



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:19 PM UTC

PDB ID : 4PJT / pdb_00004pjt
Title : Structure of PARP1 catalytic domain bound to inhibitor BMN 673
Authors : Aoyagi-Scharber, M.; Gardberg, A.S.; Arakaki, T.L.
Deposited on : 2014-05-12
Resolution : 2.35 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

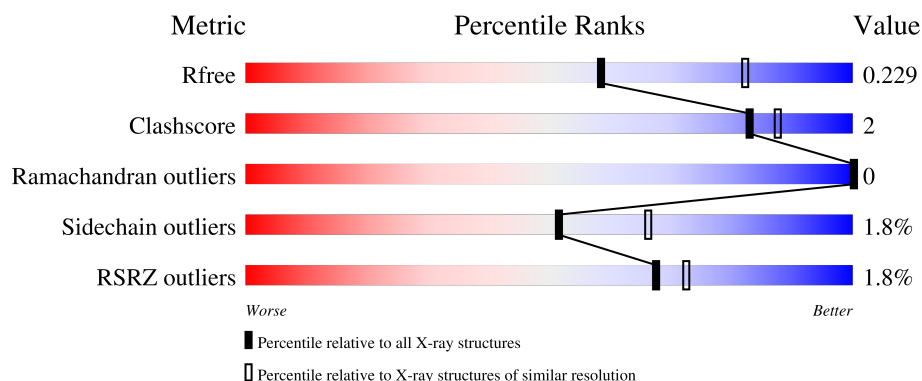
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	370	0% 85% 6% 9%
1	B	370	3% 84% 5% 10%
1	C	370	0% 88% 5% 6%
1	D	370	2% 81% 7% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10711 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	1	0
			2595	1657	428	500	10			
1	B	332	Total	C	N	O	S	0	0	0
			2504	1603	412	479	10			
1	C	346	Total	C	N	O	S	0	2	0
			2647	1690	440	506	11			
1	D	326	Total	C	N	O	S	0	0	0
			2444	1562	408	464	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	642	MET	-	expression tag	UNP P09874
A	643	GLY	-	expression tag	UNP P09874
A	644	SER	-	expression tag	UNP P09874
A	645	SER	-	expression tag	UNP P09874
A	646	HIS	-	expression tag	UNP P09874
A	647	HIS	-	expression tag	UNP P09874
A	648	HIS	-	expression tag	UNP P09874
A	649	HIS	-	expression tag	UNP P09874
A	650	HIS	-	expression tag	UNP P09874
A	651	HIS	-	expression tag	UNP P09874
A	652	SER	-	expression tag	UNP P09874
A	653	GLY	-	expression tag	UNP P09874
A	654	LEU	-	expression tag	UNP P09874
A	655	VAL	-	expression tag	UNP P09874
A	656	PRO	-	expression tag	UNP P09874
A	657	ARG	-	expression tag	UNP P09874
A	658	GLY	-	expression tag	UNP P09874
A	659	SER	-	expression tag	UNP P09874
A	660	HIS	-	expression tag	UNP P09874
A	661	MET	-	expression tag	UNP P09874
B	642	MET	-	expression tag	UNP P09874

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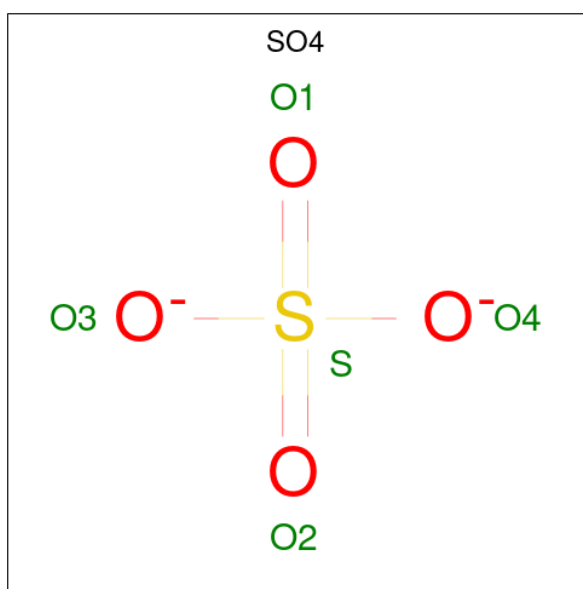
Chain	Residue	Modelled	Actual	Comment	Reference
B	643	GLY	-	expression tag	UNP P09874
B	644	SER	-	expression tag	UNP P09874
B	645	SER	-	expression tag	UNP P09874
B	646	HIS	-	expression tag	UNP P09874
B	647	HIS	-	expression tag	UNP P09874
B	648	HIS	-	expression tag	UNP P09874
B	649	HIS	-	expression tag	UNP P09874
B	650	HIS	-	expression tag	UNP P09874
B	651	HIS	-	expression tag	UNP P09874
B	652	SER	-	expression tag	UNP P09874
B	653	GLY	-	expression tag	UNP P09874
B	654	LEU	-	expression tag	UNP P09874
B	655	VAL	-	expression tag	UNP P09874
B	656	PRO	-	expression tag	UNP P09874
B	657	ARG	-	expression tag	UNP P09874
B	658	GLY	-	expression tag	UNP P09874
B	659	SER	-	expression tag	UNP P09874
B	660	HIS	-	expression tag	UNP P09874
B	661	MET	-	expression tag	UNP P09874
C	642	MET	-	expression tag	UNP P09874
C	643	GLY	-	expression tag	UNP P09874
C	644	SER	-	expression tag	UNP P09874
C	645	SER	-	expression tag	UNP P09874
C	646	HIS	-	expression tag	UNP P09874
C	647	HIS	-	expression tag	UNP P09874
C	648	HIS	-	expression tag	UNP P09874
C	649	HIS	-	expression tag	UNP P09874
C	650	HIS	-	expression tag	UNP P09874
C	651	HIS	-	expression tag	UNP P09874
C	652	SER	-	expression tag	UNP P09874
C	653	GLY	-	expression tag	UNP P09874
C	654	LEU	-	expression tag	UNP P09874
C	655	VAL	-	expression tag	UNP P09874
C	656	PRO	-	expression tag	UNP P09874
C	657	ARG	-	expression tag	UNP P09874
C	658	GLY	-	expression tag	UNP P09874
C	659	SER	-	expression tag	UNP P09874
C	660	HIS	-	expression tag	UNP P09874
C	661	MET	-	expression tag	UNP P09874
D	642	MET	-	expression tag	UNP P09874
D	643	GLY	-	expression tag	UNP P09874
D	644	SER	-	expression tag	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
D	645	SER	-	expression tag	UNP P09874
D	646	HIS	-	expression tag	UNP P09874
D	647	HIS	-	expression tag	UNP P09874
D	648	HIS	-	expression tag	UNP P09874
D	649	HIS	-	expression tag	UNP P09874
D	650	HIS	-	expression tag	UNP P09874
D	651	HIS	-	expression tag	UNP P09874
D	652	SER	-	expression tag	UNP P09874
D	653	GLY	-	expression tag	UNP P09874
D	654	LEU	-	expression tag	UNP P09874
D	655	VAL	-	expression tag	UNP P09874
D	656	PRO	-	expression tag	UNP P09874
D	657	ARG	-	expression tag	UNP P09874
D	658	GLY	-	expression tag	UNP P09874
D	659	SER	-	expression tag	UNP P09874
D	660	HIS	-	expression tag	UNP P09874
D	661	MET	-	expression tag	UNP P09874

