



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 06:18 PM EDT

PDB ID : 8V8H
Title : PI3Ka H1047R co-crystal structure with inhibitor in cryptic pocket near H1047R (compound 4).
Authors : Gunn, R.J.; Lawson, J.D.
Deposited on : 2023-12-05
Resolution : 3.58 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

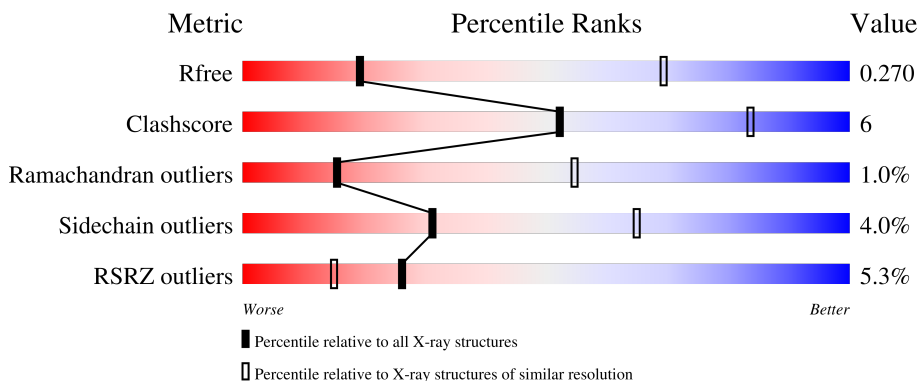
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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}	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	1072	
1	C	1072	
2	B	279	
2	D	279	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20844 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
			Total	C	N	O	S			
1	A	1020	Total	C	N	O	S	0	0	0
			8355	5352	1429	1505	69			
1	C	1012	Total	C	N	O	S	0	0	0
			8287	5304	1416	1498	69			

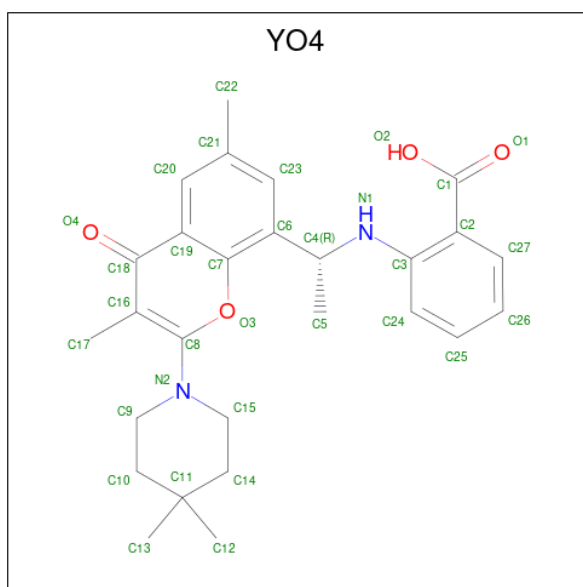
There are 10 discrepancies between the modelled and reference sequences:

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.

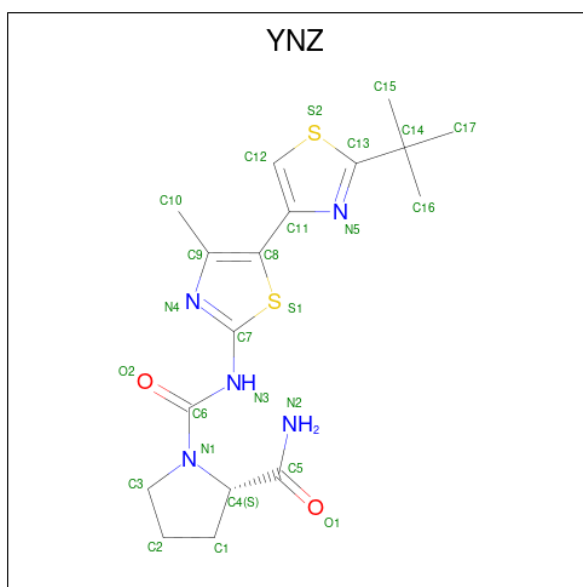
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	239	Total	C	N	O	S	0	0	0
			2042	1282	362	392	6			
2	D	239	Total	C	N	O	S	0	0	0
			2042	1282	362	392	6			

- 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 (three-letter code: YO4) (formula: C₂₇H₃₂N₂O₄) (labeled as "Ligand of Interest" by depositor).



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

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



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

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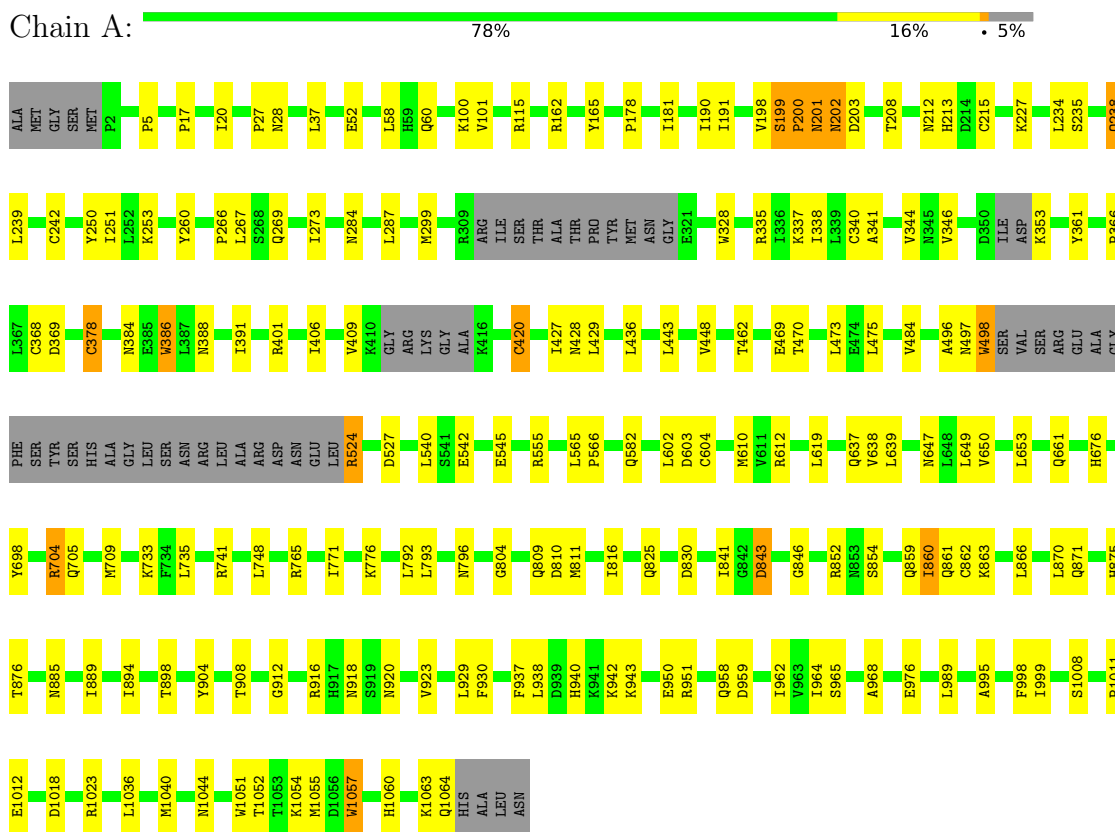
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	C	1	26	17	5	2	2	0	0

