



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:50 AM UTC

PDB ID : 5SJ4 / pdb_00005sj4
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN
COMPLEX WITH c1(ccccc1)c2cn(C)c(n2)CCC3=Nc4c(C(N3)=O)cnn4
C, micromolar IC50=0.04979
Authors : Joseph, C.; Benz, J.; Flohr, A.; Groebke-Zbinden, K.; Rudolph, M.G.
Deposited on : 2022-02-01
Resolution : 2.77 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

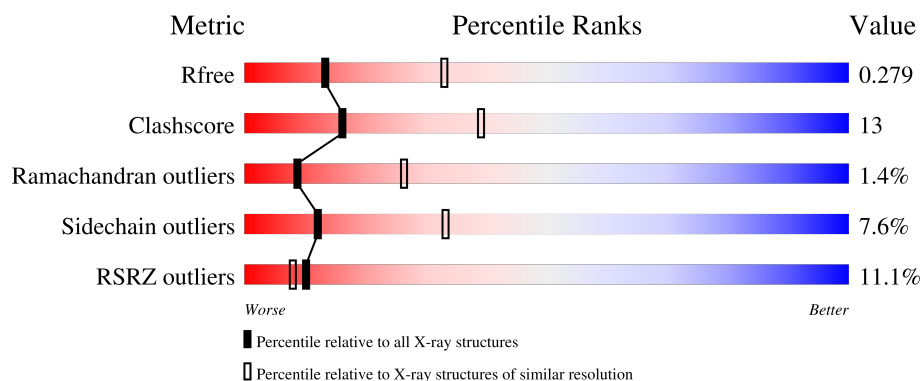
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	343	11% 56% 30% 5% • 9%
1	B	343	10% 52% 34% 6% 8%
1	C	343	7% 58% 30% • • 9%
1	D	343	12% 59% 28% • • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10464 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 cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	1	0
			2549	1629	435	461	24			
1	B	315	Total	C	N	O	S	0	1	0
			2559	1635	437	463	24			
1	C	313	Total	C	N	O	S	0	2	0
			2557	1634	438	461	24			
1	D	310	Total	C	N	O	S	0	0	0
			2519	1612	429	454	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	GLY	-	expression tag	UNP Q9Y233
A	448	SER	-	expression tag	UNP Q9Y233
B	447	GLY	-	expression tag	UNP Q9Y233
B	448	SER	-	expression tag	UNP Q9Y233
C	447	GLY	-	expression tag	UNP Q9Y233
C	448	SER	-	expression tag	UNP Q9Y233
D	447	GLY	-	expression tag	UNP Q9Y233
D	448	SER	-	expression tag	UNP Q9Y233

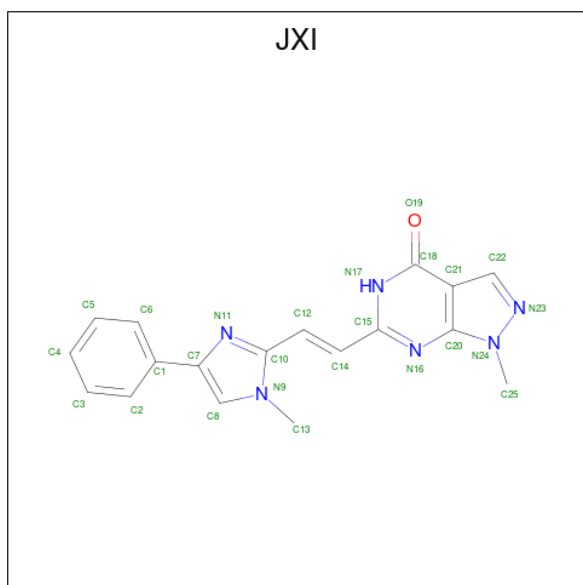
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

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

- Molecule 4 is 1-methyl-6-[(E)-2-(1-methyl-4-phenyl-1H-imidazol-2-yl)ethen-1-yl]-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one (CCD ID: JXI) (formula: C₁₈H₁₆N₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	18	6	1		
4	B	1	Total	C	N	O	0	0
			25	18	6	1		
4	C	1	Total	C	N	O	0	0
			25	18	6	1		
4	D	1	Total	C	N	O	0	0
			25	18	6	1		

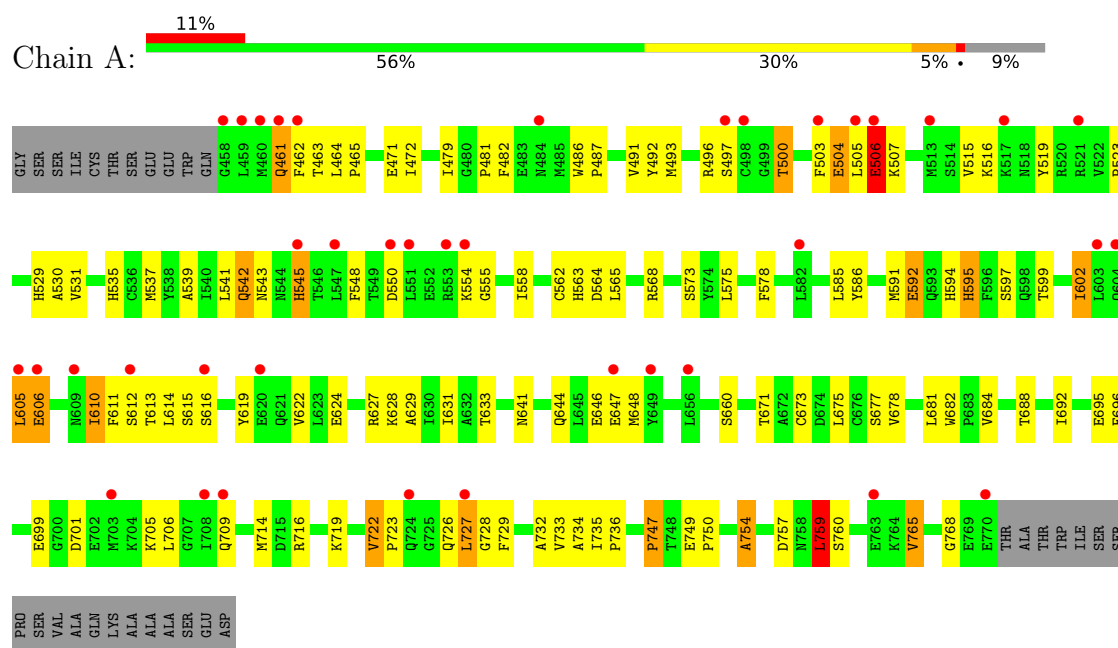
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	45	Total 45	O 45	0	0
5	B	45	Total 45	O 45	0	0
5	C	50	Total 50	O 50	0	0
5	D	32	Total 32	O 32	0	0

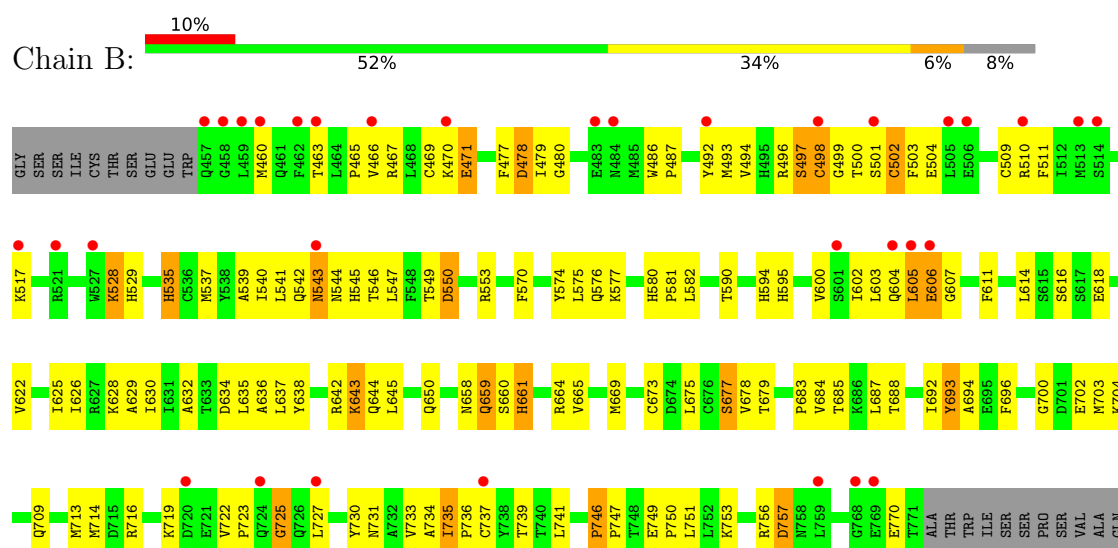
3 Residue-property plots

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: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

