



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:23 AM UTC

PDB ID : 4Q0N / pdb_00004q0n
Title : Crystal Structure of the fifth bromodomain of Human Poly-bromodomain containing protein 1 (PB1) in complex with a hydroxyphenyl-propenone ligand
Authors : Filippakopoulos, P.; Picaud, S.; Felletar, I.; Martin, S.; Monteiro, O.; Fedorov, O.; Chaikuad, A.; Yue, W.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2014-04-02
Resolution : 1.78 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](#) ①) were used in the production of this report:

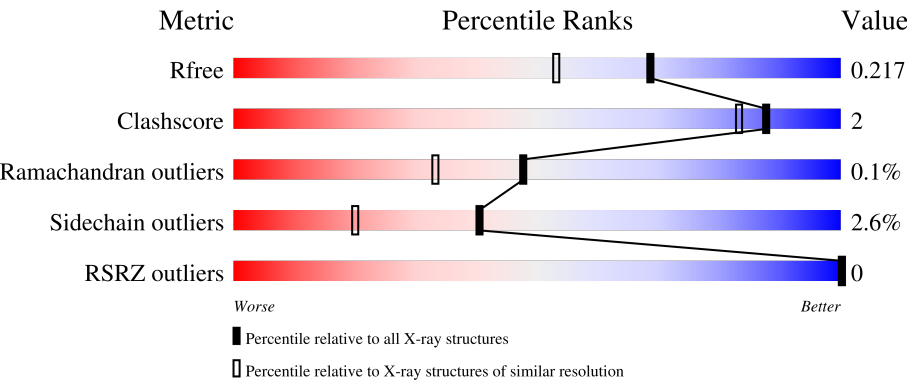
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	145	72% 5% • 22%
1	B	145	70% • • 23%
1	C	145	70% 6% • 23%
1	D	145	70% 6% • 23%
1	E	145	73% 5% 22%

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Mol	Chain	Length	Quality of chain
1	F	145	 74% • 23%
1	G	145	 70% 6% • 23%
1	H	145	 73% • 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8215 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 Protein polybromo-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	0	2	0
			948	603	162	173	10			
1	B	111	Total	C	N	O	S	0	0	0
			915	579	155	171	10			
1	C	111	Total	C	N	O	S	0	2	0
			919	585	153	170	11			
1	D	112	Total	C	N	O	S	0	2	0
			931	593	155	172	11			
1	E	113	Total	C	N	O	S	0	3	0
			943	601	157	175	10			
1	F	112	Total	C	N	O	S	0	0	0
			927	588	157	172	10			
1	G	112	Total	C	N	O	S	0	1	0
			923	587	154	172	10			
1	H	111	Total	C	N	O	S	0	1	0
			928	589	157	172	10			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	590	MET	-	expression tag	UNP Q86U86
A	591	HIS	-	expression tag	UNP Q86U86
A	592	HIS	-	expression tag	UNP Q86U86
A	593	HIS	-	expression tag	UNP Q86U86
A	594	HIS	-	expression tag	UNP Q86U86
A	595	HIS	-	expression tag	UNP Q86U86
A	596	HIS	-	expression tag	UNP Q86U86
A	597	SER	-	expression tag	UNP Q86U86
A	598	SER	-	expression tag	UNP Q86U86
A	599	GLY	-	expression tag	UNP Q86U86
A	600	VAL	-	expression tag	UNP Q86U86
A	601	ASP	-	expression tag	UNP Q86U86
A	602	LEU	-	expression tag	UNP Q86U86

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Chain	Residue	Modelled	Actual	Comment	Reference
A	603	GLY	-	expression tag	UNP Q86U86
A	604	THR	-	expression tag	UNP Q86U86
A	605	GLU	-	expression tag	UNP Q86U86
A	606	ASN	-	expression tag	UNP Q86U86
A	607	LEU	-	expression tag	UNP Q86U86
A	608	TYR	-	expression tag	UNP Q86U86
A	609	PHE	-	expression tag	UNP Q86U86
A	610	GLN	-	expression tag	UNP Q86U86
A	611	SER	-	expression tag	UNP Q86U86
A	612	MET	-	expression tag	UNP Q86U86
B	590	MET	-	expression tag	UNP Q86U86
B	591	HIS	-	expression tag	UNP Q86U86
B	592	HIS	-	expression tag	UNP Q86U86
B	593	HIS	-	expression tag	UNP Q86U86
B	594	HIS	-	expression tag	UNP Q86U86
B	595	HIS	-	expression tag	UNP Q86U86
B	596	HIS	-	expression tag	UNP Q86U86
B	597	SER	-	expression tag	UNP Q86U86
B	598	SER	-	expression tag	UNP Q86U86
B	599	GLY	-	expression tag	UNP Q86U86
B	600	VAL	-	expression tag	UNP Q86U86
B	601	ASP	-	expression tag	UNP Q86U86
B	602	LEU	-	expression tag	UNP Q86U86
B	603	GLY	-	expression tag	UNP Q86U86
B	604	THR	-	expression tag	UNP Q86U86
B	605	GLU	-	expression tag	UNP Q86U86
B	606	ASN	-	expression tag	UNP Q86U86
B	607	LEU	-	expression tag	UNP Q86U86
B	608	TYR	-	expression tag	UNP Q86U86
B	609	PHE	-	expression tag	UNP Q86U86
B	610	GLN	-	expression tag	UNP Q86U86
B	611	SER	-	expression tag	UNP Q86U86
B	612	MET	-	expression tag	UNP Q86U86
C	590	MET	-	expression tag	UNP Q86U86
C	591	HIS	-	expression tag	UNP Q86U86
C	592	HIS	-	expression tag	UNP Q86U86
C	593	HIS	-	expression tag	UNP Q86U86
C	594	HIS	-	expression tag	UNP Q86U86
C	595	HIS	-	expression tag	UNP Q86U86
C	596	HIS	-	expression tag	UNP Q86U86
C	597	SER	-	expression tag	UNP Q86U86
C	598	SER	-	expression tag	UNP Q86U86

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Chain	Residue	Modelled	Actual	Comment	Reference
C	599	GLY	-	expression tag	UNP Q86U86
C	600	VAL	-	expression tag	UNP Q86U86
C	601	ASP	-	expression tag	UNP Q86U86
C	602	LEU	-	expression tag	UNP Q86U86
C	603	GLY	-	expression tag	UNP Q86U86
C	604	THR	-	expression tag	UNP Q86U86
C	605	GLU	-	expression tag	UNP Q86U86
C	606	ASN	-	expression tag	UNP Q86U86
C	607	LEU	-	expression tag	UNP Q86U86
C	608	TYR	-	expression tag	UNP Q86U86
C	609	PHE	-	expression tag	UNP Q86U86
C	610	GLN	-	expression tag	UNP Q86U86
C	611	SER	-	expression tag	UNP Q86U86
C	612	MET	-	expression tag	UNP Q86U86
D	590	MET	-	expression tag	UNP Q86U86
D	591	HIS	-	expression tag	UNP Q86U86
D	592	HIS	-	expression tag	UNP Q86U86
D	593	HIS	-	expression tag	UNP Q86U86
D	594	HIS	-	expression tag	UNP Q86U86
D	595	HIS	-	expression tag	UNP Q86U86
D	596	HIS	-	expression tag	UNP Q86U86
D	597	SER	-	expression tag	UNP Q86U86
D	598	SER	-	expression tag	UNP Q86U86
D	599	GLY	-	expression tag	UNP Q86U86
D	600	VAL	-	expression tag	UNP Q86U86
D	601	ASP	-	expression tag	UNP Q86U86
D	602	LEU	-	expression tag	UNP Q86U86
D	603	GLY	-	expression tag	UNP Q86U86
D	604	THR	-	expression tag	UNP Q86U86
D	605	GLU	-	expression tag	UNP Q86U86
D	606	ASN	-	expression tag	UNP Q86U86
D	607	LEU	-	expression tag	UNP Q86U86
D	608	TYR	-	expression tag	UNP Q86U86
D	609	PHE	-	expression tag	UNP Q86U86
D	610	GLN	-	expression tag	UNP Q86U86
D	611	SER	-	expression tag	UNP Q86U86
D	612	MET	-	expression tag	UNP Q86U86
E	590	MET	-	expression tag	UNP Q86U86
E	591	HIS	-	expression tag	UNP Q86U86
E	592	HIS	-	expression tag	UNP Q86U86
E	593	HIS	-	expression tag	UNP Q86U86
E	594	HIS	-	expression tag	UNP Q86U86

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Chain	Residue	Modelled	Actual	Comment	Reference
E	595	HIS	-	expression tag	UNP Q86U86
E	596	HIS	-	expression tag	UNP Q86U86
E	597	SER	-	expression tag	UNP Q86U86
E	598	SER	-	expression tag	UNP Q86U86
E	599	GLY	-	expression tag	UNP Q86U86
E	600	VAL	-	expression tag	UNP Q86U86
E	601	ASP	-	expression tag	UNP Q86U86
E	602	LEU	-	expression tag	UNP Q86U86
E	603	GLY	-	expression tag	UNP Q86U86
E	604	THR	-	expression tag	UNP Q86U86
E	605	GLU	-	expression tag	UNP Q86U86
E	606	ASN	-	expression tag	UNP Q86U86
E	607	LEU	-	expression tag	UNP Q86U86
E	608	TYR	-	expression tag	UNP Q86U86
E	609	PHE	-	expression tag	UNP Q86U86
E	610	GLN	-	expression tag	UNP Q86U86
E	611	SER	-	expression tag	UNP Q86U86
E	612	MET	-	expression tag	UNP Q86U86
F	590	MET	-	expression tag	UNP Q86U86
F	591	HIS	-	expression tag	UNP Q86U86
F	592	HIS	-	expression tag	UNP Q86U86
F	593	HIS	-	expression tag	UNP Q86U86
F	594	HIS	-	expression tag	UNP Q86U86
F	595	HIS	-	expression tag	UNP Q86U86
F	596	HIS	-	expression tag	UNP Q86U86
F	597	SER	-	expression tag	UNP Q86U86
F	598	SER	-	expression tag	UNP Q86U86
F	599	GLY	-	expression tag	UNP Q86U86
F	600	VAL	-	expression tag	UNP Q86U86
F	601	ASP	-	expression tag	UNP Q86U86
F	602	LEU	-	expression tag	UNP Q86U86
F	603	GLY	-	expression tag	UNP Q86U86
F	604	THR	-	expression tag	UNP Q86U86
F	605	GLU	-	expression tag	UNP Q86U86
F	606	ASN	-	expression tag	UNP Q86U86
F	607	LEU	-	expression tag	UNP Q86U86
F	608	TYR	-	expression tag	UNP Q86U86
F	609	PHE	-	expression tag	UNP Q86U86
F	610	GLN	-	expression tag	UNP Q86U86
F	611	SER	-	expression tag	UNP Q86U86
F	612	MET	-	expression tag	UNP Q86U86
G	590	MET	-	expression tag	UNP Q86U86

