



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 02:19 PM JST

PDB ID : 9VMB / pdb\_00009vmb  
Title : The X-RAY co-crystal structure of human FGFR3 and Compound 10t  
Authors : Chen, X.J.; Liu, X.R.; Zhang, L.  
Deposited on : 2025-06-27  
Resolution : 1.97 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](mailto: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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
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

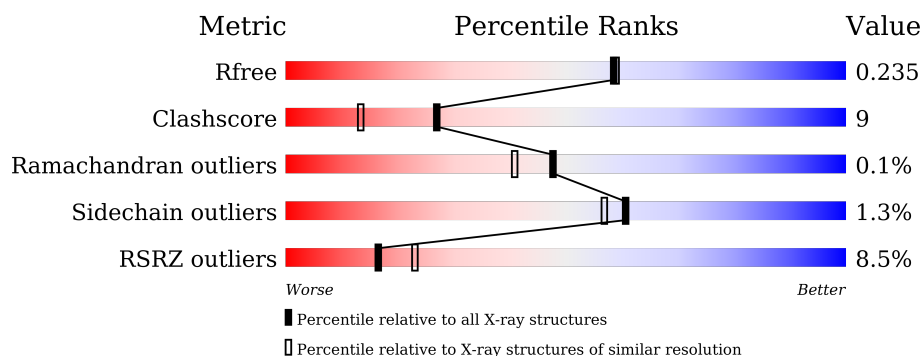
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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  $\geq 3$ , 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	292	<div> <div>8%</div> <div>81% 16% ..</div> </div>
1	B	292	<div> <div>7%</div> <div>82% 15% ..</div> </div>
1	C	292	<div> <div>9%</div> <div>78% 19% ..</div> </div>
1	D	292	<div> <div>10%</div> <div>82% 14% .</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	C	803	-	-	X	-
4	GOL	D	803	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9909 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 Fibroblast growth factor receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	1	0
			2273	1447	393	414	19			
1	B	287	Total	C	N	O	S	0	1	0
			2277	1449	393	416	19			
1	C	286	Total	C	N	O	S	0	1	0
			2268	1444	392	413	19			
1	D	281	Total	C	N	O	S	0	1	0
			2231	1419	387	406	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	453	GLY	-	expression tag	UNP P22607
A	454	PRO	-	expression tag	UNP P22607
A	584	SER	PRO	conflict	UNP P22607
A	585	GLY	PRO	conflict	UNP P22607
A	?	-	GLY	deletion	UNP P22607
A	?	-	LEU	deletion	UNP P22607
A	?	-	ASP	deletion	UNP P22607
A	?	-	TYR	deletion	UNP P22607
A	?	-	SER	deletion	UNP P22607
A	?	-	PHE	deletion	UNP P22607
A	?	-	ASP	deletion	UNP P22607
A	?	-	THR	deletion	UNP P22607
A	?	-	CYS	deletion	UNP P22607
A	?	-	LYS	deletion	UNP P22607
A	?	-	PRO	deletion	UNP P22607
A	?	-	PRO	deletion	UNP P22607
B	453	GLY	-	expression tag	UNP P22607
B	454	PRO	-	expression tag	UNP P22607
B	584	SER	PRO	conflict	UNP P22607
B	585	GLY	PRO	conflict	UNP P22607
B	?	-	GLY	deletion	UNP P22607

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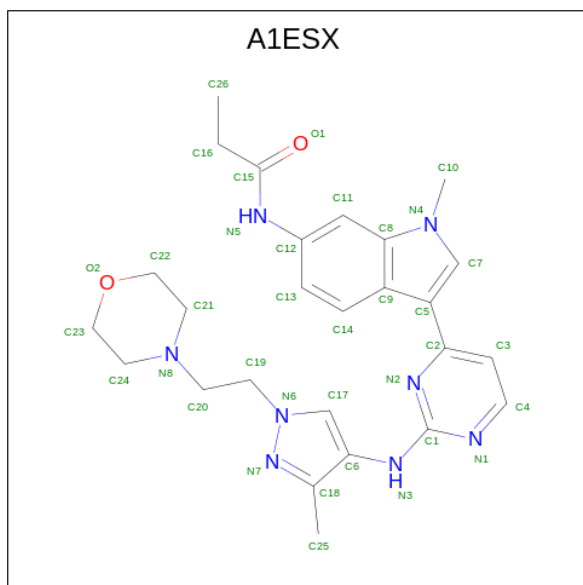
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P22607
B	?	-	ASP	deletion	UNP P22607
B	?	-	TYR	deletion	UNP P22607
B	?	-	SER	deletion	UNP P22607
B	?	-	PHE	deletion	UNP P22607
B	?	-	ASP	deletion	UNP P22607
B	?	-	THR	deletion	UNP P22607
B	?	-	CYS	deletion	UNP P22607
B	?	-	LYS	deletion	UNP P22607
B	?	-	PRO	deletion	UNP P22607
B	?	-	PRO	deletion	UNP P22607
C	453	GLY	-	expression tag	UNP P22607
C	454	PRO	-	expression tag	UNP P22607
C	584	SER	PRO	conflict	UNP P22607
C	585	GLY	PRO	conflict	UNP P22607
C	?	-	GLY	deletion	UNP P22607
C	?	-	LEU	deletion	UNP P22607
C	?	-	ASP	deletion	UNP P22607
C	?	-	TYR	deletion	UNP P22607
C	?	-	SER	deletion	UNP P22607
C	?	-	PHE	deletion	UNP P22607
C	?	-	ASP	deletion	UNP P22607
C	?	-	THR	deletion	UNP P22607
C	?	-	CYS	deletion	UNP P22607
C	?	-	LYS	deletion	UNP P22607
C	?	-	PRO	deletion	UNP P22607
C	?	-	PRO	deletion	UNP P22607
D	453	GLY	-	expression tag	UNP P22607
D	454	PRO	-	expression tag	UNP P22607
D	584	SER	PRO	conflict	UNP P22607
D	585	GLY	PRO	conflict	UNP P22607
D	?	-	GLY	deletion	UNP P22607
D	?	-	LEU	deletion	UNP P22607
D	?	-	ASP	deletion	UNP P22607
D	?	-	TYR	deletion	UNP P22607
D	?	-	SER	deletion	UNP P22607
D	?	-	PHE	deletion	UNP P22607
D	?	-	ASP	deletion	UNP P22607
D	?	-	THR	deletion	UNP P22607
D	?	-	CYS	deletion	UNP P22607
D	?	-	LYS	deletion	UNP P22607
D	?	-	PRO	deletion	UNP P22607

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P22607

- Molecule 2 is {N}-[1-methyl-3-[2-[[3-methyl-1-(2-morpholin-4-ylethyl)pyrazol-4-yl]amino]pyrimidin-4-yl]indol-6-yl]propanamide (CCD ID: A1ESX) (formula: C<sub>26</sub>H<sub>32</sub>N<sub>8</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

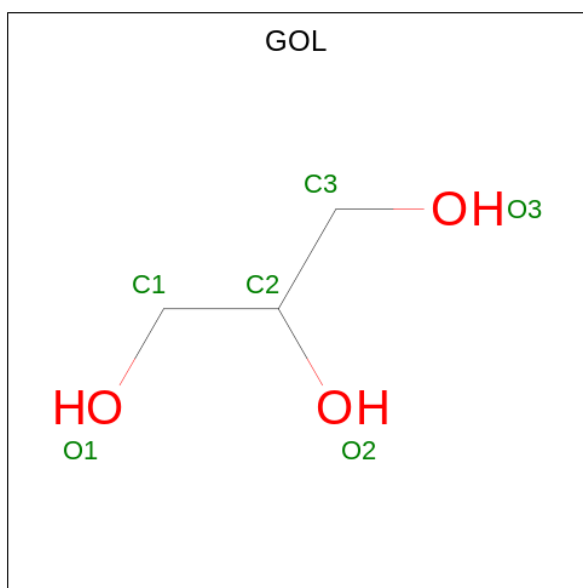


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	26	8	2		
2	B	1	Total	C	N	O	0	0
			36	26	8	2		
2	C	1	Total	C	N	O	0	0
			36	26	8	2		
2	D	1	Total	C	N	O	0	0
			36	26	8	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

