



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:56 AM UTC

PDB ID : 5SJ5 / pdb_00005sj5
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN
COMPLEX WITH c12c(nc(cn1)N)ccc(c2)Cl, micromolar IC50=41.447943
Authors : Joseph, C.; Benz, J.; Flohr, A.; Isenring, H.; Rudolph, M.G.
Deposited on : 2022-02-01
Resolution : 2.49 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

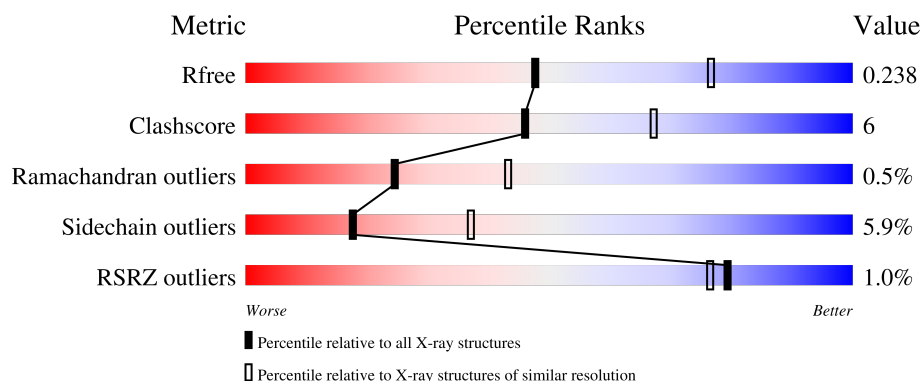
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	70% 18% 9%
1	B	343	65% 23% 8%
1	C	343	71% 18% 9%
1	D	343	70% 19% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10531 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	0	0
			2541	1624	432	461	24			
1	B	315	Total	C	N	O	S	0	0	0
			2551	1630	434	463	24			
1	C	313	Total	C	N	O	S	0	1	0
			2549	1629	435	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

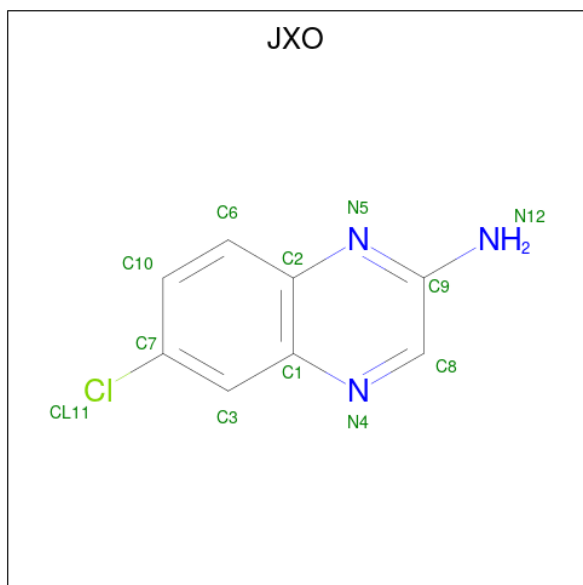
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 6-chloroquinoxalin-2-amine (CCD ID: JXO) (formula: C₈H₆ClN₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			12	8	1	3		
4	B	1	Total	C	Cl	N	0	0
			12	8	1	3		
4	C	1	Total	C	Cl	N	0	0
			12	8	1	3		
4	D	1	Total	C	Cl	N	0	0
			12	8	1	3		

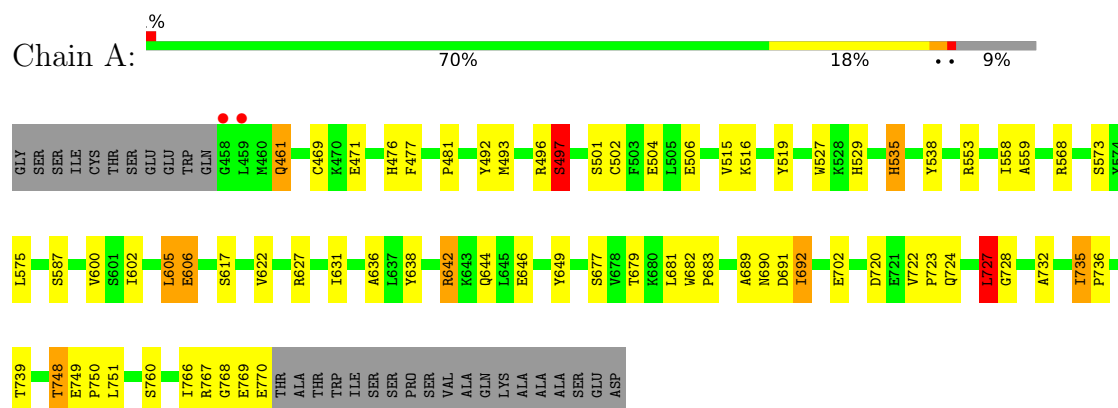
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total 82	O 82	0	0
5	B	93	Total 93	O 93	0	0
5	C	87	Total 87	O 87	0	0
5	D	53	Total 53	O 53	0	0

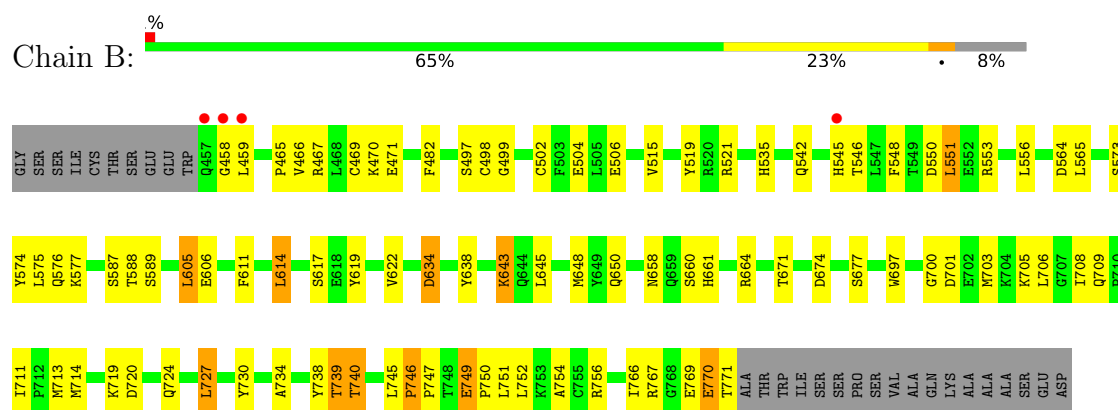
3 Residue-property plots

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.

