



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:08 PM UTC

PDB ID : 4MOE / pdb_00004moe
Title : Pyranose 2-oxidase H450G mutant with 3-fluorinated glucose
Authors : Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.
Deposited on : 2013-09-12
Resolution : 2.00 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

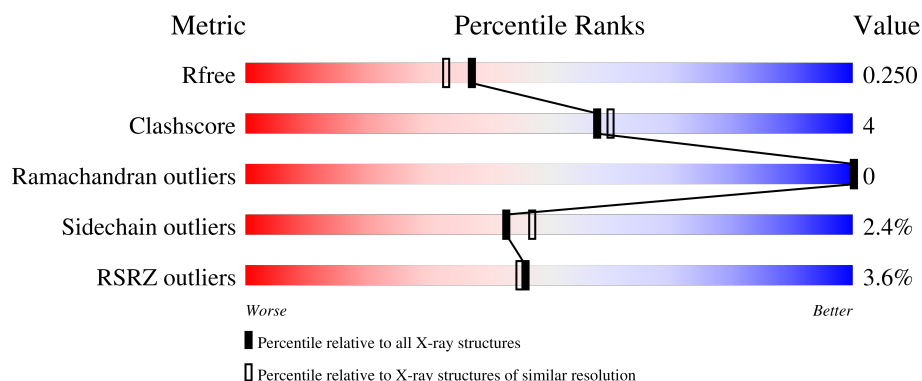
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

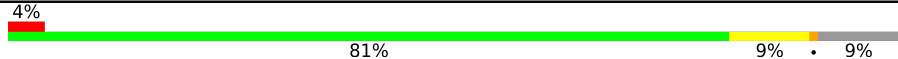
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	633	
1	B	633	
1	C	633	
1	D	633	

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
5	MES	A	804	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19611 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 Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4536	2864	775	872	25			
1	B	576	Total	C	N	O	S	0	0	0
			4536	2864	775	872	25			
1	C	574	Total	C	N	O	S	0	0	0
			4520	2855	773	868	24			
1	D	575	Total	C	N	O	S	0	0	0
			4527	2859	774	870	24			

There are 52 discrepancies between the modelled and reference sequences:

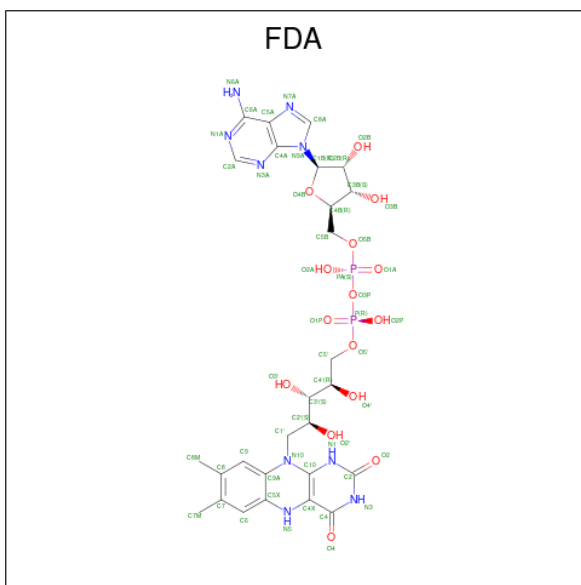
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
A	450	GLY	HIS	engineered mutation	UNP Q7ZA32
A	623	ALA	-	expression tag	UNP Q7ZA32
A	624	ALA	-	expression tag	UNP Q7ZA32
A	625	ALA	-	expression tag	UNP Q7ZA32
A	626	LEU	-	expression tag	UNP Q7ZA32
A	627	GLU	-	expression tag	UNP Q7ZA32
A	628	HIS	-	expression tag	UNP Q7ZA32
A	629	HIS	-	expression tag	UNP Q7ZA32
A	630	HIS	-	expression tag	UNP Q7ZA32
A	631	HIS	-	expression tag	UNP Q7ZA32
A	632	HIS	-	expression tag	UNP Q7ZA32
A	633	HIS	-	expression tag	UNP Q7ZA32
B	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
B	450	GLY	HIS	engineered mutation	UNP Q7ZA32
B	623	ALA	-	expression tag	UNP Q7ZA32
B	624	ALA	-	expression tag	UNP Q7ZA32
B	625	ALA	-	expression tag	UNP Q7ZA32
B	626	LEU	-	expression tag	UNP Q7ZA32
B	627	GLU	-	expression tag	UNP Q7ZA32
B	628	HIS	-	expression tag	UNP Q7ZA32

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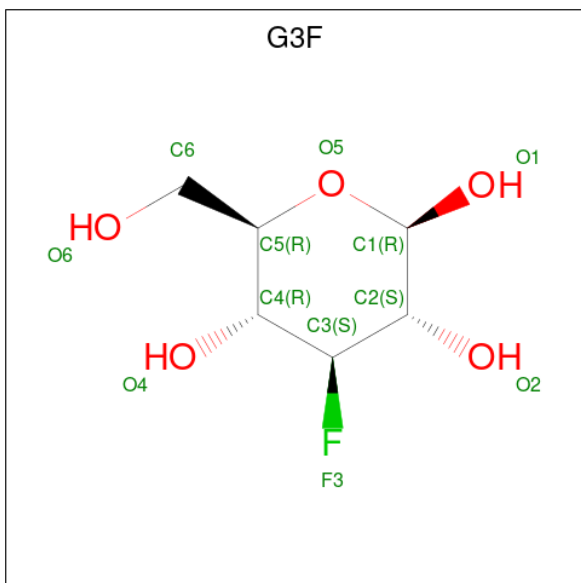
Chain	Residue	Modelled	Actual	Comment	Reference
B	629	HIS	-	expression tag	UNP Q7ZA32
B	630	HIS	-	expression tag	UNP Q7ZA32
B	631	HIS	-	expression tag	UNP Q7ZA32
B	632	HIS	-	expression tag	UNP Q7ZA32
B	633	HIS	-	expression tag	UNP Q7ZA32
C	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
C	450	GLY	HIS	engineered mutation	UNP Q7ZA32
C	623	ALA	-	expression tag	UNP Q7ZA32
C	624	ALA	-	expression tag	UNP Q7ZA32
C	625	ALA	-	expression tag	UNP Q7ZA32
C	626	LEU	-	expression tag	UNP Q7ZA32
C	627	GLU	-	expression tag	UNP Q7ZA32
C	628	HIS	-	expression tag	UNP Q7ZA32
C	629	HIS	-	expression tag	UNP Q7ZA32
C	630	HIS	-	expression tag	UNP Q7ZA32
C	631	HIS	-	expression tag	UNP Q7ZA32
C	632	HIS	-	expression tag	UNP Q7ZA32
C	633	HIS	-	expression tag	UNP Q7ZA32
D	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
D	450	GLY	HIS	engineered mutation	UNP Q7ZA32
D	623	ALA	-	expression tag	UNP Q7ZA32
D	624	ALA	-	expression tag	UNP Q7ZA32
D	625	ALA	-	expression tag	UNP Q7ZA32
D	626	LEU	-	expression tag	UNP Q7ZA32
D	627	GLU	-	expression tag	UNP Q7ZA32
D	628	HIS	-	expression tag	UNP Q7ZA32
D	629	HIS	-	expression tag	UNP Q7ZA32
D	630	HIS	-	expression tag	UNP Q7ZA32
D	631	HIS	-	expression tag	UNP Q7ZA32
D	632	HIS	-	expression tag	UNP Q7ZA32
D	633	HIS	-	expression tag	UNP Q7ZA32

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).



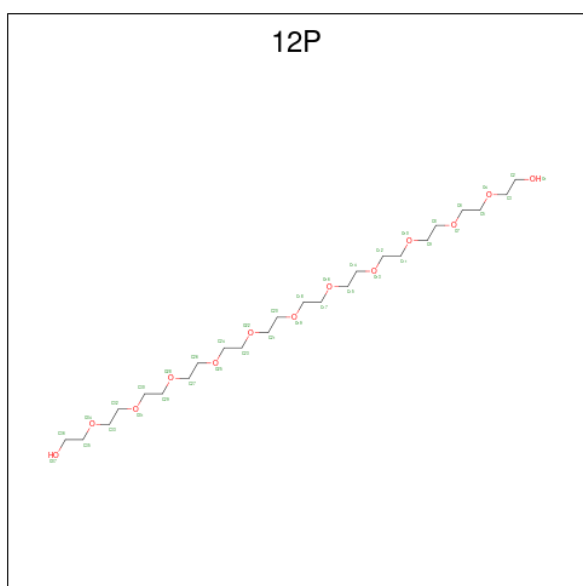
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is 3-deoxy-3-fluoro-beta-D-glucopyranose (CCD ID: G3F) (formula: $\text{C}_6\text{H}_{11}\text{FO}_5$).



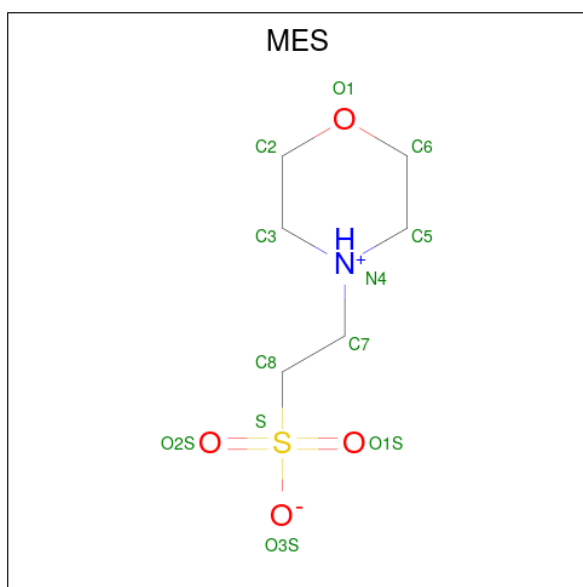
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F O 12 6 1 5	0	0
3	B	1	Total C F O 12 6 1 5	0	0
3	C	1	Total C F O 12 6 1 5	0	0
3	D	1	Total C F O 12 6 1 5	0	0

- Molecule 4 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 15 10 5	0	0
4	A	1	Total C O 14 9 5	0	0
4	B	1	Total C O 16 10 6	0	0
4	B	1	Total C O 11 8 3	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

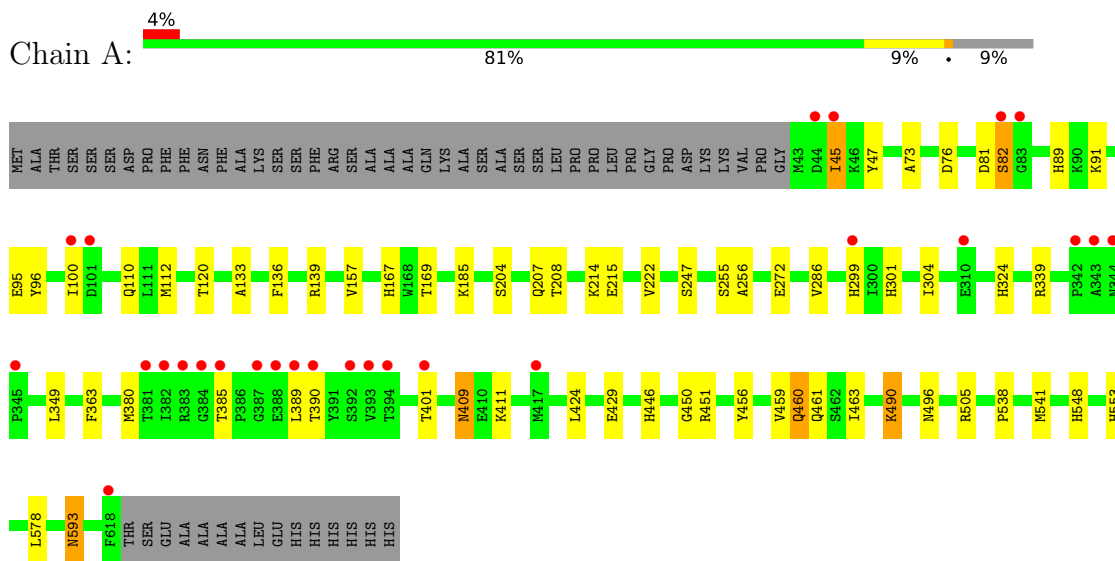
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	294	Total	O	0	0
			294	294		
6	B	369	Total	O	0	0
			369	369		
6	C	183	Total	O	0	0
			183	183		
6	D	270	Total	O	0	0
			270	270		

