



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:47 PM UTC

PDB ID : 4MOM / pdb_00004mom
Title : Pyranose 2-oxidase H450G mutant with 3-fluorinated galactose
Authors : Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.
Deposited on : 2013-09-12
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

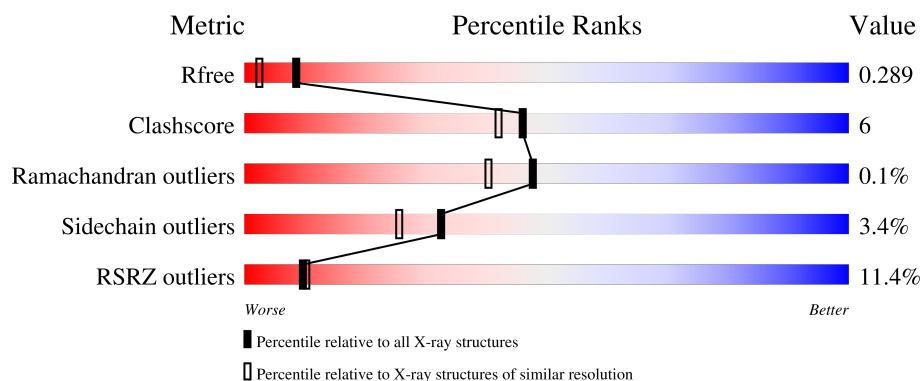
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	7% 77% 13% • 9%
1	B	633	6% 75% 15% • 9%
1	C	633	20% 73% 16% • 9%
1	D	633	9% 74% 15% • 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19522 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	574	Total	C	N	O	S	0	0	0
			4520	2855	773	868	24			

There are 52 discrepancies between the modelled and reference sequences:

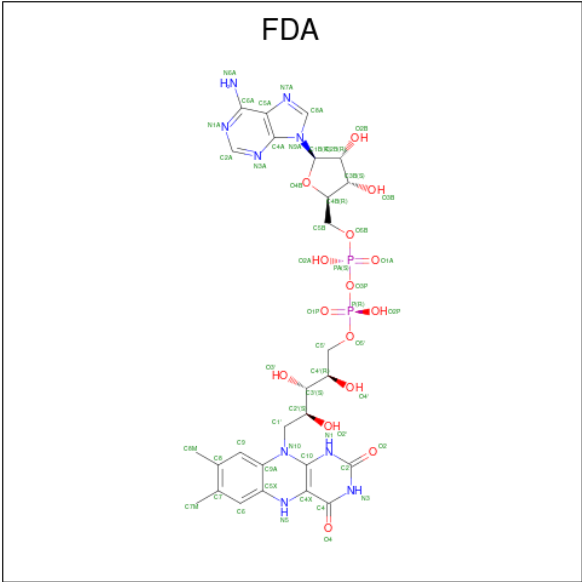
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	cloning artifact	UNP Q7ZA32
A	450	GLY	HIS	engineered mutation	UNP Q7ZA32
A	623	ALA	-	expression tag	UNP Q7ZA32
A	624	ALA	-	expression tag	UNP Q7ZA32
A	625	ALA	-	expression tag	UNP Q7ZA32
A	626	LEU	-	expression tag	UNP Q7ZA32
A	627	GLU	-	expression 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	cloning artifact	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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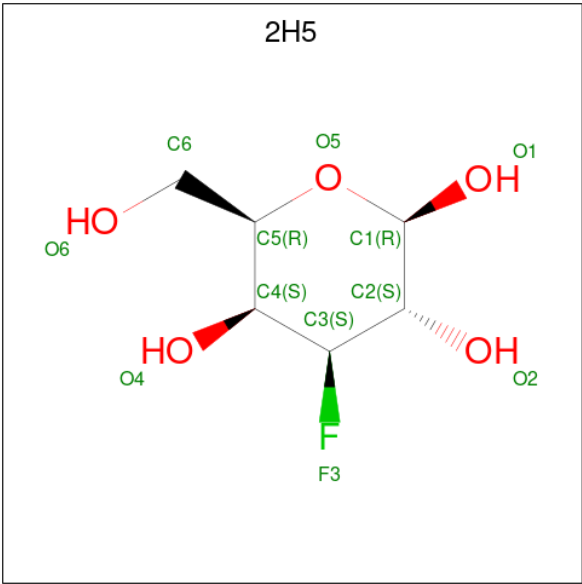
Chain	Residue	Modelled	Actual	Comment	Reference
B	629	HIS	-	expression tag	UNP Q7ZA32
B	630	HIS	-	expression tag	UNP Q7ZA32
B	631	HIS	-	expression tag	UNP Q7ZA32
B	632	HIS	-	expression tag	UNP Q7ZA32
B	633	HIS	-	expression tag	UNP Q7ZA32
C	2	ALA	SER	cloning artifact	UNP Q7ZA32
C	450	GLY	HIS	engineered 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	cloning artifact	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: $C_{27}H_{35}N_9O_{15}P_2$).



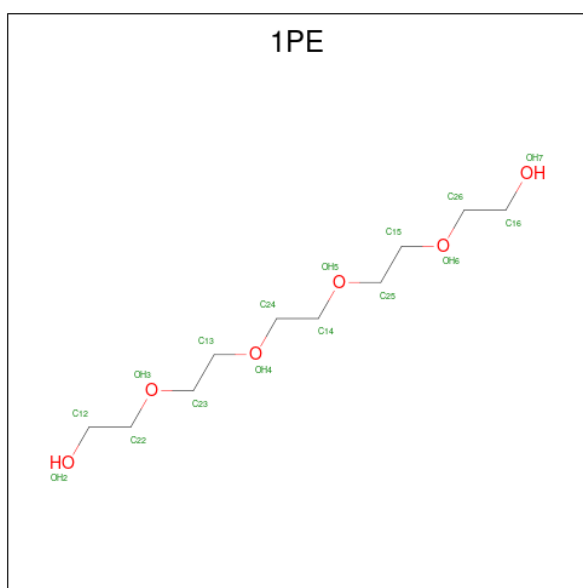
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 3-deoxy-3-fluoro-beta-D-galactopyranose (CCD ID: 2H5) (formula: C₆H₁₁FO₅).



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

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	8	4		
4	B	1	Total	C	O	0	0
			16	10	6		
4	C	1	Total	C	O	0	0
			16	10	6		
4	D	1	Total	C	O	0	0
			16	10	6		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	D	1	Total	C	N	O	S	0	0
			11	6	1	3	1		

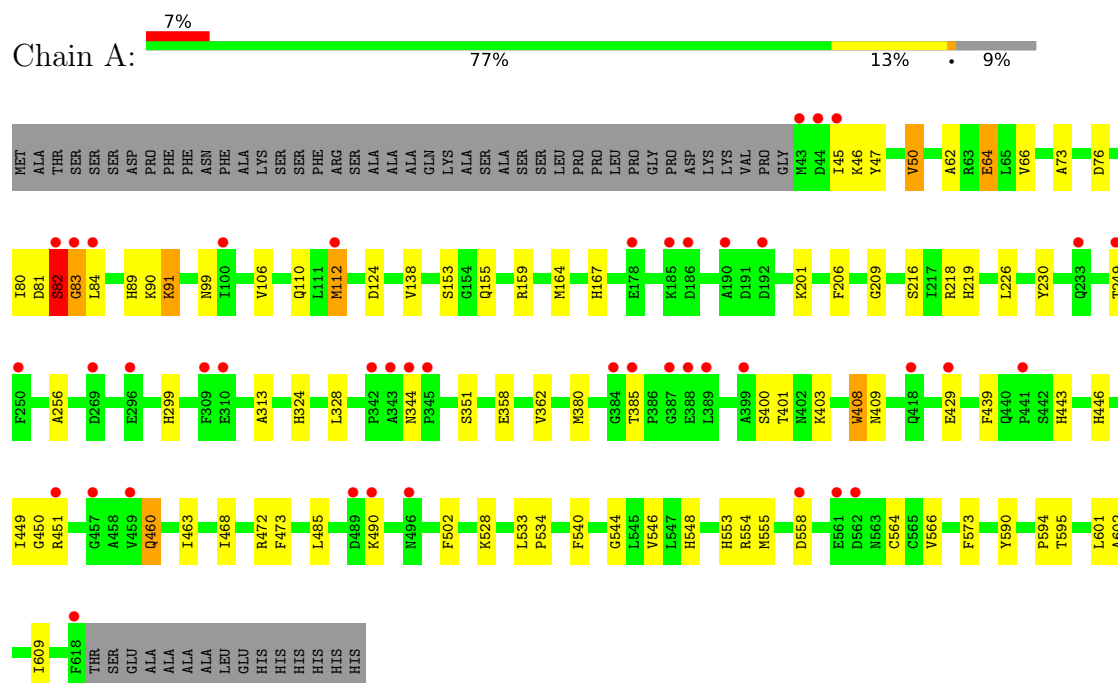
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	268	Total	O	0	0
			268	268		
6	B	348	Total	O	0	0
			348	348		
6	C	183	Total	O	0	0
			183	183		
6	D	268	Total	O	0	0
			268	268		

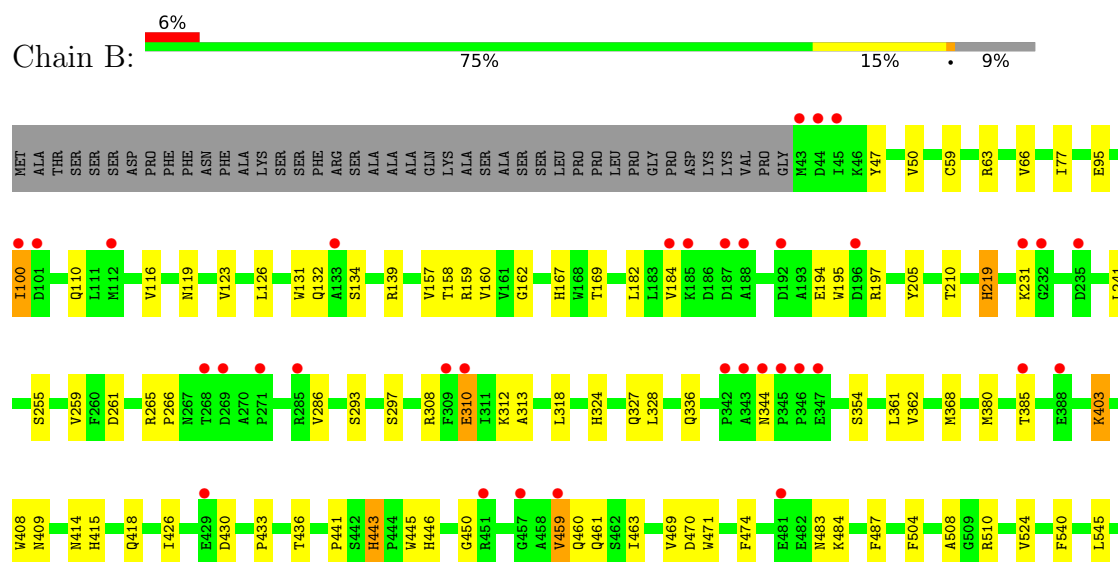
3 Residue-property plots [i](#)