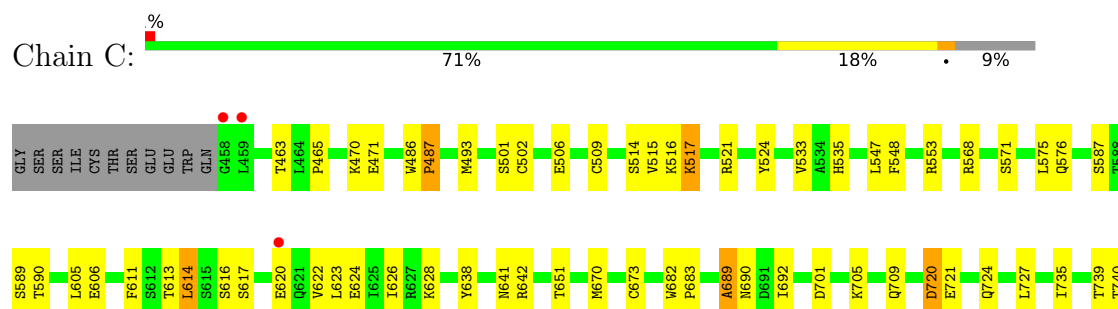
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

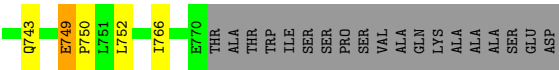


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

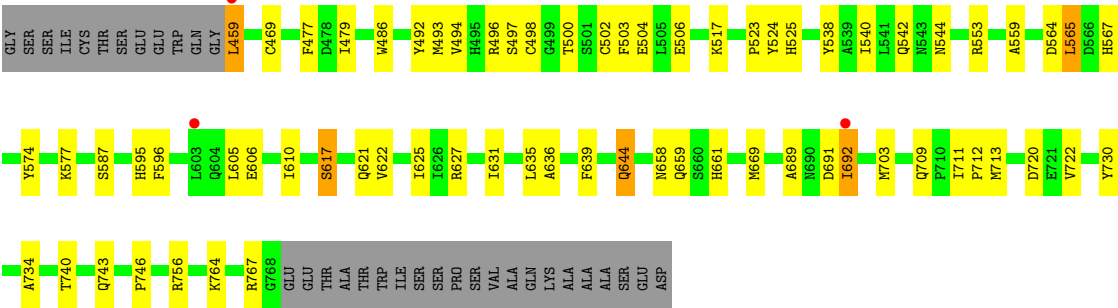


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A





● 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	134.91Å 134.91Å 234.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.40 – 2.49 43.40 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.7 (43.40-2.49) 96.7 (43.40-2.49)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.169 , 0.238 0.177 , 0.238	Depositor DCC
R_{free} test set	2754 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10531	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: ZN, JXO, CME, MG

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	8/2592 (0.3%)	1.56	15/3507 (0.4%)
1	B	1.23	4/2602 (0.2%)	1.60	21/3521 (0.6%)
1	C	1.24	7/2603 (0.3%)	1.58	27/3521 (0.8%)
1	D	1.25	0/2570	1.58	14/3478 (0.4%)
All	All	1.24	19/10367 (0.2%)	1.58	77/14027 (0.5%)

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

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	727	LEU	C-O	7.59	1.33	1.24
1	A	748	THR	C-O	7.43	1.33	1.24
1	B	754	ALA	C-O	7.01	1.32	1.24
1	A	739	THR	C-O	6.69	1.31	1.24
1	A	519	TYR	C-O	-6.46	1.16	1.23
1	A	481	PRO	C-O	-6.44	1.16	1.23
1	B	519	TYR	C-O	-5.97	1.16	1.23
1	C	589	SER	C-O	5.81	1.31	1.24
1	C	620	GLU	CD-OE1	5.59	1.35	1.25
1	B	706	LEU	C-O	-5.55	1.16	1.24
1	B	674	ASP	CG-OD2	-5.48	1.15	1.25
1	C	575	LEU	C-O	-5.44	1.17	1.24
1	A	476	HIS	CE1-NE2	5.20	1.37	1.32
1	C	514	SER	C-O	5.19	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	670	MET	C-O	5.16	1.30	1.24
1	C	689	ALA	C-O	5.14	1.30	1.24
1	A	535	HIS	CE1-NE2	5.07	1.37	1.32
1	A	527	TRP	C-O	5.05	1.30	1.24
1	C	590	THR	C-O	5.00	1.29	1.24

