



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:10 PM UTC

PDB ID : 8V8I / pdb_00008v8i
Title : PI3Ka H1047R co-crystal structure with inhibitor in cryptic pocket (compound 5).
Authors : Gunn, R.J.; Lawson, J.D.
Deposited on : 2023-12-05
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

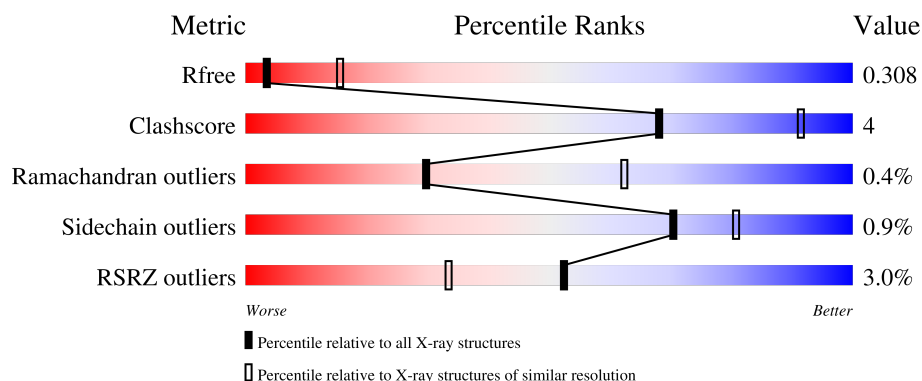
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	1072	2% 81% 11% 8%
1	C	1072	2% 80% 12% 8%
2	B	279	6% 63% 11% 24%
2	D	279	5% 68% 11% 20%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20052 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	990	Total	C	N	O	S	0	0	0
			8097	5183	1377	1469	68			
1	C	988	Total	C	N	O	S	0	0	0
			8083	5175	1375	1465	68			

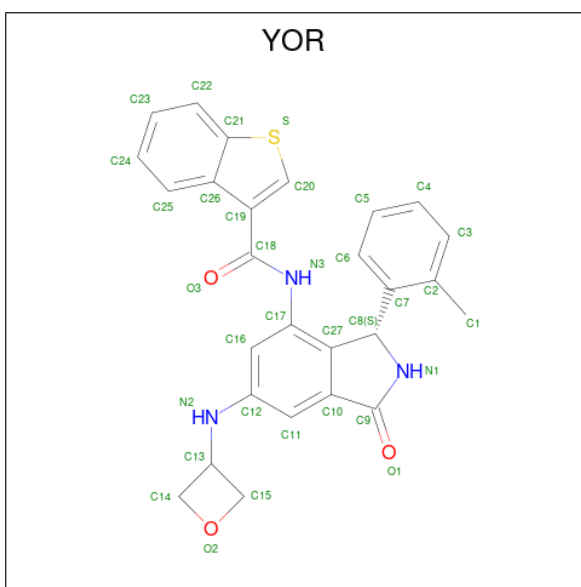
There are 10 discrepancies between the modelled and reference sequences:

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.

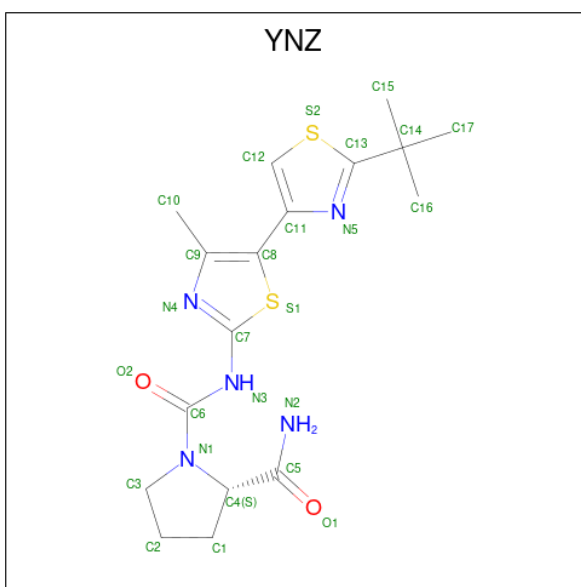
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1818	1140	326	347	5			
2	D	222	Total	C	N	O	S	0	0	0
			1903	1193	341	364	5			

- Molecule 3 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: C₂₇H₂₃N₃O₃S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 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
4	A	1	Total	C	N	O	S	0	0
			26	17	5	2	2		

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		

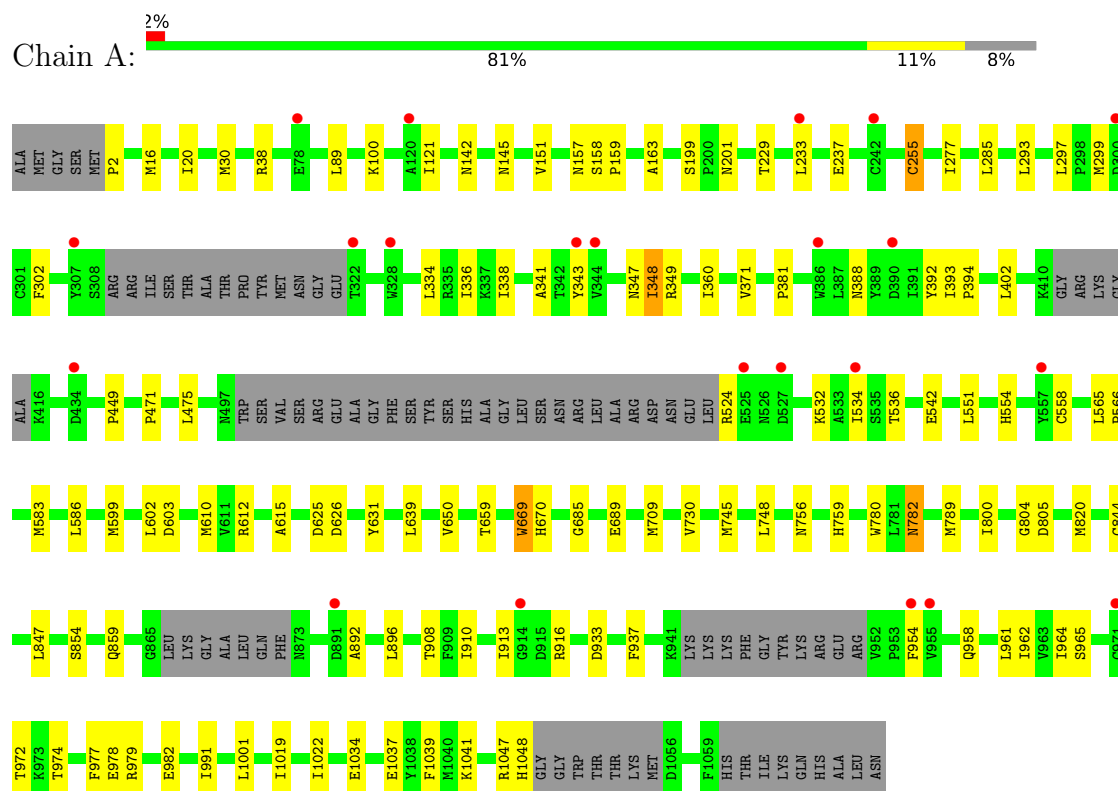
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O	0	0
			12	12		
6	C	17	Total	O	0	0
			17	17		
6	D	1	Total	O	0	0
			1	1		