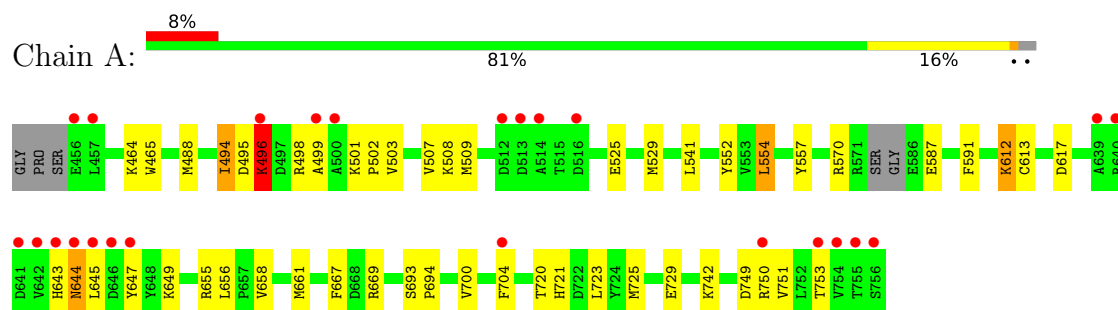
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	166	Total	O	0	0
			166	166		
5	B	185	Total	O	0	0
			185	185		
5	C	182	Total	O	0	0
			182	182		
5	D	161	Total	O	0	0
			161	161		

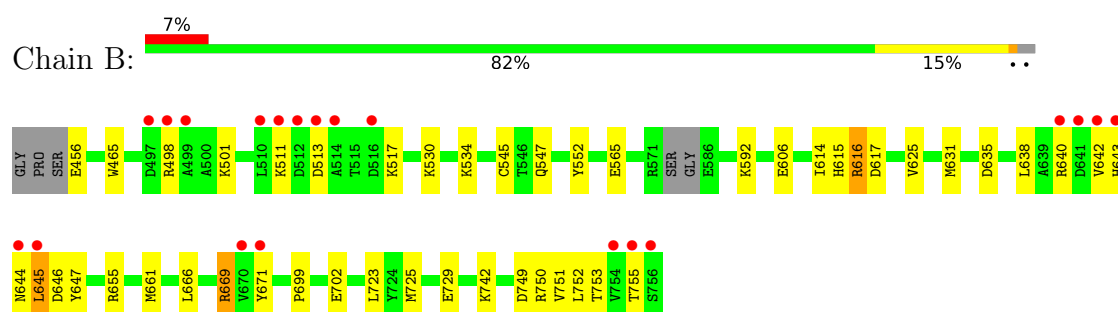
### 3 Residue-property plots [i](#)

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.

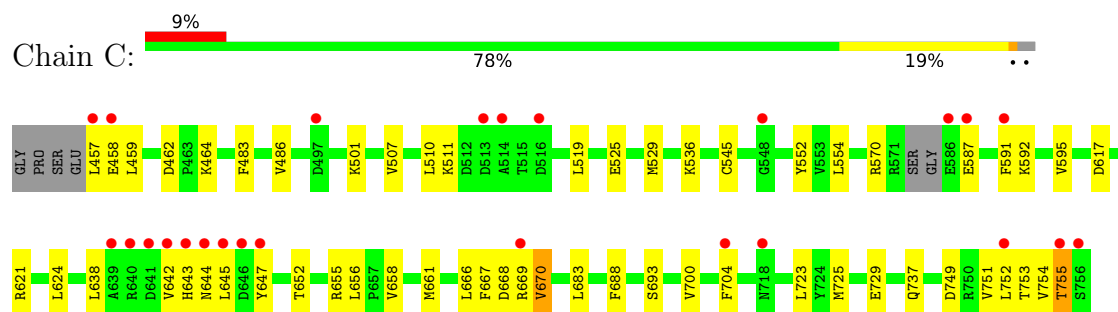
#### • Molecule 1: Fibroblast growth factor receptor 3



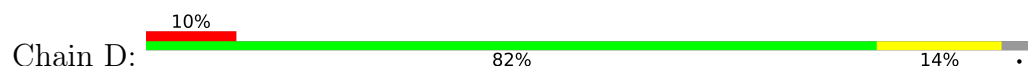
#### • Molecule 1: Fibroblast growth factor receptor 3



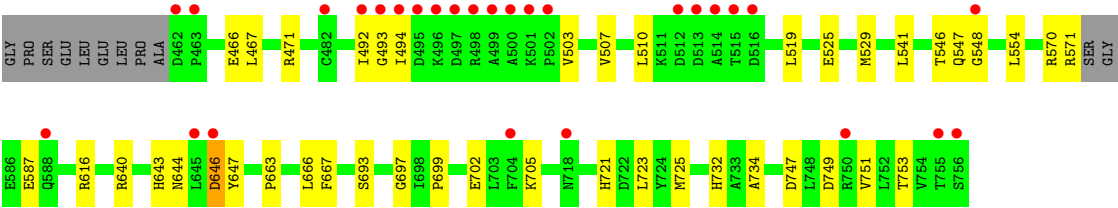
#### • Molecule 1: Fibroblast growth factor receptor 3



#### • Molecule 1: Fibroblast growth factor receptor 3







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.34Å 112.84Å 87.52Å 90.00° 94.93° 90.00°	Depositor
Resolution (Å)	19.10 – 1.97 19.10 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.10-1.97) 99.5 (19.10-1.97)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.187 , 0.237 0.187 , 0.235	Depositor DCC
$R_{free}$ test set	3896 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, A1ESX

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	0.47	2/2322 (0.1%)	0.60	1/3138 (0.0%)
1	B	0.42	3/2326 (0.1%)	0.59	0/3143
1	C	0.29	0/2317	0.55	0/3131
1	D	0.39	0/2279	0.57	1/3078 (0.0%)
All	All	0.40	5/9244 (0.1%)	0.58	2/12490 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	616	ARG	C-O	-7.38	1.14	1.24
1	B	614	ILE	C-O	-6.04	1.17	1.24
1	B	615	HIS	C-O	-5.85	1.17	1.24
1	A	613	CYS	C-O	-5.70	1.17	1.24
1	A	499	ALA	C-O	-5.04	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	548	GLY	N-CA-C	5.49	126.19	113.18
1	A	496	LYS	N-CA-C	5.25	117.75	111.71

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	2273	0	2287	45	0
1	B	2277	0	2291	45	0
1	C	2268	0	2285	50	0
1	D	2231	0	2245	33	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	1	0
2	D	36	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	0	0
4	C	6	0	8	5	0
4	D	6	0	8	5	0
5	A	166	0	0	5	0
5	B	185	0	0	4	0
5	C	182	0	0	3	0
5	D	161	0	0	9	0
All	All	9909	0	9132	168	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 9.