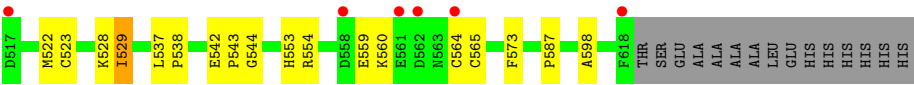
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.90Å 102.42Å 137.37Å 90.00° 91.19° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-1.90) 99.2 (50.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.238 , 0.280 0.247 , 0.289	Depositor DCC
R_{free} test set	3865 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l 0.001 for k,h,-l 0.020 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19522	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FDA, MES, 1PE, 2H5

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	1.35	23/4651 (0.5%)	1.21	7/6323 (0.1%)
1	B	1.39	20/4651 (0.4%)	1.24	19/6323 (0.3%)
1	C	1.14	7/4635 (0.2%)	1.11	6/6302 (0.1%)
1	D	1.24	8/4635 (0.2%)	1.13	17/6302 (0.3%)
All	All	1.28	58/18572 (0.3%)	1.17	49/25250 (0.2%)

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

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

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	597	THR	N-CA	-8.38	1.36	1.46
1	B	255	SER	C-O	-8.12	1.16	1.24
1	C	89	HIS	CG-ND1	-7.45	1.30	1.38
1	D	587	PRO	N-CA	-7.38	1.41	1.47
1	A	153	SER	C-O	-7.36	1.14	1.24
1	A	449	ILE	C-O	-6.91	1.16	1.24
1	A	164	MET	C-O	-6.65	1.15	1.24
1	A	443	HIS	C-O	6.29	1.31	1.24
1	D	318	LEU	C-O	-6.26	1.16	1.24
1	C	365	GLN	C-O	6.25	1.31	1.24
1	A	138	VAL	C-O	-6.23	1.17	1.24
1	B	459	VAL	C-O	-6.17	1.16	1.23
1	A	566	VAL	C-O	-6.11	1.17	1.23
1	A	553	HIS	CG-ND1	-6.08	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	HIS	CG-CD2	6.05	1.42	1.35
1	B	471	TRP	C-O	-6.04	1.17	1.24
1	D	50	VAL	C-O	-6.02	1.18	1.24
1	A	83	GLY	C-O	-6.02	1.17	1.24
1	B	286	VAL	C-O	-5.97	1.16	1.24
1	B	408	TRP	C-O	-5.79	1.17	1.24
1	B	572	VAL	C-O	5.76	1.30	1.24
1	A	609	ILE	N-CA	-5.72	1.39	1.46
1	B	443	HIS	CG-CD2	5.71	1.42	1.35
1	C	443	HIS	CG-CD2	5.70	1.42	1.35
1	D	404	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	408	TRP	NE1-CE2	-5.66	1.31	1.37
1	B	553	HIS	CE1-NE2	5.61	1.38	1.32
1	A	209	GLY	N-CA	5.59	1.50	1.45
1	B	241	LEU	C-O	-5.58	1.17	1.24
1	C	81	ASP	C-O	-5.54	1.17	1.24
1	B	131	TRP	NE1-CE2	-5.51	1.31	1.37
1	B	443	HIS	CE1-NE2	5.51	1.38	1.32
1	A	159	ARG	N-CA	-5.47	1.39	1.46
1	A	256	ALA	N-CA	-5.46	1.39	1.46
1	B	461	GLN	C-O	-5.44	1.16	1.24
1	B	195	TRP	NE1-CE2	-5.44	1.31	1.37
1	A	99	ASN	CA-C	-5.42	1.46	1.53
1	D	553	HIS	CA-C	-5.41	1.47	1.53
1	B	361	LEU	C-O	-5.39	1.17	1.24
1	A	80	ILE	C-O	-5.38	1.18	1.24
1	A	446	HIS	C-O	-5.32	1.17	1.23
1	D	278	PHE	C-O	-5.31	1.19	1.24
1	B	219	HIS	CG-ND1	-5.29	1.32	1.38
1	A	328	LEU	C-O	-5.24	1.18	1.24
1	B	510	ARG	N-CA	-5.24	1.40	1.46
1	D	386	PRO	C-O	-5.24	1.18	1.23
1	B	119	ASN	CA-C	-5.23	1.46	1.52
1	A	443	HIS	ND1-CE1	5.21	1.37	1.32
1	A	64	GLU	C-O	-5.17	1.18	1.24
1	C	554	ARG	CA-C	-5.15	1.46	1.53
1	A	50	VAL	CA-C	-5.12	1.46	1.52
1	C	89	HIS	CD2-NE2	-5.08	1.32	1.37
1	C	589	ALA	N-CA	-5.05	1.40	1.46
1	A	602	ALA	C-O	-5.03	1.18	1.24
1	A	573	PHE	CA-C	-5.02	1.46	1.52
1	B	415	HIS	CD2-NE2	-5.01	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	445	TRP	NE1-CE2	-5.01	1.31	1.37
1	D	286	VAL	C-O	-5.00	1.17	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	ILE	CA-C-N	-10.60	109.14	119.85
1	B	426	ILE	C-N-CA	-10.60	109.14	119.85
1	B	66	VAL	N-CA-C	-7.56	103.09	110.72
1	D	387	GLY	N-CA-C	7.46	125.94	115.43
1	C	81	ASP	N-CA-C	-7.09	95.70	110.80
1	B	426	ILE	N-CA-C	6.89	114.55	108.63
1	C	82	SER	N-CA-CB	6.88	122.09	111.84
1	B	430	ASP	CA-C-N	-6.79	113.31	120.03
1	B	430	ASP	C-N-CA	-6.79	113.31	120.03
1	B	586	ILE	CA-C-N	6.61	128.10	119.84
1	B	586	ILE	C-N-CA	6.61	128.10	119.84
1	D	598	ALA	N-CA-C	-6.39	104.40	111.36
1	B	116	VAL	CA-C-N	-6.33	113.03	120.11
1	B	116	VAL	C-N-CA	-6.33	113.03	120.11
1	D	388	GLU	N-CA-C	-6.19	99.52	108.07
1	B	508	ALA	N-CA-C	-6.09	102.64	110.19
1	D	409	ASN	N-CA-C	6.03	117.85	111.28
1	B	59	CYS	N-CA-C	5.92	118.52	111.71
1	D	106	VAL	CB-CA-C	-5.85	104.48	111.97
1	D	55	GLY	CA-C-N	5.84	125.71	119.28
1	D	55	GLY	C-N-CA	5.84	125.71	119.28
1	B	77	ILE	N-CA-C	-5.74	104.52	112.50
1	C	82	SER	CA-CB-OG	5.68	122.46	111.10
1	A	351	SER	N-CA-C	5.57	119.69	113.01
1	B	368	MET	N-CA-C	5.53	118.09	110.35
1	A	82	SER	N-CA-C	5.52	122.56	110.80
1	C	61	TYR	N-CA-C	-5.52	105.16	111.07
1	D	360	SER	N-CA-C	-5.52	101.54	110.32
1	D	186	ASP	N-CA-C	5.51	119.18	111.74
1	D	180	ARG	CA-C-N	-5.50	114.30	119.85
1	D	180	ARG	C-N-CA	-5.50	114.30	119.85
1	C	239	ILE	N-CA-C	-5.48	103.58	108.95
1	A	83	GLY	CA-C-O	-5.42	116.98	122.56
1	B	162	GLY	N-CA-C	-5.35	108.33	114.69
1	A	256	ALA	N-CA-C	-5.33	105.47	111.28
1	B	459	VAL	N-CA-C	5.27	115.95	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	596	LEU	N-CA-C	5.25	117.41	111.11
1	D	239	ILE	N-CA-C	-5.18	103.31	108.96
1	D	324	HIS	N-CA-C	5.17	118.74	112.23
1	A	219	HIS	N-CA-C	-5.16	105.55	111.07
1	B	524	VAL	N-CA-C	5.16	115.37	110.42
1	D	283	CYS	CA-CB-SG	-5.12	102.62	114.40
1	A	324	HIS	N-CA-C	5.11	118.67	112.23
1	D	470	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	582	GLY	N-CA-C	5.08	117.47	111.63
1	D	147	ASP	N-CA-C	-5.07	101.92	109.42
1	B	576	LYS	N-CA-C	5.06	117.46	111.33
1	D	430	ASP	N-CA-C	5.05	116.88	109.71
1	A	46	LYS	N-CA-C	5.00	117.55	109.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	436	THR	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	39	0
1	B	4536	0	4384	52	0
1	C	4520	0	4371	69	0
1	D	4520	0	4371	50	0
2	A	53	0	28	3	0
2	B	53	0	29	1	0
2	C	53	0	29	1	0
2	D	53	0	29	2	0
3	A	12	0	11	4	0
3	B	12	0	11	1	0
3	C	12	0	11	2	0
3	D	12	0	11	1	0
4	A	12	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	22	1	0
4	C	16	0	22	0	0
4	D	16	0	22	3	0
5	B	12	0	13	1	0
5	D	11	0	9	1	0
6	A	268	0	0	2	0
6	B	348	0	0	12	0
6	C	183	0	0	4	0
6	D	268	0	0	3	0
All	All	19522	0	17771	211	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 6.

