



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:22 PM UTC

PDB ID : 5TZX / pdb_00005tzz
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 2A IN
COMPLEX WITH 1-[(3-chloro-4-fluorophenyl)carbonyl]-3,3-difluoro-5-
{5-methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl}piperidine
Authors : Xu, R.; Aertgeerts, K.
Deposited on : 2016-11-22
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

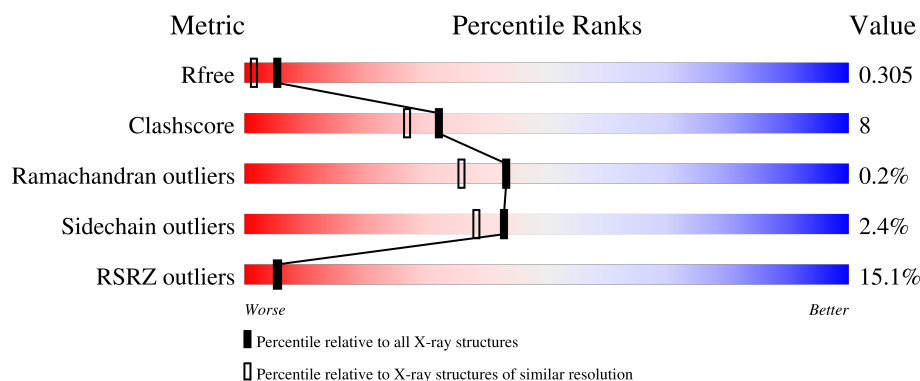
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	12% 84% 15% ..
1	B	344	13% 80% 15% ..
1	C	344	23% 73% 21% 5%
1	D	344	10% 81% 14% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11716 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.

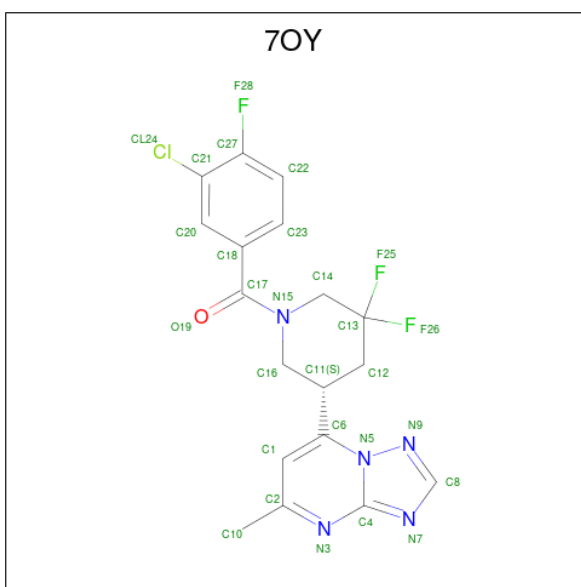
- Molecule 1 is a protein called cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2794	1778	478	512	26			
1	B	337	Total	C	N	O	S	0	0	0
			2759	1757	473	504	25			
1	C	327	Total	C	N	O	S	0	0	0
			2676	1707	460	484	25			
1	D	328	Total	C	N	O	S	0	0	0
			2684	1711	461	487	25			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	SER	-	expression tag	UNP O00408
A	577	ALA	-	expression tag	UNP O00408
A	578	MET	-	expression tag	UNP O00408
B	576	SER	-	expression tag	UNP O00408
B	577	ALA	-	expression tag	UNP O00408
B	578	MET	-	expression tag	UNP O00408
C	576	SER	-	expression tag	UNP O00408
C	577	ALA	-	expression tag	UNP O00408
C	578	MET	-	expression tag	UNP O00408
D	576	SER	-	expression tag	UNP O00408
D	577	ALA	-	expression tag	UNP O00408
D	578	MET	-	expression tag	UNP O00408

- Molecule 2 is (3-chloro-4-fluorophenyl)[(5S)-3,3-difluoro-5-(5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)piperidin-1-yl]methanone (CCD ID: 7OY) (formula: C₁₈H₁₅ClF₃N₅O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 28	C 18	Cl 1	F 3	N 5	O 1	0	0
2	B	1	Total 28	C 18	Cl 1	F 3	N 5	O 1	0	0
2	C	1	Total 28	C 18	Cl 1	F 3	N 5	O 1	0	0
2	D	1	Total 28	C 18	Cl 1	F 3	N 5	O 1	0	0

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

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

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

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

Continued on next page...

Continued from previous page...

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

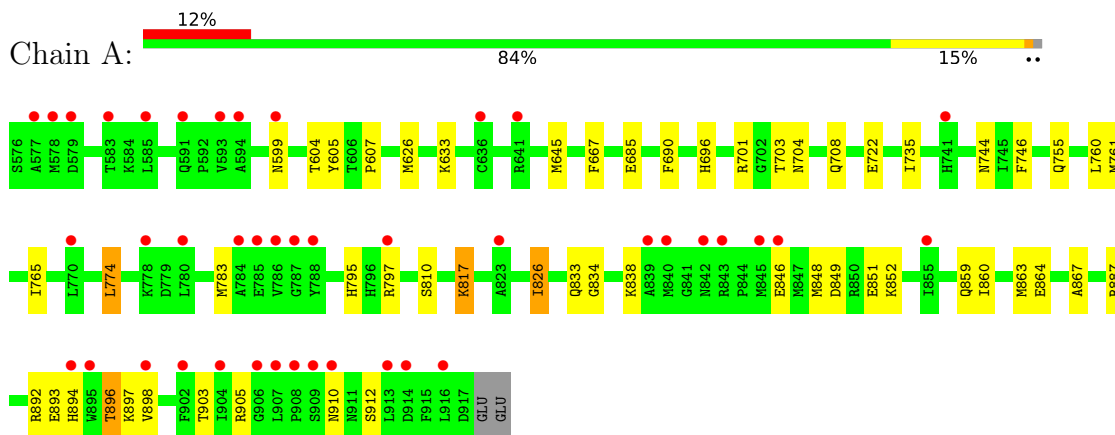
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	189	Total 189	O 189	0	0
5	B	160	Total 160	O 160	0	0
5	C	159	Total 159	O 159	0	0
5	D	175	Total 175	O 175	0	0

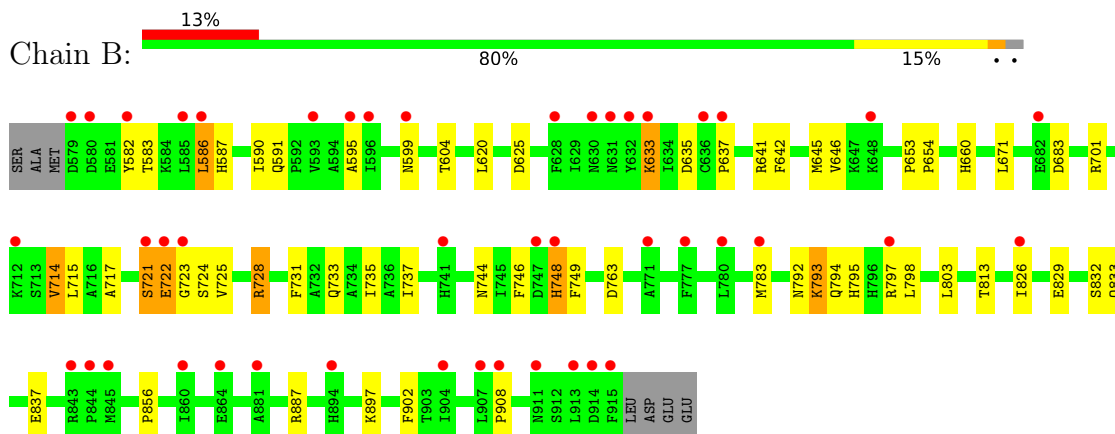
3 Residue-property plots [i](#)

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.