All (168) 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:496:LYS:HE3	1:B:534:LYS:O	1.65	0.97
1:A:529:MET:HE2	1:A:541:LEU:HB2	1.51	0.91
1:C:693:SER:H	4:D:803:GOL:H31	1.33	0.89
1:D:571:ARG:HH22	4:D:803:GOL:H11	1.36	0.89
1:B:617:ASP:OD2	1:B:655:ARG:NH2	2.05	0.88
1:C:621:ARG:HH12	4:C:803:GOL:H2	1.37	0.87
1:A:496:LYS:NZ	5:A:901:HOH:O	2.06	0.87
1:B:725:MET:HA	1:B:725:MET:HE2	1.61	0.82
1:D:663:PRO:O	5:D:901:HOH:O	2.00	0.79
1:B:645:LEU:H	1:B:645:LEU:HD12	1.47	0.77
1:A:750:ARG:NH1	5:A:902:HOH:O	2.17	0.77
1:D:747:ASP:OD2	5:D:902:HOH:O	2.02	0.77
1:D:732:HIS:HD2	1:D:734:ALA:H	1.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:ASP:CG	1:B:655:ARG:HH22	1.93	0.76
1:A:612:LYS:N	1:A:612:LYS:HD2	2.00	0.76
1:B:606:GLU:HG3	1:B:742:LYS:HD3	1.69	0.75
1:B:669:ARG:HH11	1:B:669:ARG:HG3	1.53	0.73
1:C:751:VAL:O	1:C:755:THR:OG1	2.05	0.73
1:C:617:ASP:OD2	1:C:655:ARG:NH2	2.23	0.71
1:A:617:ASP:OD2	1:A:655:ARG:NH2	2.24	0.70
1:B:498:ARG:HG2	1:B:501:LYS:HB2	1.74	0.70
1:A:494:ILE:HG22	1:A:503:VAL:HG11	1.73	0.69
1:B:456:GLU:N	5:B:902:HOH:O	2.26	0.68
1:C:525:GLU:HG2	1:C:529:MET:HE2	1.73	0.68
1:D:705:LYS:NZ	5:D:905:HOH:O	2.22	0.68
1:A:645:LEU:HD11	1:A:649:LYS:HE3	1.74	0.67
1:A:643:HIS:HB3	1:A:647:TYR:CG	2.29	0.67
1:C:617:ASP:CG	1:C:655:ARG:HH22	2.03	0.66
1:A:494:ILE:HG22	1:A:503:VAL:CG1	2.27	0.65
1:D:723:LEU:HD21	1:D:751:VAL:HG11	1.78	0.65
1:D:667:PHE:N	5:D:901:HOH:O	2.30	0.64
1:A:498:ARG:HG3	1:A:498:ARG:HH11	1.62	0.64
1:B:640:ARG:NH1	1:B:671:TYR:HD1	1.96	0.63
1:A:570:ARG:NH2	1:A:587:GLU:OE2	2.31	0.63
1:A:617:ASP:CG	1:A:655:ARG:HH22	2.07	0.62
1:B:725:MET:O	1:B:729:GLU:HG3	1.98	0.62
1:A:496:LYS:CE	1:B:534:LYS:O	2.45	0.62
1:A:525:GLU:O	1:A:529:MET:HG3	2.00	0.61
1:A:658:VAL:HA	1:A:661:MET:HG3	1.80	0.61
1:A:725:MET:O	1:A:729:GLU:HG3	2.01	0.61
1:B:511:LYS:HE3	1:B:513:ASP:HB3	1.83	0.60
1:C:667:PHE:CZ	1:C:704:PHE:HB3	2.35	0.60
1:B:643:HIS:HB3	1:B:647:TYR:CG	2.36	0.60
1:A:507:VAL:HG22	1:A:554:LEU:HD22	1.83	0.60
1:D:467:LEU:HD22	1:D:554:LEU:HD11	1.83	0.59
1:B:723:LEU:HD21	1:B:751:VAL:HG11	1.84	0.59
1:C:643:HIS:HB3	1:C:647:TYR:CG	2.38	0.59
2:C:801:A1ESX:C5	4:C:803:GOL:H32	2.31	0.59
1:D:547:GLN:O	5:D:903:HOH:O	2.17	0.58
1:C:462:ASP:OD1	1:C:464:LYS:NZ	2.36	0.58
1:B:552:TYR:OH	5:B:901:HOH:O	2.15	0.58
1:B:616:ARG:HD3	1:B:640:ARG:HG3	1.86	0.58
1:D:507:VAL:HG22	1:D:554:LEU:HD22	1.86	0.57
1:D:587:GLU:OE1	5:D:904:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:ARG:HH11	1:B:669:ARG:CG	2.17	0.56
1:D:466:GLU:OE1	1:D:546:THR:OG1	2.20	0.56
1:C:725:MET:O	1:C:729:GLU:HG3	2.05	0.56
5:A:905:HOH:O	1:B:750:ARG:HD2	2.05	0.56
1:C:668:ASP:OD2	5:C:901:HOH:O	2.18	0.56
1:C:592:LYS:HZ2	1:C:755:THR:HB	1.71	0.56
1:C:624:LEU:HD21	4:C:803:GOL:H31	1.89	0.55
1:C:656:LEU:HD13	1:C:700:VAL:HG11	1.88	0.55
1:A:612:LYS:HD2	1:A:612:LYS:H	1.68	0.55
1:C:501:LYS:NZ	5:C:903:HOH:O	2.39	0.55
1:D:466:GLU:OE2	1:D:546:THR:N	2.31	0.55
1:D:529:MET:HE2	1:D:541:LEU:HB2	1.88	0.55
1:B:465:TRP:CD1	1:B:530:LYS:HE2	2.42	0.54
1:B:606:GLU:CG	1:B:742:LYS:HD3	2.37	0.54
1:D:616:ARG:HD2	5:D:932:HOH:O	2.08	0.54
1:A:508:LYS:NZ	5:A:910:HOH:O	2.40	0.53
1:A:667:PHE:CZ	1:A:704:PHE:HB3	2.43	0.53
1:C:595:VAL:HG22	1:C:723:LEU:HD11	1.90	0.53
1:D:494:ILE:HG22	1:D:503:VAL:HG11	1.90	0.53
1:B:592:LYS:HD3	1:B:755:THR:HG23	1.91	0.52
1:D:693:SER:H	4:D:803:GOL:H32	1.74	0.52
1:C:668:ASP:HB2	1:C:670:VAL:HG13	1.90	0.52
1:A:749:ASP:O	1:A:753:THR:HG23	2.10	0.52
1:B:749:ASP:O	1:B:753:THR:HG23	2.11	0.51
1:D:721:HIS:O	1:D:725:MET:HG2	2.10	0.51
1:C:457:LEU:HD12	1:C:458:GLU:N	2.26	0.51
1:C:638:LEU:HD22	1:C:642:VAL:HG11	1.92	0.51
1:B:545:CYS:HB2	1:B:552:TYR:HB2	1.94	0.50
1:A:509:MET:HE2	1:A:552:TYR:CE1	2.46	0.50
1:D:510:LEU:HD11	1:D:519:LEU:HD13	1.92	0.50
1:D:732:HIS:CD2	1:D:734:ALA:H	2.23	0.50
1:C:749:ASP:O	1:C:753:THR:HG23	2.12	0.49
1:D:525:GLU:O	1:D:529:MET:HG3	2.13	0.49
1:A:498:ARG:HG3	1:A:498:ARG:NH1	2.28	0.49
1:D:570:ARG:HG2	1:D:587:GLU:O	2.13	0.49
1:A:750:ARG:HG3	1:A:751:VAL:N	2.27	0.48
1:B:640:ARG:HH12	1:B:671:TYR:H	1.60	0.48
1:B:534:LYS:N	1:B:534:LYS:HD2	2.28	0.48
1:B:638:LEU:HD22	1:B:642:VAL:HG11	1.95	0.48
1:A:742:LYS:HD3	1:B:753:THR:O	2.14	0.48
1:A:591:PHE:HZ	1:A:723:LEU:HD12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:LEU:HD13	1:A:700:VAL:HG11	1.95	0.47
1:D:749:ASP:O	1:D:753:THR:HG23	2.13	0.47
1:B:644:ASN:O	1:B:647:TYR:HB3	2.14	0.47
1:A:667:PHE:HZ	1:A:704:PHE:HB3	1.77	0.47
1:B:725:MET:HA	1:B:725:MET:CE	2.39	0.47
1:C:688:PHE:CZ	1:C:723:LEU:HD13	2.48	0.47
1:C:644:ASN:O	1:C:647:TYR:HB3	2.14	0.47
1:C:483:PHE:O	1:C:511:LYS:HD2	2.14	0.47
1:C:656:LEU:HG	1:D:697:GLY:O	2.13	0.47
1:B:645:LEU:HD23	1:B:669:ARG:HD3	1.96	0.47
1:C:510:LEU:HD11	1:C:519:LEU:HD13	1.97	0.47
1:A:742:LYS:NZ	5:A:917:HOH:O	2.48	0.47
1:B:640:ARG:NH2	1:C:737:GLN:HE22	2.13	0.47
1:C:592:LYS:NZ	1:C:752:LEU:O	2.43	0.47
1:C:570:ARG:HG2	1:C:587:GLU:O	2.15	0.46
1:C:658:VAL:HG22	1:C:704:PHE:CE2	2.50	0.46
1:D:666:LEU:HB3	5:D:901:HOH:O	2.14	0.46
1:D:644:ASN:HB3	1:D:646:ASP:H	1.80	0.46
1:A:495:ASP:CG	1:A:501:LYS:HD2	2.41	0.46
1:C:536:LYS:HE3	1:C:536:LYS:HB2	1.74	0.46
1:D:643:HIS:HB3	1:D:647:TYR:HB2	1.98	0.45
1:D:471:ARG:NE	1:D:492:ILE:O	2.49	0.45
1:A:496:LYS:HE3	5:B:962:HOH:O	2.17	0.45
1:C:591:PHE:CZ	1:C:723:LEU:HD12	2.51	0.45
1:B:640:ARG:HH21	1:C:737:GLN:NE2	2.15	0.45
1:C:643:HIS:HB3	1:C:647:TYR:CD2	2.52	0.45
1:C:624:LEU:CD2	4:C:803:GOL:H31	2.46	0.44
1:C:725:MET:HE3	1:C:725:MET:HB3	1.86	0.44
1:B:699:PRO:HG2	1:B:702:GLU:OE1	2.17	0.44
1:D:640:ARG:NH1	5:D:910:HOH:O	2.40	0.44
1:B:517:LYS:N	1:B:517:LYS:HD3	2.30	0.44
1:B:643:HIS:HB3	1:B:647:TYR:CD2	2.53	0.44
1:C:658:VAL:HG22	1:C:704:PHE:HE2	1.83	0.44
1:B:661:MET:HE2	1:B:661:MET:HB3	1.85	0.43
1:C:621:ARG:NH1	4:C:803:GOL:H2	2.17	0.43
1:B:640:ARG:NH2	1:C:737:GLN:NE2	2.67	0.43
1:A:494:ILE:CG2	1:A:503:VAL:HG11	2.46	0.43
1:A:721:HIS:O	1:A:725:MET:HG2	2.18	0.43
1:C:545:CYS:HB2	1:C:552:TYR:HB2	2.01	0.43
1:C:525:GLU:O	1:C:529:MET:HG3	2.18	0.43
1:A:587:GLU:H	1:A:587:GLU:HG2	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ASN:O	1:A:647:TYR:HB3	2.18	0.43
1:B:752:LEU:HA	1:B:755:THR:HG22	2.01	0.43
1:D:471:ARG:NH2	1:D:493:GLY:O	2.52	0.43
1:C:661:MET:HE1	1:C:666:LEU:HA	2.01	0.43
1:A:591:PHE:CZ	1:A:723:LEU:HD12	2.54	0.43
1:B:534:LYS:HE3	5:B:982:HOH:O	2.19	0.43
1:D:571:ARG:HH12	4:D:803:GOL:C1	2.32	0.43
1:C:652:THR:HG23	5:C:921:HOH:O	2.19	0.43
1:C:592:LYS:NZ	1:C:755:THR:O	2.43	0.42
1:A:464:LYS:HG2	1:A:465:TRP:CD1	2.53	0.42
1:C:658:VAL:HA	1:C:661:MET:HG3	2.02	0.42
1:B:644:ASN:ND2	1:B:646:ASP:OD2	2.52	0.42
1:D:699:PRO:HG2	1:D:702:GLU:CD	2.44	0.42
1:B:625:VAL:HG13	1:B:631:MET:HE1	2.01	0.42
1:D:571:ARG:NH2	4:D:803:GOL:H11	2.18	0.42
1:C:507:VAL:HG22	1:C:554:LEU:HD22	2.02	0.42
1:A:645:LEU:HD22	1:A:669:ARG:CZ	2.49	0.41
1:C:486:VAL:HA	1:C:507:VAL:O	2.20	0.41
1:B:644:ASN:OD1	1:B:645:LEU:HD12	2.21	0.41
1:A:693:SER:HA	1:A:694:PRO:HD3	1.91	0.41
1:A:643:HIS:HB3	1:A:647:TYR:CD2	2.56	0.41
1:A:725:MET:HE3	1:A:725:MET:HB3	1.92	0.41
1:B:645:LEU:H	1:B:645:LEU:CD1	2.17	0.41
1:C:591:PHE:HZ	1:C:723:LEU:HD12	1.86	0.41
1:C:645:LEU:HD22	1:C:669:ARG:NH2	2.36	0.41
1:B:635:ASP:HB3	1:B:638:LEU:HD12	2.02	0.41
1:C:459:LEU:HD12	1:C:459:LEU:HA	1.96	0.41
1:A:501:LYS:HA	1:A:502:PRO:HD3	1.97	0.40
1:A:591:PHE:CZ	1:A:720:THR:HG23	2.55	0.40
1:C:683:LEU:HD12	1:C:683:LEU:O	2.20	0.40
2:D:801:A1ESX:C17	2:D:801:A1ESX:N2	2.84	0.40
1:A:488:MET:HE3	1:A:557:TYR:CE1	2.56	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	284/292 (97%)	279 (98%)	4 (1%)	1 (0%)	30	20
1	B	284/292 (97%)	281 (99%)	3 (1%)	0	100	100
1	C	283/292 (97%)	277 (98%)	6 (2%)	0	100	100
1	D	278/292 (95%)	273 (98%)	5 (2%)	0	100	100
All	All	1129/1168 (97%)	1110 (98%)	18 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	644	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	244/248 (98%)	240 (98%)	4 (2%)	55	50
1	B	245/248 (99%)	240 (98%)	5 (2%)	48	42
1	C	244/248 (98%)	241 (99%)	3 (1%)	63	58
1	D	240/248 (97%)	239 (100%)	1 (0%)	84	82
All	All	973/992 (98%)	960 (99%)	13 (1%)	61	57