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	606	GLU	CB-CG-CD	8.33	126.76	112.60
1	C	620	GLU	CB-CG-CD	8.25	126.62	112.60
1	A	606	GLU	CB-CG-CD	7.46	125.29	112.60
1	A	692	ILE	N-CA-C	-7.42	103.23	110.72
1	D	639	PHE	CA-C-N	7.19	127.96	119.98
1	D	639	PHE	C-N-CA	7.19	127.96	119.98
1	C	617	SER	CA-C-N	6.98	129.95	120.38
1	C	617	SER	C-N-CA	6.98	129.95	120.38
1	C	506	GLU	CB-CG-CD	6.87	124.27	112.60
1	A	506	GLU	CB-CG-CD	6.86	124.26	112.60
1	C	720	ASP	CA-CB-CG	6.84	119.44	112.60
1	D	720	ASP	CA-CB-CG	6.75	119.35	112.60
1	B	746	PRO	N-CA-C	6.72	118.90	110.70
1	D	574	TYR	N-CA-C	-6.65	104.11	111.36
1	A	735	ILE	CA-C-O	6.58	123.10	118.69
1	C	606	GLU	CB-CG-CD	6.39	123.47	112.60
1	C	614	LEU	CA-C-O	-6.38	114.47	121.87
1	A	529	HIS	N-CA-C	-6.33	104.30	111.14
1	B	499	GLY	CA-C-N	6.23	129.48	120.38
1	B	499	GLY	C-N-CA	6.23	129.48	120.38
1	B	515	VAL	N-CA-C	-6.10	104.79	110.53
1	A	642	ARG	CA-C-O	-5.98	114.21	120.55
1	A	690	ASN	N-CA-CB	5.95	118.87	110.12
1	C	576	GLN	N-CA-C	-5.90	104.53	110.97
1	C	515	VAL	CA-C-O	-5.90	115.28	121.41
1	D	559	ALA	N-CA-C	-5.84	104.91	111.28
1	B	605	LEU	CA-C-O	-5.77	114.84	121.19
1	C	571	SER	CA-C-N	5.75	127.98	120.28
1	C	571	SER	C-N-CA	5.75	127.98	120.28
1	C	651	THR	CA-CB-OG1	-5.74	100.99	109.60
1	A	691	ASP	N-CA-C	-5.69	105.08	111.28
1	B	482	PHE	CA-C-N	5.66	128.13	120.38
1	B	482	PHE	C-N-CA	5.66	128.13	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	739	THR	N-CA-C	-5.65	104.76	111.03
1	C	521	ARG	CB-CA-C	5.65	120.59	112.12
1	D	544	ASN	CA-C-O	-5.61	115.37	121.20
1	D	692	ILE	N-CA-C	-5.61	105.06	110.72
1	A	690	ASN	CB-CA-C	-5.54	101.59	110.79
1	A	649	TYR	CA-C-N	5.51	127.93	120.44
1	A	649	TYR	C-N-CA	5.51	127.93	120.44
1	C	617	SER	O-C-N	5.50	128.49	122.11
1	C	587	SER	CA-C-O	-5.50	113.89	120.10
1	B	720	ASP	CA-CB-CG	5.47	118.08	112.60
1	B	706	LEU	N-CA-C	-5.46	106.39	113.16
1	D	659	GLN	CA-C-N	5.45	127.84	120.38
1	D	659	GLN	C-N-CA	5.45	127.84	120.38
1	D	712	PRO	CA-C-N	5.43	127.56	120.28
1	D	712	PRO	C-N-CA	5.43	127.56	120.28
1	B	545	HIS	CB-CA-C	5.36	119.68	110.79
1	A	636	ALA	N-CA-C	-5.33	105.47	111.28
1	C	470	LYS	CA-C-N	5.31	127.40	120.28
1	C	470	LYS	C-N-CA	5.31	127.40	120.28
1	C	735	ILE	O-C-N	-5.28	117.04	120.42
1	A	702	GLU	N-CA-C	-5.26	105.72	111.82
1	C	690	ASN	N-CA-CB	5.24	117.83	110.12
1	A	573	SER	CB-CA-C	-5.21	102.70	110.88
1	D	746	PRO	N-CA-C	5.20	117.05	110.70
1	B	588	THR	CA-CB-OG1	-5.19	101.82	109.60
1	B	740	THR	CA-CB-OG1	-5.18	101.83	109.60
1	B	574	TYR	N-CA-C	-5.17	105.54	111.07
1	C	465	PRO	CA-C-N	5.16	127.25	120.60
1	C	465	PRO	C-N-CA	5.16	127.25	120.60
1	B	658	ASN	CB-CA-C	5.14	118.81	110.22
1	C	487	PRO	O-C-N	5.11	127.95	122.17
1	B	550	ASP	N-CA-C	-5.09	105.81	111.36
1	C	641	ASN	N-CA-C	-5.08	105.65	111.14
1	B	724	GLN	CA-C-N	5.08	125.58	120.00
1	B	724	GLN	C-N-CA	5.08	125.58	120.00
1	C	516	LYS	CA-C-N	5.06	127.56	120.28
1	C	516	LYS	C-N-CA	5.06	127.56	120.28
1	B	506	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	573	SER	O-C-N	5.05	127.27	122.07
1	D	606	GLU	CB-CG-CD	5.04	121.17	112.60
1	B	634	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	506	GLU	CA-C-N	5.03	127.42	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	506	GLU	C-N-CA	5.03	127.42	120.29
1	D	506	GLU	CB-CG-CD	5.03	121.14	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	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	2541	0	2511	27	0
1	B	2551	0	2515	35	0
1	C	2549	0	2524	21	0
1	D	2519	0	2496	35	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	12	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	0	0
4	D	12	0	0	1	0
5	A	82	0	0	1	0
5	B	93	0	0	0	0
5	C	87	0	0	1	0
5	D	53	0	0	1	0
All	All	10531	0	10046	117	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 (117) 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:B:727:LEU:HD12	1:B:766:ILE:HD13	1.66	0.78
1:A:469:CYS:SG	5:A:974:HOH:O	2.45	0.73
1:A:602:ILE:HA	1:A:605:LEU:HD22	1.75	0.69
1:D:497:SER:O	1:D:553:ARG:HD2	1.93	0.69
1:D:713:MET:SD	4:D:803:JXO:N12	2.67	0.67
1:D:497:SER:HA	1:D:542:GLN:NE2	2.12	0.65
1:A:689:ALA:HA	1:A:692:ILE:HG22	1.80	0.63
1:B:498:CYS:O	1:B:502:CYS:SG	2.56	0.63
1:A:749:GLU:N	1:A:750:PRO:CD	2.62	0.61
1:C:517:LYS:O	1:C:517:LYS:HE3	2.01	0.61
1:B:467:ARG:O	1:B:471:GLU:HB2	2.03	0.59
1:C:524:TYR:CD2	1:C:692:ILE:HD13	2.38	0.59
1:C:689:ALA:HA	1:C:692:ILE:HG22	1.84	0.59
1:A:724:GLN:O	1:A:727:LEU:HB2	2.04	0.58
1:D:644:GLN:HE21	1:D:644:GLN:HA	1.67	0.58
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.87	0.57
1:C:720:ASP:OD1	1:C:721:GLU:HG3	2.04	0.57
1:B:577:LYS:HD3	1:B:703:MET:HE1	1.87	0.56
1:C:548:PHE:O	1:C:553:ARG:NH2	2.39	0.56
1:C:724:GLN:HA	1:C:766:ILE:HD11	1.87	0.56