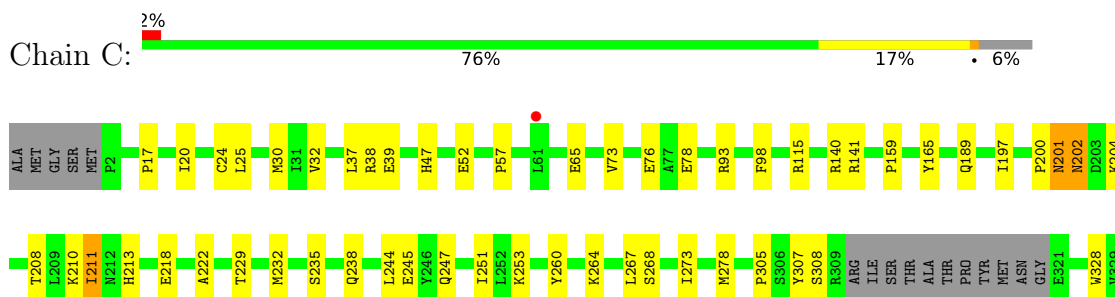
3 Residue-property plots

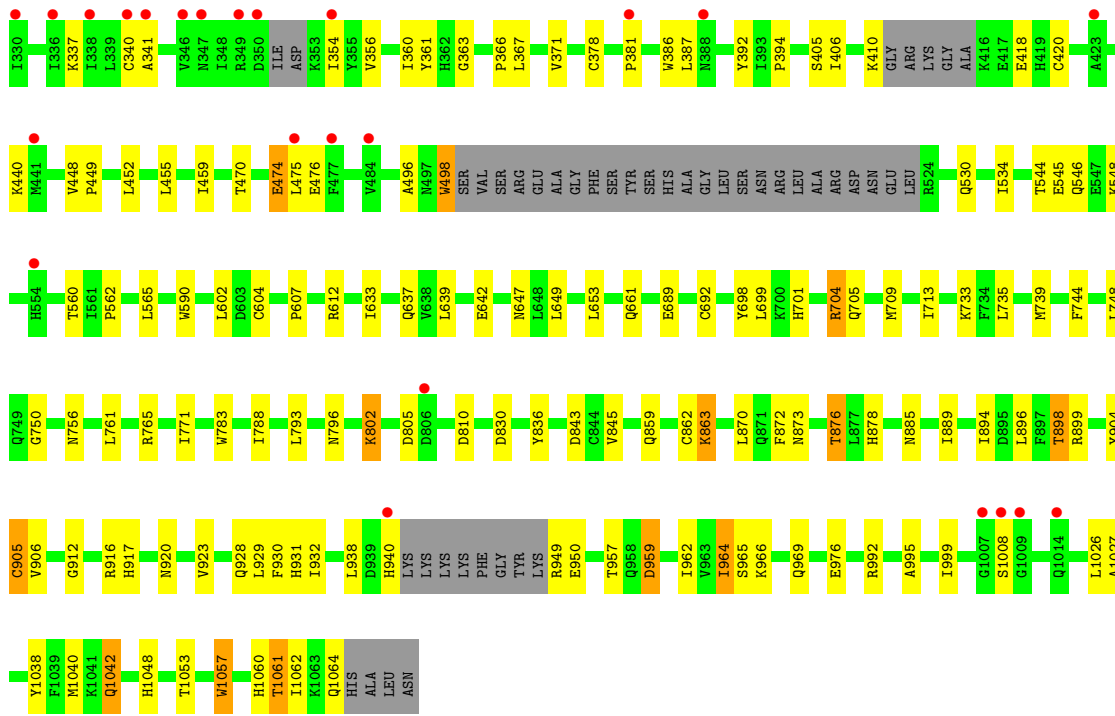
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

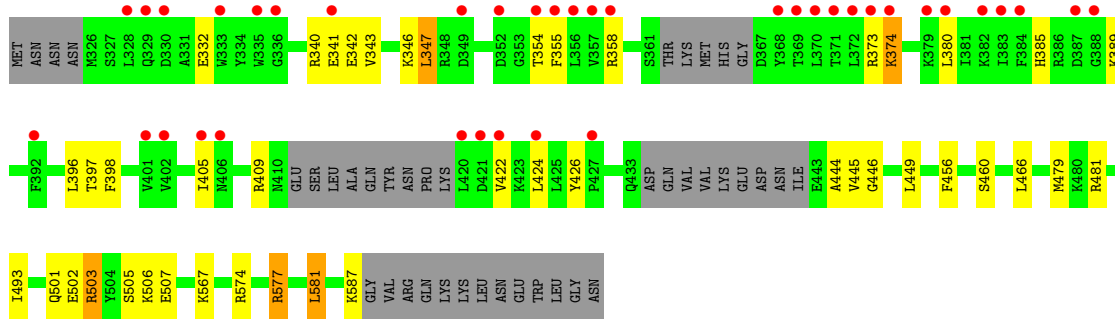


- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

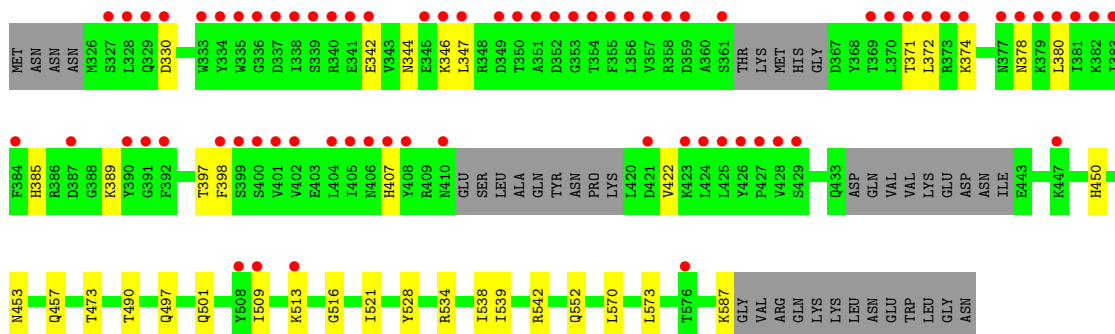
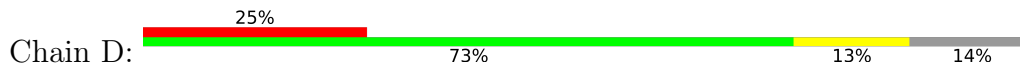




• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



• 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	233.85Å 157.77Å 121.90Å 90.00° 112.66° 90.00°	Depositor
Resolution (Å)	48.21 – 3.58 48.21 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.21-3.58) 99.5 (48.21-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.57Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.222 , 0.272 0.221 , 0.270	Depositor DCC
R_{free} test set	2353 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	104.0	Xtrriage
Anisotropy	0.427	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20844	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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

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	0.28	0/8545	0.52	0/11544
1	C	0.28	0/8474	0.52	0/11452
2	B	0.29	0/2074	0.57	0/2772
2	D	0.28	0/2074	0.57	0/2772
All	All	0.28	0/21167	0.53	0/28540