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	494	ILE
1	A	496	LYS
1	A	554	LEU
1	A	612	LYS
1	B	547	GLN

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Mol	Chain	Res	Type
1	B	565	GLU
1	B	645	LEU
1	B	666	LEU
1	B	669	ARG
1	C	670	VAL
1	C	754	VAL
1	C	755	THR
1	D	646	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	GLN
1	A	537	ASN
1	A	547	GLN
1	A	588	GLN
1	A	611	GLN
1	B	547	GLN
1	B	644	ASN
1	B	674	GLN
1	B	737	GLN
1	C	547	GLN
1	C	674	GLN
1	C	737	GLN
1	D	644	ASN
1	D	732	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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
4	GOL	D	803	-	5,5,5	0.75	0	5,5,5	0.85	0
4	GOL	A	803	-	5,5,5	0.69	0	5,5,5	1.15	1 (20%)
2	A1ESX	B	801	1	37,40,40	2.66	11 (29%)	51,56,56	5.29	19 (37%)
2	A1ESX	C	801	1	37,40,40	2.64	10 (27%)	51,56,56	5.19	19 (37%)
2	A1ESX	A	801	1	37,40,40	2.63	11 (29%)	51,56,56	5.17	19 (37%)
2	A1ESX	D	801	1	37,40,40	2.69	9 (24%)	51,56,56	5.31	19 (37%)
4	GOL	C	803	-	5,5,5	0.90	0	5,5,5	0.89	0

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	803	-	-	4/4/4/4	-
4	GOL	A	803	-	-	0/4/4/4	-
2	A1ESX	B	801	1	-	1/19/27/27	0/5/5/5
2	A1ESX	C	801	1	-	2/19/27/27	0/5/5/5
2	A1ESX	A	801	1	-	1/19/27/27	0/5/5/5
2	A1ESX	D	801	1	-	2/19/27/27	0/5/5/5
4	GOL	C	803	-	-	2/4/4/4	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	A1ESX	C20-N8	-6.76	1.31	1.47
2	A	801	A1ESX	C20-N8	-6.65	1.32	1.47
2	C	801	A1ESX	C20-N8	-6.50	1.32	1.47
2	B	801	A1ESX	C20-N8	-6.39	1.32	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	A1ESX	C9-C8	5.64	1.48	1.41
2	D	801	A1ESX	C9-C8	5.55	1.48	1.41
2	D	801	A1ESX	C1-N3	5.51	1.46	1.38
2	D	801	A1ESX	C21-N8	-5.45	1.31	1.46
2	B	801	A1ESX	C21-N8	-5.40	1.32	1.46
2	A	801	A1ESX	C9-C8	5.33	1.48	1.41
2	B	801	A1ESX	C9-C8	5.31	1.48	1.41
2	D	801	A1ESX	C24-N8	-5.29	1.32	1.46
2	B	801	A1ESX	C24-N8	-5.25	1.32	1.46
2	C	801	A1ESX	C21-N8	-5.23	1.32	1.46
2	B	801	A1ESX	C7-N4	-5.14	1.29	1.37
2	A	801	A1ESX	C21-N8	-5.11	1.32	1.46
2	A	801	A1ESX	C24-N8	-5.10	1.32	1.46
2	B	801	A1ESX	C1-N3	5.04	1.45	1.38
2	C	801	A1ESX	C24-N8	-5.02	1.33	1.46
2	A	801	A1ESX	C1-N3	5.02	1.45	1.38
2	B	801	A1ESX	C6-N3	5.01	1.46	1.36
2	D	801	A1ESX	C7-N4	-4.97	1.29	1.37
2	C	801	A1ESX	C1-N3	4.95	1.45	1.38
2	C	801	A1ESX	C7-N4	-4.81	1.29	1.37
2	A	801	A1ESX	C6-N3	4.65	1.46	1.36
2	A	801	A1ESX	C7-N4	-4.52	1.30	1.37
2	D	801	A1ESX	C6-N3	4.46	1.45	1.36
2	A	801	A1ESX	C15-N5	4.32	1.45	1.35
2	C	801	A1ESX	C6-N3	4.22	1.45	1.36
2	C	801	A1ESX	C15-N5	4.03	1.44	1.35
2	D	801	A1ESX	C15-N5	3.84	1.44	1.35
2	B	801	A1ESX	C17-N6	3.71	1.41	1.34
2	A	801	A1ESX	C17-N6	3.51	1.40	1.34
2	B	801	A1ESX	C15-N5	3.49	1.43	1.35
2	C	801	A1ESX	C17-N6	3.40	1.40	1.34
2	D	801	A1ESX	C17-N6	2.88	1.39	1.34
2	C	801	A1ESX	O1-C15	-2.23	1.18	1.23
2	A	801	A1ESX	C11-C8	-2.23	1.36	1.39
2	A	801	A1ESX	O1-C15	-2.07	1.19	1.23
2	B	801	A1ESX	O1-C15	-2.03	1.19	1.23
2	B	801	A1ESX	C11-C8	-2.02	1.36	1.39