1:B:611:PHE:HB3	1:B:614:LEU:HD22	1.88	0.55
1:C:740:THR:HA	1:C:743:GLN:NE2	2.20	0.55
1:A:749:GLU:N	1:A:750:PRO:HD2	2.20	0.55
1:D:497:SER:HA	1:D:542:GLN:HE22	1.72	0.54
1:D:524:TYR:CD2	1:D:692:ILE:HD13	2.43	0.54
1:C:493:MET:SD	1:C:535:HIS:HA	2.48	0.54
1:B:648:MET:HE2	1:B:661:HIS:NE2	2.22	0.54
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.91	0.53
1:D:493:MET:O	1:D:497:SER:CB	2.57	0.53
1:B:745:LEU:C	1:B:747:PRO:HD2	2.34	0.52
1:D:622:VAL:HA	1:D:625:ILE:HD12	1.91	0.52
1:C:533:VAL:HG13	1:C:673:CYS:HB3	1.92	0.52
1:D:740:THR:HA	1:D:743:GLN:HE21	1.74	0.52
1:B:467:ARG:O	1:B:467:ARG:HG2	2.08	0.52
1:C:486:TRP:N	1:C:487:PRO:CD	2.73	0.51
1:D:498:CYS:C	1:D:502:CYS:SG	2.93	0.51
1:C:749:GLU:HB3	1:C:750:PRO:HD3	1.93	0.51
1:D:689:ALA:HA	1:D:692:ILE:HG22	1.93	0.51
1:B:548:PHE:O	1:B:553:ARG:NH1	2.43	0.51
1:D:658:ASN:O	1:D:661:HIS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:NE2	1:A:461:GLN:HA	2.27	0.50
1:C:682:TRP:HB3	1:C:683:PRO:HD3	1.94	0.50
1:C:740:THR:HA	1:C:743:GLN:HE21	1.77	0.49
1:A:493:MET:SD	1:A:535:HIS:HA	2.53	0.49
1:B:770:GLU:HG3	1:B:771:THR:N	2.27	0.49
1:C:689:ALA:O	1:C:692:ILE:HG22	2.13	0.49
1:D:479:ILE:HD12	1:D:486:TRP:CD1	2.48	0.49
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.48	0.49
1:B:730:TYR:HA	1:B:734:ALA:HB3	1.94	0.49
1:B:546:THR:HG21	1:D:767:ARG:NH2	2.28	0.48
1:B:551:LEU:HD23	1:B:551:LEU:HA	1.69	0.48
1:D:493:MET:HB3	1:D:538:TYR:CD1	2.48	0.48
1:D:617:SER:O	1:D:621:GLN:HB2	2.13	0.48
1:D:730:TYR:HA	1:D:734:ALA:HB3	1.95	0.48
1:D:627:ARG:O	1:D:631:ILE:HG12	2.13	0.48
1:A:627:ARG:O	1:A:631:ILE:HG12	2.14	0.48
1:A:682:TRP:N	1:A:683:PRO:CD	2.77	0.48
1:B:711:ILE:HD11	1:B:713:MET:HE2	1.95	0.48
1:A:689:ALA:HA	1:A:692:ILE:CG2	2.45	0.47
1:B:497:SER:HA	1:B:542:GLN:NE2	2.29	0.47
1:B:589:SER:OG	1:B:634:ASP:OD2	2.24	0.47
1:B:645:LEU:HD21	1:B:664:ARG:HB3	1.96	0.47
1:D:494:VAL:O	1:D:498:CYS:HB3	2.15	0.46
1:D:469:CYS:SG	5:D:949:HOH:O	2.61	0.46
1:D:493:MET:O	1:D:497:SER:HB3	2.16	0.46
1:A:728:GLY:O	1:A:732:ALA:N	2.37	0.46
1:B:619:TYR:O	1:B:622:VAL:HG12	2.16	0.46
1:B:638:TYR:CD1	1:B:671:THR:HG21	2.51	0.46
1:C:628:LYS:NZ	5:C:911:HOH:O	2.49	0.46
1:C:611:PHE:HB3	1:C:614:LEU:HD22	1.96	0.46
1:D:564:ASP:O	1:D:567:HIS:HB2	2.16	0.46
1:A:766:ILE:C	1:A:768:GLY:H	2.24	0.45
1:B:703:MET:HE3	1:B:708:ILE:CG2	2.46	0.45
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.52	0.45
1:D:459:LEU:HD12	1:D:459:LEU:N	2.31	0.45
1:A:493:MET:HB3	1:A:538:TYR:CD2	2.52	0.45
1:A:515:VAL:O	1:A:516:LYS:C	2.59	0.45
1:B:700:GLY:HA3	1:B:714:MET:O	2.17	0.45
1:B:535:HIS:ND1	1:B:535:HIS:C	2.75	0.45
1:A:638:TYR:OH	1:A:642:ARG:HD3	2.16	0.44
1:A:769:GLU:O	1:A:770:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:PRO:O	1:B:466:VAL:C	2.59	0.44
1:C:701:ASP:O	1:C:705:LYS:HG3	2.17	0.44
1:D:524:TYR:CE2	1:D:692:ILE:HD13	2.52	0.44
1:D:565:LEU:O	1:D:595:HIS:ND1	2.41	0.44
1:D:577:LYS:HD3	1:D:703:MET:HE1	1.99	0.43
1:C:739:THR:HA	1:C:752:LEU:HD22	2.00	0.43
1:A:461:GLN:NE2	1:A:461:GLN:CA	2.81	0.43
1:C:624:GLU:HA	1:C:624:GLU:OE1	2.18	0.43
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.54	0.43
1:D:596:PHE:CE2	1:D:627:ARG:HG3	2.54	0.43
1:A:497:SER:O	1:A:553:ARG:HD2	2.18	0.43
1:D:493:MET:O	1:D:497:SER:HB2	2.19	0.43
1:B:697:TRP:CZ2	1:B:719:LYS:HG2	2.54	0.42
1:B:739:THR:O	1:B:740:THR:C	2.61	0.42
1:A:679:THR:HG21	1:A:751:LEU:HD22	2.01	0.42
1:B:701:ASP:O	1:B:705:LYS:HG3	2.19	0.42
1:B:564:ASP:O	1:B:565:LEU:C	2.62	0.42
1:C:638:TYR:OH	1:C:642:ARG:HD3	2.20	0.42
1:A:605:LEU:O	1:A:606:GLU:C	2.62	0.41
1:B:746:PRO:N	1:B:747:PRO:CD	2.83	0.41
1:A:558:ILE:O	1:A:559:ALA:C	2.63	0.41
1:D:540:ILE:HG21	1:D:669:MET:HE3	2.01	0.41
1:D:635:LEU:HD12	1:D:635:LEU:HA	1.95	0.41
1:C:622:VAL:O	1:C:626:ILE:HG13	2.21	0.41
1:D:525:HIS:HD2	1:D:564:ASP:OD2	2.03	0.41
1:A:748:THR:C	1:A:750:PRO:HD2	2.46	0.41
1:B:556:LEU:HD23	1:B:556:LEU:HA	1.89	0.41
1:B:752:LEU:HD21	1:B:756:ARG:NH2	2.36	0.41
1:D:523:PRO:O	1:D:691:ASP:HB3	2.20	0.41
1:D:635:LEU:O	1:D:636:ALA:C	2.62	0.41
1:B:738:TYR:CD1	1:B:751:LEU:HB3	2.56	0.41
1:B:767:ARG:NH2	1:B:769:GLU:OE1	2.54	0.40
1:D:503:PHE:CE1	1:D:610:ILE:HD12	2.55	0.40
1:B:643:LYS:HE2	1:B:643:LYS:HB3	1.91	0.40
1:B:749:GLU:N	1:B:750:PRO:CD	2.84	0.40
1:B:727:LEU:HD12	1:B:766:ILE:CD1	2.44	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	310/343 (90%)	290 (94%)	17 (6%)	3 (1%)	12	24
1	B	312/343 (91%)	301 (96%)	10 (3%)	1 (0%)	36	55
1	C	311/343 (91%)	301 (97%)	9 (3%)	1 (0%)	36	55
1	D	307/343 (90%)	290 (94%)	16 (5%)	1 (0%)	36	55
All	All	1240/1372 (90%)	1182 (95%)	52 (4%)	6 (0%)	24	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	CYS
1	B	458	GLY
1	C	502	CYS
1	A	646	GLU
1	A	767	ARG
1	D	477	PHE