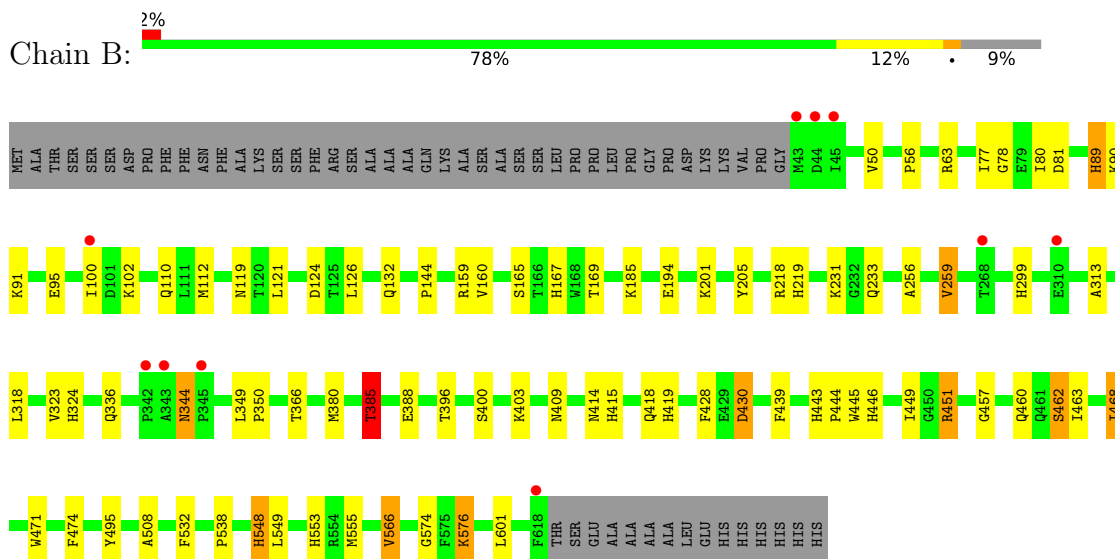
3 Residue-property plots [i](#)

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.

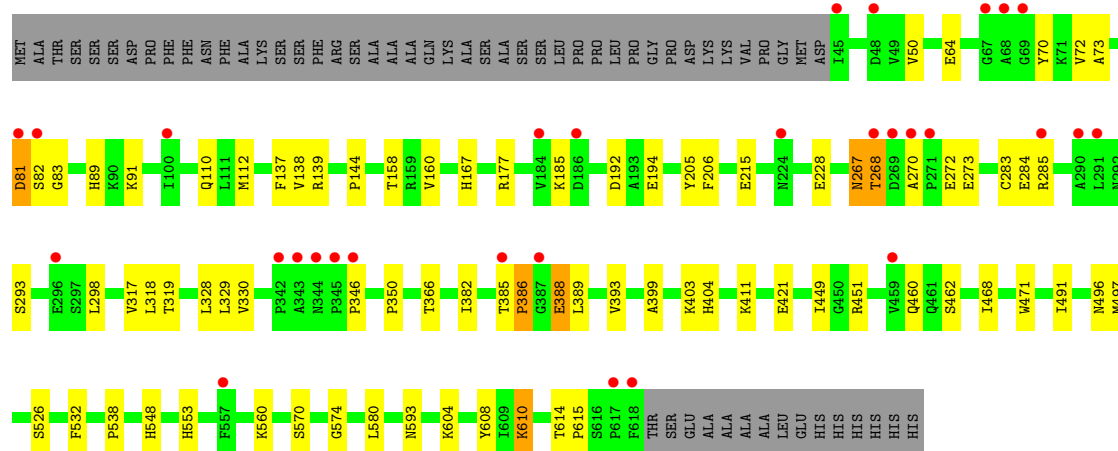
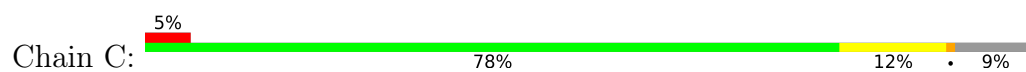
- Molecule 1: Pyranose 2-oxidase



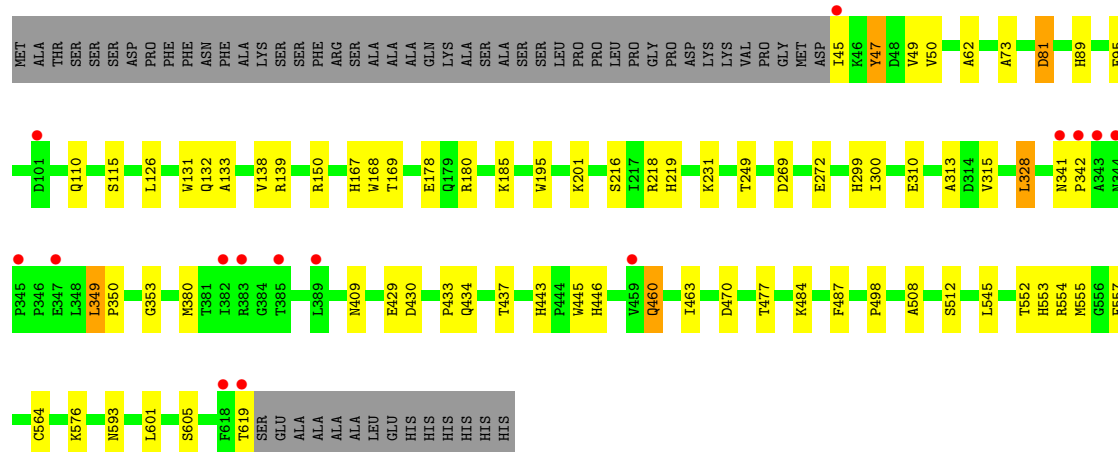
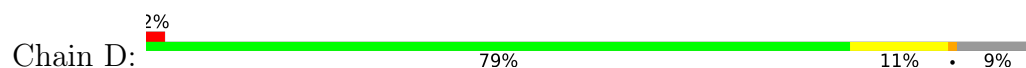
- Molecule 1: Pyranose 2-oxidase



- Molecule 1: Pyranose 2-oxidase



• Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.07Å 102.74Å 137.69Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.00) 97.7 (50.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.195 , 0.242 0.202 , 0.250	Depositor DCC
R_{free} test set	3287 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l 0.022 for k,h,-l 0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19611	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 12P, G3F, MES, FDA

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	1.39	15/4651 (0.3%)	1.21	12/6323 (0.2%)
1	B	1.49	28/4651 (0.6%)	1.23	12/6323 (0.2%)
1	C	1.20	7/4635 (0.2%)	1.11	5/6302 (0.1%)
1	D	1.34	18/4642 (0.4%)	1.14	7/6312 (0.1%)
All	All	1.36	68/18579 (0.4%)	1.17	36/25260 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	ILE	C-O	-9.41	1.14	1.24
1	B	457	GLY	N-CA	6.93	1.50	1.44
1	D	445	TRP	CA-C	-6.91	1.43	1.52
1	D	89	HIS	ND1-CE1	6.82	1.39	1.32
1	C	468	ILE	C-O	-6.57	1.16	1.24
1	A	349	LEU	C-O	6.53	1.27	1.23
1	B	299	HIS	CG-CD2	6.51	1.43	1.35
1	B	548	HIS	ND1-CE1	6.48	1.39	1.32
1	D	138	VAL	C-O	-6.43	1.17	1.24
1	A	222	VAL	C-O	-6.38	1.17	1.24
1	A	76	ASP	C-O	-6.27	1.16	1.23
1	B	443	HIS	CG-CD2	6.24	1.42	1.35
1	A	256	ALA	N-CA	-6.24	1.38	1.46
1	A	208	THR	C-O	-6.19	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	593	ASN	C-O	-6.13	1.16	1.24
1	B	219	HIS	C-O	-6.11	1.17	1.24
1	D	443	HIS	ND1-CE1	5.96	1.38	1.32
1	A	301	HIS	CG-ND1	-5.92	1.31	1.38
1	B	419	HIS	ND1-CE1	5.91	1.38	1.32
1	D	349	LEU	N-CA	5.90	1.50	1.46
1	A	578	LEU	CA-C	-5.85	1.45	1.52
1	A	363	PHE	C-O	5.85	1.30	1.23
1	A	553	HIS	CB-CG	5.85	1.58	1.50
1	D	512	SER	C-O	-5.83	1.17	1.24
1	A	255	SER	C-O	-5.81	1.18	1.24
1	B	415	HIS	ND1-CE1	5.71	1.38	1.32
1	A	89	HIS	CG-CD2	5.67	1.42	1.35
1	B	324	HIS	CD2-NE2	-5.64	1.31	1.37
1	B	428	PHE	C-O	-5.64	1.17	1.24
1	C	268	THR	N-CA	-5.63	1.39	1.46
1	A	82	SER	N-CA	5.62	1.52	1.46
1	B	256	ALA	C-O	-5.62	1.17	1.24
1	B	553	HIS	ND1-CE1	5.60	1.38	1.32
1	B	601	LEU	C-O	5.59	1.30	1.24
1	D	115	SER	CA-C	-5.55	1.46	1.52
1	B	144	PRO	C-O	-5.54	1.16	1.24
1	B	194	GLU	C-O	-5.49	1.17	1.24
1	D	605	SER	C-O	-5.47	1.17	1.24
1	B	553	HIS	CG-CD2	5.46	1.41	1.35
1	C	553	HIS	CG-CD2	5.41	1.41	1.35
1	B	350	PRO	C-O	-5.39	1.17	1.24
1	D	195	TRP	NE1-CE2	-5.39	1.31	1.37
1	B	443	HIS	CE1-NE2	5.38	1.38	1.32
1	D	446	HIS	CE1-NE2	5.37	1.38	1.32
1	B	446	HIS	C-O	-5.37	1.17	1.23
1	B	549	LEU	C-O	5.33	1.30	1.23
1	B	318	LEU	CA-C	5.33	1.59	1.52
1	D	168	TRP	CD2-CE2	5.32	1.50	1.41
1	B	89	HIS	CA-C	-5.31	1.46	1.52
1	C	267	ASN	CA-C	-5.28	1.46	1.52
1	B	474	PHE	C-O	5.21	1.29	1.24
1	A	299	HIS	ND1-CE1	5.18	1.37	1.32
1	D	62	ALA	C-O	5.18	1.30	1.24
1	D	150	ARG	C-O	-5.18	1.18	1.24
1	C	404	HIS	CG-CD2	5.17	1.41	1.35
1	A	446	HIS	CD2-NE2	-5.16	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	553	HIS	CG-CD2	5.15	1.41	1.35
1	B	256	ALA	CA-CB	5.14	1.61	1.53
1	C	491	ILE	C-O	-5.11	1.17	1.24
1	B	566	VAL	C-O	5.11	1.29	1.24
1	B	468	ILE	C-O	-5.08	1.18	1.24
1	B	78	GLY	N-CA	5.08	1.49	1.44
1	D	477	THR	C-O	5.06	1.30	1.24
1	D	552	THR	CA-C	5.04	1.59	1.52
1	B	124	ASP	C-O	-5.04	1.16	1.23
1	D	470	ASP	C-O	5.04	1.30	1.23
1	C	451	ARG	C-O	-5.04	1.17	1.23
1	D	328	LEU	C-O	-5.01	1.18	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	ASP	N-CA-C	7.20	122.06	111.34
1	B	324	HIS	N-CA-C	7.05	120.00	111.82
1	D	180	ARG	CA-C-N	-6.49	113.30	119.85
1	D	180	ARG	C-N-CA	-6.49	113.30	119.85
1	A	409	ASN	N-CA-C	6.34	118.19	111.28
1	A	385	THR	CA-C-N	6.16	126.52	119.93
1	A	385	THR	C-N-CA	6.16	126.52	119.93
1	A	82	SER	CA-CB-OG	6.11	123.32	111.10
1	C	497	MET	CA-C-N	-6.03	113.73	119.76
1	C	497	MET	C-N-CA	-6.03	113.73	119.76
1	C	267	ASN	N-CA-C	-6.02	99.99	108.96
1	A	96	TYR	CA-C-N	-5.97	110.95	122.06
1	A	96	TYR	C-N-CA	-5.97	110.95	122.06
1	B	430	ASP	CA-C-N	-5.97	113.53	119.92
1	B	430	ASP	C-N-CA	-5.97	113.53	119.92
1	B	233	GLN	N-CA-C	-5.91	106.72	114.04
1	D	47	TYR	N-CA-C	-5.74	100.63	109.52
1	D	168	TRP	N-CA-C	5.67	118.02	110.53
1	B	259	VAL	N-CA-C	-5.67	105.20	110.53
1	B	396	THR	CB-CA-C	-5.61	105.39	110.44
1	B	100	ILE	N-CA-C	5.55	116.95	110.62
1	B	385	THR	CB-CA-C	5.55	118.34	110.02
1	B	323	VAL	N-CA-C	-5.54	106.30	111.45
1	A	424	LEU	CA-C-N	5.49	125.97	120.04
1	A	424	LEU	C-N-CA	5.49	125.97	120.04
1	B	95	GLU	N-CA-C	5.44	116.89	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	SER	CB-CA-C	-5.41	102.31	111.02
1	D	508	ALA	N-CA-C	-5.37	103.80	110.41
1	B	90	LYS	N-CA-C	5.33	118.88	112.38
1	D	300	ILE	N-CA-C	5.28	117.23	108.99
1	A	339	ARG	CA-C-N	-5.28	114.33	119.76
1	A	339	ARG	C-N-CA	-5.28	114.33	119.76
1	D	81	ASP	N-CA-C	5.25	121.48	113.19
1	A	304	ILE	N-CA-C	-5.21	106.61	111.45
1	C	268	THR	N-CA-C	-5.16	105.08	111.33
1	B	508	ALA	N-CA-C	-5.06	104.00	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4536	0	4384	35	0
1	B	4536	0	4384	42	0
1	C	4520	0	4371	51	0
1	D	4527	0	4378	33	0
2	A	53	0	30	2	0
2	B	53	0	30	2	0
2	C	53	0	29	3	0
2	D	53	0	30	3	0
3	A	12	0	11	2	0
3	B	12	0	11	2	0
3	C	12	0	11	3	0
3	D	12	0	11	2	0
4	A	29	0	34	0	0
4	B	27	0	33	0	0
5	A	12	0	13	10	0
5	B	12	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	12	0	13	1	0
5	D	24	0	26	1	0
6	A	294	0	0	2	0
6	B	369	0	0	3	0
6	C	183	0	0	1	0
6	D	270	0	0	2	0
All	All	19611	0	17812	162	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 4.