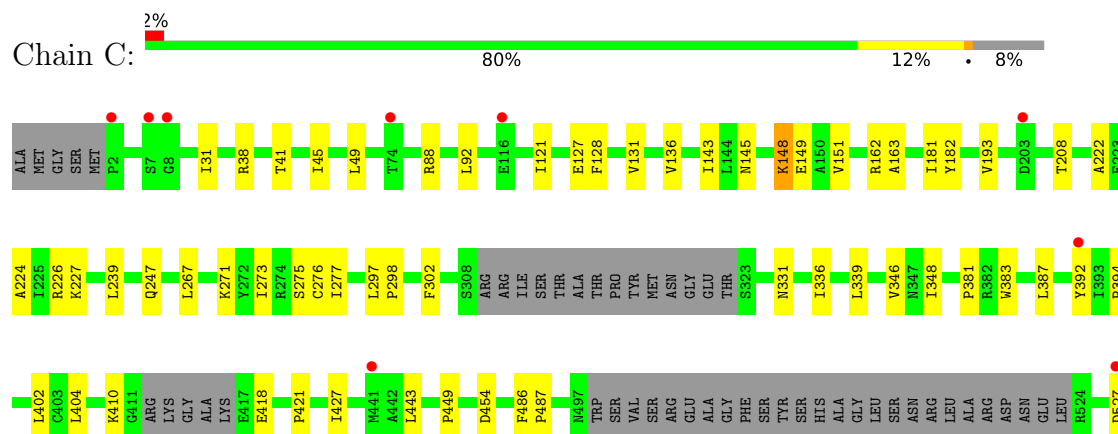
3 Residue-property plots [i](#)

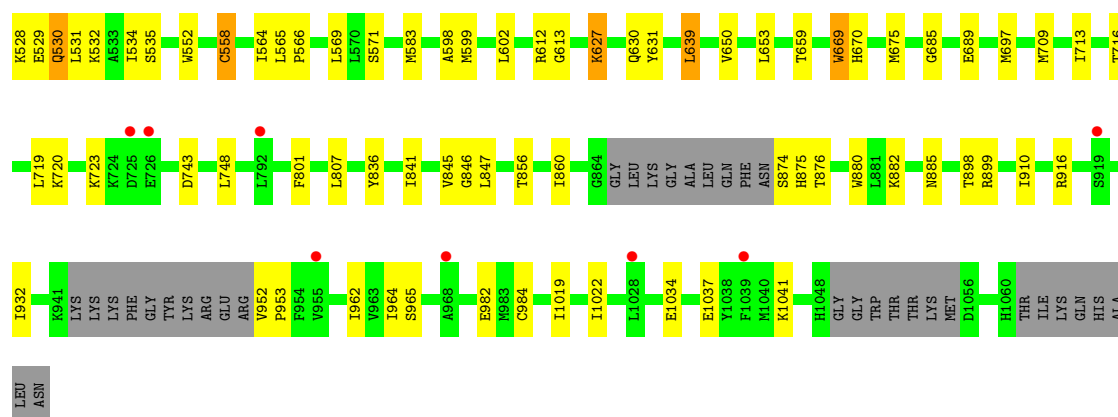
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