All (211) 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)
5:D:804:MES:C2	5:D:804:MES:C6	2.11	1.26
1:C:361:LEU:HD22	1:C:546:VAL:HG22	1.38	1.02
1:B:110:GLN:HE21	1:B:167:HIS:HD1	1.07	0.96
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.14	0.93
1:A:460:GLN:HE22	1:A:463:ILE:H	0.93	0.92
1:C:68:ALA:HB2	1:C:610:LYS:HZ1	1.32	0.91
1:C:68:ALA:HB2	1:C:610:LYS:NZ	1.88	0.88
1:D:110:GLN:HE21	1:D:167:HIS:HD1	1.24	0.81
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.47	0.80
1:A:460:GLN:NE2	1:A:463:ILE:H	1.78	0.79
1:B:459:VAL:HG23	6:B:936:HOH:O	1.84	0.76
1:C:68:ALA:CB	1:C:610:LYS:NZ	2.49	0.75
1:B:418:GLN:HG3	6:B:1064:HOH:O	1.88	0.73
1:B:100:ILE:O	1:B:100:ILE:HD13	1.89	0.73
1:C:81:ASP:OD1	1:C:81:ASP:C	2.29	0.73
1:C:507:PRO:HD2	1:C:511:THR:HG21	1.72	0.72
1:D:421:GLU:OE1	1:D:421:GLU:N	2.20	0.71
1:D:432:GLU:OE1	1:D:432:GLU:N	2.24	0.70
1:C:68:ALA:CB	1:C:610:LYS:HZ3	2.04	0.69
1:D:382:ILE:CD1	1:D:416:MET:HE1	2.23	0.69
1:B:328:LEU:HD23	1:B:328:LEU:C	2.17	0.68
1:D:382:ILE:HD13	1:D:416:MET:HE1	1.74	0.68
1:D:489:ASP:OD1	1:D:489:ASP:C	2.37	0.68
1:C:218:ARG:HD2	6:C:1033:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:GLY:O	1:B:576:LYS:NZ	2.27	0.67
1:B:126:LEU:HD12	1:B:132:GLN:CG	2.25	0.66
2:C:801:FDA:N5	3:C:802:2H5:H1	2.11	0.66
1:C:361:LEU:CD2	1:C:546:VAL:HG22	2.19	0.65
1:A:460:GLN:HE22	1:A:463:ILE:N	1.79	0.64
1:C:157:VAL:HG21	1:C:324:HIS:CE1	2.30	0.64
1:C:177:ARG:HH22	1:C:188:ALA:HB1	1.63	0.64
1:D:169:THR:O	1:D:169:THR:HG22	1.98	0.63
1:C:53:GLY:O	1:C:74:MET:HE2	1.99	0.63
4:D:803:1PE:H251	4:D:803:1PE:OH7	1.99	0.62
1:A:81:ASP:OD1	1:A:82:SER:N	2.31	0.61
1:C:112:MET:HE2	1:D:95:GLU:HG3	1.81	0.61
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.48	0.61
1:B:545:LEU:HD12	6:B:1077:HOH:O	2.01	0.61
1:B:194:GLU:OE2	1:B:197:ARG:NH2	2.32	0.61
1:D:123:VAL:HG13	6:D:1110:HOH:O	2.01	0.60
1:D:157:VAL:HG11	1:D:324:HIS:CE1	2.37	0.60
2:D:801:FDA:N5	3:D:802:2H5:H1	2.17	0.60
4:D:803:1PE:H251	4:D:803:1PE:C16	2.30	0.59
1:B:336:GLN:NE2	1:B:344:ASN:O	2.35	0.59
1:D:318:LEU:HD13	1:D:328:LEU:HD22	1.84	0.59
1:C:81:ASP:OD1	1:C:82:SER:N	2.36	0.59
1:C:112:MET:HE2	1:D:95:GLU:CG	2.32	0.58
1:C:555:MET:HE2	1:C:567:ASN:O	2.02	0.58
1:B:443:HIS:NE2	6:B:1013:HOH:O	2.32	0.58
4:B:704:1PE:H152	6:B:1094:HOH:O	2.03	0.57
1:C:95:GLU:OE1	1:D:495:TYR:OH	2.21	0.57
1:C:47:TYR:CE2	1:C:73:ALA:HB2	2.38	0.57
1:A:230:TYR:OH	1:A:528:LYS:NZ	2.38	0.56
1:C:318:LEU:HD13	1:C:328:LEU:HD23	1.87	0.55
1:C:548:HIS:CE1	1:C:593:ASN:HA	2.41	0.55
1:B:126:LEU:HD12	1:B:132:GLN:HG3	1.89	0.55
1:B:403:LYS:HD2	6:B:1023:HOH:O	2.08	0.55
1:C:199:TYR:O	1:C:203:GLU:HG3	2.07	0.55
1:C:177:ARG:NH2	1:C:188:ALA:HB1	2.21	0.54
1:C:317:VAL:HG12	1:C:319:THR:HG23	1.88	0.54
1:D:381:THR:HB	1:D:394:THR:OG1	2.08	0.54
1:C:237:GLN:NE2	1:C:238:GLN:O	2.37	0.54
1:C:548:HIS:HE2	3:C:802:2H5:H9	1.55	0.54
1:B:414:ASN:O	1:B:418:GLN:HG2	2.08	0.54
1:C:228:GLU:OE1	1:C:229:GLU:OE2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:O	1:D:543:PRO:HD3	2.08	0.54
1:B:380:MET:HE1	1:B:409:ASN:HB3	1.88	0.54
1:D:47:TYR:CE2	1:D:73:ALA:HB2	2.43	0.53
1:B:297:SER:HB2	1:B:310:GLU:HG3	1.91	0.53
1:C:49:VAL:HB	1:C:72:VAL:HG22	1.91	0.53
1:D:375:SER:HA	6:D:1101:HOH:O	2.09	0.52
1:A:230:TYR:CZ	1:A:528:LYS:NZ	2.77	0.52
1:D:528:LYS:C	1:D:529:ILE:HD13	2.34	0.52
1:D:90:LYS:NZ	1:D:110:GLN:OE1	2.43	0.52
1:D:371:GLU:CD	6:D:1039:HOH:O	2.52	0.52
1:C:110:GLN:NE2	1:C:167:HIS:HD1	1.97	0.51
1:D:177:ARG:NH2	1:D:192:ASP:OD2	2.41	0.51
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.92	0.51
1:A:533:LEU:HD12	1:A:534:PRO:HD2	1.92	0.51
1:D:537:LEU:HB3	1:D:538:PRO:HD2	1.93	0.51
1:A:358:GLU:HG2	1:A:544:GLY:HA2	1.92	0.51
1:C:555:MET:HB2	1:C:566:VAL:HG23	1.92	0.51
1:A:548:HIS:NE2	3:A:802:2H5:O2	2.36	0.50
1:B:318:LEU:HD13	1:B:328:LEU:HD22	1.92	0.50
1:B:590:TYR:CZ	6:B:1002:HOH:O	2.55	0.50
1:A:554:ARG:O	1:A:564:CYS:HB2	2.11	0.50
1:C:361:LEU:HB2	1:C:546:VAL:HG21	1.94	0.50
1:B:483:ASN:OD1	1:B:504:PHE:HA	2.13	0.49
1:C:182:LEU:HD13	1:C:185:LYS:HA	1.95	0.49
1:A:450:GLY:C	1:A:451:ARG:HG2	2.38	0.49
1:C:183:LEU:O	1:C:184:VAL:HG23	2.13	0.49
1:C:555:MET:HE2	1:C:568:THR:HA	1.95	0.49
1:A:546:VAL:O	1:A:546:VAL:HG22	2.12	0.48
1:A:249:THR:HG21	1:A:429:GLU:OE2	2.13	0.48
1:C:267:ASN:O	1:C:268:THR:C	2.55	0.48
1:A:362:VAL:HG12	1:A:540:PHE:CD1	2.49	0.47
1:B:354:SER:OG	1:B:484:LYS:NZ	2.46	0.47
1:B:548:HIS:NE2	3:B:703:2H5:O2	2.47	0.47
1:C:418:GLN:NE2	6:C:1051:HOH:O	2.37	0.47
1:D:349:LEU:HD13	1:D:565:CYS:HB3	1.95	0.47
1:A:47:TYR:CE2	1:A:73:ALA:HB2	2.50	0.47
1:A:555:MET:HE1	1:A:601:LEU:HD22	1.97	0.47
1:C:347:GLU:HG3	1:C:348:LEU:HG	1.95	0.47
1:C:52:VAL:HG22	1:C:283:CYS:SG	2.54	0.47
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.96	0.47
1:D:317:VAL:HG12	1:D:319:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:MET:HE1	1:A:409:ASN:HB3	1.97	0.47
1:C:221:LEU:HD11	1:C:372:LEU:HD22	1.96	0.47
1:C:326:THR:HG22	1:C:487:PHE:HE2	1.80	0.46
1:D:216:SER:HB3	1:D:219:HIS:HB3	1.96	0.46
1:C:47:TYR:CD2	1:C:73:ALA:HB2	2.51	0.46
1:C:158:THR:HG22	1:C:160:VAL:HG22	1.97	0.46
1:D:47:TYR:CD2	1:D:73:ALA:HB2	2.50	0.46
1:D:157:VAL:HG11	1:D:324:HIS:HE1	1.80	0.46
1:D:529:ILE:HD13	1:D:529:ILE:N	2.30	0.46
1:D:382:ILE:HD11	1:D:416:MET:HE1	1.98	0.46
1:D:559:GLU:HG3	1:D:573:PHE:CD2	2.50	0.46
1:B:210:THR:HG23	6:B:1030:HOH:O	2.15	0.45
2:A:801:FDA:N5	3:A:802:2H5:H1	2.31	0.45
1:B:47:TYR:O	1:B:313:ALA:HA	2.15	0.45
1:C:361:LEU:HB2	1:C:546:VAL:CG2	2.45	0.45
1:A:548:HIS:CE1	3:A:802:2H5:O2	2.70	0.45
1:B:63:ARG:HD2	1:B:259:VAL:O	2.17	0.45
1:C:327:GLN:HB2	1:C:487:PHE:CE1	2.52	0.45
1:B:50:VAL:HG13	1:B:313:ALA:HB2	1.98	0.45
1:B:293:SER:O	1:B:576:LYS:HG2	2.16	0.45
1:D:554:ARG:O	1:D:564:CYS:HB2	2.17	0.45
1:D:300:ILE:HD11	1:D:309:PHE:HB2	1.99	0.45
1:A:439:PHE:C	1:A:439:PHE:CD1	2.95	0.44
1:A:548:HIS:CE1	3:A:802:2H5:H9	2.31	0.44
1:A:590:TYR:CD1	1:A:590:TYR:N	2.85	0.44
1:B:380:MET:HE3	1:B:409:ASN:OD1	2.17	0.44
1:C:452:ASP:HB2	1:C:472:ARG:NH1	2.32	0.44
1:B:446:HIS:HB3	1:B:474:PHE:HB2	1.99	0.44
1:C:319:THR:HG22	1:C:581:GLY:HA3	1.99	0.44
1:A:47:TYR:O	1:A:313:ALA:HA	2.18	0.44
1:B:219:HIS:HA	1:B:433:PRO:HB3	2.00	0.44
1:C:286:VAL:HG23	1:C:286:VAL:O	2.18	0.44
1:A:62:ALA:O	1:A:66:VAL:HG23	2.18	0.43
1:C:197:ARG:NE	6:C:1019:HOH:O	2.45	0.43
1:D:296:GLU:O	1:D:312:LYS:NZ	2.34	0.43
1:A:218:ARG:HD2	6:A:1045:HOH:O	2.17	0.43
1:C:158:THR:CG2	1:C:160:VAL:HG22	2.48	0.43
1:D:169:THR:O	1:D:169:THR:CG2	2.64	0.43
1:A:112:MET:HE2	1:B:95:GLU:HG3	2.00	0.43
1:B:327:GLN:HB2	1:B:487:PHE:CE1	2.53	0.43
1:C:255:SER:O	1:C:256:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:GLY:O	1:B:470:ASP:HB2	2.18	0.43
1:B:469:VAL:HG23	6:B:939:HOH:O	2.17	0.43
1:B:380:MET:HE1	1:B:409:ASN:CB	2.48	0.43
1:C:363:PHE:HA	1:C:471:TRP:O	2.19	0.43
1:D:101:ASP:OD1	1:D:101:ASP:N	2.49	0.43
1:B:126:LEU:HD12	1:B:132:GLN:HG2	1.98	0.43
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.83	0.43
1:D:465:SER:HA	1:D:468:ILE:HD12	2.01	0.43
1:C:59:CYS:HA	1:C:62:ALA:HB3	2.00	0.42
1:C:293:SER:HA	1:C:574:GLY:O	2.19	0.42
1:D:307:ASP:N	1:D:307:ASP:OD1	2.51	0.42
1:A:451:ARG:HD3	1:A:468:ILE:O	2.19	0.42
1:B:261:ASP:OD1	1:B:261:ASP:C	2.63	0.42
1:B:308:ARG:NH2	6:B:1024:HOH:O	2.53	0.42
1:C:437:THR:HG23	1:C:437:THR:O	2.20	0.42
1:C:478:GLU:OE2	1:C:480:LYS:HE2	2.20	0.42
1:C:586:ILE:HA	1:C:587:PRO:HD3	1.69	0.42
1:D:285:ARG:O	1:D:298:LEU:HD12	2.20	0.42
1:D:355:TYR:CZ	1:D:481:GLU:HB2	2.54	0.42
1:B:265:ARG:HA	1:B:266:PRO:C	2.45	0.42
1:A:590:TYR:CE2	1:A:594:PRO:HB3	2.55	0.42
1:D:382:ILE:HD13	1:D:416:MET:CE	2.48	0.42
1:A:81:ASP:O	1:A:83:GLY:N	2.46	0.42
1:C:206:PHE:CE2	1:C:599:MET:SD	3.13	0.42
1:C:421:GLU:H	1:C:421:GLU:CD	2.28	0.41
1:C:72:VAL:O	1:C:275:PHE:HA	2.20	0.41
1:C:339:ARG:HA	1:C:340:PRO:HD3	1.94	0.41
1:D:159:ARG:HA	2:D:801:FDA:O2B	2.21	0.41
1:D:339:ARG:O	1:D:340:PRO:C	2.63	0.41
1:B:182:LEU:HD22	1:B:184:VAL:O	2.20	0.41
1:B:403:LYS:CD	6:B:1023:HOH:O	2.66	0.41
1:C:102:LYS:HG3	1:D:112:MET:HE3	2.02	0.41
1:D:59:CYS:SG	1:D:262:LEU:HD21	2.61	0.41
1:D:389:LEU:HD23	1:D:389:LEU:HA	1.79	0.41
1:B:362:VAL:HG12	1:B:540:PHE:CD1	2.55	0.41
1:B:158:THR:HG22	1:B:160:VAL:HG22	2.01	0.41
1:A:595:THR:OG1	2:A:801:FDA:O2	2.37	0.41
1:B:169:THR:O	1:B:169:THR:HG22	2.19	0.41
1:C:599:MET:O	1:C:602:ALA:HB3	2.21	0.41
1:A:472:ARG:C	1:A:473:PHE:HD1	2.28	0.41
1:B:63:ARG:NE	1:B:205:TYR:CE1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:SER:O	1:D:139:ARG:HD2	2.21	0.41
1:D:152:LEU:HD12	1:D:502:PHE:CE1	2.56	0.41
1:D:522:MET:O	1:D:523:CYS:C	2.60	0.41
1:A:90:LYS:HD2	1:A:106:VAL:CG1	2.51	0.40
1:A:155:GLN:NE2	1:A:358:GLU:OE2	2.52	0.40
1:B:219:HIS:HB2	1:B:433:PRO:HA	2.04	0.40
1:C:197:ARG:NH2	1:C:607:GLU:OE2	2.54	0.40
4:D:803:1PE:C16	4:D:803:1PE:C25	2.96	0.40
1:A:89:HIS:CE1	1:A:91:LYS:HB2	2.56	0.40
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.96	0.40
6:A:949:HOH:O	1:B:123:VAL:HG21	2.21	0.40
1:B:159:ARG:HA	2:B:702:FDA:O2B	2.22	0.40
1:B:474:PHE:CD1	1:B:474:PHE:N	2.89	0.40
1:A:485:LEU:HD13	1:A:502:PHE:CE1	2.56	0.40
1:B:132:GLN:NE2	5:B:701:MES:O1S	2.50	0.40
1:B:460:GLN:OE1	1:B:463:ILE:N	2.35	0.40
1:C:197:ARG:NH2	6:C:1019:HOH:O	2.51	0.40
1:A:76:ASP:OD1	2:A:801:FDA:O2B	2.28	0.40
1:B:418:GLN:CG	6:B:1064:HOH:O	2.60	0.40
1:C:196:ASP:O	1:C:197:ARG:C	2.65	0.40
1:C:354:SER:OG	1:C:484:LYS:NZ	2.53	0.40
1:C:372:LEU:HD11	1:C:529:ILE:HD12	2.03	0.40
1:D:358:GLU:HG2	1:D:544:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	554 (96%)	19 (3%)	1 (0%)	43	36
1	B	574/633 (91%)	555 (97%)	19 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	572/633 (90%)	547 (96%)	24 (4%)	1 (0%)	43	36
1	D	572/633 (90%)	547 (96%)	25 (4%)	0	100	100
All	All	2292/2532 (90%)	2203 (96%)	87 (4%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	C	617	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	503/547 (92%)	484 (96%)	19 (4%)	29	21
1	B	503/547 (92%)	493 (98%)	10 (2%)	48	46
1	C	501/547 (92%)	482 (96%)	19 (4%)	29	21
1	D	501/547 (92%)	481 (96%)	20 (4%)	28	20
All	All	2008/2188 (92%)	1940 (97%)	68 (3%)	32	25