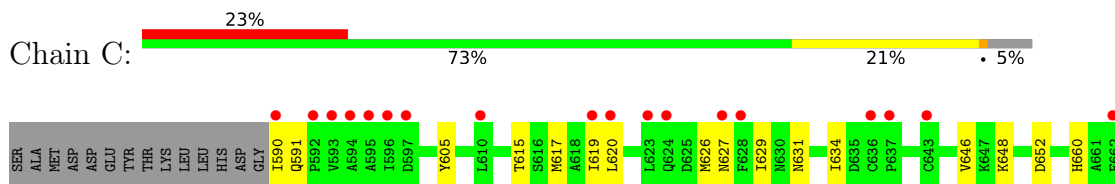
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

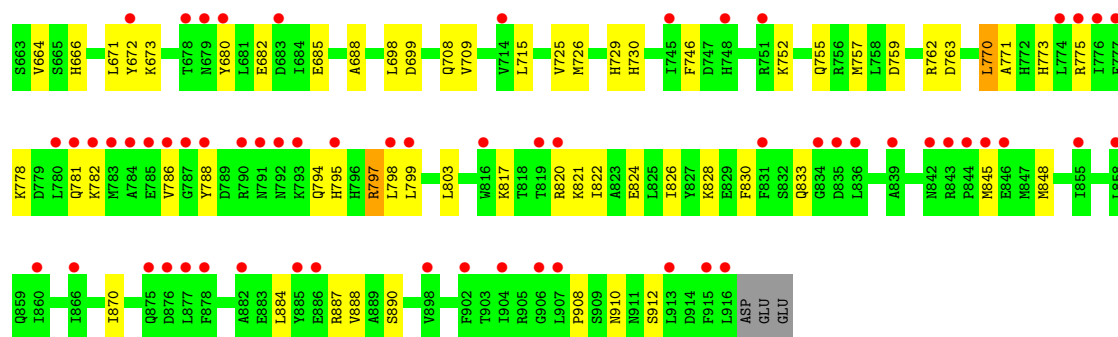


- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

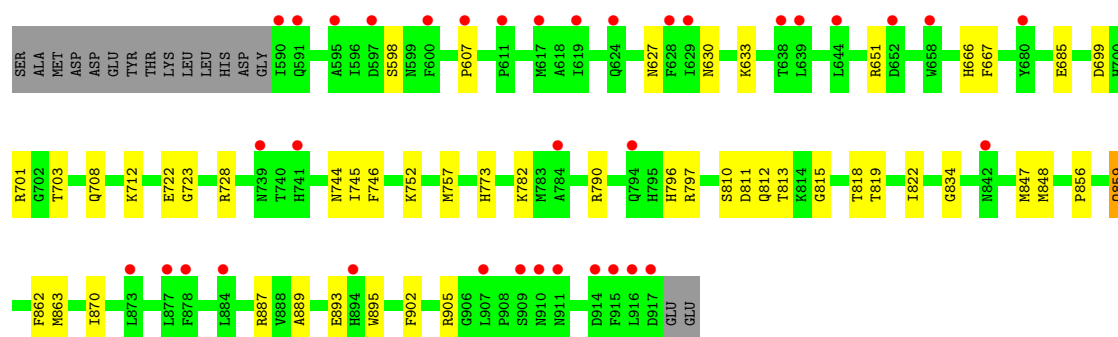
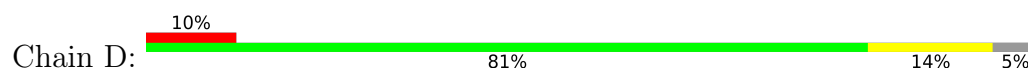


- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase





- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.67Å 72.70Å 90.36Å 109.28° 90.96° 90.97°	Depositor
Resolution (Å)	64.96 – 1.90 64.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (64.96-1.90) 97.0 (64.96-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.10.1-2155_1692: ???)	Depositor
R, R_{free}	0.247 , 0.306 0.250 , 0.305	Depositor DCC
R_{free} test set	4994 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11716	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.83% 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: MG, ZN, 7OY

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	0.35	0/2861	0.52	0/3860
1	B	0.33	0/2826	0.51	0/3813
1	C	0.30	0/2741	0.47	0/3698
1	D	0.33	0/2749	0.50	0/3709
All	All	0.33	0/11177	0.50	0/15080

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2794	0	2732	43	0
1	B	2759	0	2698	44	0
1	C	2676	0	2630	56	0
1	D	2684	0	2634	36	0
2	A	28	0	0	1	0
2	B	28	0	0	1	0
2	C	28	0	0	1	0
2	D	28	0	0	1	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	189	0	0	4	0
5	B	160	0	0	5	0
5	C	159	0	0	2	0
5	D	175	0	0	2	0
All	All	11716	0	10694	173	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 8.