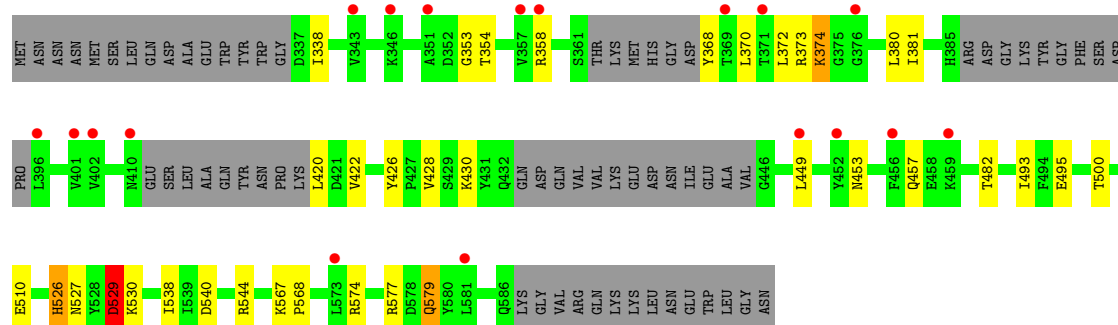


- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

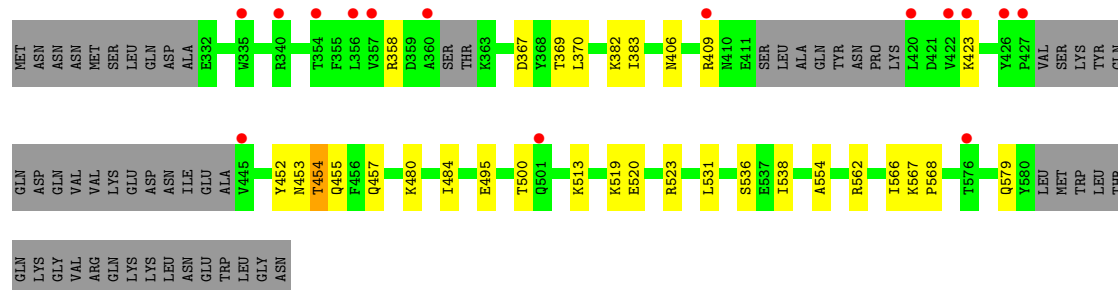




• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.56Å 124.07Å 166.47Å 90.00° 93.57° 90.00°	Depositor
Resolution (Å)	19.99 – 3.20 19.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.99-3.20) 99.2 (19.99-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.277 , 0.310 0.275 , 0.308	Depositor DCC
R_{free} test set	2741 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20052	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: YOR, YNZ, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.03	17/8277 (0.2%)	1.24	11/11187 (0.1%)
1	C	1.05	21/8264 (0.3%)	1.24	6/11170 (0.1%)
2	B	1.01	3/1841 (0.2%)	1.33	4/2455 (0.2%)
2	D	1.10	10/1933 (0.5%)	1.32	2/2580 (0.1%)
All	All	1.04	51/20315 (0.3%)	1.25	23/27392 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	LEU	C-O	-7.30	1.15	1.23
1	A	730	VAL	C-O	7.01	1.32	1.24
2	D	370	LEU	C-O	7.00	1.32	1.24
1	C	387	LEU	C-O	-6.91	1.15	1.24
1	C	162	ARG	C-O	6.85	1.31	1.24
1	C	552	TRP	C-O	6.73	1.31	1.24
1	C	583	MET	C-O	6.54	1.31	1.24
1	A	338	ILE	C-O	6.46	1.31	1.23
1	C	876	THR	C-O	6.34	1.31	1.24
1	C	598	ALA	C-O	6.31	1.31	1.24
2	D	538	ILE	C-O	6.27	1.31	1.24
1	C	627	LYS	C-O	6.26	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	610	MET	C-O	6.19	1.31	1.24
2	B	495	GLU	C-O	6.19	1.31	1.24
1	A	820	MET	C-O	6.13	1.31	1.24
2	D	513	LYS	C-O	6.09	1.31	1.24
2	D	536	SER	C-O	6.00	1.31	1.24
1	A	142	ASN	C-O	5.99	1.31	1.24
1	A	277	ILE	C-O	5.92	1.30	1.24
2	D	495	GLU	C-O	5.80	1.30	1.24
2	D	454	THR	C-O	5.76	1.30	1.24
2	B	510	GLU	C-O	5.76	1.30	1.24
2	B	538	ILE	C-O	5.75	1.30	1.24
1	C	669	TRP	C-O	5.70	1.30	1.24
2	D	562	ARG	C-O	5.61	1.30	1.24
1	C	224	ALA	C-O	5.57	1.30	1.24
1	A	978	GLU	C-O	5.54	1.30	1.24
1	C	639	LEU	C-O	5.54	1.31	1.24
1	C	181	ILE	C-O	5.53	1.30	1.24
1	C	182	TYR	C-O	5.53	1.30	1.24
2	D	519	LYS	C-O	5.49	1.31	1.24
2	D	554	ALA	C-O	5.49	1.30	1.24
1	A	896	LEU	C-O	5.46	1.30	1.24
1	C	276	CYS	C-O	5.45	1.30	1.24
1	A	145	ASN	C-O	5.44	1.30	1.24
1	A	669	TRP	C-O	5.41	1.30	1.24
1	C	148	LYS	C-O	5.40	1.30	1.24
1	C	984	CYS	C-O	5.32	1.30	1.24
1	C	277	ILE	C-O	5.26	1.30	1.24
1	C	271	LYS	C-O	5.25	1.30	1.24
1	A	685	GLY	C-O	5.22	1.30	1.23
1	C	275	SER	C-O	-5.21	1.18	1.24
1	A	293	LEU	C-O	5.21	1.29	1.24
1	A	583	MET	C-O	5.20	1.30	1.24
1	A	745	MET	C-O	5.20	1.30	1.24
1	C	613	GLY	C-O	5.20	1.30	1.23
1	A	859	GLN	C-O	5.18	1.30	1.24
2	D	566	ILE	C-O	5.10	1.30	1.24
1	A	586	LEU	C-O	5.07	1.29	1.24
1	C	239	LEU	C-O	5.05	1.30	1.24
1	C	127	GLU	C-O	5.04	1.29	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	801	PHE	CA-C-O	-8.01	111.79	120.36
1	C	836	TYR	CA-C-N	6.23	125.90	119.92
1	C	836	TYR	C-N-CA	6.23	125.90	119.92
1	A	782	ASN	CA-C-O	-6.18	113.55	120.66
1	A	1001	LEU	CA-C-O	-6.05	114.47	120.82
1	A	157	ASN	CA-C-N	5.74	127.95	120.26
1	A	157	ASN	C-N-CA	5.74	127.95	120.26
2	B	529	ASP	CA-C-O	-5.63	114.58	120.55
1	A	910	ILE	CA-C-O	-5.58	115.15	120.95
1	C	1041	LYS	CA-C-O	-5.55	114.99	120.82
1	C	298	PRO	CA-C-O	-5.45	115.32	121.43
1	A	805	ASP	CA-C-O	-5.44	114.94	120.71
1	A	615	ALA	CA-C-O	-5.41	115.12	121.07
2	B	526	HIS	N-CA-C	-5.35	104.69	111.11
1	A	892	ALA	CA-C-O	-5.33	113.51	119.79
2	B	500	THR	CA-C-O	-5.22	115.52	121.00
2	B	530	LYS	CA-C-O	-5.22	114.89	120.42
1	A	255	CYS	CA-C-O	-5.18	114.57	120.58
1	A	972	THR	N-CA-C	-5.16	104.58	111.24
2	D	500	THR	CA-C-N	5.15	127.60	120.29
2	D	500	THR	C-N-CA	5.15	127.60	120.29
1	A	1001	LEU	O-C-N	5.04	127.26	122.07
1	C	49	LEU	O-C-N	5.01	127.50	122.09

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	782	ASN	Mainchain
2	B	529	ASP	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8097	0	8110	52	0
1	C	8083	0	8091	65	0
2	B	1818	0	1822	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1903	0	1877	12	0
3	A	34	0	0	0	0
3	C	34	0	0	0	0
4	A	26	0	0	1	0
4	C	26	0	0	1	0
5	C	1	0	0	0	0
6	A	12	0	0	0	0
6	C	17	0	0	0	0
6	D	1	0	0	0	0
All	All	20052	0	19900	143	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 4.