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



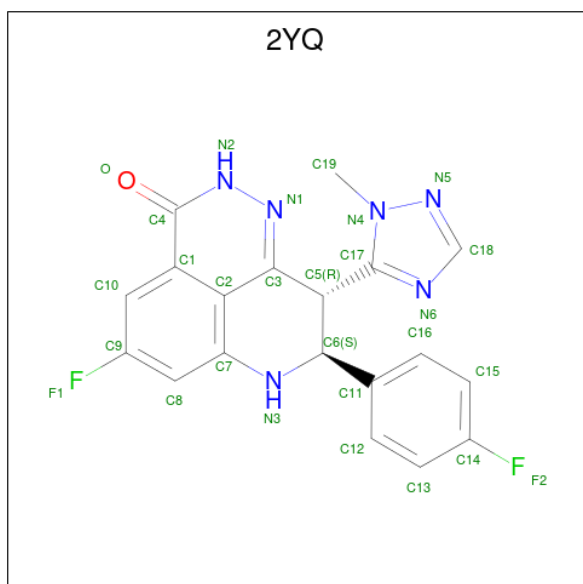
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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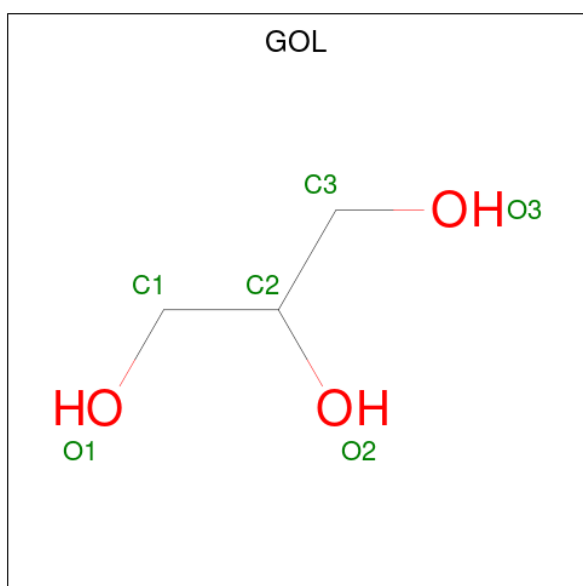
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (8S,9R)-5-fluoro-8-(4-fluorophenyl)-9-(1-methyl-1H-1,2,4-triazol-5-yl)-2,7,8,9-tetrahydro-3H-pyrido[4,3,2-de]phthalazin-3-one (CCD ID: 2YQ) (formula: C₁₉H₁₄F₂N₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			28	19	2	6	1		
3	B	1	Total	C	F	N	O	0	0
			28	19	2	6	1		
3	C	1	Total	C	F	N	O	0	0
			28	19	2	6	1		
3	D	1	Total	C	F	N	O	0	0
			28	19	2	6	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	55	Total	O	0	0
			55	55		
5	C	100	Total	O	0	0
			100	100		

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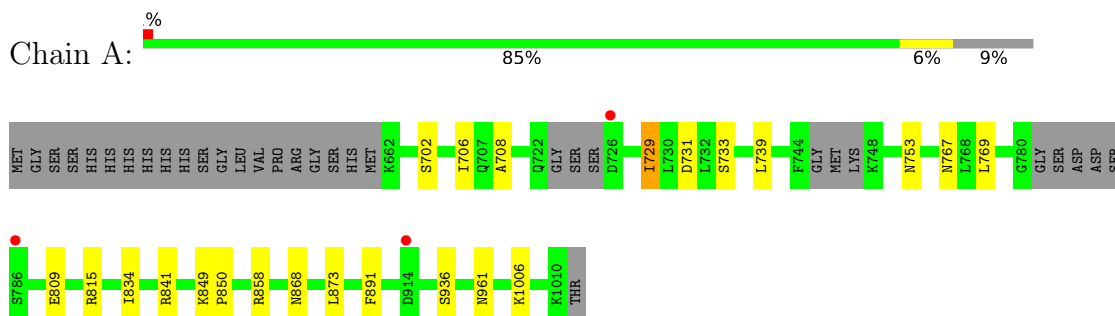
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	53	Total	O	0	0
			53	53		

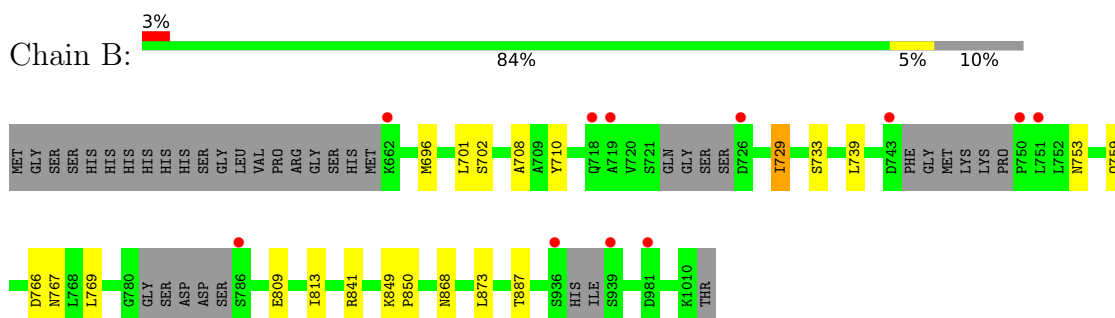
3 Residue-property plots [i](#)

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.

