



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:48 AM UTC

PDB ID : 8V8J / pdb_00008v8j
Title : PI3Ka H1047R co-crystal structure with inhibitors in two cryptic pockets (compounds 4 and 5).
Authors : Gunn, R.J.; Lawson, J.D.
Deposited on : 2023-12-05
Resolution : 3.35 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

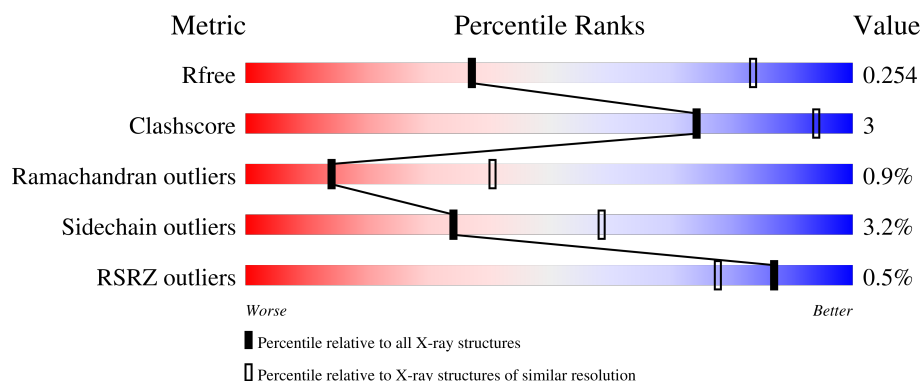
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	1072	
1	C	1072	
2	B	279	
2	D	279	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20898 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0	0
			8332	5336	1423	1504	69			
1	C	1013	Total	C	N	O	S	0	0	0
			8296	5310	1418	1499	69			

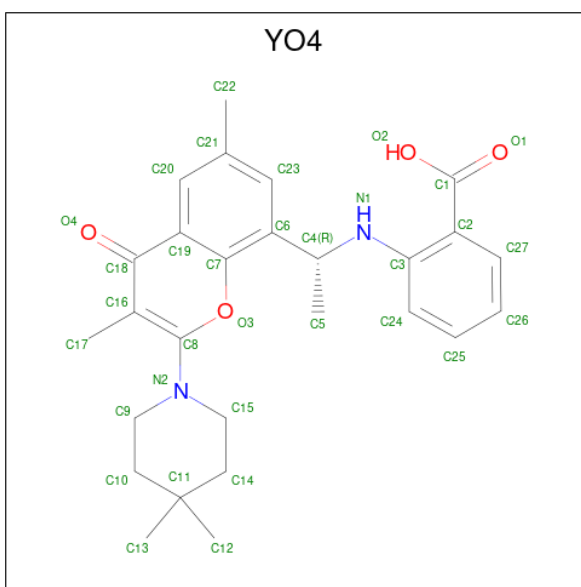
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336
A	1047	ARG	HIS	engineered mutation	UNP P42336
C	-3	ALA	-	expression tag	UNP P42336
C	-2	MET	-	expression tag	UNP P42336
C	-1	GLY	-	expression tag	UNP P42336
C	0	SER	-	expression tag	UNP P42336
C	1047	ARG	HIS	engineered mutation	UNP P42336

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

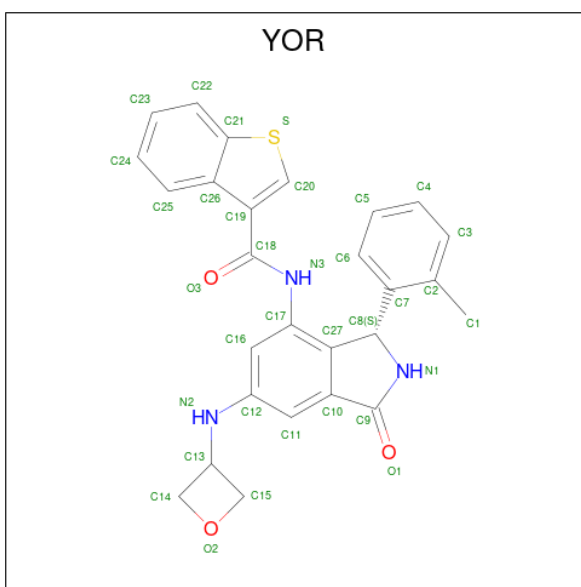
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			2042	1282	362	392	6			
2	D	239	Total	C	N	O	S	0	0	0
			2042	1282	362	392	6			

- Molecule 3 is 2-((1R)-1-[2-(4,4-dimethylpiperidin-1-yl)-3,6-dimethyl-4-oxo-4H-1-benzopyran-8-yl]ethyl)amino)benzoic acid (CCD ID: YO4) (formula: C₂₇H₃₂N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	27	2	4		
3	C	1	Total	C	N	O	0	0
			33	27	2	4		

- Molecule 4 is N-[(3S)-3-(2-methylphenyl)-6-[(oxetan-3-yl)amino]-1-oxo-2,3-dihydro-1H-indol-4-yl]-1-benzothiophene-3-carboxamide (CCD ID: YOR) (formula: $C_{27}H_{23}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



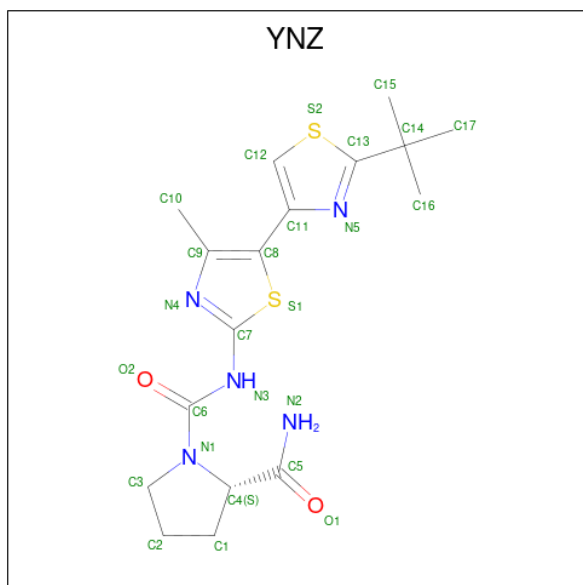
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			34	27	3	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			34	27	3	3	1		

- Molecule 5 is (2S)-N 1 -[(4P)-2-tert-butyl-4'-methyl[4,5'-bi-1,3-thiazol]-2'-yl]pyrrolidine-1,2-dicarboxamide (CCD ID: YNZ) (formula: C₁₇H₂₃N₅O₂S₂) (labeled as "Ligand of Interest" by depositor).

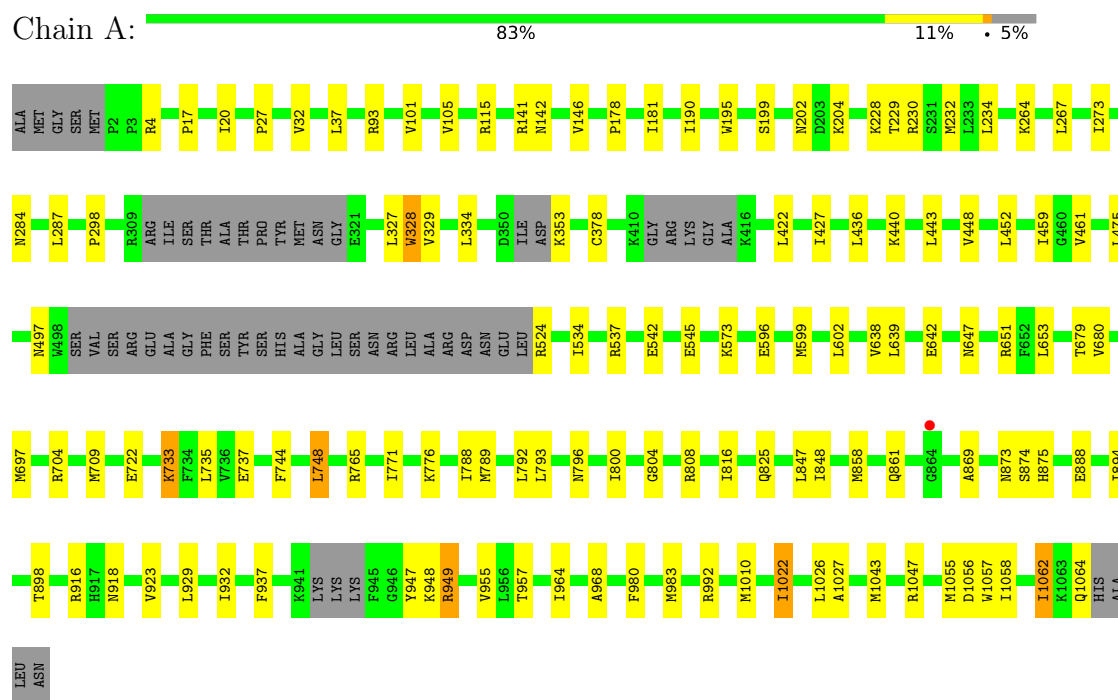


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			26	17	5	2	2		
5	C	1	Total	C	N	O	S	0	0
			26	17	5	2	2		