All (162) 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:133:ALA:CB	5:A:804:MES:H71	1.53	1.35
1:A:133:ALA:HB3	5:A:804:MES:H71	1.16	1.14
1:A:133:ALA:HB2	5:A:804:MES:H71	1.40	1.00
1:A:133:ALA:CB	5:A:804:MES:C7	2.46	0.92
1:D:460:GLN:HE22	1:D:463:ILE:H	1.13	0.92
1:A:133:ALA:HB3	5:A:804:MES:C7	2.03	0.89
1:A:460:GLN:HE22	1:A:463:ILE:H	1.14	0.87
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.23	0.86
1:D:110:GLN:HE21	1:D:167:HIS:HD1	1.25	0.85
1:D:131:TRP:CH2	1:D:133:ALA:HB2	2.17	0.80
1:C:270:ALA:HB1	1:C:273:GLU:HG3	1.65	0.78
1:B:110:GLN:HE21	1:B:167:HIS:HD1	1.31	0.76
1:B:385:THR:HG23	1:B:388:GLU:OE1	1.88	0.74
1:A:45:ILE:H	1:A:45:ILE:HD12	1.54	0.70
1:C:329:LEU:HD11	1:C:580:LEU:HD11	1.74	0.70
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.40	0.69
1:A:133:ALA:HB2	5:A:804:MES:C7	2.19	0.69
1:B:385:THR:CG2	1:B:388:GLU:OE1	2.42	0.68
1:C:460:GLN:NE2	1:C:462:SER:HB3	2.08	0.68
1:A:133:ALA:HB2	5:A:804:MES:O1S	1.93	0.68
1:C:548:HIS:NE2	3:C:802:G3F:O2	2.26	0.67
1:C:460:GLN:HE21	1:C:462:SER:HB3	1.60	0.67
1:B:451:ARG:NH1	6:B:1264:HOH:O	2.27	0.66
1:B:126:LEU:HD12	1:B:132:GLN:CG	2.26	0.66
1:B:126:LEU:HD12	1:B:132:GLN:HG3	1.77	0.65
1:C:270:ALA:HB1	1:C:273:GLU:CG	2.26	0.65
1:C:215:GLU:O	1:C:411:LYS:NZ	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ARG:HG3	1:B:430:ASP:OD2	1.97	0.65
1:B:119:ASN:HD21	1:B:121:LEU:HD12	1.62	0.65
1:B:81:ASP:OD1	1:B:81:ASP:N	2.29	0.63
1:D:216:SER:HB3	1:D:219:HIS:HB3	1.79	0.63
1:A:459:VAL:HG13	1:A:461:GLN:NE2	2.13	0.63
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.80	0.63
2:A:801:FDA:N5	3:A:802:G3F:H2	2.16	0.61
1:D:185:LYS:HE3	1:D:557:PHE:CG	2.35	0.61
1:D:555:MET:HE1	1:D:601:LEU:HD22	1.81	0.61
1:A:450:GLY:O	1:A:451:ARG:HD2	2.01	0.59
1:B:414:ASN:O	1:B:418:GLN:HG2	2.02	0.59
2:C:801:FDA:N5	3:C:802:G3F:H2	2.17	0.59
1:A:139:ARG:HD3	5:A:804:MES:H81	1.85	0.58
1:D:249:THR:HG21	1:D:429:GLU:OE1	2.03	0.58
1:B:574:GLY:O	1:B:576:LYS:NZ	2.38	0.57
1:A:91:LYS:HD2	1:A:100:ILE:HD11	1.86	0.57
1:B:63:ARG:HD2	1:B:259:VAL:O	2.06	0.56
1:C:194:GLU:OE2	1:C:604:LYS:NZ	2.35	0.56
1:C:50:VAL:HG12	1:C:73:ALA:HB3	1.87	0.55
2:D:801:FDA:N5	3:D:802:G3F:H2	2.22	0.55
1:D:132:GLN:OE1	5:D:803:MES:N4	2.38	0.55
1:B:56:PRO:HD3	1:B:165:SER:HB3	1.89	0.54
1:B:336:GLN:NE2	1:B:344:ASN:O	2.41	0.54
1:C:385:THR:O	1:C:388:GLU:HG2	2.07	0.54
1:D:341:ASN:HD22	1:D:342:PRO:HD2	1.73	0.54
1:B:380:MET:HE1	1:B:409:ASN:CB	2.38	0.53
1:A:380:MET:HE1	1:A:409:ASN:HB3	1.90	0.53
1:C:388:GLU:HA	1:C:388:GLU:OE1	2.08	0.53
1:D:126:LEU:CD1	1:D:132:GLN:CG	2.86	0.53
1:C:593:ASN:HB3	2:C:801:FDA:C2	2.38	0.53
1:A:490:LYS:HE3	1:A:490:LYS:O	2.09	0.53
1:A:538:PRO:HG2	1:C:538:PRO:HG2	1.91	0.52
1:C:158:THR:HG22	1:C:160:VAL:HG22	1.91	0.52
1:D:126:LEU:HD12	1:D:132:GLN:HG3	1.91	0.52
1:D:169:THR:H	2:D:801:FDA:HN5	1.57	0.52
1:B:201:LYS:HE2	1:B:205:TYR:OH	2.09	0.52
1:C:284:GLU:C	1:C:328:LEU:CD1	2.83	0.52
1:D:545:LEU:HD12	6:D:1109:HOH:O	2.10	0.52
1:C:112:MET:HE2	1:D:95:GLU:HG3	1.93	0.51
1:B:77:ILE:HD11	1:B:495:TYR:CD2	2.46	0.51
1:C:614:THR:HG22	1:C:615:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ASN:O	1:C:268:THR:C	2.53	0.51
1:D:49:VAL:HG22	1:D:315:VAL:HB	1.93	0.51
1:D:460:GLN:HE22	1:D:463:ILE:N	1.94	0.51
2:B:801:FDA:N5	3:B:802:G3F:H2	2.26	0.51
1:C:346:PRO:HG2	1:C:350:PRO:HA	1.93	0.50
1:B:159:ARG:HA	2:B:801:FDA:O2B	2.11	0.50
1:C:177:ARG:NH2	1:C:192:ASP:OD2	2.44	0.50
1:A:215:GLU:O	1:A:411:LYS:NZ	2.37	0.50
1:A:490:LYS:O	1:A:490:LYS:CE	2.59	0.49
1:C:283:CYS:HB3	1:C:298:LEU:HD11	1.95	0.49
1:B:169:THR:CG2	1:B:169:THR:O	2.60	0.49
1:D:185:LYS:HE3	1:D:557:PHE:CD2	2.48	0.49
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.78	0.49
1:A:95:GLU:HG3	1:B:112:MET:HE2	1.93	0.48
1:D:178:GLU:HG3	6:D:1140:HOH:O	2.14	0.48
1:A:490:LYS:HE2	1:A:490:LYS:C	2.38	0.48
1:B:89:HIS:CE1	1:B:91:LYS:HB2	2.49	0.48
1:A:120:THR:OG1	6:A:925:HOH:O	2.20	0.48
1:B:380:MET:HE1	1:B:409:ASN:HB3	1.95	0.48
1:C:385:THR:O	1:C:386:PRO:C	2.57	0.48
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.13	0.48
1:B:169:THR:O	1:B:169:THR:HG22	2.13	0.47
1:C:460:GLN:HE21	1:C:462:SER:CB	2.27	0.47
1:A:505:ARG:HD3	6:A:1120:HOH:O	2.15	0.47
1:C:421:GLU:H	1:C:421:GLU:CD	2.23	0.47
1:C:138:VAL:HG21	1:C:144:PRO:HG3	1.97	0.47
1:C:285:ARG:HA	1:C:328:LEU:HD11	1.96	0.47
1:C:329:LEU:HD11	1:C:580:LEU:CD1	2.44	0.47
1:C:548:HIS:CE1	3:C:802:G3F:HO2	2.27	0.47
1:D:554:ARG:O	1:D:564:CYS:HB2	2.15	0.47
1:B:126:LEU:CD1	1:B:132:GLN:CG	2.93	0.46
1:C:285:ARG:HA	1:C:328:LEU:CD1	2.45	0.46
1:B:167:HIS:CD2	1:B:167:HIS:C	2.93	0.46
1:C:399:ALA:O	5:C:803:MES:O3S	2.34	0.46
1:D:328:LEU:C	1:D:328:LEU:HD23	2.40	0.46
1:C:137:PHE:CE2	1:C:139:ARG:HG3	2.51	0.46
1:C:366:THR:HG21	1:C:526:SER:HB2	1.98	0.46
1:C:388:GLU:OE1	1:C:388:GLU:CA	2.63	0.46
1:C:317:VAL:HG12	1:C:319:THR:HG23	1.98	0.46
1:D:131:TRP:CZ3	1:D:133:ALA:HB2	2.50	0.46
1:D:126:LEU:HD13	1:D:132:GLN:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:SER:O	1:A:207:GLN:NE2	2.43	0.46
1:A:45:ILE:H	1:A:45:ILE:CD1	2.18	0.46
1:B:344:ASN:HD22	1:B:344:ASN:N	2.14	0.46
1:C:70:TYR:OH	1:C:610:LYS:HA	2.15	0.46
1:A:456:TYR:CD1	1:A:541:MET:HE2	2.52	0.45
1:C:270:ALA:HB1	1:C:273:GLU:CD	2.41	0.45
1:D:299:HIS:CE1	1:D:310:GLU:HG2	2.52	0.45
1:D:380:MET:HE1	1:D:409:ASN:CB	2.46	0.45
1:D:433:PRO:C	1:D:434:GLN:HG2	2.42	0.45
1:C:389:LEU:HD12	1:C:389:LEU:HA	1.65	0.45
1:C:293:SER:HA	1:C:574:GLY:O	2.16	0.45
1:C:608:TYR:CD1	1:C:608:TYR:C	2.95	0.44
1:B:532:PHE:CE1	1:B:538:PRO:HG3	2.51	0.44
1:B:548:HIS:CE1	3:B:802:G3F:HO2	2.31	0.44
1:C:167:HIS:CD2	1:C:167:HIS:C	2.95	0.44
1:C:382:ILE:HG12	1:C:393:VAL:HG22	2.00	0.44
1:B:380:MET:CE	1:B:409:ASN:OD1	2.66	0.43
1:B:444:PRO:HD2	1:B:445:TRP:CZ3	2.53	0.43
1:A:169:THR:HB	2:A:801:FDA:O4	2.19	0.43
1:D:487:PHE:HB3	1:D:498:PRO:HB2	1.99	0.43
1:B:159:ARG:C	1:B:160:VAL:HG13	2.43	0.43
1:C:81:ASP:O	1:C:83:GLY:N	2.48	0.43
5:A:804:MES:H82	1:B:462:SER:O	2.19	0.42
1:D:47:TYR:CD2	1:D:73:ALA:HB2	2.54	0.42
1:A:47:TYR:CD2	1:A:73:ALA:HB2	2.55	0.42
1:A:548:HIS:NE2	3:A:802:G3F:O2	2.38	0.42
1:B:555:MET:HA	1:B:566:VAL:O	2.19	0.42
1:C:532:PHE:CZ	1:C:538:PRO:HG3	2.55	0.42
1:D:437:THR:O	1:D:437:THR:HG23	2.20	0.42
1:A:95:GLU:CG	1:B:112:MET:HE2	2.50	0.42
1:C:70:TYR:O	1:C:72:VAL:HG23	2.20	0.42
1:C:284:GLU:C	1:C:328:LEU:HD11	2.44	0.42
1:B:366:THR:O	1:B:468:ILE:HA	2.20	0.41
1:A:120:THR:HA	1:A:136:PHE:CD1	2.55	0.41
1:B:451:ARG:CZ	6:B:1264:HOH:O	2.67	0.41
1:C:64:GLU:OE1	1:C:205:TYR:OH	2.32	0.41
1:C:449:ILE:HG12	1:C:471:TRP:CE3	2.56	0.41
2:D:801:FDA:C5X	3:D:802:G3F:H2	2.51	0.41
1:A:112:MET:HE3	1:B:102:LYS:HG3	2.03	0.41
5:A:804:MES:O3S	1:B:463:ILE:HD13	2.21	0.41
1:B:50:VAL:HG13	1:B:313:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:LEU:HB2	1:C:580:LEU:HD22	2.01	0.41
1:C:570:SER:HB3	1:C:580:LEU:O	2.20	0.41
1:D:349:LEU:N	1:D:350:PRO:HD3	2.35	0.41
1:C:89:HIS:ND1	1:C:91:LYS:HB3	2.36	0.41
1:D:380:MET:HE1	1:D:409:ASN:HB3	2.03	0.41
1:B:218:ARG:HD2	6:B:1034:HOH:O	2.22	0.40
2:C:801:FDA:H8A	6:C:933:HOH:O	2.20	0.40
1:A:214:LYS:HG3	1:A:215:GLU:HG3	2.03	0.40
1:B:449:ILE:HG12	1:B:471:TRP:CE3	2.56	0.40
1:B:439:PHE:CD1	1:B:439:PHE:C	3.00	0.40
1:D:353:GLY:O	1:D:484:LYS:HA	2.21	0.40
1:A:456:TYR:CG	1:A:541:MET:HE2	2.57	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	574/633 (91%)	560 (98%)	14 (2%)	0	100	100
1	B	574/633 (91%)	558 (97%)	16 (3%)	0	100	100
1	C	572/633 (90%)	551 (96%)	21 (4%)	0	100	100
1	D	573/633 (90%)	556 (97%)	17 (3%)	0	100	100
All	All	2293/2532 (91%)	2225 (97%)	68 (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	503/547 (92%)	489 (97%)	14 (3%)	38	41
1	B	503/547 (92%)	492 (98%)	11 (2%)	45	50
1	C	501/547 (92%)	489 (98%)	12 (2%)	43	47
1	D	502/547 (92%)	491 (98%)	11 (2%)	45	50
All	All	2009/2188 (92%)	1961 (98%)	48 (2%)	43	47