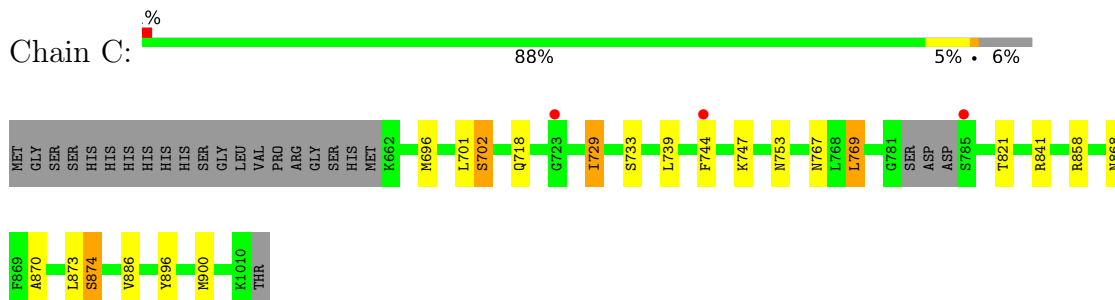
- Molecule 1: Poly [ADP-ribose] polymerase 1



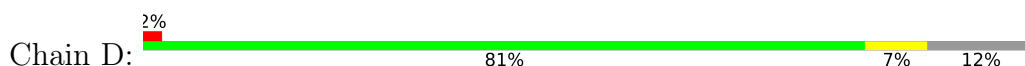
- Molecule 1: Poly [ADP-ribose] polymerase 1

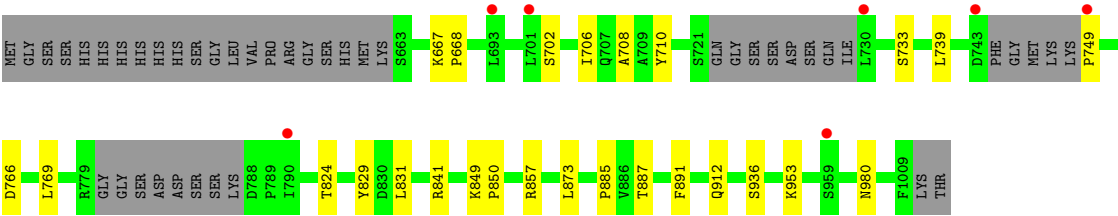


- Molecule 1: Poly [ADP-ribose] polymerase 1



- Molecule 1: Poly [ADP-ribose] polymerase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.69Å 108.15Å 142.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.35 19.94 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.94-2.35) 99.6 (19.94-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.188 , 0.228 0.192 , 0.229	Depositor DCC
R_{free} test set	3387 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10711	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: 2YQ, SO4, GOL

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	0.89	0/2647	0.90	0/3590
1	B	0.79	0/2549	0.86	0/3462
1	C	0.88	0/2706	0.90	1/3675 (0.0%)
1	D	0.72	0/2490	0.83	1/3388 (0.0%)
All	All	0.82	0/10392	0.87	2/14115 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	749	PRO	N-CA-CB	6.82	110.50	103.00
1	C	858	ARG	CG-CD-NE	-5.26	100.42	112.00

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	2595	0	2532	15	0
1	B	2504	0	2412	11	0
1	C	2647	0	2575	14	0
1	D	2444	0	2340	11	0
2	A	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	0	0	0
2	C	15	0	0	3	0
2	D	15	0	0	0	0
3	A	28	0	14	0	0
3	B	28	0	14	0	0
3	C	28	0	14	0	0
3	D	28	0	14	0	0
4	A	12	0	16	0	0
4	C	6	0	8	1	0
5	A	108	0	0	1	0
5	B	55	0	0	0	0
5	C	100	0	0	2	0
5	D	53	0	0	0	0
All	All	10711	0	9939	48	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 2.

All (48) 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:B:759:GLN:HG3	1:B:887:THR:HG22	1.48	0.92
1:A:809:GLU:CD	1:C:886:VAL:HG11	2.06	0.81
1:B:841:ARG:HD2	1:B:873:LEU:O	1.83	0.78
1:A:841:ARG:HD2	1:A:873:LEU:O	1.86	0.74
1:A:809:GLU:OE1	1:C:886:VAL:HG11	1.87	0.73
1:C:841:ARG:HD2	1:C:873:LEU:O	1.87	0.73
1:D:841:ARG:HD2	1:D:873:LEU:O	1.88	0.73
1:C:769:LEU:HD22	5:C:1283:HOH:O	1.94	0.67
1:B:729:ILE:HD11	1:B:753:ASN:CB	2.27	0.64
1:B:729:ILE:HD11	1:B:753:ASN:HB3	1.78	0.64
1:C:702:SER:HB2	2:C:1103:SO4:O1	2.01	0.61
1:B:759:GLN:CG	1:B:887:THR:HG22	2.27	0.59
1:D:829:TYR:HE1	1:D:831:LEU:HD21	1.69	0.56
1:D:885:PRO:HB2	1:D:887:THR:HG22	1.87	0.55
1:A:961:ASN:ND2	5:A:1243:HOH:O	2.39	0.55
1:C:744:PHE:HB2	1:C:747:LYS:O	2.09	0.52
1:A:767:ASN:HA	1:A:868:ASN:HD21	1.75	0.52
1:C:696:MET:HE3	1:C:701:LEU:HD21	1.92	0.51
1:B:696:MET:HE3	1:B:701:LEU:HD21	1.93	0.50
2:C:1101:SO4:O2	5:C:1266:HOH:O	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:ILE:HD11	1:A:753:ASN:CB	2.43	0.49
2:C:1102:SO4:O3	1:D:849:LYS:NZ	2.41	0.49
1:A:708:ALA:HB3	1:A:739:LEU:HD21	1.95	0.48
1:B:767:ASN:HA	1:B:868:ASN:HD21	1.78	0.48
1:C:767:ASN:HA	1:C:868:ASN:HD21	1.79	0.48
1:B:710:TYR:OH	1:B:766:ASP:OD1	2.33	0.47
1:A:858:ARG:NH2	2:A:1102:SO4:O3	2.46	0.45
1:B:849:LYS:HB3	1:B:850:PRO:HD3	1.98	0.45
1:C:896:TYR:CE2	4:C:1105:GOL:H32	2.51	0.45
1:B:809:GLU:O	1:B:813:ILE:HG13	2.17	0.45
1:B:708:ALA:HB3	1:B:739:LEU:HD21	1.98	0.44
1:C:870:ALA:O	1:C:874:SER:HB3	2.18	0.44
1:D:849:LYS:HB3	1:D:850:PRO:HD3	1.99	0.44
1:D:710:TYR:OH	1:D:766:ASP:OD1	2.30	0.43
1:A:849:LYS:HB3	1:A:850:PRO:HD3	1.99	0.43
1:A:729:ILE:HD11	1:A:753:ASN:HB3	1.99	0.42
1:C:821:THR:HB	1:C:900:MET:HA	2.02	0.42
1:A:815:ARG:NH1	1:C:718:GLN:HG2	2.35	0.42
1:D:708:ALA:HB3	1:D:739:LEU:HD21	2.00	0.42
1:A:891:PHE:HA	1:A:936:SER:O	2.20	0.42
1:A:809:GLU:OE1	1:C:886:VAL:CG1	2.62	0.41
1:D:891:PHE:HA	1:D:936:SER:O	2.21	0.41
1:A:834:ILE:HD11	1:A:1006:LYS:HB2	2.01	0.41
1:D:667:LYS:N	1:D:668:PRO:CD	2.84	0.41
1:D:953:LYS:NZ	1:D:980:ASN:O	2.51	0.41
1:D:706:ILE:HG21	1:D:769:LEU:HG	2.03	0.41
1:A:706:ILE:HG21	1:A:769:LEU:HG	2.03	0.40
1:C:729:ILE:HD11	1:C:753:ASN:CB	2.52	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	331/370 (90%)	329 (99%)	2 (1%)	0	100	100
1	B	322/370 (87%)	321 (100%)	1 (0%)	0	100	100
1	C	344/370 (93%)	342 (99%)	2 (1%)	0	100	100
1	D	318/370 (86%)	316 (99%)	2 (1%)	0	100	100
All	All	1315/1480 (89%)	1308 (100%)	7 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	279/325 (86%)	275 (99%)	4 (1%)	59	73
1	B	260/325 (80%)	256 (98%)	4 (2%)	57	72
1	C	282/325 (87%)	276 (98%)	6 (2%)	47	61
1	D	252/325 (78%)	247 (98%)	5 (2%)	48	63
All	All	1073/1300 (82%)	1054 (98%)	19 (2%)	51	66

