



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:15 AM UTC

PDB ID : 5EDE / pdb_00005ede
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN
COMPLEX WITH c13c(cc(s1)C(NCC2OCCC2)=O)c(nn3c4ccc(cc4)Cl)
C, micromolar IC50=0.217
Authors : Joseph, C.; Rudolph, M.G.
Deposited on : 2015-10-21
Resolution : 2.20 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

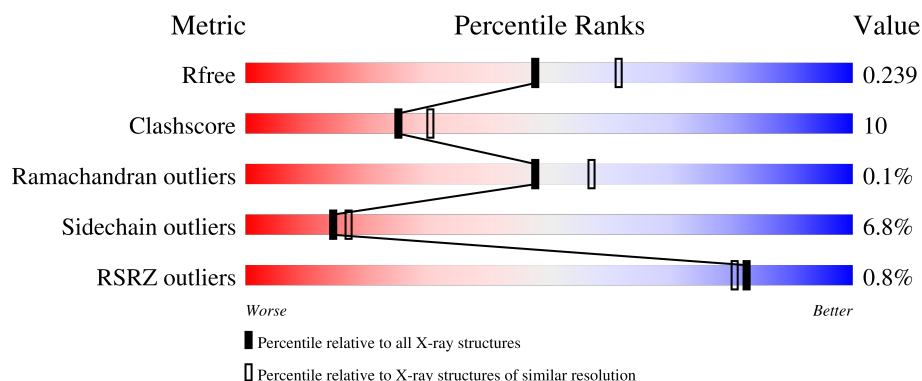
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	316	 73% 21% 5% .
1	C	316	 74% 20% 5% .
1	D	316	 74% 22% . .
2	B	315	 75% 20% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	803	-	X	-	-
5	GOL	B	803	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11207 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	314	Total	C	N	O	S	0	6	0
			2580	1648	438	468	26			
1	C	313	Total	C	N	O	S	0	7	0
			2578	1648	439	466	25			
1	D	313	Total	C	N	O	S	0	5	0
			2568	1641	439	463	25			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	ALA	-	expression tag	UNP Q9Y233
A	470	ARG	LYS	conflict	UNP Q9Y233
A	771	ALA	-	expression tag	UNP Q9Y233
C	456	ALA	-	expression tag	UNP Q9Y233
C	470	ARG	LYS	conflict	UNP Q9Y233
C	771	ALA	-	expression tag	UNP Q9Y233
D	456	ALA	-	expression tag	UNP Q9Y233
D	470	ARG	LYS	conflict	UNP Q9Y233
D	771	ALA	-	expression tag	UNP Q9Y233

- Molecule 2 is a protein called cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	315	Total	C	N	O	S	0	5	0
			2581	1648	439	469	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	457	ALA	-	expression tag	UNP Q9Y233

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Chain	Residue	Modelled	Actual	Comment	Reference
B	470	ARG	LYS	conflict	UNP Q9Y233
B	771	ALA	-	expression tag	UNP Q9Y233

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

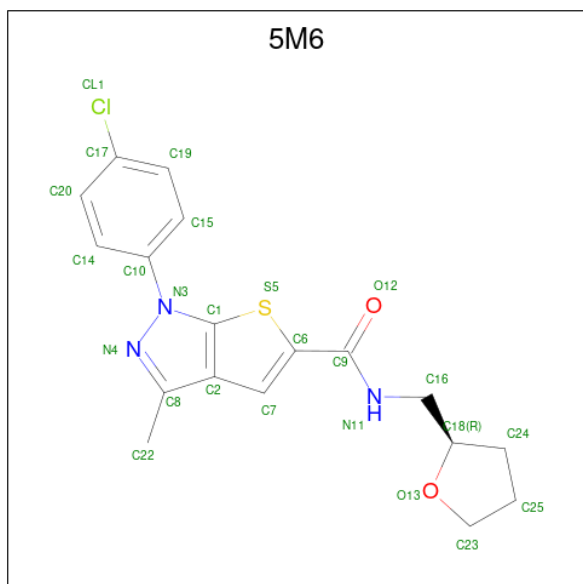
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is 1-(4-chlorophenyl)-3-methyl- {N}-[[(2 {R})-oxolan-2-yl]methyl]thieno[2,3-c]pyrazole-5-carboxamide (CCD ID: 5M6) (formula: C₁₈H₁₈ClN₃O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	S	0	0
			25	18	1	3	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 25	C 18	Cl 1	N 3	O 2	S 1	0	0
6	C	1	Total 25	C 18	Cl 1	N 3	O 2	S 1	0	0
6	D	1	Total 25	C 18	Cl 1	N 3	O 2	S 1	0	0

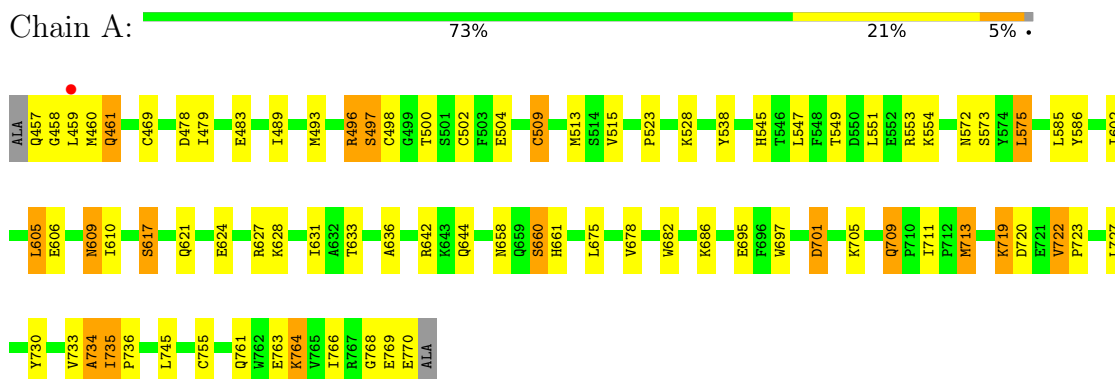
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	191	Total 191	O 191	0	0
7	B	219	Total 219	O 219	0	0
7	C	215	Total 215	O 215	0	0
7	D	155	Total 155	O 155	0	0

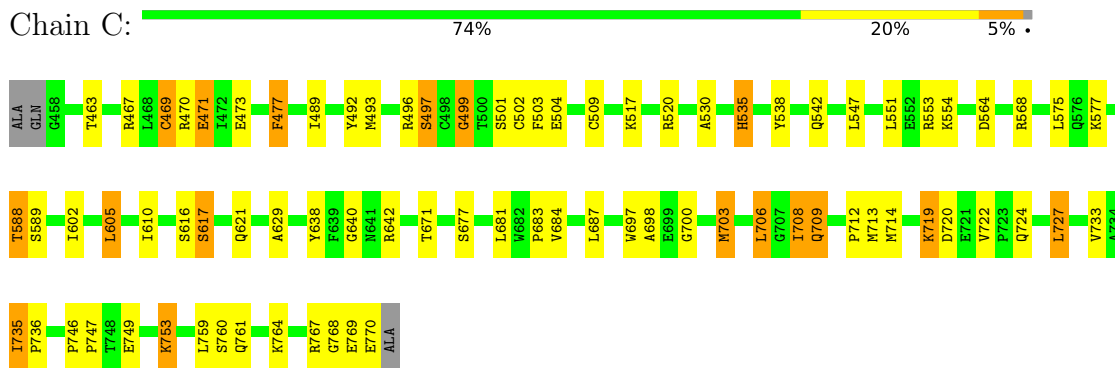
3 Residue-property plots

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.

