB	3.02	0.42
1:A:103:SER:O	1:A:111:HIS:CD2	2.71	0.42
1:A:192:ARG:HD2	1:A:207:LEU:HD11	2.02	0.42
1:B:136:SER:C	1:B:137:GLU:HG2	2.45	0.42
1:D:52:ASN:HA	1:D:178:ASN:HA	2.01	0.42
1:C:90:LEU:C	1:C:90:LEU:HD12	2.45	0.41
1:D:61:LEU:O	1:D:171:GLU:HA	2.20	0.41
1:A:7:PHE:HE2	1:A:240:ARG:HH11	1.66	0.41
1:C:119:VAL:HG11	4:C:303:WWX:F12	2.10	0.41
1:A:253:ASP:OD2	5:A:487:HOH:O	2.21	0.41
1:D:219[A]:GLN:CD	1:D:219[A]:GLN:O	2.63	0.41
1:C:114:ALA:HB3	1:C:146:ILE:HB	2.02	0.41
1:C:61:LEU:HG	1:C:70:LEU:CD1	2.51	0.40
1:C:63[B]:ASN:OD1	1:C:165:VAL:O	2.40	0.40
1:A:174:VAL:HA	1:A:175:PRO:HD3	1.98	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	264/263 (100%)	261 (99%)	3 (1%)	0	100	100
1	B	265/263 (101%)	258 (97%)	7 (3%)	0	100	100
1	C	266/263 (101%)	253 (95%)	13 (5%)	0	100	100
1	D	267/263 (102%)	258 (97%)	9 (3%)	0	100	100
All	All	1062/1052 (101%)	1030 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	238/235 (101%)	232 (98%)	6 (2%)	42	14
1	B	239/235 (102%)	231 (97%)	8 (3%)	33	7
1	C	240/235 (102%)	229 (95%)	11 (5%)	24	3
1	D	241/235 (103%)	234 (97%)	7 (3%)	37	10
All	All	958/940 (102%)	926 (97%)	32 (3%)	35	7

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	82	GLN
1	A	136	SER
1	A	156	ASP
1	A	163	GLN
1	A	166	LYS
1	B	49	GLN
1	B	89	GLN
1	B	130[A]	SER
1	B	130[B]	SER

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Mol	Chain	Res	Type
1	B	137	GLU
1	B	156	ASP
1	B	252[A]	PHE
1	B	252[B]	PHE
1	C	61	LEU
1	C	73	PRO
1	C	75	ASP
1	C	92	LEU
1	C	130	SER
1	C	154	SER
1	C	156	ASP
1	C	162	LEU
1	C	219	GLN
1	C	234	MET
1	C	235	ASP
1	D	3	LYS
1	D	49	GLN
1	D	89[A]	GLN
1	D	89[B]	GLN
1	D	156	ASP
1	D	192	ARG
1	D	232	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	33	HIS
1	A	49	GLN
1	A	58	GLN
1	A	66	HIS
1	A	82	GLN
1	A	111	HIS
1	A	164	HIS
1	A	178	ASN
1	B	49	GLN
1	B	77	HIS
1	B	82	GLN
1	B	89	GLN
1	B	96	ASN
1	B	101	HIS
1	B	111	HIS

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Mol	Chain	Res	Type
1	B	178	ASN
1	B	213	ASN
1	B	244	ASN
1	B	250	GLN
1	C	13	ASN
1	C	49	GLN
1	C	110	GLN
1	C	233	HIS
1	C	250	GLN
1	D	13	ASN
1	D	49	GLN
1	D	101	HIS
1	D	213	ASN
1	D	250	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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	302	-	3,3,3	0.81	0	2,2,2	0.25	0
3	EDO	A	302	-	3,3,3	0.66	0	2,2,2	0.11	0
3	EDO	D	302	-	3,3,3	0.42	0	2,2,2	0.32	0
3	EDO	C	302	-	3,3,3	0.30	0	2,2,2	0.78	0
3	EDO	D	304	-	3,3,3	0.94	0	2,2,2	0.67	0
4	WWX	C	303	2	37,37,37	3.11	17 (45%)	51,55,55	3.15	14 (27%)
4	WWX	D	305[A]	2	37,37,37	2.40	7 (18%)	51,55,55	2.73	12 (23%)
4	WWX	B	303	2	37,37,37	3.23	13 (35%)	51,55,55	4.63	28 (54%)
3	EDO	D	303	-	3,3,3	0.49	0	2,2,2	0.38	0
4	WWX	A	303	2	37,37,37	2.83	11 (29%)	51,55,55	3.78	20 (39%)
4	WWX	D	305[B]	2	37,37,37	2.43	7 (18%)	51,55,55	2.65	13 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	D	302	-	-	1/1/1/1	-
3	EDO	C	302	-	-	1/1/1/1	-
3	EDO	D	304	-	-	0/1/1/1	-
4	WWX	C	303	2	-	9/32/32/32	0/3/3/3
4	WWX	D	305[A]	2	-	8/32/32/32	0/3/3/3
4	WWX	B	303	2	-	18/32/32/32	0/3/3/3
3	EDO	D	303	-	-	1/1/1/1	-
4	WWX	A	303	2	-	8/32/32/32	0/3/3/3
4	WWX	D	305[B]	2	-	8/32/32/32	0/3/3/3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	WWX	O16-S14	10.10	1.57	1.44
4	A	303	WWX	O15-S14	9.34	1.56	1.44
4	B	303	WWX	O16-S14	9.18	1.56	1.44
4	C	303	WWX	S1-N4	8.92	1.77	1.60
4	B	303	WWX	O15-S14	8.88	1.56	1.44
4	A	303	WWX	O16-S14	8.51	1.55	1.44
4	D	305[B]	WWX	O16-S14	7.97	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	305[A]	WWX	O16-S14	7.78	1.54	1.44
4	B	303	WWX	C5-S1	7.56	1.90	1.78
4	D	305[B]	WWX	O15-S14	7.10	1.53	1.44
4	D	305[A]	WWX	O15-S14	6.86	1.53	1.44
4	B	303	WWX	S1-N4	6.33	1.72	1.60
4	A	303	WWX	O2-S1	5.65	1.53	1.43
4	A	303	WWX	O3-S1	5.33	1.53	1.43
4	B	303	WWX	F12-C7	5.29	1.42	1.34
4	D	305[A]	WWX	S1-N4	5.05	1.70	1.60
4	D	305[B]	WWX	S1-N4	5.05	1.70	1.60
4	D	305[A]	WWX	O2-S1	4.96	1.52	1.43
4	D	305[B]	WWX	O2-S1	4.93	1.52	1.43
4	C	303	WWX	O15-S14	4.77	1.50	1.44
4	C	303	WWX	O3-S1	4.28	1.51	1.43
4	C	303	WWX	O2-S1	4.21	1.51	1.43
4	D	305[B]	WWX	O3-S1	4.15	1.51	1.43
4	D	305[A]	WWX	O3-S1	4.09	1.50	1.43
4	C	303	WWX	C25-C26	3.64	1.46	1.38
4	C	303	WWX	C21-C22	3.61	1.60	1.54
4	B	303	WWX	C31-C30	3.35	1.44	1.39
4	C	303	WWX	C28-C23	3.35	1.44	1.39
4	C	303	WWX	F11-C6	3.28	1.39	1.34
4	A	303	WWX	C34-C35	3.25	1.44	1.38
4	B	303	WWX	O3-S1	3.20	1.49	1.43
4	B	303	WWX	C9-C10	3.15	1.44	1.39
4	B	303	WWX	C24-C23	3.14	1.44	1.39
4	C	303	WWX	C5-S1	3.08	1.83	1.78
4	A	303	WWX	C25-C26	3.04	1.44	1.38
4	D	305[A]	WWX	C17-S14	2.93	1.83	1.77
4	B	303	WWX	F11-C6	2.87	1.39	1.34
4	C	303	WWX	C31-C30	2.75	1.43	1.39
4	D	305[B]	WWX	C17-S14	2.73	1.83	1.77
4	C	303	WWX	C23-C22	-2.65	1.47	1.51
4	A	303	WWX	O29-C22	-2.63	1.37	1.42
4	C	303	WWX	C34-C35	2.54	1.43	1.38
4	C	303	WWX	C9-C10	2.45	1.43	1.39
4	A	303	WWX	F13-C10	-2.43	1.31	1.34
4	D	305[B]	WWX	C25-C24	2.42	1.43	1.38
4	B	303	WWX	C35-C30	-2.40	1.35	1.39
4	A	303	WWX	C21-N19	2.39	1.49	1.46
4	D	305[A]	WWX	C25-C24	2.36	1.42	1.38
4	C	303	WWX	C17-S14	2.30	1.82	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	WWX	C6-C5	2.17	1.43	1.39
4	A	303	WWX	C28-C23	2.13	1.42	1.39
4	B	303	WWX	C32-C31	2.07	1.42	1.38
4	A	303	WWX	F12-C7	2.06	1.37	1.34
4	C	303	WWX	C17-C18	2.05	1.55	1.50
4	C	303	WWX	C35-C30	2.01	1.42	1.39