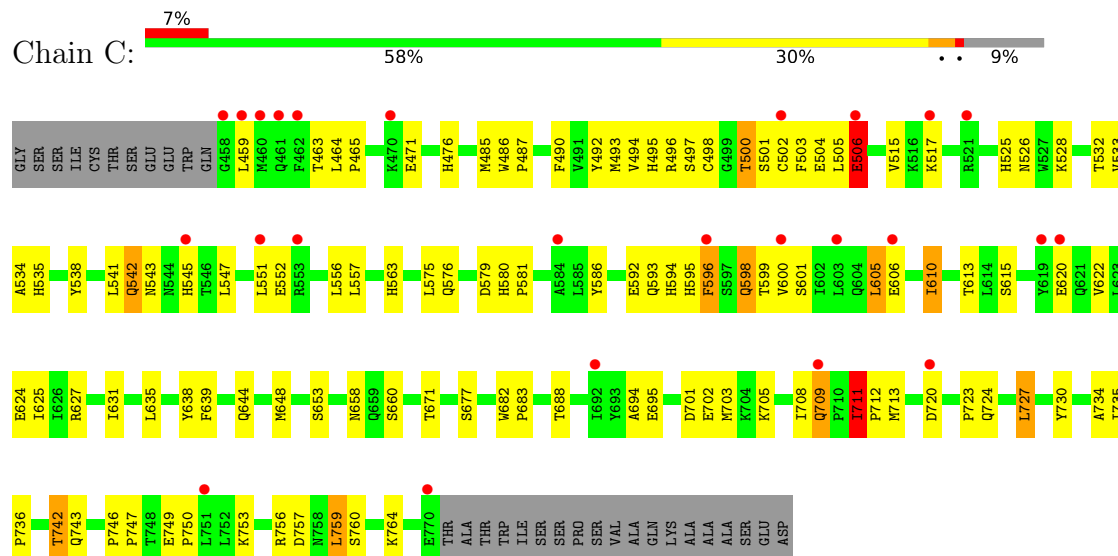


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

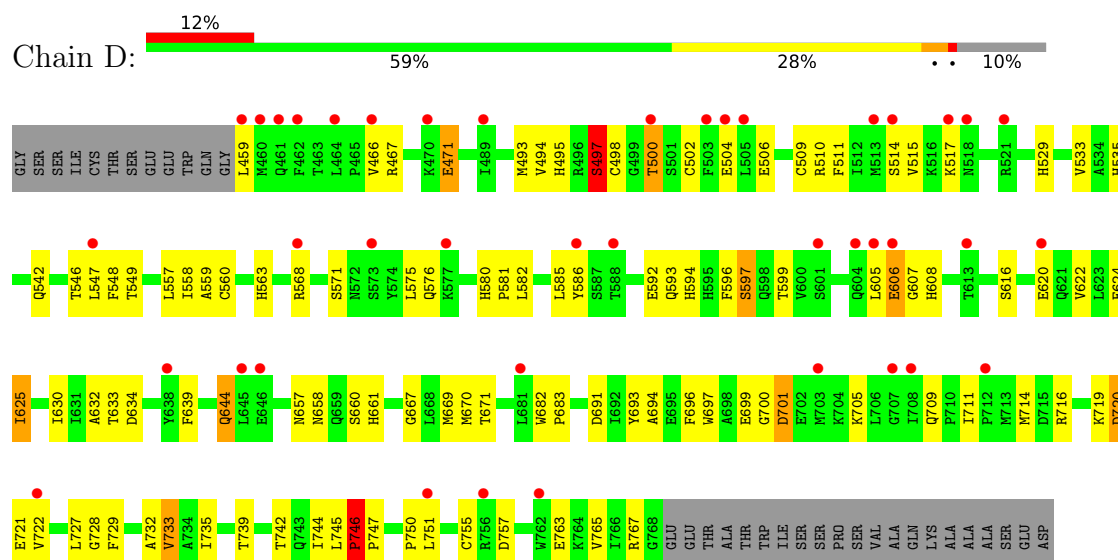


LYS
ALA
ALA
ALA
SER
GLU
ASP

- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	135.14Å 135.14Å 235.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.48 – 2.77 43.48 – 2.77	Depositor EDS
% Data completeness (in resolution range)	86.8 (43.48-2.77) 86.8 (43.48-2.77)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.195 , 0.278 0.202 , 0.279	Depositor DCC
R_{free} test set	1821 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10464	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: ZN, JXI, MG, CME

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	1.26	3/2603 (0.1%)	1.69	23/3521 (0.7%)
1	B	1.26	5/2613 (0.2%)	1.74	34/3535 (1.0%)
1	C	1.25	4/2614 (0.2%)	1.69	22/3535 (0.6%)
1	D	1.25	2/2570 (0.1%)	1.75	28/3478 (0.8%)
All	All	1.25	14/10400 (0.1%)	1.72	107/14069 (0.8%)

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	D	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	515	VAL	C-O	-6.81	1.16	1.24
1	B	595	HIS	C-O	6.74	1.32	1.24
1	A	481	PRO	C-O	-6.39	1.16	1.23
1	A	629	ALA	C-O	6.29	1.31	1.24
1	B	661	HIS	CE1-NE2	6.13	1.38	1.32
1	C	594	HIS	CE1-NE2	5.92	1.38	1.32
1	C	586	TYR	C-O	5.68	1.30	1.23
1	D	671	THR	C-O	-5.61	1.17	1.24
1	B	594	HIS	CE1-NE2	5.39	1.38	1.32
1	A	472	ILE	C-O	5.39	1.31	1.24
1	C	606	GLU	N-CA	5.25	1.52	1.46
1	B	683	PRO	C-O	-5.19	1.17	1.24
1	D	576	GLN	C-O	5.12	1.30	1.24
1	B	604	GLN	C-O	-5.11	1.17	1.24

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	620	GLU	CB-CG-CD	10.09	129.75	112.60
1	C	606	GLU	CB-CG-CD	9.42	128.61	112.60
1	C	506	GLU	CB-CG-CD	8.28	126.67	112.60
1	A	506	GLU	CB-CG-CD	8.26	126.63	112.60
1	B	606	GLU	CB-CG-CD	7.55	125.44	112.60
1	A	606	GLU	CB-CG-CD	6.98	124.46	112.60
1	A	684	VAL	N-CA-C	-6.87	104.07	110.53
1	A	726	GLN	N-CA-C	-6.86	103.73	111.14
1	B	684	VAL	CB-CA-C	-6.86	103.04	112.02
1	B	574	TYR	CA-C-O	-6.80	113.34	120.55
1	B	626	ILE	N-CA-C	-6.75	102.93	110.62
1	A	594	HIS	CA-C-O	-6.42	114.03	120.90
1	C	605	LEU	CA-C-O	-6.37	114.15	121.47
1	A	619	TYR	CA-C-N	6.28	128.99	120.38
1	A	619	TYR	C-N-CA	6.28	128.99	120.38
1	D	606	GLU	CB-CG-CD	6.25	123.22	112.60
1	A	504	GLU	CB-CG-CD	6.23	123.19	112.60
1	B	549	THR	CA-CB-OG1	6.21	118.91	109.60
1	B	741	LEU	CA-C-N	6.19	128.48	120.44
1	B	741	LEU	C-N-CA	6.19	128.48	120.44
1	D	605	LEU	CA-C-O	-6.13	113.61	120.54
1	B	605	LEU	CA-C-O	-6.11	114.09	121.05
1	B	541	LEU	CA-C-O	-6.10	114.42	120.82
1	A	564	ASP	CA-C-O	-6.02	114.34	121.32
1	D	529	HIS	CA-C-N	5.96	128.18	120.44
1	D	529	HIS	C-N-CA	5.96	128.18	120.44
1	B	693	TYR	CB-CA-C	5.95	120.97	110.85
1	B	733	VAL	CA-C-N	5.88	128.41	120.65
1	B	733	VAL	C-N-CA	5.88	128.41	120.65
1	C	711	ILE	CB-CA-C	5.87	116.64	110.88
1	D	746	PRO	N-CA-C	5.84	117.82	110.70
1	A	759	LEU	N-CA-C	-5.79	104.87	111.07
1	D	757	ASP	CA-CB-CG	5.79	118.39	112.60
1	D	765	VAL	CA-C-O	-5.77	114.95	120.95
1	B	702	GLU	CA-C-O	-5.76	114.39	120.55
1	B	600	VAL	CA-C-O	-5.75	115.29	121.27
1	D	765	VAL	CA-C-N	5.74	128.32	120.46
1	D	765	VAL	C-N-CA	5.74	128.32	120.46
1	A	754	ALA	O-C-N	5.73	127.99	122.03
1	B	550	ASP	N-CA-C	-5.72	105.12	111.36
1	C	598	GLN	CA-C-O	-5.70	114.54	120.92
1	B	725	GLY	CA-C-N	5.68	128.36	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	725	GLY	C-N-CA	5.68	128.36	120.29
1	D	750	PRO	CA-C-N	5.67	127.81	120.44
1	D	750	PRO	C-N-CA	5.67	127.81	120.44
1	B	628	LYS	N-CA-C	-5.67	105.25	111.82
1	C	658	ASN	CB-CA-C	5.66	120.16	110.81
1	C	709	GLN	N-CA-C	-5.61	102.70	109.83
1	C	545	HIS	CA-CB-CG	5.59	119.39	113.80
1	B	753	LYS	N-CA-C	-5.58	104.21	111.02
1	D	701	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	737	CYS	CA-C-O	-5.55	115.17	121.00
1	D	720	ASP	CA-C-O	-5.53	114.98	120.90
1	C	734	ALA	CA-C-N	5.52	124.75	120.33
1	C	734	ALA	C-N-CA	5.52	124.75	120.33
1	B	570	PHE	CA-C-N	5.52	131.01	120.97
1	B	570	PHE	C-N-CA	5.52	131.01	120.97
1	D	597	SER	CA-C-N	5.51	127.60	120.44
1	D	597	SER	C-N-CA	5.51	127.60	120.44
1	A	696	PHE	CA-C-O	-5.49	114.73	120.55
1	C	639	PHE	CA-C-N	5.48	127.18	120.22
1	C	639	PHE	C-N-CA	5.48	127.18	120.22
1	B	535	HIS	CA-CB-CG	-5.46	108.33	113.80
1	B	618	GLU	CB-CA-C	5.45	119.59	110.92
1	A	595	HIS	CB-CA-C	-5.45	101.74	110.79
1	C	620	GLU	CB-CA-C	5.44	121.25	110.42
1	C	702	GLU	CB-CG-CD	5.44	121.85	112.60
1	B	757	ASP	CA-C-N	5.44	127.51	120.44
1	B	757	ASP	C-N-CA	5.44	127.51	120.44
1	A	747	PRO	CB-CA-C	-5.43	102.61	111.56
1	D	639	PHE	CA-C-N	5.39	126.88	120.14
1	D	639	PHE	C-N-CA	5.39	126.88	120.14
1	A	482	PHE	CA-C-O	-5.39	116.04	122.13
1	C	592	GLU	N-CA-C	-5.37	105.46	112.23
1	D	625	ILE	CA-C-N	5.37	127.33	120.56
1	D	625	ILE	C-N-CA	5.37	127.33	120.56
1	B	746	PRO	N-CA-C	5.36	117.24	110.70
1	D	568	ARG	N-CA-C	-5.36	106.59	113.23
1	A	754	ALA	CA-C-N	5.33	127.73	120.54
1	A	754	ALA	C-N-CA	5.33	127.73	120.54
1	A	734	ALA	CA-C-O	-5.32	115.23	120.82
1	B	528	LYS	CA-C-N	5.30	127.33	120.44
1	B	528	LYS	C-N-CA	5.30	127.33	120.44
1	A	660	SER	N-CA-C	-5.30	106.77	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	529	HIS	N-CA-C	-5.29	105.16	111.03
1	A	550	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	586	TYR	CB-CA-C	-5.25	104.54	111.42
1	C	701	ASP	N-CA-C	-5.24	105.57	111.28
1	A	592	GLU	CB-CA-C	5.21	119.05	110.88
1	D	620	GLU	CB-CA-C	5.20	120.25	110.63
1	B	731	ASN	CA-C-O	-5.15	115.41	120.82
1	D	744	ILE	CA-C-N	5.15	128.66	122.89
1	D	744	ILE	C-N-CA	5.15	128.66	122.89
1	B	685	THR	CA-C-N	5.12	127.57	120.29
1	B	685	THR	C-N-CA	5.12	127.57	120.29
1	D	763	GLU	CA-C-N	5.10	127.07	120.44
1	D	763	GLU	C-N-CA	5.10	127.07	120.44
1	C	596	PHE	N-CA-C	-5.10	105.90	111.82
1	D	657	ASN	CB-CA-C	5.09	118.75	110.24
1	C	593	GLN	N-CA-C	-5.05	105.96	111.82
1	D	506	GLU	CB-CG-CD	5.05	121.19	112.60
1	C	526	ASN	CA-C-N	5.04	127.00	120.44
1	C	526	ASN	C-N-CA	5.04	127.00	120.44
1	D	549	THR	CA-C-O	-5.04	116.03	121.87
1	B	529	HIS	O-C-N	5.02	127.24	122.07
1	B	634	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	709	GLN	CB-CA-C	5.01	117.28	109.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	497	SER	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	2549	0	2524	68	1
1	B	2559	0	2528	75	1
1	C	2557	0	2537	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2519	0	2496	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	3	0
4	C	25	0	0	0	0
4	D	25	0	0	0	0
5	A	45	0	0	3	0
5	B	45	0	0	0	0
5	C	50	0	0	8	0
5	D	32	0	0	2	0
All	All	10464	0	10085	266	1