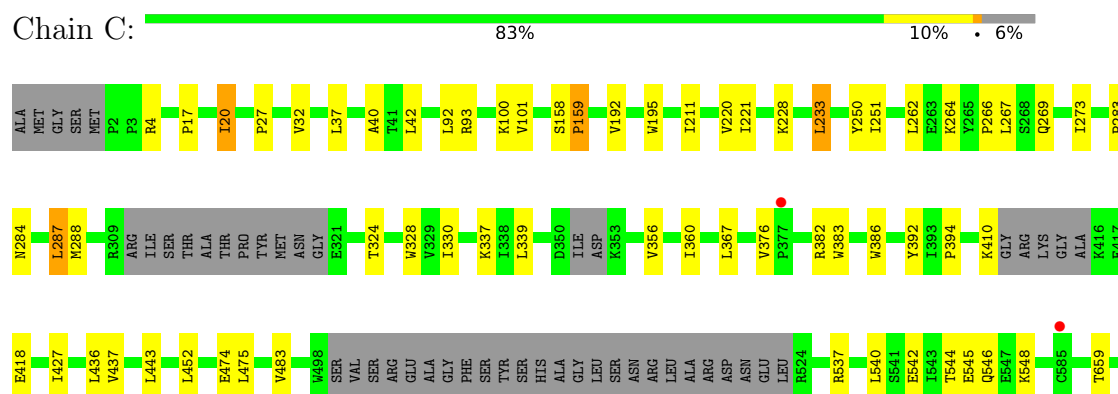
3 Residue-property plots [i](#)

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

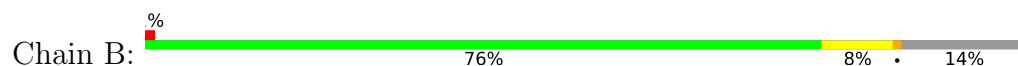


- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

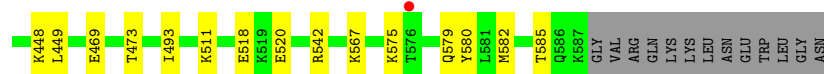
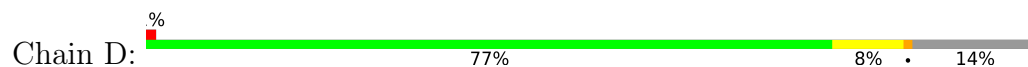




● Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



● Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	236.94Å 158.48Å 121.60Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	43.47 – 3.35 43.47 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.47-3.35) 99.8 (43.47-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.209 , 0.251 0.211 , 0.254	Depositor DCC
R_{free} test set	2940 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 86.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20898	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: YO4, YNZ, YOR

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	0.12	0/8521	0.33	0/11513
1	C	0.11	0/8483	0.34	0/11463
2	B	0.13	0/2074	0.40	0/2772
2	D	0.13	0/2074	0.40	0/2772
All	All	0.12	0/21152	0.35	0/28520

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	8332	0	8349	58	0
1	C	8296	0	8315	57	0
2	B	2042	0	2018	14	0
2	D	2042	0	2018	11	0
3	A	33	0	0	1	0
3	C	33	0	0	0	0
4	A	34	0	0	0	0
4	C	34	0	0	1	0
5	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	26	0	0	0	0
All	All	20898	0	20700	129	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 3.