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	WWX	O15-S14-O16	-18.08	99.07	118.45
4	A	303	WWX	O15-S14-O16	-15.16	102.20	118.45
4	C	303	WWX	O15-S14-O16	-13.65	103.82	118.45
4	D	305[A]	WWX	O15-S14-O16	-13.38	104.11	118.45
4	B	303	WWX	O3-S1-C5	12.85	126.16	107.28
4	D	305[B]	WWX	O15-S14-O16	-12.26	105.31	118.45
4	A	303	WWX	C5-S1-N4	9.01	124.48	108.26
4	C	303	WWX	C5-S1-N4	8.39	123.36	108.26
4	B	303	WWX	C5-S1-N4	-8.17	93.54	108.26
4	A	303	WWX	O2-S1-O3	-7.81	106.79	118.80
4	C	303	WWX	O15-S14-C17	7.08	119.77	108.18
4	B	303	WWX	F13-C10-C9	7.01	129.92	119.54
4	B	303	WWX	O2-S1-O3	-6.94	108.13	118.80
4	A	303	WWX	C23-C22-C21	-6.93	103.29	112.05
4	B	303	WWX	C6-C7-C8	-6.85	113.50	121.78
4	D	305[B]	WWX	C23-C22-C21	-6.81	103.44	112.05
4	A	303	WWX	C25-C24-C23	-6.76	112.56	120.65
4	D	305[A]	WWX	C23-C22-C21	-6.73	103.55	112.05
4	A	303	WWX	C10-C5-C6	6.72	121.25	116.65
4	D	305[A]	WWX	C5-S1-N4	6.28	119.56	108.26
4	D	305[B]	WWX	C5-S1-N4	6.25	119.52	108.26
4	B	303	WWX	O15-S14-C17	5.97	117.96	108.18
4	C	303	WWX	O2-S1-O3	-5.69	110.04	118.80
4	A	303	WWX	C24-C23-C28	5.69	125.36	118.30
4	B	303	WWX	F11-C6-C7	-5.50	108.34	119.27
4	B	303	WWX	O2-S1-N4	-5.31	99.70	107.35
4	B	303	WWX	C30-C21-C22	5.18	119.24	112.41
4	B	303	WWX	F13-C10-C5	-5.17	111.45	120.76
4	A	303	WWX	C30-C21-N19	-5.04	107.04	113.62
4	B	303	WWX	C7-C8-S14	-4.75	109.21	120.87
4	C	303	WWX	C33-C32-C31	4.72	126.06	120.24
4	C	303	WWX	C23-C22-C21	-4.66	106.16	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	WWX	O2-S1-C5	-4.62	100.49	107.28
4	B	303	WWX	C7-C6-C5	4.60	127.33	121.78
4	B	303	WWX	O16-S14-C8	-4.52	95.15	106.59
4	B	303	WWX	C28-C23-C22	-4.30	114.23	120.71
4	A	303	WWX	F13-C10-C9	4.23	125.81	119.54
4	D	305[A]	WWX	O2-S1-C5	-4.21	101.08	107.28
4	D	305[B]	WWX	O2-S1-C5	-4.21	101.09	107.28
4	B	303	WWX	O29-C22-C21	4.13	115.90	107.32
4	C	303	WWX	O15-S14-C8	-4.00	96.46	106.59
4	B	303	WWX	O2-S1-C5	3.92	113.03	107.28
4	C	303	WWX	O2-S1-C5	-3.80	101.70	107.28
4	A	303	WWX	F13-C10-C5	-3.65	114.19	120.76
4	D	305[A]	WWX	O2-S1-O3	-3.64	113.20	118.80
4	D	305[B]	WWX	O2-S1-O3	-3.63	113.22	118.80
4	D	305[A]	WWX	C25-C24-C23	-3.56	116.39	120.65
4	D	305[B]	WWX	C25-C24-C23	-3.54	116.41	120.65
4	A	303	WWX	O15-S14-C17	-3.54	102.39	108.18
4	C	303	WWX	O29-C22-C23	3.52	118.84	111.20
4	A	303	WWX	C24-C23-C22	-3.49	115.45	120.71
4	B	303	WWX	O3-S1-N4	3.42	112.29	107.35
4	B	303	WWX	C31-C30-C35	3.41	122.54	118.30
4	C	303	WWX	C32-C33-C34	-3.40	115.21	119.87
4	A	303	WWX	C26-C27-C28	-3.33	116.13	120.24
4	B	303	WWX	C31-C30-C21	-3.32	115.51	120.78
4	D	305[A]	WWX	C30-C21-N19	-3.24	109.39	113.62
4	B	303	WWX	C17-S14-C8	3.24	121.57	108.15
4	A	303	WWX	C7-C8-S14	-3.07	113.34	120.87
4	D	305[B]	WWX	C30-C21-N19	-3.07	109.61	113.62
4	B	303	WWX	C18-C17-S14	-3.06	105.77	114.27
4	A	303	WWX	O16-S14-C8	2.94	114.04	106.59
4	D	305[B]	WWX	C10-C5-C6	2.93	118.66	116.65
4	C	303	WWX	C28-C23-C22	-2.89	116.35	120.71
4	B	303	WWX	C23-C22-C21	2.88	115.69	112.05
4	A	303	WWX	O16-S14-C17	2.81	112.79	108.18
4	B	303	WWX	C24-C23-C22	2.76	124.87	120.71
4	C	303	WWX	C24-C23-C28	2.75	121.71	118.30
4	A	303	WWX	C26-C25-C24	2.70	123.58	120.24
4	D	305[A]	WWX	C10-C5-C6	2.63	118.46	116.65
4	C	303	WWX	C27-C28-C23	-2.55	117.59	120.65
4	B	303	WWX	C25-C24-C23	-2.54	117.60	120.65
4	C	303	WWX	C10-C9-C8	2.50	120.38	115.97
4	B	303	WWX	C10-C9-C8	2.49	120.36	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	305[B]	WWX	C6-C5-S1	-2.37	115.58	121.34
4	B	303	WWX	C32-C31-C30	-2.35	117.84	120.65
4	A	303	WWX	C6-C7-C8	-2.34	118.95	121.78
4	D	305[A]	WWX	C6-C5-S1	-2.33	115.69	121.34
4	D	305[B]	WWX	O16-S14-C8	2.30	112.41	106.59
4	D	305[B]	WWX	C24-C23-C28	2.27	121.11	118.30
4	D	305[A]	WWX	C24-C23-C28	2.23	121.06	118.30
4	A	303	WWX	O20-C18-C17	-2.20	104.53	109.82
4	D	305[B]	WWX	O16-S14-C17	2.14	111.69	108.18
4	D	305[B]	WWX	C28-C23-C22	-2.13	117.50	120.71
4	D	305[A]	WWX	C28-C23-C22	-2.12	117.52	120.71
4	B	303	WWX	C24-C23-C28	2.07	120.88	118.30
4	D	305[A]	WWX	O16-S14-C8	2.00	111.67	106.59