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 13.

All (266) 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:D:644:GLN:HE21	1:D:644:GLN:HA	1.23	1.02
1:B:470:LYS:HD2	1:D:742:THR:HG22	1.44	1.00
1:A:542:GLN:HA	1:A:542:GLN:NE2	1.79	0.97
1:A:542:GLN:HA	1:A:542:GLN:HE21	1.31	0.95
1:B:543:ASN:N	1:B:543:ASN:HD22	1.63	0.92
1:A:461:GLN:HE21	1:A:461:GLN:HA	1.34	0.91
1:D:497:SER:HA	1:D:542:GLN:HE22	1.37	0.89
1:D:493:MET:O	1:D:497:SER:HB3	1.77	0.85
1:B:497:SER:HA	1:B:542:GLN:HE22	1.40	0.84
1:C:542:GLN:HA	1:C:542:GLN:NE2	1.90	0.84
1:A:542:GLN:HE21	1:A:542:GLN:CA	1.92	0.82
1:A:461:GLN:HA	1:A:461:GLN:NE2	1.97	0.76
1:B:543:ASN:HD22	1:B:543:ASN:H	1.32	0.75
1:B:494:VAL:O	1:B:498:CYS:HB3	1.87	0.73
1:C:532:THR:HG23	5:C:933:HOH:O	1.87	0.73
1:A:602:ILE:HA	1:A:605:LEU:HD22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:THR:O	5:C:901:HOH:O	2.07	0.72
1:B:543:ASN:N	1:B:543:ASN:ND2	2.33	0.70
1:A:523:PRO:O	5:A:901:HOH:O	2.07	0.70
1:B:730:TYR:HA	1:B:734:ALA:HB3	1.73	0.70
1:C:492:TYR:CZ	1:C:496:ARG:HD2	2.26	0.70
1:B:470:LYS:HE2	1:D:746:PRO:HB3	1.75	0.69
1:D:691:ASP:OD2	5:D:901:HOH:O	2.09	0.69
1:D:497:SER:HA	1:D:542:GLN:NE2	2.06	0.68
1:A:461:GLN:HE22	1:A:500:THR:HG23	1.59	0.67
1:B:550:ASP:OD1	1:B:553:ARG:NH2	2.26	0.67
1:D:467:ARG:NH1	1:D:471:GLU:OE1	2.27	0.67
1:B:492:TYR:CZ	1:B:496:ARG:HD2	2.30	0.67
1:D:644:GLN:HA	1:D:644:GLN:NE2	2.04	0.67
1:C:476:HIS:ND1	5:C:906:HOH:O	2.27	0.66
1:D:622:VAL:HA	1:D:625:ILE:HD12	1.78	0.66
1:D:585:LEU:HD23	1:D:586:TYR:CE2	2.31	0.65
1:D:644:GLN:HE21	1:D:644:GLN:CA	2.05	0.65
1:D:745:LEU:C	1:D:747:PRO:HD2	2.22	0.65
1:D:547:LEU:HD13	5:D:910:HOH:O	1.96	0.65
1:A:479:ILE:HD12	1:A:486:TRP:CD1	2.33	0.64
1:C:596:PHE:O	1:C:600:VAL:HG23	1.98	0.63
1:C:760:SER:O	5:C:902:HOH:O	2.16	0.63
1:B:713:MET:HA	4:B:803:JXI:C6	2.29	0.63
1:C:542:GLN:NE2	1:C:542:GLN:CA	2.59	0.63
1:B:644:GLN:HA	1:B:644:GLN:NE2	2.15	0.62
1:B:692:ILE:HG22	1:B:696:PHE:CE2	2.34	0.62
1:C:653:SER:O	5:C:903:HOH:O	2.16	0.62
1:A:539:ALA:O	1:A:543:ASN:ND2	2.33	0.62
1:D:511:PHE:O	1:D:515:VAL:HG23	2.00	0.61
1:C:759:LEU:HD12	1:C:759:LEU:O	1.99	0.61
1:C:598:GLN:O	1:C:601:SER:HB2	2.00	0.61
1:B:675:LEU:O	1:B:678:VAL:HG22	2.01	0.60
1:C:542:GLN:HA	1:C:542:GLN:HE21	1.66	0.60
1:C:711:ILE:HD11	1:C:713:MET:HE2	1.84	0.60
1:B:644:GLN:HA	1:B:644:GLN:HE21	1.68	0.59
1:C:542:GLN:CA	1:C:542:GLN:HE21	2.15	0.58
1:B:467:ARG:HG2	1:B:471:GLU:OE1	2.04	0.57
1:C:505:LEU:O	1:C:506:GLU:C	2.46	0.57
1:B:546:THR:HG21	1:D:767:ARG:HH12	1.69	0.57
1:B:642:ARG:O	1:B:643:LYS:C	2.48	0.57
1:C:552:GLU:O	1:C:556:LEU:HG	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:648:MET:HE1	5:C:922:HOH:O	2.04	0.57
1:D:745:LEU:C	1:D:747:PRO:CD	2.78	0.57
1:D:735:ILE:HD13	1:D:755:CYS:SG	2.44	0.57
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.40	0.57
1:B:511:PHE:CE1	1:B:602:ILE:HG22	2.40	0.57
1:A:677:SER:HB2	1:A:688:THR:HG21	1.87	0.57
1:D:585:LEU:HD23	1:D:586:TYR:CZ	2.40	0.56
1:A:463:THR:O	1:A:464:LEU:HD23	2.06	0.56
1:C:543:ASN:HD22	1:C:543:ASN:N	2.04	0.56
1:A:729:PHE:O	1:A:733:VAL:N	2.37	0.56
1:D:514:SER:OG	1:D:608:HIS:NE2	2.38	0.56
1:A:461:GLN:HE21	1:A:461:GLN:CA	2.13	0.56
1:A:519:TYR:CZ	1:A:530:ALA:HB2	2.41	0.55
1:C:551:LEU:HD22	1:C:622:VAL:HB	1.86	0.55
1:C:533:VAL:HG21	1:C:563:HIS:CE1	2.41	0.55
1:B:719:LYS:O	1:B:722:VAL:HG23	2.07	0.55
1:B:635:LEU:O	1:B:636:ALA:C	2.47	0.55
1:B:692:ILE:CG2	1:B:696:PHE:CE2	2.91	0.54
1:A:723:PRO:HB3	1:A:765:VAL:HG12	1.90	0.53
1:A:505:LEU:O	1:A:506:GLU:C	2.50	0.53
1:A:585:LEU:O	1:A:585:LEU:HD12	2.08	0.53
1:B:644:GLN:HE21	1:B:644:GLN:CA	2.21	0.53
1:B:700:GLY:HA3	1:B:714:MET:O	2.09	0.53
1:D:691:ASP:O	1:D:694:ALA:HB3	2.08	0.53
1:A:541:LEU:HD23	1:A:548:PHE:CD2	2.43	0.53
1:B:677:SER:HB2	1:B:688:THR:HG21	1.91	0.53
1:B:501:SER:O	1:B:503:PHE:N	2.42	0.53
1:D:667:GLY:O	1:D:670:MET:HB2	2.09	0.53
1:C:759:LEU:HD12	1:C:759:LEU:C	2.35	0.52
1:A:671:THR:O	1:A:675:LEU:HG	2.10	0.52
1:B:700:GLY:O	1:B:704:LYS:HG3	2.10	0.52
1:C:535:HIS:O	1:C:538:TYR:HB3	2.10	0.52
1:B:645:LEU:HD21	1:B:664:ARG:CB	2.39	0.52
1:B:479:ILE:HD11	1:B:528:LYS:HG3	1.92	0.52
1:B:629:ALA:O	1:B:632:ALA:HB3	2.08	0.52
1:B:658:ASN:O	1:B:661:HIS:N	2.40	0.52
1:B:499:GLY:N	1:B:502:CYS:SG	2.83	0.52
1:B:725:GLY:HA3	4:B:803:JXI:C2	2.39	0.52
1:A:627:ARG:O	1:A:631:ILE:HG12	2.10	0.51
1:A:722:VAL:O	1:A:723:PRO:C	2.51	0.51
1:A:568:ARG:HG2	1:A:591:MET:HE1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:HIS:CE1	1:B:582:LEU:HG	2.46	0.51
1:C:730:TYR:HB3	1:C:759:LEU:HD22	1.91	0.51
1:C:533:VAL:O	1:C:534:ALA:C	2.51	0.51
1:C:635:LEU:O	1:C:638:TYR:HB3	2.11	0.51
1:A:462:PHE:CE1	1:A:491:VAL:HG11	2.46	0.51
1:B:545:HIS:CD2	1:B:546:THR:HG23	2.46	0.51
1:C:493:MET:O	1:C:497:SER:HB3	2.10	0.51
1:A:464:LEU:O	1:A:465:PRO:C	2.54	0.51
1:A:611:PHE:HB3	1:A:614:LEU:HD22	1.93	0.51
1:C:712:PRO:O	1:C:713:MET:C	2.53	0.50
1:D:624:GLU:HA	1:D:624:GLU:OE1	2.10	0.50
1:D:497:SER:OG	1:D:557:LEU:HD11	2.12	0.50
1:B:478:ASP:OD2	1:B:480:GLY:N	2.44	0.50
1:D:586:TYR:HB3	1:D:593:GLN:NE2	2.27	0.50
1:A:701:ASP:O	1:A:705:LYS:HG3	2.12	0.50
1:B:470:LYS:NZ	1:D:742:THR:O	2.33	0.50
1:D:494:VAL:O	1:D:498:CYS:HB3	2.12	0.50
1:D:735:ILE:CD1	1:D:755:CYS:SG	3.00	0.50
1:B:510:ARG:NH1	1:B:607:GLY:O	2.45	0.50
1:C:525:HIS:ND1	1:C:695:GLU:OE1	2.39	0.50
1:A:605:LEU:O	1:A:606:GLU:C	2.54	0.49
1:D:729:PHE:CE1	1:D:733:VAL:HG11	2.47	0.49
1:B:465:PRO:O	1:B:466:VAL:C	2.55	0.49
1:A:749:GLU:N	1:A:750:PRO:CD	2.76	0.49
1:B:725:GLY:HA3	4:B:803:JXI:C1	2.42	0.49
1:B:577:LYS:HD3	1:B:703:MET:HE1	1.94	0.49
1:C:682:TRP:N	1:C:683:PRO:CD	2.75	0.49
1:D:745:LEU:O	1:D:747:PRO:HD2	2.13	0.49
1:C:535:HIS:O	1:C:538:TYR:N	2.46	0.48
1:B:756[A]:ARG:HG2	1:B:756[A]:ARG:HH11	1.78	0.48
1:D:720:ASP:OD1	1:D:720:ASP:N	2.45	0.48
1:C:486:TRP:CH2	1:C:528:LYS:HB2	2.48	0.48
1:D:571:SER:HB3	1:D:699:GLU:OE1	2.12	0.48
1:A:675:LEU:O	1:A:678:VAL:HG22	2.13	0.48
1:A:699:GLU:OE2	1:A:714:MET:HE1	2.13	0.48