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	702	SER
1	A	729	ILE
1	A	731	ASP
1	A	733	SER
1	B	702	SER
1	B	729	ILE
1	B	733	SER
1	B	769	LEU
1	C	702	SER
1	C	729	ILE
1	C	733	SER
1	C	739	LEU
1	C	769	LEU

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Mol	Chain	Res	Type
1	C	874	SER
1	D	702	SER
1	D	733	SER
1	D	824	THR
1	D	857	ARG
1	D	912	GLN

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	759	GLN
1	A	868	ASN
1	A	875	GLN
1	A	961	ASN
1	B	868	ASN
1	C	670	GLN
1	C	868	ASN
1	C	875	GLN
1	D	767	ASN
1	D	909	HIS
1	D	912	GLN
1	D	998	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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$
2	SO4	D	1101	-	4,4,4	0.50	0	6,6,6	0.55	0
2	SO4	D	1103	-	4,4,4	0.46	0	6,6,6	0.29	0
3	2YQ	A	1105	-	31,32,32	2.00	7 (22%)	34,48,48	2.29	10 (29%)
2	SO4	B	1104	-	4,4,4	0.36	0	6,6,6	0.65	0
2	SO4	B	1101	-	4,4,4	0.50	0	6,6,6	0.81	0
3	2YQ	C	1104	-	31,32,32	2.12	7 (22%)	34,48,48	2.44	7 (20%)
2	SO4	A	1104	-	4,4,4	0.43	0	6,6,6	0.60	0
2	SO4	A	1101	-	4,4,4	1.13	1 (25%)	6,6,6	0.47	0
2	SO4	D	1102	-	4,4,4	0.83	0	6,6,6	0.55	0
2	SO4	A	1103	-	4,4,4	0.70	0	6,6,6	1.19	1 (16%)
3	2YQ	D	1104	-	31,32,32	2.42	12 (38%)	34,48,48	2.29	8 (23%)
2	SO4	A	1102	-	4,4,4	0.39	0	6,6,6	0.66	0
2	SO4	B	1106	-	4,4,4	0.47	0	6,6,6	0.42	0
4	GOL	A	1107	-	5,5,5	0.52	0	5,5,5	0.46	0
4	GOL	C	1105	-	5,5,5	0.87	0	5,5,5	1.57	2 (40%)
2	SO4	B	1102	-	4,4,4	0.44	0	6,6,6	0.57	0
4	GOL	A	1106	-	5,5,5	0.47	0	5,5,5	0.95	0
2	SO4	B	1103	-	4,4,4	0.30	0	6,6,6	0.41	0
2	SO4	C	1102	-	4,4,4	0.42	0	6,6,6	0.39	0
2	SO4	C	1103	-	4,4,4	0.29	0	6,6,6	0.75	0
2	SO4	C	1101	-	4,4,4	1.02	0	6,6,6	0.79	0
3	2YQ	B	1105	-	31,32,32	1.96	8 (25%)	34,48,48	2.29	9 (26%)