5.3.2 Protein sidechains [i](#)

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	281/305 (92%)	263 (94%)	18 (6%)	16	33
1	B	281/305 (92%)	260 (92%)	21 (8%)	12	26
1	C	282/305 (92%)	269 (95%)	13 (5%)	24	48
1	D	279/305 (92%)	265 (95%)	14 (5%)	22	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1123/1220 (92%)	1057 (94%)	66 (6%)	18	37

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	471	GLU
1	A	497	SER
1	A	501	SER
1	A	504	GLU
1	A	568	ARG
1	A	575	LEU
1	A	587	SER
1	A	600	VAL
1	A	605	LEU
1	A	617	SER
1	A	622	VAL
1	A	644	GLN
1	A	677	SER
1	A	681	LEU
1	A	720	ASP
1	A	727	LEU
1	A	760	SER
1	B	459	LEU
1	B	469	CYS
1	B	470	LYS
1	B	504	GLU
1	B	521	ARG
1	B	551	LEU
1	B	573	SER
1	B	575	LEU
1	B	576	GLN
1	B	587	SER
1	B	605	LEU
1	B	614	LEU
1	B	617	SER
1	B	643	LYS
1	B	650	GLN
1	B	660	SER
1	B	677	SER
1	B	709	GLN
1	B	727	LEU

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Mol	Chain	Res	Type
1	B	749	GLU
1	B	770	GLU
1	C	463	THR
1	C	471	GLU
1	C	501	SER
1	C	517	LYS
1	C	547	LEU
1	C	568	ARG
1	C	605	LEU
1	C	613	THR
1	C	616	SER
1	C	623	LEU
1	C	709	GLN
1	C	727	LEU
1	C	749	GLU
1	D	459	LEU
1	D	500	THR
1	D	504	GLU
1	D	517	LYS
1	D	565	LEU
1	D	587	SER
1	D	605	LEU
1	D	617	SER
1	D	644	GLN
1	D	709	GLN
1	D	711	ILE
1	D	722	VAL
1	D	756	ARG
1	D	764	LYS

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

Mol	Chain	Res	Type
1	A	461	GLN
1	A	484	ASN
1	A	593	GLN
1	A	604	GLN
1	A	709	GLN
1	A	726	GLN
1	A	743	GLN
1	B	484	ASN
1	B	542	GLN

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Mol	Chain	Res	Type
1	B	544	ASN
1	B	604	GLN
1	B	658	ASN
1	B	690	ASN
1	B	709	GLN
1	B	726	GLN
1	B	761	GLN
1	C	542	GLN
1	C	593	GLN
1	C	604	GLN
1	C	726	GLN
1	C	743	GLN
1	C	761	GLN
1	D	484	ASN
1	D	542	GLN
1	D	604	GLN
1	D	621	GLN
1	D	644	GLN
1	D	650	GLN
1	D	731	ASN
1	D	743	GLN
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	C	509	1	8,9,10	0.67	0	6,9,11	1.31	1 (16%)

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	0.41	0	6,9,11	0.96	0
1	CME	A	509	1	8,9,10	0.54	0	6,9,11	0.60	0
1	CME	D	509	1	8,9,10	0.40	0	6,9,11	0.89	0

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	509	CME	CB-CA-C	2.27	116.96	110.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	JXO	B	803	-	13,13,13	4.34	7 (53%)	17,18,18	3.92	11 (64%)
4	JXO	A	803	-	13,13,13	3.48	3 (23%)	17,18,18	2.01	5 (29%)
4	JXO	C	803	-	13,13,13	4.89	5 (38%)	17,18,18	5.45	12 (70%)
4	JXO	D	803	-	13,13,13	4.26	5 (38%)	17,18,18	3.44	10 (58%)

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	JXO	B	803	-	-	-	0/2/2/2
4	JXO	A	803	-	-	-	0/2/2/2
4	JXO	C	803	-	-	-	0/2/2/2
4	JXO	D	803	-	-	-	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	JXO	C8-C9	15.88	1.52	1.41
4	D	803	JXO	C8-C9	14.13	1.51	1.41
4	B	803	JXO	C8-C9	14.02	1.51	1.41
4	A	803	JXO	C8-C9	11.59	1.49	1.41
4	C	803	JXO	C3-C1	-4.94	1.34	1.41
4	C	803	JXO	C7-CL11	-3.55	1.66	1.74
4	B	803	JXO	C7-CL11	-3.38	1.66	1.74
4	A	803	JXO	C10-C7	3.19	1.43	1.38
4	B	803	JXO	C3-C1	-3.17	1.37	1.41
4	D	803	JXO	C10-C7	2.77	1.43	1.38
4	D	803	JXO	C9-N12	2.62	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	803	JXO	C3-C1	-2.59	1.37	1.41
4	A	803	JXO	C9-N12	2.52	1.42	1.35
4	B	803	JXO	C9-N12	2.33	1.41	1.35
4	B	803	JXO	C10-C7	2.32	1.42	1.38
4	D	803	JXO	C9-N5	2.25	1.36	1.33
4	C	803	JXO	C2-C1	2.17	1.46	1.42
4	B	803	JXO	C2-C1	2.11	1.46	1.42
4	B	803	JXO	C9-N5	2.10	1.36	1.33
4	C	803	JXO	C9-N5	2.03	1.36	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	803	JXO	C8-C9-N5	12.50	126.39	119.87
4	C	803	JXO	C3-C7-CL11	-9.37	108.37	119.65
4	C	803	JXO	C2-C1-N4	9.06	129.18	121.00
4	B	803	JXO	C8-C9-N5	8.07	124.08	119.87
4	B	803	JXO	C10-C7-C3	6.83	129.49	122.00
4	C	803	JXO	C10-C7-C3	6.75	129.41	122.00
4	D	803	JXO	C8-C9-N5	6.58	123.30	119.87
4	C	803	JXO	C8-N4-C1	-6.22	109.76	116.96
4	D	803	JXO	C3-C7-CL11	-5.93	112.52	119.65
4	D	803	JXO	C9-C8-N4	-5.91	119.80	122.12
4	D	803	JXO	C2-C1-N4	5.66	126.11	121.00
4	B	803	JXO	C7-C3-C1	-4.96	115.38	119.47
4	B	803	JXO	C6-C2-C1	4.90	125.04	119.25
4	C	803	JXO	N12-C9-N5	-4.73	114.32	118.24
4	B	803	JXO	C2-C1-N4	4.70	125.25	121.00
4	C	803	JXO	C6-C10-C7	-4.52	114.40	119.22
4	B	803	JXO	C10-C7-CL11	-4.27	113.06	119.36
4	B	803	JXO	C10-C6-C2	-4.04	115.97	120.80
4	C	803	JXO	C6-C2-C1	3.78	123.72	119.25
4	A	803	JXO	C8-C9-N5	3.67	121.78	119.87
4	A	803	JXO	C9-C8-N4	3.55	123.52	122.12
4	D	803	JXO	C6-C2-C1	3.46	123.34	119.25
4	B	803	JXO	C6-C2-N5	-3.32	113.85	118.69
4	C	803	JXO	C3-C1-C2	-3.30	115.83	119.50
4	B	803	JXO	C8-N4-C1	-3.27	113.17	116.96
4	D	803	JXO	C10-C7-C3	3.03	125.33	122.00
4	D	803	JXO	C8-C9-N12	-2.85	118.55	121.37
4	A	803	JXO	C8-C9-N12	-2.77	118.62	121.37
4	C	803	JXO	C3-C1-N4	-2.63	114.99	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	803	JXO	C3-C1-C2	-2.58	116.63	119.50
4	C	803	JXO	C10-C6-C2	-2.45	117.87	120.80
4	B	803	JXO	C3-C1-C2	-2.44	116.79	119.50
4	D	803	JXO	C10-C6-C2	-2.43	117.90	120.80
4	A	803	JXO	C10-C6-C2	-2.37	117.96	120.80
4	B	803	JXO	N12-C9-N5	-2.32	116.31	118.24
4	A	803	JXO	C6-C10-C7	2.21	121.58	119.22
4	C	803	JXO	C8-C9-N12	-2.11	119.28	121.37
4	D	803	JXO	C1-C2-N5	-2.00	118.73	121.18