All (143) 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:343:TYR:HB2	1:A:471:PRO:HA	1.59	0.83
2:B:353:GLY:N	2:B:373:ARG:O	2.15	0.78
1:C:131:VAL:HG21	1:C:136:VAL:HG11	1.66	0.78
2:B:354:THR:HG22	2:B:426:TYR:HB3	1.71	0.72
1:A:916:ARG:NH2	1:A:933:ASP:O	2.23	0.71
1:C:128:PHE:O	1:C:131:VAL:HG22	1.94	0.67
1:C:529:GLU:C	1:C:531:LEU:H	2.03	0.66
1:A:347:ASN:O	1:A:348:ILE:HG22	1.96	0.66
2:B:574:ARG:O	2:B:577:ARG:HB3	1.97	0.63
1:C:348:ILE:HG22	1:C:348:ILE:O	2.01	0.61
1:A:958:GLN:O	1:A:962:ILE:HG12	2.01	0.61
1:C:1019:ILE:O	1:C:1022:ILE:HG22	1.99	0.61
1:A:199:SER:O	1:A:201:ASN:O	2.19	0.60
1:A:602:LEU:O	1:A:612:ARG:NH2	2.36	0.58
2:B:449:LEU:HD13	2:B:579:GLN:CD	2.28	0.58
1:A:16:MET:HB3	1:A:20:ILE:HD11	1.86	0.58
1:C:675:MET:HE1	1:C:685:GLY:HA3	1.85	0.58
2:B:526:HIS:O	2:B:529:ASP:HB2	2.03	0.57
1:C:602:LEU:O	1:C:612:ARG:NH2	2.38	0.57
1:C:41:THR:O	1:C:45:ILE:HG12	2.04	0.57
1:C:421:PRO:HG3	1:C:454:ASP:O	2.05	0.57
1:C:675:MET:HE1	1:C:685:GLY:CA	2.35	0.56
1:C:962:ILE:HG22	1:C:962:ILE:O	2.03	0.56
1:C:410:LYS:HB3	1:C:418:GLU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:874:SER:O	1:C:875:HIS:HB2	2.06	0.56
1:A:804:GLY:C	1:A:844:CYS:HB3	2.31	0.56
2:B:453:ASN:O	2:B:457:GLN:HG2	2.06	0.56
1:C:558:CYS:SG	1:C:564:ILE:HD11	2.46	0.56
1:C:151:VAL:HG21	1:C:302:PHE:HB2	1.88	0.55
1:C:131:VAL:HG21	1:C:136:VAL:CG1	2.37	0.54
1:C:599:MET:HE1	1:C:631:TYR:CD2	2.43	0.53
1:C:713:ILE:HG12	1:C:845:VAL:HG11	1.90	0.53
1:A:121:ILE:HD11	1:A:689:GLU:HA	1.90	0.53
1:A:1047:ARG:O	1:A:1048:HIS:HB2	2.08	0.53
2:D:453:ASN:O	2:D:457:GLN:HG2	2.09	0.53
1:C:193:VAL:HG22	1:C:208:THR:HG22	1.91	0.53
1:C:121:ILE:HD11	1:C:689:GLU:HA	1.89	0.53
1:C:226:ARG:O	1:C:227:LYS:C	2.51	0.53
1:A:974:THR:H	1:A:977:PHE:HB3	1.74	0.53
1:A:542:GLU:HB2	2:B:380:LEU:CD1	2.38	0.52
1:A:2:PRO:HG2	2:B:482:THR:HG22	1.92	0.52
1:C:860:ILE:HD12	1:C:880:TRP:CD2	2.43	0.52
1:C:841:ILE:HG13	1:C:845:VAL:HG23	1.92	0.52
1:A:1019:ILE:O	1:A:1022:ILE:HG22	2.10	0.51
1:C:898:THR:HG22	1:C:964:ILE:HD13	1.92	0.51
1:A:599:MET:HE1	1:A:631:TYR:CD2	2.45	0.51
1:C:163:ALA:HB2	1:C:297:LEU:HD11	1.92	0.51
1:A:908:THR:HA	1:A:913:ILE:HG13	1.93	0.50
1:A:255:CYS:SG	1:A:789:MET:CE	3.00	0.50
2:B:372:LEU:HD21	2:B:374:LYS:HD2	1.93	0.50
1:A:38:ARG:O	1:A:89:LEU:HB3	2.12	0.50
1:A:151:VAL:HG11	1:A:302:PHE:HB3	1.92	0.49
2:D:406:ASN:HA	2:D:409:ARG:HB3	1.93	0.49
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.92	0.49
1:A:229:THR:O	1:A:229:THR:HG22	2.12	0.49
1:C:565:LEU:N	1:C:566:PRO:HD2	2.28	0.49
1:A:565:LEU:N	1:A:566:PRO:HD2	2.27	0.48
1:A:534:ILE:HD12	1:A:551:LEU:HD11	1.95	0.48
1:C:962:ILE:O	1:C:962:ILE:CG2	2.61	0.48
2:D:520:GLU:O	2:D:523:ARG:N	2.39	0.48
1:A:392:TYR:CD2	1:A:394:PRO:HD2	2.48	0.48
1:C:709:MET:HE1	1:C:847:LEU:HD21	1.96	0.48
1:A:158:SER:N	1:A:159:PRO:HD2	2.28	0.48
1:C:882:LYS:O	1:C:885:ASN:O	2.32	0.48
1:A:954:PHE:HZ	1:A:1039:PHE:CE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:LYS:N	2:B:568:PRO:HD2	2.29	0.47
1:C:88:ARG:O	1:C:92:LEU:HG	2.16	0.46
1:A:669:TRP:O	1:A:670:HIS:C	2.59	0.46
2:D:480:LYS:O	2:D:484:ILE:HD13	2.15	0.46
1:A:30:MET:HE3	2:B:527:ASN:CG	2.41	0.46
1:C:529:GLU:C	1:C:531:LEU:N	2.70	0.45
1:C:148:LYS:O	1:C:149:GLU:C	2.59	0.45
1:C:392:TYR:CD2	1:C:394:PRO:HD2	2.52	0.45
1:C:669:TRP:O	1:C:670:HIS:C	2.58	0.45
1:A:341:ALA:O	1:A:381:PRO:HG2	2.16	0.45
1:C:527:ASP:O	1:C:530:GLN:HB2	2.16	0.45
1:A:639:LEU:HD22	1:A:650:VAL:CG1	2.46	0.44
2:D:358:ARG:HB3	2:D:369:THR:OG1	2.17	0.44
1:A:255:CYS:SG	1:A:789:MET:HE3	2.58	0.44
2:D:369:THR:HG22	2:D:382:LYS:HG2	1.99	0.44
2:D:454:THR:O	2:D:455:GLN:C	2.61	0.44
1:A:336:ILE:HD13	1:A:402:LEU:HD22	2.00	0.44
1:C:531:LEU:C	1:C:531:LEU:HD12	2.43	0.44
1:C:916:ARG:NH1	1:C:932:ILE:O	2.50	0.44
1:A:780:TRP:CE3	1:A:800:ILE:HD11	2.53	0.44
1:C:856:THR:O	1:C:860:ILE:HG12	2.18	0.43
1:A:347:ASN:C	1:A:349:ARG:H	2.26	0.43
4:C:1102:YNZ:S1	4:C:1102:YNZ:O2	2.75	0.43
2:D:452:TYR:O	2:D:455:GLN:HB2	2.18	0.43
1:A:625:ASP:O	1:A:626:ASP:C	2.62	0.43
1:C:719:LEU:HA	1:C:723:LYS:HB2	2.01	0.43
1:A:1037:GLU:O	1:A:1041:LYS:HG2	2.18	0.43
1:C:486:PHE:CG	1:C:487:PRO:HD2	2.53	0.43
2:B:358:ARG:O	2:B:368:TYR:HA	2.19	0.43
1:A:524:ARG:HD2	1:A:554:HIS:NE2	2.34	0.43
1:A:916:ARG:NH1	1:A:937:PHE:HB2	2.34	0.43
1:A:371:VAL:HG11	1:A:388:ASN:O	2.18	0.43
2:B:579:GLN:HE21	2:B:579:GLN:HA	1.84	0.43
1:C:427:ILE:HD11	1:C:443:LEU:HD22	2.01	0.43
1:A:2:PRO:CG	2:B:482:THR:HG22	2.49	0.42
1:A:964:ILE:HD12	1:A:965:SER:N	2.33	0.42
2:B:574:ARG:O	2:B:577:ARG:N	2.49	0.42
1:C:528:LYS:O	1:C:531:LEU:N	2.52	0.42
2:D:367:ASP:HB3	2:D:383:ILE:O	2.18	0.42
2:D:567:LYS:N	2:D:568:PRO:HD2	2.34	0.42
1:C:38:ARG:NH1	1:C:743:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:ASN:HD22	1:A:759:HIS:CE1	2.37	0.42
1:A:709:MET:HE1	1:A:847:LEU:HD21	2.01	0.42
2:B:540:ASP:O	2:B:544:ARG:N	2.43	0.42
1:C:348:ILE:O	1:C:348:ILE:CG2	2.68	0.42
1:C:143:ILE:C	1:C:145:ASN:N	2.77	0.42
1:A:979:ARG:O	1:A:982:GLU:N	2.53	0.42
1:C:404:LEU:HD12	1:C:404:LEU:C	2.45	0.42
1:C:627:LYS:O	1:C:630:GLN:HB3	2.20	0.42
1:C:910:ILE:HG22	1:C:1022:ILE:HD11	2.02	0.42
1:A:603:ASP:C	1:A:603:ASP:OD1	2.63	0.41
1:C:532:LYS:C	1:C:534:ILE:N	2.76	0.41
1:C:331:ASN:O	1:C:392:TYR:CE1	2.73	0.41
1:C:639:LEU:HD21	1:C:653:LEU:HD12	2.02	0.41
1:A:393:ILE:HB	1:A:394:PRO:HD3	2.03	0.41
1:C:952:VAL:HA	1:C:953:PRO:HD3	1.94	0.41
1:C:1034:GLU:O	1:C:1037:GLU:HB2	2.20	0.41
1:A:804:GLY:N	1:A:844:CYS:O	2.39	0.41
1:C:860:ILE:HD12	1:C:880:TRP:CE2	2.55	0.41
2:D:454:THR:O	2:D:457:GLN:HB2	2.20	0.41
1:C:267:LEU:HG	1:C:273:ILE:HG12	2.03	0.41
1:C:535:SER:HB3	1:C:564:ILE:CG2	2.51	0.41
1:A:334:LEU:HD23	1:A:360:ILE:HD13	2.03	0.41
1:C:336:ILE:HD13	1:C:402:LEU:HD22	2.01	0.41
1:C:339:LEU:O	1:C:383:TRP:N	2.47	0.41
1:A:100:LYS:HD2	2:B:493:ILE:HG23	2.03	0.41
2:B:370:LEU:HB3	2:B:381:ILE:O	2.21	0.41
1:C:807:LEU:HD22	1:C:846:GLY:HA3	2.03	0.41
1:A:854:SER:O	4:A:1102:YNZ:N2	2.54	0.40
1:C:222:ALA:HB2	1:C:247:GLN:HE21	1.85	0.40
1:C:535:SER:CB	1:C:564:ILE:HG22	2.51	0.40
1:C:716:THR:O	1:C:720:LYS:HG3	2.22	0.40
2:B:420:LEU:O	2:B:422:VAL:HG13	2.21	0.40
1:C:569:LEU:C	1:C:571:SER:H	2.29	0.40
1:A:532:LYS:O	1:A:536:THR:HG23	2.22	0.40
1:A:1034:GLU:O	1:A:1037:GLU:HB2	2.22	0.40
1:C:31:ILE:HD12	2:D:531:LEU:HA	2.04	0.40
1:C:639:LEU:HD22	1:C:650:VAL:HG12	2.03	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	976/1072 (91%)	920 (94%)	52 (5%)	4 (0%)	30	62
1	C	974/1072 (91%)	913 (94%)	57 (6%)	4 (0%)	30	62
2	B	202/279 (72%)	196 (97%)	5 (2%)	1 (0%)	24	59
2	D	214/279 (77%)	200 (94%)	14 (6%)	0	100	100
All	All	2366/2702 (88%)	2229 (94%)	128 (5%)	9 (0%)	30	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	MET
1	A	348	ILE
1	A	558	CYS
1	C	558	CYS
1	C	530	GLN
1	A	449	PRO
2	B	338	ILE
1	C	381	PRO
1	C	449	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	912/976 (93%)	905 (99%)	7 (1%)	73	82
1	C	910/976 (93%)	903 (99%)	7 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	201/259 (78%)	197 (98%)	4 (2%)	48	72
2	D	207/259 (80%)	205 (99%)	2 (1%)	68	80
All	All	2230/2470 (90%)	2210 (99%)	20 (1%)	70	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	LEU
1	A	237	GLU
1	A	475	LEU
1	A	659	THR
1	A	748	LEU
1	A	961	LEU
1	A	991	ILE
2	B	374	LYS
2	B	428	VAL
2	B	430	LYS
2	B	579	GLN
1	C	346	VAL
1	C	659	THR
1	C	697	MET
1	C	748	LEU
1	C	899	ARG
1	C	965	SER
1	C	982	GLU
2	D	423	LYS
2	D	579	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	63	GLN
1	A	157	ASN
1	A	212	ASN
1	A	238	GLN
1	A	269	GLN
1	A	370	ASN
1	A	701	HIS
1	A	760	GLN

