



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 03:08 PM EDT

PDB ID : 5SJJ
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN COMPLEX WITH n2c(nc1[nH]cc(c1c2NCC)c3cccc(c3)C(F)(F)F)N, micromolar IC₅₀=0.256
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Deposited on : 2022-02-01
Resolution : 2.10 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

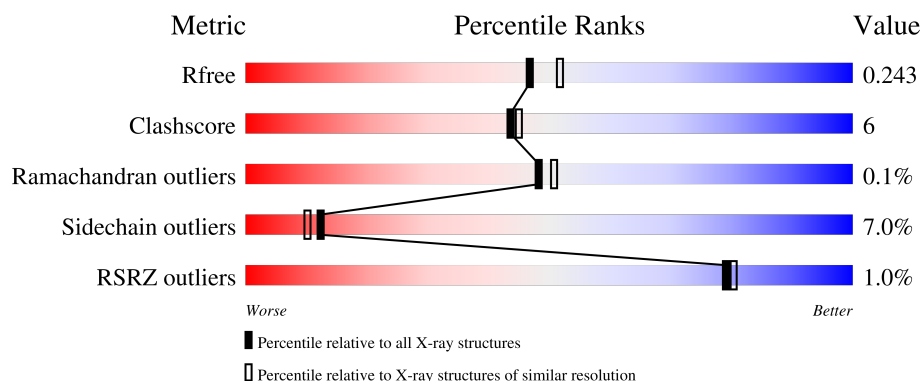
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	
1	B	343	
1	C	343	
1	D	343	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11059 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	4	0
			2561	1637	435	463	26			
1	B	315	Total	C	N	O	S	0	3	0
			2566	1640	434	467	25			
1	C	313	Total	C	N	O	S	0	6	0
			2575	1646	439	465	25			
1	D	313	Total	C	N	O	S	0	2	0
			2546	1628	434	459	25			

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

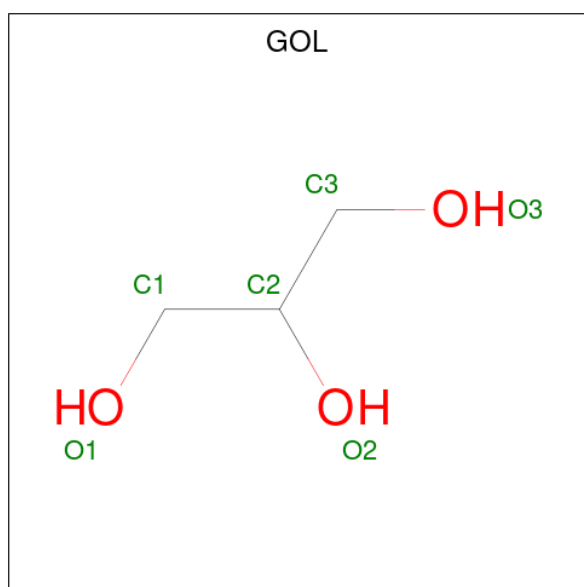
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 (three-letter code: MG) (formula: Mg).

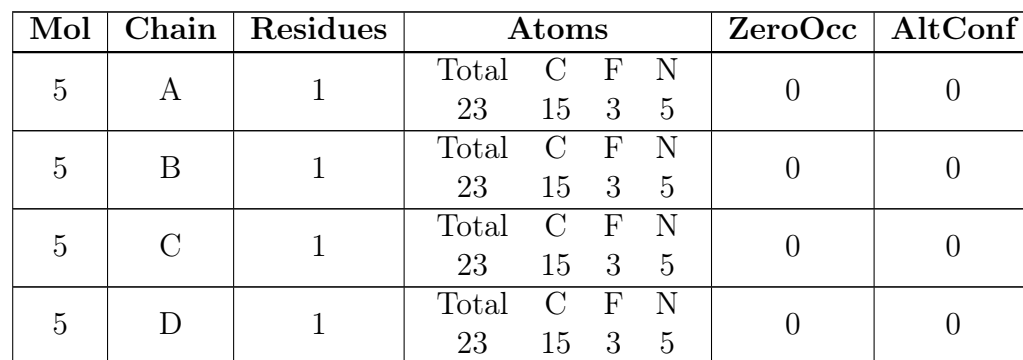
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is N 4 -ethyl-5-[3-(trifluoromethyl)phenyl]-7H-pyrrolo[2,3-d]pyrimidine-2,4-diamine (three-letter code: K3O) (formula: C₁₅H₁₄F₃N₅) (labeled as "Ligand of Interest" by depositor).

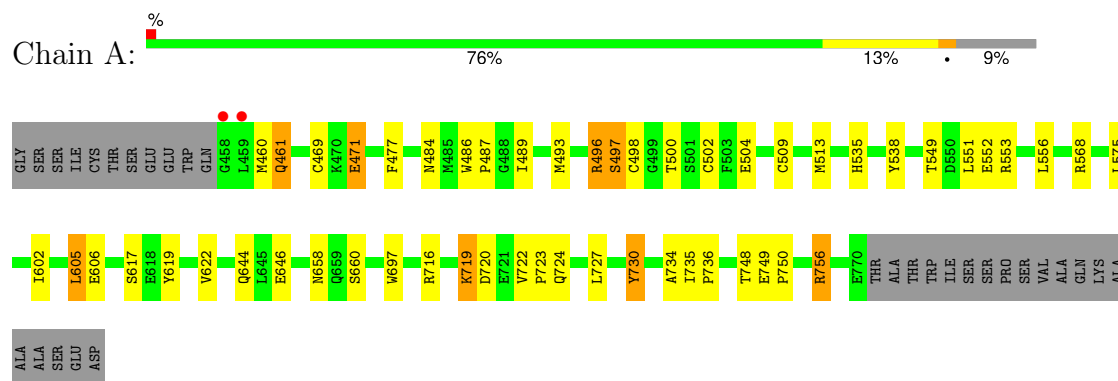


- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6 | A | 172 | Total O
172 172 | 0 | 0 |
| 6 | B | 194 | Total O
194 194 | 0 | 0 |
| 6 | C | 191 | Total O
191 191 | 0 | 0 |
| 6 | D | 148 | Total O
148 148 | 0 | 0 |

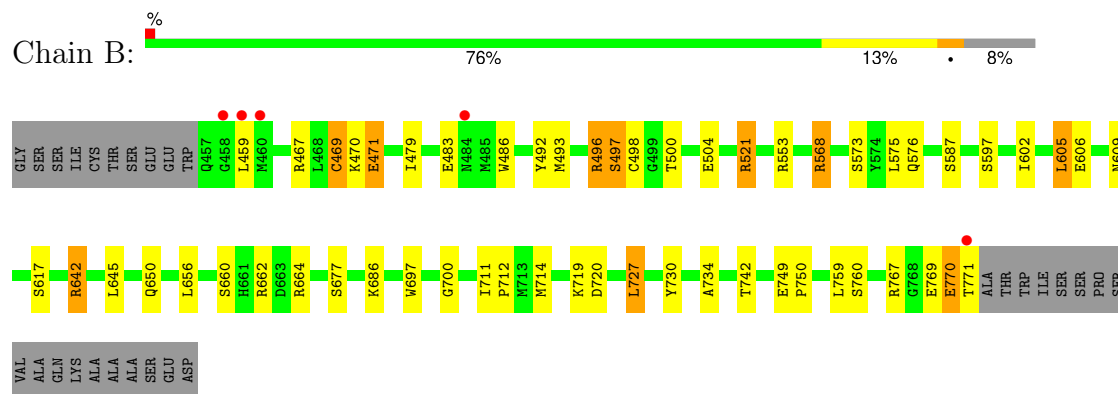
3 Residue-property plots [i](#)

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.