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	WWX	C8-C9-N19-C21
4	A	303	WWX	C10-C5-S1-N4
4	B	303	WWX	C18-C17-S14-O16
4	B	303	WWX	C18-C17-S14-O15
4	B	303	WWX	C7-C8-S14-O16
4	B	303	WWX	C9-C8-S14-O16
4	B	303	WWX	C7-C8-S14-C17
4	B	303	WWX	C9-C8-S14-C17
4	B	303	WWX	C6-C5-S1-O3
4	B	303	WWX	C6-C5-S1-N4
4	B	303	WWX	C6-C5-S1-O2
4	B	303	WWX	C10-C5-S1-O3
4	B	303	WWX	N19-C21-C22-O29
4	B	303	WWX	C30-C21-C22-O29
4	B	303	WWX	C30-C21-C22-C23
4	C	303	WWX	C9-C8-S14-O15
4	C	303	WWX	C8-C9-N19-C21
4	C	303	WWX	C10-C5-S1-N4
4	C	303	WWX	C10-C5-S1-O2
4	D	305[A]	WWX	C8-C9-N19-C21
4	D	305[A]	WWX	C10-C5-S1-N4
4	D	305[B]	WWX	S14-C17-C18-O20
4	D	305[B]	WWX	C8-C9-N19-C21
4	D	305[B]	WWX	C10-C5-S1-N4

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Mol	Chain	Res	Type	Atoms
4	D	305[A]	WWX	C10-C5-S1-O2
4	D	305[B]	WWX	C10-C5-S1-O2
4	B	303	WWX	C18-C17-S14-C8
4	A	303	WWX	S14-C17-C18-O20
4	A	303	WWX	C9-C8-S14-O15
4	D	305[A]	WWX	C9-C8-S14-O15
4	C	303	WWX	C6-C5-S1-O2
4	B	303	WWX	C30-C21-N19-C9
4	A	303	WWX	N19-C21-C30-C31
4	C	303	WWX	N19-C21-C30-C35
4	A	303	WWX	N19-C21-C30-C35
4	A	303	WWX	C22-C21-C30-C35
4	C	303	WWX	N19-C21-C30-C31
4	A	303	WWX	C22-C21-C30-C31
4	D	305[B]	WWX	N19-C21-C30-C35
4	D	305[A]	WWX	N19-C21-C30-C35
3	C	302	EDO	O1-C1-C2-O2
4	D	305[A]	WWX	N19-C21-C30-C31
4	D	305[B]	WWX	N19-C21-C30-C31
3	D	302	EDO	O1-C1-C2-O2
4	C	303	WWX	C22-C21-C30-C35
4	B	303	WWX	C10-C5-S1-O2
4	D	305[A]	WWX	C6-C5-S1-O3
4	D	305[B]	WWX	C6-C5-S1-O3
3	D	303	EDO	O1-C1-C2-O2
4	C	303	WWX	C22-C21-C30-C31
4	D	305[A]	WWX	C22-C21-C30-C31
3	B	302	EDO	O1-C1-C2-O2
4	B	303	WWX	C22-C21-N19-C9
4	D	305[B]	WWX	C22-C21-C30-C31
4	B	303	WWX	N19-C21-C22-C23