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	82	SER
1	A	185	LYS
1	A	247	SER
1	A	272	GLU
1	A	286	VAL
1	A	389	LEU
1	A	390	THR
1	A	401	THR
1	A	429	GLU
1	A	460	GLN
1	A	490	LYS
1	A	496	ASN
1	A	593	ASN
1	B	185	LYS
1	B	231	LYS
1	B	344	ASN
1	B	349	LEU
1	B	385	THR
1	B	400	SER
1	B	403	LYS
1	B	451	ARG
1	B	460	GLN
1	B	462	SER
1	B	576	LYS
1	C	82	SER
1	C	185	LYS
1	C	206	PHE

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Mol	Chain	Res	Type
1	C	228	GLU
1	C	272	GLU
1	C	330	VAL
1	C	386	PRO
1	C	388	GLU
1	C	403	LYS
1	C	496	ASN
1	C	560	LYS
1	C	610	LYS
1	D	45	ILE
1	D	81	ASP
1	D	139	ARG
1	D	201	LYS
1	D	231	LYS
1	D	269	ASP
1	D	272	GLU
1	D	460	GLN
1	D	576	LYS
1	D	593	ASN
1	D	619	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	257	ASN
1	A	263	GLN
1	A	419	HIS
1	A	460	GLN
1	B	105	ASN
1	B	110	GLN
1	B	237	GLN
1	B	257	ASN
1	B	263	GLN
1	B	341	ASN
1	B	344	ASN
1	B	418	GLN
1	B	419	HIS
1	B	461	GLN
1	B	611	GLN
1	C	105	ASN
1	C	132	GLN

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Mol	Chain	Res	Type
1	C	207	GLN
1	C	257	ASN
1	C	341	ASN
1	C	344	ASN
1	C	418	GLN
1	C	460	GLN
1	C	612	ASN
1	D	105	ASN
1	D	263	GLN
1	D	299	HIS
1	D	301	HIS
1	D	341	ASN
1	D	460	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](#)

17 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	$\# Z > 2$
3	G3F	C	802	-	12,12,12	1.20	1 (8%)	17,17,17	1.84	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MES	D	804	-	12,12,12	2.12	1 (8%)	15,16,16	1.81	5 (33%)
5	MES	B	804	-	12,12,12	1.81	1 (8%)	15,16,16	1.65	4 (26%)
3	G3F	A	802	-	12,12,12	1.17	2 (16%)	17,17,17	1.76	4 (23%)
4	12P	B	803	-	15,15,36	0.50	0	14,14,35	0.67	0
5	MES	D	803	-	12,12,12	2.00	2 (16%)	15,16,16	2.61	2 (13%)
4	12P	B	805	-	10,10,36	0.84	0	9,9,35	0.88	0
2	FDA	C	801	1	57,58,58	1.60	12 (21%)	78,89,89	2.35	32 (41%)
3	G3F	B	802	-	12,12,12	1.03	1 (8%)	17,17,17	3.08	4 (23%)
5	MES	C	803	-	12,12,12	2.31	1 (8%)	15,16,16	1.41	2 (13%)
4	12P	A	803	-	14,14,36	0.73	0	13,13,35	1.10	1 (7%)
2	FDA	A	801	1	57,58,58	1.55	7 (12%)	78,89,89	2.94	31 (39%)
4	12P	A	805	-	13,13,36	0.69	0	12,12,35	0.48	0
2	FDA	B	801	1	57,58,58	2.01	14 (24%)	78,89,89	2.42	28 (35%)
5	MES	A	804	-	12,12,12	2.10	2 (16%)	15,16,16	2.61	8 (53%)
2	FDA	D	801	1	57,58,58	1.52	13 (22%)	78,89,89	2.38	21 (26%)
3	G3F	D	802	-	12,12,12	0.90	0	17,17,17	1.48	2 (11%)

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	G3F	C	802	-	-	1/2/22/22	0/1/1/1
5	MES	D	804	-	-	2/6/14/14	0/1/1/1
5	MES	B	804	-	-	0/6/14/14	0/1/1/1
3	G3F	A	802	-	-	0/2/22/22	0/1/1/1
4	12P	B	803	-	-	3/13/13/34	-
5	MES	D	803	-	-	1/6/14/14	0/1/1/1
4	12P	B	805	-	-	4/8/8/34	-
2	FDA	C	801	1	-	0/34/50/50	0/6/6/6
3	G3F	B	802	-	-	0/2/22/22	0/1/1/1
5	MES	C	803	-	-	4/6/14/14	0/1/1/1
4	12P	A	803	-	-	3/12/12/34	-
2	FDA	A	801	1	-	1/34/50/50	0/6/6/6
4	12P	A	805	-	-	3/11/11/34	-
2	FDA	B	801	1	-	3/34/50/50	0/6/6/6
5	MES	A	804	-	-	1/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDA	D	801	1	-	3/34/50/50	0/6/6/6
3	G3F	D	802	-	-	0/2/22/22	0/1/1/1

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FDA	P-O3P	7.80	1.67	1.59
5	C	803	MES	C8-S	-7.55	1.67	1.77
5	D	804	MES	C8-S	-6.45	1.68	1.77
5	A	804	MES	C8-S	-5.98	1.69	1.77
5	D	803	MES	C8-S	-5.38	1.70	1.77
5	B	804	MES	C8-S	-5.26	1.70	1.77
2	B	801	FDA	C8A-N9A	-4.37	1.30	1.37
2	C	801	FDA	P-O3P	4.31	1.64	1.59
2	C	801	FDA	C5X-N5	-4.20	1.32	1.39
2	A	801	FDA	C2-N1	-4.20	1.30	1.37
2	A	801	FDA	C8A-N9A	-4.18	1.30	1.37
2	B	801	FDA	C8M-C8	4.14	1.58	1.51
2	B	801	FDA	C6-C5X	3.97	1.45	1.39
2	D	801	FDA	C5X-N5	-3.93	1.33	1.39
2	B	801	FDA	C5X-C9A	3.53	1.44	1.40
2	D	801	FDA	P-O3P	3.42	1.63	1.59
2	A	801	FDA	C4X-C4	3.27	1.51	1.41
2	A	801	FDA	P-O3P	3.27	1.63	1.59
2	D	801	FDA	C4'-C3'	3.27	1.59	1.53
5	A	804	MES	O1S-S	3.19	1.54	1.45
2	B	801	FDA	O4-C4	3.18	1.29	1.23
2	C	801	FDA	C6-C5X	3.14	1.44	1.39
2	C	801	FDA	O4B-C4B	-3.01	1.38	1.45
3	A	802	G3F	C3-C4	3.00	1.55	1.52
2	A	801	FDA	C4-N3	-3.00	1.33	1.38
2	B	801	FDA	O4B-C4B	-2.98	1.38	1.45
3	C	802	G3F	C3-C4	2.92	1.55	1.52
2	B	801	FDA	O3B-C3B	-2.88	1.35	1.43
2	C	801	FDA	C8A-N9A	-2.76	1.32	1.37
2	D	801	FDA	C3B-C4B	-2.72	1.46	1.53
2	B	801	FDA	C4'-C3'	2.69	1.58	1.53
2	B	801	FDA	C2A-N3A	2.65	1.38	1.33
2	C	801	FDA	C2B-C3B	-2.65	1.46	1.53
3	B	802	G3F	C3-C2	-2.57	1.50	1.52
2	D	801	FDA	C2B-C3B	-2.56	1.46	1.53
2	B	801	FDA	PA-O3P	2.48	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FDA	O3B-C3B	-2.47	1.36	1.43
2	D	801	FDA	C8A-N7A	2.47	1.36	1.31
2	A	801	FDA	C2A-N1A	2.44	1.38	1.33
2	D	801	FDA	C10-N10	-2.41	1.34	1.38
2	C	801	FDA	C2A-N1A	2.32	1.38	1.33
2	C	801	FDA	O2B-C2B	-2.31	1.37	1.43
2	D	801	FDA	C2A-N1A	2.29	1.38	1.33
2	A	801	FDA	C6-C7	2.28	1.42	1.39
2	B	801	FDA	C7M-C7	2.27	1.55	1.51
2	D	801	FDA	C6-C7	2.25	1.42	1.39
2	C	801	FDA	C8A-N7A	2.25	1.36	1.31
2	C	801	FDA	C4A-N9A	-2.24	1.33	1.37
2	C	801	FDA	C5'-C4'	2.22	1.54	1.51
3	A	802	G3F	O1-C1	2.18	1.46	1.39
5	D	803	MES	O1S-S	2.18	1.51	1.45
2	B	801	FDA	C2B-C3B	-2.17	1.47	1.53
2	D	801	FDA	PA-O3P	-2.16	1.57	1.59
2	D	801	FDA	O3B-C3B	-2.07	1.37	1.43
2	B	801	FDA	O4'-C4'	-2.04	1.39	1.43
2	D	801	FDA	C2B-C1B	-2.02	1.47	1.53
2	D	801	FDA	C8A-N9A	-2.01	1.34	1.37