All (173) 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:C:708:GLN:HG3	1:C:726:MET:HE3	1.59	0.85
1:B:783:MET:HE1	1:B:798:LEU:HB2	1.68	0.75
1:D:722:GLU:O	1:D:728:ARG:NH2	2.19	0.74
1:A:604:THR:HG22	1:A:887:ARG:HH22	1.53	0.72
1:B:582:TYR:CZ	1:B:586:LEU:HD21	2.28	0.69
1:C:759:ASP:OD1	1:C:762:ARG:NH2	2.25	0.69
1:B:637:PRO:HB2	1:B:641:ARG:NH1	2.10	0.67
1:C:680:TYR:HB3	1:C:788:TYR:CE1	2.31	0.66
1:A:744:ASN:HD22	1:A:746:PHE:H	1.43	0.66
1:D:651:ARG:HH21	1:D:701:ARG:HH12	1.43	0.66
1:C:778:LYS:HA	1:C:781:GLN:HE21	1.62	0.64
1:D:699:ASP:O	1:D:701:ARG:HD2	1.98	0.64
1:C:910:ASN:ND2	1:C:912:SER:OG	2.32	0.62
1:D:812:GLN:HG3	1:D:863:MET:HE1	1.82	0.62
1:A:760:LEU:HD23	1:A:797:ARG:HH22	1.65	0.61
1:B:637:PRO:O	1:B:641:ARG:HD3	2.01	0.61
1:B:637:PRO:HB2	1:B:641:ARG:HH11	1.64	0.60
1:C:715:LEU:CD1	1:C:726:MET:HE1	2.31	0.60
1:A:910:ASN:OD1	1:A:912:SER:HB3	2.03	0.59
1:A:863:MET:HA	1:A:867:ALA:HB3	1.85	0.59
1:D:889:ALA:O	1:D:893:GLU:HG2	2.04	0.58
1:B:733:GLN:O	1:B:737:ILE:HD13	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:680:TYR:HB3	1:C:788:TYR:HE1	1.68	0.58
1:D:744:ASN:HD22	1:D:746:PHE:H	1.51	0.58
1:C:726:MET:HA	1:C:726:MET:HE2	1.84	0.57
1:B:599:ASN:ND2	1:B:604:THR:OG1	2.38	0.57
1:C:591:GLN:H	1:C:617:MET:HE1	1.69	0.56
1:D:607:PRO:HG3	1:D:666:HIS:ND1	2.20	0.56
1:B:671:LEU:HD13	1:B:803:LEU:HD22	1.88	0.56
1:D:863:MET:HE2	1:D:863:MET:HA	1.87	0.56
1:B:783:MET:HE2	1:B:795:HIS:CD2	2.41	0.55
1:B:586:LEU:HD23	1:B:637:PRO:HA	1.89	0.55
1:D:856:PRO:HG3	1:D:902:PHE:CD1	2.42	0.55
1:C:771:ALA:O	1:C:775:ARG:HG3	2.06	0.55
1:C:778:LYS:HA	1:C:781:GLN:NE2	2.21	0.55
1:A:696:HIS:HA	1:A:765:ILE:HD12	1.89	0.54
1:C:763:ASP:OD2	1:C:797:ARG:NH1	2.39	0.54
1:C:788:TYR:CE2	1:C:795:HIS:HB3	2.43	0.54
1:B:701:ARG:CZ	1:B:715:LEU:HD11	2.38	0.54
1:C:715:LEU:HD12	1:C:726:MET:HE1	1.88	0.53
1:B:642:PHE:O	1:B:646:VAL:HG23	2.08	0.53
1:B:813:THR:O	1:B:887:ARG:HD2	2.08	0.53
1:D:797:ARG:NH2	5:D:1102:HOH:O	2.35	0.53
1:C:627:ASN:O	1:C:631:ASN:HB2	2.09	0.53
1:A:864:GLU:OE2	1:A:892:ARG:NH2	2.42	0.53
1:A:633:LYS:NZ	5:A:1103:HOH:O	2.32	0.52
1:A:703:THR:OG1	1:A:708:GLN:NE2	2.42	0.52
1:B:897:LYS:NZ	5:B:1106:HOH:O	2.43	0.52
1:C:629:ILE:HG23	1:C:634:ILE:HB	1.92	0.52
1:C:698:LEU:O	1:C:730:HIS:ND1	2.36	0.52
1:C:833:GLN:CD	1:C:848:MET:HE1	2.35	0.52
1:D:847:MET:HE1	2:D:1001:7OY:C27	2.39	0.52
1:C:746:PHE:CZ	1:C:757:MET:HE2	2.45	0.51
1:A:838:LYS:NZ	1:A:851:GLU:OE1	2.43	0.51
1:D:703:THR:OG1	1:D:708:GLN:NE2	2.43	0.51
1:B:583:THR:HA	1:B:586:LEU:HD12	1.92	0.51
1:B:731:PHE:CE1	1:B:735:ILE:HD11	2.47	0.50
1:C:591:GLN:H	1:C:617:MET:CE	2.24	0.50
1:B:591:GLN:HG2	1:B:595:ALA:HB3	1.92	0.50
1:D:723:GLY:O	1:D:728:ARG:NE	2.44	0.50
1:C:699:ASP:OD2	1:C:729:HIS:HE1	1.95	0.50
1:A:783:MET:HG3	1:A:795:HIS:CE1	2.47	0.49
1:B:590:ILE:HD13	1:B:620:LEU:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:626:MET:HE3	1:C:672:TYR:CB	2.42	0.49
5:B:1235:HOH:O	1:C:845:MET:HE3	2.12	0.49
1:C:826:ILE:HD13	2:C:1001:7OY:N5	2.27	0.48
1:B:746:PHE:HB3	1:B:749:PHE:HD2	1.77	0.48
1:D:746:PHE:CZ	1:D:757:MET:HE2	2.48	0.48
1:C:773:HIS:CE1	1:C:870:ILE:HG12	2.48	0.48
1:C:671:LEU:HD13	1:C:803:LEU:HD22	1.96	0.48
1:A:860:ILE:HD13	1:A:896:THR:HG23	1.95	0.48
1:C:794:GLN:HA	1:C:797:ARG:HG3	1.95	0.48
1:D:667:PHE:CD1	1:D:810:SER:HB2	2.49	0.48
1:D:813:THR:O	1:D:887:ARG:HD2	2.13	0.47
1:C:688:ALA:HA	1:C:757:MET:HE1	1.96	0.47
1:C:782:LYS:NZ	5:C:1104:HOH:O	2.38	0.47
1:A:797:ARG:N	1:A:797:ARG:HD2	2.30	0.47
1:B:625:ASP:O	1:C:778:LYS:HE3	2.14	0.47
1:B:723:GLY:O	1:B:725:VAL:N	2.46	0.47
1:B:744:ASN:C	1:B:744:ASN:HD22	2.23	0.47
1:C:845:MET:HG3	1:C:848:MET:HG3	1.96	0.47
1:A:599:ASN:ND2	5:A:1102:HOH:O	2.29	0.46
1:A:704:ASN:H	1:A:833:GLN:HE22	1.62	0.46
1:C:755:GLN:HE21	1:D:712:LYS:NZ	2.13	0.46
1:A:735:ILE:HG21	1:B:714:VAL:HG11	1.98	0.46
1:C:590:ILE:HD11	1:C:620:LEU:HD13	1.98	0.46
1:C:830:PHE:HA	1:C:848:MET:HE3	1.97	0.46
1:D:818:THR:O	1:D:822:ILE:HG12	2.15	0.46
1:B:645:MET:HB3	1:B:645:MET:HE3	1.72	0.46
1:A:910:ASN:ND2	1:A:910:ASN:H	2.14	0.46
1:A:910:ASN:H	1:A:910:ASN:HD22	1.63	0.46
1:B:763:ASP:OD2	1:B:797:ARG:NH2	2.49	0.46
1:C:605:TYR:HD2	1:C:666:HIS:CE1	2.33	0.46
1:A:626:MET:HE1	1:A:690:PHE:CD1	2.51	0.46
1:C:626:MET:HE3	1:C:672:TYR:CG	2.51	0.46
1:C:833:GLN:HB3	1:C:848:MET:HE1	1.99	0.45
1:D:651:ARG:NH2	1:D:701:ARG:HH12	2.10	0.45
1:A:849:ASP:OD2	1:A:852:LYS:HE2	2.17	0.45
1:A:893:GLU:O	1:A:897:LYS:HG3	2.17	0.45
1:D:722:GLU:HG3	5:D:1267:HOH:O	2.16	0.45
1:A:744:ASN:HD22	1:A:744:ASN:C	2.25	0.45
1:C:848:MET:HE2	1:C:848:MET:HB3	1.76	0.45
1:B:637:PRO:C	1:B:641:ARG:HH11	2.24	0.45
1:B:793:LYS:HD2	1:B:793:LYS:HA	1.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:LEU:CD2	1:A:797:ARG:HH22	2.30	0.44
1:B:856:PRO:HG3	1:B:902:PHE:CD1	2.52	0.44
1:B:654:PRO:HG3	5:B:1234:HOH:O	2.16	0.44
1:D:627:ASN:HD21	1:D:630:ASN:HB2	1.81	0.44
1:A:722:GLU:OE1	1:B:721:SER:HB2	2.18	0.44
1:A:817:LYS:N	1:A:817:LYS:HD3	2.32	0.44
1:C:660:HIS:HB3	5:C:1111:HOH:O	2.17	0.44
1:C:821:LYS:O	1:C:824:GLU:HB3	2.18	0.44
1:A:834:GLY:HA3	1:A:848:MET:O	2.17	0.44
1:B:660:HIS:HB3	5:B:1105:HOH:O	2.17	0.44
1:C:725:VAL:HG12	1:C:726:MET:CE	2.48	0.44
1:C:908:PRO:HB2	1:C:910:ASN:OD1	2.17	0.44
1:B:587:HIS:CD2	1:C:709:VAL:HG21	2.52	0.43
1:D:815:GLY:O	1:D:819:THR:HG23	2.17	0.43
1:A:701:ARG:N	1:A:701:ARG:HD2	2.34	0.43
1:B:633:LYS:HG3	1:B:748:HIS:HB2	2.00	0.43
1:D:745:ILE:HG13	1:D:746:PHE:CD2	2.53	0.43
1:A:604:THR:HG22	1:A:887:ARG:NH2	2.27	0.43
1:A:903:THR:HG21	1:A:905:ARG:HH21	1.82	0.43
1:C:682:GLU:HB2	1:C:685:GLU:HG3	2.01	0.43
1:D:745:ILE:HG13	1:D:746:PHE:CE2	2.54	0.43
1:A:760:LEU:HD23	1:A:797:ARG:NH2	2.32	0.43
1:A:774:LEU:HD13	1:A:774:LEU:HA	1.81	0.43
1:B:826:ILE:HD13	2:B:1001:7OY:N5	2.34	0.43
1:C:715:LEU:HD13	1:C:726:MET:HE1	2.00	0.43
1:A:704:ASN:ND2	5:A:1126:HOH:O	2.51	0.42
1:A:826:ILE:HD13	2:A:1001:7OY:C4	2.49	0.42
1:D:633:LYS:N	1:D:633:LYS:HD2	2.33	0.42
1:A:685:GLU:HA	1:A:760:LEU:HD13	2.01	0.42
1:D:862:PHE:HD2	1:D:863:MET:HE3	1.84	0.42
1:A:852:LYS:HE3	1:A:852:LYS:HB2	1.80	0.42
1:B:653:PRO:HB2	1:B:829:GLU:OE1	2.18	0.42
1:D:859:GLN:HG3	1:D:895:TRP:CZ2	2.55	0.42
1:A:859:GLN:O	1:A:863:MET:HG2	2.20	0.42
1:C:615:THR:O	1:C:619:ILE:HG12	2.20	0.42
1:C:646:VAL:HG13	1:C:698:LEU:HD21	2.01	0.42
1:D:752:LYS:HB3	1:D:752:LYS:HE3	1.92	0.42
1:A:761:MET:O	1:A:765:ILE:HG12	2.19	0.42
1:D:627:ASN:ND2	1:D:630:ASN:HB2	2.35	0.42
1:D:811:ASP:HB3	1:D:822:ILE:HG13	2.02	0.42
1:A:667:PHE:CD1	1:A:810:SER:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:770:LEU:HD12	1:C:770:LEU:HA	1.85	0.42
1:C:817:LYS:HG3	1:C:820:ARG:HH21	1.85	0.42
1:D:887:ARG:HE	1:D:887:ARG:HB2	1.63	0.42
1:B:722:GLU:OE2	1:B:728:ARG:NH1	2.52	0.42
1:B:833:GLN:NE2	1:B:837:GLU:OE1	2.38	0.41
1:C:673:LYS:HE3	1:C:673:LYS:HB3	1.88	0.41
1:D:627:ASN:HD21	1:D:630:ASN:HD22	1.67	0.41
1:D:773:HIS:CE1	1:D:870:ILE:HG12	2.55	0.41
1:B:717:ALA:N	5:B:1110:HOH:O	2.53	0.41
1:C:833:GLN:HB3	1:C:848:MET:CE	2.49	0.41
1:D:834:GLY:HA3	1:D:848:MET:O	2.20	0.41
1:C:660:HIS:O	1:C:664:VAL:HG23	2.21	0.41
1:C:884:LEU:O	1:C:888:VAL:HG23	2.20	0.41
1:A:846:GLU:HA	1:A:852:LYS:HE3	2.02	0.41
1:B:582:TYR:CE2	1:B:586:LEU:HD11	2.55	0.41
1:A:645:MET:HB3	1:A:645:MET:HE3	1.85	0.41
1:A:894:HIS:O	1:A:898:VAL:HG22	2.20	0.41
1:B:783:MET:CE	1:B:795:HIS:HA	2.51	0.41
1:D:685:GLU:OE2	1:D:796:HIS:ND1	2.41	0.41
1:B:587:HIS:NE2	1:C:709:VAL:HG21	2.36	0.41
1:B:792:ASN:OD1	1:B:794:GLN:NE2	2.54	0.41
1:D:744:ASN:HD22	1:D:744:ASN:C	2.29	0.40
1:C:824:GLU:HG2	1:C:828:LYS:HE3	2.03	0.40
1:A:605:TYR:CE2	1:A:607:PRO:HA	2.56	0.40
1:A:755:GLN:NE2	5:A:1110:HOH:O	2.39	0.40
1:B:635:ASP:OD2	1:B:637:PRO:HG2	2.21	0.40
1:B:897:LYS:HD2	1:B:897:LYS:HA	1.89	0.40
1:C:788:TYR:CE1	1:C:799:LEU:HD22	2.56	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	340/344 (99%)	334 (98%)	6 (2%)	0	100	100
1	B	335/344 (97%)	326 (97%)	7 (2%)	2 (1%)	21	13
1	C	325/344 (94%)	320 (98%)	5 (2%)	0	100	100
1	D	326/344 (95%)	320 (98%)	6 (2%)	0	100	100
All	All	1326/1376 (96%)	1300 (98%)	24 (2%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	724	SER
1	B	908	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	308/310 (99%)	304 (99%)	4 (1%)	61	61
1	B	304/310 (98%)	294 (97%)	10 (3%)	33	26
1	C	295/310 (95%)	285 (97%)	10 (3%)	32	25
1	D	296/310 (96%)	291 (98%)	5 (2%)	53	52
All	All	1203/1240 (97%)	1174 (98%)	29 (2%)	43	38