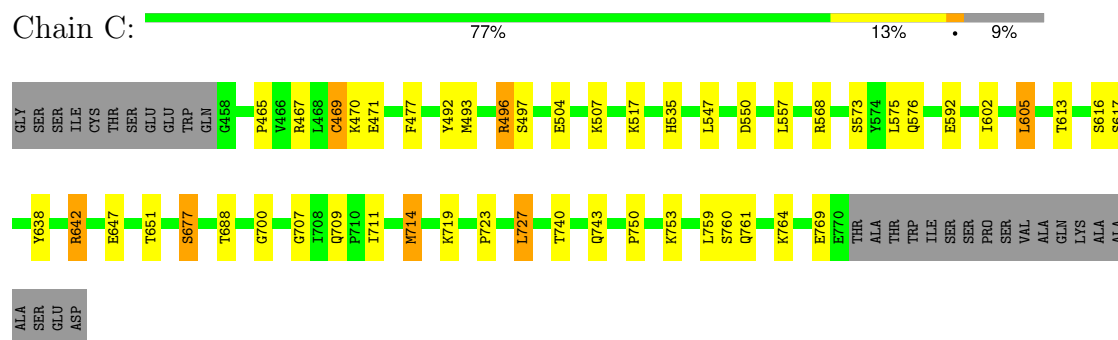
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