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	GOL	A	1107	-	-	3/4/4/4	-
4	GOL	C	1105	-	-	0/4/4/4	-
4	GOL	A	1106	-	-	2/4/4/4	-
3	2YQ	A	1105	-	-	0/6/20/20	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2YQ	B	1105	-	-	0/6/20/20	0/5/5/5
3	2YQ	C	1104	-	-	0/6/20/20	0/5/5/5
3	2YQ	D	1104	-	-	0/6/20/20	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1104	2YQ	C3-N1	8.34	1.37	1.29
3	C	1104	2YQ	C3-N1	7.05	1.35	1.29
3	B	1105	2YQ	C3-N1	5.48	1.34	1.29
3	A	1105	2YQ	C2-C3	-5.47	1.38	1.47
3	C	1104	2YQ	C2-C3	-5.39	1.38	1.47
3	D	1104	2YQ	C17-N6	4.87	1.38	1.32
3	A	1105	2YQ	C3-N1	4.67	1.33	1.29
3	A	1105	2YQ	C1-C4	-4.06	1.40	1.47
3	B	1105	2YQ	C2-C3	-3.88	1.40	1.47
3	A	1105	2YQ	C5-C17	-3.83	1.45	1.50
3	D	1104	2YQ	C2-C3	-3.75	1.41	1.47
3	D	1104	2YQ	C11-C6	-3.68	1.47	1.52
3	B	1105	2YQ	C17-N6	3.19	1.36	1.32
3	C	1104	2YQ	C5-C3	-3.16	1.48	1.51
3	B	1105	2YQ	C1-C4	-3.14	1.41	1.47
3	D	1104	2YQ	C5-C3	-3.14	1.48	1.51
3	B	1105	2YQ	C19-N4	3.02	1.51	1.46
3	C	1104	2YQ	C19-N4	2.86	1.51	1.46
3	B	1105	2YQ	C5-C3	-2.84	1.48	1.51
3	C	1104	2YQ	C5-C17	-2.61	1.47	1.50
3	A	1105	2YQ	C5-C3	-2.61	1.48	1.51
3	C	1104	2YQ	O-C4	2.55	1.29	1.23
3	D	1104	2YQ	C17-N4	-2.54	1.32	1.34
3	D	1104	2YQ	C18-N5	2.46	1.36	1.32
3	D	1104	2YQ	C19-N4	2.35	1.50	1.46
3	B	1105	2YQ	O-C4	2.32	1.28	1.23
3	B	1105	2YQ	N4-N5	2.31	1.40	1.36
3	D	1104	2YQ	N4-N5	2.30	1.40	1.36
3	D	1104	2YQ	C10-C9	2.27	1.41	1.37
3	A	1105	2YQ	C7-N3	-2.24	1.35	1.39
3	A	1105	2YQ	C17-N6	2.17	1.35	1.32
3	D	1104	2YQ	C1-C4	-2.13	1.43	1.47
3	D	1104	2YQ	N2-N1	2.10	1.43	1.38
2	A	1101	SO4	O2-S	2.04	1.57	1.44
3	C	1104	2YQ	C1-C4	-2.03	1.43	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1104	2YQ	C4-N2-N1	-8.63	118.35	127.98
3	D	1104	2YQ	C4-N2-N1	-7.23	119.92	127.98
3	A	1105	2YQ	C4-N2-N1	-7.05	120.11	127.98
3	B	1105	2YQ	C4-N2-N1	-6.86	120.33	127.98
3	B	1105	2YQ	N5-C18-N6	-5.52	108.02	116.78
3	B	1105	2YQ	C2-C3-N1	-5.36	119.31	122.78
3	D	1104	2YQ	N5-C18-N6	-5.34	108.32	116.78
3	C	1104	2YQ	C3-N1-N2	5.27	123.24	117.20
3	A	1105	2YQ	C2-C3-N1	-5.22	119.40	122.78
3	D	1104	2YQ	C1-C4-N2	4.74	120.50	115.04
3	C	1104	2YQ	C2-C3-N1	-4.74	119.71	122.78
3	B	1105	2YQ	C3-N1-N2	4.57	122.43	117.20
3	C	1104	2YQ	N5-C18-N6	-4.57	109.54	116.78
3	A	1105	2YQ	N5-C18-N6	-4.20	110.13	116.78
3	A	1105	2YQ	C1-C4-N2	4.09	119.75	115.04
3	A	1105	2YQ	C3-N1-N2	4.04	121.83	117.20
3	D	1104	2YQ	C2-C3-N1	-4.01	120.18	122.78
3	C	1104	2YQ	C1-C4-N2	3.41	118.97	115.04
3	D	1104	2YQ	F1-C9-C10	3.17	122.78	118.28
3	C	1104	2YQ	C1-C2-C7	3.09	121.78	118.86
3	D	1104	2YQ	C3-N1-N2	2.99	120.63	117.20
3	C	1104	2YQ	C5-C17-N4	2.99	128.25	123.61
3	B	1105	2YQ	C1-C2-C7	2.92	121.62	118.86
3	B	1105	2YQ	C1-C4-N2	2.83	118.30	115.04
3	A	1105	2YQ	C16-C15-C14	2.76	121.21	118.38
3	A	1105	2YQ	C1-C2-C7	2.74	121.45	118.86
3	D	1104	2YQ	O-C4-N2	-2.74	117.37	120.88
3	D	1104	2YQ	C10-C9-C8	-2.72	120.19	123.50
3	A	1105	2YQ	O-C4-N2	-2.56	117.60	120.88
4	C	1105	GOL	O2-C2-C3	-2.52	98.74	109.18
3	B	1105	2YQ	O-C4-N2	-2.34	117.87	120.88
3	B	1105	2YQ	C5-C17-N4	2.23	127.07	123.61
3	A	1105	2YQ	C15-C14-C13	-2.22	119.89	122.80
4	C	1105	GOL	C3-C2-C1	2.21	119.91	111.80
3	B	1105	2YQ	C10-C1-C2	-2.17	117.55	120.33
3	A	1105	2YQ	F2-C14-C13	2.06	121.84	118.55
2	A	1103	SO4	O3-S-O2	2.05	120.30	109.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1106	GOL	O1-C1-C2-C3
4	A	1107	GOL	O1-C1-C2-O2
4	A	1107	GOL	O1-C1-C2-C3
4	A	1106	GOL	O1-C1-C2-O2
4	A	1107	GOL	O2-C2-C3-O3

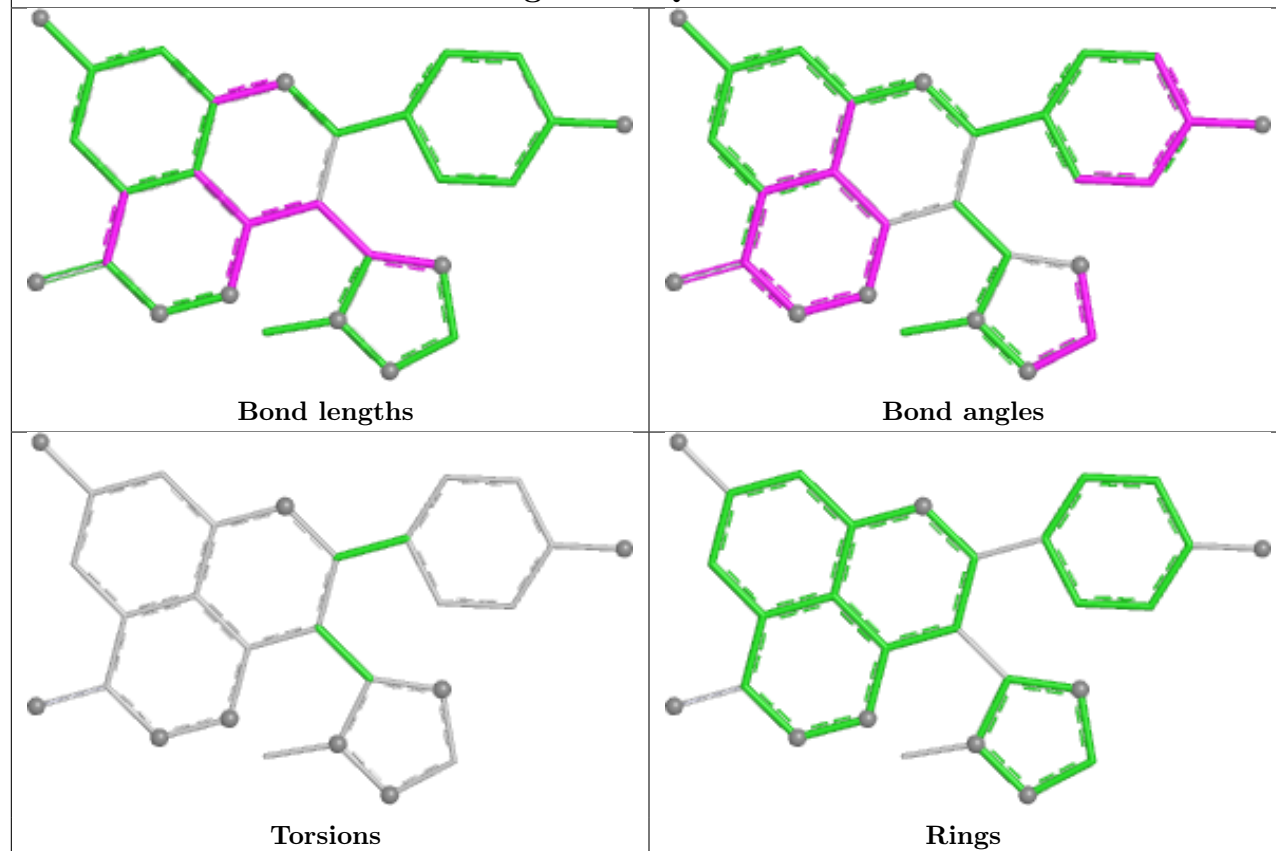
There are no ring outliers.