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	774	LEU
1	A	817	LYS
1	A	826	ILE
1	A	896	THR
1	B	586	LEU
1	B	633	LYS
1	B	683	ASP
1	B	714	VAL
1	B	721	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	722	GLU
1	B	728	ARG
1	B	748	HIS
1	B	793	LYS
1	B	832	SER
1	C	648	LYS
1	C	652	ASP
1	C	752	LYS
1	C	770	LEU
1	C	786	VAL
1	C	797	ARG
1	C	798	LEU
1	C	822	ILE
1	C	887	ARG
1	C	890	SER
1	D	598	SER
1	D	782	LYS
1	D	790	ARG
1	D	859	GLN
1	D	905	ARG

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	631	ASN
1	A	679	ASN
1	A	708	GLN
1	A	744	ASN
1	A	755	GLN
1	A	772	HIS
1	A	812	GLN
1	A	833	GLN
1	A	865	HIS
1	A	910	ASN
1	B	599	ASN
1	B	624	GLN
1	B	627	ASN
1	B	744	ASN
1	B	772	HIS
1	B	791	ASN
1	B	794	GLN
1	B	812	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	591	GLN
1	C	599	ASN
1	C	627	ASN
1	C	630	ASN
1	C	733	GLN
1	C	755	GLN
1	C	894	HIS
1	C	910	ASN
1	D	624	GLN
1	D	627	ASN
1	D	708	GLN
1	D	744	ASN
1	D	791	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	7OY	C	1001	-	29,31,31	1.34	5 (17%)	40,47,47	1.53	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7OY	A	1001	-	29,31,31	1.12	3 (10%)	40,47,47	1.68	11 (27%)
2	7OY	D	1001	-	29,31,31	1.29	4 (13%)	40,47,47	1.84	11 (27%)
2	7OY	B	1001	-	29,31,31	1.30	5 (17%)	40,47,47	1.45	6 (15%)

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
2	7OY	C	1001	-	-	0/12/26/26	0/4/4/4
2	7OY	A	1001	-	-	0/12/26/26	0/4/4/4
2	7OY	D	1001	-	-	0/12/26/26	0/4/4/4
2	7OY	B	1001	-	-	0/12/26/26	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	7OY	C1-C2	3.17	1.48	1.41
2	D	1001	7OY	C1-C2	3.03	1.47	1.41
2	A	1001	7OY	C1-C2	3.01	1.47	1.41
2	B	1001	7OY	C2-N3	-2.97	1.29	1.33
2	B	1001	7OY	C1-C2	2.87	1.47	1.41
2	D	1001	7OY	C2-N3	-2.72	1.29	1.33
2	C	1001	7OY	C2-N3	-2.67	1.29	1.33
2	B	1001	7OY	C14-N15	-2.61	1.43	1.46
2	C	1001	7OY	C14-N15	-2.56	1.43	1.46
2	D	1001	7OY	C18-C17	-2.46	1.45	1.50
2	A	1001	7OY	C2-N3	-2.42	1.30	1.33
2	C	1001	7OY	C18-C17	-2.35	1.46	1.50
2	B	1001	7OY	N5-N9	-2.30	1.34	1.37
2	B	1001	7OY	C18-C17	-2.24	1.46	1.50
2	D	1001	7OY	N5-N9	-2.22	1.34	1.37
2	C	1001	7OY	N5-N9	-2.20	1.34	1.37
2	A	1001	7OY	C18-C17	-2.01	1.46	1.50

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	7OY	C12-C13-C14	-4.57	109.95	114.30
2	A	1001	7OY	C18-C20-C21	-3.67	117.06	120.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	7OY	C18-C20-C21	-3.67	117.06	120.26
2	B	1001	7OY	C18-C20-C21	-3.64	117.08	120.26
2	A	1001	7OY	C23-C18-C20	3.36	123.13	119.25
2	D	1001	7OY	C18-C20-C21	-3.32	117.36	120.26
2	D	1001	7OY	C23-C18-C20	3.22	122.97	119.25
2	C	1001	7OY	C23-C18-C20	3.16	122.91	119.25
2	A	1001	7OY	C12-C13-C14	-3.01	111.43	114.30
2	C	1001	7OY	C12-C13-C14	-3.01	111.43	114.30
2	D	1001	7OY	C10-C2-C1	-2.97	116.55	120.44
2	C	1001	7OY	C10-C2-C1	-2.93	116.61	120.44
2	B	1001	7OY	C23-C18-C20	2.93	122.64	119.25
2	A	1001	7OY	C20-C21-CL24	2.89	123.19	118.45
2	D	1001	7OY	O19-C17-C18	-2.86	114.62	120.29
2	A	1001	7OY	C8-N9-N5	2.79	103.14	100.86
2	D	1001	7OY	C20-C21-CL24	2.66	122.81	118.45
2	D	1001	7OY	N5-C4-N3	-2.62	120.33	122.61
2	B	1001	7OY	C14-N15-C17	-2.57	115.25	121.44
2	D	1001	7OY	C1-C2-N3	2.56	125.23	122.71
2	A	1001	7OY	C27-C21-CL24	-2.53	116.59	119.79
2	A	1001	7OY	C10-C2-C1	-2.50	117.18	120.44
2	D	1001	7OY	C8-N9-N5	2.44	102.85	100.86
2	A	1001	7OY	C16-N15-C14	2.41	119.38	114.42
2	D	1001	7OY	C27-C21-CL24	-2.39	116.78	119.79
2	B	1001	7OY	O19-C17-C18	-2.29	115.75	120.29
2	A	1001	7OY	C14-N15-C17	-2.24	116.06	121.44
2	C	1001	7OY	C8-N7-C4	2.23	103.85	102.36
2	B	1001	7OY	C23-C18-C17	-2.18	114.68	120.28
2	B	1001	7OY	N5-C4-N3	-2.13	120.76	122.61
2	A	1001	7OY	C23-C18-C17	-2.06	115.00	120.28
2	A	1001	7OY	C22-C23-C18	-2.05	118.61	120.80
2	C	1001	7OY	F25-C13-C14	2.02	113.49	106.49
2	D	1001	7OY	C22-C23-C18	-2.01	118.66	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