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	64	GLU
1	A	82	SER
1	A	84	LEU
1	A	91	LYS
1	A	112	MET
1	A	201	LYS
1	A	206	PHE
1	A	216	SER
1	A	299	HIS

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Mol	Chain	Res	Type
1	A	344	ASN
1	A	385	THR
1	A	400	SER
1	A	401	THR
1	A	403	LYS
1	A	408	TRP
1	A	460	GLN
1	A	490	LYS
1	A	558	ASP
1	B	100	ILE
1	B	134	SER
1	B	139	ARG
1	B	231	LYS
1	B	310	GLU
1	B	312	LYS
1	B	385	THR
1	B	403	LYS
1	B	441	PRO
1	B	587	PRO
1	C	45	ILE
1	C	50	VAL
1	C	79	GLU
1	C	82	SER
1	C	177	ARG
1	C	185	LYS
1	C	210	THR
1	C	216	SER
1	C	228	GLU
1	C	312	LYS
1	C	318	LEU
1	C	385	THR
1	C	492	THR
1	C	496	ASN
1	C	555	MET
1	C	560	LYS
1	C	576	LYS
1	C	586	ILE
1	C	593	ASN
1	D	45	ILE
1	D	101	ASP
1	D	201	LYS
1	D	204	SER

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Mol	Chain	Res	Type
1	D	206	PHE
1	D	217	ILE
1	D	231	LYS
1	D	341	ASN
1	D	344	ASN
1	D	347	GLU
1	D	377	LYS
1	D	385	THR
1	D	388	GLU
1	D	392	SER
1	D	403	LYS
1	D	460	GLN
1	D	462	SER
1	D	529	ILE
1	D	542	GLU
1	D	560	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	263	GLN
1	A	341	ASN
1	A	365	GLN
1	A	419	HIS
1	A	460	GLN
1	A	585	ASN
1	B	108	GLN
1	B	110	GLN
1	B	257	ASN
1	B	419	HIS
1	B	499	GLN
1	B	611	GLN
1	C	110	GLN
1	C	207	GLN
1	C	233	GLN
1	C	263	GLN
1	C	409	ASN
1	C	419	HIS
1	C	499	GLN
1	C	563	ASN
1	C	612	ASN

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Mol	Chain	Res	Type
1	D	105	ASN
1	D	132	GLN
1	D	299	HIS
1	D	324	HIS
1	D	419	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 ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	1PE	C	803	-	15,15,15	0.51	0	14,14,14	0.22	0
2	FDA	A	801	1	57,58,58	1.78	11 (19%)	78,89,89	2.66	24 (30%)
3	2H5	B	703	-	12,12,12	1.15	1 (8%)	17,17,17	2.35	7 (41%)
5	MES	B	701	-	12,12,12	2.48	1 (8%)	15,16,16	1.37	1 (6%)
2	FDA	B	702	1	57,58,58	1.90	16 (28%)	78,89,89	2.30	26 (33%)
2	FDA	C	801	1	57,58,58	1.57	10 (17%)	78,89,89	3.09	29 (37%)
4	1PE	A	803	-	11,11,15	0.68	0	10,10,14	0.26	0
4	1PE	D	803	-	15,15,15	0.62	0	14,14,14	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MES	D	804	-	10,10,12	2.05	1 (10%)	12,13,16	1.47	3 (25%)
4	1PE	B	704	-	15,15,15	0.63	0	14,14,14	0.28	0
3	2H5	C	802	-	12,12,12	0.83	0	17,17,17	2.77	7 (41%)
2	FDA	D	801	1	57,58,58	1.38	7 (12%)	78,89,89	2.60	28 (35%)
3	2H5	D	802	-	12,12,12	0.67	0	17,17,17	1.74	5 (29%)
3	2H5	A	802	-	12,12,12	1.14	1 (8%)	17,17,17	1.71	4 (23%)

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	1PE	C	803	-	-	6/13/13/13	-
2	FDA	A	801	1	-	1/34/50/50	0/6/6/6
3	2H5	B	703	-	-	0/2/22/22	0/1/1/1
5	MES	B	701	-	-	0/6/14/14	0/1/1/1
2	FDA	B	702	1	-	3/34/50/50	0/6/6/6
2	FDA	C	801	1	-	3/34/50/50	0/6/6/6
4	1PE	A	803	-	-	4/9/9/13	-
4	1PE	D	803	-	-	7/13/13/13	-
5	MES	D	804	-	-	2/10/10/14	-
4	1PE	B	704	-	-	7/13/13/13	-
3	2H5	C	802	-	-	2/2/22/22	0/1/1/1
2	FDA	D	801	1	-	1/34/50/50	0/6/6/6
3	2H5	D	802	-	-	2/2/22/22	0/1/1/1
3	2H5	A	802	-	-	0/2/22/22	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	701	MES	C8-S	-8.16	1.66	1.77
5	D	804	MES	C8-S	-6.18	1.68	1.77
2	B	702	FDA	PA-O3P	5.73	1.65	1.59
2	A	801	FDA	C2-N1	-4.53	1.30	1.37
2	A	801	FDA	C4A-N9A	-4.44	1.28	1.37
2	D	801	FDA	C4'-C3'	4.30	1.60	1.53
2	B	702	FDA	C2-N3	-4.13	1.30	1.37
2	B	702	FDA	C8A-N9A	-4.09	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FDA	C5X-N5	-4.02	1.33	1.39
2	C	801	FDA	C6-C5X	3.99	1.45	1.39
2	C	801	FDA	PA-O3P	3.94	1.63	1.59
2	A	801	FDA	O3B-C3B	-3.83	1.33	1.43
2	D	801	FDA	C8A-N9A	-3.81	1.31	1.37
2	B	702	FDA	O3B-C3B	-3.58	1.34	1.43
2	B	702	FDA	P-O3P	-3.43	1.55	1.59
2	C	801	FDA	C2A-N1A	3.41	1.40	1.33
2	A	801	FDA	C2'-C3'	-3.36	1.47	1.53
2	A	801	FDA	C1'-C2'	3.34	1.57	1.52
2	A	801	FDA	C5X-C9A	-3.29	1.36	1.40
2	B	702	FDA	C10-N1	-3.10	1.31	1.37
2	B	702	FDA	C4X-N5	-3.05	1.30	1.35
2	C	801	FDA	C8A-N9A	-2.95	1.32	1.37
2	C	801	FDA	C5X-C9A	2.85	1.43	1.40
2	B	702	FDA	C8A-N7A	2.85	1.37	1.31
2	C	801	FDA	C4X-C4	2.84	1.50	1.41
2	A	801	FDA	C5A-N7A	-2.83	1.33	1.39
2	B	702	FDA	O4B-C4B	-2.82	1.38	1.45
2	C	801	FDA	O4B-C4B	-2.80	1.38	1.45
2	C	801	FDA	C2A-N3A	2.65	1.38	1.33
2	A	801	FDA	C8A-N7A	2.63	1.36	1.31
3	A	802	2H5	C3-C4	2.60	1.55	1.52
2	B	702	FDA	C4X-C4	2.56	1.49	1.41
2	D	801	FDA	C2B-C3B	-2.54	1.46	1.53
2	D	801	FDA	C4X-C4	2.45	1.49	1.41
2	D	801	FDA	C5X-N5	-2.36	1.35	1.39
2	B	702	FDA	C5'-C4'	2.29	1.54	1.51
2	C	801	FDA	P-O3P	2.23	1.61	1.59
2	A	801	FDA	O4B-C4B	-2.22	1.40	1.45
3	B	703	2H5	C3-C2	-2.18	1.50	1.52
2	D	801	FDA	C2-N3	-2.16	1.33	1.37
2	B	702	FDA	PA-O1A	-2.13	1.43	1.50
2	B	702	FDA	O4B-C1B	-2.12	1.37	1.42
2	B	702	FDA	C2A-N1A	2.11	1.37	1.33
2	A	801	FDA	C6-C5X	2.10	1.42	1.39
2	B	702	FDA	C4A-N9A	-2.07	1.33	1.37
2	B	702	FDA	C7M-C7	-2.03	1.47	1.51
2	A	801	FDA	C2-N3	-2.03	1.34	1.37
2	D	801	FDA	C9A-N10	-2.02	1.37	1.41