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	8355	0	8385	101	0
1	C	8287	0	8302	96	0
2	B	2042	0	2018	29	0
2	D	2042	0	2018	20	0
3	A	33	0	0	0	0
3	C	33	0	0	0	0
4	A	26	0	0	1	0
4	C	26	0	0	0	0
All	All	20844	0	20723	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (229) 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	1.65	0.94
1:A:859:GLN:O	1:A:862:CYS:N	2.20	0.74
2:B:574:ARG:O	2:B:577:ARG:NE	2.21	0.74
1:A:17:PRO:HD2	1:A:20:ILE:HD11	1.71	0.72
1:A:555:ARG:NH2	1:A:582:GLN:OE1	2.24	0.69
1:A:940:HIS:HB3	1:A:943:LYS:HB2	1.74	0.69
1:A:765:ARG:NH1	1:A:796:ASN:OD1	2.25	0.69
1:A:937:PHE:HB2	1:A:1012:GLU:HB2	1.75	0.68
1:A:1054:LYS:HD2	1:A:1063:LYS:HB3	1.74	0.68
1:C:545:GLU:HA	1:C:548:LYS:HB2	1.75	0.67
1:C:859:GLN:O	1:C:863:LYS:N	2.27	0.67
1:A:234:LEU:HB3	1:A:238:GLN:HB3	1.76	0.67
2:B:343:VAL:HG21	2:B:358:ARG:HH11	1.61	0.65
1:A:639:LEU:HD21	1:A:653:LEU:HD12	1.77	0.65
1:C:140:ARG:NH2	1:C:689:GLU:OE2	2.24	0.65
2:D:453:ASN:ND2	2:D:457:GLN:OE1	2.30	0.65
1:A:361:TYR:HA	1:A:366:PRO:HA	1.78	0.63
1:C:765:ARG:NH1	1:C:796:ASN:OD1	2.32	0.62
1:C:639:LEU:HD21	1:C:653:LEU:HD12	1.82	0.62
1:C:1038:TYR:O	1:C:1042:GLN:HG2	2.00	0.61
1:A:602:LEU:O	1:A:612:ARG:NH2	2.33	0.60
1:A:340:CYS:SG	1:A:341:ALA:N	2.74	0.60
1:A:989:LEU:HD11	1:A:1036:LEU:HD11	1.83	0.59
1:C:141:ARG:HG3	1:C:308:SER:HA	1.83	0.59
2:B:397:THR:HG23	2:B:398:PHE:CE2	2.37	0.59
1:C:17:PRO:HD2	1:C:20:ILE:HD11	1.85	0.59
2:B:501:GLN:O	2:B:503:ARG:N	2.32	0.59
1:C:340:CYS:SG	1:C:341:ALA:N	2.77	0.58
1:A:266:PRO:HD2	1:A:269:GLN:NE2	2.17	0.58
1:C:704:ARG:NH1	1:C:750:GLY:O	2.36	0.58
1:A:898:THR:HG22	1:A:964:ILE:HG12	1.85	0.57
1:A:200:PRO:O	1:A:202:ASN:N	2.37	0.57
1:C:530:GLN:O	1:C:534:ILE:HG12	2.04	0.57
2:D:372:LEU:HD21	2:D:374:LYS:HE3	1.85	0.57
1:C:360:ILE:HG22	1:C:367:LEU:HD12	1.87	0.57
1:A:436:LEU:HB3	1:A:484:VAL:HB	1.87	0.57
1:C:965:SER:HB3	1:C:976:GLU:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ARG:HH11	1:A:704:ARG:HB3	1.71	0.56
1:C:862:CYS:SG	1:C:863:LYS:N	2.79	0.56
1:A:337:LYS:HB2	1:A:386:TRP:HD1	1.72	0.55
1:C:76:GLU:OE1	1:C:93:ARG:NH2	2.39	0.55
1:C:802:LYS:NZ	1:C:805:ASP:OD2	2.36	0.55
1:A:28:ASN:ND2	1:A:58:LEU:O	2.40	0.54
1:A:854:SER:O	4:A:1102:YNZ:N2	2.41	0.54
1:C:354:ILE:HD11	1:C:381:PRO:HB3	1.90	0.54
1:A:1040:MET:O	1:A:1044:ASN:ND2	2.29	0.54
1:A:337:LYS:HB2	1:A:386:TRP:CD1	2.43	0.54
1:A:203:ASP:H	1:C:949:ARG:HH22	1.57	0.53
2:B:581:LEU:HD13	2:B:581:LEU:H	1.72	0.53
1:A:958:GLN:NE2	1:A:1051:TRP:HA	2.24	0.53
1:C:894:ILE:O	1:C:898:THR:OG1	2.27	0.52
1:A:923:VAL:HG22	1:A:929:LEU:HD12	1.91	0.52
2:B:374:LYS:HD3	2:B:422:VAL:HB	1.91	0.52
1:A:809:GLN:HE22	1:A:1011:PRO:HD2	1.75	0.52
1:C:200:PRO:O	1:C:202:ASN:N	2.42	0.52
1:A:735:LEU:HD22	1:A:771:ILE:HG13	1.91	0.52
1:C:363:GLY:HA3	1:C:607:PRO:HG3	1.92	0.52
1:C:661:GLN:NE2	1:C:698:TYR:HB2	2.25	0.52
1:A:950:GLU:OE1	1:A:951:ARG:NH2	2.43	0.52
1:A:965:SER:HB3	1:A:976:GLU:HB2	1.92	0.52
1:C:633:ILE:HD12	1:C:633:ILE:H	1.75	0.52
1:C:923:VAL:HG22	1:C:929:LEU:HD12	1.91	0.51
1:C:25:LEU:HD23	2:D:497:GLN:HB2	1.92	0.51
1:C:410:LYS:N	1:C:418:GLU:O	2.41	0.51
1:C:859:GLN:O	1:C:862:CYS:N	2.43	0.51
1:A:661:GLN:NE2	1:A:698:TYR:HB2	2.26	0.51
1:A:201:ASN:HB3	1:C:949:ARG:CD	2.41	0.51
2:D:509:ILE:HG12	2:D:521:ILE:HG23	1.91	0.51
1:A:344:VAL:HG12	1:A:346:VAL:HG13	1.93	0.51
1:A:198:VAL:O	1:C:1061:THR:OG1	2.23	0.50
1:C:371:VAL:HG23	1:C:387:LEU:HD13	1.93	0.50
1:A:267:LEU:HG	1:A:273:ILE:HG12	1.93	0.50
1:A:266:PRO:HD2	1:A:269:GLN:HE21	1.76	0.50
2:D:539:ILE:HG23	2:D:542:ARG:HH12	1.76	0.50
1:A:212:ASN:HB2	1:A:215:CYS:SG	2.52	0.49
1:C:222:ALA:HB2	1:C:247:GLN:HG2	1.93	0.49
2:B:405:ILE:O	2:B:409:ARG:HB2	2.12	0.49
1:C:253:LYS:HB2	1:C:260:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:LEU:HD13	1:A:1018:ASP:O	2.13	0.49
1:C:448:VAL:HG13	1:C:452:LEU:HD22	1.93	0.49
1:A:602:LEU:HB3	1:A:638:VAL:HG11	1.94	0.49
1:C:544:THR:O	1:C:548:LYS:N	2.40	0.49
1:A:937:PHE:HB3	1:A:938:LEU:HG	1.95	0.49
2:B:505:SER:C	2:B:507:GLU:H	2.17	0.49
1:C:449:PRO:HD2	1:C:452:LEU:HD13	1.95	0.49
1:A:338:ILE:O	1:A:384:ASN:N	2.46	0.48
1:A:250:TYR:HB3	1:A:287:LEU:HD22	1.95	0.48
2:B:374:LYS:NZ	2:B:422:VAL:O	2.46	0.48
2:B:505:SER:O	2:B:507:GLU:N	2.46	0.48
1:C:140:ARG:HB3	1:C:307:TYR:CE2	2.48	0.48
1:C:602:LEU:O	1:C:612:ARG:NH2	2.46	0.48
1:C:30:MET:HE2	1:C:57:PRO:HD2	1.95	0.48
1:A:199:SER:C	1:C:949:ARG:HH21	2.17	0.48
1:A:816:ILE:HG23	1:A:998:PHE:CE2	2.49	0.48
1:C:165:TYR:CZ	1:C:661:GLN:HG3	2.48	0.48
2:B:444:ALA:O	2:B:446:GLY:N	2.45	0.48
1:C:995:ALA:O	1:C:999:ILE:HG12	2.13	0.48
1:A:235:SER:HB2	1:A:238:GLN:HB2	1.94	0.48
1:A:353:LYS:O	1:A:409:VAL:HG22	2.14	0.48
1:A:958:GLN:HE22	1:A:1051:TRP:HA	1.79	0.48
1:C:885:ASN:HD22	1:C:889:ILE:HG22	1.78	0.48
2:B:347:LEU:O	2:B:373:ARG:NH1	2.46	0.47
1:A:540:LEU:O	2:B:340:ARG:NH1	2.40	0.47
2:D:397:THR:HG23	2:D:398:PHE:CE2	2.50	0.47
1:C:872:PHE:O	1:C:876:THR:OG1	2.22	0.47
1:C:896:LEU:HD21	1:C:928:GLN:HB2	1.96	0.47
2:D:374:LYS:HD3	2:D:422:VAL:HB	1.97	0.47
2:B:385:HIS:HA	2:B:389:LYS:O	2.14	0.47
1:A:776:LYS:HD2	1:A:804:GLY:HA3	1.97	0.47
2:D:501:GLN:NE2	2:D:528:TYR:HB2	2.30	0.47
2:B:342:GLU:HG3	2:B:346:LYS:HE3	1.96	0.47
1:A:165:TYR:CZ	1:A:661:GLN:HG3	2.50	0.47
1:A:5:PRO:HG3	2:B:479:MET:HG2	1.96	0.46
1:C:904:TYR:CE2	1:C:930:PHE:HA	2.50	0.46
1:C:912:GLY:HA3	1:C:938:LEU:HA	1.96	0.46