1:A:493:MET:O	1:A:497:SER:HB2	2.13	0.48
1:D:592:GLU:HG2	1:D:634:ASP:HB2	1.95	0.47
1:C:485:MET:HE2	1:C:485:MET:HB3	1.68	0.47
1:C:503:PHE:CD1	1:C:610:ILE:HB	2.49	0.47
1:A:515:VAL:HG13	1:A:565:LEU:HD21	1.96	0.47
1:B:756[B]:ARG:HH11	1:B:756[B]:ARG:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:VAL:HA	1:C:625:ILE:HD12	1.97	0.47
1:C:753:LYS:NZ	1:C:757:ASP:OD2	2.47	0.47
1:D:580:HIS:ND1	1:D:581:PRO:HD2	2.29	0.47
1:A:612:SER:OG	1:A:613:THR:N	2.48	0.47
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.95	0.47
1:B:735:ILE:HB	1:B:736:PRO:HD3	1.97	0.47
1:A:503:PHE:CD1	1:A:610:ILE:HB	2.49	0.47
1:A:716:ARG:O	1:A:719:LYS:HG3	2.15	0.47
1:C:495:HIS:CD2	1:C:500:THR:HA	2.50	0.47
1:D:548:PHE:CZ	1:D:669:MET:HE1	2.49	0.47
1:D:563:HIS:HA	1:D:630:ILE:HG12	1.95	0.47
1:D:580:HIS:CE1	1:D:582:LEU:HD12	2.50	0.47
1:D:535:HIS:ND1	1:D:535:HIS:C	2.73	0.47
1:C:694:ALA:O	5:C:904:HOH:O	2.20	0.46
1:C:638:TYR:CD1	1:C:671:THR:HG21	2.50	0.46
1:D:596:PHE:O	1:D:599:THR:HB	2.14	0.46
1:B:645:LEU:HD21	1:B:664:ARG:HB3	1.98	0.46
1:C:486:TRP:N	1:C:487:PRO:CD	2.79	0.46
1:A:562:CYS:SG	1:A:599:THR:HG23	2.56	0.46
1:B:501:SER:O	1:B:502:CYS:C	2.58	0.46
1:D:466:VAL:O	1:D:467:ARG:C	2.59	0.46
1:D:745:LEU:O	1:D:746:PRO:C	2.57	0.46
1:D:745:LEU:O	1:D:747:PRO:N	2.49	0.46
1:B:470:LYS:HE2	1:D:746:PRO:CB	2.44	0.46
1:A:479:ILE:HD13	1:A:531:VAL:CG1	2.45	0.46
1:C:595:HIS:O	1:C:599:THR:OG1	2.31	0.46
1:C:735:ILE:HB	1:C:736:PRO:HD3	1.97	0.46
1:B:492:TYR:CE1	1:B:496:ARG:HD2	2.50	0.46
1:B:580:HIS:CG	1:B:581:PRO:HD2	2.50	0.46
1:C:749:GLU:N	1:C:750:PRO:CD	2.79	0.46
1:D:585:LEU:CD2	1:D:586:TYR:CZ	2.99	0.45
1:A:759:LEU:C	1:A:759:LEU:HD12	2.42	0.45
1:C:627:ARG:O	1:C:631:ILE:HG12	2.15	0.45
1:A:545:HIS:CD2	1:A:545:HIS:C	2.93	0.45
1:D:658:ASN:ND2	1:D:661:HIS:CD2	2.85	0.45
1:A:523:PRO:HD2	1:A:695:GLU:HG2	1.97	0.45
1:B:544:ASN:HB3	1:B:547:LEU:HD22	1.98	0.45
1:B:645:LEU:HD21	1:B:664:ARG:HB2	1.98	0.45
1:A:624:GLU:HG3	1:A:628:LYS:HE3	1.99	0.45
1:A:644:GLN:HE21	1:A:648:MET:HE3	1.81	0.45
1:A:735:ILE:N	1:A:736:PRO:CD	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:GLN:HE21	1:C:542:GLN:N	2.15	0.45
1:C:724:GLN:HA	1:C:724:GLN:NE2	2.31	0.45
1:D:728:GLY:O	1:D:732:ALA:HB3	2.16	0.45
1:A:563:HIS:HD2	1:A:633:THR:HG21	1.82	0.45
1:B:611:PHE:HB3	1:B:614:LEU:HD22	1.99	0.45
1:D:533:VAL:HG12	1:D:560:CYS:HB3	1.98	0.45
1:C:624:GLU:HA	1:C:624:GLU:OE1	2.17	0.45
1:D:693:TYR:HA	1:D:696:PHE:HB2	1.99	0.44
1:A:461:GLN:NE2	1:A:500:THR:CG2	2.80	0.44
1:A:461:GLN:NE2	1:A:500:THR:HG23	2.30	0.44
1:A:728:GLY:O	1:A:732:ALA:N	2.46	0.44
1:B:722:VAL:HB	1:B:723:PRO:HD3	2.00	0.44
1:C:543:ASN:N	1:C:543:ASN:ND2	2.66	0.44
1:D:745:LEU:O	1:D:747:PRO:CD	2.65	0.44
1:A:486:TRP:N	1:A:487:PRO:CD	2.81	0.44
1:B:749:GLU:N	1:B:750:PRO:CD	2.81	0.44
1:B:537:MET:HE2	1:B:673:CYS:SG	2.58	0.44
1:B:693:TYR:O	1:B:694:ALA:C	2.60	0.44
1:B:539:ALA:O	1:B:543:ASN:ND2	2.51	0.44
1:B:679:THR:HG21	1:B:751:LEU:HD22	2.00	0.44
1:C:644:GLN:HA	1:C:644:GLN:NE2	2.33	0.44
1:A:505:LEU:O	1:A:507:LYS:N	2.51	0.44
1:A:537:MET:HE2	1:A:673:CYS:SG	2.58	0.44
1:B:658:ASN:O	1:B:659:GLN:C	2.60	0.44
1:C:580:HIS:ND1	1:C:581:PRO:HD2	2.33	0.44
1:B:493:MET:SD	1:B:535:HIS:HA	2.58	0.43
1:C:756[A]:ARG:HG2	1:C:756[A]:ARG:HH11	1.83	0.43
1:D:493:MET:O	1:D:497:SER:CB	2.59	0.43
1:B:716:ARG:O	1:B:719:LYS:HG3	2.19	0.43
1:C:677:SER:HB2	1:C:688:THR:HG21	2.00	0.43
1:A:735:ILE:N	1:A:736:PRO:HD2	2.33	0.43
1:B:687:LEU:HD13	1:C:705:LYS:HE3	2.00	0.43
1:B:746:PRO:N	1:B:747:PRO:CD	2.81	0.43
1:B:540:ILE:HG21	1:B:669:MET:HE3	2.00	0.43
1:D:682:TRP:N	1:D:683:PRO:CD	2.81	0.43
1:C:501:SER:O	1:C:503:PHE:N	2.52	0.43
1:C:541:LEU:O	1:C:542:GLN:C	2.59	0.43
1:D:594:HIS:O	1:D:597:SER:N	2.52	0.43
1:D:716:ARG:O	1:D:719:LYS:HG3	2.18	0.43
1:D:495:HIS:CD2	1:D:500:THR:HA	2.53	0.43
1:A:461:GLN:HE22	1:A:500:THR:CG2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:ALA:O	1:A:757:ASP:HB2	2.18	0.42
1:A:646:GLU:O	1:A:647:GLU:C	2.62	0.42
1:B:629:ALA:O	1:B:630:ILE:C	2.61	0.42
1:A:493:MET:SD	1:A:535:HIS:HA	2.60	0.42
1:A:592:GLU:HA	1:A:595:HIS:CD2	2.55	0.42
1:A:479:ILE:HD13	1:A:531:VAL:HG12	2.02	0.42
1:B:486:TRP:N	1:B:487:PRO:CD	2.83	0.42
1:C:486:TRP:HB2	1:C:487:PRO:HD3	2.01	0.42
1:C:764:LYS:HG3	5:C:902:HOH:O	2.19	0.42
1:D:746:PRO:N	1:D:747:PRO:CD	2.82	0.42
1:B:497:SER:HA	1:B:542:GLN:NE2	2.21	0.41
1:C:525:HIS:HD1	1:C:695:GLU:CD	2.24	0.41
1:C:557:LEU:HD23	1:C:557:LEU:HA	1.97	0.41
1:D:558:ILE:O	1:D:559:ALA:C	2.63	0.41
1:D:693:TYR:O	1:D:697:TRP:N	2.47	0.41
1:A:727:LEU:O	1:A:728:GLY:C	2.63	0.41
1:B:696:PHE:CZ	1:B:713:MET:HE3	2.54	0.41
1:C:703:MET:HE3	1:C:708:ILE:HB	2.01	0.41
1:D:632:ALA:C	1:D:634:ASP:H	2.27	0.41
1:A:648:MET:HE1	5:A:938:HOH:O	2.20	0.41
1:B:486:TRP:HB2	1:B:487:PRO:HD3	2.03	0.41
1:B:658:ASN:ND2	1:B:661:HIS:CD2	2.89	0.41
1:A:681:LEU:O	1:A:682:TRP:C	2.63	0.41
1:B:638:TYR:OH	1:B:642:ARG:HD3	2.20	0.41
1:D:701:ASP:O	1:D:705:LYS:HG3	2.21	0.41
1:C:746:PRO:N	1:C:747:PRO:CD	2.84	0.41
1:D:510:ARG:NH1	1:D:607:GLY:O	2.53	0.41
1:A:578:PHE:HA	1:A:706:LEU:HD11	2.03	0.41
1:C:720:ASP:O	1:C:723:PRO:HD2	2.21	0.41
1:B:637:LEU:HD23	1:B:637:LEU:HA	1.89	0.41
1:D:700:GLY:HA3	1:D:714:MET:O	2.20	0.41
1:A:515:VAL:O	1:A:516:LYS:C	2.64	0.41
1:C:742:THR:O	1:C:746:PRO:HA	2.21	0.41
1:A:641:ASN:ND2	5:A:911:HOH:O	2.52	0.40
1:C:490:PHE:HA	1:C:493:MET:HE2	2.04	0.40
1:C:743:GLN:HE21	1:C:743:GLN:HB2	1.57	0.40
1:A:578:PHE:O	1:A:578:PHE:CG	2.74	0.40
1:C:631:ILE:HD13	1:C:631:ILE:HA	1.82	0.40
1:B:471:GLU:HB3	1:B:477:PHE:CD1	2.55	0.40
1:B:603:LEU:HA	1:B:603:LEU:HD23	1.82	0.40
1:B:622:VAL:HA	1:B:625:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:LEU:O	1:C:465:PRO:C	2.64	0.40
1:C:727:LEU:CD2	1:C:759:LEU:HD11	2.51	0.40
1:C:494:VAL:O	1:C:498:CYS:HB3	2.21	0.40
1:A:519:TYR:CE2	1:A:530:ALA:HB2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:GLU:OE1	1:B:606:GLU:OE2[3_555]	2.01	0.19