There are no chirality outliers.

There are no torsion outliers.

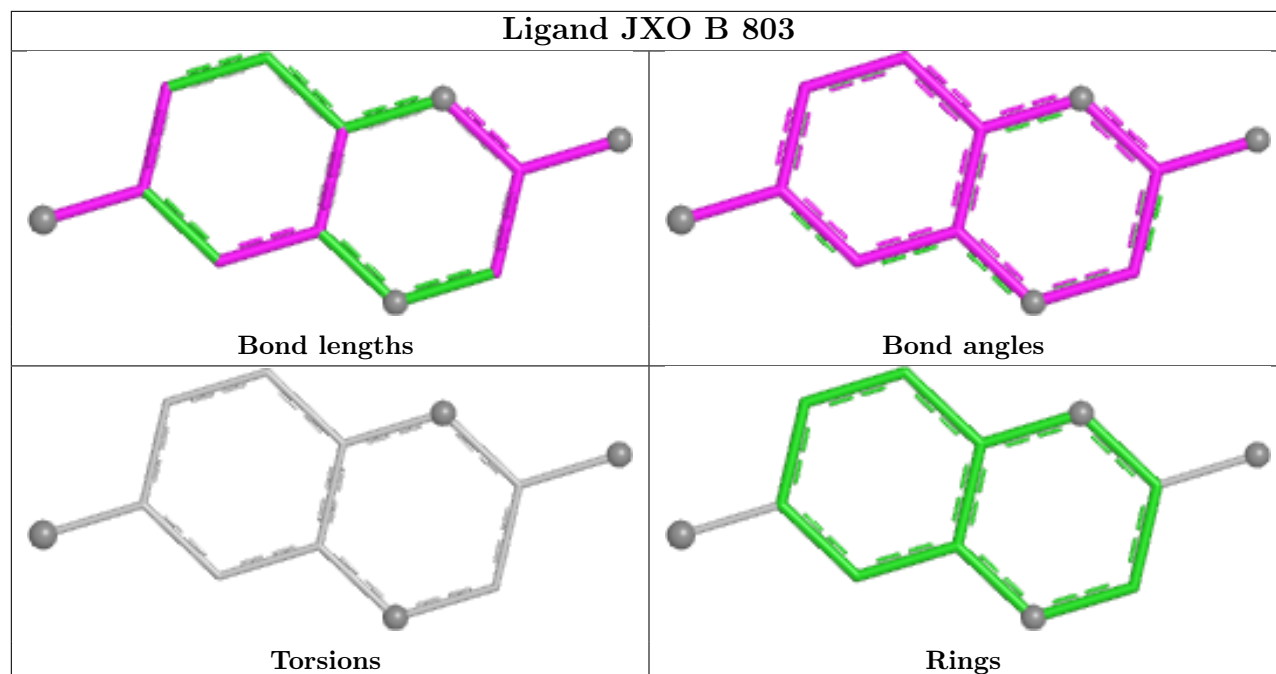
There are no ring outliers.

1 monomer is involved in 1 short contact:

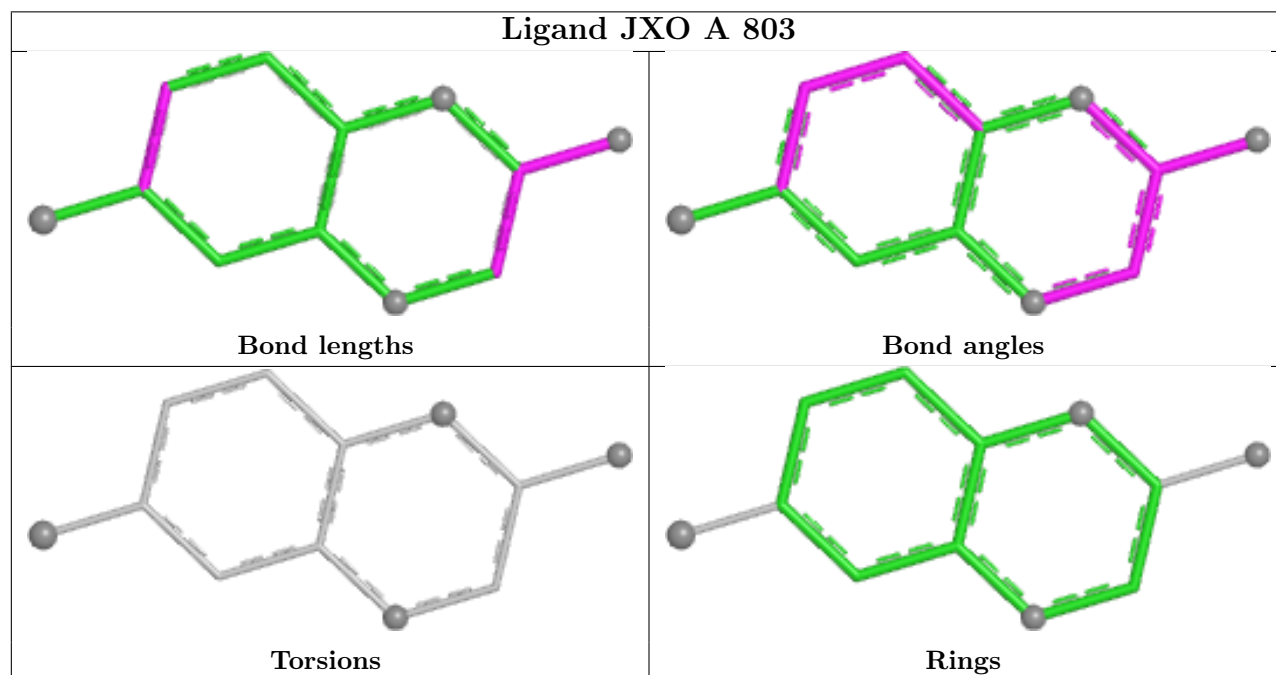
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	803	JXO	1	0