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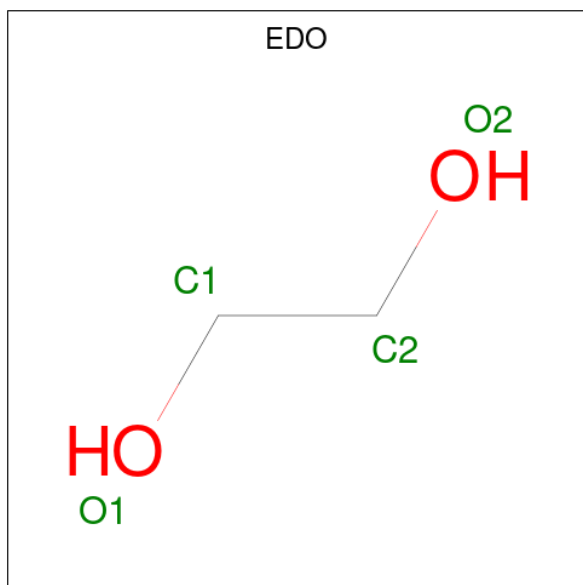
Chain	Residue	Modelled	Actual	Comment	Reference
G	591	HIS	-	expression tag	UNP Q86U86
G	592	HIS	-	expression tag	UNP Q86U86
G	593	HIS	-	expression tag	UNP Q86U86
G	594	HIS	-	expression tag	UNP Q86U86
G	595	HIS	-	expression tag	UNP Q86U86
G	596	HIS	-	expression tag	UNP Q86U86
G	597	SER	-	expression tag	UNP Q86U86
G	598	SER	-	expression tag	UNP Q86U86
G	599	GLY	-	expression tag	UNP Q86U86
G	600	VAL	-	expression tag	UNP Q86U86
G	601	ASP	-	expression tag	UNP Q86U86
G	602	LEU	-	expression tag	UNP Q86U86
G	603	GLY	-	expression tag	UNP Q86U86
G	604	THR	-	expression tag	UNP Q86U86
G	605	GLU	-	expression tag	UNP Q86U86
G	606	ASN	-	expression tag	UNP Q86U86
G	607	LEU	-	expression tag	UNP Q86U86
G	608	TYR	-	expression tag	UNP Q86U86
G	609	PHE	-	expression tag	UNP Q86U86
G	610	GLN	-	expression tag	UNP Q86U86
G	611	SER	-	expression tag	UNP Q86U86
G	612	MET	-	expression tag	UNP Q86U86
H	590	MET	-	expression tag	UNP Q86U86
H	591	HIS	-	expression tag	UNP Q86U86
H	592	HIS	-	expression tag	UNP Q86U86
H	593	HIS	-	expression tag	UNP Q86U86
H	594	HIS	-	expression tag	UNP Q86U86
H	595	HIS	-	expression tag	UNP Q86U86
H	596	HIS	-	expression tag	UNP Q86U86
H	597	SER	-	expression tag	UNP Q86U86
H	598	SER	-	expression tag	UNP Q86U86
H	599	GLY	-	expression tag	UNP Q86U86
H	600	VAL	-	expression tag	UNP Q86U86
H	601	ASP	-	expression tag	UNP Q86U86
H	602	LEU	-	expression tag	UNP Q86U86
H	603	GLY	-	expression tag	UNP Q86U86
H	604	THR	-	expression tag	UNP Q86U86
H	605	GLU	-	expression tag	UNP Q86U86
H	606	ASN	-	expression tag	UNP Q86U86
H	607	LEU	-	expression tag	UNP Q86U86
H	608	TYR	-	expression tag	UNP Q86U86
H	609	PHE	-	expression tag	UNP Q86U86

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Chain	Residue	Modelled	Actual	Comment	Reference
H	610	GLN	-	expression tag	UNP Q86U86
H	611	SER	-	expression tag	UNP Q86U86
H	612	MET	-	expression tag	UNP Q86U86

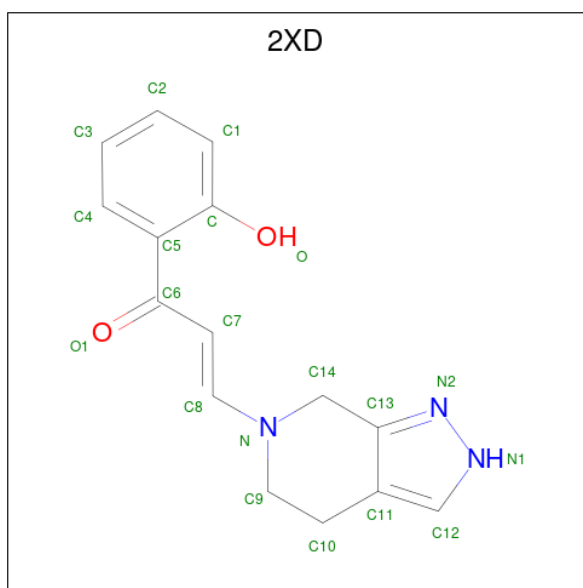
- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is (2E)-1-(2-hydroxyphenyl)-3-(2,4,5,7-tetrahydro-6H-pyrazolo[3,4-c]pyridin-6-yl

)prop-2-en-1-one (CCD ID: 2XD) (formula: C₁₅H₁₅N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			30	22	6	2		
3	B	1	Total	C	N	O	0	0
			20	15	3	2		
3	C	1	Total	C	N	O	0	1
			30	22	6	2		
3	D	1	Total	C	N	O	0	1
			30	22	6	2		
3	E	1	Total	C	N	O	0	1
			30	22	6	2		
3	F	1	Total	C	N	O	0	0
			20	15	3	2		
3	G	1	Total	C	N	O	0	0
			20	15	3	2		
3	H	1	Total	C	N	O	0	0
			20	15	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	65	Total	O	0	0
			65	65		
4	C	61	Total	O	0	0
			61	61		

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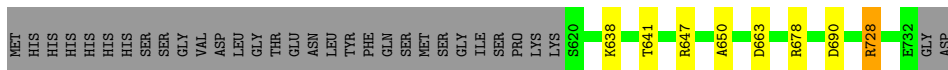
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	69	Total 69	O 69	0	0
4	E	76	Total 76	O 76	0	0
4	F	58	Total 58	O 58	0	0
4	G	72	Total 72	O 72	0	0
4	H	80	Total 80	O 80	0	0

3 Residue-property plots [i](#)

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

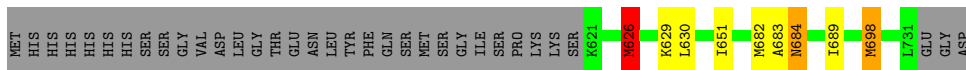
- Molecule 1: Protein polybromo-1

Chain A: 



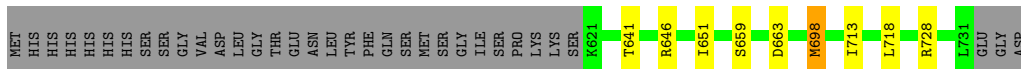
- Molecule 1: Protein polybromo-1

Chain B: 



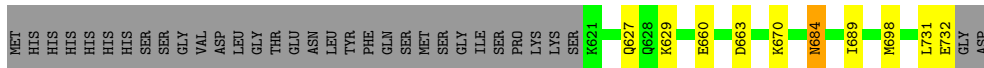
- Molecule 1: Protein polybromo-1

Chain C: 



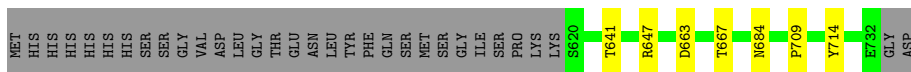
- Molecule 1: Protein polybromo-1

Chain D: 



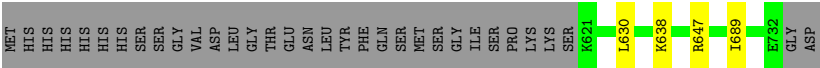
- Molecule 1: Protein polybromo-1

Chain E: 

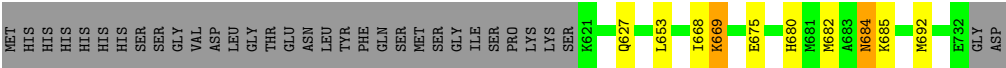


- Molecule 1: Protein polybromo-1

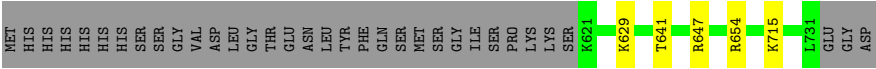
Chain F: 



● Molecule 1: Protein polybromo-1



● Molecule 1: Protein polybromo-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.02Å 136.72Å 114.41Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	26.69 – 1.78 26.69 – 1.78	Depositor EDS
% Data completeness (in resolution range)	96.9 (26.69-1.78) 96.9 (26.69-1.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.176 , 0.214 0.186 , 0.217	Depositor DCC
R_{free} test set	1938 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8215	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 21.15 % 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 7.4557e-03.*

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: 2XD, EDO

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	1.02	0/971	1.02	1/1304 (0.1%)
1	B	0.90	0/932	0.97	2/1255 (0.2%)
1	C	0.92	1/942 (0.1%)	0.92	0/1269
1	D	0.97	0/954	0.98	0/1283
1	E	1.05	1/969 (0.1%)	0.98	0/1303
1	F	0.92	0/944	0.93	0/1270
1	G	1.04	2/944 (0.2%)	0.95	2/1273 (0.2%)
1	H	0.94	0/948	0.93	0/1274
All	All	0.97	4/7604 (0.1%)	0.96	5/10231 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	667	THR	N-CA	5.47	1.52	1.46
1	G	668	ILE	C-O	5.14	1.29	1.24
1	G	692	MET	SD-CE	-5.13	1.66	1.79
1	C	718	LEU	N-CA	5.07	1.52	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	698	MET	CG-SD-CE	-8.45	82.32	100.90
1	G	692	MET	CG-SD-CE	-6.29	87.06	100.90
1	A	650	ALA	N-CA-C	5.95	118.25	111.11
1	B	626	MET	CG-SD-CE	5.72	113.49	100.90
1	G	669	LYS	N-CA-C	5.51	118.21	111.82

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	948	0	955	4	0
1	B	915	0	901	5	0
1	C	919	0	908	4	0
1	D	931	0	928	5	0
1	E	943	0	950	3	0
1	F	927	0	923	2	0
1	G	923	0	903	3	0
1	H	928	0	935	3	0
2	A	4	0	6	0	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
2	E	8	0	12	1	0
2	F	4	0	6	0	0
2	G	8	0	12	0	0
2	H	4	0	6	0	0
3	A	30	0	20	1	0
3	B	20	0	14	0	0
3	C	30	0	20	0	0
3	D	30	0	20	1	0
3	E	30	0	20	0	0
3	F	20	0	15	0	0
3	G	20	0	15	0	0
3	H	20	0	15	0	0
4	A	64	0	0	1	0
4	B	65	0	0	0	0
4	C	61	0	0	1	2
4	D	69	0	0	0	0
4	E	76	0	0	0	0
4	F	58	0	0	3	2
4	G	72	0	0	0	0
4	H	80	0	0	2	0
All	All	8215	0	7596	30	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:638:LYS:NZ	4:F:942:HOH:O	1.97	0.83
1:G:680[A]:HIS:CE1	1:G:685:LYS:CB	2.70	0.73
1:B:626:MET:CE	1:B:626:MET:HA	2.32	0.60
1:F:630:LEU:HD23	1:F:689:ILE:HD13	1.82	0.60
1:A:647[A]:ARG:HD3	4:F:907:HOH:O	2.02	0.60
1:A:641:THR:HG22	1:A:647[B]:ARG:HG3	1.84	0.59
1:D:627:GLN:HE21	1:D:684:ASN:HD21	1.53	0.56
1:G:627:GLN:NE2	1:G:684:ASN:OD1	2.42	0.53
1:A:647[A]:ARG:HB2	4:F:907:HOH:O	2.08	0.53
1:E:647:ARG:HD3	4:H:909:HOH:O	2.09	0.53
1:C:698[A]:MET:HE1	4:C:959:HOH:O	2.10	0.52
3:A:802[B]:2XD:N1	4:A:919:HOH:O	2.32	0.51
1:C:651[B]:ILE:HD11	1:C:713:ILE:HG23	1.92	0.51
1:B:626:MET:HE2	1:B:629:LYS:HB3	1.93	0.51
1:E:709:PRO:HA	1:E:714:TYR:CG	2.49	0.48
1:A:690:ASP:OD1	1:A:728:ARG:NH2	2.47	0.46
1:G:653:LEU:O	1:G:675:GLU:HG2	2.17	0.45
1:D:731:LEU:O	1:D:732:GLU:C	2.60	0.45
1:H:654:ARG:NH1	4:H:946:HOH:O	2.49	0.44
2:E:802:EDO:H22	1:H:715:LYS:CE	2.48	0.44
1:H:641:THR:HG22	1:H:647:ARG:HG2	2.00	0.44
1:E:641:THR:HG22	1:E:647:ARG:HG3	2.00	0.43
1:B:683:ALA:O	1:B:684:ASN:C	2.61	0.43
1:C:698[A]:MET:HB2	1:C:698[A]:MET:HE3	1.77	0.43
1:C:641:THR:HA	1:C:646:ARG:O	2.19	0.42
1:D:629:LYS:HB3	1:D:689:ILE:HD11	2.00	0.42
1:B:626:MET:HA	1:B:626:MET:HE3	2.01	0.42
1:D:670:LYS:CG	1:D:698[A]:MET:SD	3.09	0.41
1:D:660:GLU:OE2	3:D:802[A]:2XD:N1	2.51	0.40
1:B:630:LEU:HD23	1:B:689:ILE:HD13	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:934:HOH:O	4:F:915:HOH:O[2_546]	2.04	0.16
4:C:956:HOH:O	4:F:928:HOH:O[2_546]	2.16	0.04