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	311/343 (91%)	282 (91%)	23 (7%)	6 (2%)	6	19
1	B	313/343 (91%)	284 (91%)	25 (8%)	4 (1%)	9	28
1	C	312/343 (91%)	284 (91%)	26 (8%)	2 (1%)	21	47
1	D	307/343 (90%)	276 (90%)	26 (8%)	5 (2%)	7	23
All	All	1243/1372 (91%)	1126 (91%)	100 (8%)	17 (1%)	9	26

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	LYS
1	B	502	CYS
1	A	506	GLU
1	B	659	GLN
1	C	502	CYS
1	D	721	GLU

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Mol	Chain	Res	Type
1	D	502	CYS
1	A	616	SER
1	B	770	GLU
1	C	579	ASP
1	D	606	GLU
1	D	633	THR
1	B	498	CYS
1	A	555	GLY
1	D	746	PRO
1	A	768	GLY
1	A	747	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	282/305 (92%)	260 (92%)	22 (8%)	11	32
1	B	282/305 (92%)	257 (91%)	25 (9%)	9	26
1	C	283/305 (93%)	263 (93%)	20 (7%)	13	36
1	D	279/305 (92%)	261 (94%)	18 (6%)	15	40
All	All	1126/1220 (92%)	1041 (92%)	85 (8%)	12	34

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	471	GLU
1	A	500	THR
1	A	504	GLU
1	A	542	GLN
1	A	545	HIS
1	A	558	ILE
1	A	573	SER
1	A	575	LEU
1	A	597	SER

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Mol	Chain	Res	Type
1	A	602	ILE
1	A	605	LEU
1	A	610	ILE
1	A	615	SER
1	A	622	VAL
1	A	692	ILE
1	A	709	GLN
1	A	722	VAL
1	A	727	LEU
1	A	759	LEU
1	A	760	SER
1	A	765	VAL
1	B	460	MET
1	B	463	THR
1	B	469	CYS
1	B	471	GLU
1	B	478	ASP
1	B	497	SER
1	B	500	THR
1	B	504	GLU
1	B	517	LYS
1	B	543	ASN
1	B	575	LEU
1	B	576	GLN
1	B	590	THR
1	B	605	LEU
1	B	616	SER
1	B	643	LYS
1	B	650	GLN
1	B	660	SER
1	B	665	VAL
1	B	677	SER
1	B	709	GLN
1	B	727	LEU
1	B	735	ILE
1	B	739	THR
1	B	757	ASP
1	C	459	LEU
1	C	463	THR
1	C	471	GLU
1	C	500	THR
1	C	504	GLU

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Mol	Chain	Res	Type
1	C	506	GLU
1	C	517	LYS
1	C	542	GLN
1	C	547	LEU
1	C	575	LEU
1	C	576	GLN
1	C	605	LEU
1	C	610	ILE
1	C	615	SER
1	C	660	SER
1	C	709	GLN
1	C	711	ILE
1	C	727	LEU
1	C	742	THR
1	C	759	LEU
1	D	459	LEU
1	D	471	GLU
1	D	497	SER
1	D	500	THR
1	D	504	GLU
1	D	517	LYS
1	D	546	THR
1	D	575	LEU
1	D	616	SER
1	D	644	GLN
1	D	660	SER
1	D	709	GLN
1	D	711	ILE
1	D	722	VAL
1	D	727	LEU
1	D	733	VAL
1	D	739	THR
1	D	751	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	542	GLN
1	A	545	HIS
1	A	576	GLN
1	A	593	GLN