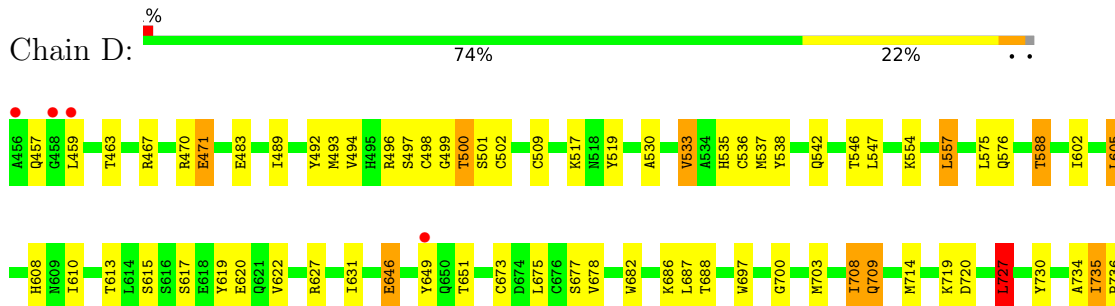
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



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

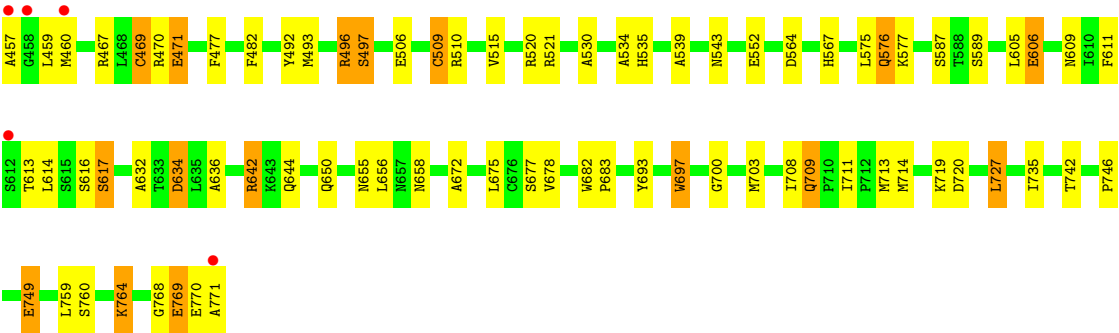


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A





● Molecule 2: 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	135.61Å 135.61Å 235.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.73 – 2.20 43.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.73-2.20) 96.0 (43.73-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.242 0.186 , 0.239	Depositor DCC
R_{free} test set	4074 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11207	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: GOL, CME, MG, ZN, 5M6

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	1.50	9/2649 (0.3%)	1.40	13/3583 (0.4%)
1	C	1.52	12/2650 (0.5%)	1.42	11/3584 (0.3%)
1	D	1.37	5/2634 (0.2%)	1.43	12/3563 (0.3%)
2	B	1.54	14/2647 (0.5%)	1.45	9/3581 (0.3%)
All	All	1.48	40/10580 (0.4%)	1.42	45/14311 (0.3%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	530	ALA	CA-CB	8.40	1.66	1.53
1	D	735	ILE	CA-CB	7.28	1.58	1.54
2	B	672	ALA	CA-CB	7.12	1.64	1.53
1	A	734	ALA	CA-CB	6.68	1.64	1.53
2	B	515	VAL	CA-CB	6.65	1.62	1.54
2	B	530	ALA	N-CA	6.42	1.54	1.46
1	A	733	VAL	CA-C	-6.31	1.44	1.52
2	B	735	ILE	N-CA	6.30	1.54	1.46
1	C	629	ALA	CA-CB	6.29	1.63	1.53
1	A	610	ILE	CA-CB	6.08	1.61	1.54
2	B	606	GLU	CG-CD	6.08	1.67	1.52
1	A	735	ILE	N-CA	5.92	1.53	1.46
1	A	545	HIS	C-O	5.70	1.31	1.24
1	D	610	ILE	CA-CB	5.68	1.62	1.54
1	A	633	THR	N-CA	5.66	1.53	1.46
1	D	530	ALA	CA-CB	5.66	1.62	1.53
1	D	519	TYR	C-O	-5.62	1.17	1.23
2	B	534	ALA	CA-CB	-5.61	1.44	1.53
2	B	634	ASP	C-O	-5.59	1.17	1.23
1	C	722	VAL	CA-CB	5.46	1.57	1.54
1	C	588	THR	N-CA	5.45	1.52	1.45
2	B	617	SER	CA-C	-5.44	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	632	ALA	CA-CB	5.44	1.62	1.53
2	B	521	ARG	CA-C	-5.41	1.47	1.53
1	C	698	ALA	CA-CB	-5.39	1.44	1.53
1	A	764	LYS	C-O	-5.37	1.17	1.24
2	B	697	TRP	C-O	-5.37	1.17	1.24
1	C	733	VAL	CA-CB	5.37	1.61	1.54
1	C	640	GLY	C-O	5.35	1.30	1.23
2	B	636	ALA	CA-CB	5.30	1.62	1.53
1	C	735	ILE	C-O	-5.27	1.20	1.24
1	A	722	VAL	CA-CB	5.26	1.57	1.54
1	C	477	PHE	N-CA	5.24	1.52	1.46
1	C	564	ASP	CA-C	5.17	1.59	1.53
1	A	478	ASP	C-O	-5.15	1.17	1.24
1	C	727	LEU	N-CA	5.12	1.52	1.46
1	D	533	VAL	N-CA	5.11	1.52	1.46
1	C	499	GLY	N-CA	5.10	1.50	1.45
2	B	764	LYS	CA-C	-5.05	1.46	1.52
2	B	693	TYR	C-O	-5.05	1.17	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	609	ASN	N-CA-C	7.26	121.59	108.17
2	B	769	GLU	N-CA-C	-7.18	104.25	112.87
1	D	646	GLU	N-CA-C	-7.03	103.31	110.97
1	C	709	GLN	CA-C-N	-6.85	113.60	120.31
1	C	709	GLN	C-N-CA	-6.85	113.60	120.31
2	B	746	PRO	N-CA-C	6.84	119.05	110.70
1	C	708	ILE	N-CA-C	6.34	116.99	107.80
2	B	709	GLN	CA-C-N	-6.28	113.81	120.03
2	B	709	GLN	C-N-CA	-6.28	113.81	120.03
1	D	537	MET	N-CA-C	-6.09	104.72	111.36
2	B	642	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	C	706	LEU	N-CA-C	-5.93	106.00	113.18
1	D	709	GLN	CA-C-N	-5.85	114.58	120.31
1	D	709	GLN	C-N-CA	-5.85	114.58	120.31
1	C	735	ILE	N-CA-CB	5.79	114.96	110.45
1	D	536	CYS	N-CA-C	-5.78	105.06	111.36
1	D	557	LEU	N-CA-C	-5.76	105.08	111.36
1	C	703	MET	N-CA-C	-5.73	105.11	111.36
1	A	636	ALA	N-CA-C	-5.71	105.42	112.38
1	C	617	SER	O-C-N	5.62	128.10	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	LEU	N-CA-C	-5.59	106.67	112.93
2	B	617	SER	CB-CA-C	-5.59	102.28	110.95
1	C	671	THR	CA-C-O	5.53	126.41	120.55
1	A	735	ILE	CA-C-O	5.37	122.29	118.69
1	D	500	THR	CA-C-O	5.37	125.98	119.11
1	D	746	PRO	CA-C-N	-5.28	114.26	120.12
1	D	746	PRO	C-N-CA	-5.28	114.26	120.12
1	C	683	PRO	CB-CA-C	-5.27	104.41	112.11
1	D	727	LEU	N-CA-C	-5.22	104.85	111.11
1	A	609	ASN	N-CA-C	5.19	117.75	107.98
2	B	642	ARG	N-CA-C	5.19	116.93	111.28
1	C	535	HIS	N-CA-CB	5.16	117.80	110.16
1	A	682	TRP	CA-C-N	-5.15	114.44	119.64
1	A	682	TRP	C-N-CA	-5.15	114.44	119.64
1	A	515	VAL	N-CA-C	-5.15	105.48	110.42
1	A	572	ASN	N-CA-C	-5.11	105.71	111.28
1	A	701	ASP	N-CA-C	-5.10	105.80	111.36
1	A	573	SER	CB-CA-C	-5.09	102.88	110.88
1	A	709	GLN	CA-C-N	-5.09	115.48	120.52
1	A	709	GLN	C-N-CA	-5.09	115.48	120.52
1	D	708	ILE	N-CA-C	5.07	115.27	108.17
1	A	575	LEU	N-CA-C	-5.05	105.86	111.36
2	B	552	GLU	N-CA-C	-5.03	105.88	111.36
1	D	620	GLU	CA-C-O	5.02	125.74	119.97
1	C	473	GLU	N-CA-C	-5.01	107.17	113.28

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	2580	0	2554	55	0
1	C	2578	0	2566	54	0
1	D	2568	0	2550	44	0
2	B	2581	0	2555	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	8	3	0
5	B	6	0	8	4	0
6	A	25	0	0	0	0
6	B	25	0	0	1	0
6	C	25	0	0	1	0
6	D	25	0	0	2	0
7	A	191	0	0	6	0
7	B	219	0	0	3	0
7	C	215	0	0	8	0
7	D	155	0	0	4	0
All	All	11207	0	10241	198	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 10.