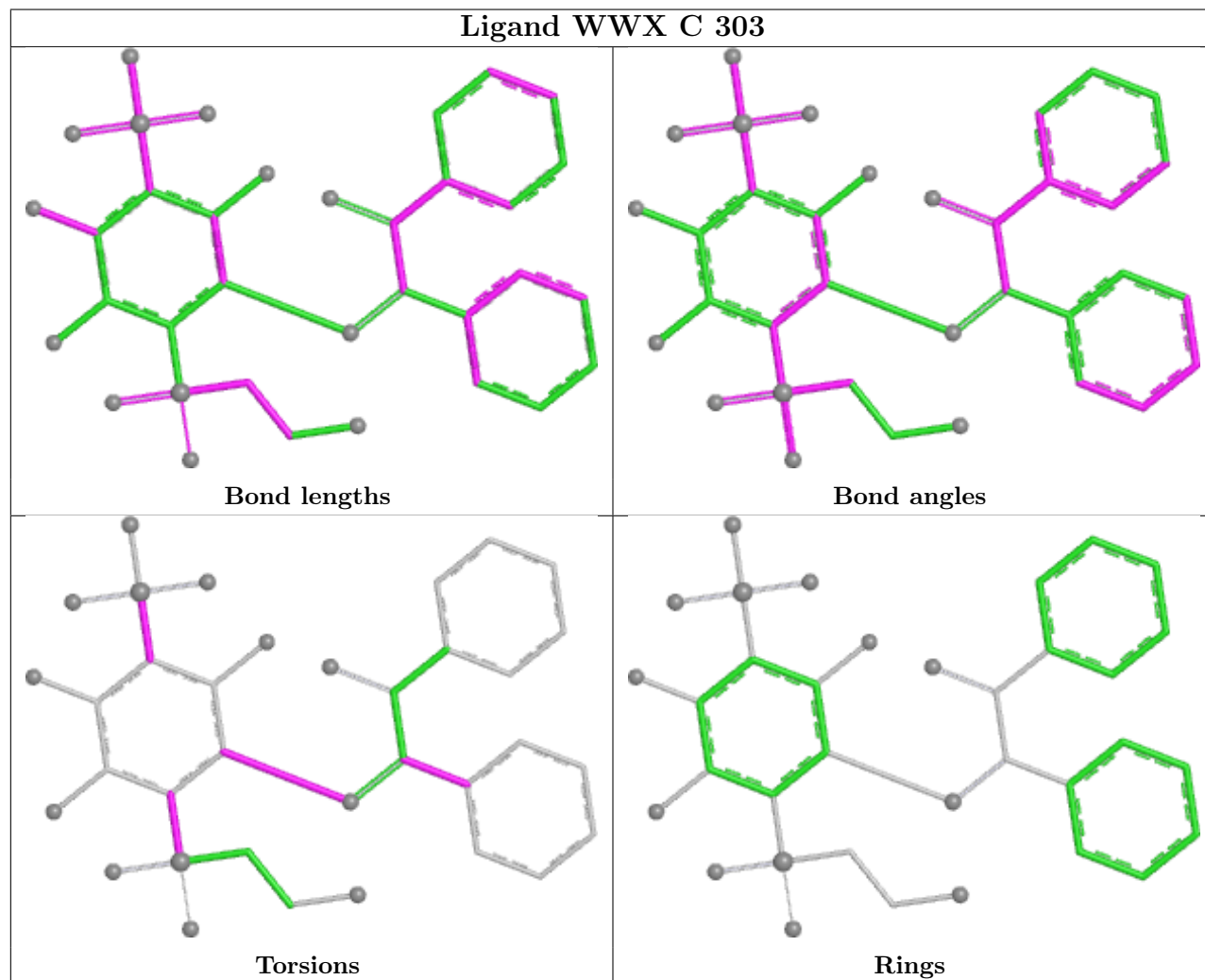
There are no ring outliers.

3 monomers are involved in 9 short contacts:

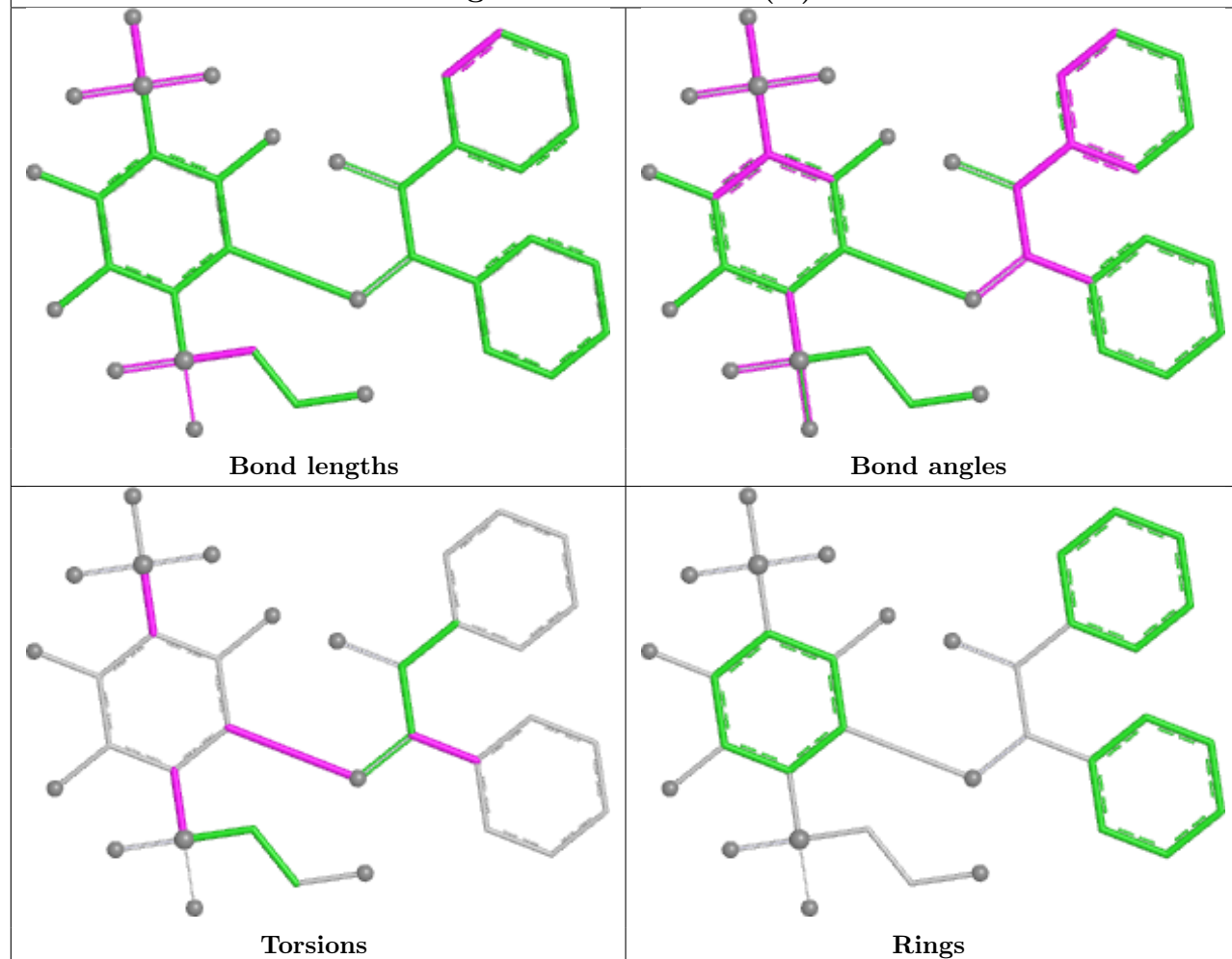
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	EDO	3	0
4	C	303	WWX	1	0
4	B	303	WWX	5	0