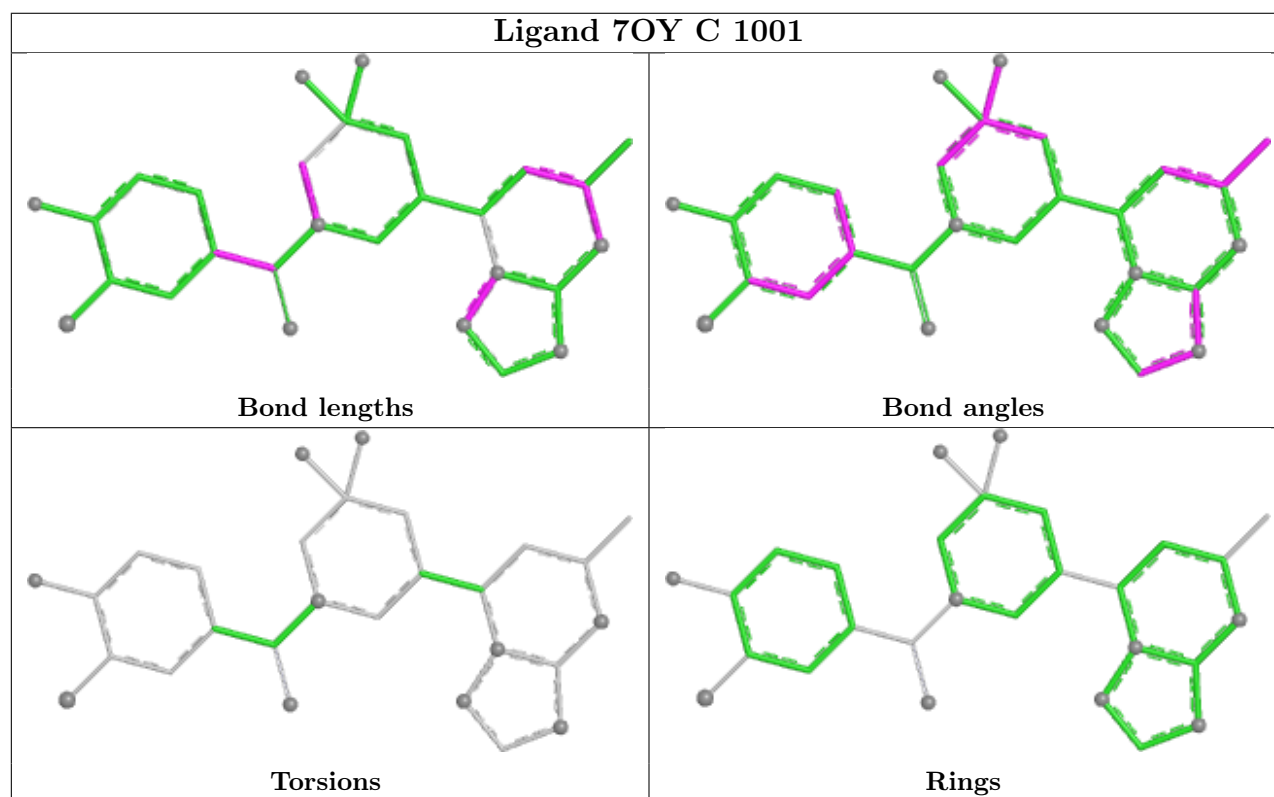
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	7OY	1	0
2	A	1001	7OY	1	0

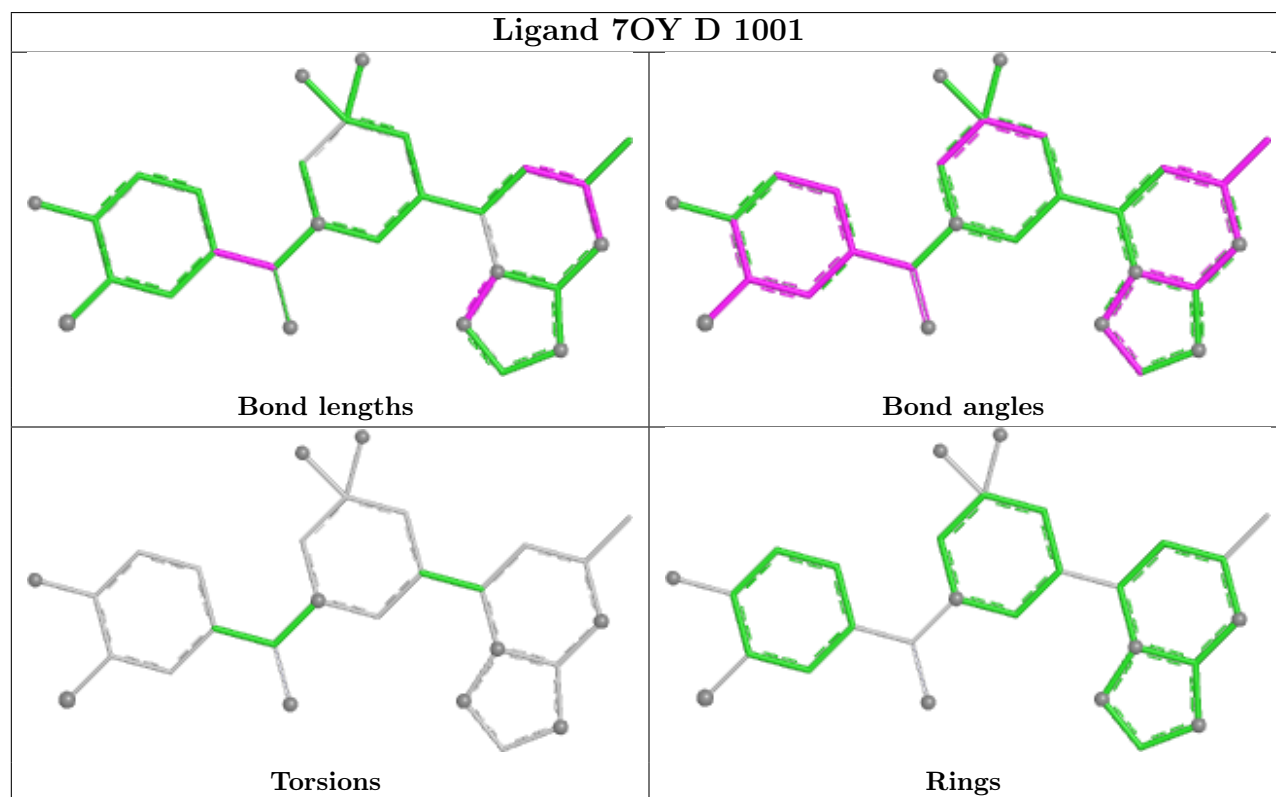
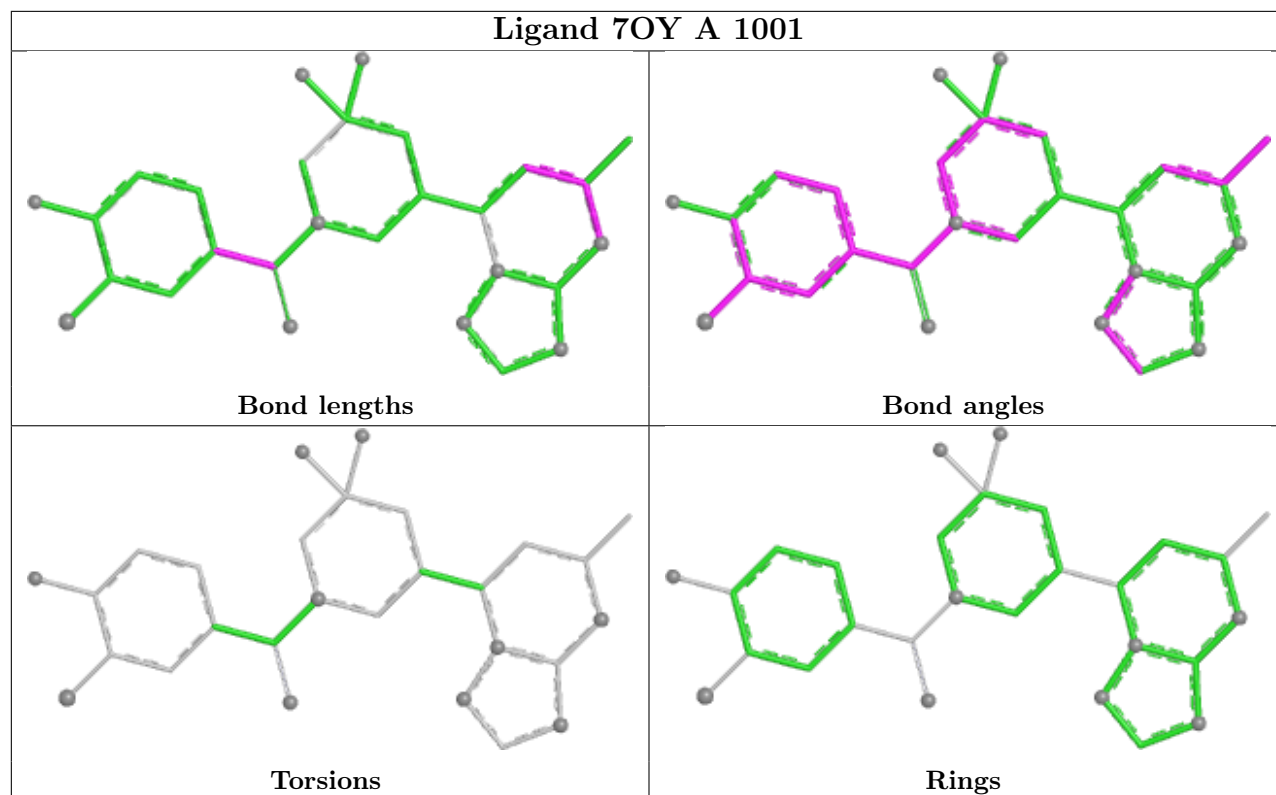
Continued on next page...