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	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
1	B	109/145 (75%)	107 (98%)	1 (1%)	1 (1%)	14	4
1	C	111/145 (77%)	111 (100%)	0	0	100	100
1	D	112/145 (77%)	112 (100%)	0	0	100	100
1	E	114/145 (79%)	114 (100%)	0	0	100	100
1	F	110/145 (76%)	110 (100%)	0	0	100	100
1	G	111/145 (77%)	111 (100%)	0	0	100	100
1	H	110/145 (76%)	110 (100%)	0	0	100	100
All	All	890/1160 (77%)	887 (100%)	2 (0%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	684	ASN

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	105/135 (78%)	100 (95%)	5 (5%)	23	5
1	B	101/135 (75%)	97 (96%)	4 (4%)	28	8
1	C	101/135 (75%)	96 (95%)	5 (5%)	22	5
1	D	103/135 (76%)	101 (98%)	2 (2%)	50	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	106/135 (78%)	104 (98%)	2 (2%)	50	32
1	F	103/135 (76%)	102 (99%)	1 (1%)	68	55
1	G	101/135 (75%)	98 (97%)	3 (3%)	36	15
1	H	105/135 (78%)	104 (99%)	1 (1%)	68	55
All	All	825/1080 (76%)	802 (97%)	23 (3%)	40	17

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	638[A]	LYS
1	A	638[B]	LYS
1	A	663	ASP
1	A	678	ARG
1	A	728	ARG
1	B	626	MET
1	B	651	ILE
1	B	682	MET
1	B	698	MET
1	C	659	SER
1	C	663	ASP
1	C	698[A]	MET
1	C	698[B]	MET
1	C	728	ARG
1	D	663	ASP
1	D	684	ASN
1	E	663	ASP
1	E	684	ASN
1	F	647	ARG
1	G	669	LYS
1	G	682	MET
1	G	684	ASN
1	H	629	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	631	ASN
1	B	627	GLN
1	B	639	ASN
1	B	684	ASN

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Mol	Chain	Res	Type
1	C	631	ASN
1	D	707	ASN
1	G	628	GLN
1	G	631	ASN
1	G	707	ASN

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](#)

21 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	$\# Z > 2$
2	EDO	H	801	-	3,3,3	0.58	0	2,2,2	0.18	0
3	2XD	A	802[A]	-	21,22,22	2.21	7 (33%)	24,30,30	1.62	3 (12%)
3	2XD	C	802[A]	-	21,22,22	1.99	7 (33%)	24,30,30	1.48	5 (20%)
2	EDO	D	801	-	3,3,3	0.45	0	2,2,2	0.31	0
2	EDO	G	801	-	3,3,3	0.54	0	2,2,2	0.52	0
2	EDO	A	801	-	3,3,3	0.28	0	2,2,2	1.14	0
3	2XD	B	801	-	21,22,22	1.91	6 (28%)	24,30,30	1.78	4 (16%)
3	2XD	H	802	-	21,22,22	2.31	10 (47%)	24,30,30	1.93	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	G	802	-	3,3,3	0.31	0	2,2,2	0.81	0
3	2XD	C	802[B]	-	21,22,22	2.03	7 (33%)	24,30,30	1.63	6 (25%)
3	2XD	A	802[B]	-	21,22,22	2.22	7 (33%)	24,30,30	1.59	3 (12%)
3	2XD	E	803[B]	-	21,22,22	2.43	8 (38%)	24,30,30	1.79	7 (29%)
2	EDO	E	802	-	3,3,3	0.19	0	2,2,2	0.42	0
3	2XD	D	802[A]	-	21,22,22	2.20	8 (38%)	24,30,30	1.74	5 (20%)
3	2XD	F	802	-	21,22,22	2.11	6 (28%)	24,30,30	1.55	3 (12%)
2	EDO	C	801	-	3,3,3	0.37	0	2,2,2	0.57	0
3	2XD	D	802[B]	-	21,22,22	2.20	7 (33%)	24,30,30	1.81	6 (25%)
2	EDO	F	801	-	3,3,3	0.35	0	2,2,2	0.53	0
3	2XD	G	803	-	21,22,22	2.02	7 (33%)	24,30,30	1.76	6 (25%)
2	EDO	E	801	-	3,3,3	0.72	0	2,2,2	0.24	0
3	2XD	E	803[A]	-	21,22,22	2.45	8 (38%)	24,30,30	1.83	7 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	H	801	-	-	1/1/1/1	-
3	2XD	A	802[A]	-	-	0/9/18/18	0/3/3/3
3	2XD	C	802[A]	-	-	1/9/18/18	0/3/3/3
2	EDO	D	801	-	-	0/1/1/1	-
2	EDO	G	801	-	-	0/1/1/1	-
2	EDO	A	801	-	-	1/1/1/1	-
3	2XD	B	801	-	-	0/9/18/18	0/3/3/3
3	2XD	H	802	-	-	0/9/18/18	0/3/3/3
2	EDO	G	802	-	-	0/1/1/1	-
3	2XD	C	802[B]	-	-	0/9/18/18	0/3/3/3
3	2XD	A	802[B]	-	-	0/9/18/18	0/3/3/3
3	2XD	E	803[B]	-	-	0/9/18/18	0/3/3/3
2	EDO	E	802	-	-	1/1/1/1	-
3	2XD	D	802[A]	-	-	0/9/18/18	0/3/3/3
3	2XD	F	802	-	-	0/9/18/18	0/3/3/3
2	EDO	C	801	-	-	0/1/1/1	-
3	2XD	D	802[B]	-	-	0/9/18/18	0/3/3/3
2	EDO	F	801	-	-	1/1/1/1	-
3	2XD	G	803	-	-	0/9/18/18	0/3/3/3
2	EDO	E	801	-	-	0/1/1/1	-
3	2XD	E	803[A]	-	-	0/9/18/18	0/3/3/3

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	803[A]	2XD	O-C	5.30	1.47	1.36
3	E	803[B]	2XD	O-C	5.30	1.47	1.36
3	D	802[A]	2XD	O-C	5.07	1.46	1.36
3	D	802[B]	2XD	O-C	5.07	1.46	1.36
3	F	802	2XD	C14-C13	-5.05	1.44	1.50
3	B	801	2XD	C14-C13	-4.86	1.44	1.50
3	H	802	2XD	C4-C5	4.85	1.47	1.39
3	A	802[A]	2XD	O-C	4.55	1.45	1.36
3	A	802[B]	2XD	O-C	4.55	1.45	1.36
3	A	802[B]	2XD	C12-C11	4.54	1.44	1.38
3	C	802[A]	2XD	C4-C5	4.53	1.46	1.39
3	C	802[B]	2XD	C4-C5	4.53	1.46	1.39
3	H	802	2XD	C14-C13	-4.34	1.45	1.50
3	G	803	2XD	C12-C11	4.19	1.44	1.38
3	E	803[A]	2XD	C4-C5	3.95	1.45	1.39
3	E	803[B]	2XD	C4-C5	3.95	1.45	1.39
3	E	803[A]	2XD	C2-C3	3.91	1.46	1.38
3	E	803[B]	2XD	C2-C3	3.91	1.46	1.38
3	D	802[A]	2XD	C9-N	3.90	1.52	1.46
3	G	803	2XD	C9-N	3.83	1.52	1.46
3	F	802	2XD	C10-C11	-3.82	1.43	1.50
3	H	802	2XD	C5-C6	-3.76	1.41	1.48
3	B	801	2XD	C4-C5	3.76	1.45	1.39
3	E	803[A]	2XD	O1-C6	3.73	1.32	1.24
3	E	803[B]	2XD	O1-C6	3.73	1.32	1.24
3	G	803	2XD	O1-C6	3.68	1.32	1.24
3	F	802	2XD	C9-N	3.67	1.52	1.46
3	E	803[A]	2XD	C12-C11	3.58	1.43	1.38
3	D	802[B]	2XD	C12-C11	3.57	1.43	1.38
3	C	802[A]	2XD	C2-C1	3.50	1.44	1.38
3	C	802[B]	2XD	C2-C1	3.50	1.44	1.38
3	A	802[A]	2XD	C12-N1	3.42	1.39	1.34
3	F	802	2XD	C12-N1	3.31	1.39	1.34
3	A	802[B]	2XD	C10-C11	-3.31	1.44	1.50
3	A	802[A]	2XD	C5-C	-3.30	1.35	1.40
3	A	802[B]	2XD	C5-C	-3.30	1.35	1.40
3	A	802[A]	2XD	C12-C11	3.19	1.42	1.38
3	C	802[A]	2XD	O-C	3.18	1.42	1.36
3	C	802[B]	2XD	O-C	3.18	1.42	1.36
3	A	802[A]	2XD	C10-C11	-3.17	1.45	1.50
3	D	802[B]	2XD	C9-N	3.16	1.51	1.46
3	B	801	2XD	C9-N	3.10	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802[A]	2XD	C2-C3	3.09	1.45	1.38
3	D	802[B]	2XD	C2-C3	3.09	1.45	1.38
3	H	802	2XD	O1-C6	3.08	1.31	1.24
3	E	803[A]	2XD	C7-C6	-3.04	1.42	1.47
3	E	803[B]	2XD	C7-C6	-3.04	1.42	1.47
3	C	802[B]	2XD	C9-N	2.98	1.51	1.46
3	C	802[B]	2XD	C12-C11	2.90	1.42	1.38
3	B	801	2XD	C12-N1	2.89	1.38	1.34
3	E	803[B]	2XD	C13-N2	2.86	1.39	1.33
3	H	802	2XD	C12-N1	2.83	1.38	1.34
3	A	802[A]	2XD	C14-C13	-2.81	1.47	1.50
3	E	803[B]	2XD	C12-C11	2.80	1.42	1.38
3	E	803[A]	2XD	C13-N2	2.77	1.39	1.33
3	D	802[A]	2XD	C7-C6	-2.70	1.42	1.47
3	D	802[B]	2XD	C7-C6	-2.70	1.42	1.47
3	D	802[A]	2XD	C12-C11	2.63	1.42	1.38
3	F	802	2XD	C4-C5	2.62	1.43	1.39
3	A	802[B]	2XD	C13-N2	2.58	1.39	1.33
3	H	802	2XD	C9-N	2.58	1.50	1.46
3	A	802[A]	2XD	C2-C3	2.52	1.43	1.38
3	A	802[B]	2XD	C2-C3	2.52	1.43	1.38
3	H	802	2XD	C2-C1	2.48	1.43	1.38
3	B	801	2XD	O1-C6	2.47	1.29	1.24
3	C	802[A]	2XD	O1-C6	2.44	1.29	1.24
3	C	802[B]	2XD	O1-C6	2.44	1.29	1.24
3	C	802[A]	2XD	C10-C11	-2.35	1.46	1.50
3	G	803	2XD	O-C	2.35	1.41	1.36
3	G	803	2XD	C7-C6	-2.34	1.43	1.47
3	A	802[B]	2XD	C9-N	2.33	1.50	1.46
3	E	803[A]	2XD	C3-C4	-2.30	1.35	1.38
3	E	803[B]	2XD	C3-C4	-2.30	1.35	1.38
3	C	802[A]	2XD	C13-N2	2.29	1.38	1.33
3	D	802[A]	2XD	C4-C5	2.27	1.43	1.39
3	D	802[B]	2XD	C4-C5	2.27	1.43	1.39
3	H	802	2XD	C2-C3	2.27	1.43	1.38
3	H	802	2XD	C1-C	2.24	1.43	1.39
3	B	801	2XD	C10-C11	-2.22	1.46	1.50
3	D	802[A]	2XD	C10-C11	-2.21	1.46	1.50
3	C	802[B]	2XD	C13-N2	2.21	1.38	1.33
3	G	803	2XD	C4-C5	2.16	1.43	1.39
3	G	803	2XD	C14-C13	-2.16	1.48	1.50
3	F	802	2XD	O1-C6	2.09	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802[A]	2XD	C12-N1	2.08	1.37	1.34
3	C	802[A]	2XD	C9-N	2.07	1.49	1.46
3	D	802[B]	2XD	C10-C11	-2.07	1.47	1.50
3	H	802	2XD	C5-C	2.06	1.44	1.40