1:A:637:GLN:NE2	1:A:1008:SER:HB3	2.31	0.46
1:A:816:ILE:HG23	1:A:998:PHE:HE2	1.81	0.46
1:C:197:ILE:HD13	1:C:204:LYS:HG2	1.97	0.46
1:C:761:LEU:HB3	1:C:783:TRP:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:HB2	1:A:260:TYR:CE2	2.51	0.46
1:A:540:LEU:HB2	1:A:1023:ARG:HD2	1.98	0.46
2:D:385:HIS:HA	2:D:389:LYS:O	2.16	0.46
2:D:344:ASN:OD1	2:D:378:ASN:ND2	2.49	0.45
1:C:189:GLN:NE2	1:C:210:LYS:HE2	2.31	0.45
1:A:238:GLN:HE22	1:C:863:LYS:HE3	1.82	0.45
1:A:524:ARG:N	1:A:524:ARG:HD2	2.30	0.45
1:C:356:VAL:HG22	1:C:406:ILE:HG12	1.98	0.45
1:C:992:ARG:NH1	1:C:1027:ALA:O	2.40	0.45
1:A:496:ALA:C	1:A:498:TRP:H	2.19	0.45
1:C:959:ASP:HA	1:C:962:ILE:HD12	1.98	0.45
1:C:496:ALA:O	1:C:498:TRP:N	2.47	0.45
1:A:401:ARG:HA	1:A:429:LEU:HG	1.99	0.45
1:A:1055:MET:O	1:A:1060:HIS:HA	2.17	0.45
1:C:878:HIS:HE2	1:C:966:LYS:HG3	1.81	0.45
1:A:841:ILE:HG12	1:A:846:GLY:HA2	1.99	0.44
2:B:587:LYS:HD3	2:B:587:LYS:HA	1.68	0.44
1:A:647:ASN:HD22	1:A:649:LEU:H	1.65	0.44
1:C:862:CYS:HB3	1:C:1057:TRP:CH2	2.53	0.44
1:A:904:TYR:CE2	1:A:930:PHE:HA	2.53	0.44
1:A:875:HIS:ND1	1:A:962:ILE:HD13	2.31	0.44
1:A:162:ARG:NH1	1:A:299:MET:HG2	2.32	0.44
1:A:199:SER:HB2	1:C:949:ARG:NH2	2.33	0.44
2:B:354:THR:HA	2:B:426:TYR:O	2.17	0.44
1:C:949:ARG:HB3	1:C:950:GLU:H	1.55	0.44
1:A:406:ILE:HD11	1:A:473:LEU:HD13	1.99	0.44
1:A:676:HIS:CG	1:A:843:ASP:HB2	2.53	0.44
2:D:473:THR:HG23	2:D:552:GLN:HG2	1.99	0.44
1:C:47:HIS:HA	1:C:65:GLU:OE1	2.18	0.44
1:C:735:LEU:HD22	1:C:771:ILE:HG13	2.00	0.44
1:C:788:ILE:HD12	1:C:788:ILE:H	1.83	0.44
1:C:830:ASP:O	1:C:899:ARG:HD3	2.18	0.44
1:C:917:HIS:CD2	1:C:1060:HIS:CD2	3.06	0.44
1:A:284:ASN:HB3	1:A:792:LEU:HD13	2.00	0.43
1:C:637:GLN:CD	1:C:1008:SER:HB3	2.39	0.43
1:C:705:GLN:O	1:C:709:MET:HG2	2.18	0.43
1:A:178:PRO:HD2	1:A:181:ILE:HD12	2.00	0.43
1:A:908:THR:HG21	1:A:916:ARG:HG3	2.00	0.43
1:A:995:ALA:O	1:A:999:ILE:HG12	2.19	0.43
1:A:234:LEU:HD12	1:A:239:LEU:HD23	2.00	0.43
1:C:836:TYR:CE2	1:C:932:ILE:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:916:ARG:NH1	1:C:931:HIS:HB3	2.33	0.43
2:D:450:HIS:NE2	2:D:587:LYS:HA	2.34	0.43
2:D:342:GLU:HG2	2:D:346:LYS:HE3	1.99	0.43
1:C:560:THR:O	1:C:562:PRO:HD3	2.19	0.43
1:A:469:GLU:HG3	2:B:481:ARG:HH21	1.84	0.43
1:C:642:GLU:HG2	1:C:647:ASN:CG	2.39	0.43
1:C:361:TYR:CE2	1:C:366:PRO:HG3	2.54	0.43
1:A:100:LYS:HD2	2:B:493:ILE:HG23	2.01	0.43
1:A:238:GLN:NE2	1:C:863:LYS:HB2	2.34	0.43
1:C:739:MET:HG2	1:C:744:PHE:CZ	2.53	0.42
1:A:894:ILE:O	1:A:898:THR:HG23	2.19	0.42
1:C:268:SER:HA	1:C:273:ILE:HG22	2.00	0.42
1:C:713:ILE:HG12	1:C:845:VAL:HG11	2.01	0.42
1:C:862:CYS:HB3	1:C:1057:TRP:HH2	1.83	0.42
2:D:534:ARG:O	2:D:538:ILE:HG13	2.19	0.42
2:B:385:HIS:CG	2:B:385:HIS:O	2.72	0.42
2:B:389:LYS:HB3	2:B:396:LEU:HD21	2.01	0.42
1:A:885:ASN:HB3	1:A:889:ILE:HG22	2.02	0.42
1:A:705:GLN:O	1:A:709:MET:HG2	2.20	0.42
1:A:859:GLN:O	1:A:861:GLN:N	2.53	0.42
1:A:866:LEU:HD13	1:A:870:LEU:HA	2.02	0.42
1:C:38:ARG:HG2	1:C:39:GLU:OE1	2.19	0.42
1:C:701:HIS:O	1:C:705:GLN:HG3	2.20	0.42
1:C:218:GLU:OE1	1:C:264:LYS:NZ	2.53	0.42
1:C:392:TYR:CD2	1:C:394:PRO:HD2	2.54	0.42
1:C:692:CYS:HB3	1:C:699:LEU:HD13	2.02	0.42
2:D:385:HIS:O	2:D:385:HIS:CG	2.72	0.42
1:A:428:ASN:CG	1:A:462:THR:HG21	2.39	0.42
1:C:267:LEU:HG	1:C:273:ILE:HG12	2.02	0.42
1:C:405:SER:OG	1:C:455:LEU:O	2.30	0.42
2:D:570:LEU:HD23	2:D:573:LEU:HD12	2.02	0.42
1:A:912:GLY:HA3	1:A:938:LEU:CA	2.50	0.42
2:B:456:PHE:O	2:B:460:SER:N	2.49	0.42
1:A:335:ARG:HG2	1:A:388:ASN:HA	2.02	0.41
1:C:337:LYS:HB3	1:C:476:GLU:HB3	2.01	0.41
1:A:825:GLN:NE2	1:A:830:ASP:HA	2.35	0.41
1:C:565:LEU:HD22	1:C:590:TRP:CD1	2.54	0.41
1:A:190:ILE:HG12	1:A:191:ILE:N	2.36	0.41
1:A:859:GLN:O	1:A:860:ILE:C	2.58	0.41
1:C:98:PHE:CZ	2:D:490:THR:HG23	2.54	0.41
1:C:189:GLN:HB2	1:C:211:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:992:ARG:HH12	1:C:1027:ALA:C	2.22	0.41
1:C:73:VAL:HA	1:C:78:GLU:O	2.21	0.41
1:C:992:ARG:NH1	1:C:1026:LEU:O	2.52	0.41
1:C:1053:THR:HA	1:C:1064:GLN:HA	2.02	0.41
1:A:27:PRO:HD3	1:A:101:VAL:HB	2.02	0.41
1:A:427:ILE:HD11	1:A:443:LEU:HD13	2.03	0.41
1:A:565:LEU:N	1:A:566:PRO:HD2	2.36	0.41
2:D:371:THR:HG22	2:D:380:LEU:HD23	2.02	0.41
2:D:398:PHE:HE1	2:D:407:HIS:HB2	1.85	0.41
1:A:420:CYS:SG	2:B:567:LYS:HG2	2.60	0.41
2:B:449:LEU:HA	2:B:449:LEU:HD12	1.85	0.41
1:A:253:LYS:HD2	1:A:260:TYR:CZ	2.56	0.41
1:C:24:CYS:HB2	1:C:32:VAL:HG23	2.02	0.41
1:C:898:THR:HG23	1:C:964:ILE:HG12	2.03	0.41
1:A:337:LYS:O	1:A:475:LEU:HB2	2.21	0.40
2:B:355:PHE:CG	2:B:424:LEU:HD22	2.56	0.40
1:C:440:LYS:HZ2	1:C:474:GLU:HB2	1.87	0.40
1:A:545:GLU:HG2	2:B:380:LEU:O	2.21	0.40
1:C:647:ASN:HD22	1:C:649:LEU:H	1.70	0.40
1:A:368:CYS:HB3	1:A:391:ILE:HB	2.02	0.40
1:A:542:GLU:HG3	2:B:380:LEU:HD13	2.02	0.40
1:A:639:LEU:HD22	1:A:650:VAL:HG12	2.03	0.40
1:A:448:VAL:HG11	2:B:567:LYS:NZ	2.36	0.40
1:C:229:THR:HA	1:C:232:MET:CG	2.51	0.40
2:D:509:ILE:HG22	2:D:513:LYS:HE2	2.04	0.40
1:A:811:MET:HB3	1:A:811:MET:HE2	1.96	0.40
1:A:912:GLY:HA3	1:A:938:LEU:HA	2.02	0.40
1:C:905:CYS:SG	1:C:906:VAL:N	2.95	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	1010/1072 (94%)	930 (92%)	71 (7%)	9 (1%)	17	57
1	C	1000/1072 (93%)	921 (92%)	69 (7%)	10 (1%)	15	55
2	B	231/279 (83%)	196 (85%)	31 (13%)	4 (2%)	9	44
2	D	231/279 (83%)	205 (89%)	25 (11%)	1 (0%)	34	71
All	All	2472/2702 (92%)	2252 (91%)	196 (8%)	24 (1%)	15	55