All (198) 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:457:GLN:CB	1:A:458:GLY:HA2	1.67	1.22
2:B:770:GLU:HG3	2:B:771:ALA:H	1.10	1.08
1:A:457:GLN:CB	1:A:458:GLY:CA	2.29	1.07
2:B:770:GLU:HG3	2:B:771:ALA:N	1.59	1.05
1:D:727:LEU:CD1	1:D:766:ILE:HD12	1.88	1.03
2:B:469[B]:CYS:SG	7:B:1087:HOH:O	2.21	0.96
1:D:727:LEU:HD12	1:D:766:ILE:CD1	1.96	0.95
1:C:764[B]:LYS:HG3	1:C:769:GLU:HB2	1.52	0.89
1:D:727:LEU:CD1	1:D:766:ILE:CD1	2.51	0.88
1:C:469[B]:CYS:SG	7:C:1087:HOH:O	2.34	0.86
2:B:770:GLU:CG	2:B:771:ALA:N	2.40	0.85
1:A:461:GLN:NE2	1:A:500:THR:HG21	1.95	0.81
1:C:493:MET:O	1:C:497:SER:HB2	1.84	0.78
2:B:711:ILE:HD11	2:B:713:MET:HE2	1.65	0.78
1:A:769:GLU:O	1:A:770:GLU:HB3	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:727:LEU:HD12	1:D:766:ILE:HD11	1.64	0.77
1:D:727:LEU:HD12	1:D:766:ILE:HD12	1.59	0.75
2:B:764:LYS:HD3	2:B:769:GLU:HG2	1.68	0.74
1:D:677:SER:HB2	6:D:803:5M6:CL1	2.25	0.74
2:B:677:SER:HB2	6:B:804:5M6:CL1	2.26	0.72
1:A:461:GLN:HE22	1:A:500:THR:CG2	2.01	0.72
1:A:493:MET:O	1:A:497:SER:HB2	1.89	0.72
2:B:493:MET:O	2:B:497:SER:HB2	1.90	0.71
1:C:502:CYS:HB3	1:C:554:LYS:HE2	1.72	0.71
1:A:461:GLN:NE2	1:A:461:GLN:HA	2.07	0.68
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.75	0.68
1:C:714:MET:HE2	7:C:1056:HOH:O	1.94	0.68
2:B:727:LEU:CD2	2:B:759:LEU:HD11	2.24	0.68
2:B:457:ALA:HB1	2:B:460:MET:HE3	1.77	0.67
2:B:682:TRP:HB3	2:B:683:PRO:HD3	1.78	0.66
1:D:493:MET:O	1:D:497:SER:HB2	1.95	0.66
2:B:697:TRP:CZ2	2:B:719:LYS:HG2	2.32	0.65
1:D:761:GLN:HE22	1:D:764:LYS:NZ	1.94	0.65
1:C:714:MET:CE	7:C:1056:HOH:O	2.46	0.64
1:C:470:ARG:HG3	1:C:470:ARG:HH11	1.63	0.63
2:B:727:LEU:HD23	2:B:759:LEU:CD1	2.28	0.63
1:C:769:GLU:O	1:C:770:GLU:HB2	1.99	0.62
1:A:642:ARG:NH2	7:A:908:HOH:O	2.33	0.62
1:D:675:LEU:O	1:D:678:VAL:HG22	2.00	0.62
1:C:767:ARG:HH21	1:C:769:GLU:CD	2.07	0.61
1:A:523:PRO:HD2	1:A:695:GLU:HG2	1.83	0.61
1:A:469[A]:CYS:SG	7:A:995:HOH:O	2.50	0.61
1:A:461:GLN:NE2	1:A:500:THR:CG2	2.61	0.60
2:B:727:LEU:HD23	2:B:759:LEU:HD11	1.82	0.60
1:D:766:ILE:HG22	1:D:766:ILE:O	2.00	0.60
1:C:768:GLY:C	1:C:770:GLU:H	2.09	0.59
1:D:602:ILE:O	1:D:605:LEU:HB2	2.01	0.59
2:B:700:GLY:HA3	2:B:714:MET:O	2.02	0.59
1:A:549:THR:O	1:A:553:ARG:HG3	2.03	0.59
1:A:711:ILE:HD11	1:A:713:MET:HE2	1.84	0.58
1:C:700:GLY:HA3	1:C:714:MET:O	2.03	0.58
1:D:588:THR:CG2	7:D:967:HOH:O	2.52	0.58
1:A:727:LEU:HD21	1:A:763:GLU:HG3	1.85	0.58
2:B:742:THR:HG21	2:B:749:GLU:HG2	1.85	0.57
1:C:677:SER:HB2	6:C:803:5M6:CL1	2.40	0.57
2:B:470:ARG:HG3	2:B:471:GLU:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:GLY:C	1:A:770:GLU:H	2.12	0.57
2:B:742:THR:CG2	2:B:749:GLU:HG2	2.36	0.56
1:C:503:PHE:CE2	1:C:610:ILE:HD12	2.41	0.56
1:D:762:TRP:O	1:D:766:ILE:HG13	2.05	0.56
1:D:493:MET:O	1:D:497:SER:CB	2.54	0.56
1:C:727:LEU:CD2	1:C:759:LEU:HD11	2.36	0.55
1:C:602:ILE:HA	1:C:605:LEU:HD22	1.87	0.55
1:C:496:ARG:NH1	7:C:907:HOH:O	2.40	0.54
1:D:627:ARG:O	1:D:631:ILE:HG12	2.07	0.54
1:A:461:GLN:HE22	1:A:500:THR:HG22	1.70	0.54
2:B:457:ALA:HB1	2:B:460:MET:CE	2.38	0.54
2:B:703:MET:HE3	2:B:708:ILE:CG2	2.38	0.54
2:B:577:LYS:HD3	2:B:703:MET:HE1	1.88	0.54
1:C:542:GLN:NE2	1:C:542:GLN:HA	2.22	0.54
1:A:602:ILE:HA	1:A:605:LEU:HD22	1.91	0.53
2:B:457:ALA:CB	2:B:460:MET:HE3	2.39	0.53
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.44	0.53
1:D:483[B]:GLU:OE1	7:D:901:HOH:O	2.18	0.53
1:D:730:TYR:HA	1:D:734:ALA:HB3	1.91	0.53
2:B:611:PHE:HB3	2:B:614:LEU:HD22	1.91	0.52
1:D:542:GLN:NE2	7:D:906:HOH:O	2.42	0.52
1:D:761:GLN:HE22	1:D:764:LYS:HZ2	1.58	0.52
1:A:461:GLN:HE22	1:A:500:THR:HG21	1.61	0.52
1:A:769:GLU:O	1:A:770:GLU:CB	2.56	0.51
1:D:700:GLY:HA3	1:D:714:MET:O	2.11	0.51
1:C:697:TRP:CZ2	1:C:719:LYS:HG3	2.45	0.51
1:A:658:ASN:O	1:A:661:HIS:HB2	2.09	0.51
2:B:482:PHE:HA	5:B:803:GOL:H2	1.92	0.51
5:A:803:GOL:H2	2:B:520:ARG:NH1	2.26	0.51
2:B:644:GLN:HE21	2:B:644:GLN:HA	1.76	0.51
1:A:624:GLU:HG3	1:A:628:LYS:HE3	1.93	0.51
1:C:764[A]:LYS:NZ	7:C:910:HOH:O	2.44	0.51
1:D:677:SER:OG	1:D:688:THR:HG21	2.10	0.51
2:B:768:GLY:C	2:B:770:GLU:N	2.67	0.51
1:D:467:ARG:O	1:D:471:GLU:HB2	2.11	0.50
1:C:727:LEU:HD23	1:C:759:LEU:HD12	1.94	0.50
1:C:577:LYS:HD3	1:C:703:MET:HE1	1.94	0.49
1:A:496:ARG:HD3	1:A:538:TYR:OH	2.12	0.49
1:C:642:ARG:NH2	7:C:914:HOH:O	2.45	0.49
2:B:644:GLN:HA	2:B:644:GLN:NE2	2.28	0.49
1:D:727:LEU:HD13	1:D:766:ILE:CD1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:727:LEU:HD23	1:C:759:LEU:CD1	2.41	0.49
1:C:769:GLU:O	1:C:770:GLU:CB	2.59	0.49
2:B:770:GLU:CG	2:B:771:ALA:H	2.00	0.49
1:A:498:CYS:SG	1:A:502[A]:CYS:CB	3.01	0.48