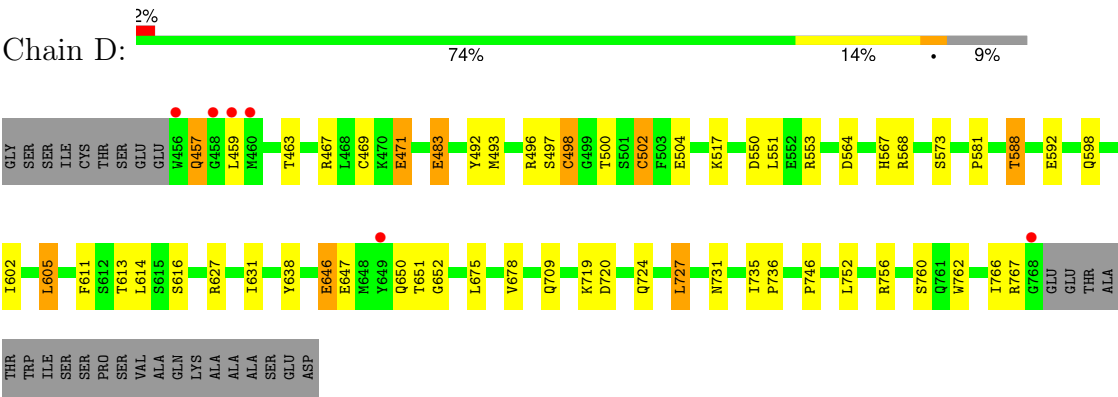
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- 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	136.49Å 136.49Å 236.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.85 – 2.10 43.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	85.9 (43.85-2.10) 85.9 (43.85-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.174 , 0.240 0.183 , 0.243	Depositor DCC
R_{free} test set	4793 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11059	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, K3O, GOL, 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	0.90	1/2624 (0.0%)	1.03	5/3549 (0.1%)
1	B	0.91	1/2626 (0.0%)	1.05	4/3553 (0.1%)
1	C	0.87	1/2644 (0.0%)	1.01	3/3576 (0.1%)
1	D	0.87	2/2603 (0.1%)	0.98	0/3522
All	All	0.89	5/10497 (0.0%)	1.02	12/14200 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	730	TYR	C-O	7.93	1.38	1.23
1	D	483	GLU	CD-OE2	5.91	1.32	1.25
1	C	592	GLU	CD-OE2	5.89	1.32	1.25
1	D	592	GLU	CD-OE1	-5.65	1.19	1.25
1	B	504	GLU	CD-OE2	5.20	1.31	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	467	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	756[A]	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	756[B]	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	B	642	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	C	642	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	A	496	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	568	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	471[A]	GLU	CB-CA-C	5.15	120.70	110.40
1	A	471[B]	GLU	CB-CA-C	5.15	120.70	110.40
1	B	496	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	470	LYS	N-CA-CB	-5.12	101.38	110.60
1	B	609	ASN	N-CA-CB	5.11	119.79	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2561	0	2540	39	0
1	B	2566	0	2532	25	0
1	C	2575	0	2561	28	0
1	D	2546	0	2522	32	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	6	0	8	1	0
5	A	23	0	0	0	0
5	B	23	0	0	0	0
5	C	23	0	0	1	0
5	D	23	0	0	0	0
6	A	172	0	0	4	0
6	B	194	0	0	3	0
6	C	191	0	0	9	0
6	D	148	0	0	7	0
All	All	11059	0	10163	123	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 (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469[A]:CYS:SG	6:A:1035:HOH:O	2.19	0.98
1:C:469[B]:CYS:SG	6:C:1069:HOH:O	2.25	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:GLN:HB2	6:D:932:HOH:O	1.70	0.89
1:B:469[B]:CYS:SG	6:B:1067:HOH:O	2.30	0.88
1:C:709:GLN:OE1	6:C:901:HOH:O	2.00	0.79
1:C:493:MET:O	1:C:497:SER:HB2	1.84	0.77
1:D:727:LEU:HD12	1:D:766:ILE:HD12	1.69	0.74
1:A:756[B]:ARG:HD2	6:A:903:HOH:O	1.87	0.73
1:A:646:GLU:HG3	6:A:924:HOH:O	1.89	0.71
1:D:727:LEU:HD12	1:D:766:ILE:CD1	2.22	0.70
1:A:461:GLN:HE22	1:A:500:THR:CG2	2.06	0.69
1:B:483:GLU:HB2	6:B:975:HOH:O	1.95	0.66
1:A:461:GLN:NE2	1:A:461:GLN:HA	2.10	0.65
1:D:719:LYS:NZ	6:D:904:HOH:O	2.31	0.64
1:A:461:GLN:NE2	1:A:500:THR:HG21	2.13	0.64
1:C:550:ASP:OD1	6:C:902:HOH:O	2.15	0.64
1:D:568:ARG:NH1	6:D:902:HOH:O	2.30	0.63
1:A:749:GLU:N	1:A:750:PRO:CD	2.62	0.63
4:A:803:GOL:O2	1:B:568:ARG:HD2	1.98	0.62
1:C:764:LYS:HG3	1:C:769:GLU:HB2	1.82	0.61
1:B:493:MET:O	1:B:497:SER:HB2	2.02	0.60
1:D:724:GLN:HB2	6:D:956:HOH:O	2.02	0.59
1:B:497:SER:O	1:B:553:ARG:HD2	2.02	0.59
1:A:497:SER:O	1:A:553:ARG:HD2	2.03	0.58
1:D:467:ARG:O	1:D:471:GLU:HB2	2.03	0.58
1:B:770:GLU:HG3	1:B:771:THR:N	2.19	0.58
1:A:461:GLN:HE22	1:A:500:THR:HG21	1.69	0.56
1:C:507:LYS:HE2	6:C:1012:HOH:O	2.06	0.55
1:D:493:MET:O	1:D:497:SER:HB2	2.07	0.55
1:D:550:ASP:HB3	6:D:993:HOH:O	2.06	0.55
1:A:461:GLN:HE22	1:A:500:THR:HG22	1.70	0.55
1:A:493:MET:O	1:A:497:SER:HB2	2.07	0.54
1:B:492:TYR:CZ	1:B:496:ARG:HD2	2.42	0.54
1:B:467:ARG:O	1:B:471:GLU:HB2	2.08	0.54
1:A:730:TYR:HA	1:A:734:ALA:HB3	1.90	0.54
1:D:498:CYS:HB2	1:D:553:ARG:HB3	1.89	0.53
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.42	0.53
1:A:756[B]:ARG:CD	6:A:903:HOH:O	2.50	0.53
1:C:647:GLU:O	1:C:651:THR:HG23	2.09	0.53
1:B:742:THR:HG21	1:B:749:GLU:HG2	1.90	0.53
1:A:498:CYS:SG	1:A:502[A]:CYS:SG	3.08	0.52
1:A:602:ILE:HA	1:A:605:LEU:HD22	1.92	0.52
1:C:642:ARG:NH2	6:C:912:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:GLY:HA3	1:C:714:MET:O	2.10	0.51
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.92	0.51
1:B:742:THR:CG2	1:B:749:GLU:HG2	2.41	0.50
1:D:469:CYS:SG	6:D:1021:HOH:O	2.59	0.50
1:A:658:ASN:OD1	1:A:660:SER:HB3	2.11	0.50
1:C:740:THR:HA	1:C:743:GLN:HE21	1.77	0.49
1:C:677:SER:HB2	1:C:688:THR:HG21	1.94	0.49
1:A:724:GLN:O	1:A:727:LEU:HB2	2.13	0.48
1:B:602:ILE:HA	1:B:605:LEU:HD22	1.95	0.48
1:A:498:CYS:SG	1:A:502[A]:CYS:CB	3.01	0.48
1:D:735:ILE:HB	1:D:736:PRO:HD3	1.95	0.48
1:D:727:LEU:CD1	1:D:766:ILE:HD12	2.41	0.48
1:A:749:GLU:O	1:A:749:GLU:HG3	2.14	0.48
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.96	0.47
1:A:619:TYR:O	1:A:622:VAL:HG12	2.15	0.47
1:D:627:ARG:O	1:D:631:ILE:HG12	2.15	0.47
1:D:493:MET:O	1:D:497:SER:CB	2.62	0.47
1:B:656:LEU:O	1:B:662:ARG:HG3	2.14	0.47
1:A:461:GLN:NE2	1:A:500:THR:CG2	2.72	0.47
1:A:486:TRP:N	1:A:487:PRO:CD	2.78	0.46
1:B:727:LEU:HD23	1:B:759:LEU:CD1	2.45	0.46
1:B:767:ARG:NH1	1:B:769:GLU:OE2	2.48	0.46
1:B:749:GLU:N	1:B:750:PRO:CD	2.79	0.46
1:D:498:CYS:C	1:D:502[B]:CYS:SG	2.94	0.46
1:D:602:ILE:O	1:D:605:LEU:HB2	2.15	0.46
1:D:675:LEU:O	1:D:678:VAL:HG22	2.16	0.46
1:A:697:TRP:HB3	1:A:716:ARG:HB3	1.98	0.46
1:C:557:LEU:HD23	1:C:557:LEU:HA	1.86	0.46
1:B:697:TRP:CZ2	1:B:719:LYS:HG2	2.51	0.45
1:C:753:LYS:HE2	6:C:1044:HOH:O	2.15	0.45
1:D:598:GLN:O	1:D:602:ILE:HG13	2.16	0.45
1:D:647:GLU:O	1:D:651:THR:HG23	2.15	0.45
1:D:762:TRP:O	1:D:766:ILE:HG13	2.16	0.45
1:A:461:GLN:NE2	1:A:461:GLN:CA	2.77	0.45
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.52	0.45
1:C:714:MET:HE2	6:C:1023:HOH:O	2.16	0.45
1:B:470:LYS:HE2	1:D:746:PRO:HG3	1.98	0.45
1:C:677:SER:HB3	6:C:962:HOH:O	2.15	0.45
1:A:644:GLN:HE21	1:A:644:GLN:HA	1.81	0.45
1:C:740:THR:HA	1:C:743:GLN:NE2	2.32	0.44
1:D:611:PHE:HB3	1:D:614:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:THR:OG1	1:A:552:GLU:HG3	2.17	0.44
1:B:700:GLY:HA3	1:B:714:MET:O	2.17	0.44
1:D:727:LEU:HD12	1:D:766:ILE:HD11	1.99	0.43
1:A:489:ILE:O	1:A:493:MET:HG3	2.18	0.43
1:B:521:ARG:NH1	1:B:521:ARG:HG3	2.32	0.43
1:C:477:PHE:HB3	1:C:535:HIS:CE1	2.54	0.43
1:B:730:TYR:HA	1:B:734:ALA:HB3	2.01	0.42
1:A:484:ASN:HD22	1:A:484:ASN:HA	1.53	0.42
1:A:509:CME:O	1:A:513:MET:HG2	2.19	0.42
1:C:638:TYR:OH	1:C:642:ARG:HD3	2.19	0.42
5:C:803:K3O:C15	5:C:803:K3O:N21	2.82	0.42
1:D:646:GLU:O	1:D:650:GLN:HG3	2.20	0.42
1:C:602:ILE:O	1:C:605:LEU:HB2	2.18	0.42
1:D:564:ASP:O	1:D:567:HIS:HB2	2.19	0.42
1:B:727:LEU:HD23	1:B:759:LEU:HD11	2.01	0.42
1:C:707:GLY:O	1:D:652:GLY:HA3	2.19	0.42
1:B:479:ILE:HD12	1:B:486:TRP:CD1	2.54	0.42
1:C:727:LEU:HD22	1:C:759:LEU:HD11	2.01	0.42
1:C:761:GLN:HA	1:C:761:GLN:OE1	2.19	0.42
1:B:711:ILE:HA	1:B:712:PRO:HD3	1.86	0.42
1:C:492:TYR:CZ	1:C:496:ARG:HD2	2.55	0.42
1:D:588:THR:CG2	6:D:982:HOH:O	2.68	0.42
1:A:493:MET:HB3	1:A:538:TYR:CD1	2.55	0.42
1:C:727:LEU:CD2	1:C:759:LEU:HD11	2.50	0.41
1:D:752:LEU:HD21	1:D:756:ARG:NH2	2.35	0.41
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.78	0.41
1:A:727:LEU:HD23	1:A:727:LEU:HA	1.88	0.41
1:B:469[A]:CYS:HB3	6:B:1067:HOH:O	2.19	0.41
1:C:568[A]:ARG:NH1	6:C:928:HOH:O	2.54	0.41
1:A:748:THR:C	1:A:750:PRO:HD2	2.41	0.41
1:D:727:LEU:HD23	1:D:731:ASN:HD21	1.85	0.41
1:A:749:GLU:N	1:A:750:PRO:HD3	2.35	0.41
1:A:697:TRP:CH2	1:A:719:LYS:HG2	2.56	0.41
1:D:551:LEU:HD23	1:D:551:LEU:HA	1.86	0.41
1:C:492:TYR:CE2	1:C:496:ARG:HD2	2.56	0.41
1:B:645:LEU:HD21	1:B:664:ARG:HB3	2.02	0.40
1:C:711:ILE:HG12	1:C:714:MET:HG3	2.03	0.40
1:A:556:LEU:HD23	1:A:556:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/343 (92%)	304 (97%)	10 (3%)	0	100	100
1	B	315/343 (92%)	305 (97%)	10 (3%)	0	100	100
1	C	316/343 (92%)	308 (98%)	7 (2%)	1 (0%)	37	37
1	D	312/343 (91%)	302 (97%)	10 (3%)	0	100	100
All	All	1257/1372 (92%)	1219 (97%)	37 (3%)	1 (0%)	48	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	465	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	285/305 (93%)	271 (95%)	14 (5%)	21	20
1	B	284/305 (93%)	259 (91%)	25 (9%)	8	5
1	C	287/305 (94%)	265 (92%)	22 (8%)	10	8
1	D	282/305 (92%)	258 (92%)	24 (8%)	8	6
All	All	1138/1220 (93%)	1053 (92%)	85 (8%)	12	9