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Mol	Chain	Res	Type
1	A	598	GLN
1	A	604	GLN
1	A	609	ASN
1	A	644	GLN
1	A	661	HIS
1	A	743	GLN
1	B	484	ASN
1	B	495	HIS
1	B	542	GLN
1	B	543	ASN
1	B	545	HIS
1	B	604	GLN
1	B	609	ASN
1	B	644	GLN
1	B	655	ASN
1	B	657	ASN
1	B	658	ASN
1	B	726	GLN
1	B	761	GLN
1	C	476	HIS
1	C	495	HIS
1	C	542	GLN
1	C	543	ASN
1	C	593	GLN
1	C	604	GLN
1	C	644	GLN
1	C	743	GLN
1	D	461	GLN
1	D	495	HIS
1	D	542	GLN
1	D	543	ASN
1	D	593	GLN
1	D	598	GLN
1	D	604	GLN
1	D	644	GLN
1	D	650	GLN
1	D	658	ASN
1	D	709	GLN
1	D	731	ASN
1	D	761	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CME	B	509	1	8,9,10	0.60	0	6,9,11	1.20	1 (16%)
1	CME	D	509	1	8,9,10	0.55	0	6,9,11	1.03	1 (16%)
1	CME	A	509	1	8,9,10	0.64	0	6,9,11	0.79	0
1	CME	C	509	1	8,9,10	0.49	0	6,9,11	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	B	509	1	-	2/5/8/10	-
1	CME	D	509	1	-	2/5/8/10	-
1	CME	A	509	1	-	1/5/8/10	-
1	CME	C	509	1	-	1/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	509	CME	CB-SG-SD	2.36	109.97	103.86
1	D	509	CME	CB-SG-SD	2.02	109.09	103.86

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	509	CME	SD-CE-CZ-OH
1	C	509	CME	SD-CE-CZ-OH
1	D	509	CME	N-CA-CB-SG
1	B	509	CME	SD-CE-CZ-OH
1	D	509	CME	SD-CE-CZ-OH
1	B	509	CME	CE-SD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	JXI	D	803	-	28,28,28	2.26	13 (46%)	32,40,40	2.26	10 (31%)
4	JXI	C	803	-	28,28,28	2.27	9 (32%)	32,40,40	2.78	18 (56%)
4	JXI	A	803	-	28,28,28	2.12	6 (21%)	32,40,40	2.42	9 (28%)
4	JXI	B	803	-	28,28,28	2.38	10 (35%)	32,40,40	2.79	15 (46%)

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	JXI	D	803	-	-	4/9/9/9	0/4/4/4
4	JXI	C	803	-	-	2/9/9/9	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	JXI	A	803	-	-	4/9/9/9	0/4/4/4
4	JXI	B	803	-	-	4/9/9/9	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	JXI	C15-N17	6.37	1.44	1.37
4	A	803	JXI	C15-N17	6.30	1.44	1.37
4	C	803	JXI	C15-N17	5.90	1.43	1.37
4	D	803	JXI	C14-C12	5.25	1.48	1.33
4	A	803	JXI	C14-C12	4.53	1.46	1.33
4	D	803	JXI	C8-C7	4.44	1.44	1.37
4	C	803	JXI	C8-C7	4.41	1.44	1.37
4	B	803	JXI	C14-C12	4.34	1.46	1.33
4	B	803	JXI	C10-N11	4.07	1.40	1.33
4	C	803	JXI	C14-C12	3.99	1.45	1.33
4	B	803	JXI	C8-C7	3.76	1.43	1.37
4	A	803	JXI	C14-C15	3.28	1.49	1.45
4	D	803	JXI	C12-C10	3.18	1.49	1.45
4	C	803	JXI	C18-N17	3.15	1.44	1.38
4	C	803	JXI	C10-N11	3.13	1.38	1.33
4	A	803	JXI	C10-N9	2.96	1.43	1.36
4	A	803	JXI	C8-C7	2.96	1.42	1.37
4	C	803	JXI	C22-N23	2.85	1.37	1.32
4	D	803	JXI	C15-N17	2.85	1.40	1.37
4	B	803	JXI	C18-N17	2.82	1.44	1.38
4	B	803	JXI	C8-N9	2.81	1.42	1.37
4	D	803	JXI	C10-N11	2.80	1.38	1.33
4	A	803	JXI	C1-C7	-2.62	1.43	1.47
4	D	803	JXI	C6-C1	2.56	1.43	1.39
4	D	803	JXI	C10-N9	2.53	1.42	1.36
4	D	803	JXI	C20-N24	2.50	1.39	1.35
4	D	803	JXI	C14-C15	2.49	1.48	1.45
4	C	803	JXI	C22-C21	2.48	1.44	1.41
4	D	803	JXI	C8-N9	2.48	1.42	1.37
4	B	803	JXI	O19-C18	2.29	1.27	1.23
4	D	803	JXI	C22-N23	2.27	1.36	1.32
4	D	803	JXI	C15-N16	-2.24	1.29	1.32
4	B	803	JXI	C15-N16	-2.18	1.29	1.32
4	B	803	JXI	C5-C6	2.17	1.42	1.38
4	C	803	JXI	C5-C6	2.13	1.42	1.38
4	B	803	JXI	C2-C1	2.07	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	803	JXI	C2-C1	2.04	1.42	1.39
4	C	803	JXI	C8-N9	2.04	1.41	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	JXI	C15-N16-C20	-7.58	106.42	117.18
4	A	803	JXI	C15-N16-C20	-7.36	106.73	117.18
4	C	803	JXI	C25-N24-N23	6.55	132.28	119.22
4	A	803	JXI	C25-N24-N23	5.47	130.13	119.22
4	C	803	JXI	C25-N24-C20	-5.45	116.53	128.76
4	D	803	JXI	C13-N9-C8	5.07	132.29	123.98
4	B	803	JXI	C25-N24-N23	4.94	129.07	119.22
4	C	803	JXI	C15-N16-C20	-4.92	110.20	117.18
4	D	803	JXI	C15-N16-C20	-4.85	110.29	117.18
4	D	803	JXI	C25-N24-N23	4.85	128.88	119.22
4	D	803	JXI	C13-N9-C10	-4.67	123.61	127.84
4	B	803	JXI	C8-C7-N11	-4.46	106.48	110.75
4	A	803	JXI	C25-N24-C20	-4.42	118.84	128.76
4	D	803	JXI	C22-N23-N24	4.31	109.17	105.06
4	C	803	JXI	C13-N9-C8	4.24	130.93	123.98
4	C	803	JXI	C8-C7-N11	-4.14	106.79	110.75
4	B	803	JXI	C21-C18-N17	-4.08	107.30	114.45
4	B	803	JXI	C18-C21-C20	4.07	120.86	118.35
4	B	803	JXI	C1-C7-N11	4.03	126.12	119.95
4	B	803	JXI	C21-C20-N16	4.00	130.47	127.44
4	B	803	JXI	C25-N24-C20	-3.90	120.00	128.76
4	A	803	JXI	C21-C20-N16	3.88	130.38	127.44
4	B	803	JXI	C12-C10-N11	3.82	129.57	125.03
4	C	803	JXI	C18-N17-C15	-3.46	120.19	123.36
4	C	803	JXI	C1-C7-N11	3.45	125.23	119.95
4	C	803	JXI	C12-C10-N9	-3.32	118.21	122.69
4	C	803	JXI	C21-C22-N23	-3.31	108.34	112.45
4	B	803	JXI	C12-C10-N9	-3.21	118.36	122.69
4	A	803	JXI	C18-C21-C20	3.19	120.31	118.35
4	D	803	JXI	C25-N24-C20	-3.12	121.76	128.76
4	C	803	JXI	C21-C20-N16	2.98	129.70	127.44
4	A	803	JXI	C22-N23-N24	2.73	107.66	105.06
4	C	803	JXI	C7-N11-C10	-2.69	104.39	105.64
4	D	803	JXI	C21-C22-N23	-2.63	109.19	112.45
4	C	803	JXI	C18-C21-C20	-2.60	116.74	118.35
4	C	803	JXI	C22-N23-N24	2.49	107.44	105.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	JXI	C21-C18-N17	-2.42	110.21	114.45
4	D	803	JXI	C7-N11-C10	-2.40	104.53	105.64
4	B	803	JXI	C22-N23-N24	2.34	107.29	105.06
4	A	803	JXI	C21-C22-N23	-2.31	109.58	112.45
4	C	803	JXI	C6-C1-C2	-2.31	115.62	118.57
4	B	803	JXI	C14-C12-C10	-2.30	117.27	124.08
4	C	803	JXI	N9-C10-N11	2.29	114.22	111.29
4	B	803	JXI	C7-C8-N9	2.26	109.09	106.82
4	D	803	JXI	C21-C18-N17	-2.20	110.59	114.45
4	B	803	JXI	C13-N9-C8	2.17	127.53	123.98
4	A	803	JXI	C3-C2-C1	-2.16	118.24	120.36
4	C	803	JXI	C12-C10-N11	2.12	127.56	125.03
4	C	803	JXI	C6-C1-C7	2.11	123.24	120.87
4	D	803	JXI	C12-C10-N9	-2.08	119.89	122.69
4	B	803	JXI	O19-C18-C21	2.02	130.42	125.98
4	C	803	JXI	C5-C4-C3	-2.01	117.11	119.87

There are no chirality outliers.