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Mol	Chain	Res	Type
1	A	763	ASN
1	A	826	ASN
1	A	936	HIS
1	A	1014	GLN
1	A	1033	GLN
2	B	455	GLN
2	B	564	ASN
1	C	47	HIS
1	C	63	GLN
1	C	114	ASN
1	C	189	GLN
1	C	247	GLN
1	C	269	GLN
1	C	530	GLN
1	C	630	GLN
1	C	701	HIS
1	C	756	ASN
1	C	760	GLN
1	C	763	ASN
1	C	855	HIS
1	C	875	HIS
2	D	407	HIS
2	D	455	GLN
2	D	501	GLN
2	D	564	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is 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
4	YNZ	C	1102	-	28,28,28	1.20	3 (10%)	37,42,42	3.44	11 (29%)
3	YOR	A	1101	-	34,39,39	0.64	0	46,57,57	2.36	8 (17%)
4	YNZ	A	1102	-	28,28,28	1.22	3 (10%)	37,42,42	3.58	14 (37%)
3	YOR	C	1101	-	34,39,39	0.66	0	46,57,57	2.38	8 (17%)

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	YNZ	C	1102	-	-	6/22/32/32	0/3/3/3
3	YOR	A	1101	-	-	5/16/34/34	0/6/6/6
4	YNZ	A	1102	-	-	6/22/32/32	0/3/3/3
3	YOR	C	1101	-	-	3/16/34/34	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	YNZ	C9-N4	-3.03	1.32	1.38
4	C	1102	YNZ	C9-N4	-2.92	1.32	1.38
4	C	1102	YNZ	C11-N5	-2.65	1.32	1.38
4	A	1102	YNZ	C11-C8	2.44	1.49	1.44
4	A	1102	YNZ	C11-N5	-2.42	1.33	1.38
4	C	1102	YNZ	C11-C8	2.00	1.48	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	YNZ	C7-N4-C9	13.19	118.43	110.38
4	C	1102	YNZ	C7-N4-C9	12.56	118.04	110.38
3	C	1101	YOR	C8-N1-C9	-9.25	108.78	114.03
3	A	1101	YOR	C8-N1-C9	-9.18	108.82	114.03
3	C	1101	YOR	C10-C9-N1	9.06	110.44	106.51
3	A	1101	YOR	C10-C9-N1	8.90	110.37	106.51
4	A	1102	YNZ	S1-C7-N4	-8.73	107.97	115.78
4	C	1102	YNZ	C11-N5-C13	8.54	118.22	110.97
4	C	1102	YNZ	S1-C7-N4	-8.39	108.27	115.78
4	A	1102	YNZ	C11-N5-C13	8.36	118.06	110.97
4	C	1102	YNZ	N3-C6-N1	5.33	121.61	115.57
4	A	1102	YNZ	C9-C8-S1	-5.19	106.70	109.94
4	A	1102	YNZ	C7-S1-C8	5.14	91.24	88.34
4	A	1102	YNZ	N3-C6-N1	4.95	121.18	115.57
3	A	1101	YOR	C19-C18-N3	4.68	120.35	114.89
4	C	1102	YNZ	C7-S1-C8	4.39	90.81	88.34
3	C	1101	YOR	C19-C18-N3	4.36	119.98	114.89
4	C	1102	YNZ	C9-C8-S1	-4.02	107.43	109.94
4	A	1102	YNZ	C4-N1-C6	3.75	125.31	119.26
4	A	1102	YNZ	S1-C7-N3	3.52	128.43	123.72
4	C	1102	YNZ	C4-N1-C6	3.39	124.74	119.26
4	C	1102	YNZ	C1-C4-N1	3.35	107.93	103.02
4	A	1102	YNZ	C1-C4-N1	3.31	107.87	103.02
3	A	1101	YOR	C21-S-C20	3.12	92.85	91.16
3	C	1101	YOR	C21-S-C20	3.03	92.80	91.16
3	C	1101	YOR	C26-C19-C20	2.97	113.01	111.63
3	A	1101	YOR	C11-C10-C9	2.85	132.55	129.66
3	C	1101	YOR	C11-C10-C9	2.81	132.51	129.66
3	A	1101	YOR	C11-C10-C27	-2.78	119.50	122.79
3	C	1101	YOR	C11-C10-C27	-2.67	119.63	122.79
4	C	1102	YNZ	S1-C7-N3	2.56	127.15	123.72
3	A	1101	YOR	C26-C19-C20	2.54	112.81	111.63
4	C	1102	YNZ	C14-C13-S2	2.36	125.46	121.51
4	A	1102	YNZ	C3-N1-C4	-2.35	108.32	112.01
4	C	1102	YNZ	C3-N1-C4	-2.27	108.44	112.01
4	A	1102	YNZ	C4-C5-N2	2.25	121.61	116.57
3	C	1101	YOR	C14-O2-C15	2.19	93.42	91.34
4	A	1102	YNZ	C12-C11-N5	-2.18	112.44	115.43
4	A	1102	YNZ	C2-C3-N1	2.17	106.97	103.24
3	A	1101	YOR	C26-C21-S	-2.11	110.02	111.46
4	A	1102	YNZ	O1-C5-N2	-2.06	119.40	123.04

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1101	YOR	C2-C7-C8-N1
4	A	1102	YNZ	S2-C13-C14-C17
4	A	1102	YNZ	S2-C13-C14-C16
4	A	1102	YNZ	S2-C13-C14-C15
4	A	1102	YNZ	N1-C4-C5-N2
4	A	1102	YNZ	N1-C4-C5-O1
4	C	1102	YNZ	N1-C4-C5-N2
3	C	1101	YOR	C6-C7-C8-N1
4	A	1102	YNZ	N4-C7-N3-C6
4	C	1102	YNZ	N1-C4-C5-O1
3	A	1101	YOR	C2-C7-C8-N1
3	A	1101	YOR	C2-C7-C8-C27
3	A	1101	YOR	C6-C7-C8-N1
4	C	1102	YNZ	N5-C13-C14-C17
4	C	1102	YNZ	N5-C13-C14-C16
4	C	1102	YNZ	N5-C13-C14-C15
4	C	1102	YNZ	N5-C11-C8-C9
3	A	1101	YOR	C16-C17-N3-C18
3	A	1101	YOR	C27-C17-N3-C18
3	C	1101	YOR	C27-C17-N3-C18