All (129) 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:353:LYS:N	1:A:378:CYS:HG	1.77	0.81
1:A:765:ARG:NH1	1:A:796:ASN:OD1	2.26	0.69
1:C:1038:TYR:O	1:C:1042:GLN:NE2	2.26	0.68
1:A:461:VAL:HG11	1:A:679:THR:HB	1.78	0.66
1:C:968:ALA:O	1:C:970:GLU:N	2.29	0.65
1:A:735:LEU:HD22	1:A:771:ILE:HG13	1.79	0.63
1:C:992:ARG:NH1	1:C:1027:ALA:O	2.32	0.62
1:A:545:GLU:OE2	2:B:379:LYS:HD2	2.01	0.61
1:A:898:THR:HG22	1:A:964:ILE:HG12	1.84	0.59
1:C:284:ASN:HD22	1:C:792:LEU:HD13	1.67	0.59
1:C:735:LEU:HD22	1:C:771:ILE:HG13	1.84	0.59
1:A:923:VAL:HG22	1:A:929:LEU:HD12	1.84	0.58
1:C:709:MET:HE1	1:C:847:LEU:HD21	1.87	0.57
1:A:955:VAL:HG11	1:A:1055:MET:HB2	1.87	0.57
2:D:372:LEU:HD21	2:D:374:LYS:HE3	1.87	0.56
1:A:199:SER:OG	1:C:949:ARG:NH2	2.38	0.56
1:A:534:ILE:HA	1:A:537:ARG:HD3	1.86	0.56
1:A:992:ARG:NH1	1:A:1027:ALA:O	2.38	0.56
1:C:904:TYR:O	1:C:908:THR:OG1	2.10	0.55
1:A:709:MET:HE1	1:A:847:LEU:HD21	1.88	0.54
1:C:376:VAL:HG11	1:C:382:ARG:O	2.07	0.54
1:A:234:LEU:HD21	1:C:858:MET:HG2	1.90	0.54
1:C:765:ARG:NH1	1:C:796:ASN:OD1	2.42	0.53
1:C:545:GLU:HA	1:C:548:LYS:HB2	1.90	0.53
1:C:913:ILE:HD11	4:C:1102:YOR:C20	2.39	0.53
1:A:542:GLU:OE1	2:B:358:ARG:NH2	2.40	0.53
1:C:192:VAL:HG22	1:C:283:PRO:HG2	1.90	0.53
1:C:964:ILE:O	1:C:965:SER:OG	2.24	0.53
1:C:100:LYS:HD2	2:D:493:ILE:HG23	1.89	0.52
1:C:37:LEU:HB2	1:C:40:ALA:HB2	1.92	0.52
2:B:372:LEU:HD12	2:B:424:LEU:HD21	1.91	0.52
1:C:965:SER:HB3	1:C:976:GLU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:PRO:HD3	1:C:101:VAL:HB	1.92	0.51
1:C:540:LEU:O	2:D:340:ARG:NH1	2.44	0.51
1:A:733:LYS:NZ	1:A:737:GLU:OE2	2.43	0.51
2:D:469:GLU:O	2:D:473:THR:OG1	2.18	0.51
1:C:195:TRP:CG	1:C:789:MET:HE1	2.46	0.51
1:C:267:LEU:HG	1:C:273:ILE:HG12	1.93	0.51
1:C:264:LYS:O	1:C:264:LYS:HG3	2.10	0.50
1:C:858:MET:HE3	1:C:1057:TRP:CH2	2.47	0.50
1:C:251:ILE:HD11	1:C:262:LEU:CD2	2.42	0.50
1:A:916:ARG:NH1	1:A:932:ILE:O	2.44	0.50
1:A:602:LEU:HB3	1:A:638:VAL:HG11	1.92	0.50
1:A:17:PRO:HD2	1:A:20:ILE:HD11	1.94	0.50
1:A:873:ASN:O	1:A:875:HIS:N	2.44	0.50
1:C:955:VAL:HG11	1:C:1055:MET:HB3	1.94	0.50
1:A:267:LEU:HG	1:A:273:ILE:HG12	1.92	0.50
2:B:347:LEU:O	2:B:373:ARG:NH1	2.44	0.49
1:A:229:THR:HA	1:A:232:MET:HE2	1.94	0.49
1:C:42:LEU:HD21	1:C:92:LEU:HD11	1.95	0.49
1:A:204:LYS:HD3	1:A:789:MET:HE3	1.95	0.49
1:A:448:VAL:HG13	1:A:452:LEU:HD23	1.95	0.49
1:C:856:THR:HG22	1:C:922:MET:HG2	1.95	0.49
1:C:360:ILE:HG22	1:C:367:LEU:HD12	1.96	0.48
1:C:17:PRO:HD2	1:C:20:ILE:HD11	1.94	0.48
1:C:542:GLU:OE1	2:D:358:ARG:NH2	2.47	0.48
1:A:178:PRO:HD2	1:A:181:ILE:HD12	1.96	0.48
1:A:776:LYS:HD2	1:A:804:GLY:HA3	1.96	0.47
1:A:327:LEU:C	1:A:329:VAL:H	2.22	0.47
1:A:916:ARG:NH2	1:A:937:PHE:HB2	2.29	0.47
1:A:1062:ILE:H	1:A:1062:ILE:HG13	1.45	0.47
1:A:284:ASN:HD22	1:A:792:LEU:HD13	1.79	0.47
2:B:459:LYS:HE3	2:B:566:ILE:HG23	1.97	0.47
1:A:861:GLN:OE1	1:A:1057:TRP:HZ3	1.97	0.47
1:A:800:ILE:HB	1:A:848:ILE:HB	1.96	0.46
1:C:337:LYS:HB2	1:C:386:TRP:CD1	2.49	0.46
1:A:146:VAL:HG21	1:A:651:ARG:HG2	1.97	0.46
2:D:374:LYS:HD3	2:D:422:VAL:HB	1.96	0.46
1:C:913:ILE:HA	1:C:937:PHE:CE2	2.50	0.46
1:A:537:ARG:NH2	1:A:542:GLU:O	2.48	0.46
2:B:577:ARG:HG2	2:B:577:ARG:O	2.16	0.46
1:A:1043:MET:HB3	3:A:1101:YO4:C3	2.46	0.46
1:A:596:GLU:HA	1:A:599:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:GLU:OE2	1:C:548:LYS:HD2	2.17	0.45
1:C:392:TYR:CD2	1:C:394:PRO:HD2	2.52	0.45
1:A:1022:ILE:HG23	1:A:1026:LEU:HD12	1.99	0.45
1:C:211:ILE:HD12	1:C:220:VAL:HG22	1.99	0.45
1:C:537:ARG:NH2	1:C:542:GLU:O	2.50	0.44
2:B:518:GLU:C	2:B:520:GLU:H	2.25	0.44
1:C:4:ARG:NH1	1:C:93:ARG:HG2	2.31	0.44
1:C:452:LEU:O	2:D:567:LYS:NZ	2.45	0.44
1:C:914:GLY:O	1:C:916:ARG:N	2.51	0.44
1:C:1019:ILE:O	1:C:1022:ILE:HG12	2.18	0.44
1:A:353:LYS:N	1:A:378:CYS:SG	2.85	0.44
1:A:230:ARG:HG3	1:C:773:SER:O	2.18	0.44
1:A:298:PRO:HG2	1:A:697:MET:HG3	2.00	0.44
1:A:733:LYS:HZ2	1:A:737:GLU:CD	2.25	0.43
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.43	0.43
1:C:287:LEU:HD23	1:C:287:LEU:HA	1.83	0.43
1:C:356:VAL:HG23	1:C:383:TRP:CZ2	2.53	0.43
1:C:427:ILE:HD11	1:C:443:LEU:HD22	2.01	0.43
1:A:980:PHE:HA	1:A:983:MET:HE2	1.99	0.43
1:C:158:SER:HB2	1:C:159:PRO:HD3	2.01	0.43
1:A:27:PRO:HD3	1:A:101:VAL:HB	1.99	0.43
1:C:251:ILE:CG2	1:C:288:MET:HB3	2.49	0.43
2:B:468:GLU:O	2:B:472:ARG:HG3	2.19	0.43
1:A:808:ARG:HB3	1:A:1010:MET:HE2	2.02	0.42
1:A:639:LEU:HD21	1:A:653:LEU:HD12	2.01	0.42
1:A:744:PHE:CZ	1:A:748:LEU:HD13	2.55	0.42
1:A:888:GLU:OE1	1:A:888:GLU:N	2.44	0.42
1:A:957:THR:HG21	1:A:1047:ARG:HG3	2.01	0.42
1:C:324:THR:HG22	1:C:483:VAL:HB	2.01	0.42
2:B:397:THR:HG23	2:B:398:PHE:CD2	2.55	0.42
2:D:449:LEU:HD21	2:D:579:GLN:O	2.20	0.41
1:A:427:ILE:HD11	1:A:443:LEU:HD22	2.02	0.41
1:A:948:LYS:HB3	1:A:949:ARG:H	1.67	0.41
1:C:266:PRO:HG2	1:C:269:GLN:HB2	2.01	0.41
1:C:721:GLN:O	1:C:722:GLU:C	2.63	0.41
1:A:542:GLU:CD	2:B:380:LEU:HD13	2.45	0.41
1:C:544:THR:O	1:C:548:LYS:N	2.48	0.41
2:B:574:ARG:O	2:B:577:ARG:NE	2.53	0.41
1:C:800:ILE:HG13	1:C:850:VAL:HG22	2.02	0.41
1:A:858:MET:HG3	1:A:1057:TRP:CZ2	2.55	0.41
1:C:221:ILE:HG21	1:C:250:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:LYS:N	1:C:418:GLU:O	2.49	0.41
1:A:141:ARG:NH1	1:A:142:ASN:OD1	2.53	0.41
1:C:917:HIS:O	1:C:921:ILE:HD12	2.21	0.41
1:A:1057:TRP:HD1	1:A:1058:ILE:HG13	1.86	0.41
2:B:587:LYS:HD3	2:B:587:LYS:HA	1.83	0.41
1:A:195:TRP:CG	1:A:789:MET:HE1	2.56	0.41
1:C:233:LEU:HD22	1:C:233:LEU:HA	1.87	0.41
2:D:350:THR:HG21	2:D:354:THR:HG21	2.03	0.41
2:D:518:GLU:C	2:D:520:GLU:H	2.29	0.41
1:A:545:GLU:HG2	2:B:380:LEU:O	2.22	0.40
1:A:4:ARG:CZ	1:A:93:ARG:HG2	2.52	0.40
2:D:448:LYS:HD2	2:D:448:LYS:H	1.86	0.40
2:B:326:MET:HB3	2:B:402:VAL:HB	2.04	0.40
1:C:251:ILE:HG22	1:C:288:MET:HB3	2.03	0.40
1:A:894:ILE:O	1:A:898:THR:HG23	2.22	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	1005/1072 (94%)	938 (93%)	59 (6%)	8 (1%)	16	44
1	C	1001/1072 (93%)	926 (92%)	66 (7%)	9 (1%)	14	41
2	B	231/279 (83%)	207 (90%)	21 (9%)	3 (1%)	9	32
2	D	231/279 (83%)	209 (90%)	20 (9%)	2 (1%)	14	41
All	All	2468/2702 (91%)	2280 (92%)	166 (7%)	22 (1%)	14	41

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	722	GLU
1	A	874	SER
1	C	722	GLU
1	C	874	SER
1	C	969	GLN
2	D	338	ILE
1	A	968	ALA
1	A	202	ASN
1	A	328	TRP
1	A	793	LEU
2	B	331	ALA
1	C	793	LEU
1	C	868	GLY
1	C	869	ALA
1	C	1056	ASP
1	A	869	ALA
2	B	511	LYS
2	B	585	THR
1	A	1056	ASP
1	C	159	PRO
1	C	339	LEU
2	D	336	GLY