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

Mol	Chain	Res	Type
1	A	460	MET
1	A	461	GLN
1	A	471[A]	GLU
1	A	471[B]	GLU
1	A	496	ARG
1	A	497	SER
1	A	504	GLU
1	A	568	ARG
1	A	575	LEU
1	A	605	LEU
1	A	606	GLU
1	A	617	SER
1	A	719	LYS
1	A	720	ASP
1	B	459	LEU
1	B	469[A]	CYS
1	B	469[B]	CYS
1	B	471	GLU
1	B	497	SER
1	B	498	CYS
1	B	500	THR
1	B	521	ARG
1	B	573	SER
1	B	575	LEU
1	B	576	GLN
1	B	587	SER
1	B	597	SER
1	B	605	LEU
1	B	606	GLU
1	B	617	SER
1	B	642	ARG
1	B	650	GLN
1	B	660	SER
1	B	677	SER
1	B	686	LYS
1	B	720	ASP
1	B	727	LEU
1	B	760	SER
1	B	770	GLU
1	C	469[A]	CYS
1	C	469[B]	CYS
1	C	471	GLU
1	C	496	ARG

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Mol	Chain	Res	Type
1	C	504	GLU
1	C	517	LYS
1	C	547	LEU
1	C	573[A]	SER
1	C	573[B]	SER
1	C	575	LEU
1	C	576[A]	GLN
1	C	576[B]	GLN
1	C	605	LEU
1	C	613	THR
1	C	616	SER
1	C	617	SER
1	C	677	SER
1	C	714	MET
1	C	719	LYS
1	C	723	PRO
1	C	727	LEU
1	C	760	SER
1	D	457	GLN
1	D	459	LEU
1	D	463	THR
1	D	471	GLU
1	D	483	GLU
1	D	498	CYS
1	D	500	THR
1	D	502[A]	CYS
1	D	502[B]	CYS
1	D	504	GLU
1	D	517	LYS
1	D	573	SER
1	D	581	PRO
1	D	588	THR
1	D	605	LEU
1	D	613	THR
1	D	616	SER
1	D	638	TYR
1	D	646	GLU
1	D	709	GLN
1	D	720	ASP
1	D	727	LEU
1	D	760	SER
1	D	767	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	484	ASN
1	A	495	HIS
1	A	604	GLN
1	A	644	GLN
1	A	743	GLN
1	A	761	GLN
1	B	604	GLN
1	B	621	GLN
1	B	644	GLN
1	B	709	GLN
1	B	743	GLN
1	C	542	GLN
1	C	604	GLN
1	C	743	GLN
1	D	542	GLN
1	D	604	GLN
1	D	609	ASN
1	D	621	GLN
1	D	644	GLN
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	0.51	0	6,9,11	1.09	0
1	CME	D	509	1	8,9,10	0.81	0	6,9,11	0.81	0
1	CME	A	509	1	8,9,10	0.77	0	6,9,11	0.98	0
1	CME	C	509	1	8,9,10	0.61	0	6,9,11	1.08	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	-	1/5/8/10	-
1	CME	D	509	1	-	1/5/8/10	-
1	CME	A	509	1	-	1/5/8/10	-
1	CME	C	509	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	509	CME	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	803	-	5,5,5	0.34	0	5,5,5	0.62	0
5	K3O	B	803	-	24,25,25	1.69	7 (29%)	25,37,37	2.15	7 (28%)
5	K3O	A	804	-	24,25,25	2.11	9 (37%)	25,37,37	2.19	6 (24%)
5	K3O	C	803	-	24,25,25	1.89	8 (33%)	25,37,37	2.29	10 (40%)
5	K3O	D	803	-	24,25,25	1.69	6 (25%)	25,37,37	2.05	9 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	803	-	-	4/4/4/4	-
5	K3O	B	803	-	-	1/13/13/13	0/3/3/3
5	K3O	A	804	-	-	2/13/13/13	0/3/3/3
5	K3O	C	803	-	-	3/13/13/13	0/3/3/3
5	K3O	D	803	-	-	1/13/13/13	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804	K3O	C7-C8	4.80	1.49	1.41
5	A	804	K3O	C4-N21	4.43	1.41	1.34
5	C	803	K3O	C2-N10	3.49	1.40	1.33
5	D	803	K3O	C9-N5	3.40	1.41	1.34
5	D	803	K3O	C2-N10	3.31	1.40	1.33
5	C	803	K3O	F18-C17	3.28	1.44	1.33
5	D	803	K3O	C17-C13	3.19	1.56	1.49
5	B	803	K3O	C15-C12	3.15	1.45	1.39
5	C	803	K3O	C15-C13	3.13	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804	K3O	C2-N10	3.07	1.40	1.33
5	A	804	K3O	F19-C17	3.00	1.43	1.33
5	B	803	K3O	C7-C8	2.99	1.46	1.41
5	B	803	K3O	F20-C17	2.88	1.43	1.33
5	A	804	K3O	C17-C13	2.82	1.55	1.49
5	B	803	K3O	C2-N10	2.81	1.39	1.33
5	D	803	K3O	C7-C8	2.74	1.46	1.41
5	C	803	K3O	F20-C17	2.73	1.42	1.33
5	A	804	K3O	F18-C17	2.66	1.42	1.33
5	C	803	K3O	C4-N21	2.65	1.38	1.34
5	C	803	K3O	C16-C11	2.63	1.43	1.38
5	B	803	K3O	C17-C13	2.50	1.55	1.49
5	B	803	K3O	F19-C17	2.44	1.41	1.33
5	A	804	K3O	C15-C12	2.35	1.43	1.39
5	C	803	K3O	C4-N1	2.30	1.36	1.33
5	D	803	K3O	F20-C17	2.25	1.41	1.33
5	B	803	K3O	C4-N21	2.23	1.38	1.34
5	A	804	K3O	F20-C17	2.20	1.40	1.33
5	D	803	K3O	F19-C17	2.17	1.40	1.33
5	A	804	K3O	C4-N1	-2.10	1.30	1.33
5	C	803	K3O	C17-C13	2.03	1.54	1.49