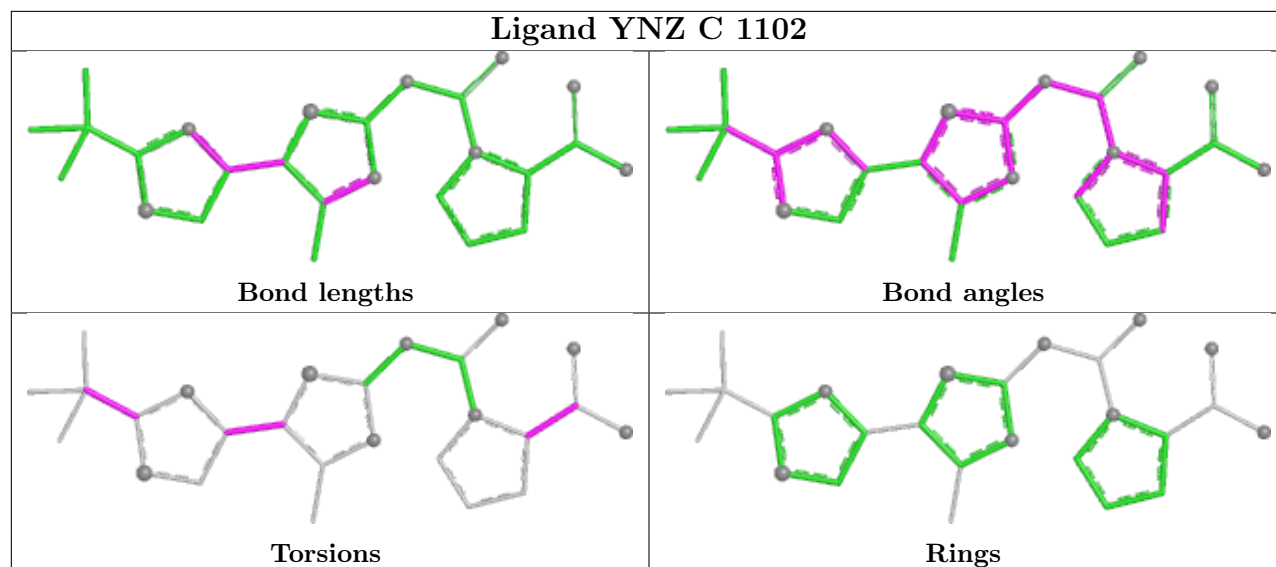
There are no ring outliers.

2 monomers are involved in 2 short contacts:

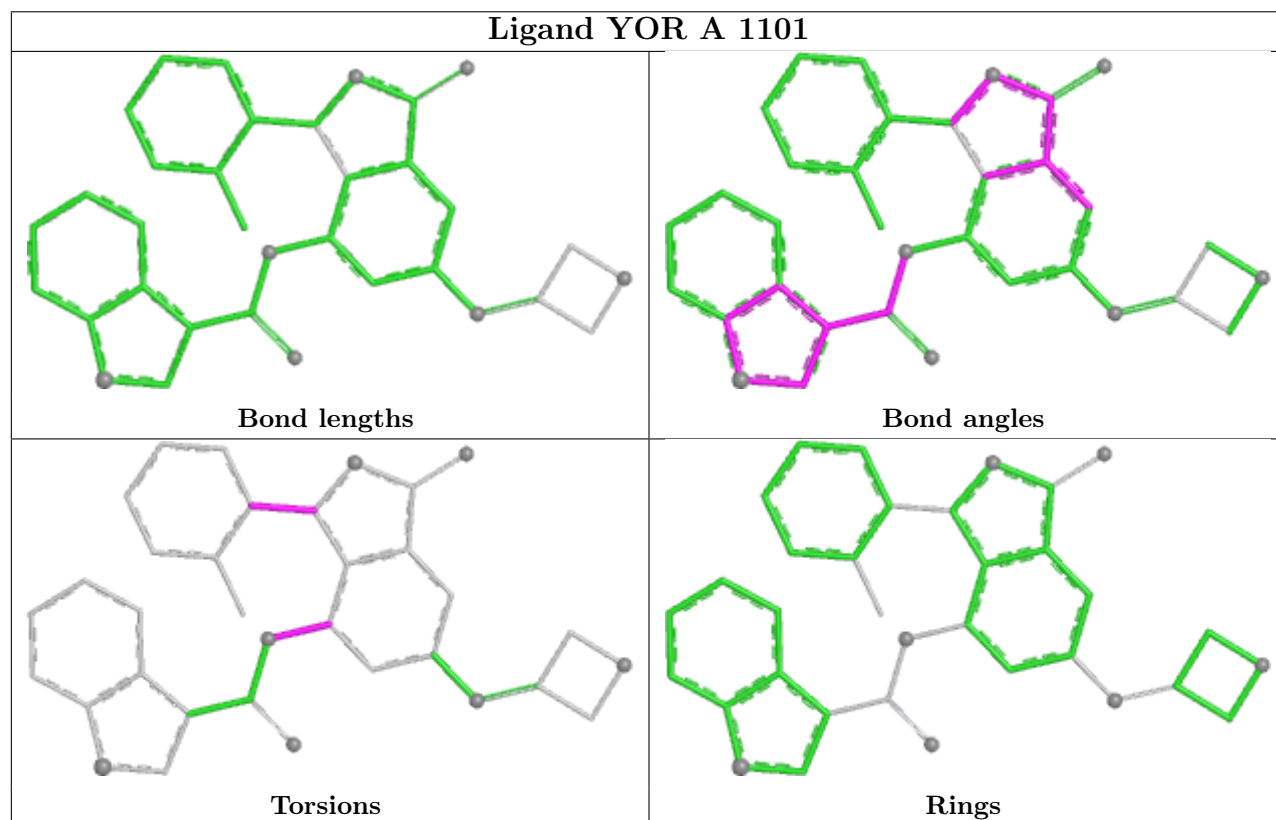
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1102	YNZ	1	0
4	A	1102	YNZ	1	0