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FDA	O4-C4-N3	9.73	138.41	120.11
2	A	801	FDA	C4-N3-C2	9.62	139.61	126.37
2	A	801	FDA	C4A-N9A-C8A	9.19	115.39	105.74
2	C	801	FDA	C4A-N9A-C8A	8.25	114.40	105.74
5	D	803	MES	O2S-S-C8	8.21	119.13	106.73
3	B	802	G3F	F3-C3-C2	-8.19	101.72	108.81
2	A	801	FDA	N3A-C2A-N1A	-7.86	116.69	128.58
3	B	802	G3F	F3-C3-C4	7.80	115.57	108.81
2	D	801	FDA	O4B-C1B-N9A	7.69	122.85	108.09
2	B	801	FDA	C4-N3-C2	7.43	136.60	126.37
2	B	801	FDA	C4A-N9A-C8A	7.12	113.22	105.74
2	D	801	FDA	C4A-N9A-C8A	6.52	112.58	105.74
2	D	801	FDA	C4-N3-C2	6.25	134.97	126.37
2	C	801	FDA	N9A-C8A-N7A	-6.08	105.30	113.94
2	D	801	FDA	N9A-C8A-N7A	-5.79	105.72	113.94
2	C	801	FDA	C2B-C1B-N9A	5.67	127.38	113.30
2	B	801	FDA	N3A-C2A-N1A	-5.66	120.01	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FDA	N3A-C2A-N1A	-5.56	120.17	128.58
2	A	801	FDA	N9A-C8A-N7A	-5.50	106.13	113.94
5	A	804	MES	O1S-S-C8	5.48	115.01	106.73
5	A	804	MES	O2S-S-C8	5.29	114.72	106.73
2	A	801	FDA	C7M-C7-C6	-4.96	110.83	119.57
2	A	801	FDA	C2B-C1B-N9A	4.94	125.59	113.30
2	C	801	FDA	N3A-C2A-N1A	-4.75	121.39	128.58
2	D	801	FDA	C2B-C1B-N9A	4.41	124.27	113.30
2	B	801	FDA	N9A-C8A-N7A	-4.40	107.70	113.94
2	B	801	FDA	O2P-P-O3P	-4.35	95.51	107.27
2	B	801	FDA	C2B-C1B-N9A	4.27	123.92	113.30
2	B	801	FDA	O4B-C4B-C5B	4.23	122.87	109.33
2	B	801	FDA	O2B-C2B-C1B	4.15	124.38	110.10
2	A	801	FDA	C4X-C4-N3	-4.04	101.04	112.13
5	D	804	MES	O2S-S-C8	-4.00	100.69	106.73
5	D	803	MES	O3S-S-C8	-3.96	98.25	106.00
5	B	804	MES	C6-C5-N4	3.96	116.14	110.12
3	D	802	G3F	F3-C3-C4	3.94	112.22	108.81
2	D	801	FDA	O4B-C4B-C5B	3.87	121.72	109.33
2	A	801	FDA	N3-C2-N1	-3.86	109.67	115.74
2	B	801	FDA	O2B-C2B-C3B	3.83	124.09	111.82
2	C	801	FDA	O2-C2-N1	-3.81	115.09	121.86
2	C	801	FDA	O2P-P-O3P	-3.71	97.24	107.27
2	D	801	FDA	N3A-C4A-N9A	3.68	133.43	127.17
3	C	802	G3F	C4-C3-C2	-3.63	107.28	111.50
2	D	801	FDA	O3B-C3B-C4B	3.61	121.45	111.08
2	A	801	FDA	C1B-N9A-C8A	-3.60	119.10	127.09
2	B	801	FDA	C1'-N10-C9A	3.60	127.63	120.63
2	C	801	FDA	O3P-P-O1P	3.59	121.51	110.70
3	B	802	G3F	O2-C2-C1	3.57	117.48	109.25
2	A	801	FDA	N3A-C4A-N9A	3.52	133.16	127.17
3	A	802	G3F	C3-C4-C5	3.52	113.85	109.68
2	D	801	FDA	C5A-C4A-N3A	-3.50	121.90	126.72
2	B	801	FDA	C5X-C9A-N10	3.49	121.96	118.01
2	A	801	FDA	C2A-N3A-C4A	3.46	120.28	111.83
2	C	801	FDA	O4-C4-C4X	-3.45	118.93	127.26
2	D	801	FDA	C9A-C5X-N5	-3.45	115.17	119.37
2	D	801	FDA	O2B-C2B-C1B	3.40	121.80	110.10
2	D	801	FDA	C5A-N7A-C8A	3.31	108.66	103.45
2	B	801	FDA	O4B-C1B-N9A	3.30	114.42	108.09
2	C	801	FDA	C4-C4X-N5	3.27	124.73	116.37
2	C	801	FDA	N3A-C4A-N9A	3.17	132.55	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	MES	O1-C2-C3	-3.14	105.00	111.77
2	C	801	FDA	O2-C2-N3	-3.11	116.34	121.86
5	C	803	MES	O2S-S-C8	3.10	111.41	106.73
5	D	804	MES	O1S-S-C8	-3.05	102.13	106.73
2	C	801	FDA	O4B-C4B-C5B	3.04	119.08	109.33
2	B	801	FDA	N3A-C4A-N9A	3.04	132.34	127.17
2	C	801	FDA	C1B-N9A-C8A	-3.03	120.38	127.09
2	B	801	FDA	C4X-C4-N3	-3.00	103.89	112.13
2	D	801	FDA	C5B-C4B-C3B	3.00	126.02	115.21
5	A	804	MES	O1-C6-C5	-3.00	105.31	111.77
2	A	801	FDA	C5A-C4A-N9A	-3.00	102.54	105.81
2	C	801	FDA	O2B-C2B-C1B	2.97	120.35	110.10
2	A	801	FDA	O2B-C2B-C3B	2.92	121.17	111.82
2	B	801	FDA	C2B-C3B-C4B	2.92	108.25	102.61
2	C	801	FDA	C5B-C4B-C3B	2.91	125.67	115.21
2	C	801	FDA	C4-N3-C2	-2.90	122.38	126.37
2	D	801	FDA	C2A-N3A-C4A	2.89	118.89	111.83
2	B	801	FDA	C4A-C5A-N7A	-2.89	107.28	110.58
3	C	802	G3F	O6-C6-C5	-2.89	101.49	111.33
2	A	801	FDA	O4-C4-C4X	-2.86	120.36	127.26
2	A	801	FDA	C5'-C4'-C3'	-2.86	106.83	112.22
3	C	802	G3F	C3-C4-C5	2.85	113.06	109.68
3	A	802	G3F	O2-C2-C3	2.84	114.87	109.63
2	B	801	FDA	O2-C2-N1	2.83	126.90	121.86
2	C	801	FDA	O4-C4-N3	-2.83	114.79	120.11
2	B	801	FDA	C1B-N9A-C8A	-2.82	120.83	127.09
2	B	801	FDA	C5A-N7A-C8A	2.82	107.88	103.45
2	A	801	FDA	C2A-N1A-C6A	2.81	123.34	118.73
5	D	804	MES	C6-C5-N4	2.80	114.38	110.12
2	C	801	FDA	O4B-C1B-C2B	2.79	112.59	106.62
2	B	801	FDA	O5'-C5'-C4'	-2.79	101.91	109.36
2	A	801	FDA	O4B-C4B-C5B	2.76	118.18	109.33
2	D	801	FDA	N3-C2-N1	-2.68	111.52	115.74
2	A	801	FDA	O4B-C4B-C3B	2.68	110.47	105.15
2	C	801	FDA	O4B-C4B-C3B	2.68	110.47	105.15
2	A	801	FDA	O4B-C1B-C2B	2.67	112.32	106.62
2	B	801	FDA	C5B-C4B-C3B	2.65	124.77	115.21
2	A	801	FDA	C9-C8-C7	-2.65	115.80	119.69
2	B	801	FDA	C9-C9A-C5X	-2.59	116.33	119.95
2	A	801	FDA	O2A-PA-O3P	2.58	114.25	107.27
2	C	801	FDA	C5X-C9A-N10	2.56	120.91	118.01
2	C	801	FDA	C5A-C4A-N3A	-2.56	123.20	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	G3F	O5-C1-C2	-2.55	105.82	110.30
5	A	804	MES	O3S-S-O2S	-2.53	105.08	111.40
3	A	802	G3F	C3-C2-C1	2.52	114.90	110.84
2	C	801	FDA	C5A-N7A-C8A	2.52	107.41	103.45
2	C	801	FDA	O2B-C2B-C3B	2.50	119.83	111.82
2	B	801	FDA	C7M-C7-C6	-2.49	115.18	119.57
3	C	802	G3F	F3-C3-C4	2.48	110.97	108.81
2	C	801	FDA	O2P-P-O1P	2.48	123.98	112.44
5	D	804	MES	C2-C3-N4	-2.47	106.37	110.12
2	D	801	FDA	O3'-C3'-C4'	-2.46	103.34	108.93
2	A	801	FDA	C9-C9A-N10	2.46	125.16	121.85
2	A	801	FDA	C5A-C4A-N3A	-2.45	123.34	126.72
2	C	801	FDA	C8M-C8-C9	-2.45	115.26	119.57
3	C	802	G3F	O5-C1-C2	2.44	114.59	110.30
5	B	804	MES	O1-C2-C3	-2.44	106.51	111.77
2	C	801	FDA	C9-C9A-N10	-2.42	118.60	121.85
2	B	801	FDA	C5A-C4A-N3A	-2.41	123.39	126.72
2	A	801	FDA	C9A-C9-C8	2.40	124.05	119.22
2	D	801	FDA	O3P-PA-O1A	-2.39	103.50	110.70
2	C	801	FDA	C4X-C4-N3	2.39	118.68	112.13
2	C	801	FDA	O4B-C1B-N9A	2.37	112.64	108.09
5	A	804	MES	C6-C5-N4	-2.35	106.55	110.12
2	A	801	FDA	C8M-C8-C9	-2.33	115.46	119.57
2	B	801	FDA	C2A-N3A-C4A	2.33	117.52	111.83
5	C	803	MES	O1S-S-C8	2.31	110.22	106.73
2	A	801	FDA	O2'-C2'-C3'	2.31	114.65	109.25
2	C	801	FDA	O3B-C3B-C4B	2.30	117.70	111.08
5	B	804	MES	O2S-S-C8	2.29	110.19	106.73
2	C	801	FDA	C2A-N3A-C4A	2.26	117.35	111.83
2	A	801	FDA	N6A-C6A-N1A	2.25	123.39	118.38
2	A	801	FDA	O3B-C3B-C4B	2.25	117.55	111.08
2	D	801	FDA	C4B-O4B-C1B	-2.24	104.52	109.47
2	B	801	FDA	N3-C2-N1	-2.24	112.22	115.74
5	A	804	MES	O3S-S-C8	-2.23	101.63	106.00
2	D	801	FDA	O2A-PA-O3P	2.23	113.30	107.27
5	A	804	MES	C2-C3-N4	-2.23	106.73	110.12
3	D	802	G3F	O5-C1-C2	-2.22	106.40	110.30
2	B	801	FDA	O4B-C1B-C2B	2.21	111.36	106.62
5	B	804	MES	O3S-S-O1S	-2.19	105.91	111.40
5	D	804	MES	O3S-S-O1S	2.18	116.86	111.40
2	A	801	FDA	C5B-C4B-C3B	2.17	123.03	115.21
2	D	801	FDA	O2A-PA-O1A	2.15	122.44	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FDA	O2A-PA-O1A	2.14	122.41	112.44
4	A	803	12P	C3-O4-C5	2.14	120.55	113.06
2	A	801	FDA	O3P-PA-O1A	-2.05	104.53	110.70
2	C	801	FDA	O2'-C2'-C3'	2.05	114.04	109.25
3	B	802	G3F	O4-C4-C5	2.04	114.36	109.32
2	B	801	FDA	O2A-PA-O3P	2.03	112.77	107.27
3	C	802	G3F	O1-C1-C2	-2.01	103.14	108.98

There are no chirality outliers.