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FDA	O4-C4-N3	-13.31	95.09	120.11
2	A	801	FDA	O4-C4-C4X	-12.08	98.14	127.26
2	C	801	FDA	C4A-N9A-C8A	11.28	117.58	105.74
3	C	802	2H5	F3-C3-C4	8.41	116.10	108.81
2	B	702	FDA	C4A-N9A-C8A	8.40	114.56	105.74
2	D	801	FDA	C4A-N9A-C8A	8.12	114.27	105.74
2	C	801	FDA	N9A-C8A-N7A	-7.36	103.50	113.94
2	D	801	FDA	N9A-C8A-N7A	-7.30	103.58	113.94
2	A	801	FDA	C4A-N9A-C8A	7.08	113.17	105.74
2	C	801	FDA	C4-N3-C2	-6.84	116.95	126.37
2	D	801	FDA	C2B-C1B-N9A	6.27	128.88	113.30
2	A	801	FDA	O4-C4-N3	6.20	131.76	120.11
2	D	801	FDA	O2B-C2B-C1B	6.18	131.38	110.10
2	C	801	FDA	C2B-C1B-N9A	5.95	128.09	113.30
2	A	801	FDA	C2B-C1B-N9A	5.95	128.08	113.30
2	C	801	FDA	N3A-C2A-N1A	-5.85	119.73	128.58
2	B	702	FDA	N9A-C8A-N7A	-5.80	105.71	113.94
2	B	702	FDA	N3A-C2A-N1A	-5.69	119.97	128.58
2	A	801	FDA	N9A-C8A-N7A	-5.67	105.90	113.94
2	D	801	FDA	C5A-N7A-C8A	5.62	112.29	103.45
2	A	801	FDA	N3A-C2A-N1A	-5.61	120.08	128.58
2	B	702	FDA	O2B-C2B-C3B	5.52	129.51	111.82
2	D	801	FDA	C4A-C5A-N7A	-5.02	104.84	110.58
2	D	801	FDA	N3A-C2A-N1A	-4.97	121.06	128.58
2	B	702	FDA	C2B-C1B-N9A	4.94	125.57	113.30
2	C	801	FDA	C5A-C4A-N9A	-4.87	100.50	105.81
2	D	801	FDA	O3B-C3B-C4B	4.80	124.86	111.08
2	C	801	FDA	N3A-C4A-N9A	4.63	135.05	127.17
3	A	802	2H5	F3-C3-C2	-4.58	104.84	108.81
2	B	702	FDA	C1'-N10-C9A	4.57	129.51	120.63
2	A	801	FDA	O4B-C1B-N9A	4.51	116.75	108.09
3	B	703	2H5	O5-C5-C4	4.46	117.73	109.70
2	D	801	FDA	C5B-C4B-C3B	4.36	130.90	115.21
2	C	801	FDA	O2B-C2B-C3B	4.34	125.72	111.82
3	B	703	2H5	F3-C3-C2	-4.25	105.14	108.81
2	B	702	FDA	O4B-C1B-N9A	4.13	116.03	108.09
3	D	802	2H5	F3-C3-C4	4.04	112.31	108.81
5	B	701	MES	O3S-S-C8	4.00	113.82	106.00
2	D	801	FDA	O4-C4-C4X	-3.96	117.72	127.26
3	B	703	2H5	C3-C4-C5	3.90	114.29	109.68
2	A	801	FDA	C6-C5X-C9A	-3.84	115.59	119.80
2	B	702	FDA	C7M-C7-C6	-3.84	112.81	119.57
2	D	801	FDA	C5A-C4A-N3A	-3.83	121.44	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	2H5	F3-C3-C2	-3.82	105.51	108.81
2	D	801	FDA	N3A-C4A-N9A	3.74	133.53	127.17
2	A	801	FDA	O2B-C2B-C1B	3.67	122.74	110.10
2	C	801	FDA	C4A-N9A-C1B	-3.58	118.27	126.63
3	B	703	2H5	C3-C2-C1	3.52	116.51	110.84
2	C	801	FDA	C5A-N7A-C8A	3.50	108.95	103.45
2	D	801	FDA	C1B-N9A-C8A	-3.45	119.44	127.09
2	C	801	FDA	O4-C4-C4X	-3.45	118.94	127.26
2	C	801	FDA	O2B-C2B-C1B	3.44	121.96	110.10
2	D	801	FDA	C5'-C4'-C3'	-3.42	105.76	112.22
3	C	802	2H5	O6-C6-C5	-3.40	99.76	111.33
2	A	801	FDA	C9-C8-C7	-3.40	114.70	119.69
2	A	801	FDA	O3P-PA-O1A	-3.37	100.56	110.70
2	B	702	FDA	C1B-N9A-C8A	-3.36	119.65	127.09
2	B	702	FDA	C5B-C4B-C3B	3.30	127.09	115.21
2	A	801	FDA	C5B-C4B-C3B	3.28	127.00	115.21
2	C	801	FDA	O2-C2-N1	-3.23	116.12	121.86
2	C	801	FDA	C5B-C4B-C3B	3.19	126.70	115.21
2	A	801	FDA	N3A-C4A-N9A	3.19	132.59	127.17
2	D	801	FDA	C4-N3-C2	-3.18	121.99	126.37
2	B	702	FDA	O4-C4-N3	-3.12	114.25	120.11
2	A	801	FDA	O2B-C2B-C3B	3.12	121.80	111.82
2	D	801	FDA	O4B-C1B-N9A	3.03	113.91	108.09
2	C	801	FDA	O4B-C1B-C2B	3.03	113.09	106.62
2	D	801	FDA	C2A-N3A-C4A	2.99	119.13	111.83
2	A	801	FDA	C5A-C4A-N3A	-2.94	122.66	126.72
2	B	702	FDA	O3B-C3B-C4B	2.91	119.43	111.08
2	A	801	FDA	O4B-C4B-C3B	2.88	110.86	105.15
2	A	801	FDA	O4B-C4B-C5B	2.85	118.46	109.33
2	B	702	FDA	O4B-C4B-C5B	2.81	118.33	109.33
3	B	703	2H5	F3-C3-C4	2.79	111.23	108.81
2	B	702	FDA	O2B-C2B-C1B	2.77	119.64	110.10
2	B	702	FDA	C5A-N7A-C8A	2.75	107.77	103.45
5	D	804	MES	O1S-S-C8	2.73	110.86	106.73
2	C	801	FDA	C4-C4X-N5	2.70	123.28	116.37
2	B	702	FDA	N3A-C4A-N9A	2.67	131.70	127.17
2	C	801	FDA	C7M-C7-C6	-2.66	114.88	119.57
2	A	801	FDA	O2P-P-O5'	2.63	119.47	107.57
2	C	801	FDA	C5X-C9A-N10	2.61	120.97	118.01
5	D	804	MES	O2S-S-C8	2.59	110.65	106.73
2	A	801	FDA	C2A-N3A-C4A	2.59	118.16	111.83
2	B	702	FDA	C2A-N3A-C4A	2.59	118.16	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	2H5	C3-C4-C5	-2.56	106.66	109.68
3	C	802	2H5	O5-C5-C4	2.45	114.12	109.70
3	D	802	2H5	O5-C5-C6	2.45	112.50	106.44
2	C	801	FDA	O3P-PA-O1A	-2.44	103.35	110.70
2	D	801	FDA	N6A-C6A-N1A	-2.44	112.94	118.38
3	B	703	2H5	C4-C3-C2	-2.44	108.67	111.50
2	C	801	FDA	C9-C9A-C5X	-2.43	116.56	119.95
2	A	801	FDA	C2A-N1A-C6A	2.42	122.70	118.73
2	D	801	FDA	C4-C4X-N5	2.42	122.55	116.37
2	D	801	FDA	O2A-PA-O1A	2.40	123.59	112.44
3	D	802	2H5	O4-C4-C3	2.39	114.04	109.63
2	D	801	FDA	O4B-C4B-C3B	2.38	109.87	105.15
2	D	801	FDA	O4-C4-N3	2.36	124.55	120.11
3	C	802	2H5	C3-C2-C1	2.35	114.63	110.84
2	D	801	FDA	C5A-C6A-N6A	2.33	129.06	123.29
2	C	801	FDA	N6A-C6A-N1A	2.29	123.49	118.38
2	D	801	FDA	O4B-C1B-C2B	2.28	111.49	106.62
2	C	801	FDA	O3B-C3B-C4B	2.25	117.54	111.08
2	C	801	FDA	O2A-PA-O1A	2.25	122.89	112.44
2	B	702	FDA	O5'-P-O1P	-2.22	100.14	108.94
2	B	702	FDA	O3P-PA-O1A	-2.21	104.04	110.70
2	C	801	FDA	O4B-C4B-C3B	2.21	109.53	105.15
3	D	802	2H5	C3-C4-C5	-2.20	107.08	109.68
2	B	702	FDA	O2-C2-N3	-2.18	117.98	121.86
2	A	801	FDA	C6-C5X-N5	2.18	123.54	119.76
2	B	702	FDA	C5X-C6-C7	-2.18	115.28	119.92
3	C	802	2H5	C6-C5-C4	2.17	118.36	113.02
2	D	801	FDA	N3-C2-N1	2.15	119.12	115.74
2	B	702	FDA	O2A-PA-O3P	2.15	113.09	107.27
3	A	802	2H5	F3-C3-C4	2.15	110.68	108.81
2	A	801	FDA	C1B-N9A-C8A	-2.15	122.32	127.09
5	D	804	MES	O3S-S-O2S	-2.14	106.05	111.40
3	A	802	2H5	O2-C2-C1	2.14	114.17	109.25
3	B	703	2H5	O1-C1-C2	-2.11	102.86	108.98
2	C	801	FDA	C2A-N3A-C4A	2.10	116.96	111.83
2	D	801	FDA	O3'-C3'-C4'	-2.08	104.20	108.93
2	C	801	FDA	C2A-N1A-C6A	2.08	122.15	118.73
2	C	801	FDA	O3B-C3B-C2B	2.08	118.49	111.82
3	A	802	2H5	O2-C2-C3	2.08	113.47	109.63
2	A	801	FDA	C9A-C9-C8	2.07	123.39	119.22
3	D	802	2H5	C3-C2-C1	2.07	114.17	110.84
2	B	702	FDA	C5A-C4A-N9A	-2.06	103.56	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	FDA	C5A-C4A-N3A	-2.05	123.89	126.72
2	D	801	FDA	C6A-C5A-N7A	2.05	136.05	132.09
2	C	801	FDA	O2A-PA-O3P	2.05	112.82	107.27
2	A	801	FDA	O4'-C4'-C3'	2.04	114.02	109.25
2	D	801	FDA	O3P-P-O1P	2.03	116.82	110.70
2	B	702	FDA	C4A-C5A-N7A	-2.01	108.28	110.58
2	B	702	FDA	C4-N3-C2	2.01	129.13	126.37