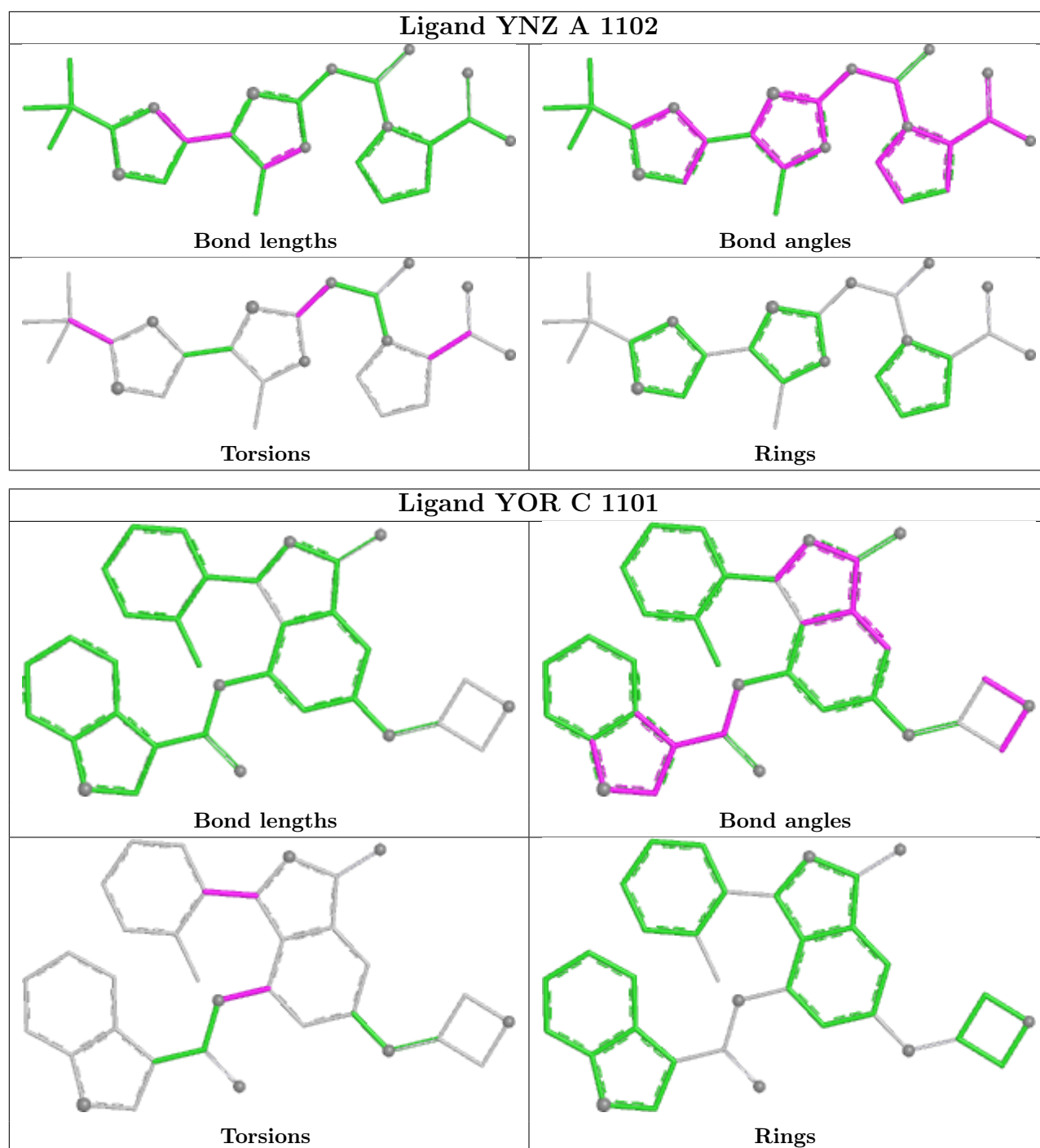
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand YNZ C 1102



Ligand YOR 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 ⓘ

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	990/1072 (92%)	0.42	22 (2%)	62 42	60, 90, 125, 150	0
1	C	988/1072 (92%)	0.28	17 (1%)	69 49	48, 79, 111, 139	0
2	B	212/279 (75%)	0.69	18 (8%)	16 11	67, 126, 168, 176	0
2	D	222/279 (79%)	0.70	15 (6%)	23 15	73, 121, 160, 171	0
All	All	2412/2702 (89%)	0.41	72 (2%)	52 33	48, 87, 145, 176	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	356	LEU	4.6
1	A	328	TRP	4.0
1	A	954	PHE	3.9
2	D	576	THR	3.8
2	B	357	VAL	3.4
2	D	445	VAL	3.4
2	D	357	VAL	3.3
1	A	955	VAL	3.1
2	B	351	ALA	3.1
2	D	335	TRP	3.1
1	A	78	GLU	3.0
1	A	914	GLY	3.0
2	B	358	ARG	3.0
2	B	456	PHE	3.0
1	C	392	TYR	2.9
1	C	7	SER	2.9
2	B	396	LEU	2.9
2	D	360	ALA	2.8
2	B	346	LYS	2.8
1	C	792	LEU	2.7
1	A	343	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	971	CYS	2.7
2	B	459	LYS	2.7
1	C	116	GLU	2.6
1	A	557	TYR	2.6
1	A	233	LEU	2.6
2	B	376	GLY	2.6
2	B	343	VAL	2.6
2	B	402	VAL	2.6
1	C	1028	LEU	2.5
2	B	401	VAL	2.5
1	A	434	ASP	2.5
1	A	322	THR	2.4
2	B	369	THR	2.4
2	B	371	THR	2.4
2	D	420	LEU	2.4
1	C	8	GLY	2.4
2	D	501	GLN	2.4
1	C	441	MET	2.4
2	B	581	LEU	2.4
1	C	919	SER	2.4
2	D	427	PRO	2.4
1	A	300	ASP	2.4
1	A	390	ASP	2.4
1	A	525	GLU	2.4
1	C	203	ASP	2.3
1	A	307	TYR	2.3
1	A	534	ILE	2.3
2	D	422	VAL	2.3
2	B	410	ASN	2.2
1	A	891	ASP	2.2
2	B	573	LEU	2.2
2	D	354	THR	2.2
2	B	449	LEU	2.2
1	C	968	ALA	2.2
1	A	386	TRP	2.2
2	D	426	TYR	2.2
1	C	725	ASP	2.2
2	D	423	LYS	2.1
1	C	955	VAL	2.1
1	C	726	GLU	2.1
2	D	340	ARG	2.1
2	B	452	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	527	ASP	2.1
1	C	527	ASP	2.1
1	A	242	CYS	2.1
1	C	1039	PHE	2.1
1	A	120	ALA	2.0
1	A	344	VAL	2.0
1	C	74	THR	2.0
1	C	2	PRO	2.0
2	D	409	ARG	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](#)

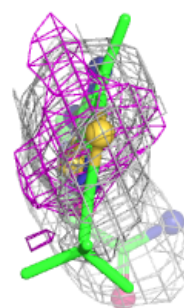
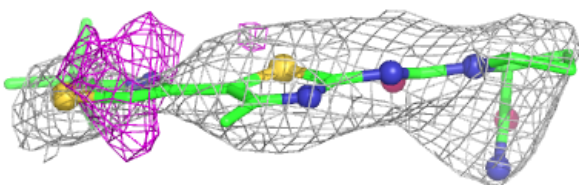
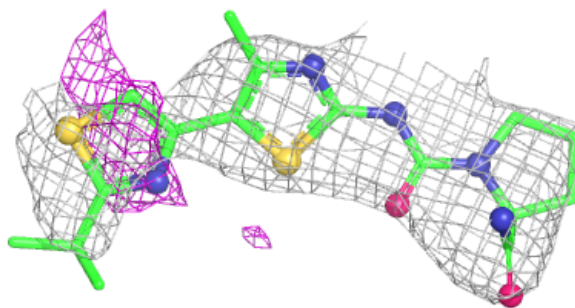
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	YNZ	A	1102	26/26	0.77	0.16	92,97,106,106	0
3	YOR	A	1101	34/34	0.88	0.11	79,80,82,82	0
3	YOR	C	1101	34/34	0.89	0.11	60,66,69,70	0
4	YNZ	C	1102	26/26	0.93	0.10	70,71,72,72	0
5	CL	C	1103	1/1	0.95	0.18	69,69,69,69	0