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	968	ALA
1	A	1057	TRP
2	B	445	VAL
1	C	202	ASN
2	D	516	GLY
1	A	202	ASN
2	B	502	GLU
2	B	506	LYS
1	C	201	ASN
1	C	305	PRO
1	C	1057	TRP
1	A	201	ASN
1	C	969	GLN
1	A	793	LEU
2	B	503	ARG
1	C	793	LEU
1	A	200	PRO
1	A	497	ASN
1	A	843	ASP
1	C	843	ASP
1	A	860	ILE
1	C	459	ILE
1	C	159	PRO
1	C	964	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	936/976 (96%)	896 (96%)	40 (4%)	29	63
1	C	930/976 (95%)	886 (95%)	44 (5%)	26	61
2	B	223/259 (86%)	216 (97%)	7 (3%)	40	71
2	D	223/259 (86%)	221 (99%)	2 (1%)	78	90
All	All	2312/2470 (94%)	2219 (96%)	93 (4%)	31	65

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	52	GLU
1	A	60	GLN
1	A	115	ARG
1	A	199	SER
1	A	208	THR
1	A	213	HIS
1	A	227	LYS
1	A	238	GLN
1	A	242	CYS
1	A	251	ILE
1	A	328	TRP
1	A	369	ASP
1	A	378	CYS
1	A	386	TRP
1	A	420	CYS
1	A	470	THR
1	A	498	TRP
1	A	524	ARG
1	A	527	ASP
1	A	603	ASP
1	A	604	CYS
1	A	610	MET
1	A	619	LEU
1	A	704	ARG
1	A	733	LYS
1	A	741	ARG
1	A	748	LEU
1	A	810	ASP
1	A	852	ARG
1	A	863	LYS
1	A	871	GLN
1	A	876	THR

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Mol	Chain	Res	Type
1	A	918	ASN
1	A	920	ASN
1	A	942	LYS
1	A	959	ASP
1	A	1052	THR
1	A	1057	TRP
1	A	1064	GLN
2	B	332	GLU
2	B	341	GLU
2	B	347	LEU
2	B	374	LYS
2	B	466	LEU
2	B	577	ARG
2	B	581	LEU
1	C	37	LEU
1	C	52	GLU
1	C	115	ARG
1	C	201	ASN
1	C	208	THR
1	C	211	ILE
1	C	213	HIS
1	C	235	SER
1	C	238	GLN
1	C	244	LEU
1	C	245	GLU
1	C	251	ILE
1	C	278	MET
1	C	328	TRP
1	C	378	CYS
1	C	386	TRP
1	C	420	CYS
1	C	470	THR
1	C	474	GLU
1	C	475	LEU
1	C	498	TRP
1	C	546	GLN
1	C	604	CYS
1	C	704	ARG
1	C	733	LYS
1	C	748	LEU
1	C	756	ASN
1	C	802	LYS

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Mol	Chain	Res	Type
1	C	810	ASP
1	C	863	LYS
1	C	870	LEU
1	C	873	ASN
1	C	876	THR
1	C	898	THR
1	C	905	CYS
1	C	920	ASN
1	C	940	HIS
1	C	957	THR
1	C	959	ASP
1	C	1040	MET
1	C	1042	GLN
1	C	1048	HIS
1	C	1061	THR
1	C	1062	ILE
2	D	330	ASP
2	D	347	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	A	362	HIS
1	A	647	ASN
1	A	670	HIS
1	A	825	GLN
2	B	432	GLN
2	B	453	ASN
1	C	647	ASN
1	C	756	ASN
1	C	885	ASN
2	D	453	ASN
2	D	478	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
3	YO4	C	1101	-	36,36,36	0.93	2 (5%)	47,54,54	1.74	7 (14%)
4	YNZ	A	1102	-	21,28,28	1.17	2 (9%)	21,42,42	1.40	6 (28%)
4	YNZ	C	1102	-	21,28,28	1.18	2 (9%)	21,42,42	1.33	3 (14%)
3	YO4	A	1101	-	36,36,36	0.91	2 (5%)	47,54,54	1.85	9 (19%)

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
3	YO4	C	1101	-	-	8/16/28/28	0/4/4/4
4	YNZ	A	1102	-	-	2/13/32/32	0/3/3/3
4	YNZ	C	1102	-	-	2/13/32/32	0/3/3/3
3	YO4	A	1101	-	-	8/16/28/28	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1102	YNZ	C12-S2	3.91	1.76	1.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	YNZ	C12-S2	3.84	1.76	1.70
3	C	1101	YO4	C16-C18	-3.65	1.40	1.48
3	A	1101	YO4	C16-C18	-3.47	1.40	1.48
4	A	1102	YNZ	C7-N3	2.48	1.41	1.36
3	C	1101	YO4	O3-C7	-2.36	1.34	1.38
4	C	1102	YNZ	C7-N3	2.35	1.40	1.36
3	A	1101	YO4	O3-C7	-2.26	1.35	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	YO4	O3-C7-C6	7.65	123.50	115.22
3	C	1101	YO4	O3-C7-C6	6.74	122.52	115.22
3	C	1101	YO4	O3-C8-N2	4.08	116.64	111.55
3	A	1101	YO4	O3-C8-N2	3.97	116.50	111.55
3	A	1101	YO4	C7-O3-C8	3.86	124.26	118.03
3	C	1101	YO4	C9-N2-C15	3.61	119.56	112.62
3	C	1101	YO4	C7-O3-C8	3.31	123.38	118.03
3	A	1101	YO4	O3-C7-C19	-3.31	117.32	121.27
3	C	1101	YO4	C5-C4-N1	3.24	115.10	108.95
4	A	1102	YNZ	C14-C13-N5	3.02	125.68	122.93
3	C	1101	YO4	C5-C4-C6	-2.94	107.37	111.60
3	A	1101	YO4	C5-C4-C6	-2.91	107.41	111.60
3	A	1101	YO4	C5-C4-N1	2.83	114.31	108.95
4	C	1102	YNZ	C1-C4-N1	2.78	107.15	103.03
4	C	1102	YNZ	C11-C12-S2	-2.62	108.58	111.79
4	C	1102	YNZ	C3-N1-C4	-2.46	108.09	112.00
3	A	1101	YO4	C10-C9-N2	-2.46	106.06	110.92
4	A	1102	YNZ	C1-C4-N1	2.30	106.44	103.03
3	C	1101	YO4	O3-C7-C19	-2.28	118.54	121.27
4	A	1102	YNZ	C3-N1-C4	-2.25	108.43	112.00
4	A	1102	YNZ	C2-C3-N1	2.24	107.18	103.25
3	A	1101	YO4	C9-N2-C15	2.24	116.93	112.62
4	A	1102	YNZ	O1-C5-N2	-2.17	119.22	123.00
4	A	1102	YNZ	C11-C12-S2	-2.12	109.18	111.79
3	A	1101	YO4	C17-C16-C18	2.09	119.73	116.27