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1ESX	C5-C7-N4	-25.32	103.19	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	A1ESX	C5-C7-N4	-25.00	103.29	111.05
2	A	801	A1ESX	C5-C7-N4	-24.61	103.41	111.05
2	C	801	A1ESX	C5-C7-N4	-24.29	103.51	111.05
2	D	801	A1ESX	C8-N4-C7	17.23	121.05	108.54
2	C	801	A1ESX	C8-N4-C7	16.89	120.80	108.54
2	B	801	A1ESX	C8-N4-C7	16.63	120.61	108.54
2	A	801	A1ESX	C8-N4-C7	16.47	120.49	108.54
2	B	801	A1ESX	C9-C5-C7	11.29	112.61	106.00
2	D	801	A1ESX	C9-C5-C7	10.89	112.37	106.00
2	A	801	A1ESX	C9-C5-C7	10.78	112.31	106.00
2	B	801	A1ESX	C8-C9-C5	-10.39	101.14	106.92
2	C	801	A1ESX	C9-C5-C7	10.39	112.08	106.00
2	A	801	A1ESX	C8-C9-C5	-10.08	101.31	106.92
2	D	801	A1ESX	C8-C9-C5	-10.04	101.33	106.92
2	C	801	A1ESX	C8-C9-C5	-9.76	101.49	106.92
2	D	801	A1ESX	C9-C8-N4	-9.41	101.96	107.89
2	C	801	A1ESX	C9-C8-N4	-9.18	102.10	107.89
2	B	801	A1ESX	C9-C8-N4	-8.65	102.43	107.89
2	A	801	A1ESX	C9-C8-N4	-8.60	102.47	107.89
2	C	801	A1ESX	C10-N4-C8	-6.65	119.13	125.69
2	A	801	A1ESX	C10-N4-C8	-6.63	119.15	125.69
2	D	801	A1ESX	C10-N4-C7	-6.39	118.79	125.71
2	B	801	A1ESX	C10-N4-C8	-6.05	119.72	125.69
2	D	801	A1ESX	C10-N4-C8	-5.61	120.16	125.69
2	B	801	A1ESX	C10-N4-C7	-5.58	119.67	125.71
2	C	801	A1ESX	C10-N4-C7	-5.21	120.07	125.71
2	A	801	A1ESX	C10-N4-C7	-4.94	120.36	125.71
2	D	801	A1ESX	C19-N6-N7	4.83	124.59	119.57
2	C	801	A1ESX	C22-C21-N8	3.96	116.11	110.10
2	B	801	A1ESX	C23-C24-N8	3.46	115.35	110.10
2	C	801	A1ESX	C24-N8-C21	3.45	116.61	108.83
2	D	801	A1ESX	C11-C8-N4	3.38	136.92	131.25
2	A	801	A1ESX	C22-C21-N8	3.29	115.09	110.10
2	C	801	A1ESX	C11-C8-N4	3.24	136.68	131.25
2	A	801	A1ESX	C9-C5-C2	-3.23	121.66	126.32
2	A	801	A1ESX	C24-N8-C21	3.21	116.04	108.83
2	A	801	A1ESX	C2-N2-C1	3.16	119.35	116.80
2	B	801	A1ESX	C9-C5-C2	-3.11	121.82	126.32
2	B	801	A1ESX	C11-C8-N4	3.10	136.45	131.25
2	A	801	A1ESX	N1-C1-N2	-3.10	123.61	126.55
2	D	801	A1ESX	N1-C1-N2	-3.06	123.65	126.55
2	A	801	A1ESX	C14-C9-C5	2.96	139.22	132.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	A1ESX	C19-N6-N7	2.90	122.58	119.57
2	C	801	A1ESX	C23-C24-N8	2.88	114.47	110.10
2	C	801	A1ESX	C14-C9-C5	2.88	139.03	132.39
2	D	801	A1ESX	C14-C9-C5	2.87	139.00	132.39
2	C	801	A1ESX	C2-N2-C1	2.85	119.10	116.80
2	A	801	A1ESX	C11-C8-N4	2.85	136.02	131.25
2	C	801	A1ESX	C9-C5-C2	-2.84	122.21	126.32
2	B	801	A1ESX	C19-N6-N7	2.82	122.50	119.57
2	B	801	A1ESX	C14-C9-C5	2.81	138.88	132.39
2	D	801	A1ESX	C25-C18-N7	2.75	124.78	119.33
2	C	801	A1ESX	C3-C2-N2	-2.72	119.73	122.92
2	C	801	A1ESX	N1-C1-N2	-2.72	123.97	126.55
2	B	801	A1ESX	C13-C12-C11	2.69	122.84	119.65
2	D	801	A1ESX	C9-C5-C2	-2.67	122.47	126.32
2	B	801	A1ESX	N1-C1-N2	-2.58	124.11	126.55
2	D	801	A1ESX	C1-N3-C6	-2.56	123.10	128.09
2	C	801	A1ESX	C25-C18-N7	2.54	124.38	119.33
2	B	801	A1ESX	C25-C18-N7	2.52	124.34	119.33
2	D	801	A1ESX	C19-N6-C17	-2.51	124.06	128.83
2	D	801	A1ESX	C4-N1-C1	2.50	117.67	115.45
2	A	801	A1ESX	C3-C2-N2	-2.49	120.00	122.92
2	D	801	A1ESX	C3-C2-N2	-2.46	120.03	122.92
2	D	801	A1ESX	C2-N2-C1	2.44	118.77	116.80
2	D	801	A1ESX	C13-C12-C11	2.30	122.38	119.65
2	B	801	A1ESX	C2-N2-C1	2.26	118.62	116.80
2	A	801	A1ESX	C13-C12-C11	2.25	122.31	119.65
2	B	801	A1ESX	C3-C2-N2	-2.20	120.35	122.92
2	B	801	A1ESX	C17-N6-N7	-2.16	110.82	113.62
2	A	801	A1ESX	C4-N1-C1	2.11	117.32	115.45
2	C	801	A1ESX	C13-C12-C11	2.10	122.14	119.65
4	A	803	GOL	C3-C2-C1	-2.08	103.61	111.70
2	A	801	A1ESX	C25-C18-N7	2.07	123.44	119.33
2	A	801	A1ESX	C19-N6-N7	2.04	121.69	119.57
2	B	801	A1ESX	C13-C12-N5	-2.01	113.63	120.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	A1ESX	N6-C19-C20-N8
4	C	803	GOL	O1-C1-C2-C3
4	C	803	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	803	GOL	C1-C2-C3-O3
2	A	801	A1ESX	N2-C2-C5-C9
2	B	801	A1ESX	N2-C2-C5-C9
2	C	801	A1ESX	N2-C2-C5-C9
2	D	801	A1ESX	N2-C2-C5-C9
4	D	803	GOL	O1-C1-C2-O2
4	D	803	GOL	O2-C2-C3-O3
2	D	801	A1ESX	N6-C19-C20-N8
4	D	803	GOL	O1-C1-C2-C3