All (29) torsion outliers are listed below:

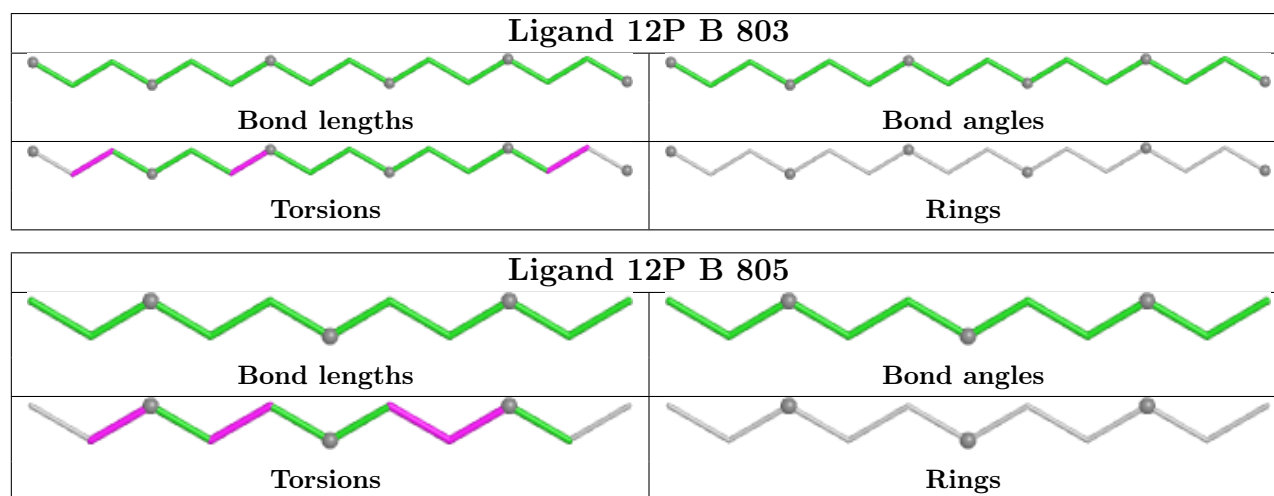
Mol	Chain	Res	Type	Atoms
2	B	801	FDA	PA-O3P-P-O5'
5	C	803	MES	N4-C7-C8-S
5	C	803	MES	C7-C8-S-O2S
5	D	803	MES	N4-C7-C8-S
5	D	804	MES	C8-C7-N4-C5
4	B	805	12P	O10-C11-C12-O13
4	B	803	12P	O13-C14-C15-O16
4	B	803	12P	O1-C2-C3-O4
4	A	805	12P	O13-C14-C15-O16
4	B	805	12P	C5-C6-O7-C8
4	A	805	12P	O10-C11-C12-O13
4	B	805	12P	O7-C8-C9-O10
3	C	802	G3F	C4-C5-C6-O6
2	D	801	FDA	PA-O3P-P-O5'
5	C	803	MES	C7-C8-S-O1S
4	A	803	12P	C15-C14-O13-C12
4	A	805	12P	O7-C8-C9-O10
2	D	801	FDA	O4B-C4B-C5B-O5B
4	B	803	12P	C5-C6-O7-C8
5	C	803	MES	C7-C8-S-O3S
2	B	801	FDA	P-O3P-PA-O1A
5	A	804	MES	N4-C7-C8-S
4	A	803	12P	C11-C12-O13-C14
4	B	805	12P	C11-C12-O13-C14
4	A	803	12P	O10-C11-C12-O13
5	D	804	MES	N4-C7-C8-S
2	B	801	FDA	P-O3P-PA-O2A
2	D	801	FDA	O4B-C1B-N9A-C8A
2	A	801	FDA	P-O3P-PA-O2A

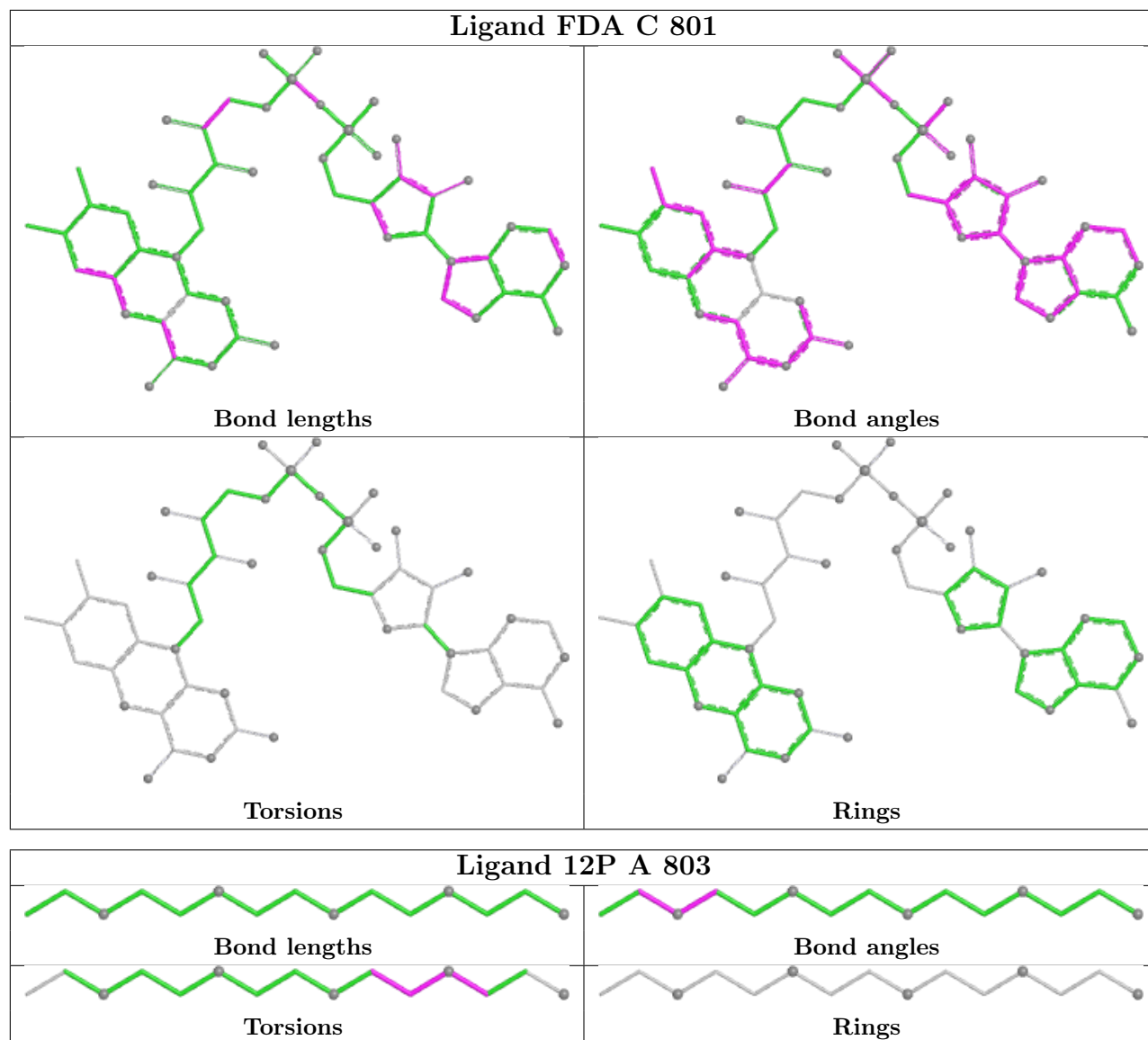
There are no ring outliers.

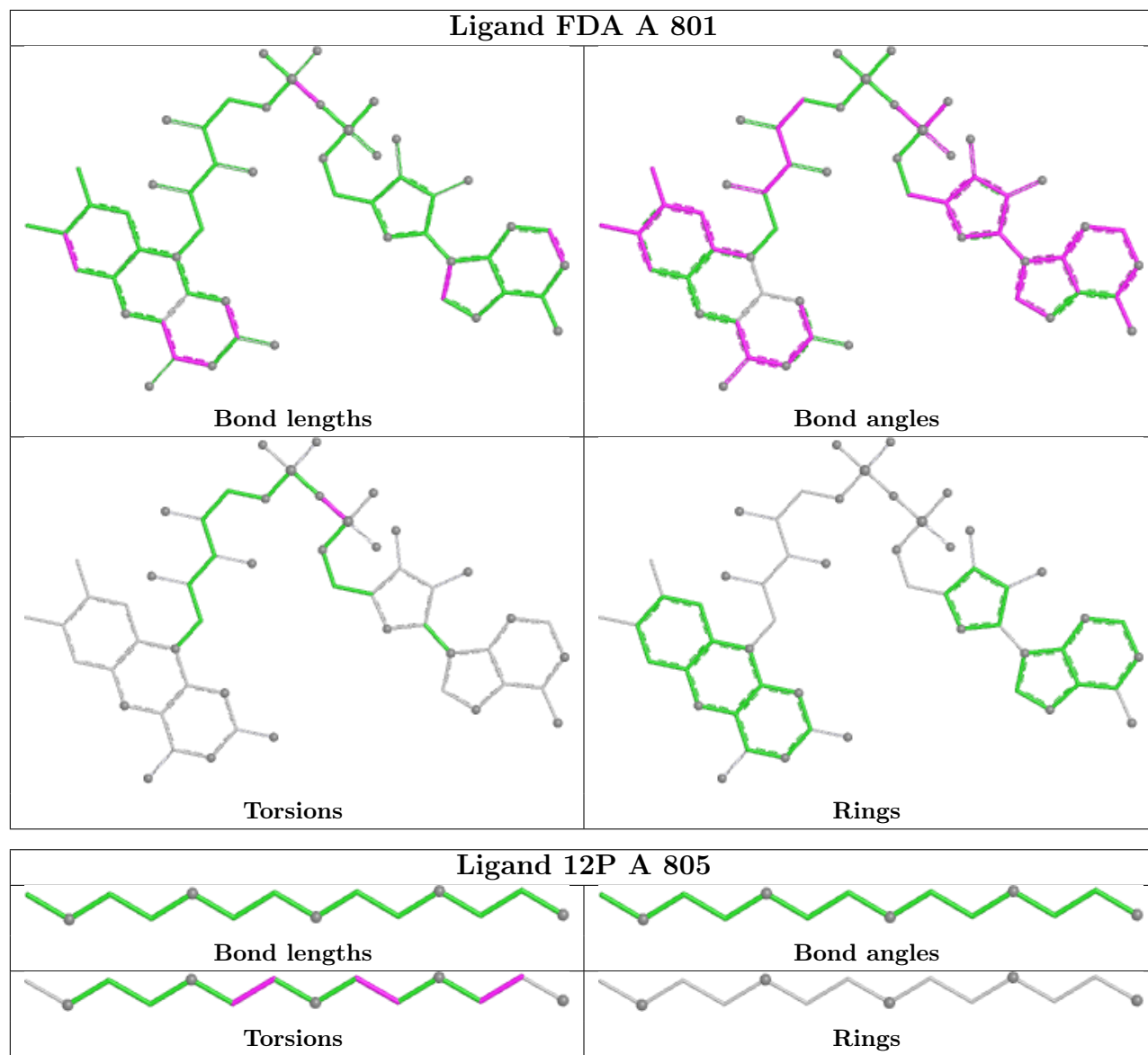
11 monomers are involved in 26 short contacts:

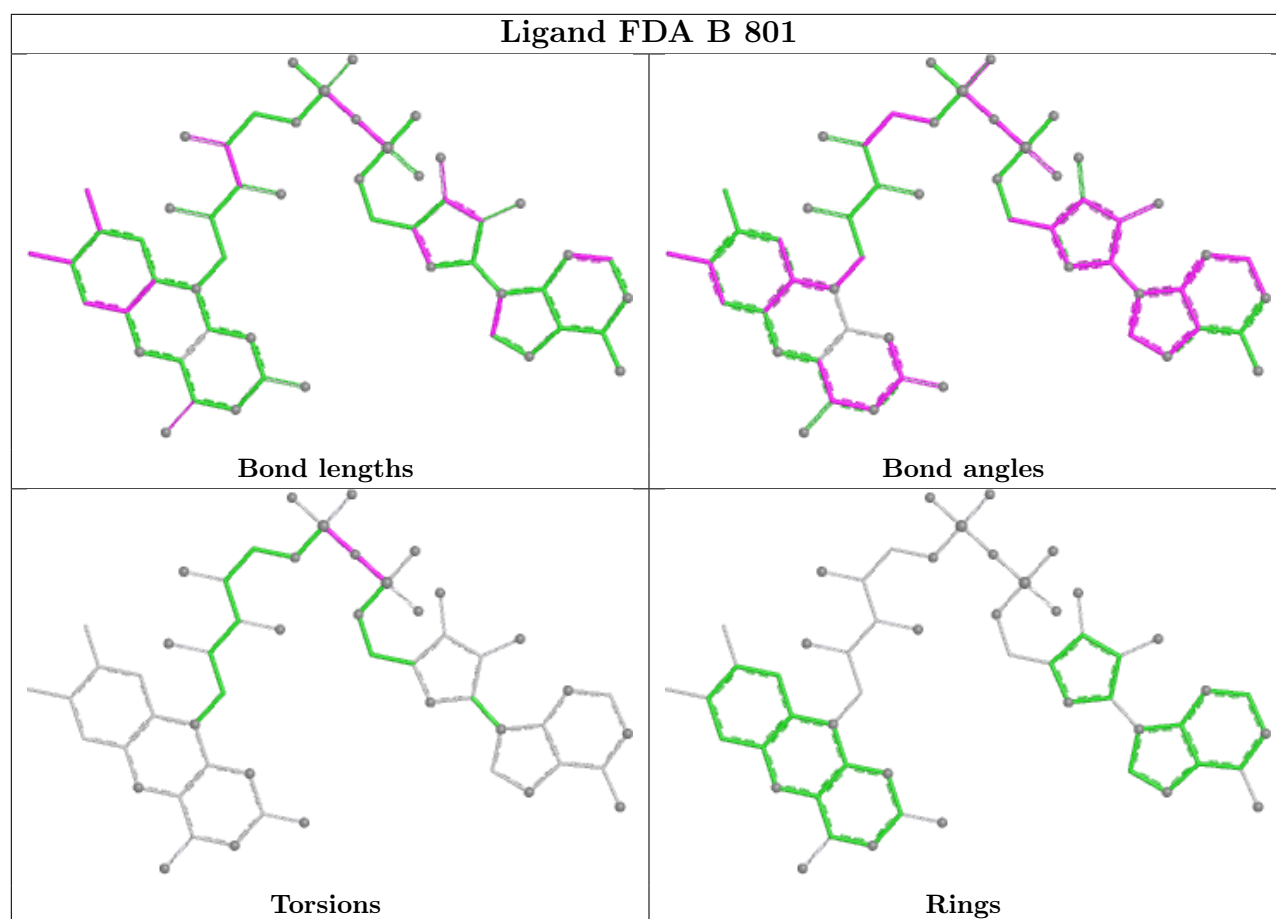
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	G3F	3	0
3	A	802	G3F	2	0
5	D	803	MES	1	0
2	C	801	FDA	3	0
3	B	802	G3F	2	0
5	C	803	MES	1	0
2	A	801	FDA	2	0
2	B	801	FDA	2	0
5	A	804	MES	10	0
2	D	801	FDA	3	0
3	D	802	G3F	2	0

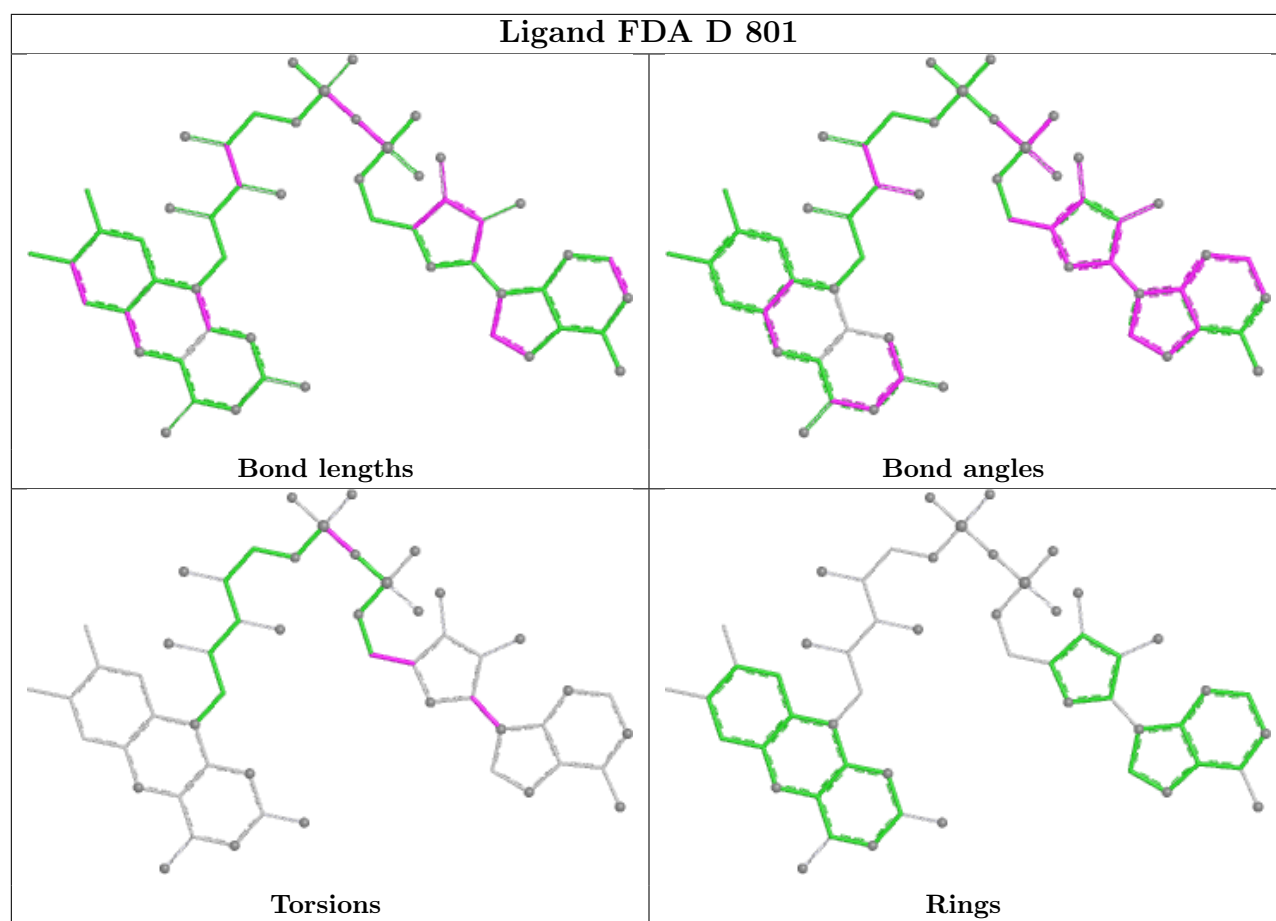
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	576/633 (90%)	-0.01	27 (4%) 36 35	12, 19, 43, 72	0
1	B	576/633 (90%)	-0.17	10 (1%) 69 68	11, 18, 34, 59	0
1	C	574/633 (90%)	0.48	30 (5%) 33 31	15, 33, 56, 81	0
1	D	575/633 (90%)	-0.03	15 (2%) 57 56	13, 23, 44, 71	0
All	All	2301/2532 (90%)	0.07	82 (3%) 46 45	11, 23, 49, 81	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	45	ILE	5.7
1	B	45	ILE	5.6
1	A	382	ILE	5.5
1	A	389	LEU	4.7
1	D	389	LEU	4.4
1	A	343	ALA	4.1
1	C	343	ALA	4.0
1	C	618	PHE	4.0
1	C	345	PRO	4.0
1	A	393	VAL	3.9
1	C	45	ILE	3.9
1	C	290	ALA	3.9
1	B	618	PHE	3.8
1	A	390	THR	3.6
1	C	82	SER	3.4
1	A	44	ASP	3.4
1	A	82	SER	3.3
1	A	387	GLY	3.2
1	B	343	ALA	3.2
1	A	618	PHE	3.1
1	A	384	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	385	THR	3.1
1	A	342	PRO	3.1
1	C	68	ALA	3.0
1	C	270	ALA	3.0
1	A	345	PRO	3.0
1	B	44	ASP	3.0
1	C	271	PRO	3.0
1	C	344	ASN	2.9
1	D	619	THR	2.9
1	B	342	PRO	2.9
1	A	388	GLU	2.9
1	D	345	PRO	2.8
1	D	347	GLU	2.8
1	C	48	ASP	2.8
1	C	291	LEU	2.8
1	D	459	VAL	2.8
1	D	343	ALA	2.7
1	B	100	ILE	2.7
1	C	81	ASP	2.7
1	D	344	ASN	2.7
1	B	268	THR	2.6
1	D	618	PHE	2.6
1	C	459	VAL	2.6
1	D	382	ILE	2.6
1	A	344	ASN	2.6
1	A	381	THR	2.6
1	A	385	THR	2.6
1	A	45	ILE	2.6
1	A	383	ARG	2.6
1	C	385	THR	2.6
1	D	342	PRO	2.6
1	A	310	GLU	2.5
1	C	296	GLU	2.5
1	A	417	MET	2.5
1	B	345	PRO	2.5
1	C	617	PRO	2.5
1	C	184	VAL	2.4
1	A	401	THR	2.4
1	D	383	ARG	2.4
1	C	268	THR	2.4
1	A	299	HIS	2.4
1	C	269	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	310	GLU	2.3
1	C	224	ASN	2.3
1	D	341	ASN	2.3
1	C	387	GLY	2.3
1	C	557	PHE	2.3
1	A	392	SER	2.2
1	A	100	ILE	2.2
1	C	342	PRO	2.2
1	C	346	PRO	2.2
1	A	101	ASP	2.2
1	D	101	ASP	2.2
1	C	100	ILE	2.1
1	A	83	GLY	2.1
1	C	67	GLY	2.1
1	C	285	ARG	2.1
1	B	43	MET	2.1
1	A	394	THR	2.1
1	C	186	ASP	2.1
1	C	69	GLY	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
5	MES	C	803	12/12	0.65	0.21	74,83,106,113	0
4	12P	B	805	11/37	0.73	0.21	38,44,46,47	0
5	MES	A	804	12/12	0.82	0.16	28,41,47,53	0
4	12P	A	803	15/37	0.84	0.16	27,32,45,47	0

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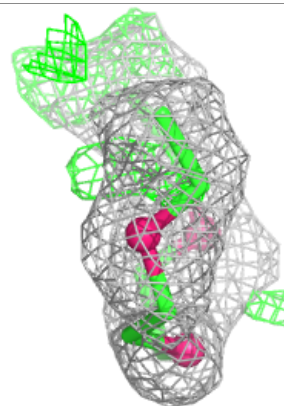
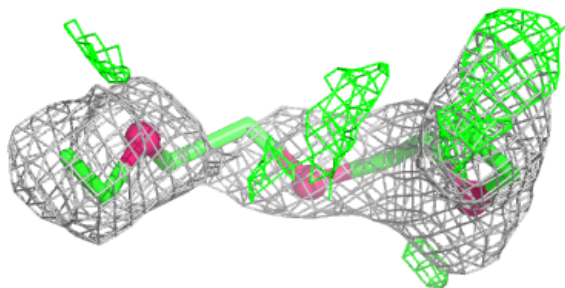
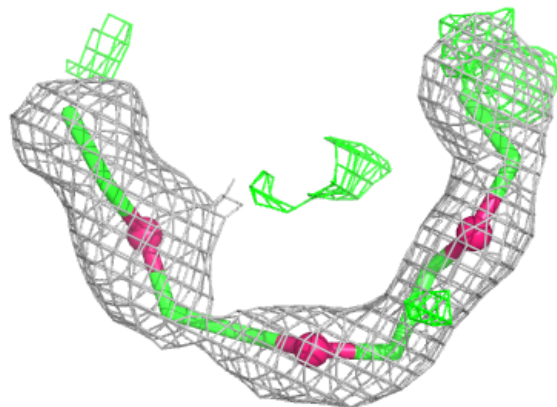
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MES	D	804	12/12	0.85	0.14	31,34,40,40	0
4	12P	A	805	14/37	0.88	0.12	27,32,37,39	0
3	G3F	C	802	12/12	0.89	0.10	29,35,37,38	0
4	12P	B	803	16/37	0.91	0.12	31,34,65,69	0
5	MES	D	803	12/12	0.94	0.10	24,30,32,33	0
3	G3F	A	802	12/12	0.94	0.07	20,22,25,26	0
2	FDA	C	801	53/53	0.95	0.07	16,24,29,33	0
3	G3F	D	802	12/12	0.95	0.07	23,24,28,28	0
5	MES	B	804	12/12	0.96	0.08	27,29,36,36	0
3	G3F	B	802	12/12	0.96	0.06	22,24,25,25	0
2	FDA	D	801	53/53	0.97	0.06	10,15,21,31	0
2	FDA	B	801	53/53	0.98	0.05	7,10,14,17	0
2	FDA	A	801	53/53	0.98	0.05	6,10,14,17	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.