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	801	FDA	PA-O3P-P-O5'
3	C	802	2H5	O5-C5-C6-O6
4	D	803	1PE	OH7-C16-C26-OH6
4	A	803	1PE	OH6-C15-C25-OH5
4	D	803	1PE	OH2-C12-C22-OH3
4	B	704	1PE	OH6-C15-C25-OH5
3	D	802	2H5	O5-C5-C6-O6
4	C	803	1PE	OH2-C12-C22-OH3
4	C	803	1PE	OH4-C13-C23-OH3
5	D	804	MES	N4-C7-C8-S
4	B	704	1PE	OH2-C12-C22-OH3
2	B	702	FDA	C3B-C4B-C5B-O5B
4	D	803	1PE	OH4-C13-C23-OH3
4	B	704	1PE	OH5-C14-C24-OH4
4	D	803	1PE	C25-C15-OH6-C26
2	B	702	FDA	PA-O3P-P-O5'
2	D	801	FDA	PA-O3P-P-O5'
3	C	802	2H5	C4-C5-C6-O6
4	A	803	1PE	C23-C13-OH4-C24
4	C	803	1PE	C13-C23-OH3-C22
4	A	803	1PE	C15-C25-OH5-C14
4	B	704	1PE	OH7-C16-C26-OH6
4	C	803	1PE	OH6-C15-C25-OH5
4	C	803	1PE	C16-C26-OH6-C15
4	A	803	1PE	C24-C14-OH5-C25
4	C	803	1PE	C14-C24-OH4-C13
2	A	801	FDA	C3B-C4B-C5B-O5B
4	D	803	1PE	C12-C22-OH3-C23
5	D	804	MES	C2-C3-N4-C5
4	D	803	1PE	OH5-C14-C24-OH4

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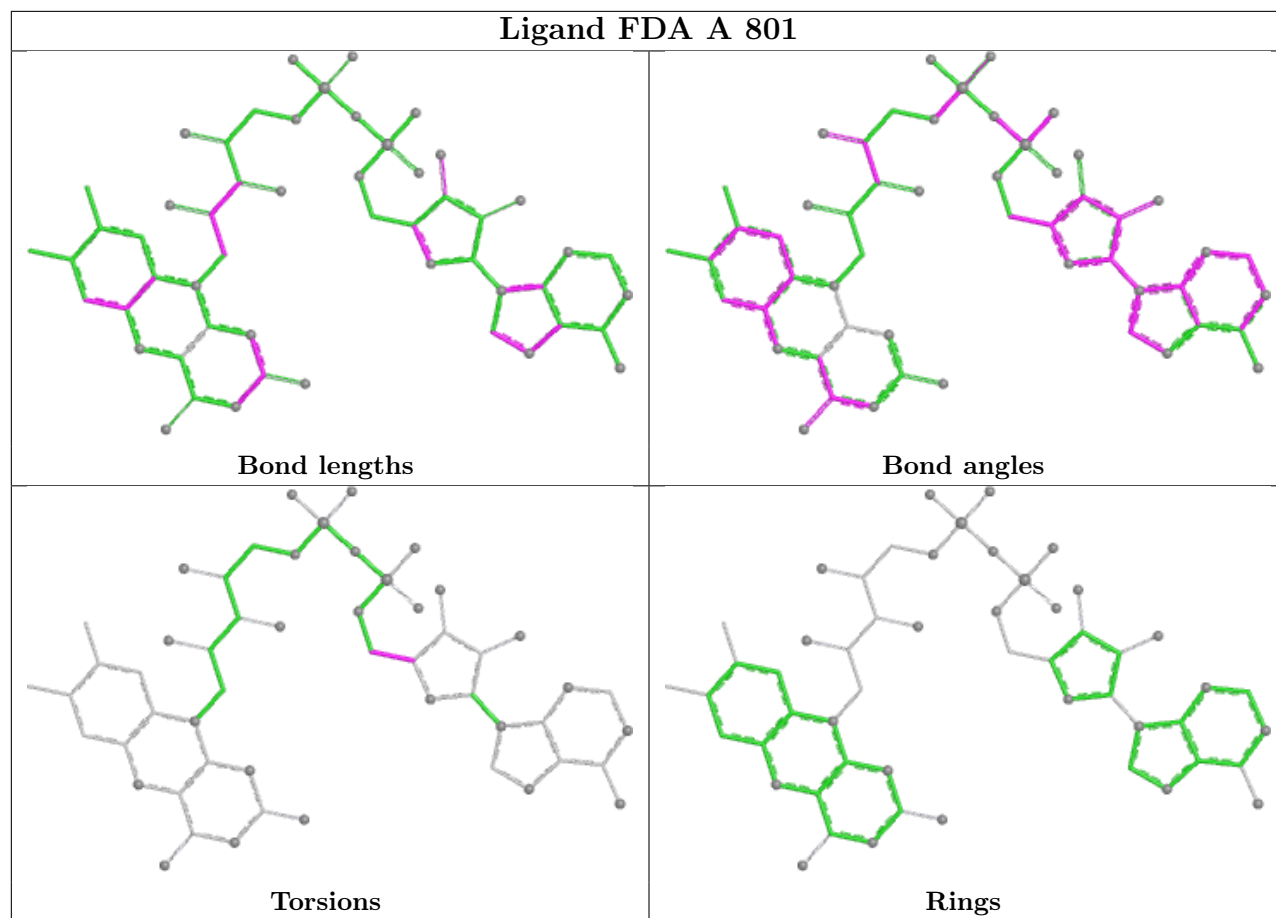
Mol	Chain	Res	Type	Atoms
4	B	704	1PE	C13-C23-OH3-C22
2	B	702	FDA	C5B-O5B-PA-O1A
4	B	704	1PE	C15-C25-OH5-C14
3	D	802	2H5	C4-C5-C6-O6
4	B	704	1PE	C12-C22-OH3-C23
4	D	803	1PE	C24-C14-OH5-C25
2	C	801	FDA	P-O3P-PA-O2A
2	C	801	FDA	O4B-C4B-C5B-O5B

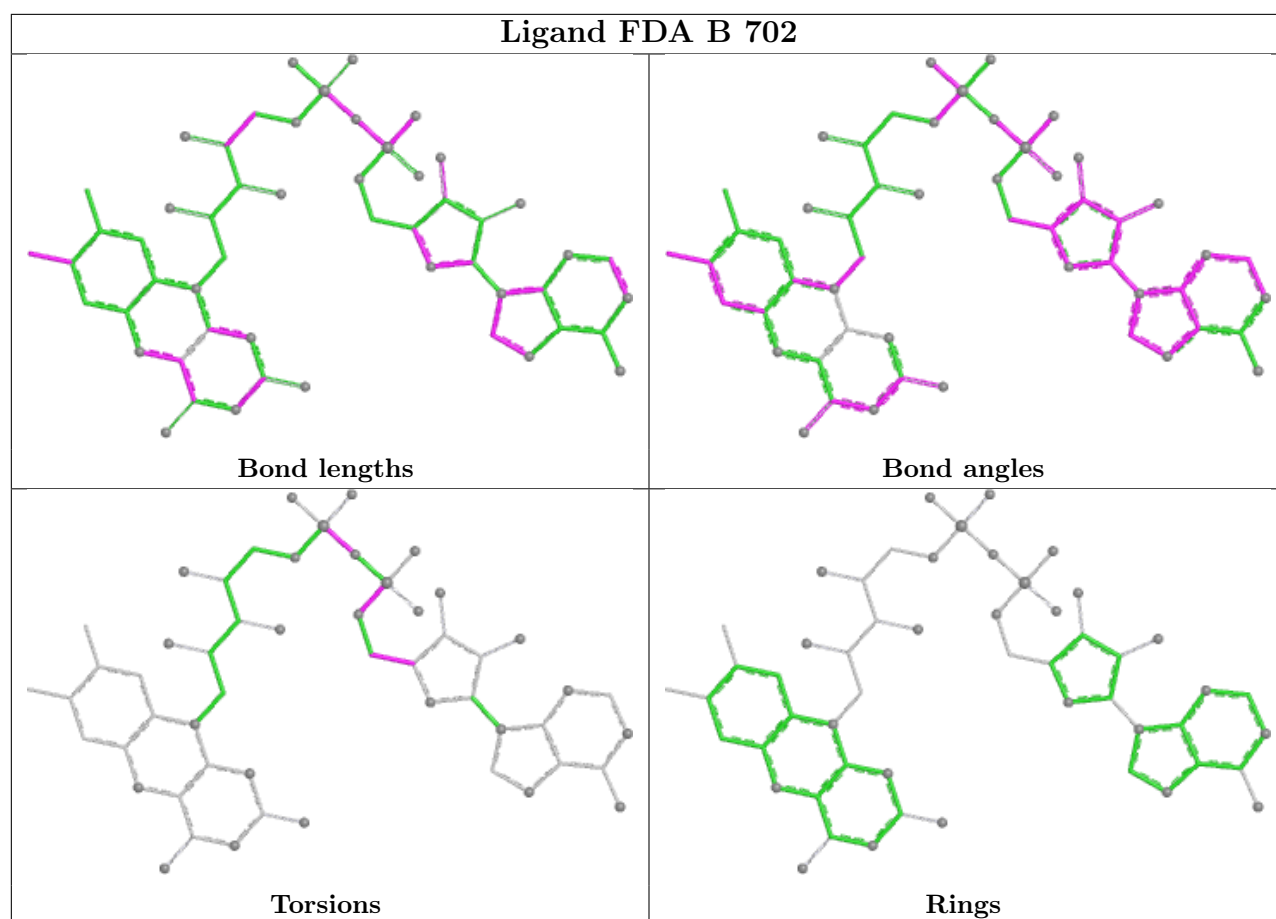
There are no ring outliers.