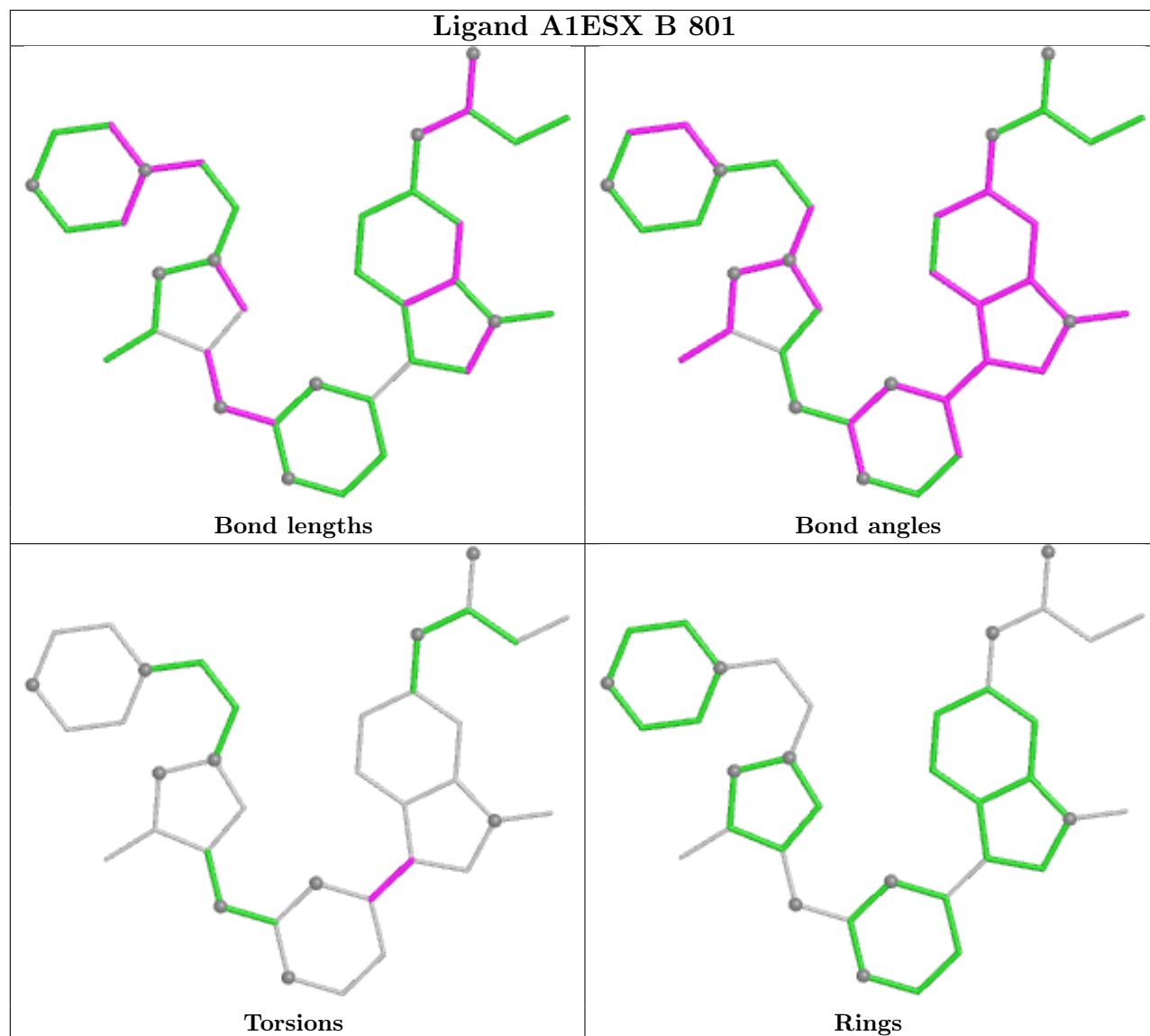
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	803	GOL	5	0
2	C	801	A1ESX	1	0
2	D	801	A1ESX	1	0
4	C	803	GOL	5	0

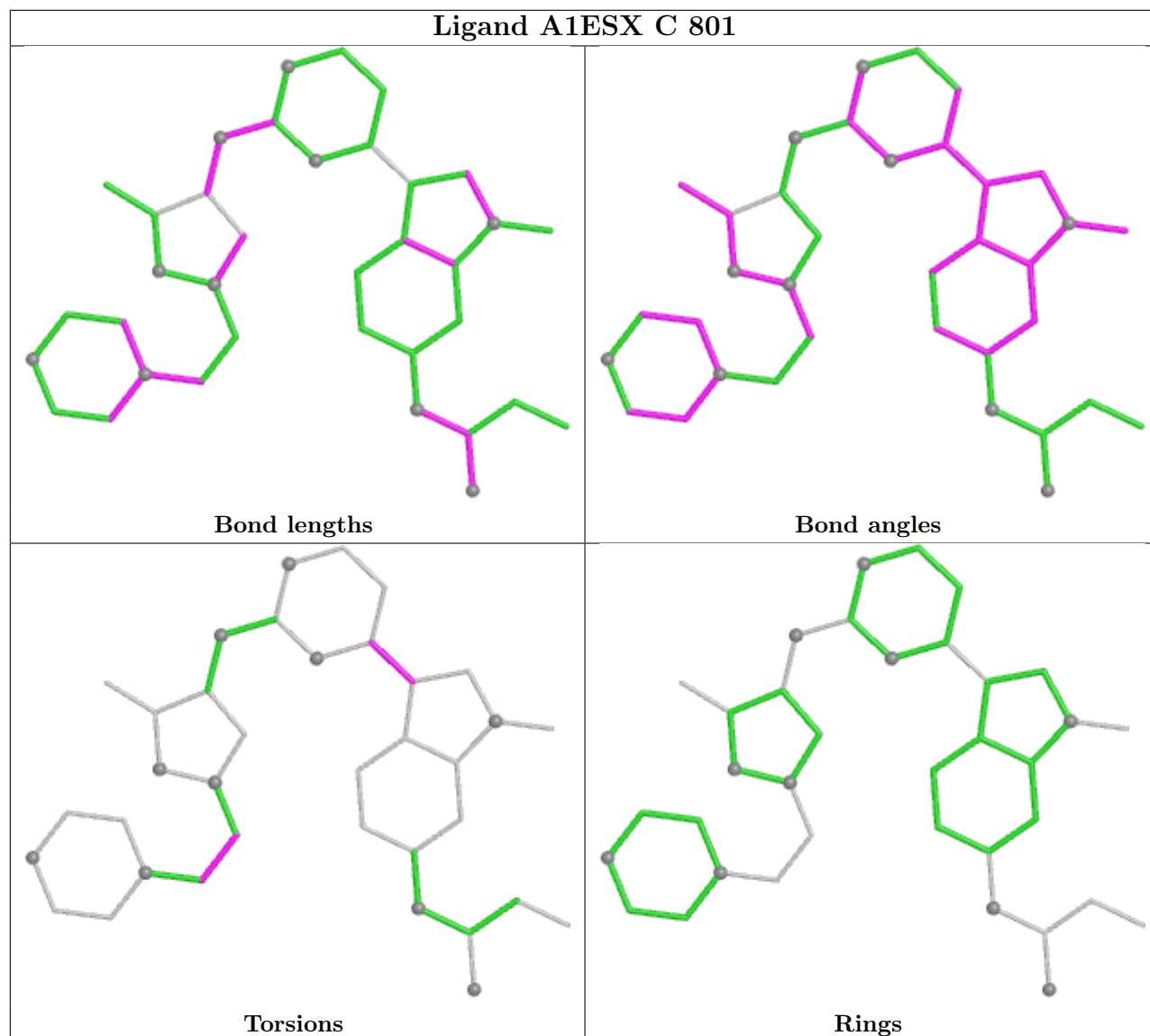
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A1ESX B 801