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	YO4	C16-C8-N2-C15

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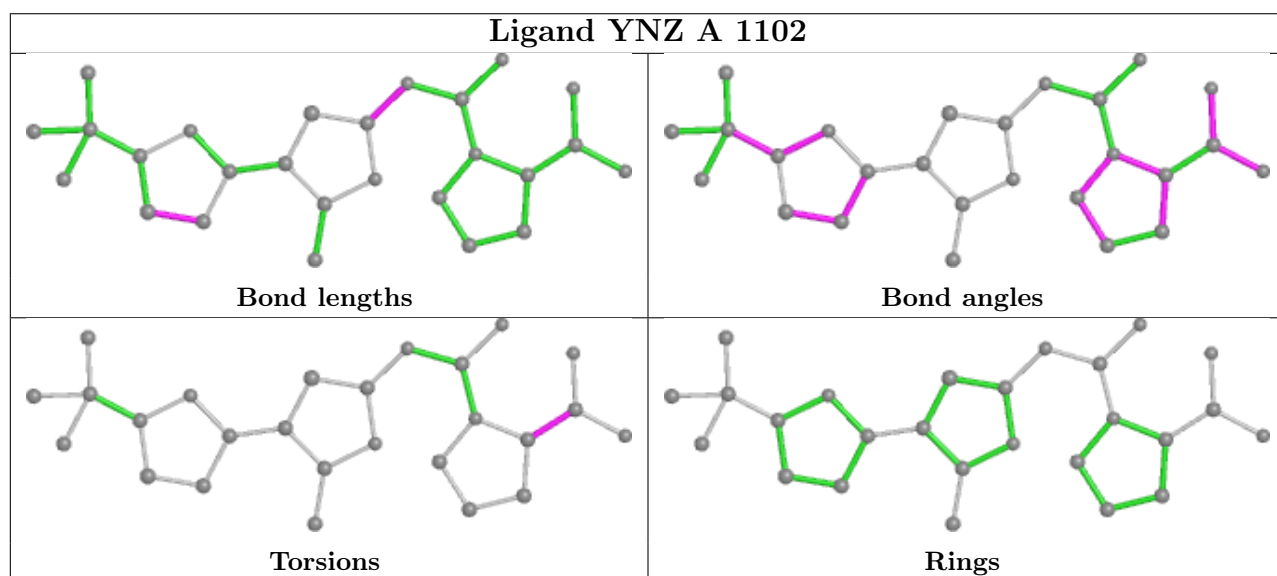
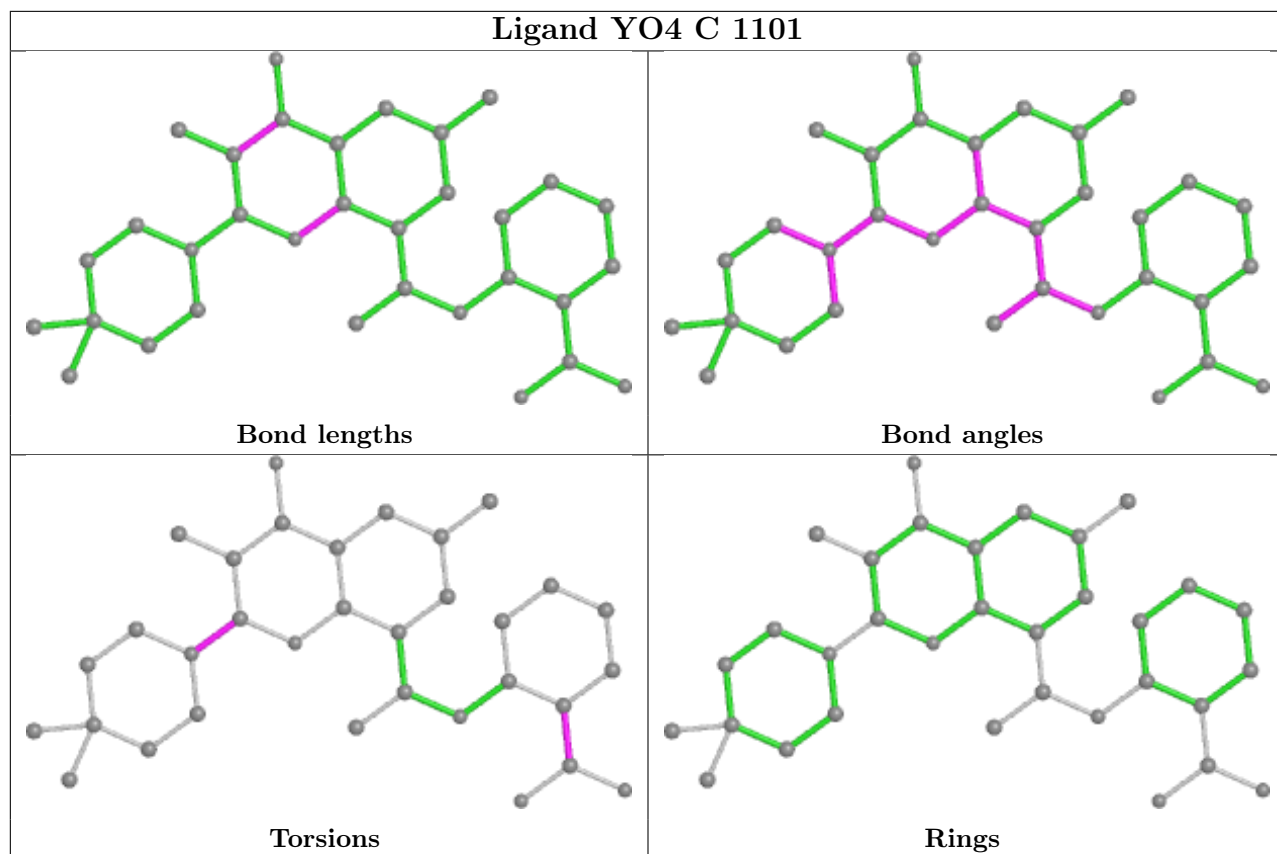
Mol	Chain	Res	Type	Atoms
3	A	1101	YO4	C16-C8-N2-C9
3	A	1101	YO4	O3-C8-N2-C15
3	A	1101	YO4	O3-C8-N2-C9
3	C	1101	YO4	C16-C8-N2-C15
3	C	1101	YO4	C16-C8-N2-C9
3	C	1101	YO4	O3-C8-N2-C15
3	C	1101	YO4	O3-C8-N2-C9
4	C	1102	YNZ	N1-C4-C5-N2
3	C	1101	YO4	O2-C1-C2-C3
4	A	1102	YNZ	N1-C4-C5-N2
4	A	1102	YNZ	N1-C4-C5-O1
4	C	1102	YNZ	N1-C4-C5-O1
3	C	1101	YO4	O1-C1-C2-C3
3	A	1101	YO4	O2-C1-C2-C3
3	A	1101	YO4	O1-C1-C2-C3
3	C	1101	YO4	O2-C1-C2-C27
3	C	1101	YO4	O1-C1-C2-C27
3	A	1101	YO4	O1-C1-C2-C27
3	A	1101	YO4	O2-C1-C2-C27