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	802	2XD	C12-N1-N2	-6.02	103.37	112.59
3	B	801	2XD	C12-N1-N2	-5.69	103.88	112.59
3	B	801	2XD	C13-N2-N1	4.54	113.08	104.75
3	G	803	2XD	C12-N1-N2	-4.42	105.82	112.59
3	D	802[B]	2XD	C12-N1-N2	-4.35	105.93	112.59
3	D	802[B]	2XD	C13-N2-N1	4.12	112.30	104.75
3	A	802[A]	2XD	C12-N1-N2	-4.08	106.35	112.59
3	F	802	2XD	C12-N1-N2	-4.07	106.36	112.59
3	H	802	2XD	C13-N2-N1	3.93	111.96	104.75
3	E	803[B]	2XD	C12-N1-N2	-3.88	106.66	112.59
3	D	802[A]	2XD	C12-N1-N2	-3.86	106.69	112.59
3	C	802[B]	2XD	C12-N1-N2	-3.82	106.74	112.59
3	D	802[A]	2XD	C13-N2-N1	3.80	111.72	104.75
3	A	802[B]	2XD	C13-N2-N1	3.77	111.66	104.75
3	E	803[A]	2XD	C13-N2-N1	3.71	111.55	104.75
3	A	802[A]	2XD	C13-N2-N1	3.70	111.53	104.75
3	E	803[A]	2XD	C12-N1-N2	-3.68	106.95	112.59
3	E	803[B]	2XD	C13-N2-N1	3.65	111.44	104.75
3	G	803	2XD	C13-N2-N1	3.57	111.29	104.75
3	A	802[B]	2XD	C12-N1-N2	-3.56	107.14	112.59
3	H	802	2XD	C11-C12-N1	3.56	110.74	107.30
3	C	802[B]	2XD	C13-N2-N1	3.54	111.24	104.75
3	E	803[A]	2XD	C14-C13-N2	3.52	129.65	124.72
3	F	802	2XD	C13-N2-N1	3.46	111.09	104.75
3	A	802[B]	2XD	C14-C13-N2	3.44	129.55	124.72
3	D	802[A]	2XD	C-C5-C6	-3.40	117.63	119.82
3	D	802[B]	2XD	C-C5-C6	-3.40	117.63	119.82
3	A	802[A]	2XD	C8-C7-C6	-3.36	116.60	119.72
3	C	802[A]	2XD	C13-N2-N1	3.34	110.87	104.75
3	G	803	2XD	C8-C7-C6	-3.20	116.75	119.72
3	C	802[A]	2XD	C12-N1-N2	-3.05	107.93	112.59
3	E	803[B]	2XD	C14-C13-N2	2.87	128.74	124.72
3	C	802[B]	2XD	C11-C12-N1	2.85	110.06	107.30
3	B	801	2XD	C11-C12-N1	2.75	109.97	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	803[B]	2XD	C11-C12-N1	2.69	109.90	107.30
3	C	802[B]	2XD	C14-C13-N2	2.58	128.33	124.72
3	B	801	2XD	O-C-C5	-2.55	116.98	121.71
3	E	803[A]	2XD	C-C5-C6	2.51	121.43	119.82
3	E	803[B]	2XD	C-C5-C6	2.51	121.43	119.82
3	E	803[A]	2XD	C3-C2-C1	-2.51	117.14	120.24
3	E	803[B]	2XD	C3-C2-C1	-2.51	117.14	120.24
3	E	803[A]	2XD	C2-C3-C4	2.45	123.27	120.24
3	E	803[B]	2XD	C2-C3-C4	2.45	123.27	120.24
3	C	802[A]	2XD	O1-C6-C5	-2.44	116.26	119.47
3	C	802[B]	2XD	O1-C6-C5	-2.44	116.26	119.47
3	G	803	2XD	C14-C13-N2	2.35	128.01	124.72
3	D	802[A]	2XD	O-C-C5	-2.32	117.42	121.71
3	D	802[B]	2XD	O-C-C5	-2.32	117.42	121.71
3	C	802[A]	2XD	C-C5-C6	-2.31	118.33	119.82
3	C	802[B]	2XD	C-C5-C6	-2.31	118.33	119.82
3	E	803[A]	2XD	C11-C12-N1	2.29	109.52	107.30
3	F	802	2XD	C3-C2-C1	2.25	123.02	120.24
3	G	803	2XD	C10-C9-N	2.23	117.55	111.83
3	G	803	2XD	O-C-C5	-2.19	117.65	121.71
3	H	802	2XD	C8-C7-C6	-2.15	117.72	119.72
3	D	802[B]	2XD	C11-C12-N1	2.09	109.32	107.30
3	D	802[B]	2XD	C14-C13-N2	2.07	127.62	124.72
3	C	802[A]	2XD	C14-C13-N2	2.07	127.62	124.72
3	D	802[A]	2XD	C11-C12-N1	2.05	109.29	107.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	802[A]	2XD	C7-C8-N-C14
2	E	802	EDO	O1-C1-C2-O2
2	F	801	EDO	O1-C1-C2-O2
2	A	801	EDO	O1-C1-C2-O2
2	H	801	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

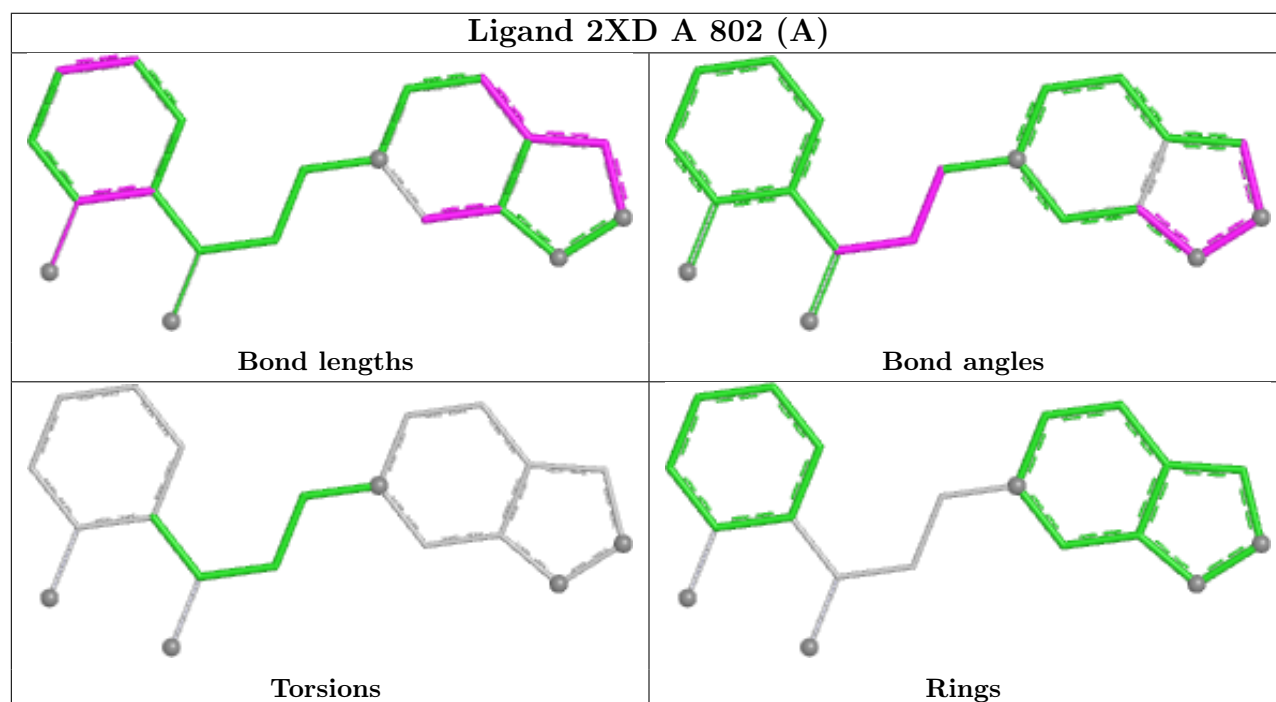
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802[B]	2XD	1	0

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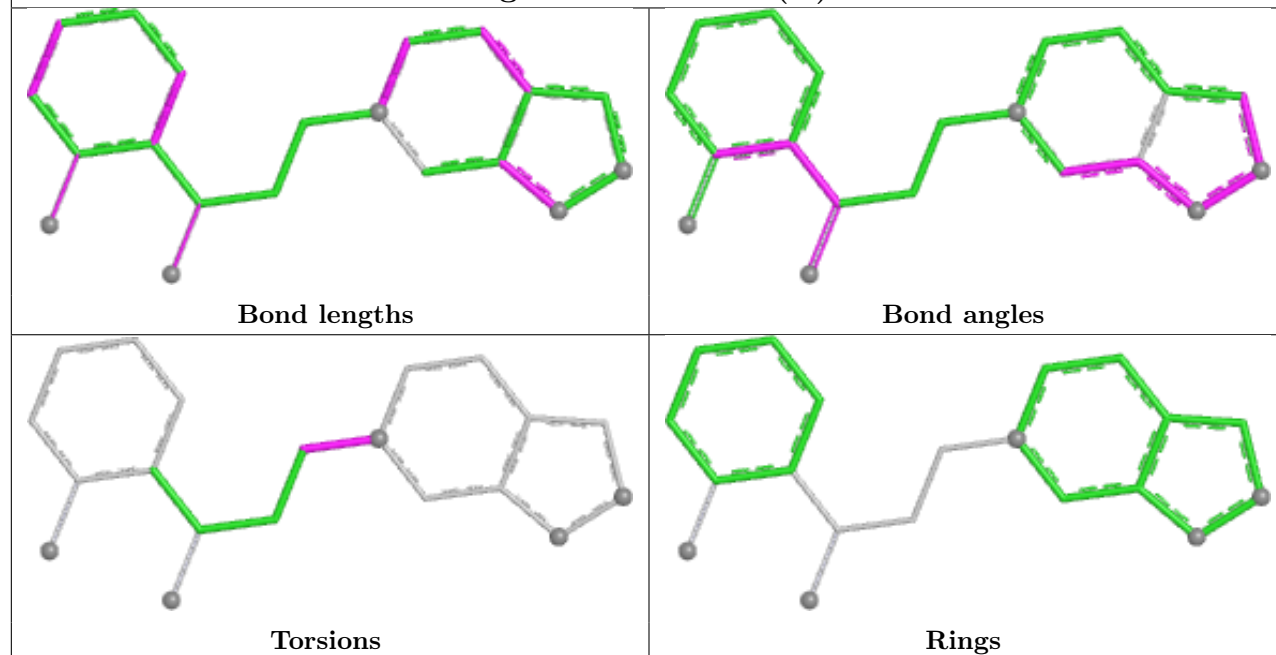
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	802	EDO	1	0
3	D	802[A]	2XD	1	0