1:A:686:LYS:HD3	7:A:997:HOH:O	2.13	0.48
2:B:644:GLN:HE21	2:B:644:GLN:CA	2.26	0.48
1:C:727:LEU:CD2	1:C:759:LEU:CD1	2.90	0.48
1:D:499:GLY:C	1:D:501:SER:H	2.22	0.48
1:C:553:ARG:NH1	7:C:916:HOH:O	2.47	0.48
2:B:457:ALA:CA	2:B:460:MET:HE3	2.44	0.48
1:D:697:TRP:CZ2	1:D:719:LYS:HG3	2.48	0.48
1:C:467:ARG:O	1:C:471:GLU:HB2	2.13	0.47
1:A:617:SER:O	1:A:621:GLN:HG3	2.14	0.47
1:D:619:TYR:O	1:D:622:VAL:HG12	2.15	0.47
5:B:803:GOL:H12	1:C:568:ARG:HH11	1.80	0.47
1:C:602:ILE:O	1:C:605:LEU:HB2	2.14	0.47
1:C:471:GLU:HB3	1:C:477:PHE:CD1	2.49	0.46
1:A:766:ILE:C	1:A:768:GLY:H	2.21	0.46
1:A:483[A]:GLU:H	5:A:803:GOL:H31	1.80	0.46
2:B:564:ASP:O	2:B:567:HIS:HB2	2.15	0.46
1:C:735:ILE:HB	1:C:736:PRO:HD3	1.98	0.46
1:D:649:TYR:CD2	1:D:649:TYR:C	2.91	0.46
1:A:489:ILE:O	1:A:493:MET:HG3	2.16	0.46
1:A:461:GLN:NE2	1:A:461:GLN:CA	2.76	0.46
1:D:766:ILE:O	1:D:766:ILE:CG2	2.63	0.46
1:A:719:LYS:O	1:A:722:VAL:HG23	2.16	0.46
1:A:730:TYR:HA	1:A:734:ALA:HB3	1.98	0.46
1:A:509:CME:O	1:A:513:MET:HG2	2.17	0.45
2:B:509:CME:HB2	7:B:1077:HOH:O	2.16	0.45
1:C:492:TYR:CE2	1:C:496:ARG:HD2	2.52	0.45
1:D:727:LEU:HD13	1:D:766:ILE:HD12	1.90	0.45
1:D:605:LEU:HB3	1:D:608:HIS:ND1	2.32	0.45
2:B:656:LEU:HD23	2:B:656:LEU:HA	1.80	0.45
1:A:483[B]:GLU:H	5:A:803:GOL:H31	1.81	0.45
2:B:492:TYR:CZ	2:B:496:ARG:HD2	2.52	0.45
1:C:724:GLN:HB2	7:C:1034:HOH:O	2.17	0.45
1:A:458:GLY:C	1:A:460:MET:H	2.24	0.45
1:A:735:ILE:N	1:A:736:PRO:HD2	2.32	0.45
2:B:477:PHE:HB3	2:B:535:HIS:CE1	2.51	0.45
2:B:655:ASN:O	2:B:658:ASN:HB3	2.17	0.45
2:B:768:GLY:C	2:B:770:GLU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:546:THR:OG1	1:D:547:LEU:HD12	2.17	0.45
1:C:489:ILE:O	1:C:493:MET:HG3	2.17	0.44
1:A:553:ARG:HD2	7:A:1058:HOH:O	2.18	0.44
1:A:705:LYS:HG2	1:C:684:VAL:HG22	2.00	0.44
1:D:740:THR:O	1:D:743[A]:GLN:HB2	2.16	0.44
1:D:605:LEU:HD12	1:D:605:LEU:HA	1.86	0.44
1:A:697:TRP:CZ2	1:A:719:LYS:HG2	2.53	0.44
1:C:764[B]:LYS:HE2	1:C:769:GLU:O	2.18	0.44
1:A:585:LEU:HD23	1:A:586:TYR:CE1	2.53	0.43
1:D:703:MET:HE3	1:D:708:ILE:CG2	2.48	0.43
2:B:675:LEU:O	2:B:678:VAL:HG22	2.18	0.43
1:C:703:MET:HE3	1:C:708:ILE:CG2	2.48	0.43
1:A:722:VAL:CB	1:A:723:PRO:HD3	2.47	0.43
1:C:746:PRO:N	1:C:747:PRO:CD	2.82	0.43
1:D:489:ILE:O	1:D:493:MET:HG3	2.19	0.43
1:C:499:GLY:C	1:C:501:SER:H	2.26	0.43
1:D:533:VAL:HG13	1:D:673:CYS:HB3	1.99	0.43
1:D:502[A]:CYS:HB2	1:D:554:LYS:HE2	2.00	0.43
1:C:687:LEU:HD23	1:C:687:LEU:HA	1.88	0.42
1:C:535:HIS:O	1:C:538:TYR:HB3	2.19	0.42
1:A:735:ILE:HD13	1:A:755:CYS:SG	2.59	0.42
1:A:658:ASN:OD1	1:A:660:SER:HB3	2.20	0.42
1:A:675:LEU:O	1:A:678:VAL:HG22	2.19	0.42
1:C:588:THR:O	1:C:589:SER:C	2.62	0.42
1:D:682:TRP:CZ2	1:D:686:LYS:HD3	2.54	0.42
1:A:498:CYS:C	1:A:502[B]:CYS:SG	3.03	0.42
1:C:761:GLN:HA	1:C:761:GLN:OE1	2.19	0.42
1:A:605:LEU:HD12	1:A:605:LEU:HA	1.90	0.42
2:B:471:GLU:HB3	2:B:477:PHE:CD1	2.54	0.42
5:B:803:GOL:C1	1:C:568:ARG:HH11	2.33	0.42
1:C:749[B]:GLU:OE2	1:C:753:LYS:HB2	2.19	0.42
1:A:547:LEU:HD22	1:A:745:LEU:CD2	2.50	0.42
1:C:764[A]:LYS:HG2	1:C:767:ARG:NH2	2.35	0.42
1:A:627:ARG:O	1:A:631:ILE:HG12	2.20	0.42
6:D:803:5M6:O12	7:D:902:HOH:O	2.21	0.42
1:A:502[A]:CYS:HB2	1:A:554:LYS:HE2	2.01	0.41
1:C:638:TYR:OH	1:C:642:ARG:HD3	2.20	0.41
1:D:535:HIS:O	1:D:538:TYR:HB3	2.20	0.41
2:B:576:GLN:HB2	7:B:1080:HOH:O	2.20	0.41
1:A:553:ARG:CD	7:A:1058:HOH:O	2.69	0.41
1:A:479:ILE:HD11	1:A:528:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ARG:HD3	1:C:538:TYR:OH	2.20	0.41
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.74	0.41
1:A:701:ASP:HB3	1:C:687:LEU:HD13	2.03	0.41
1:A:761:GLN:HE22	1:A:764:LYS:HZ3	1.69	0.41
1:A:727:LEU:HD13	7:A:1063:HOH:O	2.21	0.41
2:B:506[B]:GLU:HG2	2:B:510:ARG:NH1	2.36	0.41
2:B:539:ALA:O	2:B:543:ASN:ND2	2.41	0.41
2:B:703:MET:HE3	2:B:708:ILE:HG21	2.03	0.41
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.81	0.41
1:D:687:LEU:HD23	1:D:687:LEU:HA	1.95	0.41
2:B:467:ARG:O	2:B:467:ARG:HG2	2.18	0.41
1:C:706:LEU:HD23	1:C:706:LEU:HA	1.91	0.41
1:D:735:ILE:HB	1:D:736:PRO:HD3	2.02	0.40
1:C:767:ARG:NE	1:C:769:GLU:OE2	2.51	0.40
1:D:492:TYR:CE2	1:D:496:ARG:HD2	2.56	0.40
2:B:589:SER:OG	2:B:634:ASP:OD2	2.36	0.40
1:C:727:LEU:HD22	1:C:759:LEU:HD11	2.02	0.40
5:B:803:GOL:H11	1:C:520:ARG:NH1	2.37	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	317/316 (100%)	306 (96%)	11 (4%)	0	100	100
1	C	317/316 (100%)	310 (98%)	7 (2%)	0	100	100
1	D	315/316 (100%)	308 (98%)	6 (2%)	1 (0%)	36	42
2	B	317/315 (101%)	310 (98%)	7 (2%)	0	100	100
All	All	1266/1263 (100%)	1234 (98%)	31 (2%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	615	SER