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	K3O	C8-C4-N21	6.57	127.26	120.79
5	C	803	K3O	C16-C14-C13	-6.24	114.41	120.75
5	A	804	K3O	C7-C8-C9	-5.32	103.30	107.54
5	B	803	K3O	C2-N3-C9	5.09	120.97	115.48
5	D	803	K3O	C2-N3-C9	4.55	120.39	115.48
5	C	803	K3O	C8-C4-N21	-4.43	116.43	120.79
5	B	803	K3O	C15-C13-C17	4.39	125.37	119.57
5	B	803	K3O	N3-C2-N1	-4.08	122.02	127.21
5	A	804	K3O	F20-C17-C13	-3.96	104.42	112.90
5	D	803	K3O	C7-C8-C9	-3.34	104.88	107.54
5	B	803	K3O	F18-C17-C13	-3.28	105.88	112.90
5	B	803	K3O	N10-C2-N1	3.26	122.11	117.22
5	C	803	K3O	C14-C16-C11	3.24	124.42	120.24
5	D	803	K3O	N3-C2-N1	-2.99	123.41	127.21
5	C	803	K3O	F20-C17-C13	-2.92	106.63	112.90
5	D	803	K3O	F20-C17-C13	-2.90	106.68	112.90
5	C	803	K3O	C2-N3-C9	2.90	118.61	115.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	803	K3O	C14-C13-C15	2.89	123.42	117.86
5	D	803	K3O	C8-C4-N21	2.72	123.47	120.79
5	C	803	K3O	F20-C17-F18	2.57	115.04	105.77
5	C	803	K3O	C7-C8-C9	-2.57	105.49	107.54
5	C	803	K3O	F19-C17-F18	2.56	115.01	105.77
5	D	803	K3O	C15-C13-C17	2.54	122.92	119.57
5	C	803	K3O	F20-C17-F19	-2.54	96.61	105.77
5	D	803	K3O	C11-C12-C7	2.52	125.06	120.87
5	A	804	K3O	C15-C12-C7	-2.50	116.61	120.60
5	B	803	K3O	C14-C13-C17	-2.48	115.98	119.96
5	B	803	K3O	C7-C8-C9	-2.47	105.57	107.54
5	D	803	K3O	C2-N1-C4	2.46	120.44	114.59
5	A	804	K3O	C2-N1-C4	2.35	120.17	114.59
5	D	803	K3O	C15-C12-C7	-2.23	117.04	120.60
5	A	804	K3O	C23-C22-N21	-2.10	104.79	111.45

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	GOL	C1-C2-C3-O3
4	A	803	GOL	O1-C1-C2-C3
5	B	803	K3O	C23-C22-N21-C4
4	A	803	GOL	O2-C2-C3-O3
5	C	803	K3O	N1-C4-N21-C22
4	A	803	GOL	O1-C1-C2-O2
5	C	803	K3O	C23-C22-N21-C4
5	A	804	K3O	C23-C22-N21-C4
5	C	803	K3O	C8-C4-N21-C22
5	D	803	K3O	C23-C22-N21-C4
5	A	804	K3O	C11-C12-C7-C8

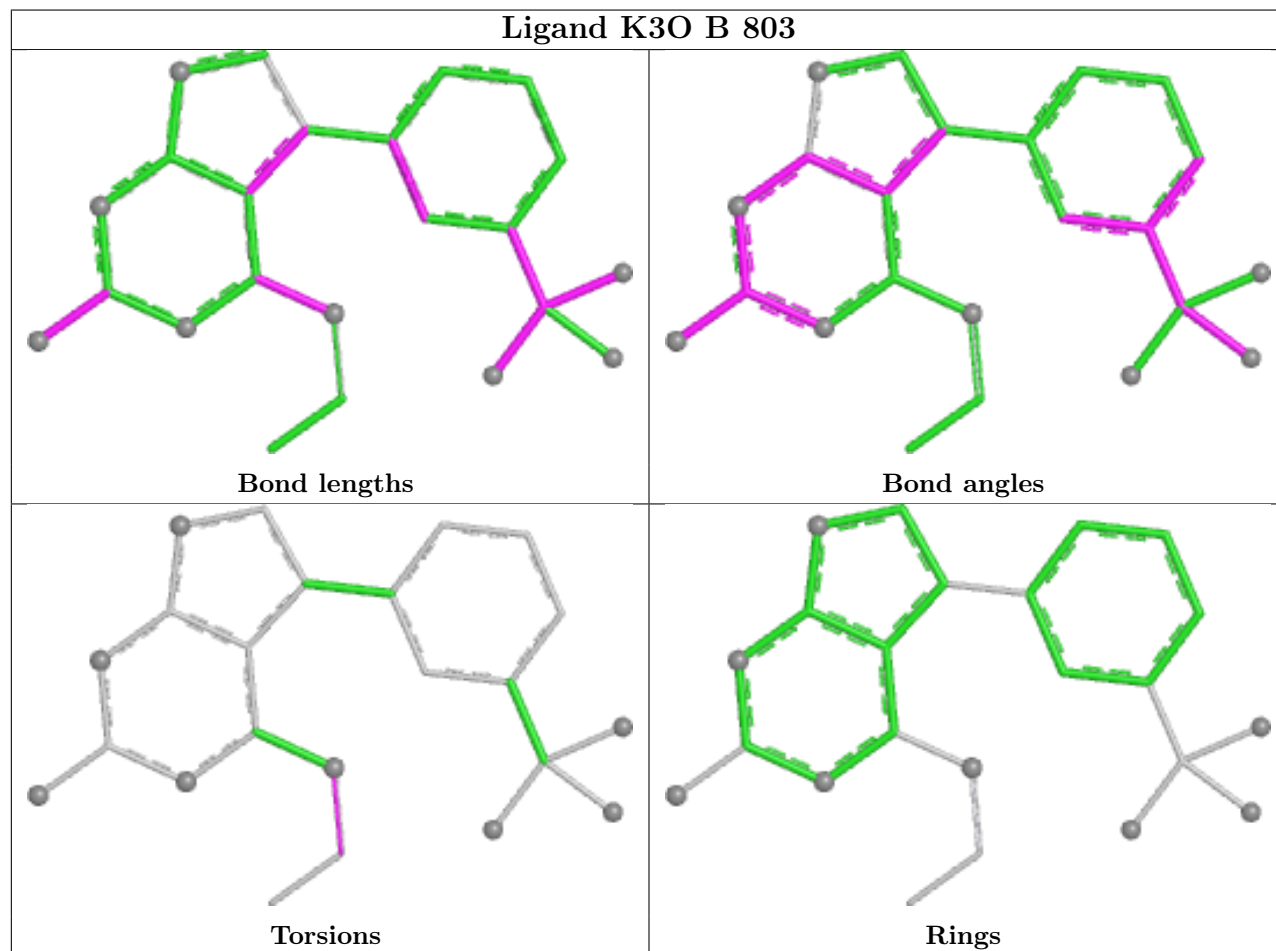
There are no ring outliers.