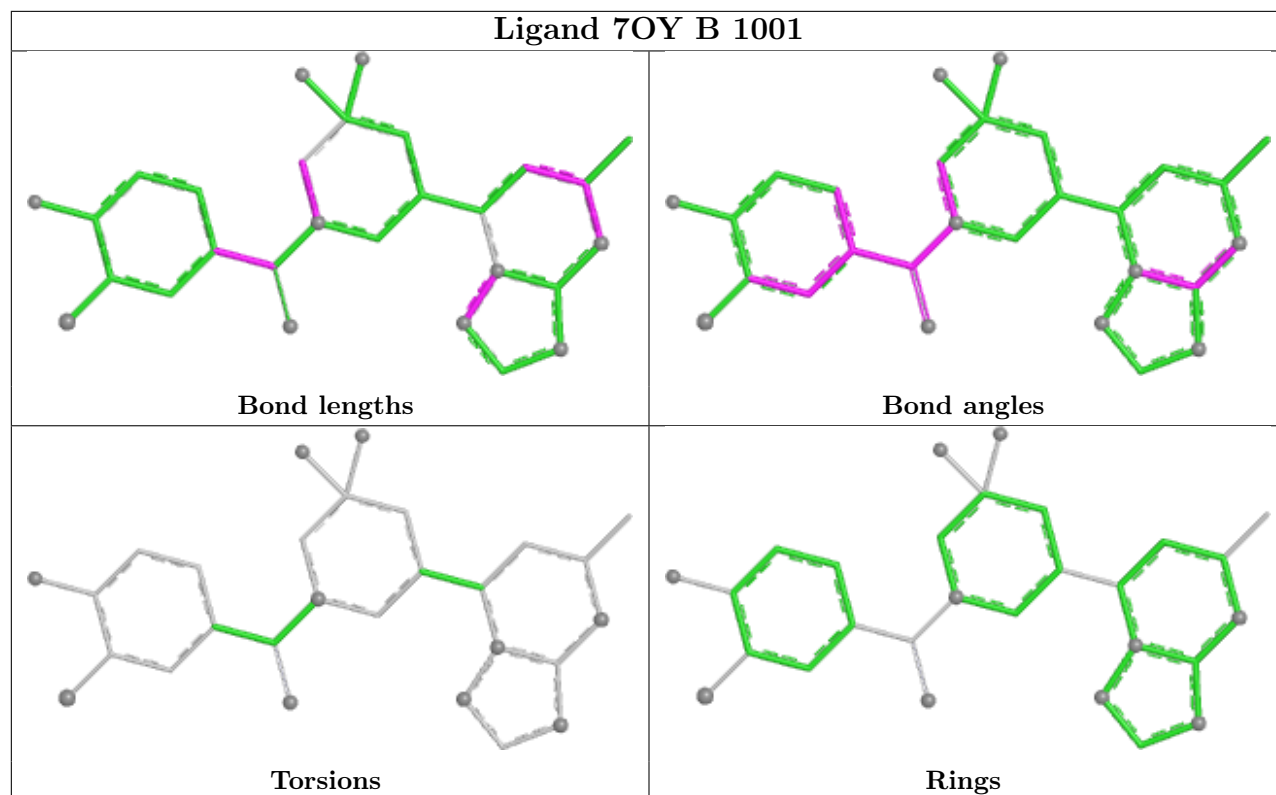
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	7OY	1	0
2	B	1001	7OY	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