5 monomers are involved in 5 short contacts:

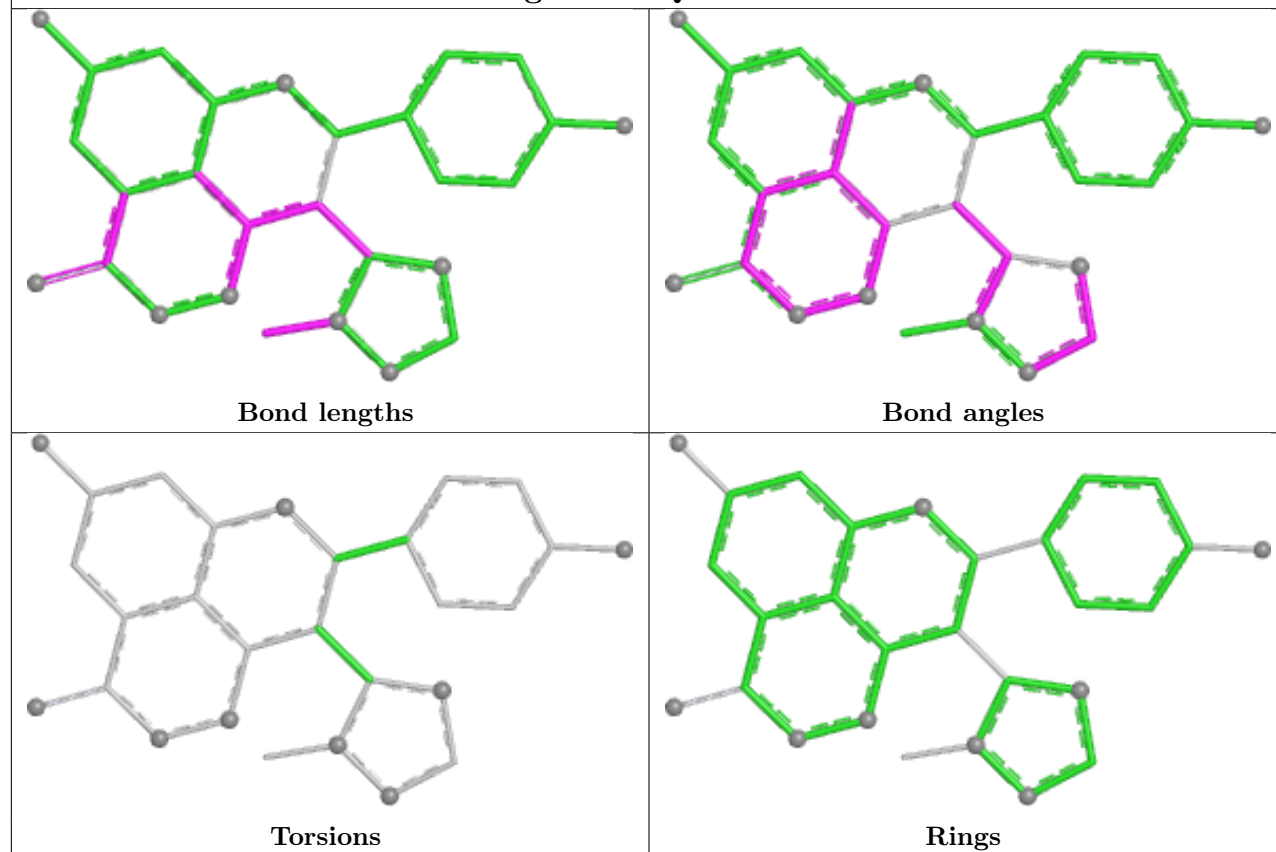
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1102	SO4	1	0
4	C	1105	GOL	1	0
2	C	1102	SO4	1	0
2	C	1103	SO4	1	0
2	C	1101	SO4	1	0

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.