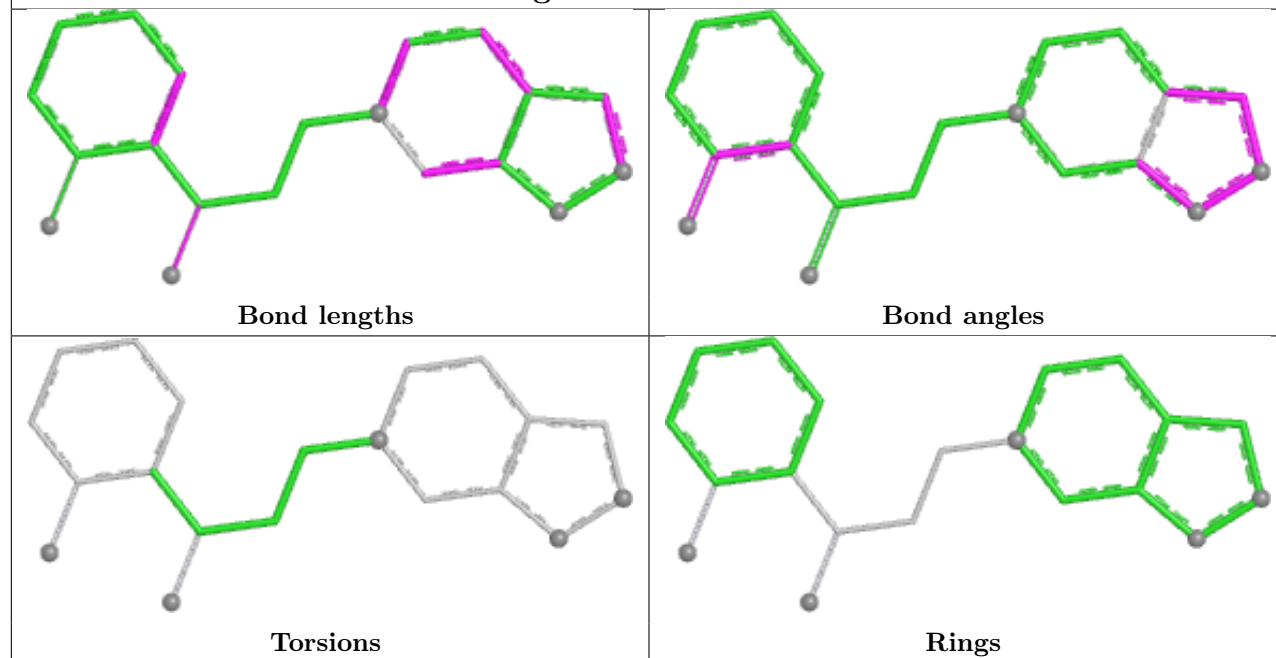
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



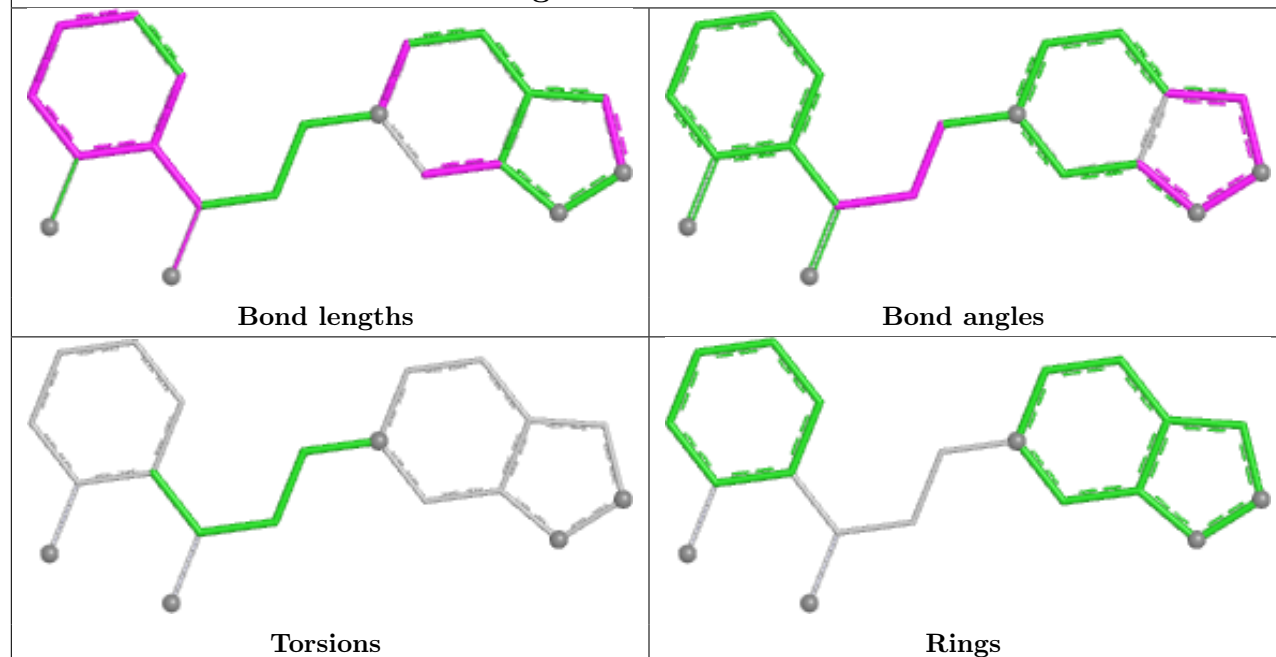
Ligand 2XD C 802 (A)