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	287/282 (102%)	272 (95%)	15 (5%)	21	26
1	C	288/282 (102%)	267 (93%)	21 (7%)	13	15
1	D	285/282 (101%)	264 (93%)	21 (7%)	13	14
2	B	286/281 (102%)	265 (93%)	21 (7%)	13	15
All	All	1146/1127 (102%)	1068 (93%)	78 (7%)	14	17

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	496	ARG
1	A	497	SER
1	A	504	GLU
1	A	575	LEU
1	A	605	LEU
1	A	606	GLU
1	A	609	ASN
1	A	617	SER
1	A	644	GLN
1	A	660	SER
1	A	709	GLN
1	A	713	MET
1	A	719	LYS
1	A	720	ASP
2	B	459	LEU
2	B	469[A]	CYS
2	B	469[B]	CYS
2	B	471	GLU
2	B	496	ARG
2	B	497	SER

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Mol	Chain	Res	Type
2	B	575	LEU
2	B	576	GLN
2	B	587	SER
2	B	605	LEU
2	B	606	GLU
2	B	613	THR
2	B	616	SER
2	B	617	SER
2	B	642	ARG
2	B	650	GLN
2	B	709	GLN
2	B	720	ASP
2	B	727	LEU
2	B	749	GLU
2	B	760	SER
1	C	463	THR
1	C	469[A]	CYS
1	C	469[B]	CYS
1	C	471	GLU
1	C	497	SER
1	C	504	GLU
1	C	517	LYS
1	C	547	LEU
1	C	575	LEU
1	C	605	LEU
1	C	616	SER
1	C	617	SER
1	C	621	GLN
1	C	681	LEU
1	C	709	GLN
1	C	712	PRO
1	C	713	MET
1	C	719	LYS
1	C	720	ASP
1	C	753	LYS
1	C	760	SER
1	D	457	GLN
1	D	459	LEU
1	D	463	THR
1	D	470	ARG
1	D	471	GLU
1	D	494	VAL

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Mol	Chain	Res	Type
1	D	498	CYS
1	D	500	THR
1	D	517	LYS
1	D	557	LEU
1	D	575	LEU
1	D	576	GLN
1	D	588	THR
1	D	605	LEU
1	D	613	THR
1	D	617	SER
1	D	646	GLU
1	D	709	GLN
1	D	720	ASP
1	D	727	LEU
1	D	767	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	484	ASN
1	A	542	GLN
1	A	604	GLN
1	A	644	GLN
1	A	650	GLN
1	A	761	GLN
2	B	484	ASN
2	B	495	HIS
2	B	545	HIS
2	B	604	GLN
2	B	644	GLN
2	B	724	GLN
2	B	726	GLN
2	B	761	GLN
1	C	461	GLN
1	C	542	GLN
1	C	545	HIS
1	C	604	GLN
1	C	621	GLN
1	C	659	GLN
1	C	709	GLN
1	D	484	ASN

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Mol	Chain	Res	Type
1	D	542	GLN
1	D	604	GLN
1	D	621	GLN
1	D	644	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	A	509	1	8,9,10	0.74	0	6,9,11	2.93	1 (16%)
1	CME	D	509	1	8,9,10	0.73	0	6,9,11	2.97	2 (33%)
1	CME	C	509	1	8,9,10	0.78	0	6,9,11	2.69	1 (16%)
2	CME	B	509	2	8,9,10	0.68	0	6,9,11	3.25	2 (33%)

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	A	509	1	-	2/5/8/10	-
1	CME	D	509	1	-	2/5/8/10	-
1	CME	C	509	1	-	2/5/8/10	-
2	CME	B	509	2	-	1/5/8/10	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	509	CME	CE-SD-SG	7.39	135.90	103.46
1	A	509	CME	CE-SD-SG	7.01	134.25	103.46
1	D	509	CME	CE-SD-SG	6.63	132.57	103.46
1	C	509	CME	CE-SD-SG	5.90	129.38	103.46
2	B	509	CME	CB-SG-SD	-2.65	97.01	103.86
1	D	509	CME	CA-CB-SG	-2.03	106.12	114.45

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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
6	5M6	A	804	-	28,28,28	1.33	4 (14%)	37,40,40	1.99	10 (27%)
5	GOL	B	803	-	5,5,5	0.95	0	5,5,5	1.24	1 (20%)
5	GOL	A	803	-	5,5,5	0.92	0	5,5,5	1.46	2 (40%)
6	5M6	D	803	-	28,28,28	1.12	2 (7%)	37,40,40	2.38	17 (45%)
6	5M6	C	803	-	28,28,28	1.22	4 (14%)	37,40,40	1.98	14 (37%)
6	5M6	B	804	-	28,28,28	1.36	5 (17%)	37,40,40	2.07	12 (32%)

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
6	5M6	A	804	-	-	2/13/20/20	0/4/4/4
5	GOL	B	803	-	-	2/4/4/4	-
5	GOL	A	803	-	-	4/4/4/4	-
6	5M6	D	803	-	-	2/13/20/20	0/4/4/4
6	5M6	C	803	-	-	2/13/20/20	0/4/4/4
6	5M6	B	804	-	-	3/13/20/20	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	804	5M6	C16-C18	3.10	1.55	1.51
6	B	804	5M6	C16-C18	3.01	1.55	1.51
6	C	803	5M6	C10-N3	-2.51	1.38	1.43
6	A	804	5M6	C10-N3	-2.50	1.38	1.43
6	D	803	5M6	C16-C18	2.45	1.54	1.51
6	B	804	5M6	C6-S5	2.44	1.79	1.73
6	D	803	5M6	C20-C17	2.33	1.42	1.38
6	A	804	5M6	C17-CL1	2.31	1.79	1.74
6	C	803	5M6	C16-C18	2.30	1.54	1.51
6	B	804	5M6	C20-C17	2.23	1.42	1.38
6	C	803	5M6	C9-N11	2.21	1.37	1.33
6	C	803	5M6	O13-C23	2.10	1.49	1.43
6	B	804	5M6	C10-N3	-2.03	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	804	5M6	C9-N11	2.02	1.37	1.33
6	B	804	5M6	O13-C23	2.01	1.48	1.43

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	803	5M6	C10-N3-N4	6.82	128.55	118.67
6	C	803	5M6	C10-N3-N4	6.25	127.72	118.67
6	B	804	5M6	C6-C9-N11	5.22	123.32	117.09
6	D	803	5M6	C22-C8-N4	5.17	129.43	119.39
6	A	804	5M6	C10-N3-N4	5.14	126.12	118.67
6	D	803	5M6	C18-C16-N11	-4.60	102.83	111.98
6	B	804	5M6	C18-C16-N11	-4.49	103.06	111.98
6	D	803	5M6	C22-C8-C2	-4.13	121.48	127.84
6	A	804	5M6	C22-C8-C2	-4.01	121.65	127.84
6	B	804	5M6	C22-C8-N4	3.82	126.81	119.39
6	A	804	5M6	C22-C8-N4	3.70	126.56	119.39
6	A	804	5M6	C14-C20-C17	3.69	122.95	119.24
6	B	804	5M6	O12-C9-C6	-3.61	114.05	120.62
6	B	804	5M6	C10-N3-N4	3.57	123.85	118.67
6	A	804	5M6	C10-N3-C1	-3.43	122.57	129.70
6	A	804	5M6	C6-C9-N11	3.41	121.17	117.09
6	C	803	5M6	C22-C8-N4	3.23	125.66	119.39
6	B	804	5M6	C20-C14-C10	-3.17	116.28	120.30
6	C	803	5M6	C14-C10-N3	-3.15	114.98	119.72
6	D	803	5M6	C8-N4-N3	3.09	109.68	105.75
6	D	803	5M6	C1-N3-N4	-3.01	107.06	112.83
6	B	804	5M6	C6-S5-C1	-3.00	87.04	90.94
6	C	803	5M6	C19-C15-C10	-2.98	116.52	120.30
6	B	804	5M6	C22-C8-C2	-2.95	123.29	127.84
6	C	803	5M6	C1-N3-N4	-2.93	107.21	112.83
6	D	803	5M6	C10-N3-C1	-2.77	123.93	129.70
6	B	804	5M6	C7-C6-S5	2.65	116.02	111.55
6	C	803	5M6	C14-C10-C15	2.52	123.98	119.18
6	D	803	5M6	C6-C9-N11	2.47	120.05	117.09
6	A	804	5M6	C14-C10-N3	-2.35	116.19	119.72
6	D	803	5M6	C2-C1-N3	2.35	109.03	105.54
6	D	803	5M6	C14-C10-C15	2.32	123.59	119.18
6	C	803	5M6	C20-C14-C10	-2.31	117.38	120.30
6	D	803	5M6	C2-C1-S5	-2.28	109.05	112.72
6	C	803	5M6	C19-C17-CL1	2.27	122.71	119.36
6	D	803	5M6	C20-C14-C10	-2.27	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	803	5M6	C2-C1-N3	2.26	108.91	105.54
6	C	803	5M6	C10-N3-C1	-2.26	124.99	129.70
6	D	803	5M6	C14-C10-N3	-2.26	116.32	119.72
6	A	804	5M6	C20-C14-C10	-2.25	117.44	120.30
5	B	803	GOL	O2-C2-C1	2.25	118.48	109.18
6	C	803	5M6	C20-C17-CL1	-2.24	116.06	119.36
6	B	804	5M6	C7-C2-C1	2.23	115.33	110.41
5	A	803	GOL	O2-C2-C1	-2.22	99.99	109.18
6	C	803	5M6	C8-N4-N3	2.20	108.54	105.75
6	A	804	5M6	C18-C16-N11	-2.19	107.62	111.98
6	B	804	5M6	C7-C6-C9	-2.18	126.62	130.38
6	D	803	5M6	C19-C15-C10	-2.16	117.56	120.30
6	D	803	5M6	C19-C17-CL1	2.16	122.55	119.36
5	A	803	GOL	C3-C2-C1	2.14	119.65	111.80
6	C	803	5M6	C22-C8-C2	-2.10	124.60	127.84
6	C	803	5M6	C7-C6-C9	-2.07	126.80	130.38
6	A	804	5M6	C7-C6-C9	-2.07	126.81	130.38
6	D	803	5M6	O12-C9-C6	-2.06	116.87	120.62
6	D	803	5M6	C7-C2-C1	2.06	114.95	110.41
6	B	804	5M6	C14-C20-C17	2.05	121.30	119.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	803	GOL	O1-C1-C2-C3
5	A	803	GOL	C1-C2-C3-O3
5	B	803	GOL	O2-C2-C3-O3
5	B	803	GOL	C1-C2-C3-O3
5	A	803	GOL	O1-C1-C2-O2
5	A	803	GOL	O2-C2-C3-O3
6	A	804	5M6	C15-C10-N3-C1
6	A	804	5M6	C14-C10-N3-C1
6	B	804	5M6	C15-C10-N3-C1
6	B	804	5M6	C14-C10-N3-C1
6	D	803	5M6	C14-C10-N3-C1
6	C	803	5M6	C15-C10-N3-C1
6	C	803	5M6	C14-C10-N3-C1
6	D	803	5M6	C15-C10-N3-C1
6	B	804	5M6	N11-C16-C18-O13