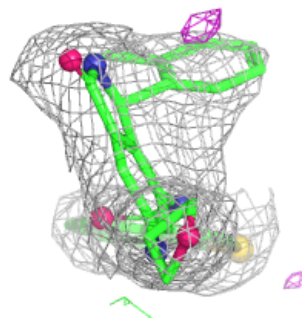
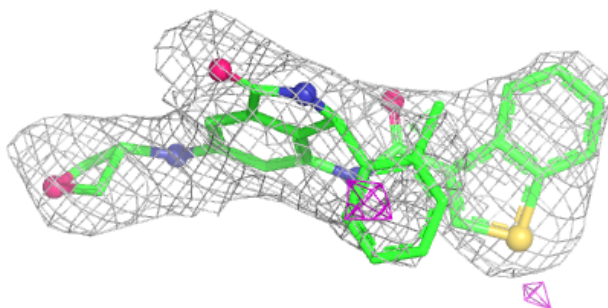
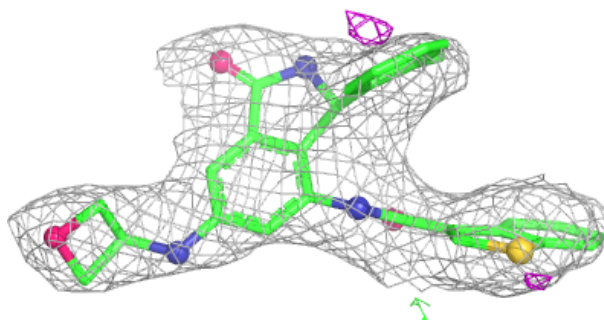
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

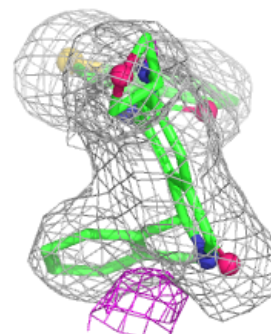
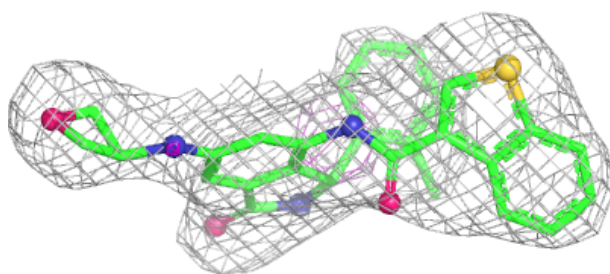
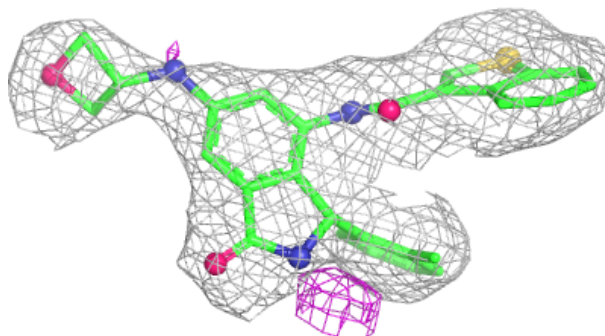
**Electron density around YOR A 1101:**

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

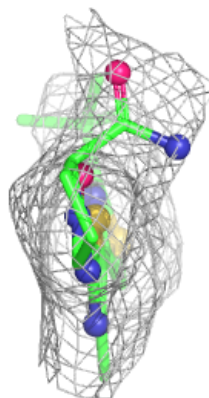
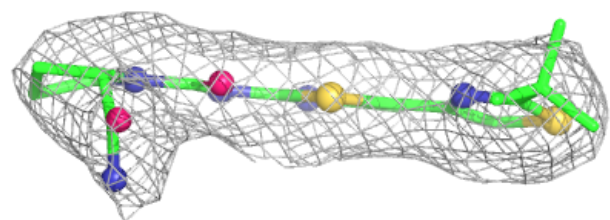
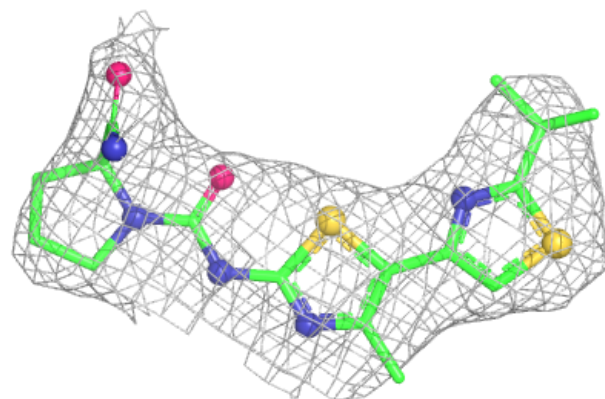


Electron density around YOR C 1101:

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

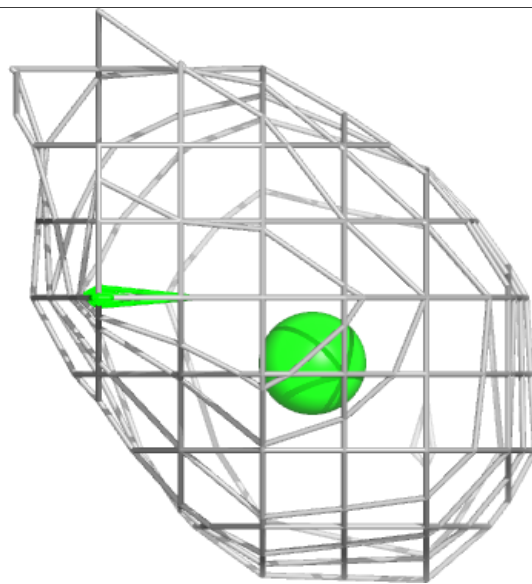
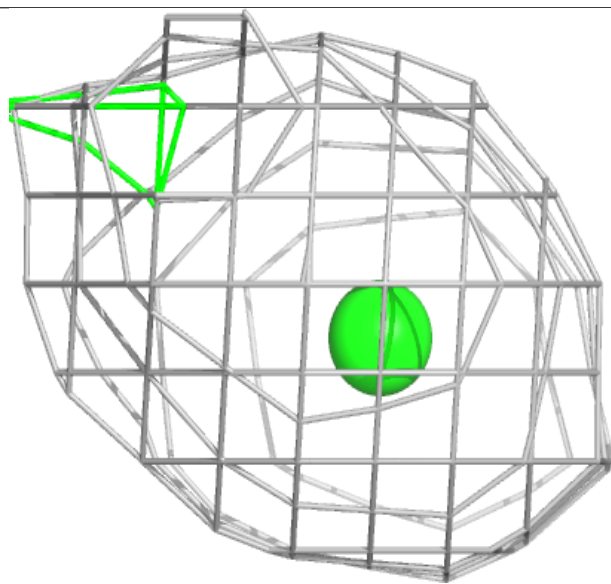
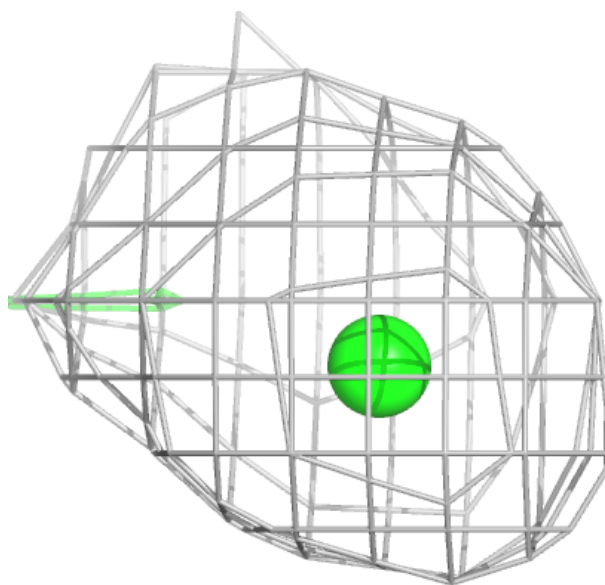
**Electron density around YNZ C 1102:**

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



Electron density around CL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.