All (14) torsion outliers are listed below:

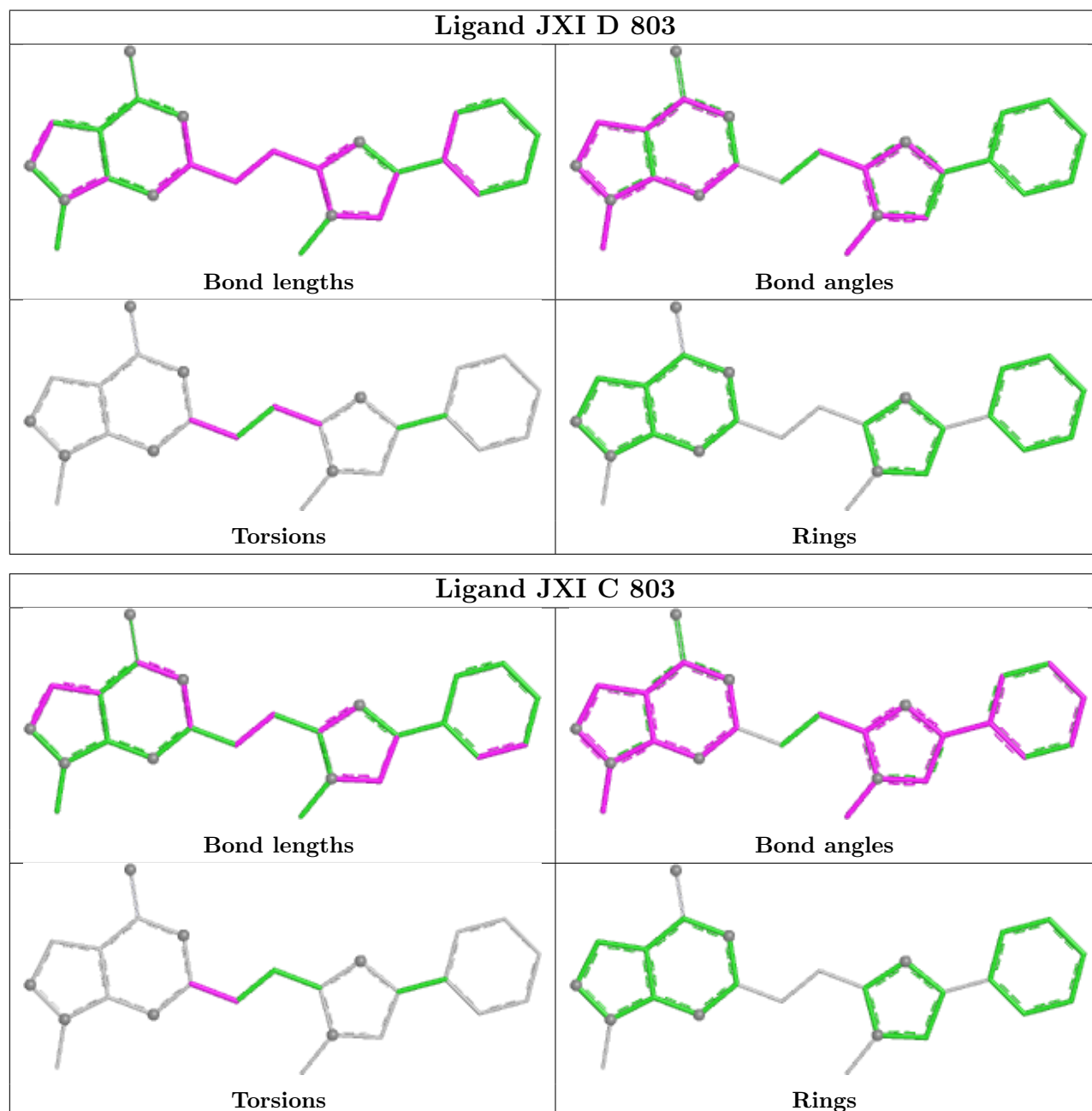
Mol	Chain	Res	Type	Atoms
4	A	803	JXI	N9-C10-C12-C14
4	A	803	JXI	N11-C10-C12-C14
4	A	803	JXI	C12-C14-C15-N16
4	A	803	JXI	C12-C14-C15-N17
4	B	803	JXI	C12-C14-C15-N16
4	B	803	JXI	C12-C14-C15-N17
4	C	803	JXI	C12-C14-C15-N16
4	C	803	JXI	C12-C14-C15-N17
4	D	803	JXI	N9-C10-C12-C14
4	D	803	JXI	N11-C10-C12-C14
4	D	803	JXI	C12-C14-C15-N16
4	D	803	JXI	C12-C14-C15-N17
4	B	803	JXI	N11-C10-C12-C14
4	B	803	JXI	N9-C10-C12-C14

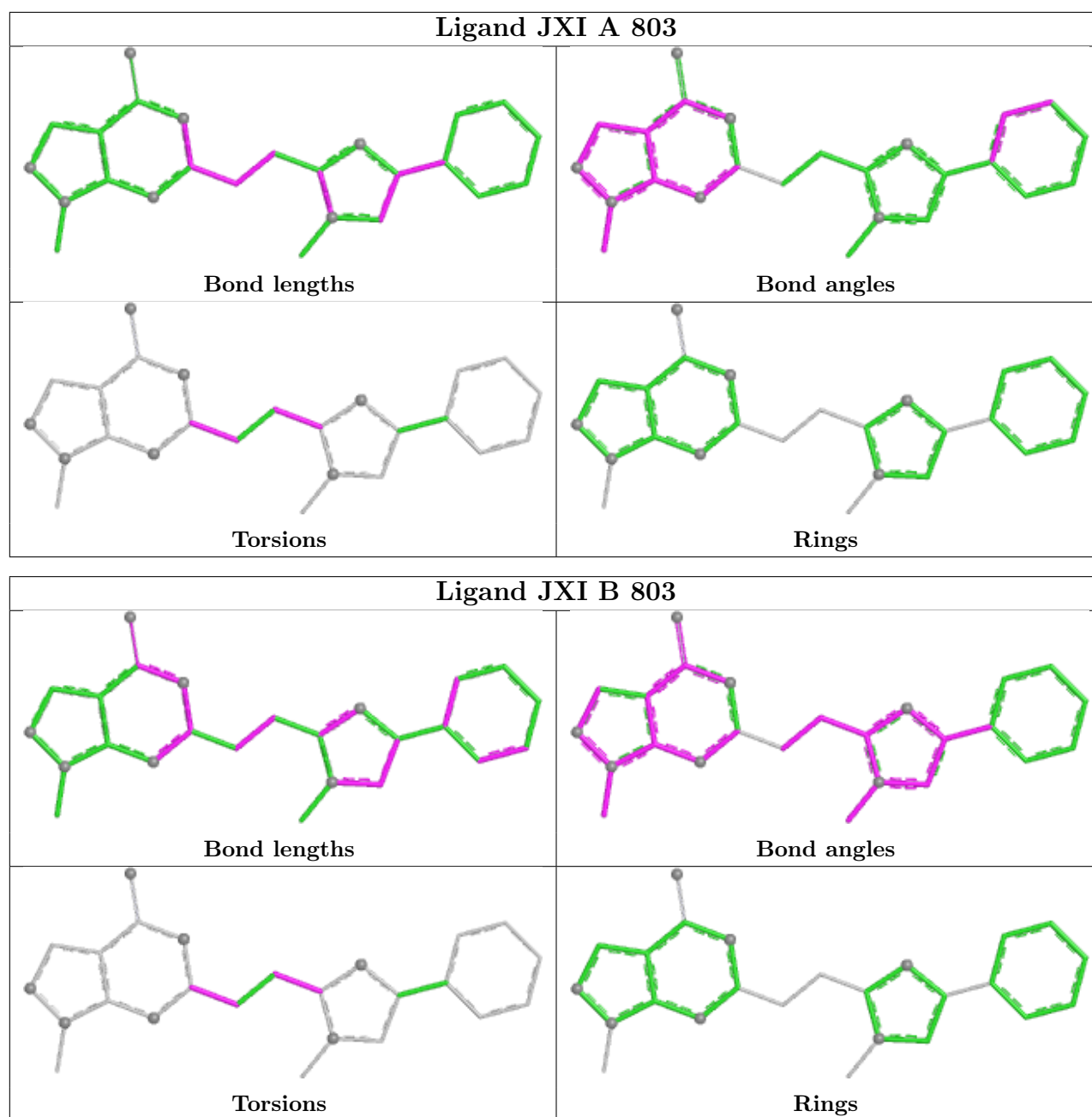
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	JXI	3	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	312/343 (90%)	0.98	39 (12%) 8 6	32, 62, 91, 112	1 (0%)
1	B	314/343 (91%)	0.98	33 (10%) 11 9	40, 62, 97, 118	1 (0%)
1	C	312/343 (90%)	0.93	25 (8%) 18 14	40, 64, 92, 121	2 (0%)
1	D	309/343 (90%)	1.23	41 (13%) 7 6	50, 73, 98, 111	0
All	All	1247/1372 (90%)	1.03	138 (11%) 10 8	32, 66, 97, 121	4 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	458	GLY	4.6
1	D	459	LEU	4.5
1	A	459	LEU	4.2
1	B	460	MET	4.1
1	C	606	GLU	3.9
1	A	458	GLY	3.8
1	A	462	PHE	3.6
1	D	620	GLU	3.6
1	B	459	LEU	3.6
1	A	551	LEU	3.5
1	B	601	SER	3.4
1	A	708	ILE	3.4
1	C	462	PHE	3.4
1	C	521	ARG	3.3
1	D	505	LEU	3.3
1	B	513	MET	3.2
1	B	605	LEU	3.2
1	D	462	PHE	3.2
1	B	458	GLY	3.2
1	B	510	ARG	3.2
1	D	756	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	459	LEU	3.1
1	D	708	ILE	3.1
1	B	727	LEU	3.0
1	A	521	ARG	3.0
1	C	620	GLU	3.0
1	B	457	GLN	3.0
1	A	484	ASN	3.0
1	D	461	GLN	3.0
1	A	605	LEU	2.9
1	D	517	LYS	2.9
1	B	514	SER	2.9
1	D	500	THR	2.9
1	C	596	PHE	2.9
1	D	460	MET	2.8
1	B	604	GLN	2.8
1	A	553	ARG	2.8
1	B	466	VAL	2.8
1	B	470	LYS	2.8
1	C	460	MET	2.8
1	D	606	GLU	2.7
1	D	613	THR	2.7
1	A	649	TYR	2.7
1	B	517	LYS	2.7
1	D	489	ILE	2.6
1	A	612	SER	2.6
1	B	484	ASN	2.6
1	A	724	GLN	2.6
1	B	506	GLU	2.6
1	A	513	MET	2.6
1	C	600	VAL	2.6
1	D	464	LEU	2.6
1	A	506	GLU	2.6
1	A	460	MET	2.5
1	B	505	LEU	2.5
1	C	751	LEU	2.5
1	D	470	LYS	2.5
1	B	498	CYS	2.5
1	C	619	TYR	2.5
1	D	466	VAL	2.5
1	B	462	PHE	2.5
1	A	497	SER	2.5
1	D	605	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	545	HIS	2.5
1	A	770	GLU	2.5
1	B	768	GLY	2.5
1	D	503	PHE	2.5
1	A	505	LEU	2.4
1	D	568	ARG	2.4
1	C	603	LEU	2.4
1	D	518	ASN	2.4
1	D	751	LEU	2.4
1	A	616	SER	2.4
1	A	461	GLN	2.4
1	D	604	GLN	2.4
1	C	584	ALA	2.4
1	C	551	LEU	2.3
1	D	586	TYR	2.3
1	C	461	GLN	2.3
1	C	770	GLU	2.3
1	D	646	GLU	2.3
1	A	603	LEU	2.3
1	A	647	GLU	2.3
1	C	517	LYS	2.3
1	B	527	TRP	2.3
1	C	692	ILE	2.3
1	C	470	LYS	2.3
1	A	609	ASN	2.2
1	D	521	ARG	2.2
1	D	712	PRO	2.2
1	C	502	CYS	2.2
1	B	606	GLU	2.2
1	A	656	LEU	2.2
1	A	554	LYS	2.2
1	A	503	PHE	2.2
1	C	506	GLU	2.2
1	D	577	LYS	2.2
1	D	645	LEU	2.2
1	D	722	VAL	2.2
1	A	545	HIS	2.2
1	A	606	GLU	2.2
1	A	547	LEU	2.2
1	D	513	MET	2.2
1	D	573	SER	2.2
1	B	521	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	737	CYS	2.1
1	B	724	GLN	2.1
1	D	681	LEU	2.1
1	A	550	ASP	2.1
1	B	501	SER	2.1
1	D	514	SER	2.1
1	B	769	GLU	2.1
1	A	604	GLN	2.1
1	A	582	LEU	2.1
1	B	492	TYR	2.1
1	D	707	GLY	2.1
1	A	517	LYS	2.1
1	A	703	MET	2.1
1	A	498	CYS	2.1
1	B	720	ASP	2.1
1	C	720	ASP	2.1
1	A	620	GLU	2.1
1	C	553	ARG	2.1
1	A	709	GLN	2.1
1	C	709	GLN	2.1
1	B	759	LEU	2.1
1	D	504	GLU	2.0
1	D	601	SER	2.0
1	D	588	THR	2.0
1	D	638	TYR	2.0
1	A	763	GLU	2.0
1	B	483	GLU	2.0
1	B	463	THR	2.0
1	D	703	MET	2.0
1	D	762	TRP	2.0
1	A	727	LEU	2.0
1	D	547	LEU	2.0
1	B	543	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	CME	D	509	10/11	0.69	0.25	61,91,129,132	0
1	CME	C	509	10/11	0.75	0.19	64,78,126,127	0
1	CME	A	509	10/11	0.79	0.20	58,93,131,135	0
1	CME	B	509	10/11	0.80	0.32	66,94,102,109	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