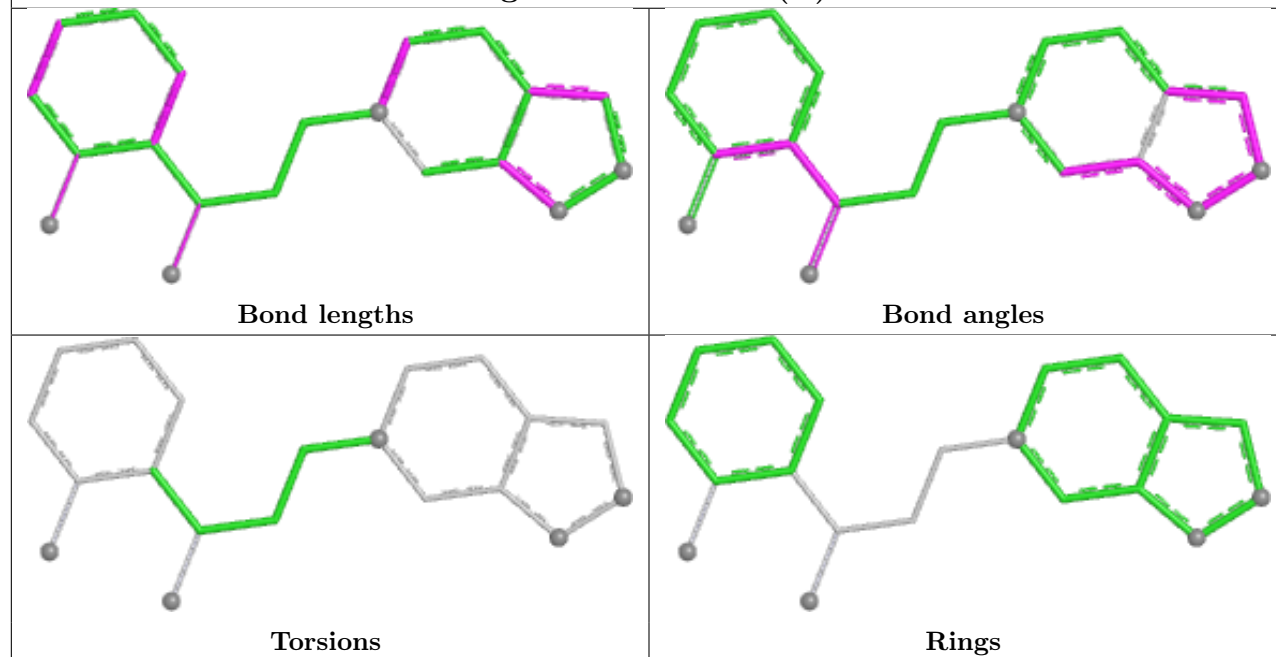
Ligand 2XD B 801



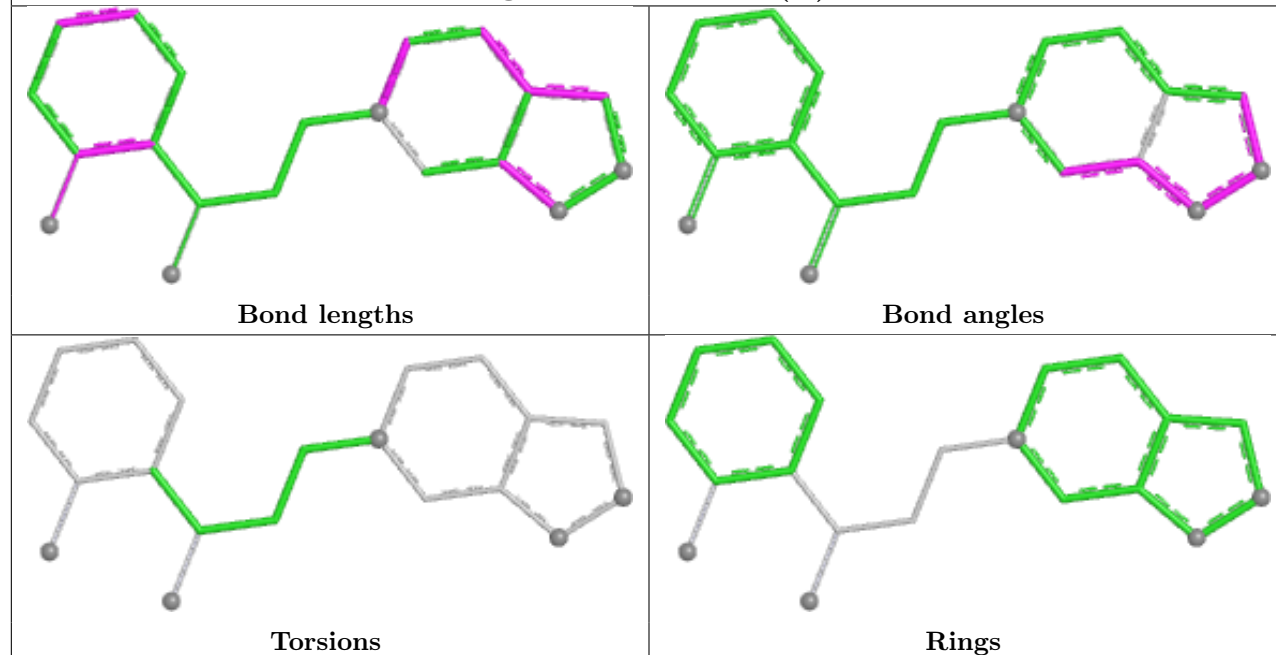
Ligand 2XD H 802



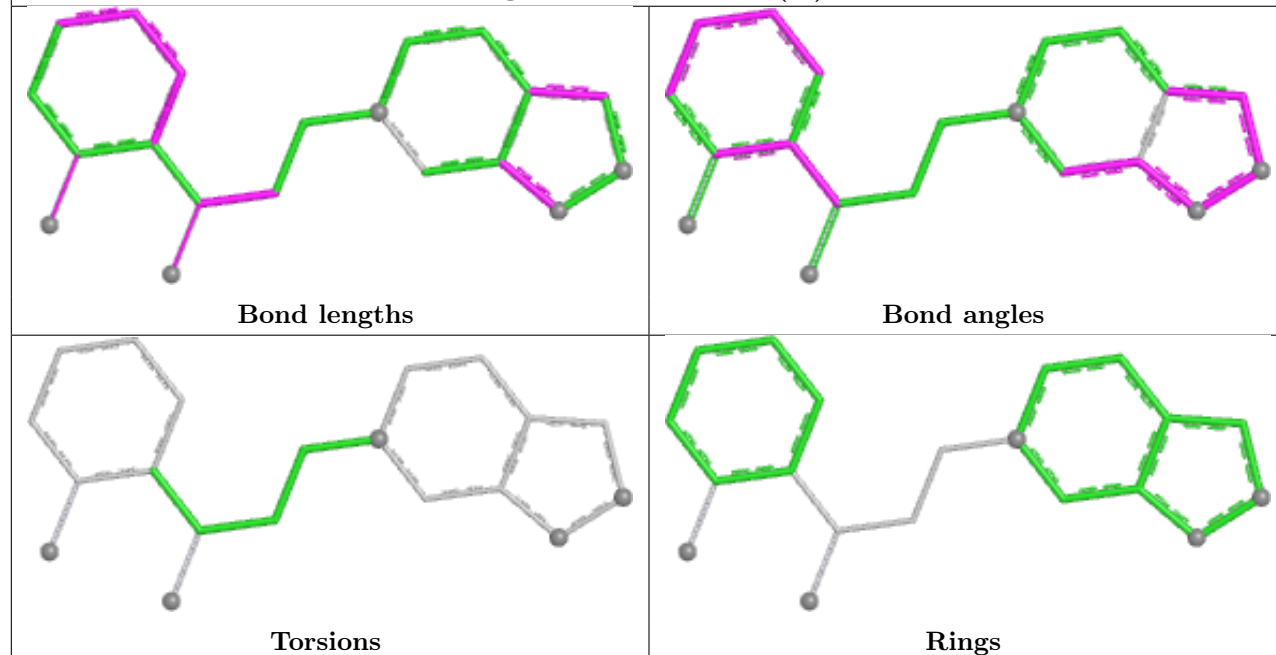
Ligand 2XD C 802 (B)



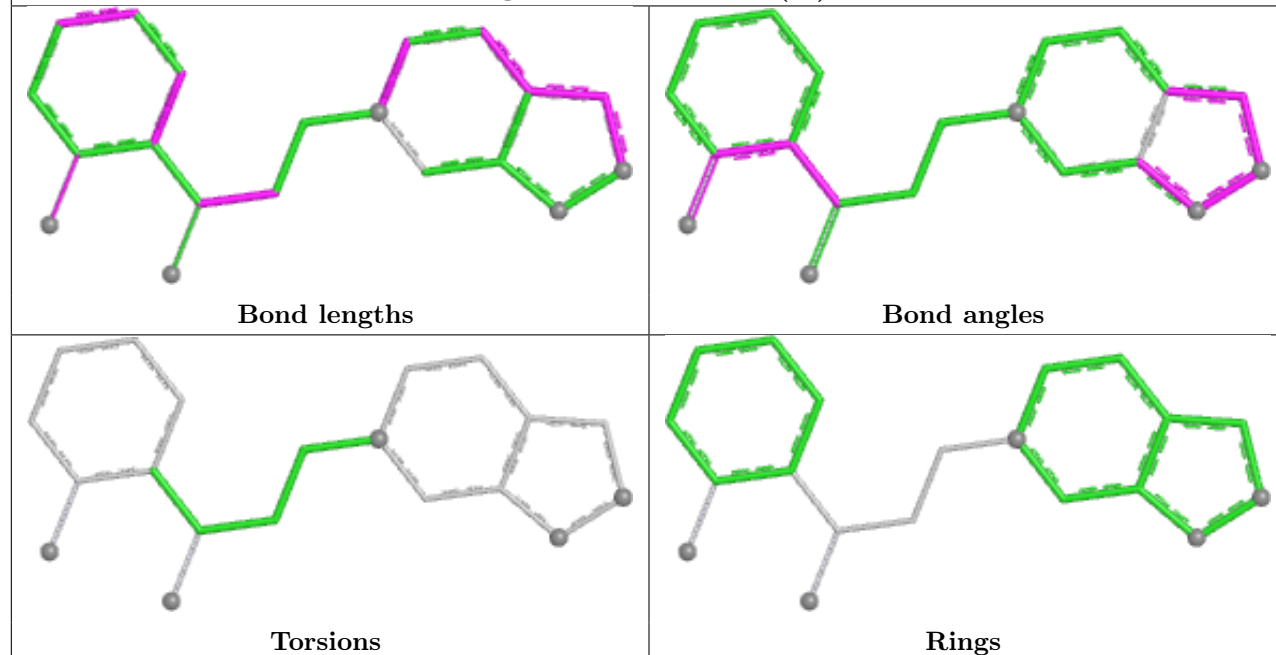
Ligand 2XD A 802 (B)



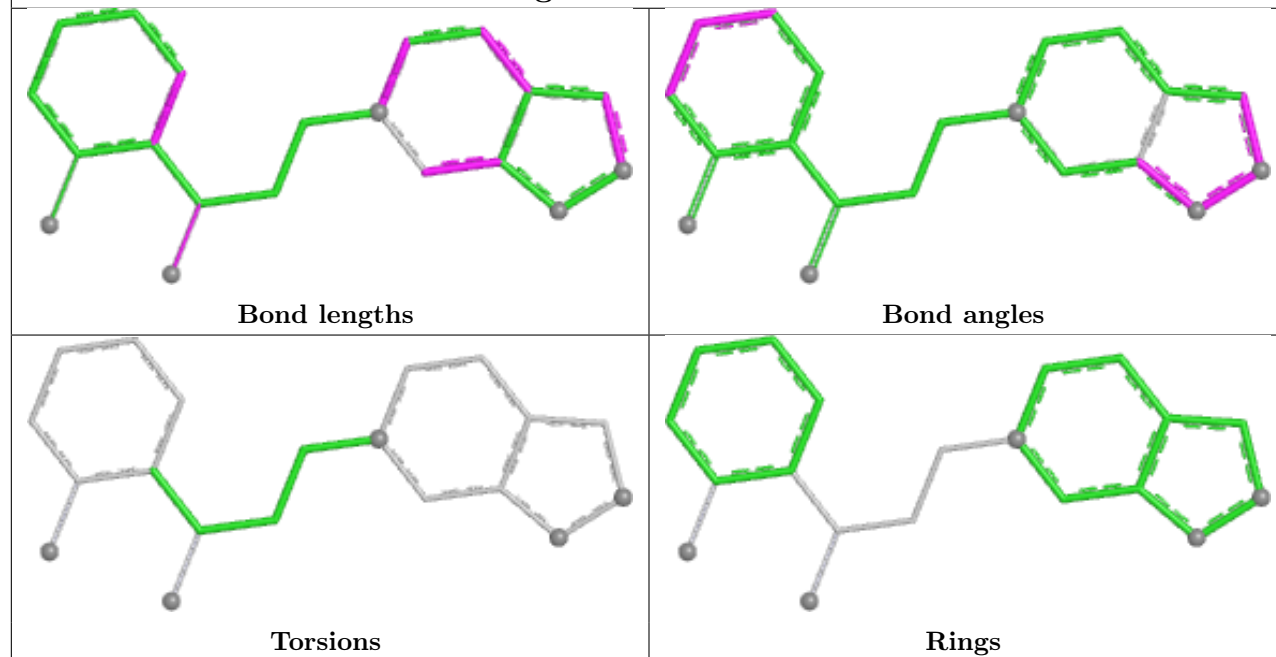
Ligand 2XD E 803 (B)



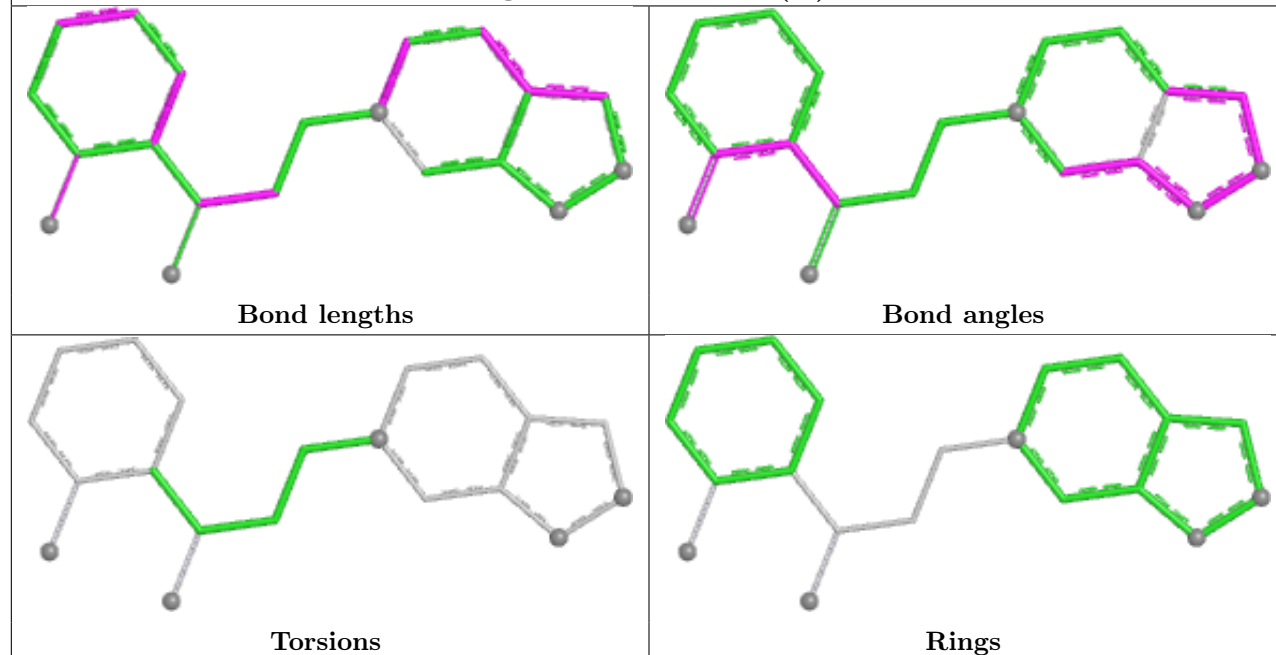
Ligand 2XD D 802 (A)