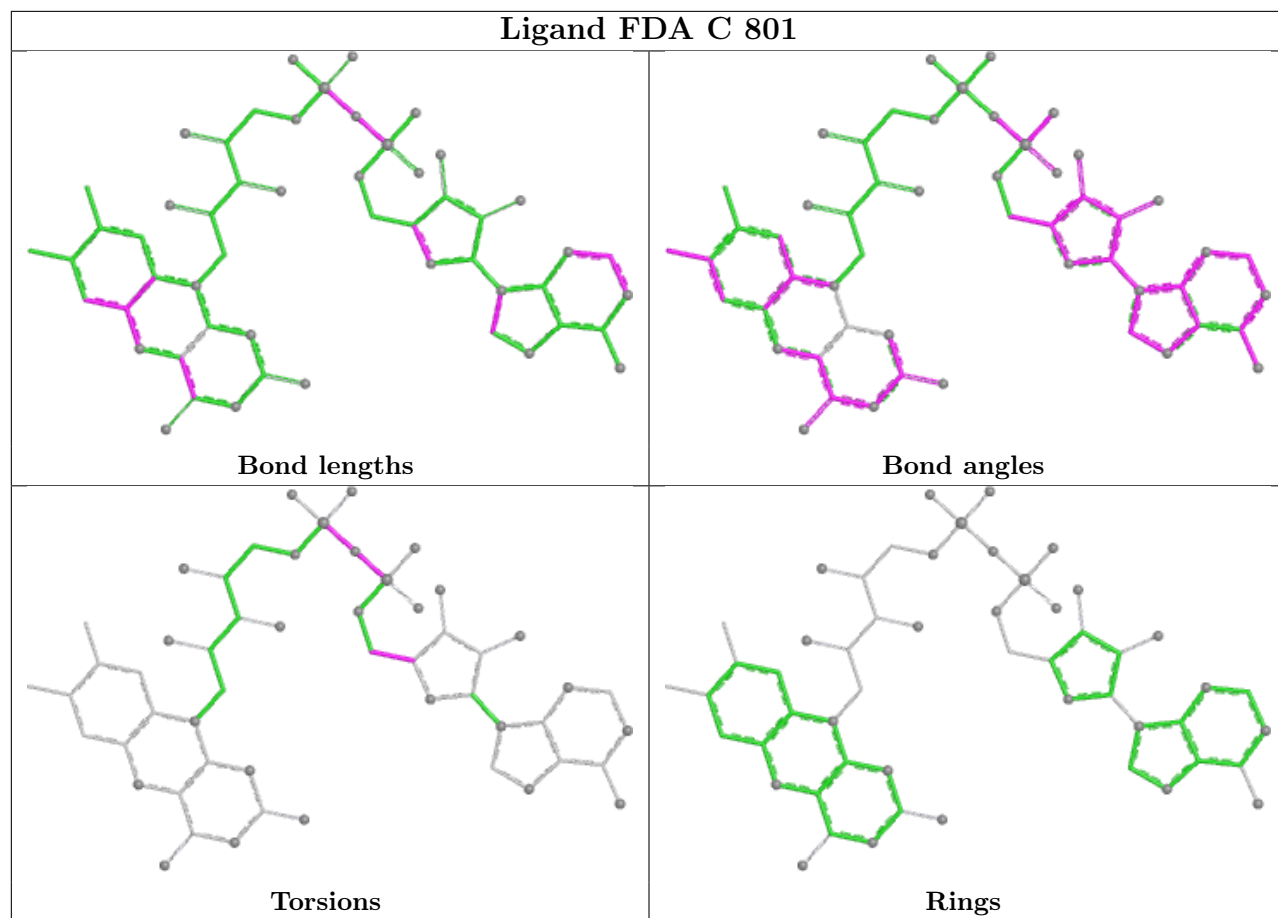
12 monomers are involved in 18 short contacts:

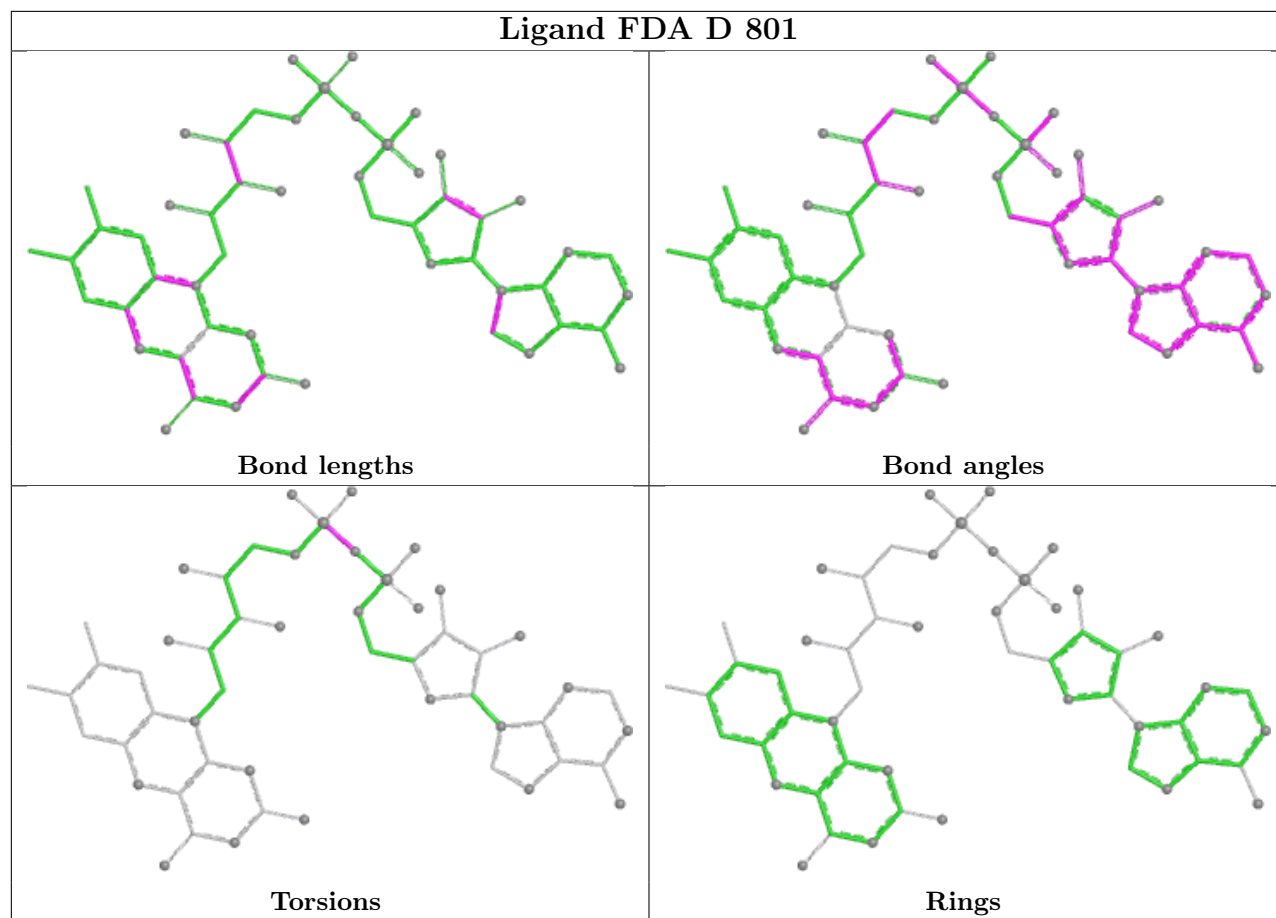
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FDA	3	0
3	B	703	2H5	1	0
5	B	701	MES	1	0
2	B	702	FDA	1	0
2	C	801	FDA	1	0
4	D	803	1PE	3	0
5	D	804	MES	1	0
4	B	704	1PE	1	0
3	C	802	2H5	2	0
2	D	801	FDA	2	0
3	D	802	2H5	1	0
3	A	802	2H5	4	0

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%)	0.62	43 (7%)	20 21	11, 19, 37, 62	0
1	B	576/633 (90%)	0.61	39 (6%)	23 24	10, 18, 35, 61	0
1	C	574/633 (90%)	1.27	125 (21%)	2 2	14, 29, 51, 88	0
1	D	574/633 (90%)	0.82	55 (9%)	13 14	12, 22, 43, 64	0
All	All	2300/2532 (90%)	0.83	262 (11%)	10 10	10, 22, 44, 88	0