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	934/976 (96%)	903 (97%)	31 (3%)	33	58
1	C	931/976 (95%)	905 (97%)	26 (3%)	38	60
2	B	223/259 (86%)	215 (96%)	8 (4%)	31	56
2	D	223/259 (86%)	214 (96%)	9 (4%)	28	53
All	All	2311/2470 (94%)	2237 (97%)	74 (3%)	34	58

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	37	LEU
1	A	105	VAL
1	A	115	ARG
1	A	190	ILE
1	A	228	LYS
1	A	264	LYS
1	A	287	LEU
1	A	328	TRP
1	A	334	LEU
1	A	422	LEU
1	A	436	LEU
1	A	440	LYS
1	A	459	ILE
1	A	475	LEU
1	A	497	ASN
1	A	524	ARG
1	A	573	LYS
1	A	680	VAL
1	A	704	ARG
1	A	733	LYS
1	A	748	LEU
1	A	788	ILE
1	A	816	ILE
1	A	825	GLN
1	A	918	ASN
1	A	947	TYR
1	A	949	ARG
1	A	1022	ILE
1	A	1062	ILE
1	A	1064	GLN
2	B	332	GLU
2	B	338	ILE
2	B	347	LEU
2	B	372	LEU
2	B	542	ARG
2	B	574	ARG
2	B	577	ARG
2	B	581	LEU
1	C	20	ILE
1	C	32	VAL
1	C	228	LYS
1	C	233	LEU

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Mol	Chain	Res	Type
1	C	287	LEU
1	C	328	TRP
1	C	330	ILE
1	C	436	LEU
1	C	437	VAL
1	C	474	GLU
1	C	475	LEU
1	C	546	GLN
1	C	659	THR
1	C	663	ILE
1	C	748	LEU
1	C	770	ARG
1	C	829	LEU
1	C	858	MET
1	C	908	THR
1	C	929	LEU
1	C	949	ARG
1	C	961	LEU
1	C	1022	ILE
1	C	1041	LYS
1	C	1055	MET
1	C	1062	ILE
2	D	338	ILE
2	D	347	LEU
2	D	372	LEU
2	D	511	LYS
2	D	542	ARG
2	D	575	LYS
2	D	580	TYR
2	D	582	MET
2	D	585	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	384	ASN
1	A	444	ASN
1	A	647	ASN
1	A	855	HIS
1	A	918	ASN
1	A	1044	ASN

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Mol	Chain	Res	Type
1	A	1048	HIS
1	A	1064	GLN
2	B	579	GLN
1	C	284	ASN
1	C	296	GLN
1	C	345	ASN
1	C	370	ASN
1	C	467	ASN
1	C	661	GLN
1	C	855	HIS
1	C	879	GLN
2	D	455	GLN
2	D	475	GLN

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](#)

6 ligands 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	$\# Z > 2$
4	YOR	A	1102	-	34,39,39	0.71	0	46,57,57	2.50	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	YO4	C	1101	-	36,36,36	0.86	2 (5%)	44,54,54	1.31	6 (13%)
5	YNZ	A	1103	-	28,28,28	1.23	3 (10%)	37,42,42	3.52	11 (29%)
3	YO4	A	1101	-	36,36,36	0.91	2 (5%)	44,54,54	1.39	6 (13%)
4	YOR	C	1102	-	34,39,39	0.69	0	46,57,57	2.52	8 (17%)
5	YNZ	C	1103	-	28,28,28	1.23	3 (10%)	37,42,42	3.45	13 (35%)

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	YOR	A	1102	-	-	5/16/34/34	0/6/6/6
3	YO4	C	1101	-	-	7/16/28/28	0/4/4/4
5	YNZ	A	1103	-	-	4/22/32/32	0/3/3/3
3	YO4	A	1101	-	-	7/16/28/28	0/4/4/4
4	YOR	C	1102	-	-	2/16/34/34	0/6/6/6
5	YNZ	C	1103	-	-	6/22/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	YO4	C16-C18	-3.24	1.40	1.47
3	C	1101	YO4	C16-C18	-3.17	1.40	1.47
5	C	1103	YNZ	C9-N4	-2.91	1.32	1.38
5	A	1103	YNZ	C9-N4	-2.83	1.32	1.38
3	A	1101	YO4	O3-C7	-2.60	1.34	1.38
5	A	1103	YNZ	C11-N5	-2.59	1.33	1.38
5	C	1103	YNZ	C11-N5	-2.54	1.33	1.38
5	C	1103	YNZ	C11-C8	2.24	1.49	1.44
5	A	1103	YNZ	C11-C8	2.22	1.49	1.44
3	C	1101	YO4	O3-C7	-2.14	1.35	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1103	YNZ	C7-N4-C9	13.27	118.48	110.38
5	C	1103	YNZ	C7-N4-C9	13.09	118.37	110.38
4	C	1102	YOR	C8-N1-C9	-10.41	108.12	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	YOR	C8-N1-C9	-10.01	108.35	114.03
4	C	1102	YOR	C10-C9-N1	9.51	110.63	106.51
4	A	1102	YOR	C10-C9-N1	9.31	110.55	106.51
5	A	1103	YNZ	S1-C7-N4	-9.02	107.71	115.78
5	C	1103	YNZ	S1-C7-N4	-8.73	107.97	115.78
5	A	1103	YNZ	C11-N5-C13	8.09	117.83	110.97
5	C	1103	YNZ	C11-N5-C13	8.01	117.77	110.97
5	A	1103	YNZ	C7-S1-C8	5.35	91.35	88.34
5	C	1103	YNZ	C4-N1-C6	4.98	127.32	119.26
5	C	1103	YNZ	C7-S1-C8	4.96	91.13	88.34
4	A	1102	YOR	C26-C19-C20	4.57	113.76	111.63
5	A	1103	YNZ	C9-C8-S1	-4.47	107.15	109.94
5	A	1103	YNZ	C4-N1-C6	4.36	126.31	119.26
5	C	1103	YNZ	C9-C8-S1	-4.34	107.23	109.94
5	A	1103	YNZ	N3-C6-N1	4.07	120.18	115.57
4	C	1102	YOR	C26-C19-C20	3.91	113.45	111.63
3	C	1101	YO4	O3-C7-C19	-3.46	117.46	121.25
3	A	1101	YO4	C14-C15-N2	-3.37	104.53	110.82
3	A	1101	YO4	O3-C7-C19	-3.36	117.57	121.25
3	C	1101	YO4	C5-C4-N1	3.30	114.78	108.91
5	C	1103	YNZ	S1-C7-N3	3.18	127.97	123.72
4	C	1102	YOR	C11-C10-C27	-3.17	119.03	122.79
3	A	1101	YO4	C5-C4-N1	3.16	114.53	108.91
5	A	1103	YNZ	S1-C7-N3	3.14	127.92	123.72
4	C	1102	YOR	C11-C10-C9	3.11	132.81	129.66
4	A	1102	YOR	C11-C10-C27	-3.05	119.17	122.79
4	A	1102	YOR	C21-S-C20	3.03	92.80	91.16
4	A	1102	YOR	C11-C10-C9	2.95	132.65	129.66
3	A	1101	YO4	C10-C9-N2	-2.94	105.32	110.82
5	C	1103	YNZ	N3-C6-N1	2.89	118.85	115.57
4	C	1102	YOR	C19-C18-N3	2.80	118.16	114.89
4	A	1102	YOR	C14-O2-C15	2.79	93.99	91.34
3	C	1101	YO4	C5-C4-C6	-2.78	107.65	111.58
3	C	1101	YO4	C14-C15-N2	-2.66	105.85	110.82
4	C	1102	YOR	C21-S-C20	2.58	92.56	91.16
4	C	1102	YOR	C14-O2-C15	2.54	93.75	91.34
5	A	1103	YNZ	C1-C4-N1	2.52	106.70	103.02
3	A	1101	YO4	C5-C4-C6	-2.44	108.13	111.58
5	C	1103	YNZ	C2-C3-N1	2.37	107.31	103.24
5	C	1103	YNZ	C3-N1-C4	-2.33	108.35	112.01
4	A	1102	YOR	C19-C20-S	-2.32	112.60	114.16
5	A	1103	YNZ	C3-N1-C4	-2.30	108.40	112.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1101	YO4	C10-C9-N2	-2.25	106.62	110.82
5	A	1103	YNZ	C14-C13-S2	2.12	125.07	121.51
4	A	1102	YOR	C26-C21-S	-2.10	110.03	111.46
5	C	1103	YNZ	C1-C4-N1	2.09	106.09	103.02
5	C	1103	YNZ	C1-C4-C5	-2.08	108.53	111.29
3	A	1101	YO4	C9-N2-C15	2.06	116.89	112.68
3	C	1101	YO4	C2-C3-N1	-2.05	119.27	121.08
5	C	1103	YNZ	C14-C13-S2	2.01	124.87	121.51