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	342/344 (99%)	1.07	42 (12%) 8 9	9, 19, 35, 47	0
1	B	337/344 (97%)	1.19	45 (13%) 7 7	10, 20, 34, 46	0
1	C	327/344 (95%)	1.40	79 (24%) 2 1	11, 26, 43, 53	0
1	D	328/344 (95%)	1.10	36 (10%) 10 11	11, 20, 36, 49	0
All	All	1334/1376 (96%)	1.19	202 (15%) 5 5	9, 21, 39, 53	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	636	CYS	6.2
1	C	784	ALA	5.8
1	C	590	ILE	5.7
1	C	786	VAL	5.4
1	A	636	CYS	4.8
1	B	915	PHE	4.3
1	A	577	ALA	4.2
1	C	680	TYR	4.2
1	C	595	ALA	4.2
1	C	594	ALA	4.1
1	B	723	GLY	3.8
1	A	578	MET	3.8
1	C	785	GLU	3.8
1	D	909	SER	3.8
1	C	845	MET	3.7
1	B	586	LEU	3.6
1	C	620	LEU	3.6
1	C	683	ASP	3.5
1	D	628	PHE	3.4
1	D	617	MET	3.4
1	A	785	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	894	HIS	3.3
1	D	590	ILE	3.3
1	A	787	GLY	3.3
1	B	747	ASP	3.2
1	B	894	HIS	3.2
1	A	839	ALA	3.2
1	B	593	VAL	3.2
1	B	579	ASP	3.2
1	A	842	ASN	3.1
1	C	793	LYS	3.1
1	C	672	TYR	3.1
1	C	907	LEU	3.1
1	C	787	GLY	3.1
1	B	907	LEU	3.1
1	D	629	ILE	3.0
1	C	628	PHE	3.0
1	C	678	THR	3.0
1	B	904	ILE	3.0
1	C	627	ASN	3.0
1	C	916	LEU	3.0
1	C	788	TYR	3.0
1	C	839	ALA	3.0
1	B	722	GLU	3.0
1	C	842	ASN	3.0
1	C	898	VAL	2.9
1	D	680	TYR	2.9
1	C	783	MET	2.9
1	D	842	ASN	2.9
1	A	907	LEU	2.9
1	D	914	ASP	2.9
1	D	652	ASP	2.9
1	B	630	ASN	2.8
1	B	741	HIS	2.8
1	C	902	PHE	2.8
1	D	595	ALA	2.8
1	B	777	PHE	2.8
1	A	894	HIS	2.8
1	C	593	VAL	2.8
1	B	631	ASN	2.8
1	D	658	TRP	2.8
1	D	784	ALA	2.7
1	C	877	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	712	LYS	2.7
1	C	834	GLY	2.7
1	C	831	PHE	2.7
1	C	843	ARG	2.7
1	B	648	LYS	2.7
1	C	636	CYS	2.7
1	C	624	GLN	2.7
1	A	913	LEU	2.6
1	A	916	LEU	2.6
1	A	906	GLY	2.6
1	C	791	ASN	2.6
1	C	592	PRO	2.6
1	B	596	ILE	2.6
1	B	637	PRO	2.6
1	D	915	PHE	2.6
1	D	644	LEU	2.6
1	C	776	ILE	2.6
1	D	619	ILE	2.6
1	C	795	HIS	2.5
1	B	844	PRO	2.5
1	A	902	PHE	2.5
1	C	875	GLN	2.5
1	A	855	ILE	2.5
1	C	855	ILE	2.5
1	B	913	LEU	2.5
1	C	836	LEU	2.5
1	C	860	ILE	2.5
1	B	797	ARG	2.5
1	B	783	MET	2.5
1	A	843	ARG	2.5
1	D	741	HIS	2.5
1	B	864	GLU	2.5
1	D	794	GLN	2.5
1	A	784	ALA	2.5
1	B	582	TYR	2.4
1	D	624	GLN	2.4
1	B	721	SER	2.4
1	C	619	ILE	2.4
1	B	881	ALA	2.4
1	C	782	LYS	2.4
1	A	585	LEU	2.4
1	C	885	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	884	LEU	2.4
1	B	826	ILE	2.4
1	C	835	ASP	2.4
1	C	844	PRO	2.4
1	B	682	GLU	2.4
1	C	679	ASN	2.4
1	B	748	HIS	2.4
1	C	798	LEU	2.4
1	C	858	LEU	2.4
1	B	632	TYR	2.4
1	A	583	THR	2.4
1	C	816	TRP	2.4
1	A	770	LEU	2.3
1	A	797	ARG	2.3
1	B	585	LEU	2.3
1	C	820	ARG	2.3
1	C	777	PHE	2.3
1	B	599	ASN	2.3
1	C	790	ARG	2.3
1	A	594	ALA	2.3
1	C	913	LEU	2.3
1	D	739	ASN	2.3
1	B	628	PHE	2.3
1	A	904	ILE	2.3
1	B	860	ILE	2.3
1	D	597	ASP	2.3
1	C	748	HIS	2.3
1	D	910	ASN	2.3
1	A	778	LYS	2.3
1	A	780	LEU	2.3
1	B	780	LEU	2.3
1	B	771	ALA	2.2
1	D	611	PRO	2.2
1	D	878	PHE	2.2
1	A	909	SER	2.2
1	C	596	ILE	2.2
1	C	745	ILE	2.2
1	C	876	ASP	2.2
1	D	917	ASP	2.2
1	A	908	PRO	2.2
1	B	914	ASP	2.2
1	A	895	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	866	ILE	2.2
1	A	593	VAL	2.2
1	C	714	VAL	2.2
1	C	610	LEU	2.2
1	C	774	LEU	2.2
1	C	780	LEU	2.2
1	D	916	LEU	2.2
1	A	579	ASP	2.2
1	A	788	TYR	2.2
1	C	915	PHE	2.2
1	D	911	ASN	2.2
1	A	591	GLN	2.2
1	C	623	LEU	2.2
1	D	907	LEU	2.2
1	A	823	ALA	2.2
1	C	751	ARG	2.2
1	B	911	ASN	2.1
1	C	878	PHE	2.1
1	C	886	GLU	2.1
1	C	904	ILE	2.1
1	B	843	ARG	2.1
1	A	840	MET	2.1
1	A	845	MET	2.1
1	A	599	ASN	2.1
1	D	591	GLN	2.1
1	B	580	ASP	2.1
1	C	819	THR	2.1
1	A	641	ARG	2.1
1	C	906	GLY	2.1
1	A	846	GLU	2.1
1	C	846	GLU	2.1
1	A	741	HIS	2.1
1	C	643	CYS	2.1
1	C	792	ASN	2.1
1	D	600	PHE	2.1
1	C	597	ASP	2.1
1	D	638	THR	2.1
1	A	786	VAL	2.1
1	C	799	LEU	2.1
1	D	639	LEU	2.1
1	D	877	LEU	2.1
1	B	595	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	882	ALA	2.1
1	A	914	ASP	2.1
1	C	637	PRO	2.0
1	D	607	PRO	2.0
1	D	873	LEU	2.0
1	C	775	ARG	2.0
1	B	633	LYS	2.0
1	B	845	MET	2.0
1	C	662	PHE	2.0
1	C	781	GLN	2.0
1	A	910	ASN	2.0
1	B	908	PRO	2.0
1	A	898	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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.

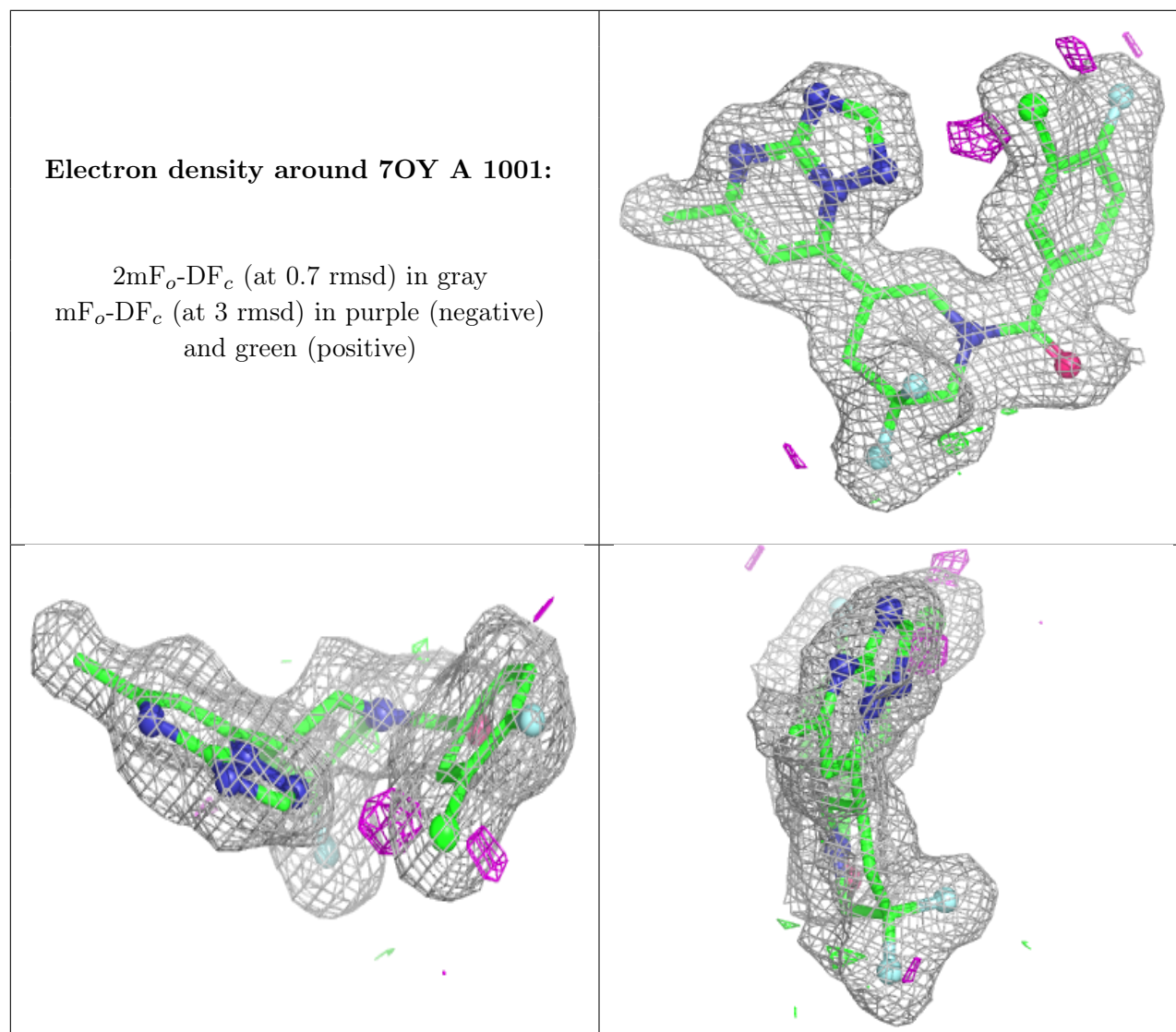
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	B	1003	1/1	0.89	0.07	5,5,5,5	0
4	MG	C	1003	1/1	0.90	0.04	4,4,4,4	0
2	7OY	A	1001	28/28	0.91	0.08	4,15,23,25	0
2	7OY	D	1001	28/28	0.92	0.08	5,14,19,21	0
2	7OY	B	1001	28/28	0.92	0.09	4,15,22,28	0
2	7OY	C	1001	28/28	0.92	0.08	6,18,24,30	0
4	MG	D	1003	1/1	0.93	0.05	4,4,4,4	0
4	MG	A	1003	1/1	0.94	0.06	3,3,3,3	0
3	ZN	B	1002	1/1	0.99	0.04	11,11,11,11	0
3	ZN	C	1002	1/1	0.99	0.02	12,12,12,12	0

Continued on next page...