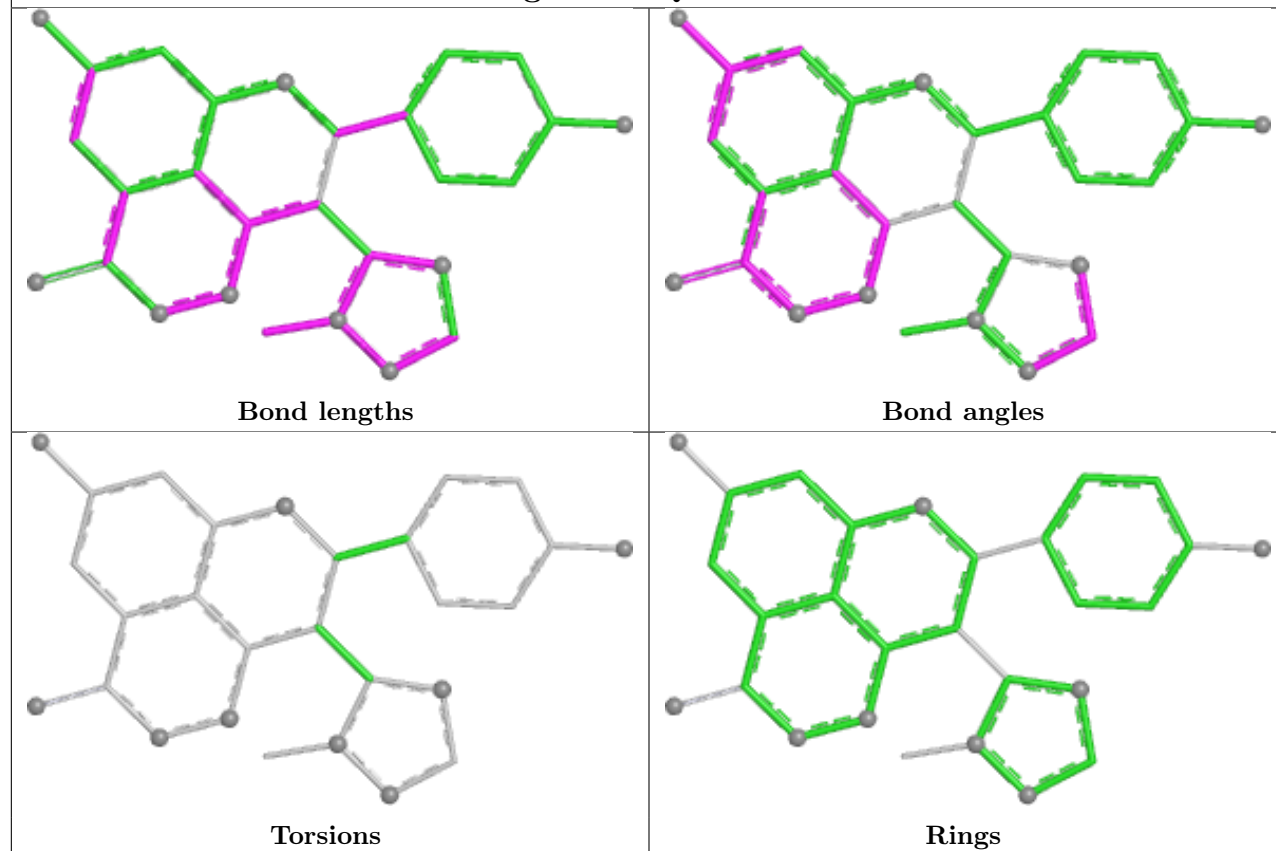
Ligand 2YQ A 1105



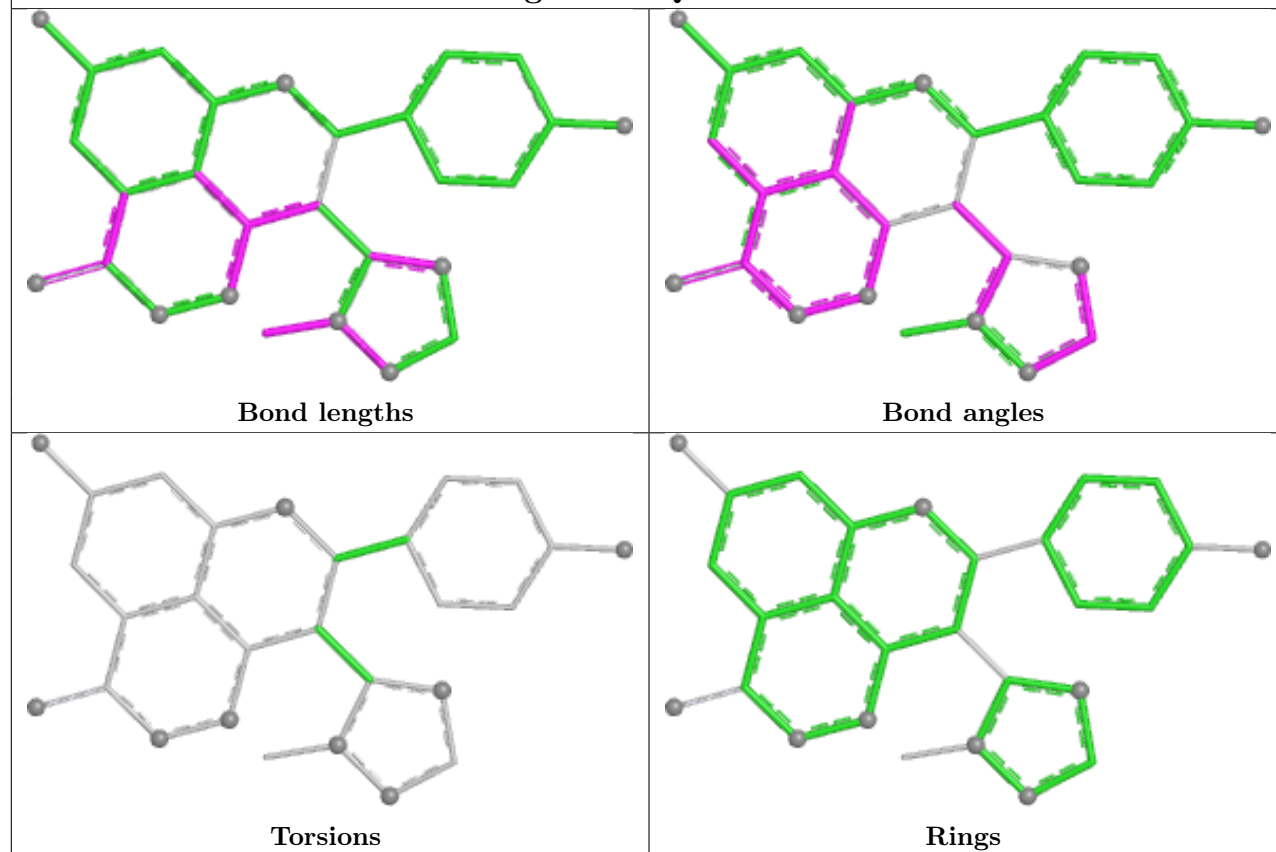
Ligand 2YQ C 1104



Ligand 2YQ D 1104



Ligand 2YQ B 1105



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	338/370 (91%)	-0.22	3 (0%) 81 84	16, 34, 61, 91	1 (0%)
1	B	332/370 (89%)	0.10	11 (3%) 49 56	22, 46, 72, 86	0
1	C	346/370 (93%)	-0.21	3 (0%) 81 84	17, 34, 60, 81	2 (0%)
1	D	326/370 (88%)	0.23	7 (2%) 63 68	26, 51, 80, 91	0
All	All	1342/1480 (90%)	-0.03	24 (1%) 67 72	16, 40, 72, 91	3 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	743	ASP	3.8
1	A	726	ASP	3.8
1	D	749	PRO	3.7
1	B	786	SER	3.6
1	B	750	PRO	3.4
1	B	726	ASP	3.2
1	A	786	SER	2.8
1	C	744	PHE	2.6
1	D	701	LEU	2.6
1	C	785	SER	2.5
1	D	790	ILE	2.5
1	B	939	SER	2.4
1	D	730	LEU	2.4
1	D	959	SER	2.4
1	B	936	SER	2.3
1	D	693	LEU	2.3
1	C	723	GLY	2.2
1	A	914	ASP	2.2
1	B	981	ASP	2.1
1	B	718	GLN	2.1
1	B	719	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	751	LEU	2.0
1	D	743	ASP	2.0
1	B	662	LYS	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.