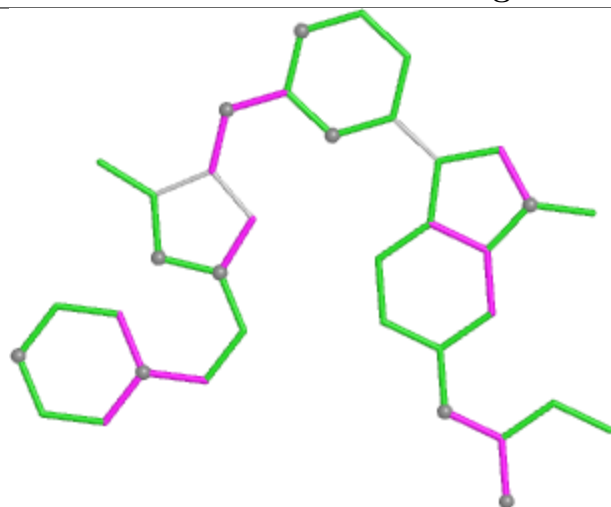




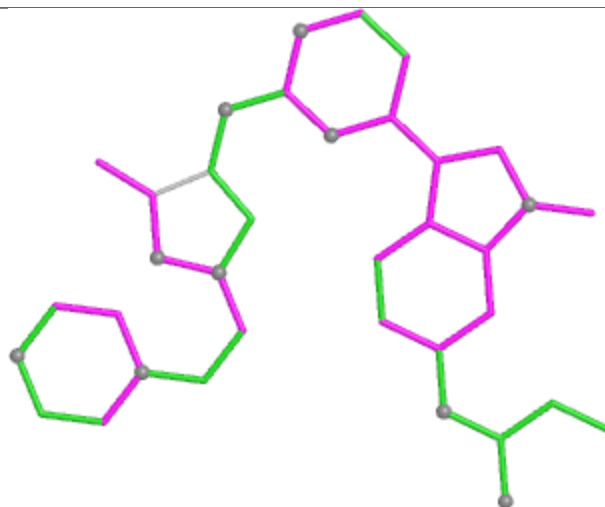
## Ligand A1ESX C 801



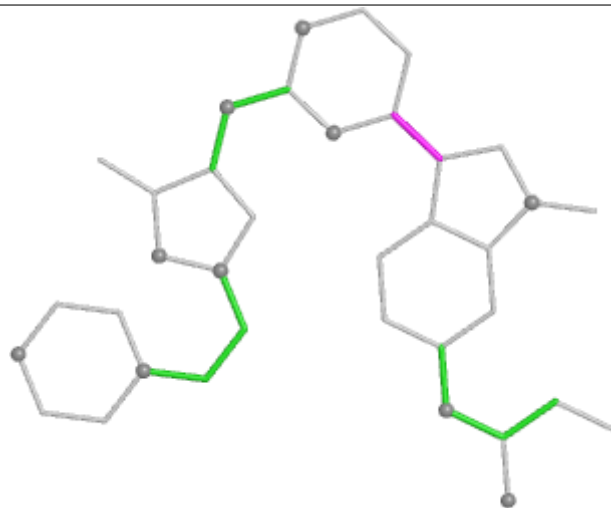
## Ligand A1ESX A 801



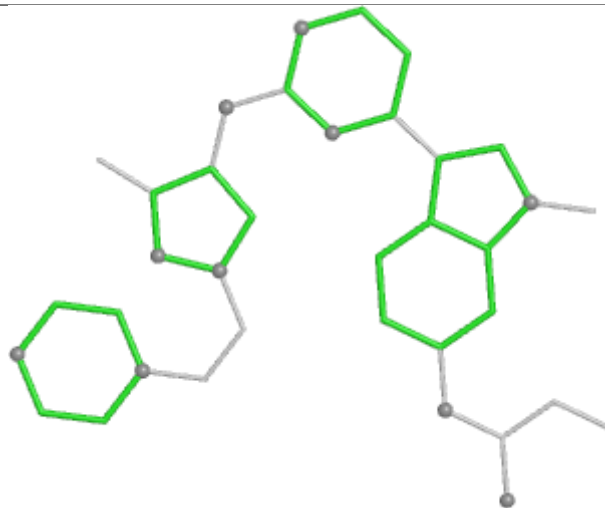
Bond lengths



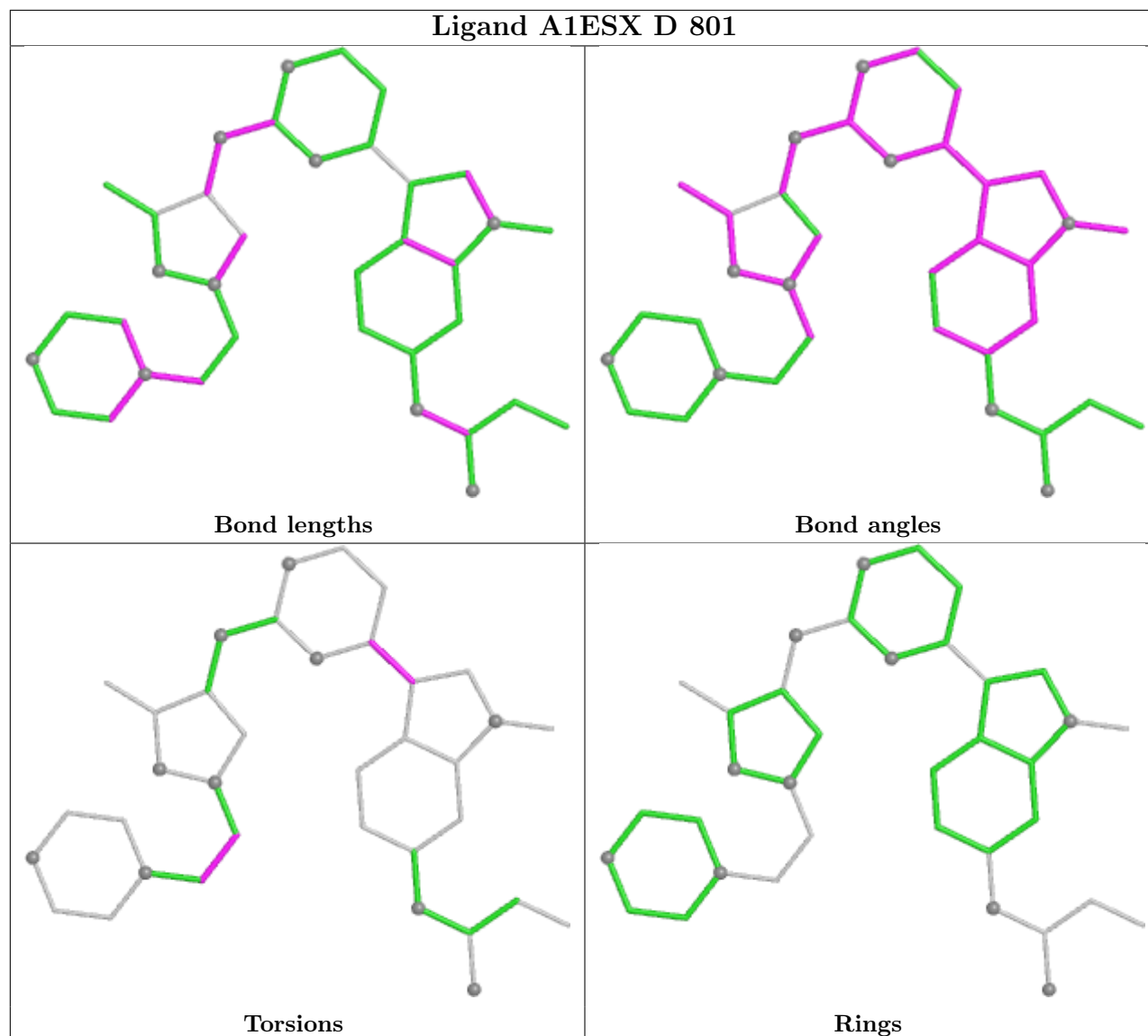
Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	287/292 (98%)	0.25	24 (8%)	17 23	7, 19, 55, 74	1 (0%)
1	B	287/292 (98%)	0.18	20 (6%)	22 30	6, 18, 52, 71	1 (0%)
1	C	286/292 (97%)	0.26	25 (8%)	16 22	8, 19, 56, 83	1 (0%)
1	D	281/292 (96%)	0.36	28 (9%)	12 18	8, 20, 62, 97	1 (0%)
All	All	1141/1168 (97%)	0.26	97 (8%)	16 23	6, 19, 57, 97	4 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	645	LEU	6.0
1	B	755	THR	5.7
1	D	514	ALA	5.4
1	C	643	HIS	4.9
1	D	495	ASP	4.8
1	C	644	ASN	4.7
1	B	642	VAL	4.6
1	B	644	ASN	4.6
1	D	494	ILE	4.5
1	B	643	HIS	4.5
1	C	756	SER	4.5
1	D	516	ASP	4.4
1	D	718	ASN	4.4
1	D	499	ALA	4.4
1	B	756	SER	4.4
1	A	457	LEU	4.3
1	C	640	ARG	4.3
1	D	756	SER	4.3
1	C	642	VAL	4.2
1	D	492	ILE	4.2
1	B	498	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	496	LYS	4.0
1	B	513	ASP	4.0
1	C	641	ASP	3.9
1	A	644	ASN	3.8
1	C	645	LEU	3.8
1	C	513	ASP	3.8
1	D	500	ALA	3.8
1	C	718	ASN	3.8
1	D	496	LYS	3.7
1	B	640	ARG	3.7
1	A	643	HIS	3.6
1	C	457	LEU	3.6
1	A	642	VAL	3.6
1	A	647	TYR	3.5
1	D	498	ARG	3.5
1	C	647	TYR	3.5
1	B	670	VAL	3.5
1	A	639	ALA	3.4
1	B	512	ASP	3.4
1	B	754	VAL	3.3
1	A	513	ASP	3.3
1	B	671	TYR	3.3
1	A	516	ASP	3.2
1	A	646	ASP	3.2
1	B	641	ASP	3.1
1	D	513	ASP	3.1
1	A	456	GLU	3.1
1	A	645	LEU	3.0
1	A	754	VAL	3.0
1	A	641	ASP	3.0
1	B	514	ALA	2.9
1	B	497	ASP	2.9
1	D	645	LEU	2.9
1	D	482	CYS	2.8
1	D	515	THR	2.8
1	C	639	ALA	2.7
1	C	587	GLU	2.7
1	D	512	ASP	2.7
1	D	502	PRO	2.7
1	D	501	LYS	2.7
1	D	493	GLY	2.7
1	B	516	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	646	ASP	2.6
1	D	462	ASP	2.5
1	B	499	ALA	2.5
1	D	704	PHE	2.5
1	A	514	ALA	2.5
1	A	704	PHE	2.4
1	B	510	LEU	2.4
1	C	458	GLU	2.4
1	A	499	ALA	2.4
1	C	514	ALA	2.4
1	C	591	PHE	2.4
1	A	512	ASP	2.4
1	D	497	ASP	2.4
1	C	755	THR	2.4
1	A	750	ARG	2.4
1	C	586	GLU	2.4
1	C	704	PHE	2.4
1	A	500	ALA	2.3
1	A	756	SER	2.3
1	C	497	ASP	2.3
1	D	646	ASP	2.3
1	A	753	THR	2.3
1	D	463	PRO	2.2
1	A	640	ARG	2.2
1	D	588	GLN	2.2
1	C	516	ASP	2.2
1	A	755	THR	2.2
1	D	548	GLY	2.2
1	D	755	THR	2.1
1	B	511	LYS	2.1
1	C	669	ARG	2.1
1	D	750	ARG	2.1
1	C	752	LEU	2.1
1	C	548	GLY	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 [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