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	618	PHE	6.0
1	D	343	ALA	6.0
1	B	45	ILE	6.0
1	B	343	ALA	5.7
1	D	345	PRO	5.3
1	C	343	ALA	5.2
1	A	343	ALA	5.1
1	C	45	ILE	5.1
1	D	45	ILE	5.0
1	B	345	PRO	5.0
1	D	385	THR	4.9
1	D	389	LEU	4.8
1	A	344	ASN	4.7
1	C	617	PRO	4.7
1	B	43	MET	4.7
1	B	100	ILE	4.6
1	C	270	ALA	4.5
1	C	82	SER	4.3
1	C	290	ALA	4.2
1	B	342	PRO	4.2
1	B	459	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	382	ILE	4.2
1	C	187	ASP	4.2
1	C	345	PRO	4.2
1	C	342	PRO	4.1
1	C	346	PRO	4.1
1	D	398	GLY	4.1
1	A	45	ILE	4.1
1	C	459	VAL	4.1
1	A	342	PRO	4.1
1	A	44	ASP	4.0
1	B	618	PHE	4.0
1	C	309	PHE	4.0
1	C	266	PRO	4.0
1	C	400	SER	4.0
1	C	492	THR	3.9
1	D	618	PHE	3.9
1	C	494	ALA	3.9
1	C	291	LEU	3.8
1	D	564	CYS	3.8
1	C	184	VAL	3.7
1	C	188	ALA	3.7
1	C	312	LYS	3.7
1	D	387	GLY	3.7
1	D	562	ASP	3.6
1	C	249	THR	3.5
1	D	184	VAL	3.4
1	B	188	ALA	3.4
1	A	82	SER	3.4
1	B	44	ASP	3.4
1	B	385	THR	3.4
1	C	271	PRO	3.4
1	D	558	ASP	3.3
1	B	271	PRO	3.3
1	D	188	ALA	3.3
1	D	100	ILE	3.3
1	C	573	PHE	3.3
1	D	185	LYS	3.2
1	C	268	THR	3.2
1	C	451	ARG	3.2
1	C	347	GLU	3.2
1	C	204	SER	3.2
1	A	490	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	47	TYR	3.2
1	C	269	ASP	3.2
1	C	68	ALA	3.2
1	C	310	GLU	3.2
1	C	267	ASN	3.2
1	C	603	ILE	3.1
1	A	496	ASN	3.1
1	B	344	ASN	3.1
1	C	66	VAL	3.1
1	B	231	LYS	3.1
1	C	259	VAL	3.0
1	D	378	SER	3.0
1	A	385	THR	3.0
1	C	385	THR	3.0
1	C	489	ASP	3.0
1	C	576	LYS	3.0
1	A	250	PHE	3.0
1	C	606	CYS	3.0
1	C	201	LYS	3.0
1	C	387	GLY	3.0
1	C	190	ALA	3.0
1	A	451	ARG	2.9
1	D	384	GLY	2.9
1	C	322	ALA	2.9
1	D	347	GLU	2.9
1	D	383	ARG	2.9
1	A	388	GLU	2.9
1	C	399	ALA	2.9
1	D	307	ASP	2.9
1	B	309	PHE	2.8
1	B	451	ARG	2.8
1	C	441	PRO	2.8
1	A	429	GLU	2.8
1	B	133	ALA	2.8
1	A	387	GLY	2.8
1	D	309	PHE	2.8
1	A	418	GLN	2.8
1	C	491	ILE	2.8
1	C	250	PHE	2.7
1	C	215	GLU	2.7
1	C	481	GLU	2.7
1	C	307	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	561	GLU	2.7
1	C	185	LYS	2.7
1	D	458	ALA	2.7
1	A	384	GLY	2.7
1	B	232	GLY	2.7
1	C	265	ARG	2.7
1	C	205	TYR	2.7
1	A	112	MET	2.7
1	C	192	ASP	2.7
1	C	545	LEU	2.7
1	C	605	SER	2.7
1	C	344	ASN	2.7
1	A	83	GLY	2.6
1	C	313	ALA	2.6
1	A	43	MET	2.6
1	A	249	THR	2.6
1	D	371	GLU	2.6
1	C	193	ALA	2.6
1	B	457	GLY	2.6
1	C	48	ASP	2.6
1	C	176	ASP	2.6
1	C	611	GLN	2.6
1	D	457	GLY	2.6
1	C	186	ASP	2.6
1	C	561	GLU	2.6
1	C	70	TYR	2.5
1	C	564	CYS	2.5
1	C	260	PHE	2.5
1	D	561	GLU	2.5
1	C	62	ALA	2.5
1	C	341	ASN	2.5
1	B	184	VAL	2.5
1	D	388	GLU	2.5
1	C	314	ASP	2.5
1	D	517	ASP	2.5
1	C	428	PHE	2.5
1	C	439	PHE	2.5
1	D	344	ASN	2.5
1	A	233	GLN	2.5
1	C	122	VAL	2.5
1	D	393	VAL	2.5
1	D	346	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	269	ASP	2.5
1	D	235	ASP	2.5
1	A	309	PHE	2.5
1	A	457	GLY	2.5
1	C	557	PHE	2.5
1	D	390	THR	2.5
1	D	231	LYS	2.5
1	C	275	PHE	2.4
1	C	406	ASP	2.4
1	C	67	GLY	2.4
1	B	310	GLU	2.4
1	D	481	GLU	2.4
1	D	391	TYR	2.4
1	C	300	ILE	2.4
1	C	381	THR	2.4
1	D	429	GLU	2.4
1	C	84	LEU	2.4
1	C	282	ALA	2.4
1	C	559	GLU	2.4
1	D	397	PRO	2.4
1	D	418	GLN	2.4
1	A	459	VAL	2.4
1	D	355	TYR	2.3
1	C	272	GLU	2.3
1	C	388	GLU	2.3
1	A	100	ILE	2.3
1	B	112	MET	2.3
1	C	287	VAL	2.3
1	A	489	ASP	2.3
1	C	246	ARG	2.3
1	C	328	LEU	2.3
1	C	389	LEU	2.3
1	C	429	GLU	2.3
1	C	183	LEU	2.3
1	A	185	LYS	2.3
1	C	69	GLY	2.3
1	C	288	ARG	2.3
1	A	192	ASP	2.3
1	B	101	ASP	2.3
1	B	269	ASP	2.3
1	C	566	VAL	2.3
1	B	268	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	490	LYS	2.3
1	D	249	THR	2.3
1	D	268	THR	2.3
1	A	618	PHE	2.2
1	C	403	LYS	2.2
1	C	614	THR	2.2
1	A	84	LEU	2.2
1	A	561	GLU	2.2
1	B	481	GLU	2.2
1	C	65	LEU	2.2
1	B	346	PRO	2.2
1	A	399	ALA	2.2
1	B	192	ASP	2.2
1	D	186	ASP	2.2
1	C	80	ILE	2.2
1	D	46	LYS	2.2
1	D	490	LYS	2.2
1	B	429	GLU	2.2
1	A	186	ASP	2.2
1	A	562	ASP	2.2
1	C	101	ASP	2.2
1	A	345	PRO	2.2
1	B	617	PRO	2.2
1	C	214	LYS	2.2
1	A	310	GLU	2.2
1	C	336	GLN	2.2
1	D	317	VAL	2.2
1	C	401	THR	2.2
1	A	558	ASP	2.2
1	D	189	ASP	2.2
1	A	389	LEU	2.2
1	C	457	GLY	2.2
1	A	190	ALA	2.2
1	C	602	ALA	2.2
1	B	347	GLU	2.1
1	B	557	PHE	2.1
1	C	75	PHE	2.1
1	C	608	TYR	2.1
1	C	311	ILE	2.1
1	B	196	ASP	2.1
1	B	185	LYS	2.1
1	B	285	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	438	LEU	2.1
1	D	250	PHE	2.1
1	D	96	TYR	2.1
1	D	304	ILE	2.1
1	C	568	THR	2.1
1	C	141	GLY	2.1
1	C	560	LYS	2.1
1	A	178	GLU	2.1
1	A	296	GLU	2.1
1	C	112	MET	2.1
1	A	441	PRO	2.1
1	C	299	HIS	2.1
1	C	198	LEU	2.1
1	C	496	ASN	2.1
1	D	291	LEU	2.1
1	B	187	ASP	2.1
1	C	302	ASP	2.1
1	C	274	ARG	2.1
1	C	308	ARG	2.1
1	D	516	GLU	2.1
1	C	497	MET	2.1
1	D	101	ASP	2.1
1	B	388	GLU	2.0
1	C	228	GLU	2.0
1	C	83	GLY	2.0
1	C	251	VAL	2.0
1	B	235	ASP	2.0
1	C	211	ASP	2.0
1	D	442	SER	2.0
1	D	380	MET	2.0
1	C	556	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

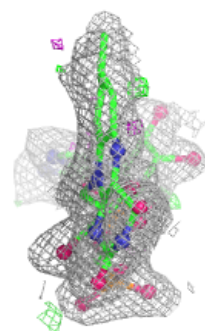
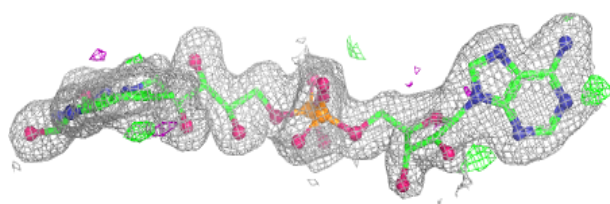
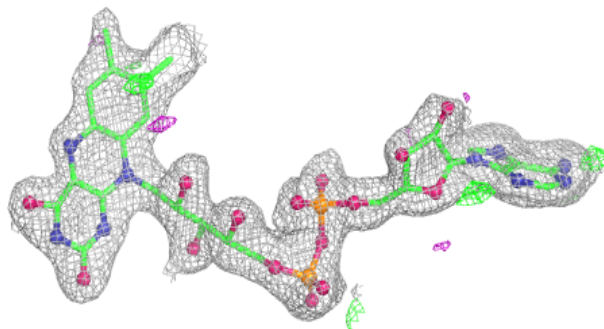
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	1PE	C	803	16/16	0.72	0.20	43,50,64,69	0
4	1PE	A	803	12/16	0.79	0.15	27,31,36,36	0
5	MES	D	804	11/12	0.79	0.15	31,38,44,49	0
4	1PE	D	803	16/16	0.80	0.16	31,37,48,51	0
3	2H5	C	802	12/12	0.81	0.16	39,42,47,50	0
4	1PE	B	704	16/16	0.83	0.16	28,41,53,54	0
3	2H5	A	802	12/12	0.83	0.12	29,31,34,34	0
3	2H5	B	703	12/12	0.89	0.10	24,26,28,29	0
5	MES	B	701	12/12	0.90	0.14	28,38,41,44	0
3	2H5	D	802	12/12	0.90	0.10	26,30,33,34	0
2	FDA	C	801	53/53	0.94	0.09	18,20,28,32	0
2	FDA	B	702	53/53	0.96	0.06	6,9,15,20	0
2	FDA	A	801	53/53	0.96	0.06	7,9,12,16	0
2	FDA	D	801	53/53	0.97	0.06	11,13,19,25	0

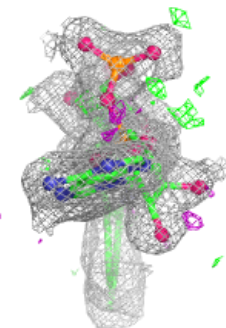
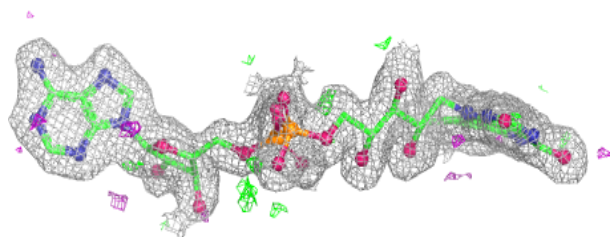
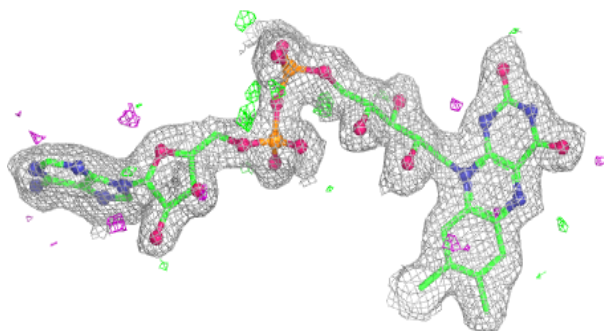
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

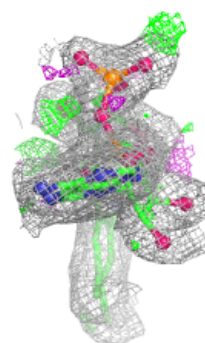
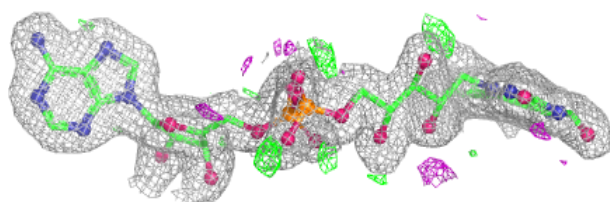
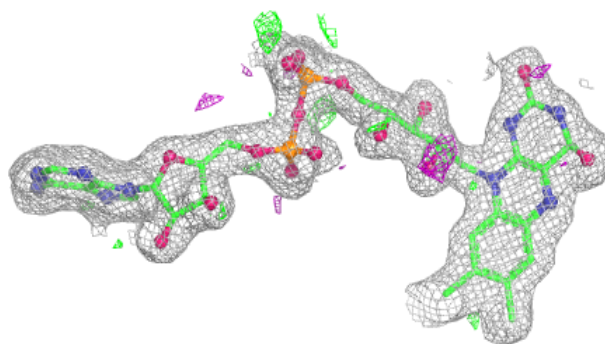
**Electron density around FDA B 702:**

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

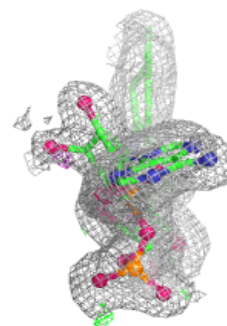
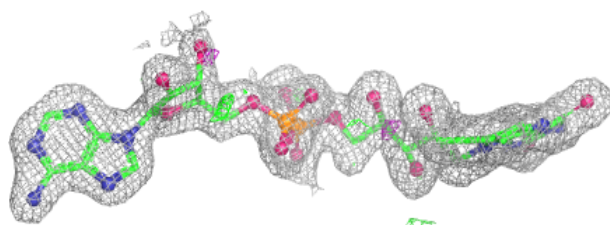
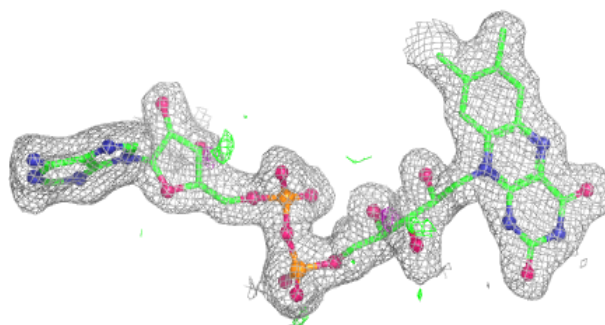


Electron density around FDA A 801:

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

**Electron density around FDA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.