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

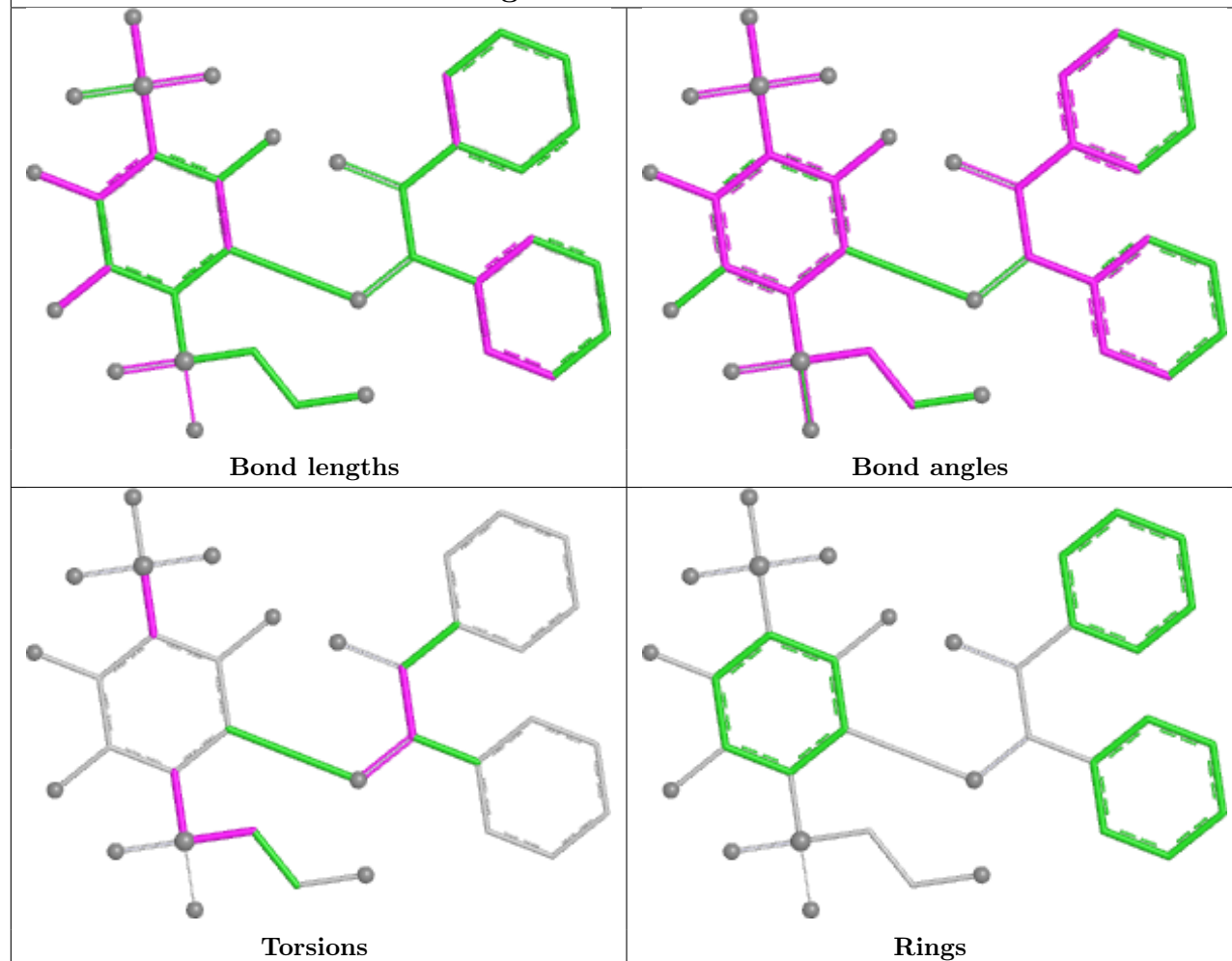
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



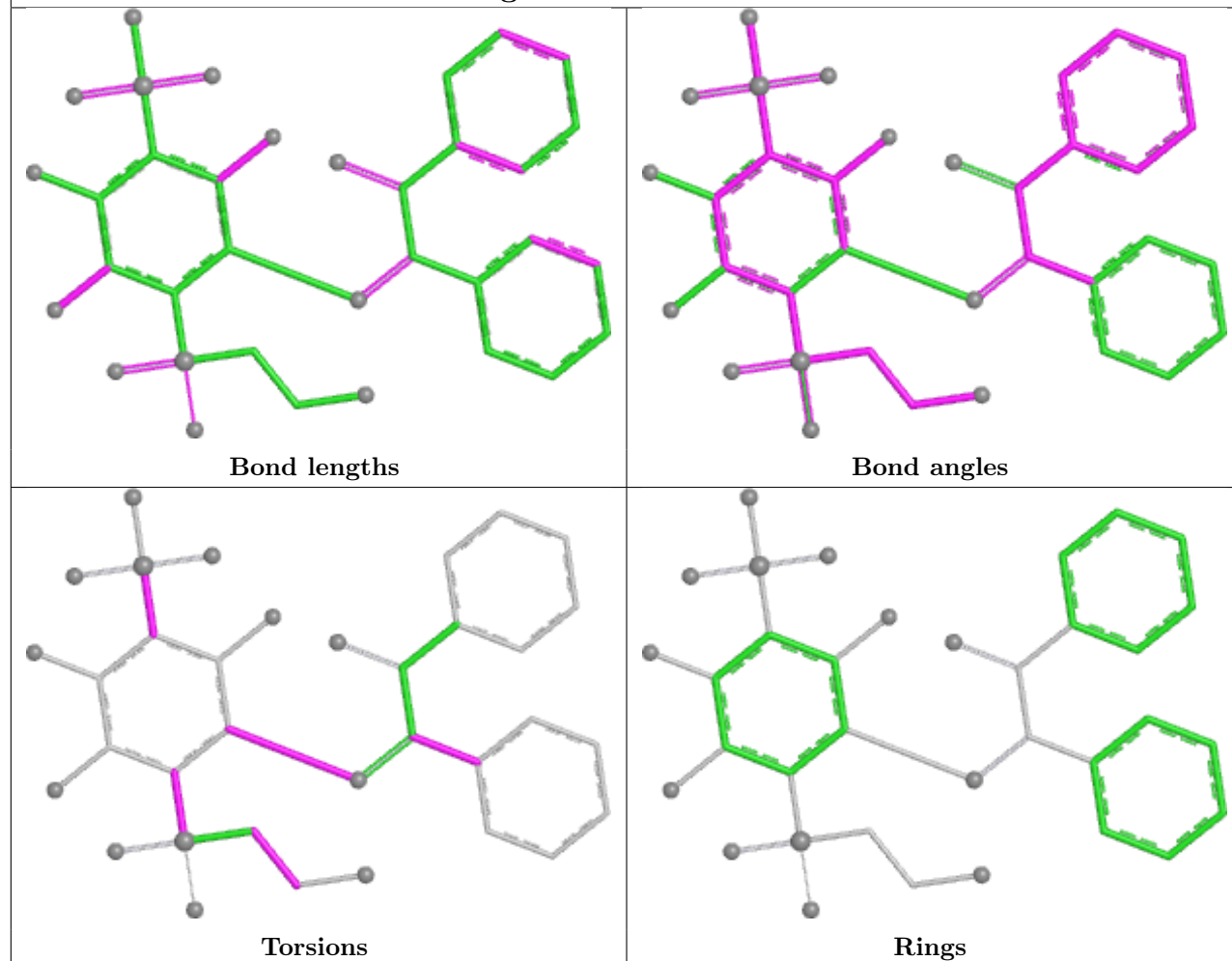
Ligand WWX D 305 (A)