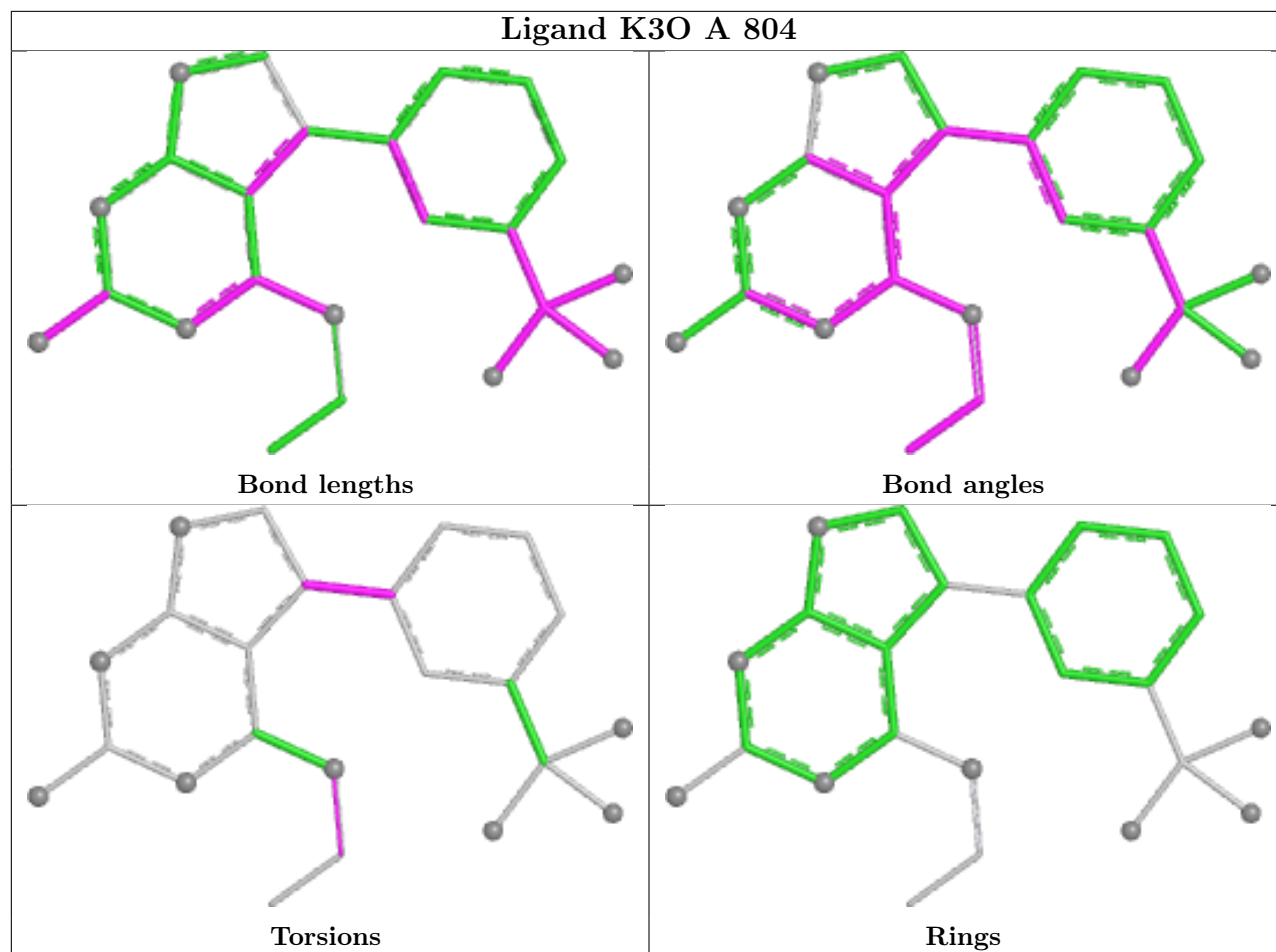
2 monomers are involved in 2 short contacts:

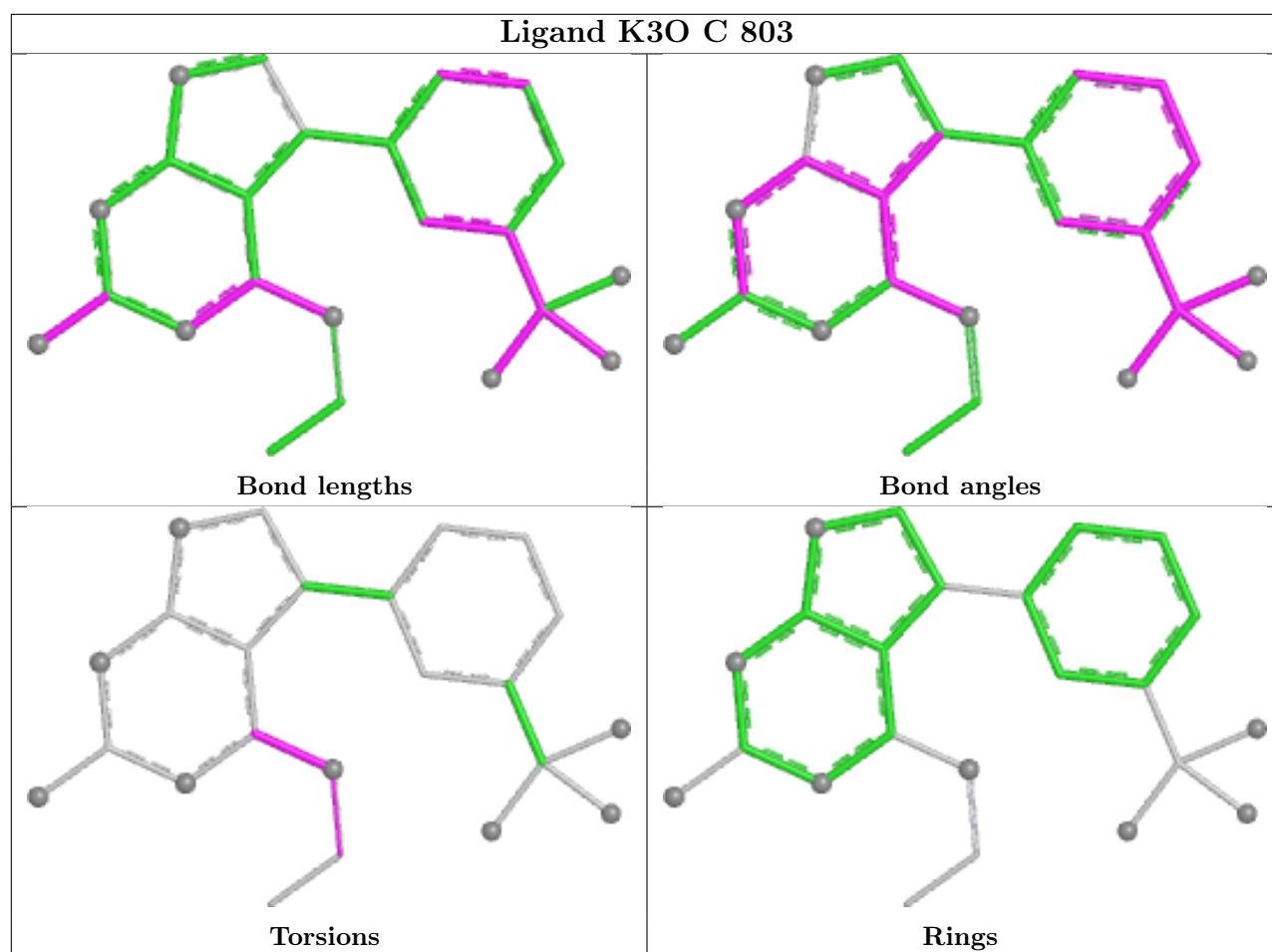
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	GOL	1	0
5	C	803	K3O	1	0