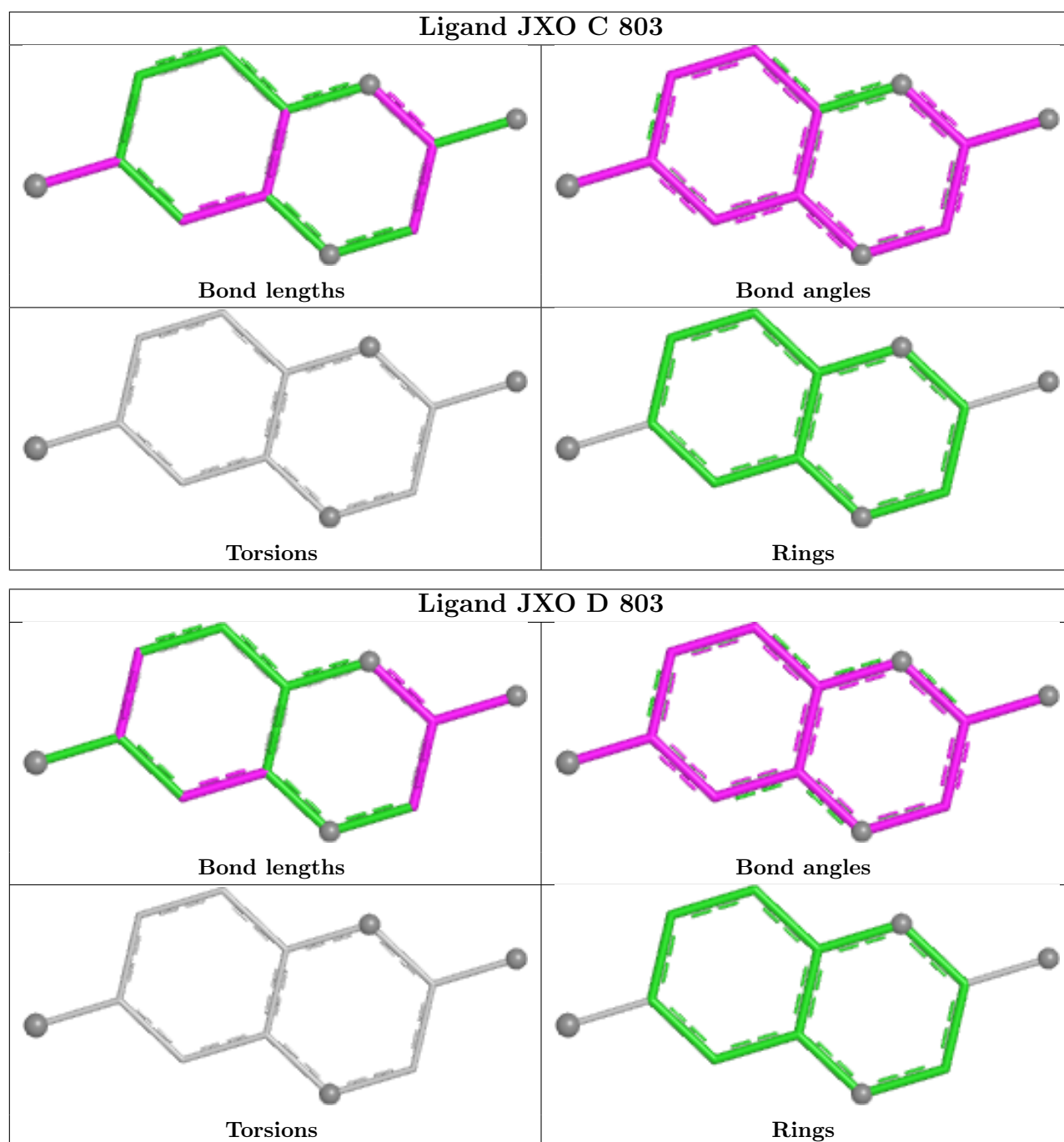
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand JXO B 803



Ligand JXO A 803





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.41	2 (0%) 85 83	33, 47, 79, 113	0
1	B	314/343 (91%)	-0.34	4 (1%) 75 71	32, 47, 80, 116	0
1	C	312/343 (90%)	-0.42	3 (0%) 79 76	27, 49, 76, 107	1 (0%)
1	D	309/343 (90%)	-0.20	3 (0%) 79 76	39, 58, 82, 108	0
All	All	1247/1372 (90%)	-0.34	12 (0%) 79 76	27, 51, 81, 116	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	459	LEU	6.5
1	C	620	GLU	3.8
1	B	457	GLN	3.7
1	B	458	GLY	3.5
1	A	459	LEU	3.3
1	C	459	LEU	3.1
1	A	458	GLY	3.0
1	D	692	ILE	2.6
1	B	459	LEU	2.2
1	D	603	LEU	2.2
1	B	545	HIS	2.1
1	C	458	GLY	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	B	509	10/11	0.89	0.14	47,68,103,103	0
1	CME	C	509	10/11	0.90	0.12	52,60,99,104	0
1	CME	D	509	10/11	0.91	0.12	49,72,103,105	0
1	CME	A	509	10/11	0.94	0.10	50,66,97,98	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