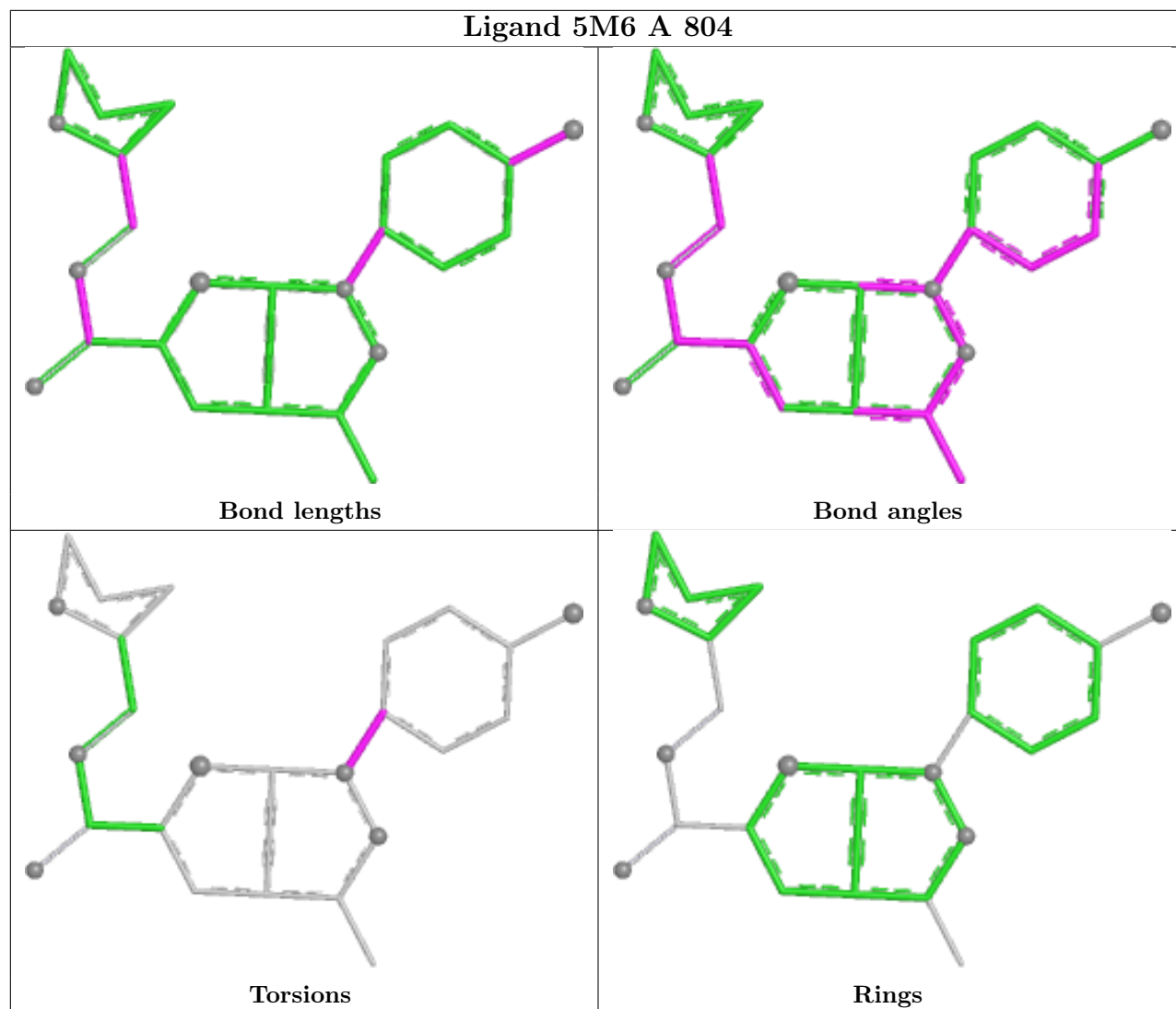
There are no ring outliers.

5 monomers are involved in 11 short contacts:

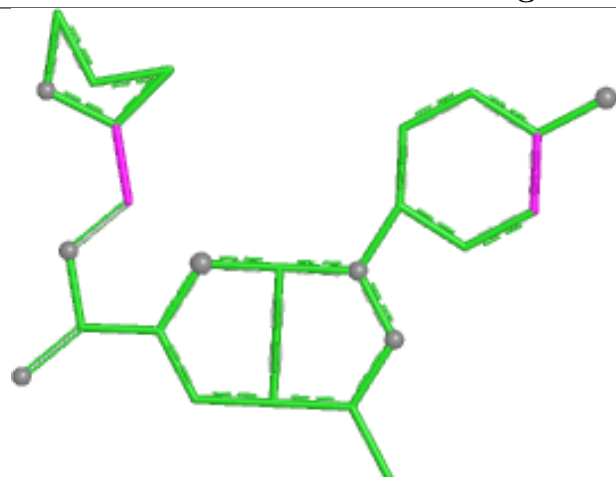
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	803	GOL	4	0
5	A	803	GOL	3	0
6	D	803	5M6	2	0
6	C	803	5M6	1	0
6	B	804	5M6	1	0

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.