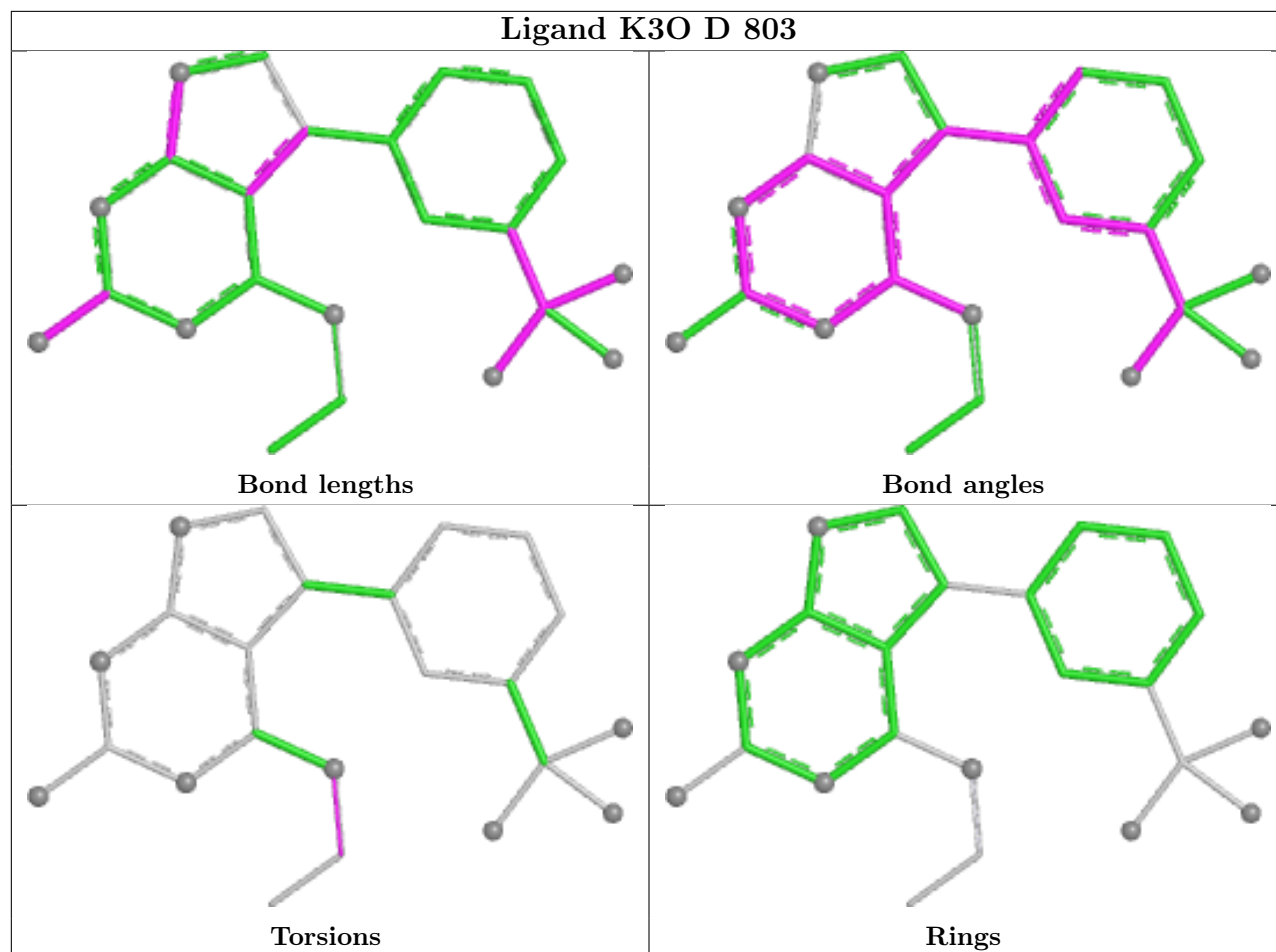
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.35	2 (0%) 85 86	16, 35, 62, 94	4 (1%)
1	B	314/343 (91%)	-0.34	5 (1%) 70 71	21, 33, 61, 97	3 (0%)
1	C	312/343 (90%)	-0.38	0 100 100	18, 34, 59, 88	6 (1%)
1	D	312/343 (90%)	-0.14	6 (1%) 66 67	26, 42, 65, 120	2 (0%)
All	All	1250/1372 (91%)	-0.30	13 (1%) 79 80	16, 37, 62, 120	15 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	456	TRP	5.9
1	B	459	LEU	3.4
1	A	459	LEU	3.4
1	B	458	GLY	3.3
1	D	459	LEU	3.2
1	D	649	TYR	3.0
1	B	771	THR	2.9
1	D	458	GLY	2.9
1	B	460	MET	2.5
1	A	458	GLY	2.2
1	B	484	ASN	2.0
1	D	460	MET	2.0
1	D	768	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	CME	D	509	10/11	0.89	0.12	41,50,73,76	0
1	CME	A	509	10/11	0.91	0.12	39,44,78,82	0
1	CME	C	509	10/11	0.93	0.12	37,42,79,90	0
1	CME	B	509	10/11	0.93	0.12	32,50,78,83	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

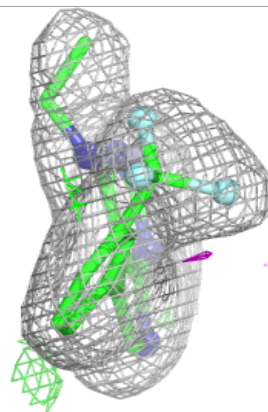
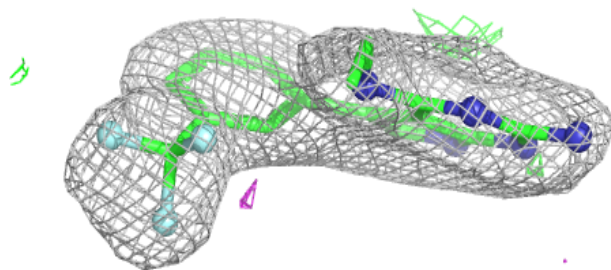
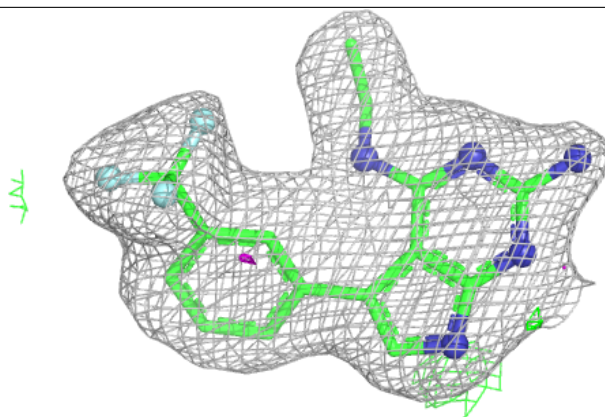
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	803	6/6	0.78	0.18	65,67,73,75	0
5	K3O	C	803	23/23	0.95	0.07	28,36,51,60	0
5	K3O	B	803	23/23	0.97	0.05	26,31,47,47	0
5	K3O	A	804	23/23	0.97	0.06	25,33,52,60	0
5	K3O	D	803	23/23	0.97	0.06	31,38,44,47	0
3	MG	C	802	1/1	0.99	0.02	23,23,23,23	0
2	ZN	A	801	1/1	1.00	0.01	30,30,30,30	0
3	MG	D	802	1/1	1.00	0.04	27,27,27,27	0
2	ZN	B	801	1/1	1.00	0.01	30,30,30,30	0
2	ZN	C	801	1/1	1.00	0.01	32,32,32,32	0
2	ZN	D	801	1/1	1.00	0.01	37,37,37,37	0
3	MG	A	802	1/1	1.00	0.03	24,24,24,24	0
3	MG	B	802	1/1	1.00	0.02	19,19,19,19	0