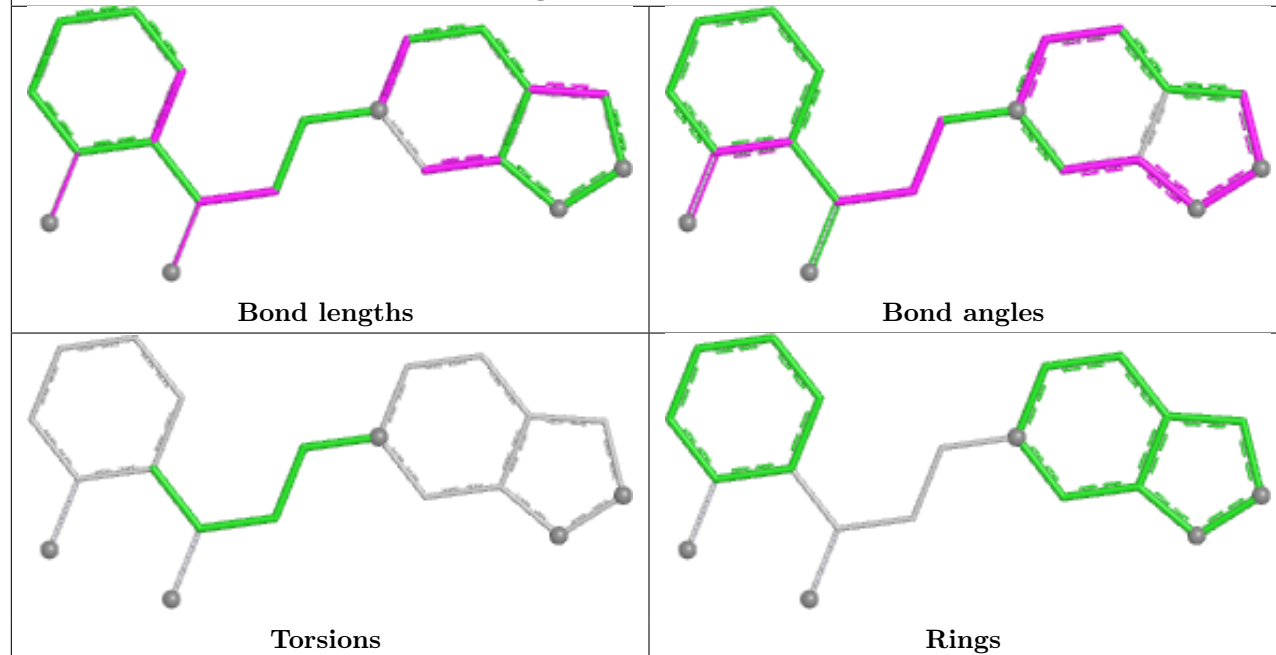
Ligand 2XD F 802

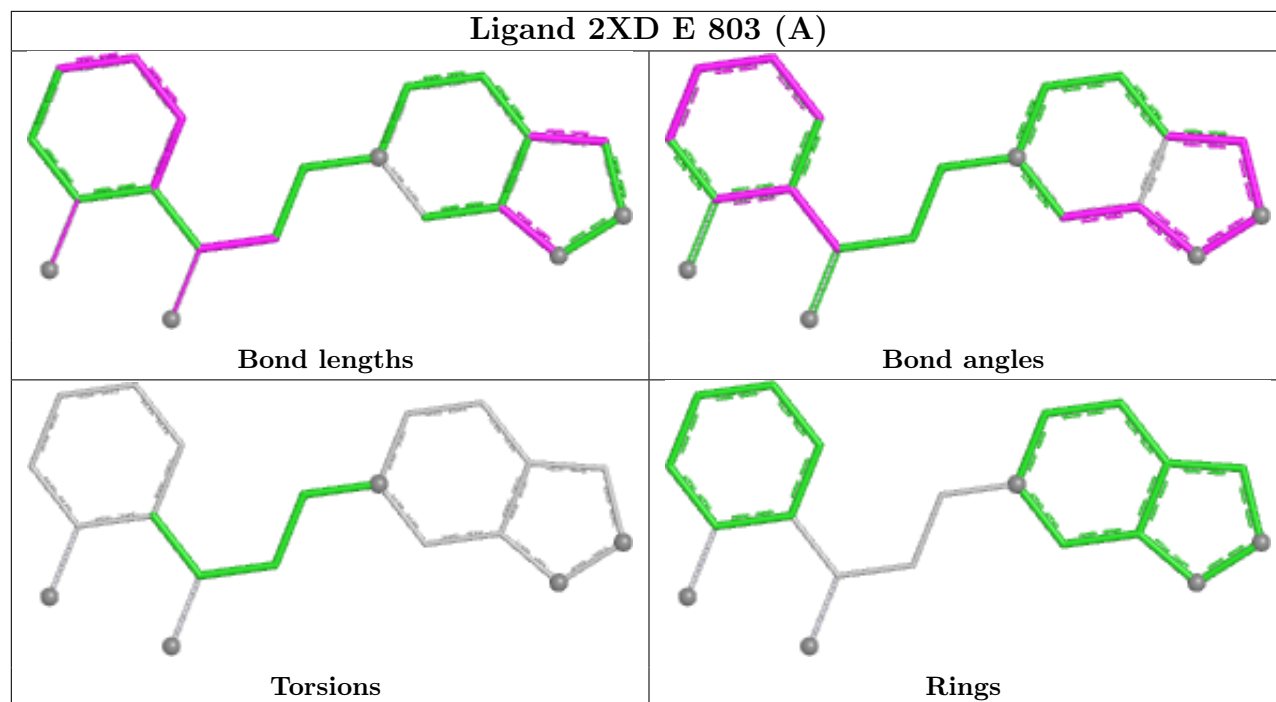


Ligand 2XD D 802 (B)



Ligand 2XD G 803





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	113/145 (77%)	-1.29	0 100 100	12, 26, 54, 72	2 (1%)
1	B	111/145 (76%)	-1.24	0 100 100	16, 29, 64, 72	0
1	C	111/145 (76%)	-1.26	0 100 100	14, 29, 57, 75	2 (1%)
1	D	112/145 (77%)	-1.28	0 100 100	11, 27, 60, 75	2 (1%)
1	E	113/145 (77%)	-1.35	0 100 100	12, 23, 53, 70	3 (2%)
1	F	112/145 (77%)	-1.27	0 100 100	15, 28, 56, 72	0
1	G	112/145 (77%)	-1.34	0 100 100	12, 24, 49, 66	1 (0%)
1	H	111/145 (76%)	-1.34	0 100 100	13, 25, 47, 64	1 (0%)
All	All	895/1160 (77%)	-1.30	0 100 100	11, 27, 56, 75	11 (1%)

There are no RSRZ outliers to report.

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](#)

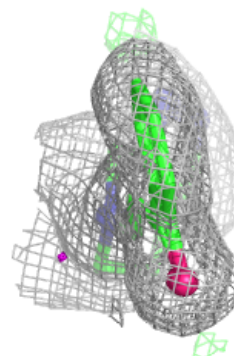
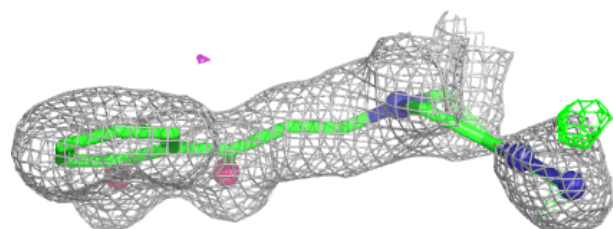
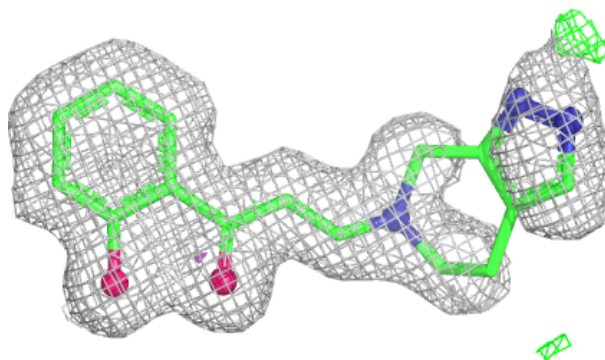
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
2	EDO	C	801	4/4	0.99	0.04	32,35,35,39	0
2	EDO	D	801	4/4	0.99	0.03	22,24,26,28	0
2	EDO	E	802	4/4	0.99	0.04	29,30,35,59	0
2	EDO	G	802	4/4	0.99	0.03	20,21,32,35	0
2	EDO	H	801	4/4	0.99	0.04	23,29,30,33	0
3	2XD	C	802[A]	20/20	0.99	0.04	19,28,44,50	10
3	2XD	C	802[B]	20/20	0.99	0.04	19,25,34,41	10
3	2XD	D	802[A]	20/20	0.99	0.03	13,20,30,32	10
3	2XD	D	802[B]	20/20	0.99	0.03	13,20,38,39	10
3	2XD	E	803[A]	20/20	0.99	0.03	12,16,24,24	10
3	2XD	E	803[B]	20/20	0.99	0.03	12,17,34,49	10
3	2XD	F	802	20/20	0.99	0.03	14,18,21,22	0
2	EDO	F	801	4/4	1.00	0.03	22,33,39,41	0
2	EDO	G	801	4/4	1.00	0.02	19,25,26,29	0
2	EDO	E	801	4/4	1.00	0.02	19,21,21,24	0
2	EDO	A	801	4/4	1.00	0.02	13,17,17,18	0
3	2XD	A	802[A]	20/20	1.00	0.03	13,17,24,34	10
3	2XD	A	802[B]	20/20	1.00	0.03	13,19,35,41	10
3	2XD	B	801	20/20	1.00	0.02	13,17,22,23	0
3	2XD	G	803	20/20	1.00	0.02	11,17,28,30	0
3	2XD	H	802	20/20	1.00	0.02	10,16,19,19	0

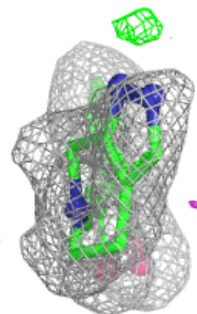
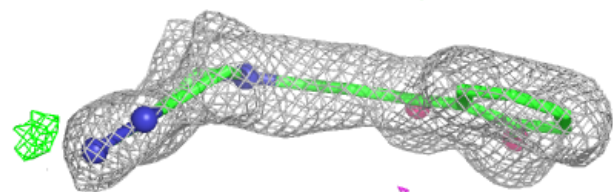
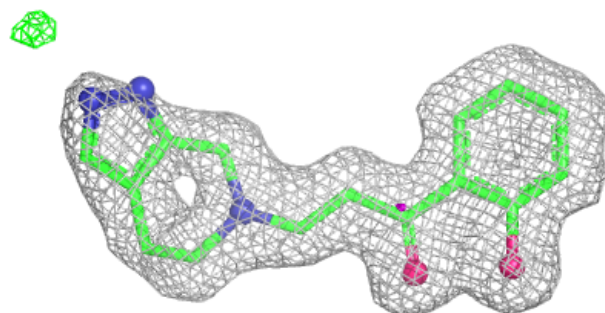
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2XD C 802 (A):

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

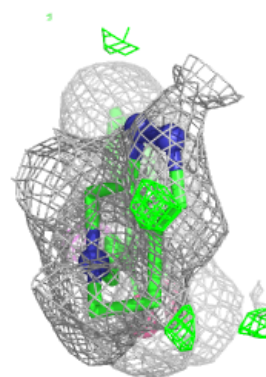
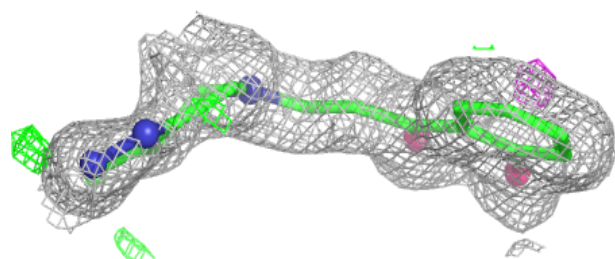
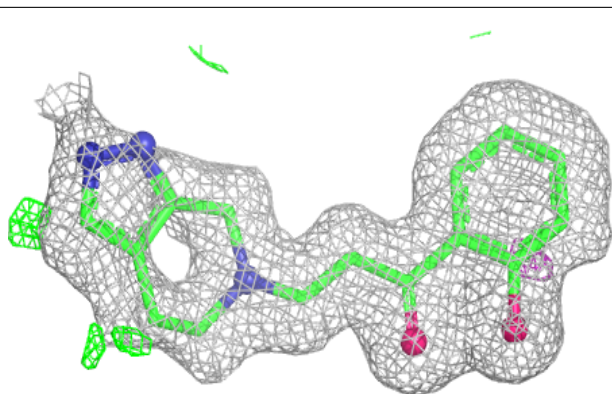
**Electron density around 2XD C 802 (B):**

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

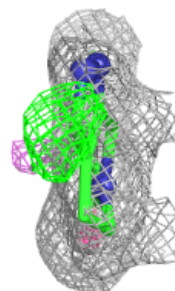
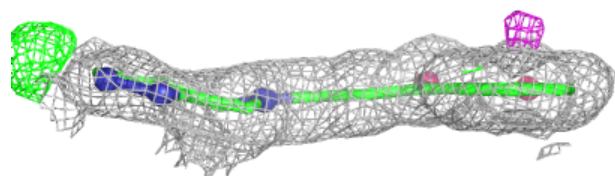
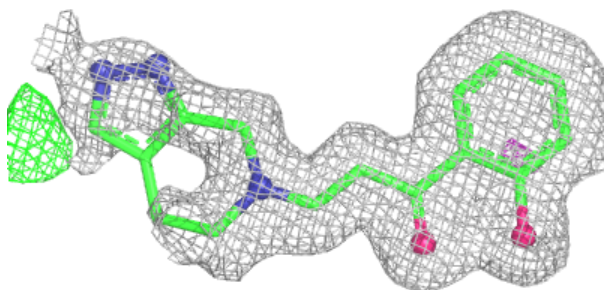