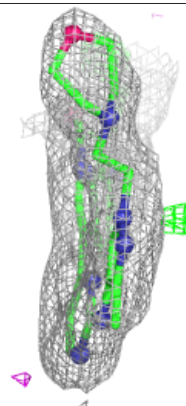
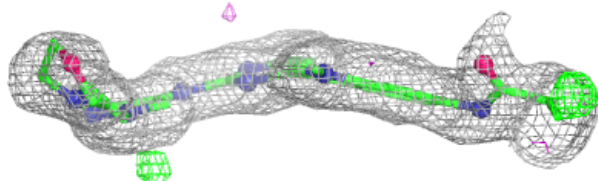
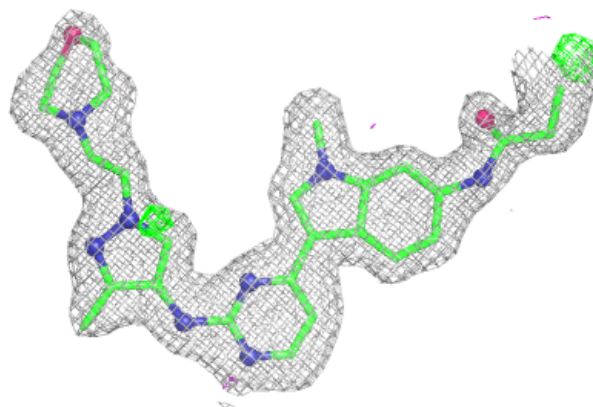
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	GOL	C	803	6/6	0.75	0.17	19,32,36,41	0
4	GOL	D	803	6/6	0.78	0.13	20,28,33,34	0
4	GOL	A	803	6/6	0.89	0.11	12,31,32,35	0
2	A1ESX	A	801	36/36	0.92	0.08	12,20,40,47	0
2	A1ESX	D	801	36/36	0.93	0.09	11,22,49,53	0
2	A1ESX	B	801	36/36	0.93	0.08	9,17,40,42	0
2	A1ESX	C	801	36/36	0.94	0.08	9,17,39,42	0
3	MG	D	802	1/1	0.98	0.06	14,14,14,14	0
3	MG	C	802	1/1	0.98	0.08	14,14,14,14	0
3	MG	B	802	1/1	0.99	0.05	14,14,14,14	0
3	MG	A	802	1/1	0.99	0.05	14,14,14,14	0

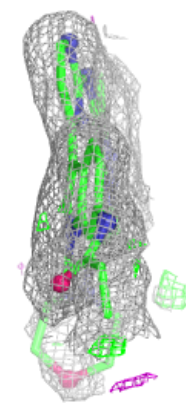
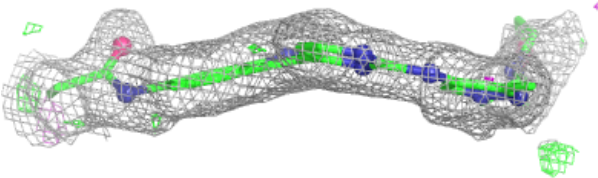
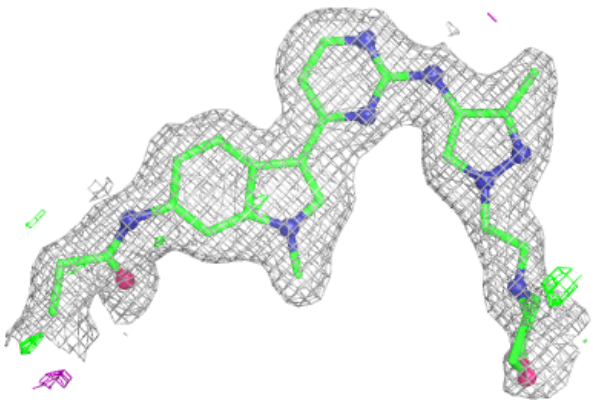
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1ESX A 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 A1ESX D 801:**

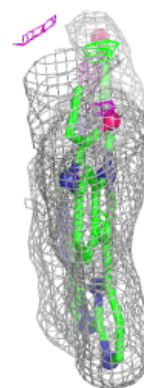
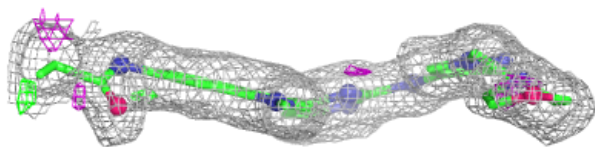
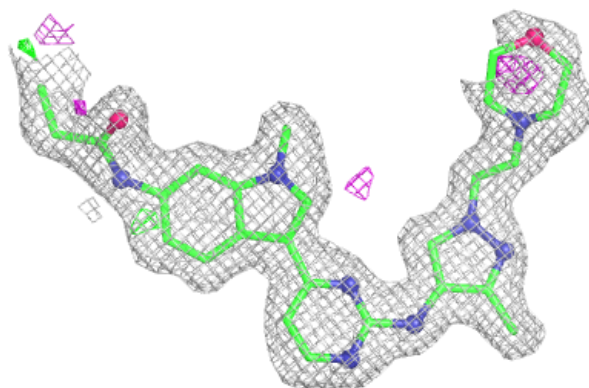
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



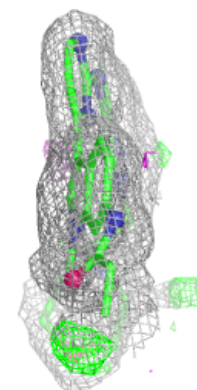
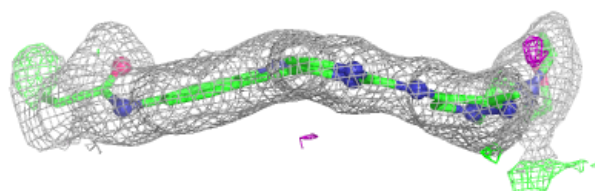
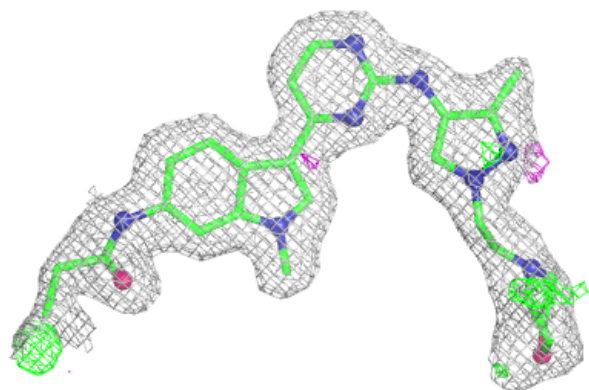


**Electron density around A1ESX B 801:**

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

**Electron density around A1ESX C 801:**

$2mF_o-DF_c$  (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.