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	YO4	C16-C8-N2-C9
3	A	1101	YO4	O3-C8-N2-C15
3	A	1101	YO4	O3-C8-N2-C9
3	C	1101	YO4	C16-C8-N2-C9
3	C	1101	YO4	O3-C8-N2-C15
3	C	1101	YO4	O3-C8-N2-C9
4	A	1102	YOR	C6-C7-C8-N1
4	A	1102	YOR	C2-C7-C8-N1
4	C	1102	YOR	C6-C7-C8-N1
4	C	1102	YOR	C2-C7-C8-N1
5	A	1103	YNZ	N1-C4-C5-N2
5	A	1103	YNZ	N1-C4-C5-O1
5	A	1103	YNZ	N5-C11-C8-C9
5	C	1103	YNZ	N5-C11-C8-C9
4	A	1102	YOR	C15-C13-N2-C12
5	C	1103	YNZ	N1-C4-C5-N2
5	C	1103	YNZ	N1-C4-C5-O1
5	C	1103	YNZ	C1-C4-C5-N2
5	C	1103	YNZ	C1-C4-C5-O1
3	A	1101	YO4	O1-C1-C2-C3
3	C	1101	YO4	O1-C1-C2-C3
3	A	1101	YO4	O2-C1-C2-C3
3	C	1101	YO4	O2-C1-C2-C3
5	A	1103	YNZ	N5-C11-C8-S1
5	C	1103	YNZ	N5-C11-C8-S1
3	A	1101	YO4	O2-C1-C2-C27
3	C	1101	YO4	O2-C1-C2-C27
3	A	1101	YO4	O1-C1-C2-C27
3	C	1101	YO4	O1-C1-C2-C27

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Mol	Chain	Res	Type	Atoms
4	A	1102	YOR	C16-C17-N3-C18
4	A	1102	YOR	C27-C17-N3-C18

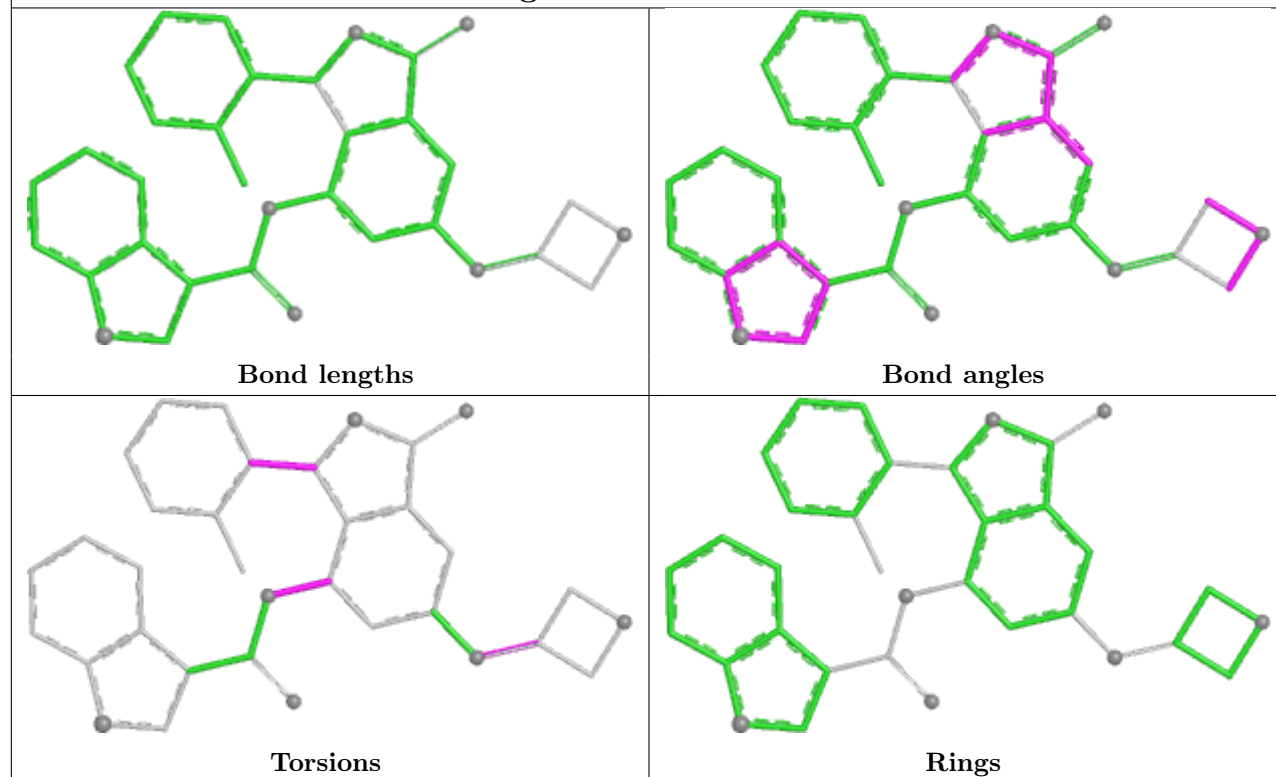
There are no ring outliers.

2 monomers are involved in 2 short contacts:

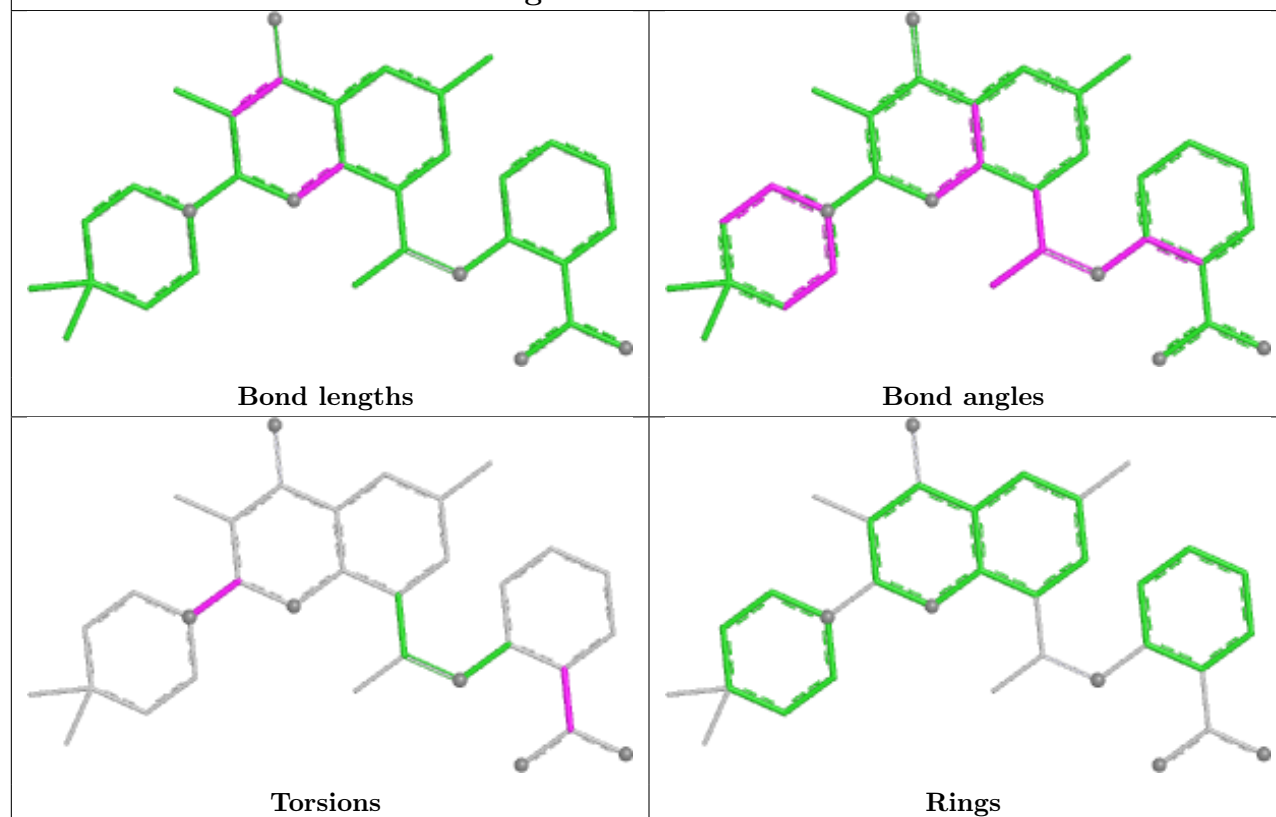
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	YO4	1	0
4	C	1102	YOR	1	0

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.