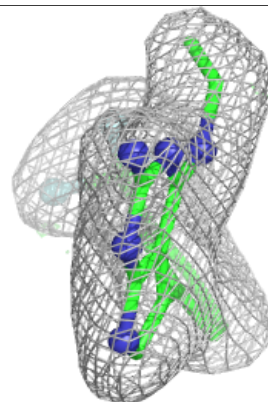
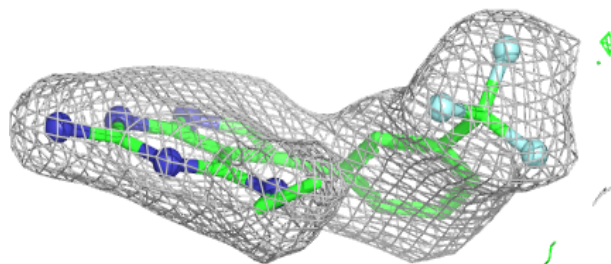
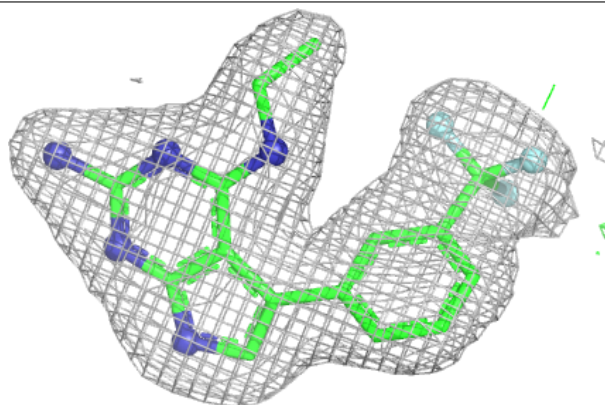
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around K3O 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)

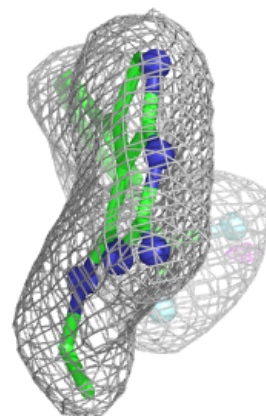
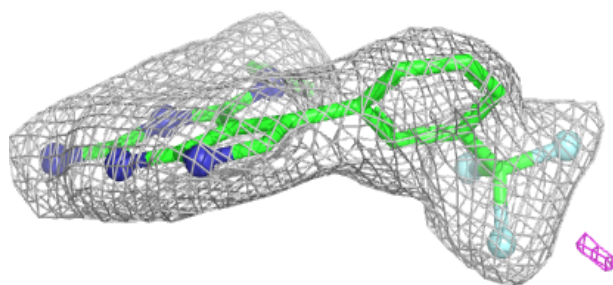
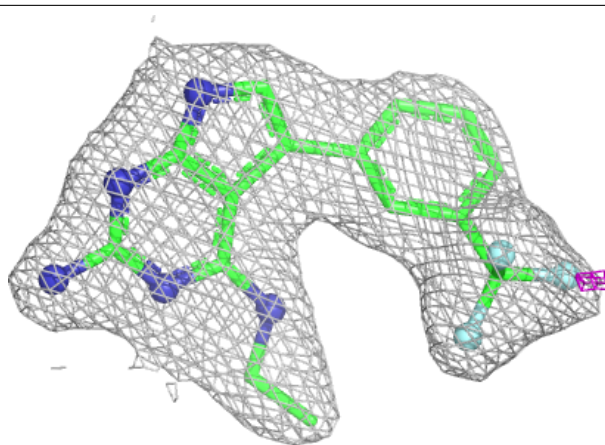
**Electron density around K3O B 803:**

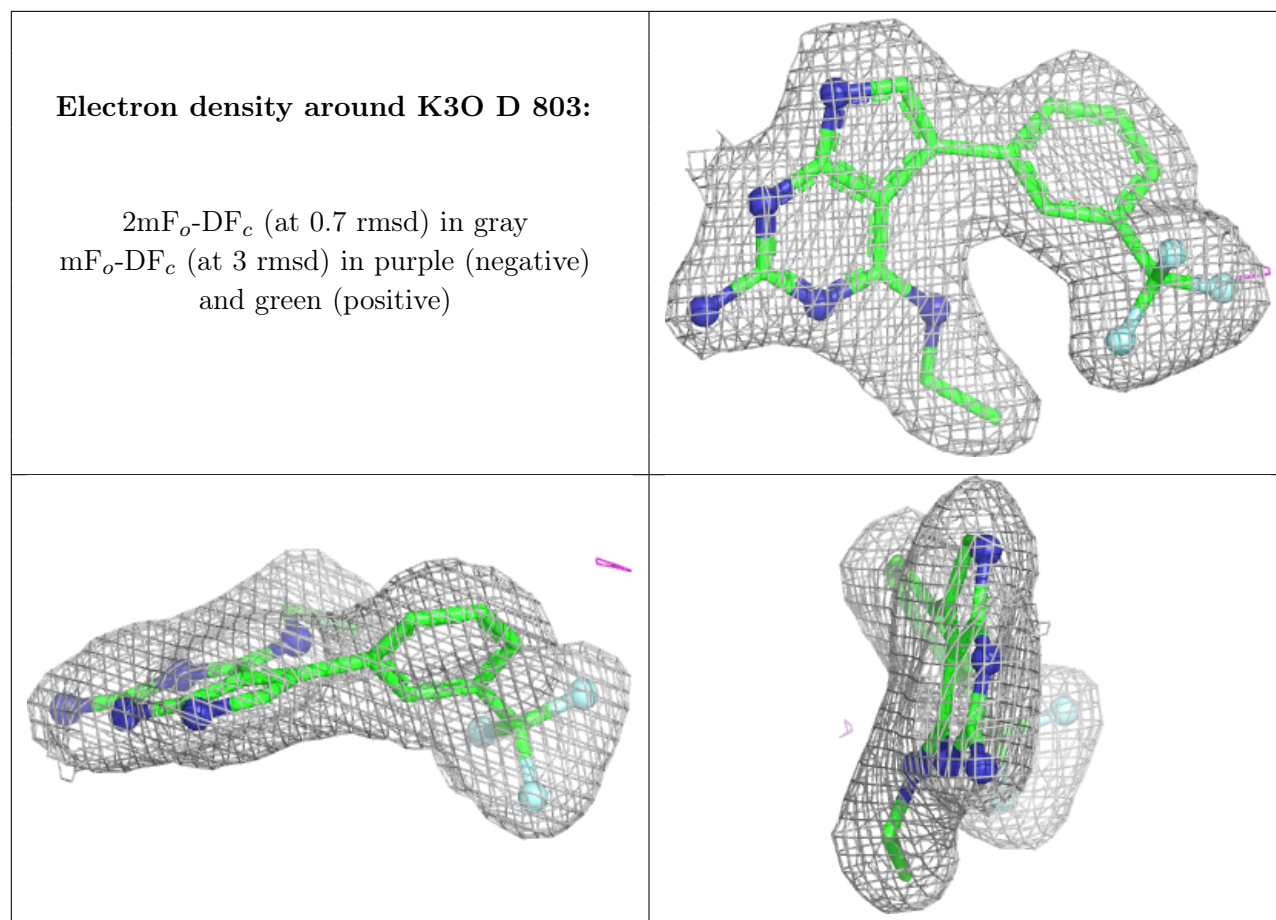
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around K3O A 804:

$2mF_o-DF_c$ (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.