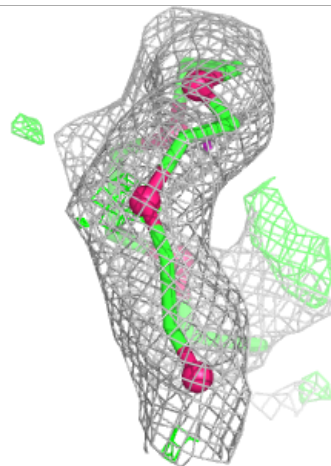
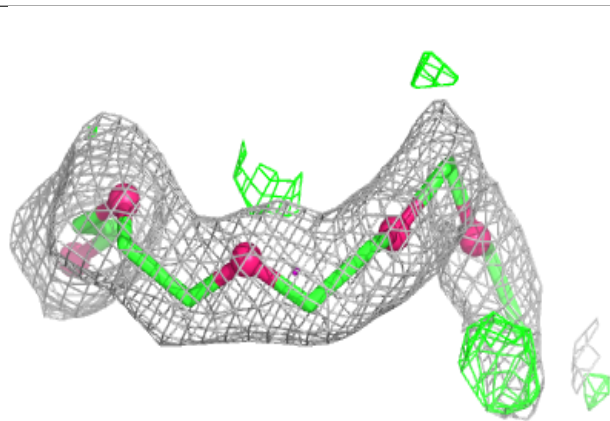
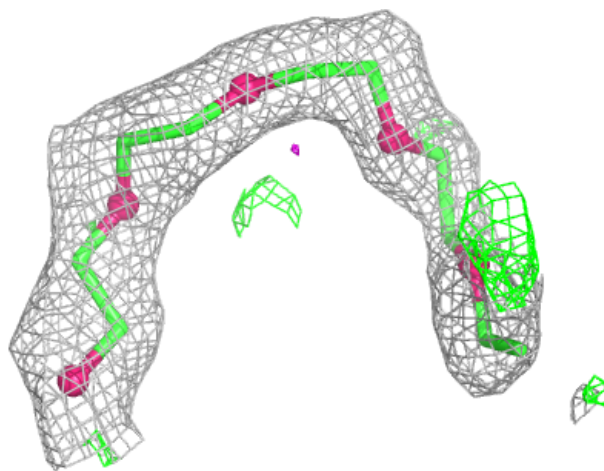
Electron density around 12P B 805:

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



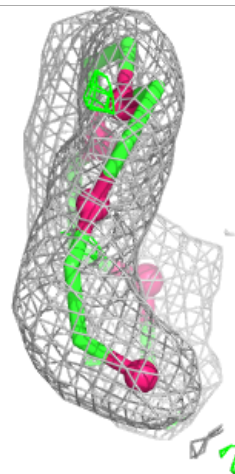
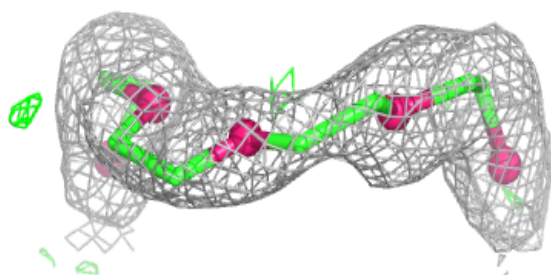
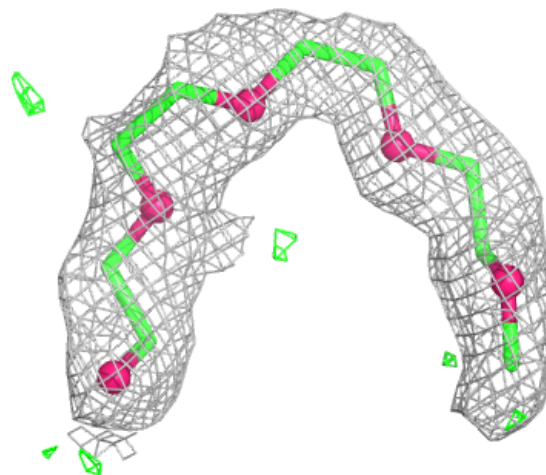
Electron density around 12P A 803:

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



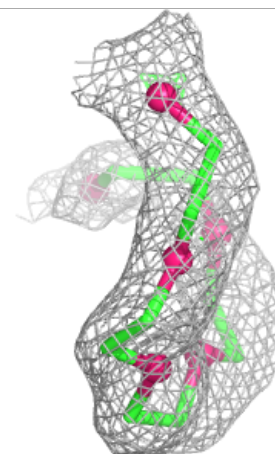
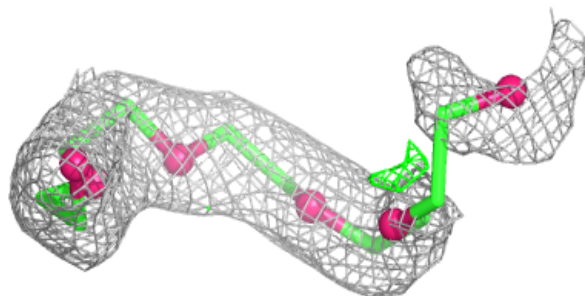
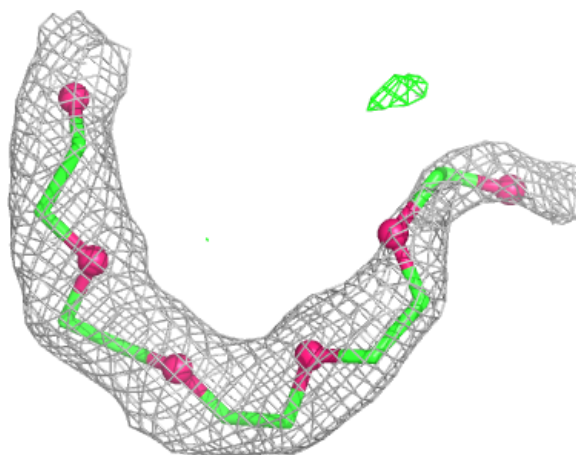
Electron density around 12P A 805:

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



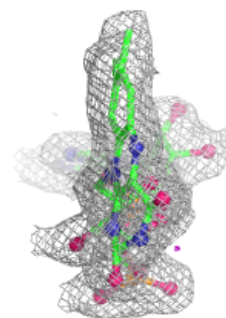
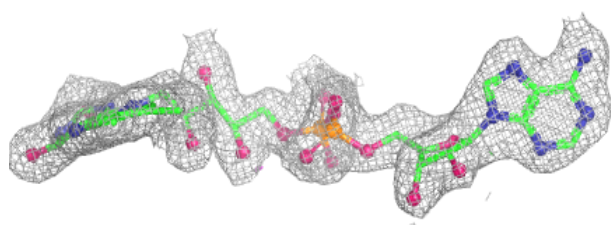
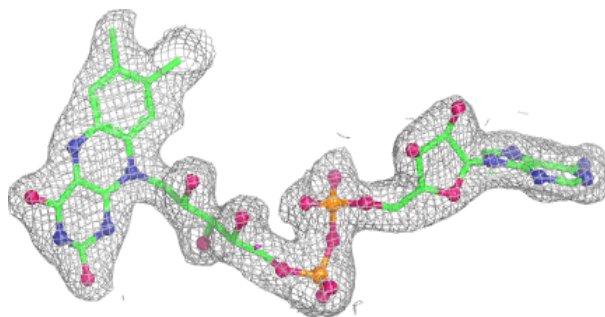
Electron density around 12P B 803:

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and green (positive)

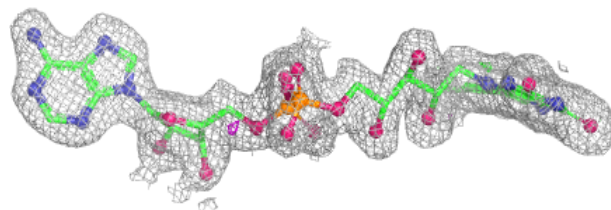
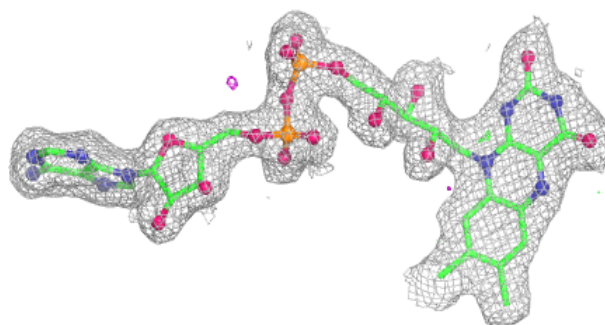


Electron density around FDA C 801:

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

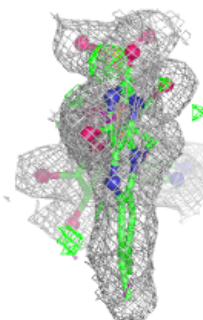
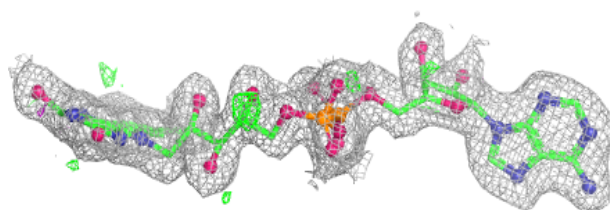
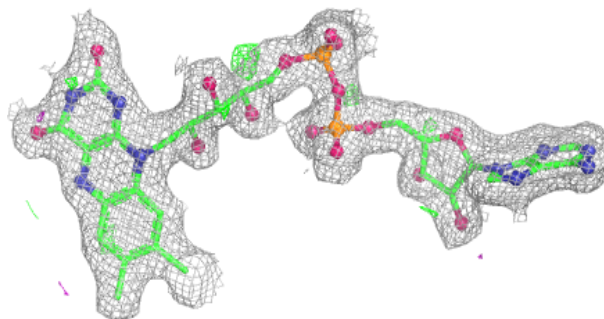
**Electron density around FDA D 801:**

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

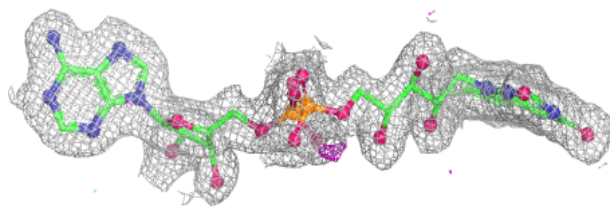
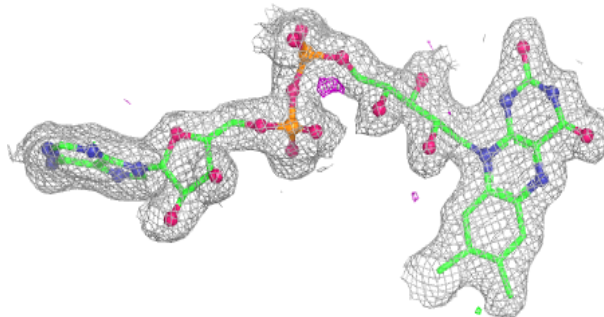


Electron density around FDA B 801:

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

**Electron density around FDA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.