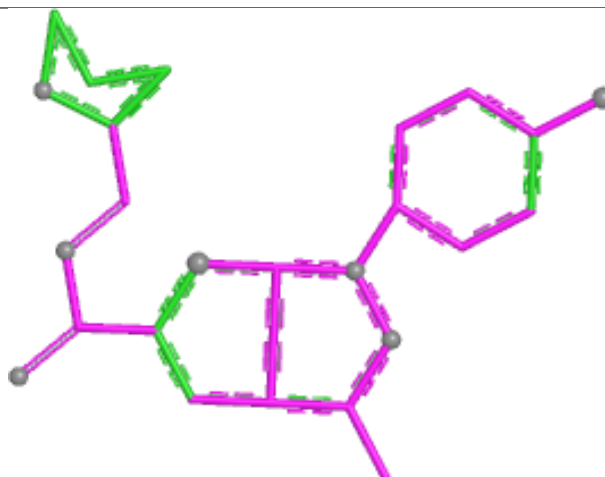
Ligand 5M6 A 804



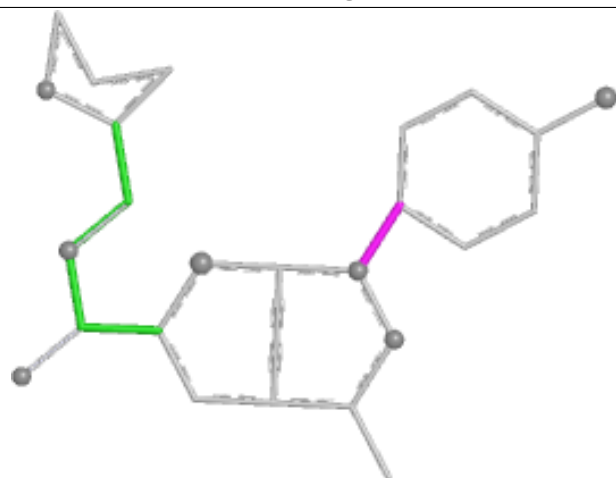
Ligand 5M6 D 803



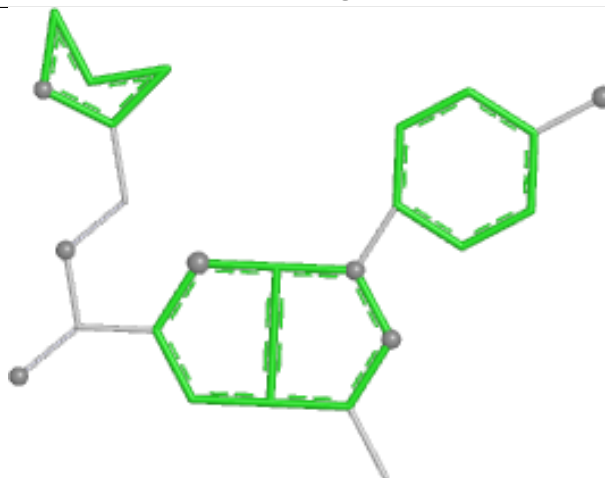
Bond lengths



Bond angles

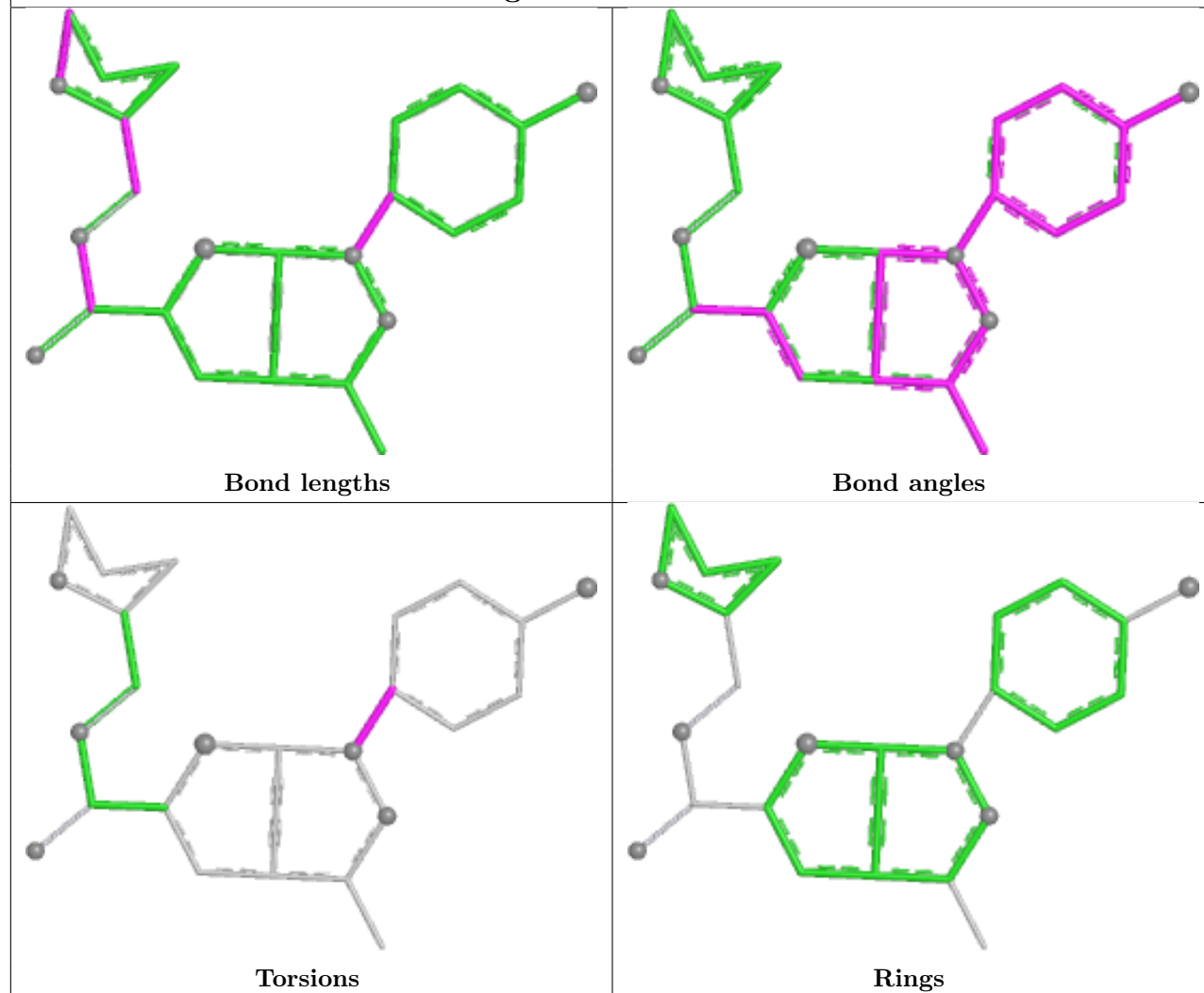


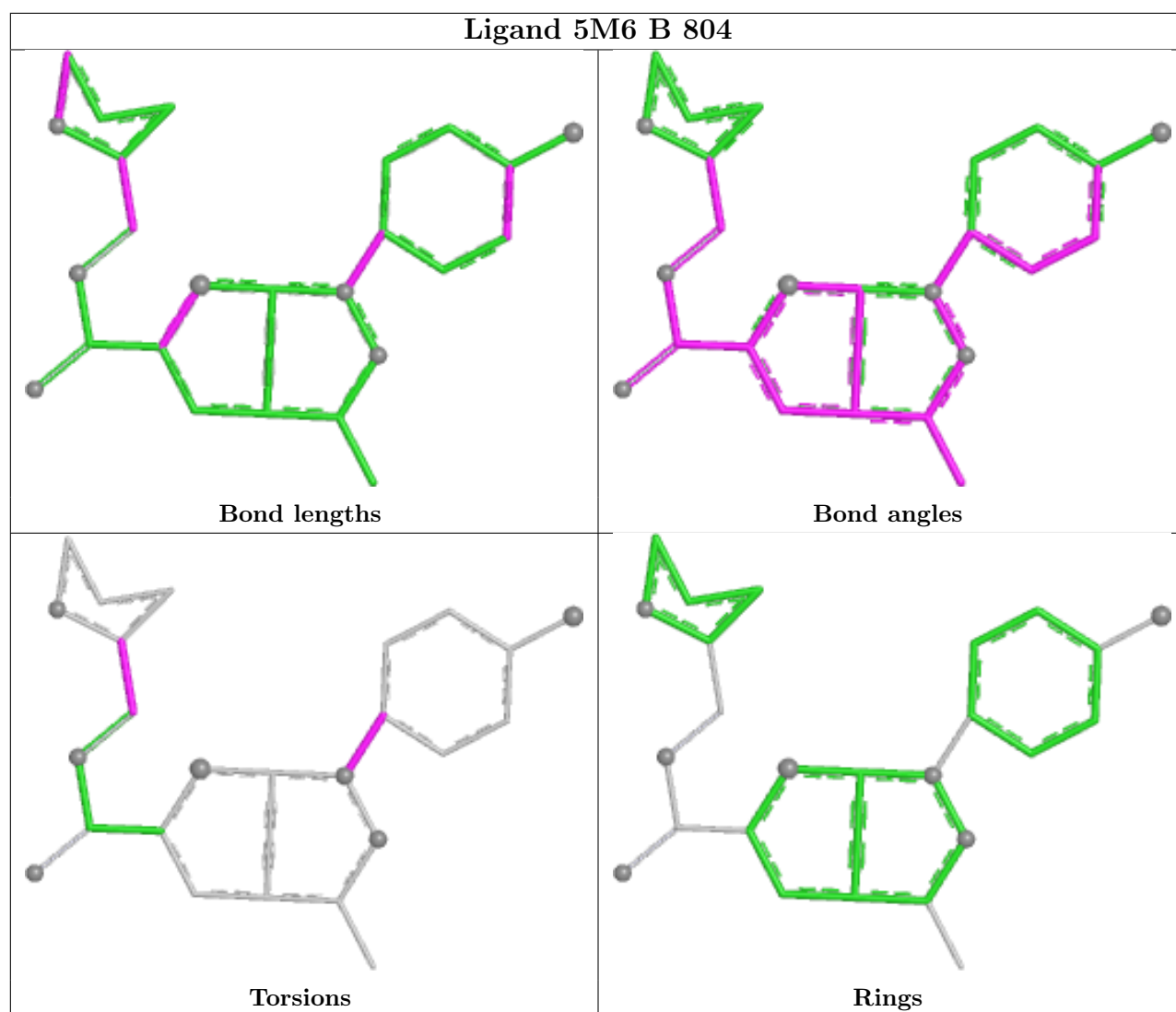
Torsions



Rings

Ligand 5M6 C 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 [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	313/316 (99%)	-0.21	1 (0%) 90 88	16, 32, 53, 80	6 (1%)
1	C	312/316 (98%)	-0.24	0 100 100	18, 32, 52, 73	7 (2%)
1	D	312/316 (98%)	0.10	4 (1%) 75 73	24, 40, 60, 80	5 (1%)
2	B	314/315 (99%)	-0.15	5 (1%) 70 67	18, 31, 53, 75	5 (1%)
All	All	1251/1263 (99%)	-0.12	10 (0%) 82 80	16, 34, 56, 80	23 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	456	ALA	4.9
1	A	459	LEU	2.9
1	D	649	TYR	2.9
2	B	458	GLY	2.9
2	B	771	ALA	2.7
1	D	459	LEU	2.4
1	D	458	GLY	2.3
2	B	457	ALA	2.2
2	B	460	MET	2.1
2	B	612	SER	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(Å ²)	Q<0.9
1	CME	A	509	10/11	0.87	0.14	38,43,65,66	0
2	CME	B	509	10/11	0.89	0.13	32,40,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CME	D	509	10/11	0.89	0.12	40,43,69,71	0
1	CME	C	509	10/11	0.91	0.12	35,38,64,67	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

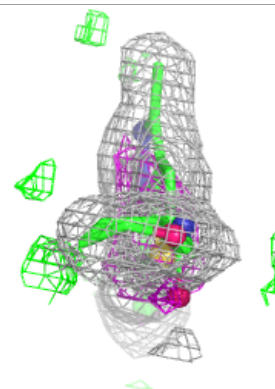
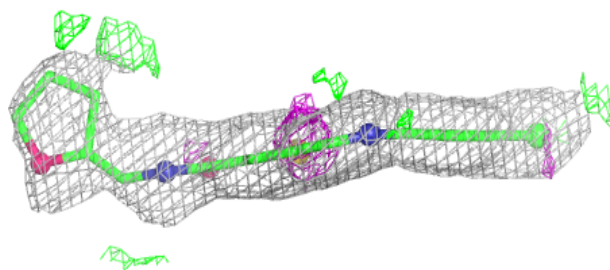
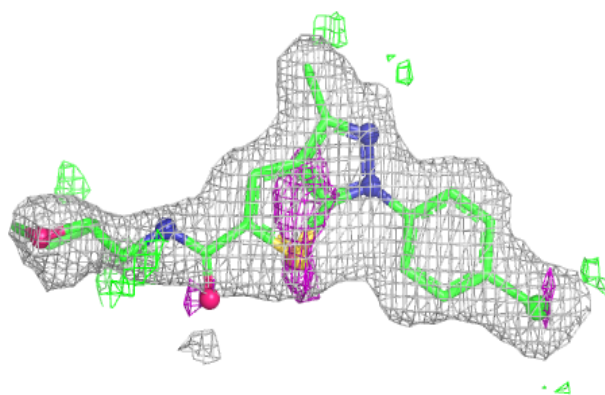