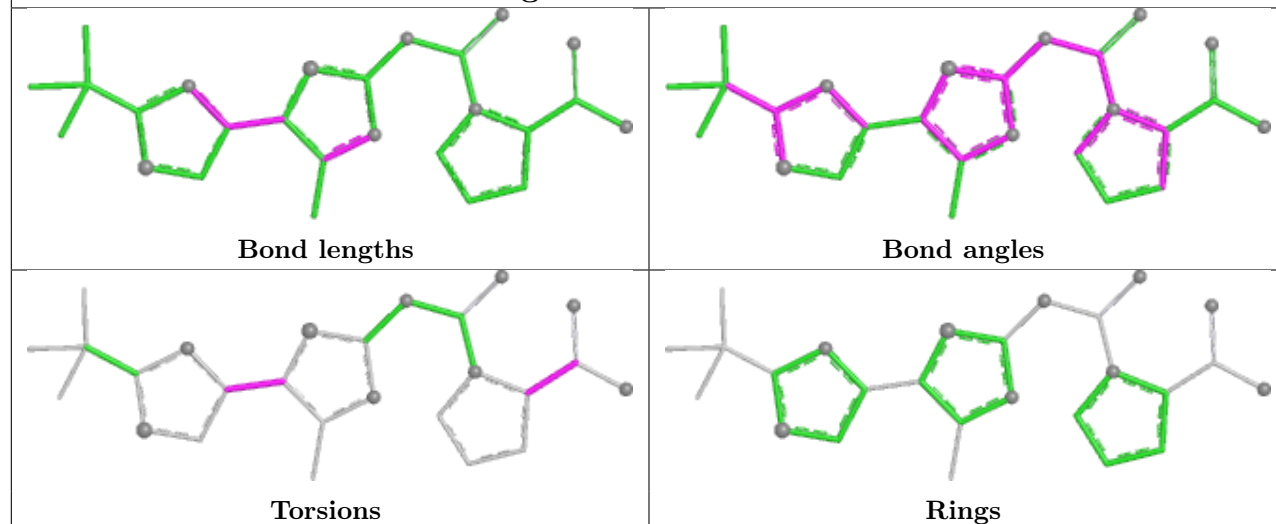
Ligand YOR A 1102



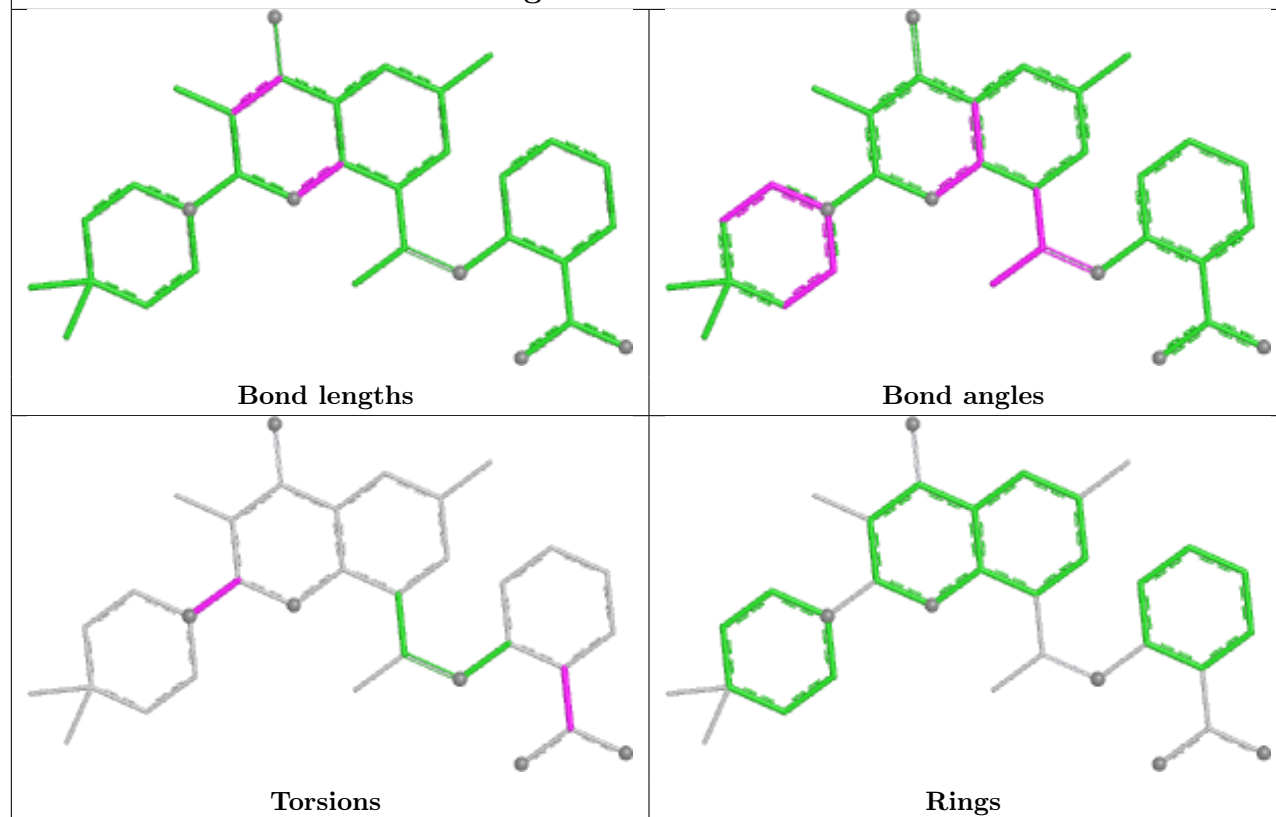
Ligand YO4 C 1101

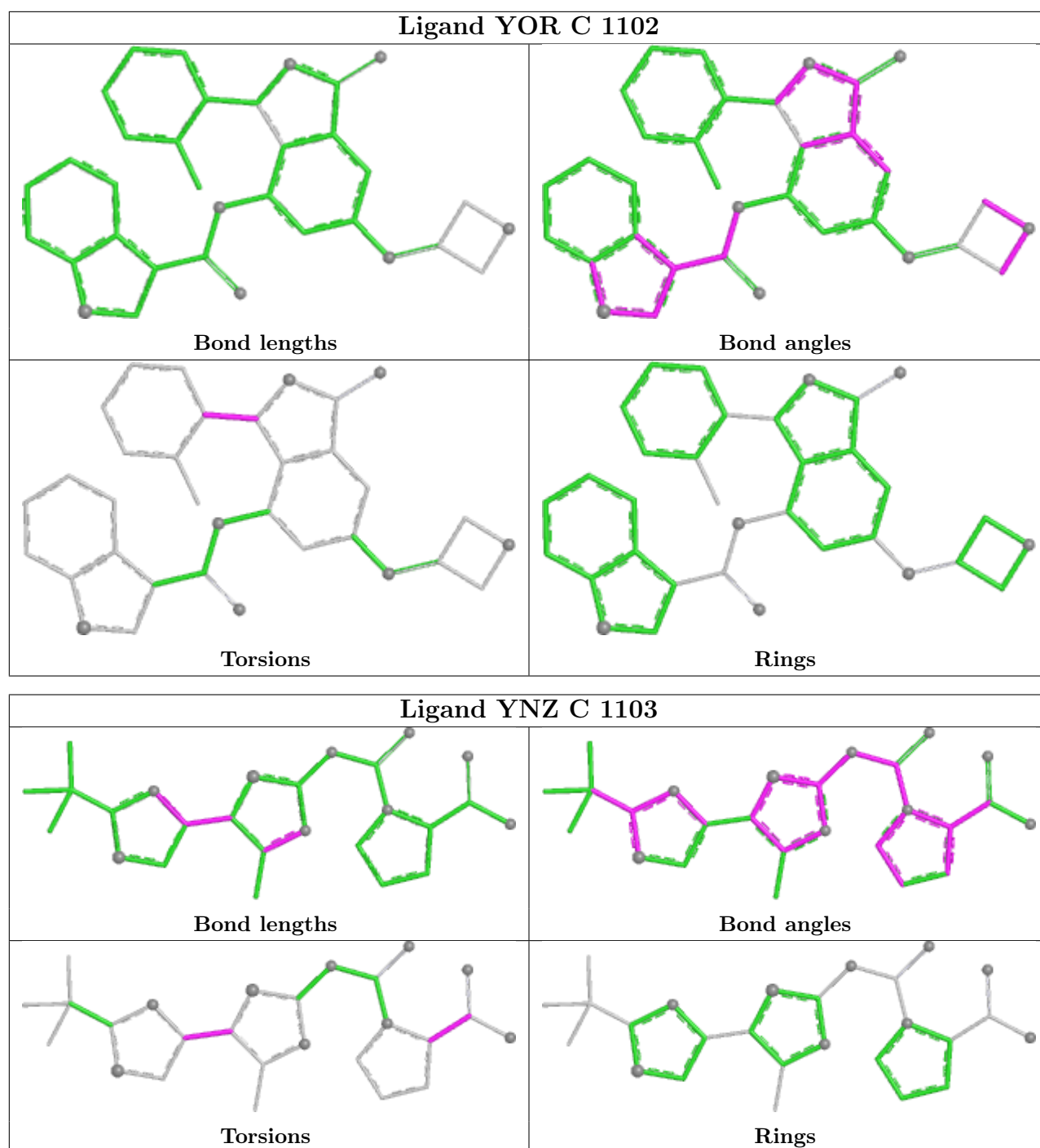


Ligand YNZ A 1103



Ligand YO4 A 1101





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	1017/1072 (94%)	-0.24	1 (0%) 92 92	49, 86, 150, 258	0
1	C	1013/1072 (94%)	-0.17	4 (0%) 88 81	50, 96, 181, 239	0
2	B	239/279 (85%)	0.09	4 (1%) 69 53	74, 147, 282, 329	0
2	D	239/279 (85%)	0.21	3 (1%) 75 61	100, 185, 310, 353	0