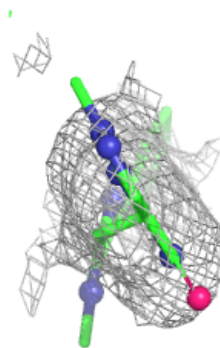
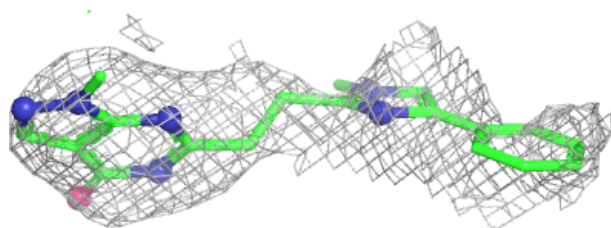
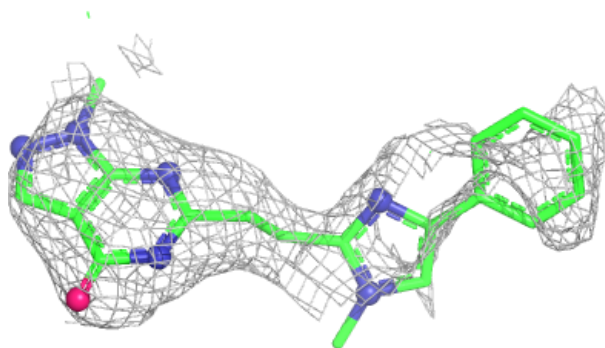
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	JXI	D	803	25/25	0.80	0.20	58,102,135,145	0
4	JXI	B	803	25/25	0.87	0.15	53,76,95,102	0
4	JXI	A	803	25/25	0.87	0.14	54,67,78,86	0
4	JXI	C	803	25/25	0.88	0.17	51,72,117,121	0
3	MG	B	802	1/1	0.93	0.07	58,58,58,58	0
3	MG	C	802	1/1	0.96	0.05	44,44,44,44	0
3	MG	D	802	1/1	0.96	0.07	54,54,54,54	0
2	ZN	D	801	1/1	0.97	0.04	60,60,60,60	0
2	ZN	A	801	1/1	0.99	0.03	51,51,51,51	0
3	MG	A	802	1/1	0.99	0.03	90,90,90,90	0
2	ZN	C	801	1/1	0.99	0.02	46,46,46,46	0
2	ZN	B	801	1/1	1.00	0.02	51,51,51,51	0

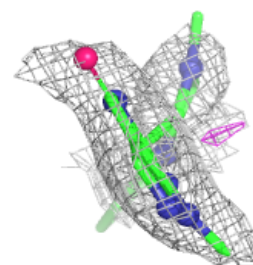
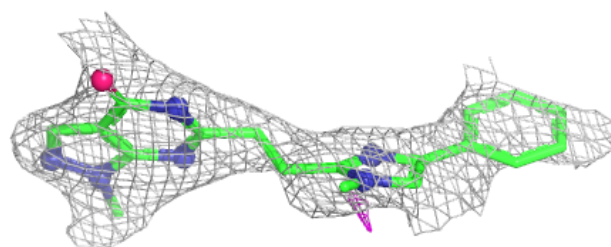
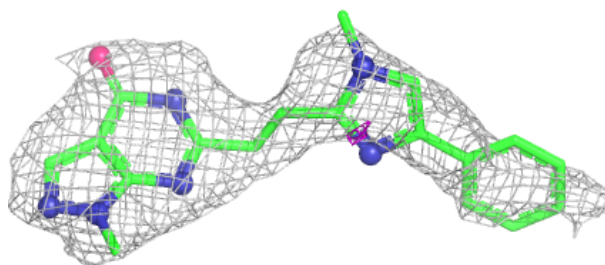
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JXI D 803:

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

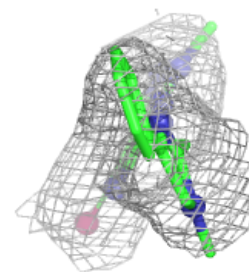
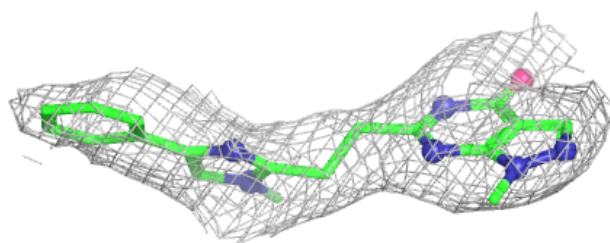
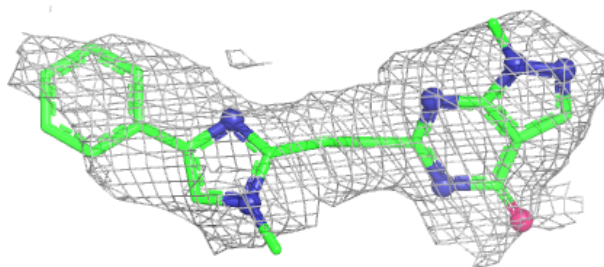
**Electron density around JXI B 803:**

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

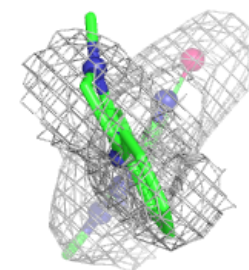
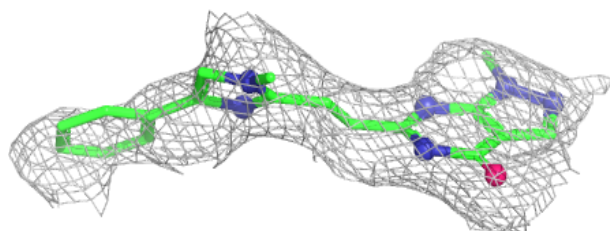
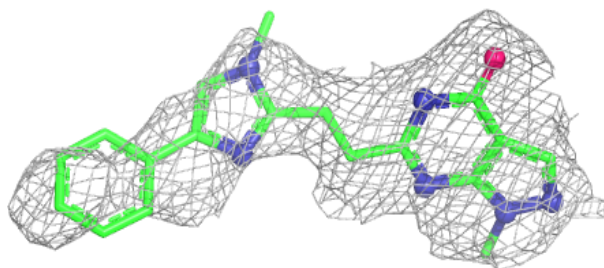


Electron density around JXI A 803:

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

**Electron density around JXI C 803:**

$2mF_o-DF_c$ (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.