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	GOL	B	803	6/6	0.86	0.12	37,42,43,44	0
5	GOL	A	803	6/6	0.87	0.15	43,46,49,49	0
6	5M6	D	803	25/25	0.88	0.14	36,43,69,71	0
6	5M6	B	804	25/25	0.92	0.11	29,38,58,62	0
6	5M6	C	803	25/25	0.92	0.11	32,36,58,63	0
6	5M6	A	804	25/25	0.92	0.11	32,36,58,61	0
4	MG	A	802	1/1	0.99	0.01	25,25,25,25	0
4	MG	B	802	1/1	0.99	0.02	12,12,12,12	0
4	MG	D	802	1/1	0.99	0.03	31,31,31,31	0
3	ZN	A	801	1/1	1.00	0.01	28,28,28,28	0
3	ZN	B	801	1/1	1.00	0.01	24,24,24,24	0
4	MG	C	802	1/1	1.00	0.01	22,22,22,22	0
3	ZN	C	801	1/1	1.00	0.01	26,26,26,26	0
3	ZN	D	801	1/1	1.00	0.01	33,33,33,33	0

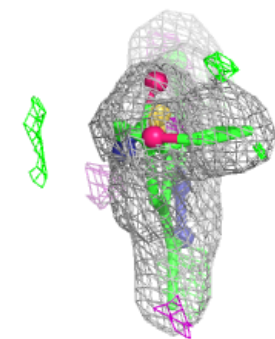
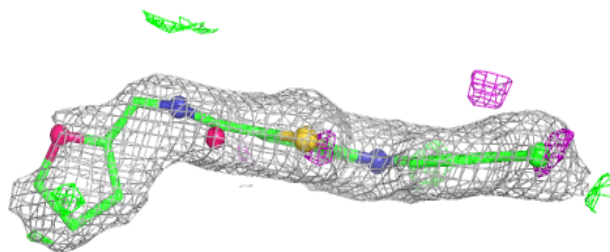
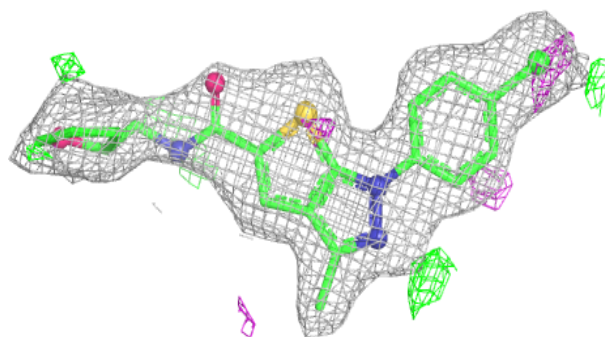
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5M6 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)

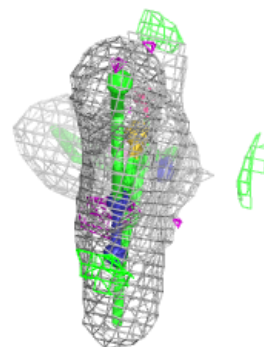
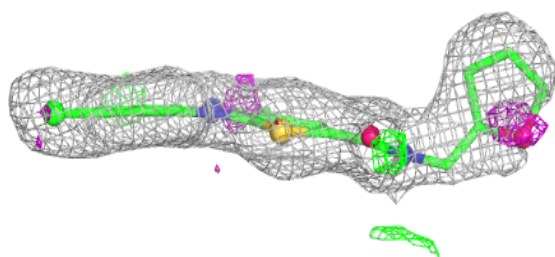
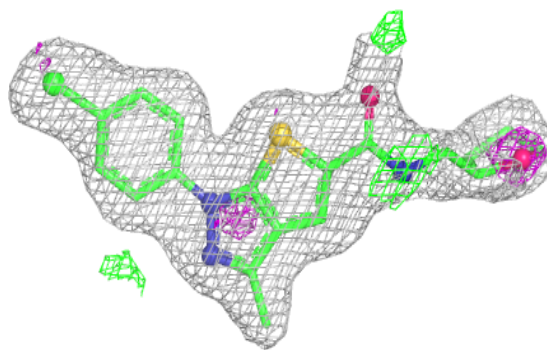
**Electron density around 5M6 B 804:**

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

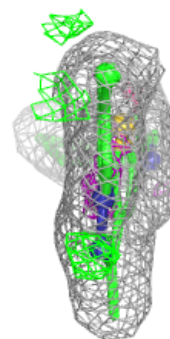
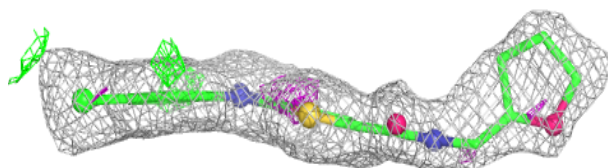
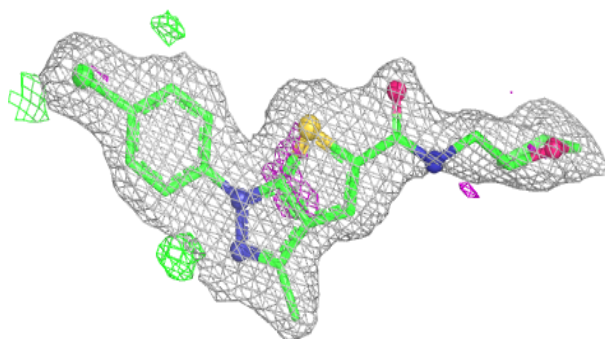


Electron density around 5M6 C 803:

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

**Electron density around 5M6 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 [i](#)

There are no such residues in this entry.