All	All	2508/2702 (92%)	-0.14	12 (0%) 87 78	49, 100, 239, 353	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	585	CYS	2.6
2	D	335	TRP	2.6
2	D	405	ILE	2.6
2	D	576	THR	2.4
2	B	335	TRP	2.4
2	B	585	THR	2.3
2	B	356	LEU	2.3
1	C	377	PRO	2.3
2	B	587	LYS	2.3
1	C	952	VAL	2.2
1	C	962	ILE	2.2
1	A	864	GLY	2.1

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](#)

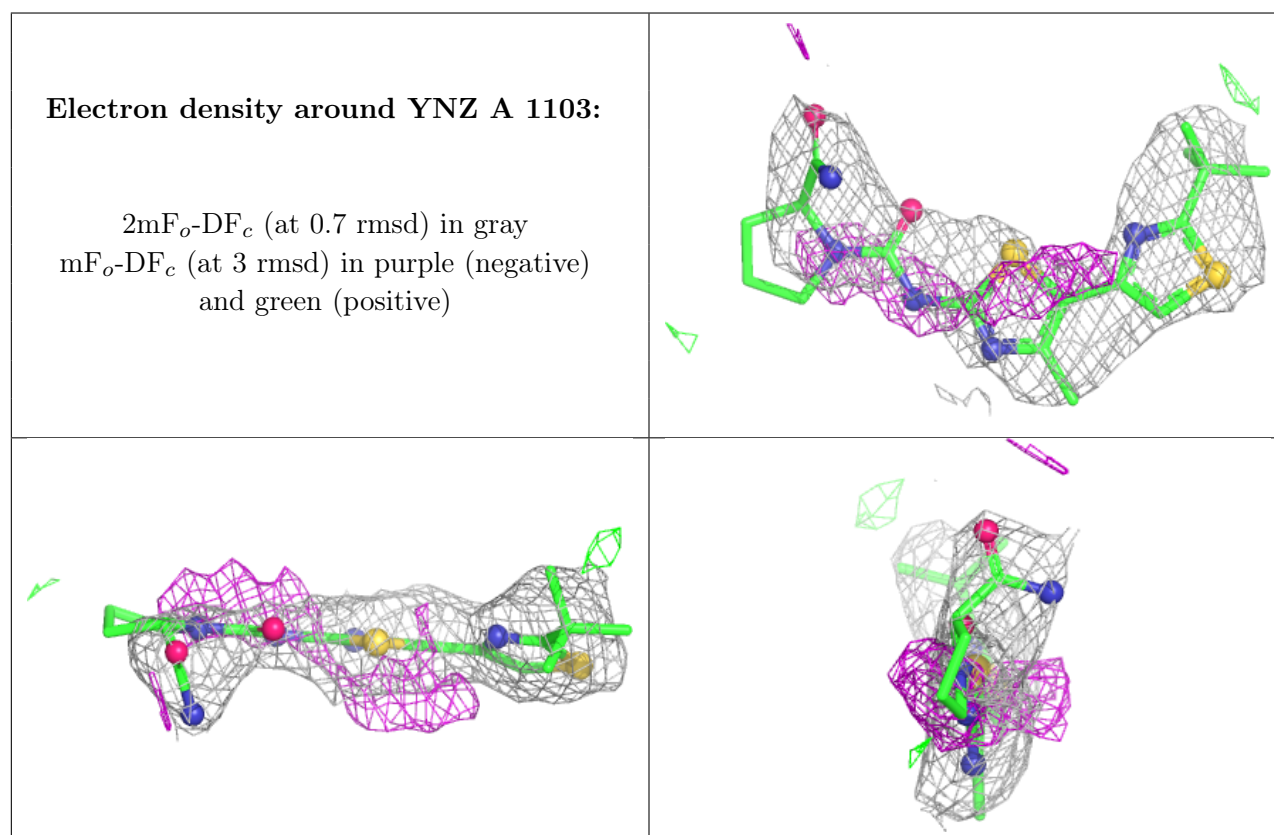
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