Electron density around 2XD D 802 (A):

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

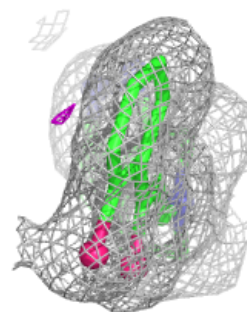
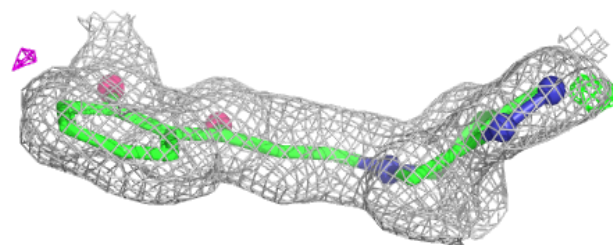
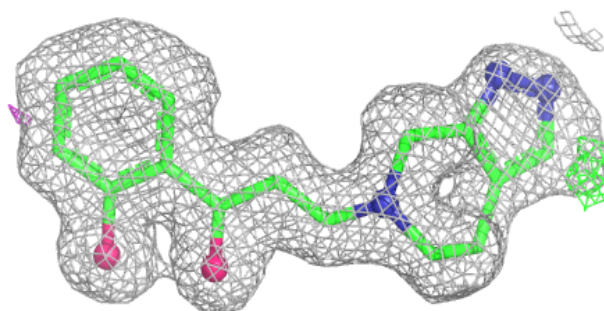
**Electron density around 2XD D 802 (B):**

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

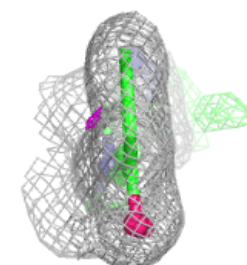
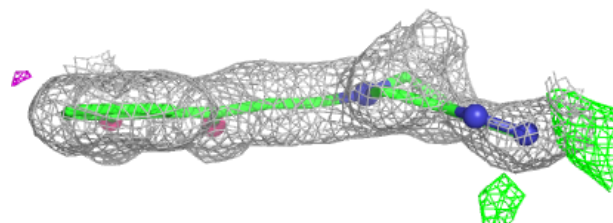
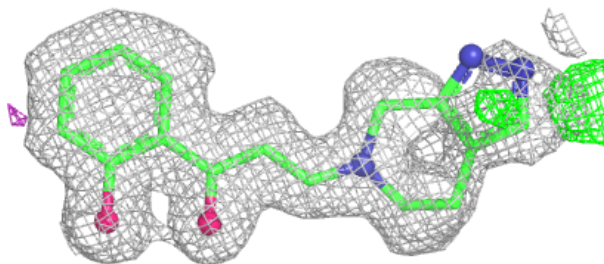


Electron density around 2XD E 803 (A):

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

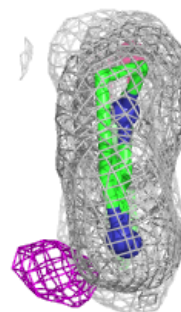
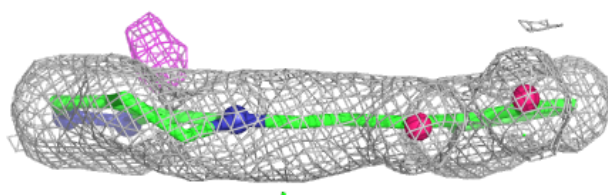
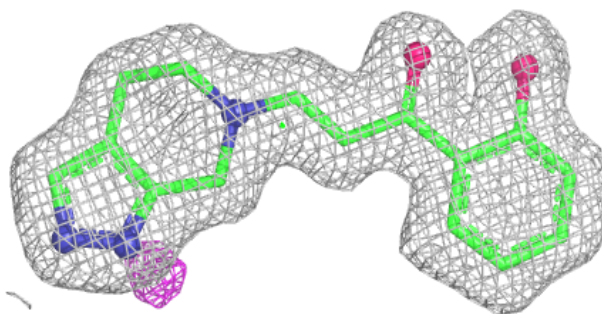
**Electron density around 2XD E 803 (B):**

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and green (positive)

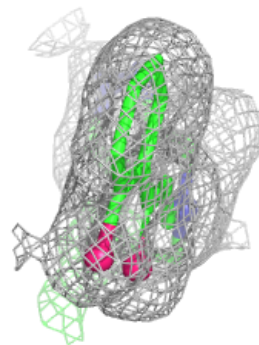
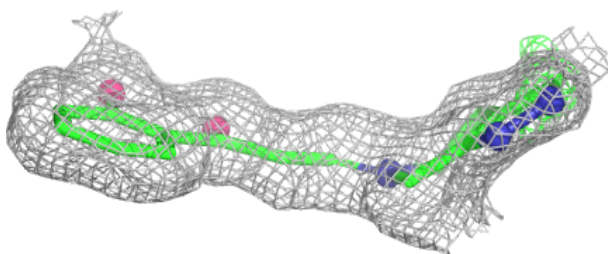
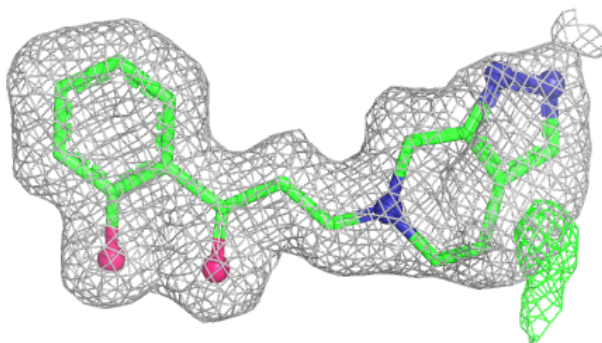


Electron density around 2XD F 802:

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and green (positive)

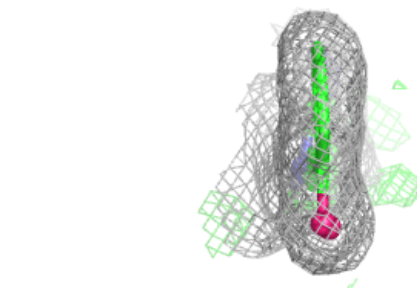
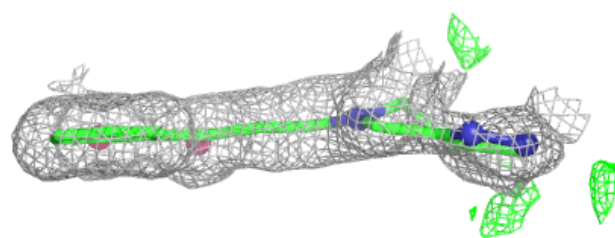
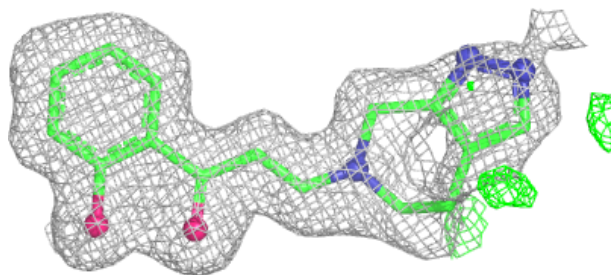
**Electron density around 2XD A 802 (A):**

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

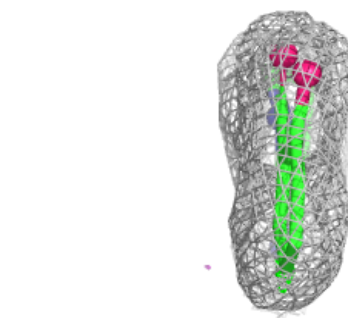
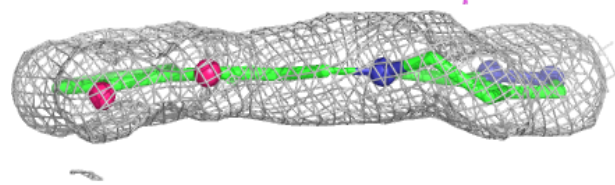
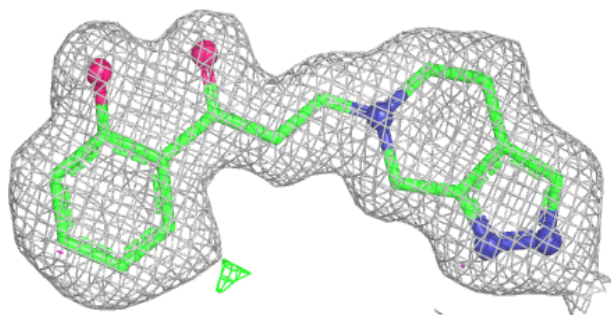


Electron density around 2XD A 802 (B):

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

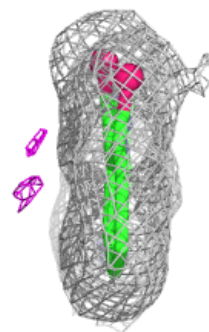
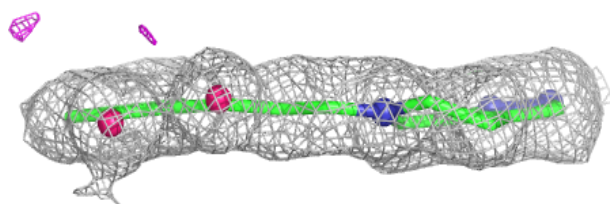
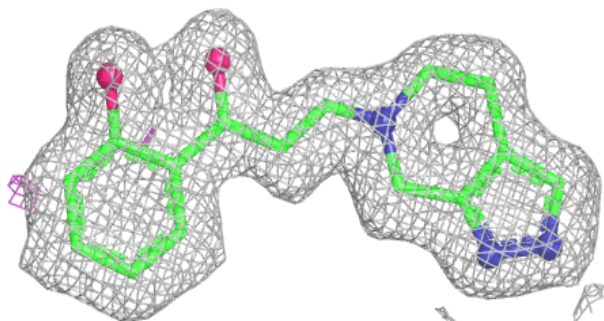
**Electron density around 2XD B 801:**

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

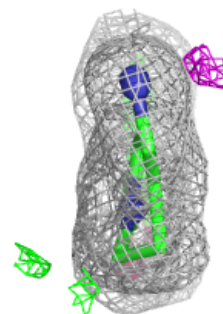
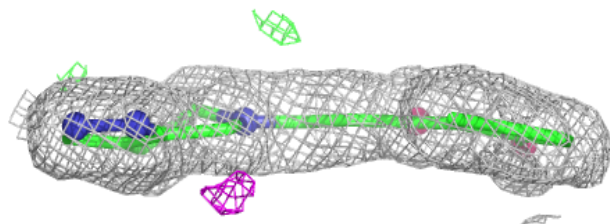
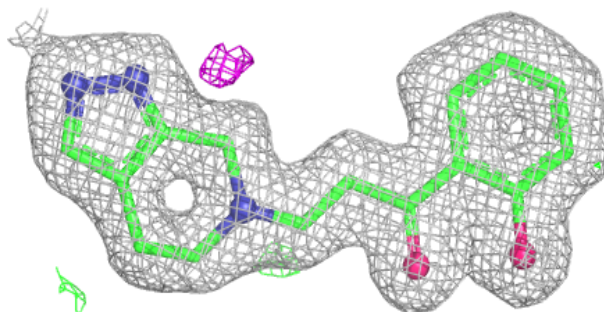


Electron density around 2XD G 803:

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

**Electron density around 2XD H 802:**

$2mF_o-DF_c$ (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.