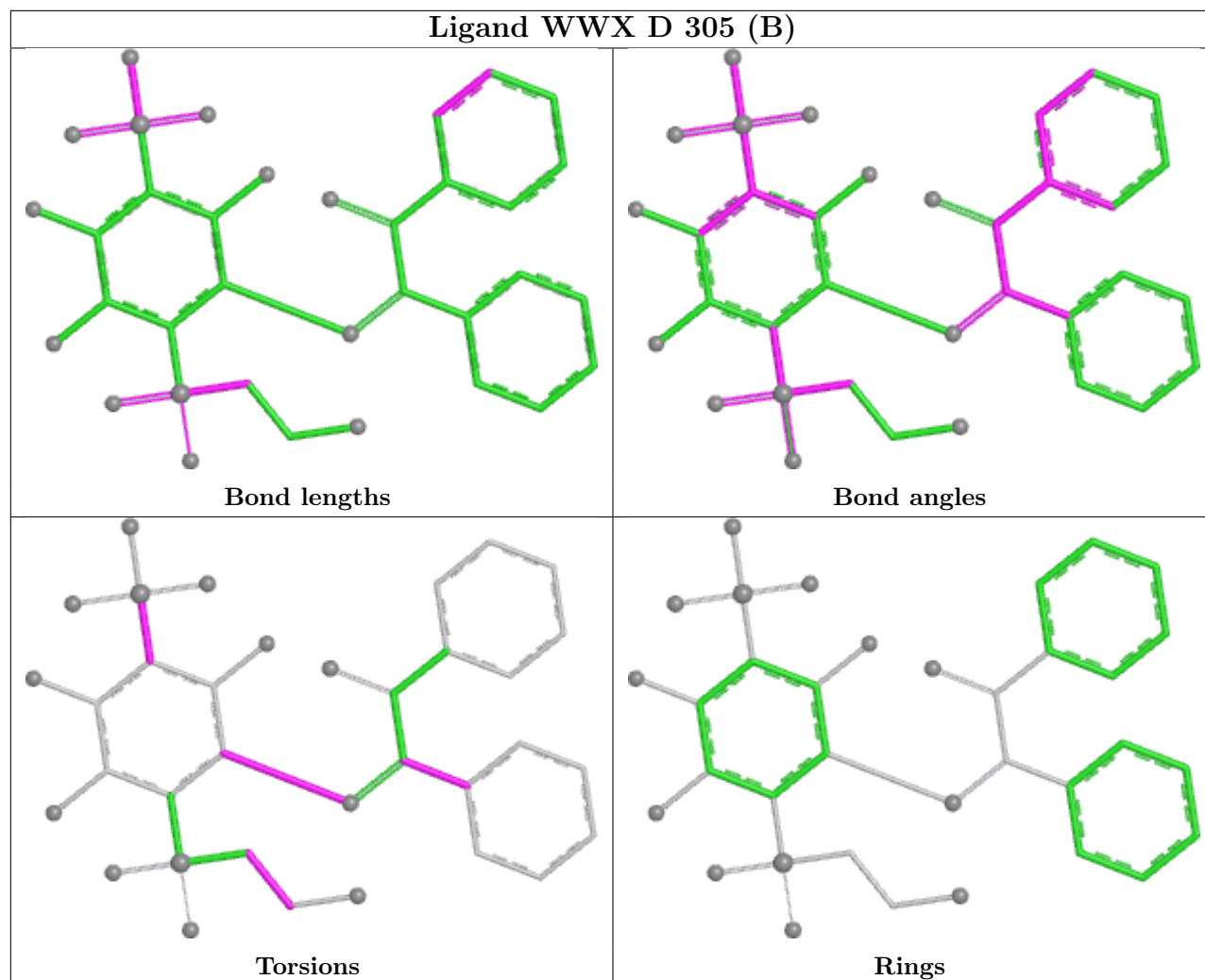


Ligand WWX B 303



Ligand WWX A 303





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	260/263 (98%)	0.00	7 (2%) 56 64	6, 17, 34, 47	6 (2%)
1	B	261/263 (99%)	-0.05	13 (4%) 34 41	5, 13, 39, 52	6 (2%)
1	C	260/263 (98%)	0.77	45 (17%) 4 5	7, 21, 41, 65	8 (3%)
1	D	260/263 (98%)	-0.29	3 (1%) 76 83	6, 13, 25, 37	9 (3%)
All	All	1041/1052 (98%)	0.11	68 (6%) 25 29	5, 15, 35, 65	29 (2%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	PRO	6.2
1	C	55	ALA	4.8
1	C	61	LEU	4.4
1	C	8	GLY	4.3
1	B	252[A]	PHE	4.0
1	C	173	PHE	3.9
1	C	3	LYS	3.8
1	A	8	GLY	3.8
1	C	177	PHE	3.4
1	B	125	LEU	3.4
1	C	174	VAL	3.3
1	D	262	SER	3.2
1	C	51	TYR	3.0
1	C	169	GLY	2.9
1	B	253	ASP	2.9
1	C	70	LEU	2.9
1	C	230[A]	TYR	2.9
1	C	151	PHE	2.8
1	C	234	MET	2.8
1	B	164	HIS	2.8
1	C	10	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	228	ALA	2.7
1	C	165	VAL	2.7
1	C	56	ASN	2.7
1	C	237	PRO	2.7
1	C	158	ILE	2.7
1	A	82	GLN	2.6
1	B	136	SER	2.6
1	D	252	PHE	2.6
1	B	3	LYS	2.6
1	C	162	LEU	2.6
1	A	3	LYS	2.6
1	A	7	PHE	2.5
1	C	159	PHE	2.5
1	C	167	TYR	2.5
1	C	262	SER	2.5
1	C	155	TYR	2.5
1	C	59	PHE	2.5
1	C	53	LEU	2.4
1	B	126	TYR	2.4
1	B	137	GLU	2.4
1	A	55	ALA	2.3
1	C	148	MET	2.3
1	B	81	LEU	2.3
1	C	172	ALA	2.3
1	C	233	HIS	2.3
1	C	7	PHE	2.3
1	B	131	THR	2.3
1	C	152	ASN	2.3
1	C	179	ILE	2.3
1	C	175	PRO	2.2
1	C	217	ILE	2.2
1	C	52	ASN	2.2
1	C	235	ASP	2.2
1	D	3	LYS	2.2
1	C	63[A]	ASN	2.2
1	C	50	GLY	2.2
1	B	127	PRO	2.1
1	A	262	SER	2.1
1	C	58	GLN	2.1
1	A	9	PRO	2.1
1	C	75	ASP	2.1
1	C	229	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	68	VAL	2.0
1	B	124	ASP	2.0
1	C	176	GLY	2.0
1	C	57	LYS	2.0
1	B	123	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