Continued from previous page...

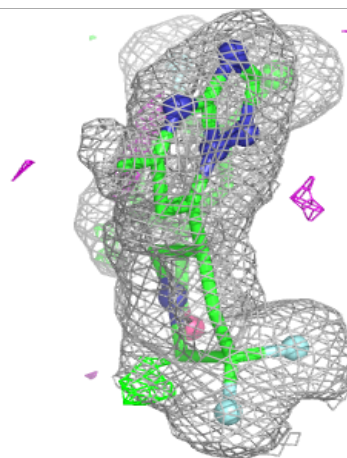
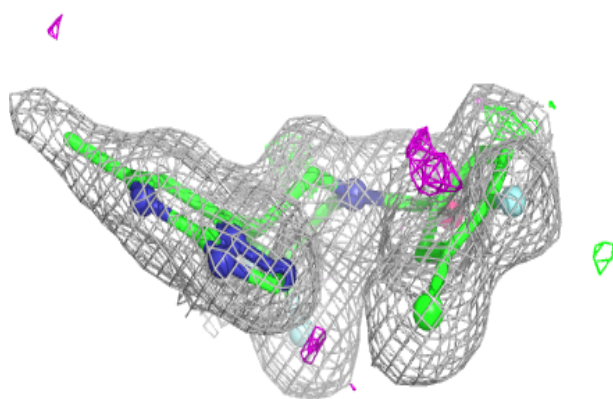
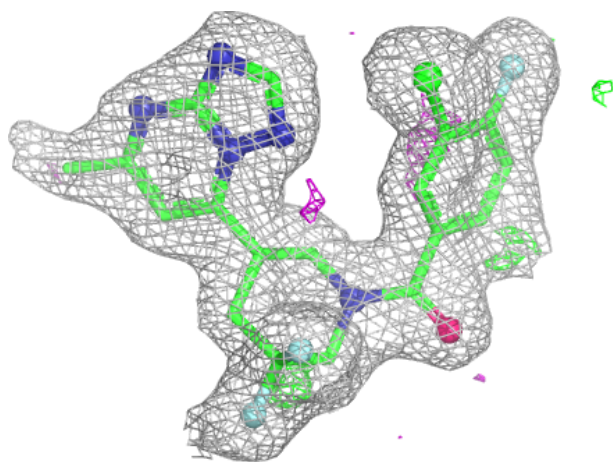
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1002	1/1	0.99	0.05	11,11,11,11	0
3	ZN	D	1002	1/1	1.00	0.03	12,12,12,12	0

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.



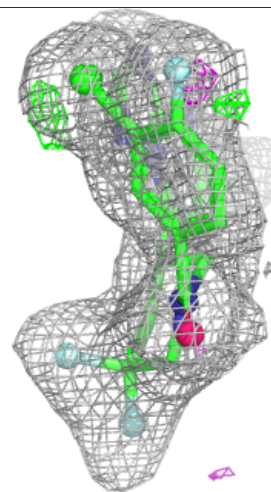
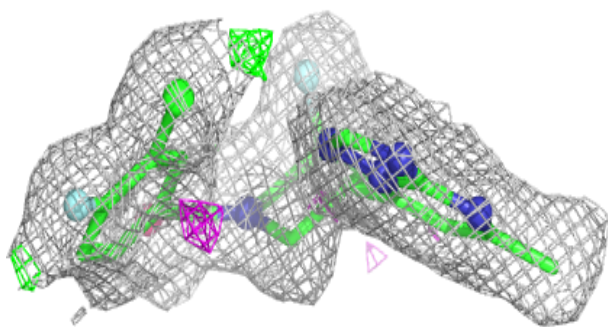
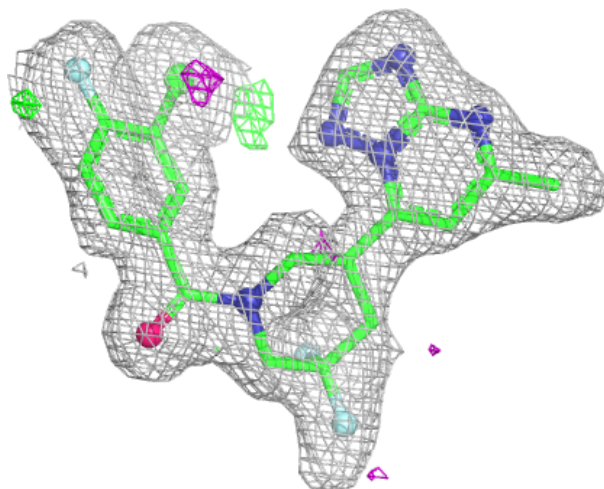
Electron density around 7OY D 1001:

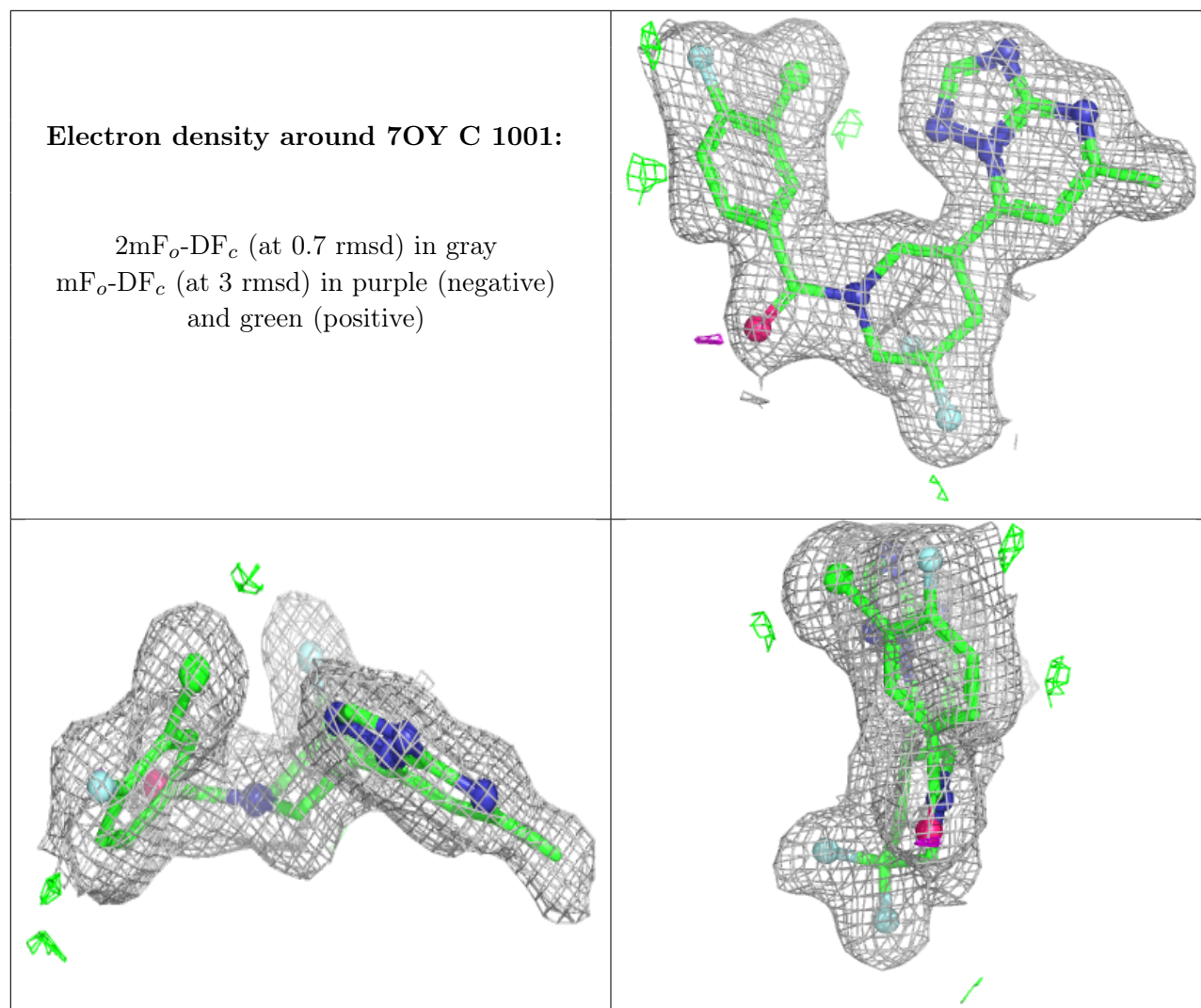
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7OY B 1001:

$2mF_o-DF_c$ (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.