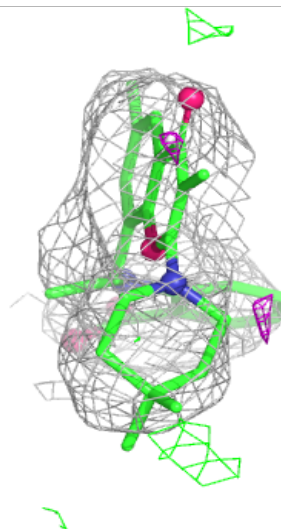
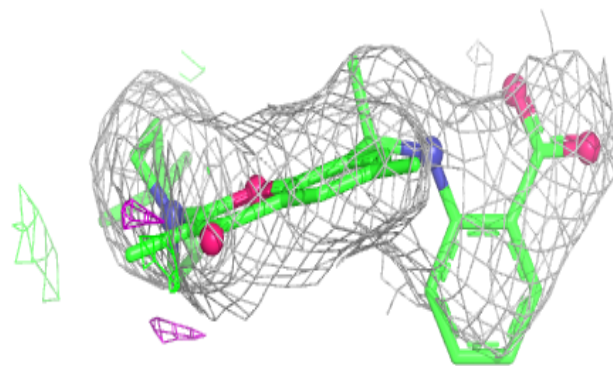
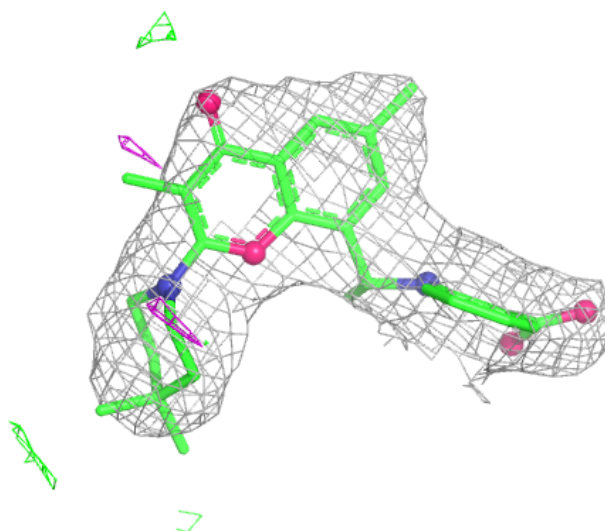
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	YNZ	A	1103	26/26	0.85	0.16	78,107,125,132	0
3	YO4	A	1101	33/33	0.94	0.12	48,85,100,102	0
4	YOR	C	1102	34/34	0.95	0.09	63,91,113,117	0
4	YOR	A	1102	34/34	0.95	0.09	45,81,93,117	0
5	YNZ	C	1103	26/26	0.95	0.08	65,81,88,93	0
3	YO4	C	1101	33/33	0.96	0.11	75,96,112,125	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.



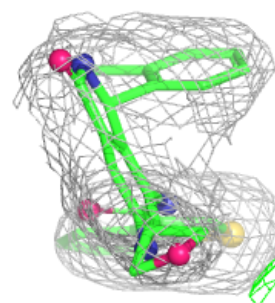
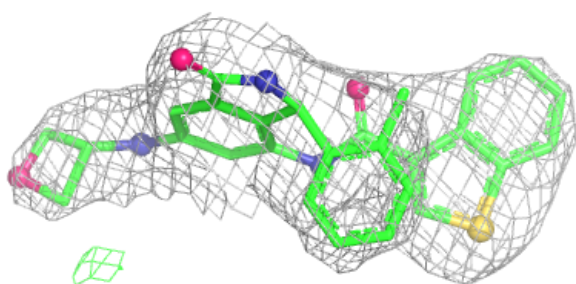
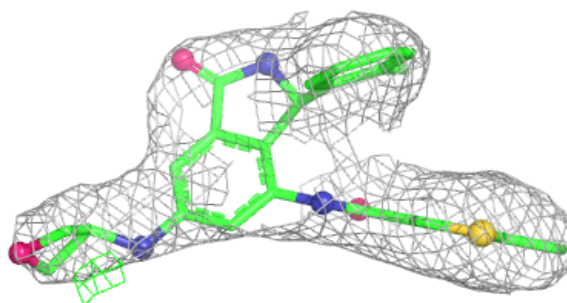
Electron density around YO4 A 1101:

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

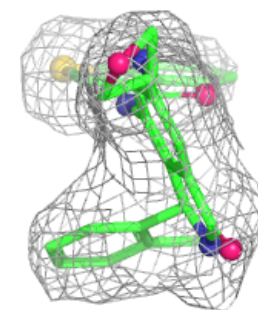
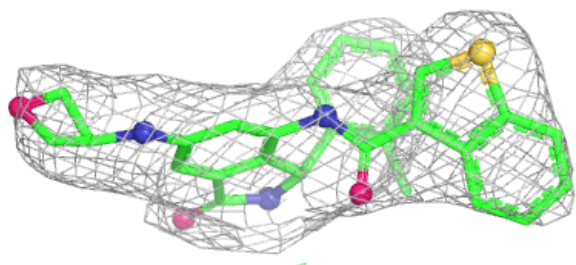
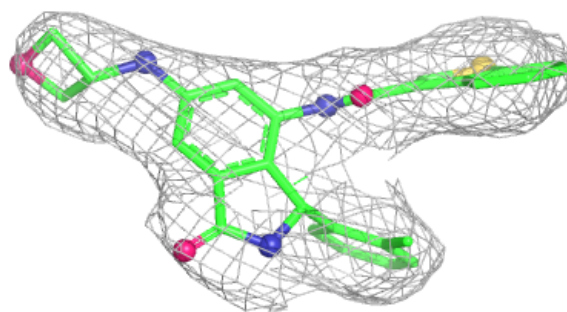


Electron density around YOR C 1102:

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

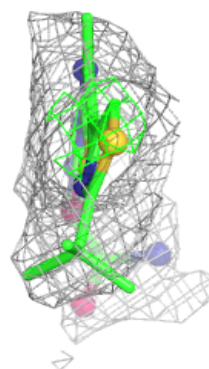
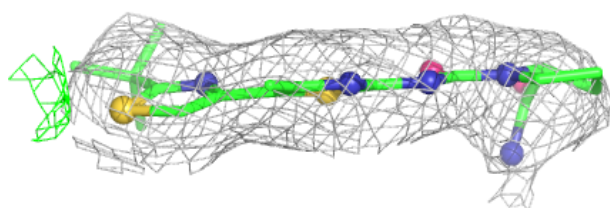
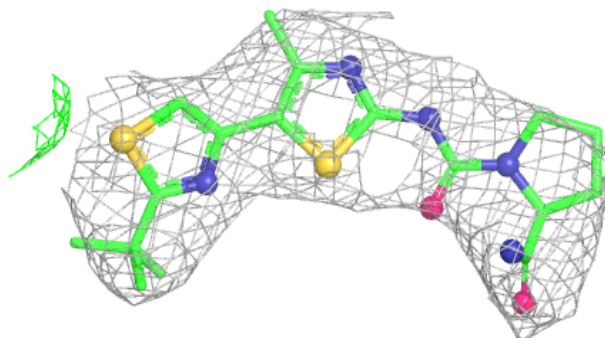
**Electron density around YOR A 1102:**

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

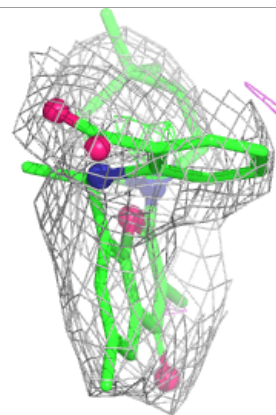
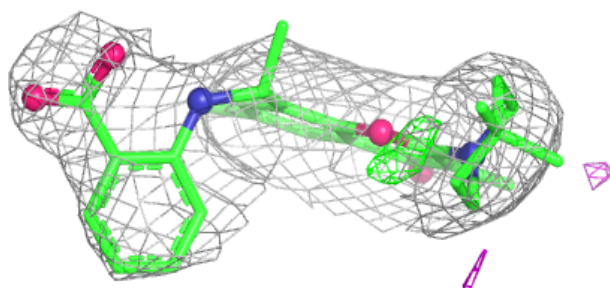
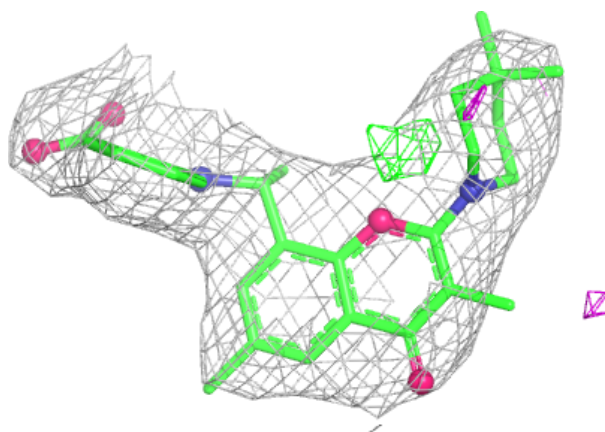


Electron density around YNZ C 1103:

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

**Electron density around YO4 C 1101:**

$2mF_o-DF_c$ (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.