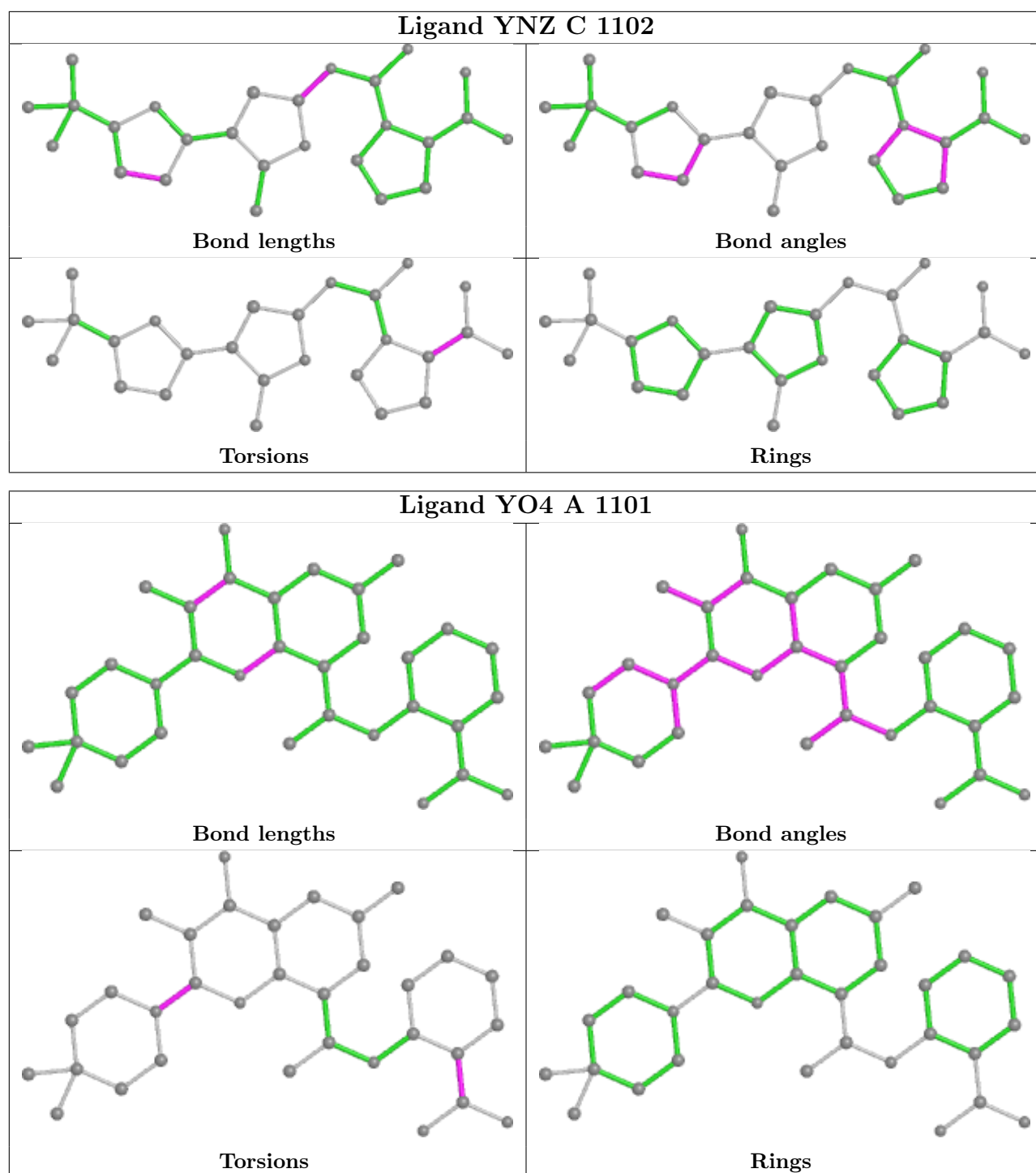
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1102	YNZ	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	1020/1072 (95%)	-0.16	0 100 100	68, 116, 188, 264	0
1	C	1012/1072 (94%)	-0.04	25 (2%) 57 39	64, 124, 220, 307	0
2	B	239/279 (85%)	0.57	38 (15%) 1 1	95, 167, 292, 350	0
2	D	239/279 (85%)	1.21	71 (29%) 0 0	135, 228, 338, 405	0
All	All	2510/2702 (92%)	0.09	134 (5%) 26 15	64, 130, 259, 405	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	371	THR	9.0
2	D	372	LEU	7.2
2	D	424	LEU	7.2
2	B	372	LEU	7.1
2	D	369	THR	6.5
2	D	381	ILE	6.3
2	D	371	THR	6.2
2	D	370	LEU	6.0
2	D	404	LEU	5.9
2	D	337	ASP	5.4
1	C	341	ALA	5.4
2	D	405	ILE	5.3
2	D	354	THR	5.3
2	D	357	VAL	5.1
2	D	335	TRP	5.1
2	B	349	ASP	4.9
2	B	421	ASP	4.8
2	D	346	LYS	4.8
1	C	340	CYS	4.7
2	B	335	TRP	4.6
2	D	359	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	D	358	ARG	4.6
2	B	356	LEU	4.5
2	B	329	GLN	4.5
2	D	390	TYR	4.5
2	D	347	LEU	4.4
2	D	355	PHE	4.3
2	D	356	LEU	4.3
2	D	425	LEU	4.1
2	D	392	PHE	4.1
2	D	401	VAL	4.1
2	D	339	SER	4.1
2	D	406	ASN	4.0
2	B	402	VAL	4.0
2	B	352	ASP	4.0
2	D	329	GLN	4.0
2	D	378	ASN	3.9
2	D	391	GLY	3.9
2	D	402	VAL	3.8
1	C	423	ALA	3.8
2	D	427	PRO	3.8
2	D	328	LEU	3.7
2	B	341	GLU	3.7
2	B	355	PHE	3.6
2	B	392	PHE	3.5
2	B	379	LYS	3.5
2	D	429	SER	3.5
2	D	513	LYS	3.4
2	B	401	VAL	3.3
1	C	350	ASP	3.3
2	D	408	TYR	3.3
2	B	380	LEU	3.2
2	D	334	TYR	3.2
2	D	423	LYS	3.1
2	B	328	LEU	3.1
1	C	484	VAL	3.1
2	B	374	LYS	3.1
2	B	358	ARG	3.1
1	C	347	ASN	3.0
2	B	405	ILE	3.0
1	C	338	ILE	3.0
2	D	336	GLY	3.0
2	D	374	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	361	SER	3.0
2	B	424	LEU	3.0
2	D	327	SER	2.9
2	D	338	ILE	2.9
2	D	426	TYR	2.9
2	D	351	ALA	2.9
2	B	354	THR	2.9
2	D	380	LEU	2.9
2	D	400	SER	2.9
2	D	382	LYS	2.8
2	D	342	GLU	2.8
1	C	61	LEU	2.8
2	D	407	HIS	2.8
2	D	379	LYS	2.8
1	C	940	HIS	2.8
2	D	421	ASP	2.7
2	B	388	GLY	2.7
2	D	383	ILE	2.7
2	D	428	VAL	2.7
2	B	368	TYR	2.7
2	B	369	THR	2.7
2	B	336	GLY	2.7
2	D	384	PHE	2.7
2	D	353	GLY	2.7
2	D	350	THR	2.6
2	D	447	LYS	2.6
1	C	354	ILE	2.6
1	C	441	MET	2.6
2	B	382	LYS	2.6
2	D	341	GLU	2.6
2	D	399	SER	2.6
1	C	1007	GLY	2.6
2	D	352	ASP	2.5
2	B	370	LEU	2.5
1	C	346	VAL	2.5
2	B	427	PRO	2.5
2	D	349	ASP	2.5
2	B	422	VAL	2.5
2	D	387	ASP	2.5
2	D	576	THR	2.5
2	D	373	ARG	2.5
1	C	806	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	477	PHE	2.4
1	C	381	PRO	2.4
2	D	377	ASN	2.4
2	B	406	ASN	2.4
2	B	387	ASP	2.4
1	C	349	ARG	2.3
2	B	384	PHE	2.3
2	B	373	ARG	2.3
2	B	383	ILE	2.3
1	C	1009	GLY	2.3
1	C	388	ASN	2.3
2	D	340	ARG	2.3
2	B	357	VAL	2.3
1	C	475	LEU	2.2
2	D	345	GLU	2.2
1	C	554	HIS	2.2
1	C	336	ILE	2.2
2	B	330	ASP	2.2
2	B	333	TRP	2.2
1	C	330	ILE	2.2
2	B	420	LEU	2.2
2	D	508	TYR	2.1
2	D	410	ASN	2.1
2	D	333	TRP	2.1
2	D	509	ILE	2.1
1	C	1014	GLN	2.1
1	C	1008	SER	2.0
2	D	330	ASP	2.0
2	D	398	PHE	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](#)

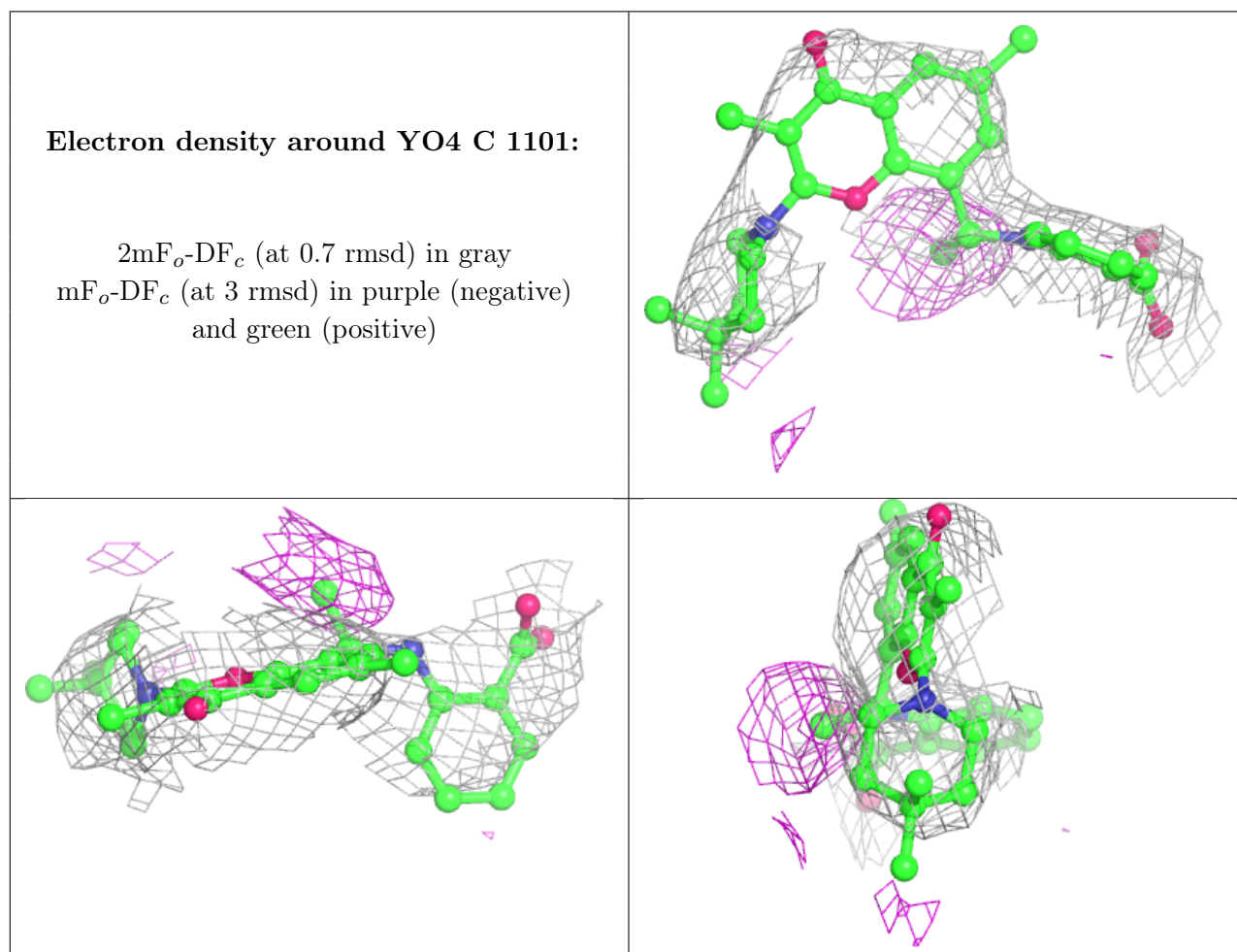
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