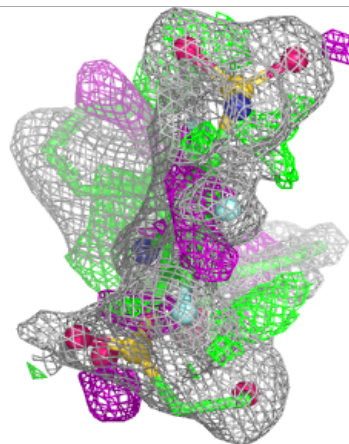
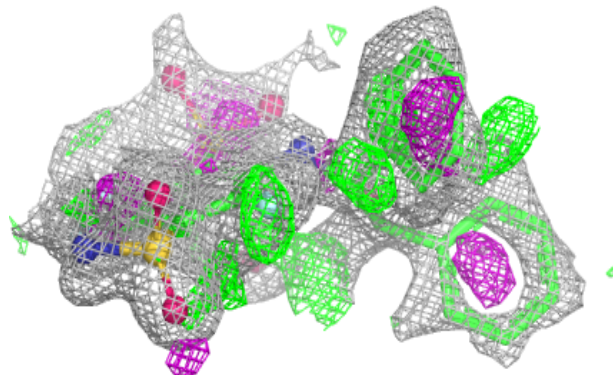
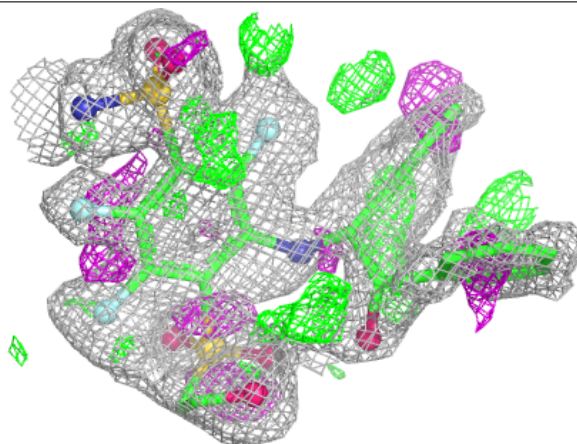
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	C	302	4/4	0.81	0.15	33,38,38,41	0
3	EDO	D	303	4/4	0.83	0.14	35,39,40,43	0
3	EDO	B	302	4/4	0.86	0.13	25,26,33,35	0
3	EDO	D	302	4/4	0.88	0.11	28,32,33,36	0
3	EDO	A	302	4/4	0.89	0.11	30,32,33,34	0
3	EDO	D	304	4/4	0.90	0.10	26,28,28,33	0
4	WWX	B	303	35/35	0.91	0.14	14,31,44,47	0
4	WWX	A	303	35/35	0.94	0.10	12,22,29,38	0
4	WWX	C	303	35/35	0.94	0.09	10,21,26,33	0
2	ZN	C	301	1/1	0.95	0.05	14,14,14,14	0
4	WWX	D	305[A]	35/35	0.95	0.08	11,17,19,20	35
4	WWX	D	305[B]	35/35	0.95	0.08	11,17,19,23	35
2	ZN	D	301	1/1	1.00	0.01	8,8,8,8	0
2	ZN	B	301	1/1	1.00	0.01	8,8,8,8	0
2	ZN	A	301	1/1	1.00	0.01	9,9,9,9	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.

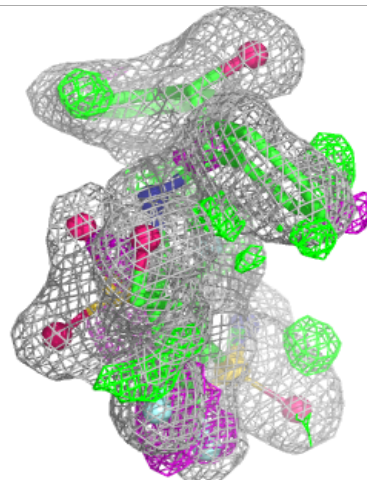
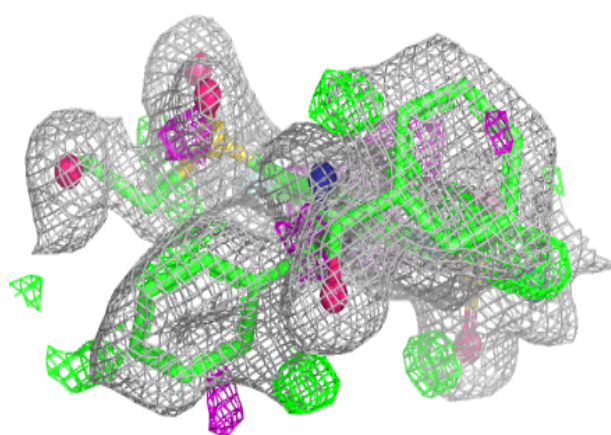
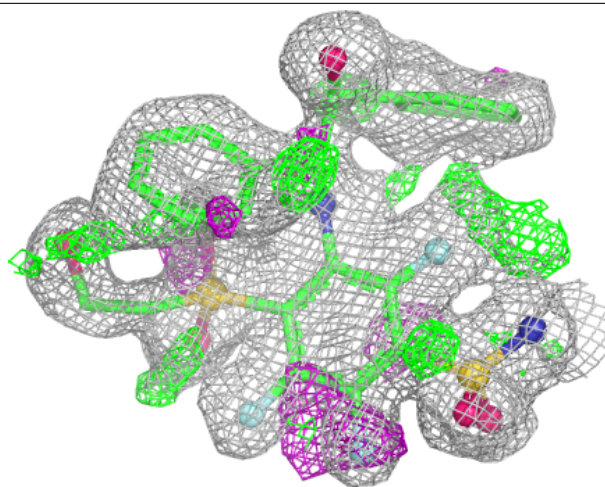
Electron density around WWX B 303:

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



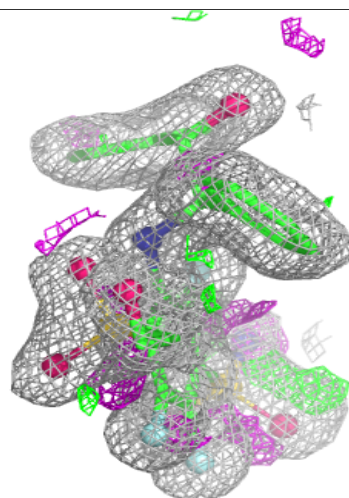
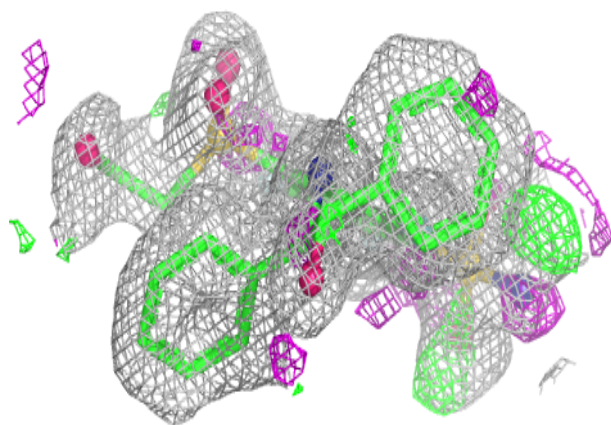
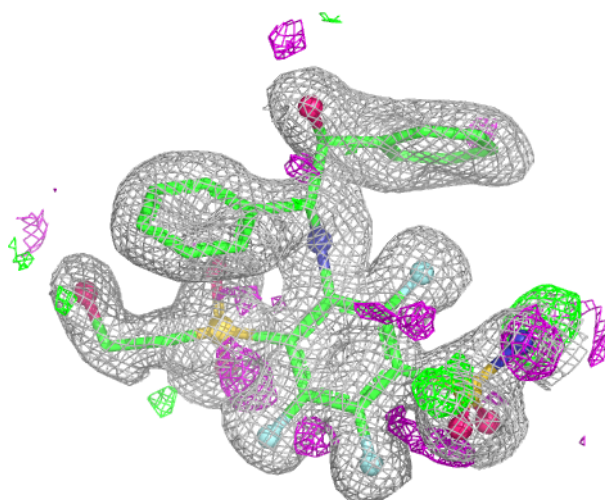
Electron density around WWX A 303:

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



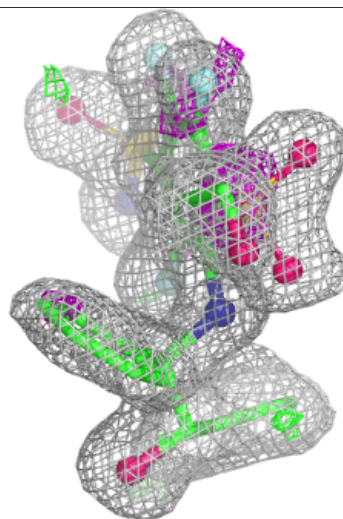
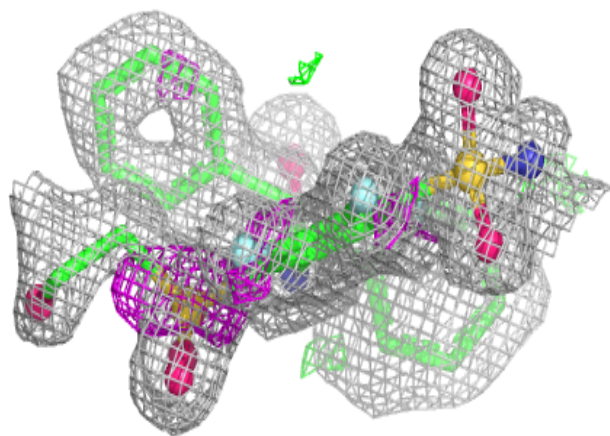
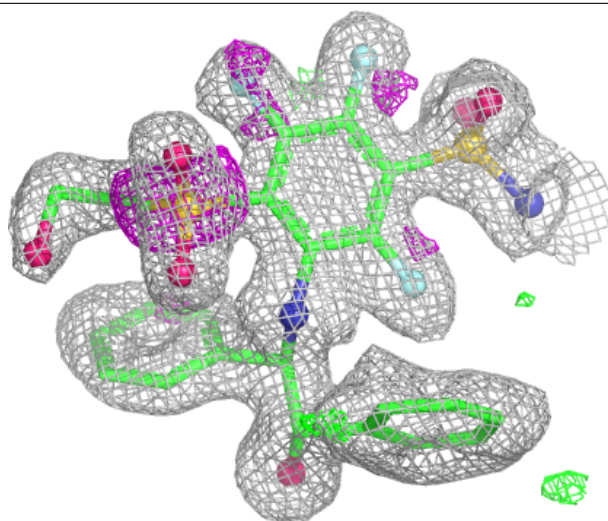
Electron density around WWX C 303:

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



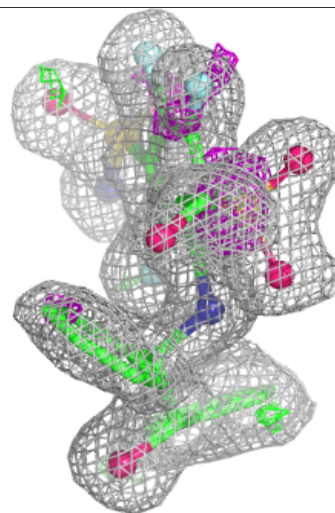
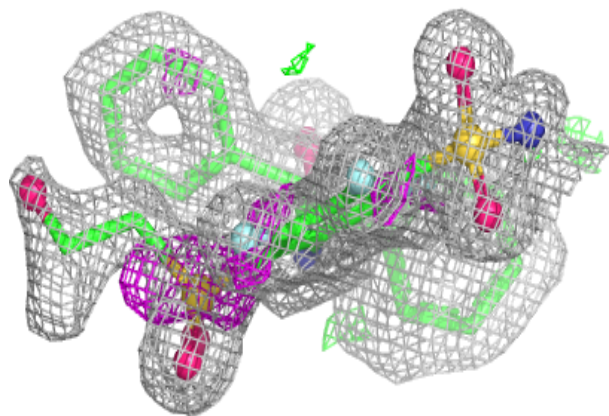
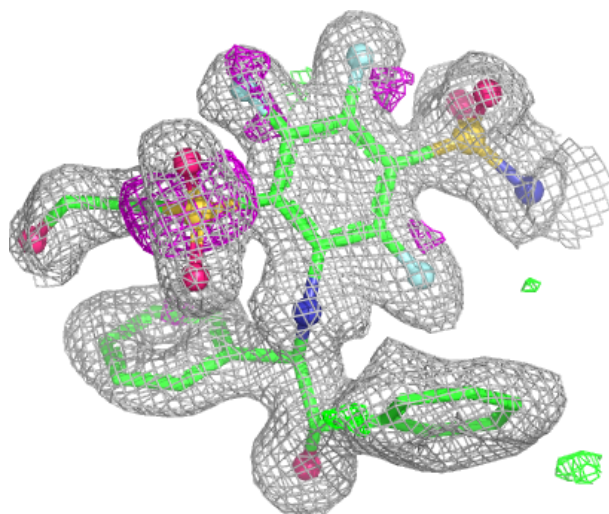
Electron density around WWX D 305 (A):

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



Electron density around WWX D 305 (B):

$2mF_o-DF_c$ (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.