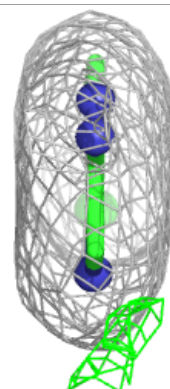
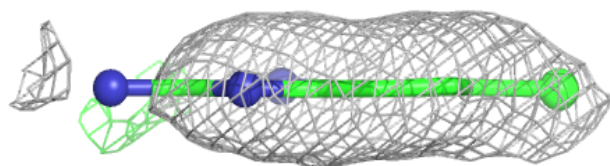
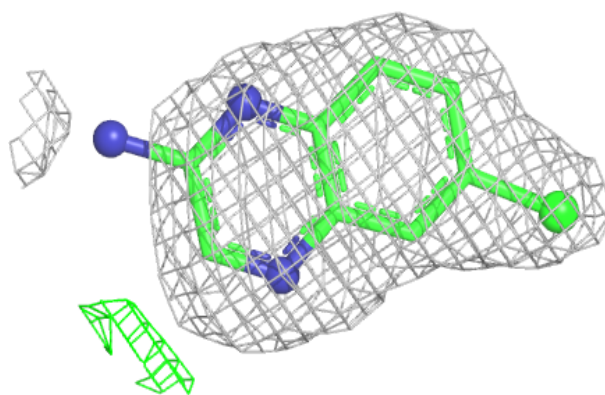
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	JXO	D	803	12/12	0.91	0.10	47,57,79,93	0
4	JXO	B	803	12/12	0.93	0.10	45,50,63,96	0
4	JXO	C	803	12/12	0.94	0.09	44,52,85,87	0
4	JXO	A	803	12/12	0.94	0.09	43,49,61,75	0
3	MG	D	802	1/1	0.99	0.02	49,49,49,49	0
3	MG	B	802	1/1	1.00	0.02	31,31,31,31	0
3	MG	C	802	1/1	1.00	0.02	33,33,33,33	0
2	ZN	A	801	1/1	1.00	0.01	45,45,45,45	0
2	ZN	B	801	1/1	1.00	0.01	37,37,37,37	0
2	ZN	C	801	1/1	1.00	0.01	45,45,45,45	0
2	ZN	D	801	1/1	1.00	0.01	50,50,50,50	0
3	MG	A	802	1/1	1.00	0.01	39,39,39,39	0

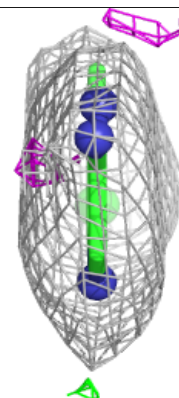
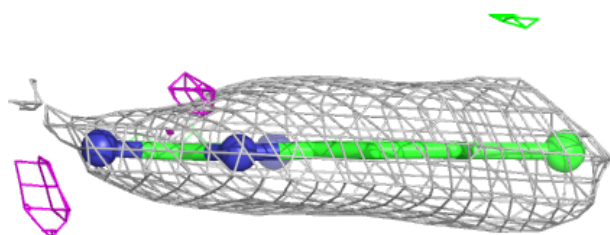
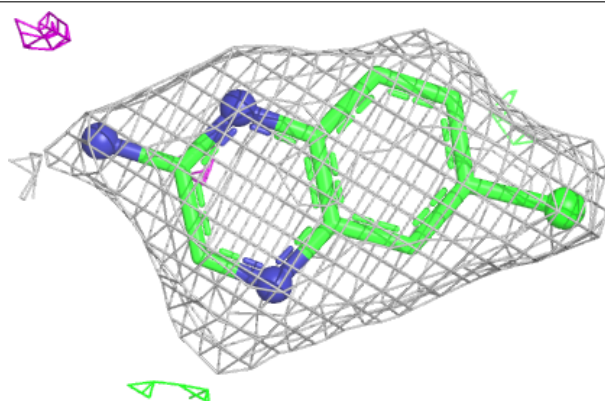
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JXO 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)

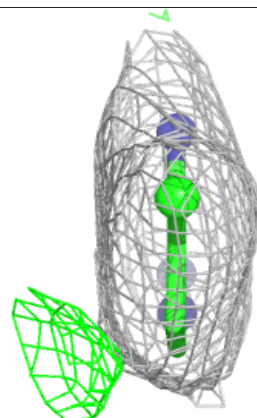
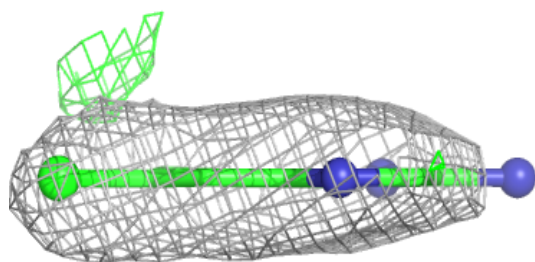
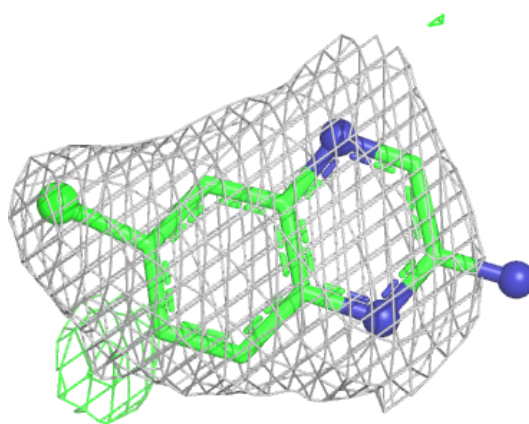
**Electron density around JXO B 803:**

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

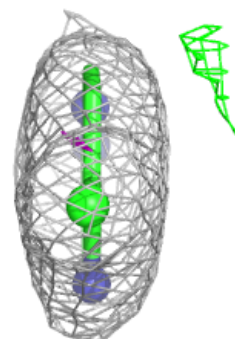
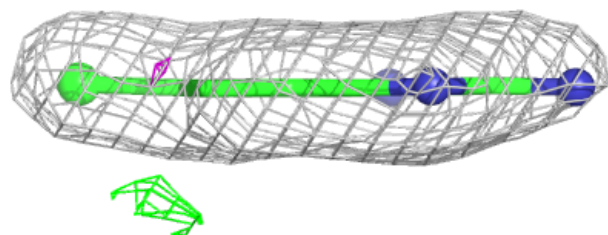
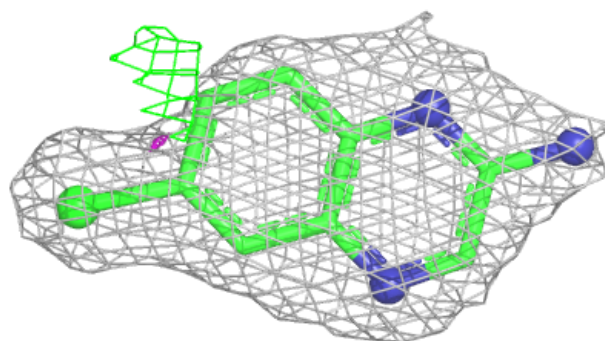


Electron density around JXO C 803:

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

**Electron density around JXO 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)



6.5 Other polymers

There are no such residues in this entry.