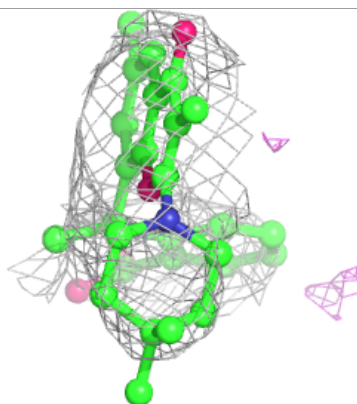
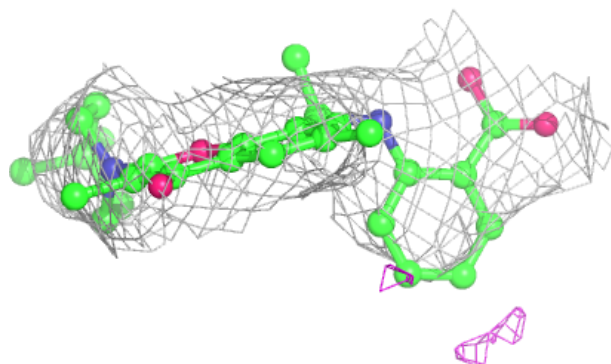
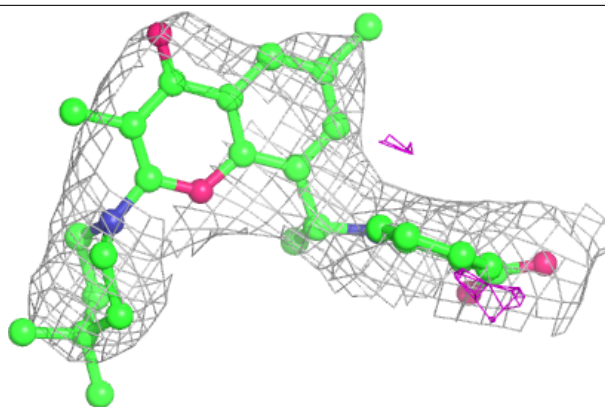
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	YO4	C	1101	33/33	0.91	0.54	98,116,151,161	0
3	YO4	A	1101	33/33	0.94	0.44	89,107,121,131	0
4	YNZ	A	1102	26/26	0.94	0.28	91,107,115,120	0
4	YNZ	C	1102	26/26	0.94	0.29	91,101,109,113	0

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.

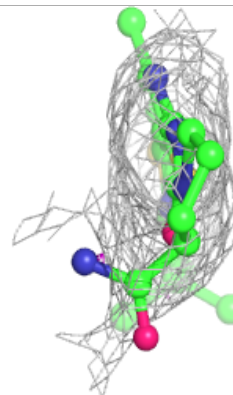
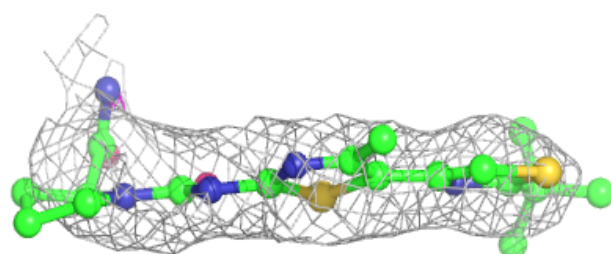
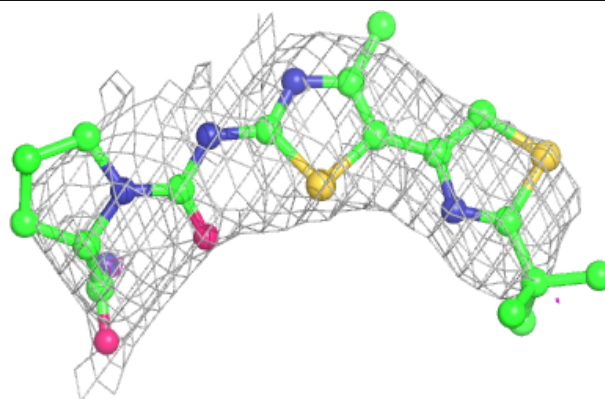


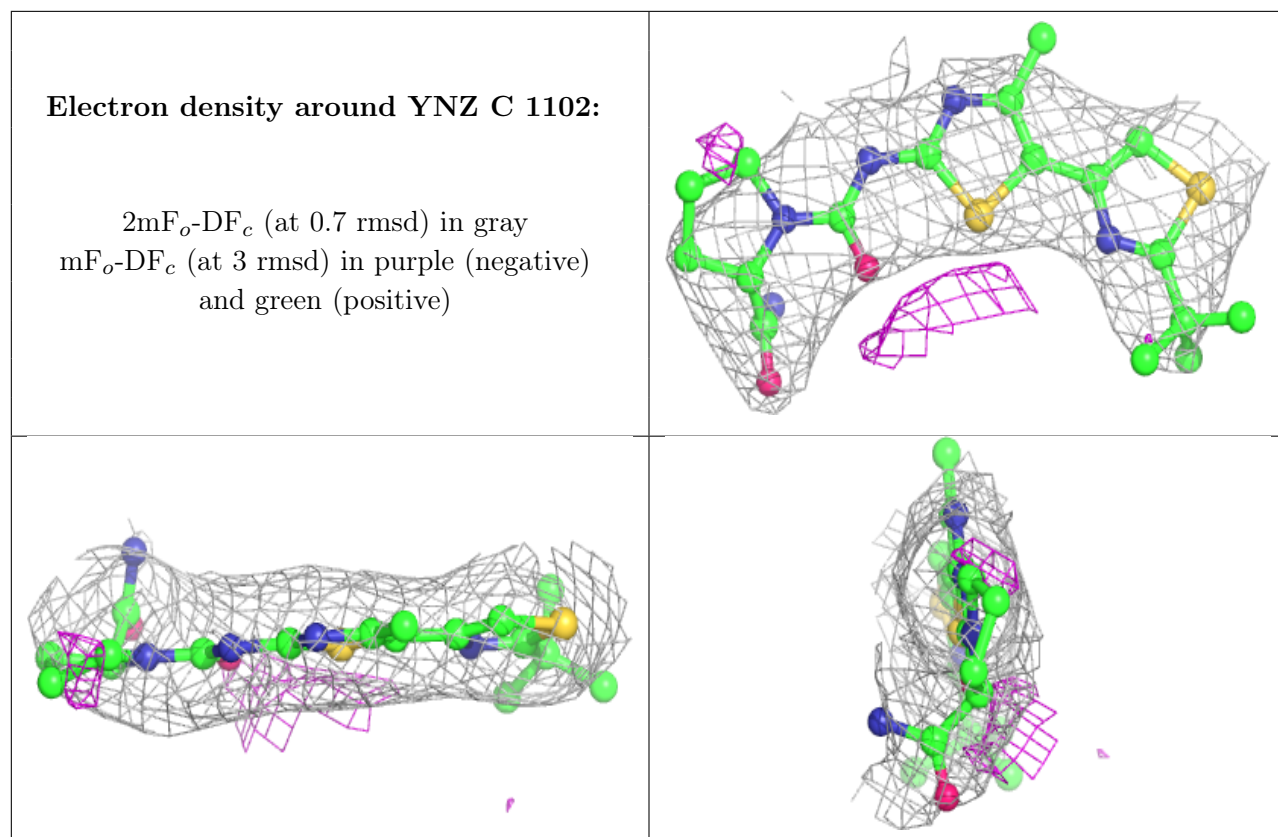
Electron density around YO4 A 1101:

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

**Electron density around YNZ 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.