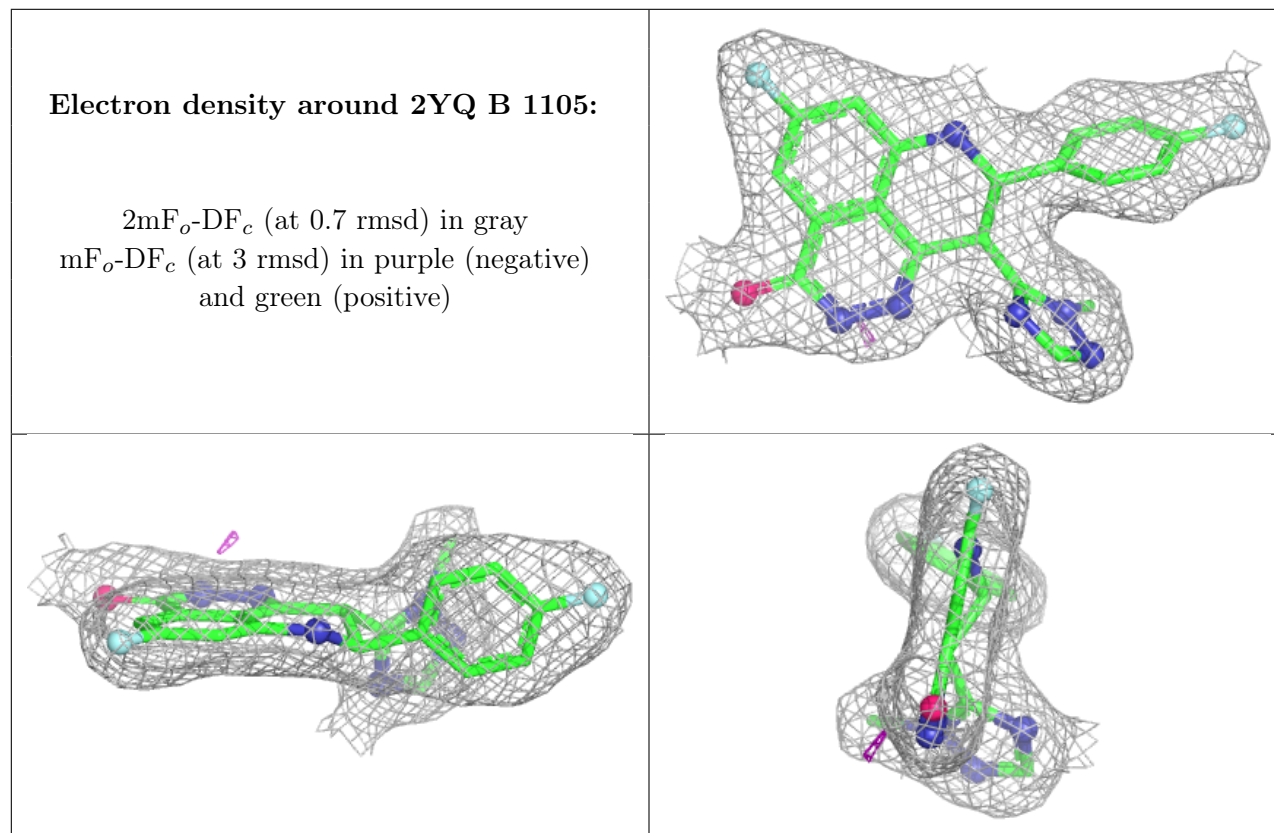
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	1106	5/5	0.80	0.17	46,49,54,54	5
4	GOL	A	1107	6/6	0.83	0.15	54,60,62,65	0
2	SO4	D	1102	5/5	0.84	0.13	50,51,61,66	0
4	GOL	A	1106	6/6	0.88	0.13	42,53,56,62	0
2	SO4	B	1101	5/5	0.88	0.12	47,54,56,60	0
2	SO4	C	1101	5/5	0.89	0.10	36,40,53,54	0
2	SO4	A	1101	5/5	0.90	0.14	29,37,37,41	0
4	GOL	C	1105	6/6	0.91	0.09	28,31,35,36	0
2	SO4	C	1103	5/5	0.92	0.14	30,31,33,33	5
2	SO4	A	1102	5/5	0.92	0.13	30,31,33,34	5
2	SO4	D	1103	5/5	0.92	0.12	37,37,40,42	5
2	SO4	A	1104	5/5	0.93	0.14	28,28,29,32	5
2	SO4	B	1103	5/5	0.95	0.16	31,31,34,34	5
2	SO4	B	1104	5/5	0.95	0.14	25,26,28,29	5
2	SO4	C	1102	5/5	0.95	0.13	55,59,64,67	0
2	SO4	A	1103	5/5	0.96	0.13	37,39,44,50	0
2	SO4	D	1101	5/5	0.96	0.14	43,44,50,51	0
3	2YQ	B	1105	28/28	0.96	0.05	22,27,37,45	0
3	2YQ	D	1104	28/28	0.97	0.05	23,27,32,34	0
3	2YQ	A	1105	28/28	0.97	0.04	18,19,23,24	0

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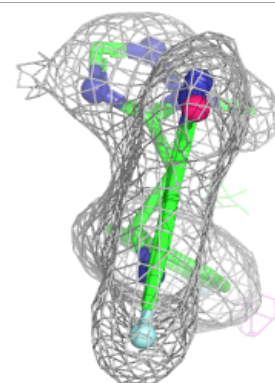
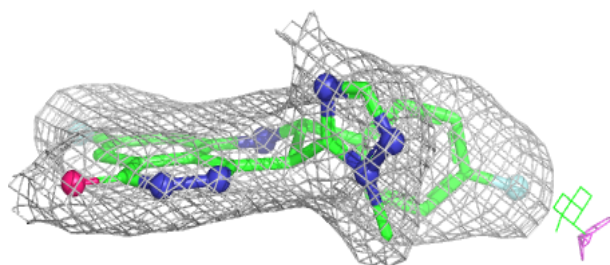
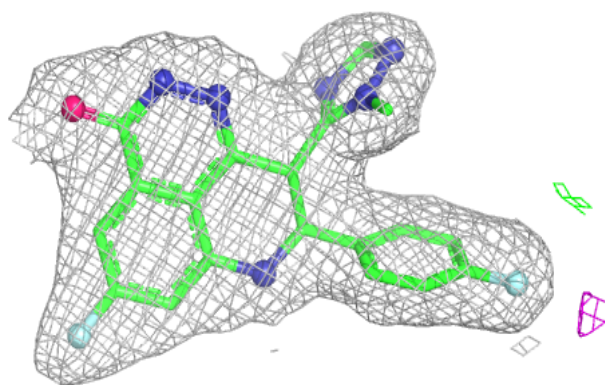
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1102	5/5	0.97	0.08	52,52,57,57	0
3	2YQ	C	1104	28/28	0.97	0.05	17,19,23,28	0

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.

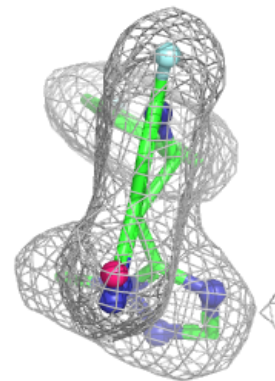
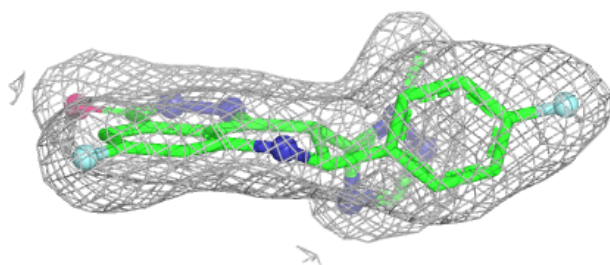
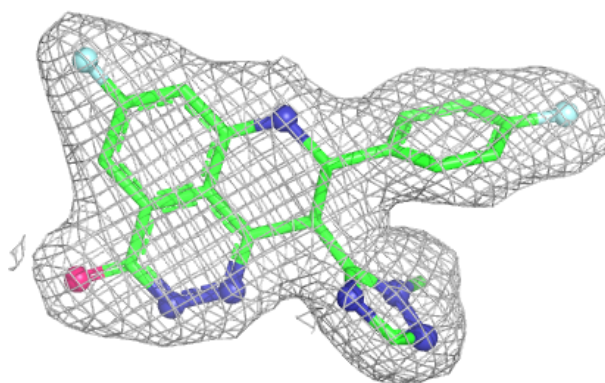


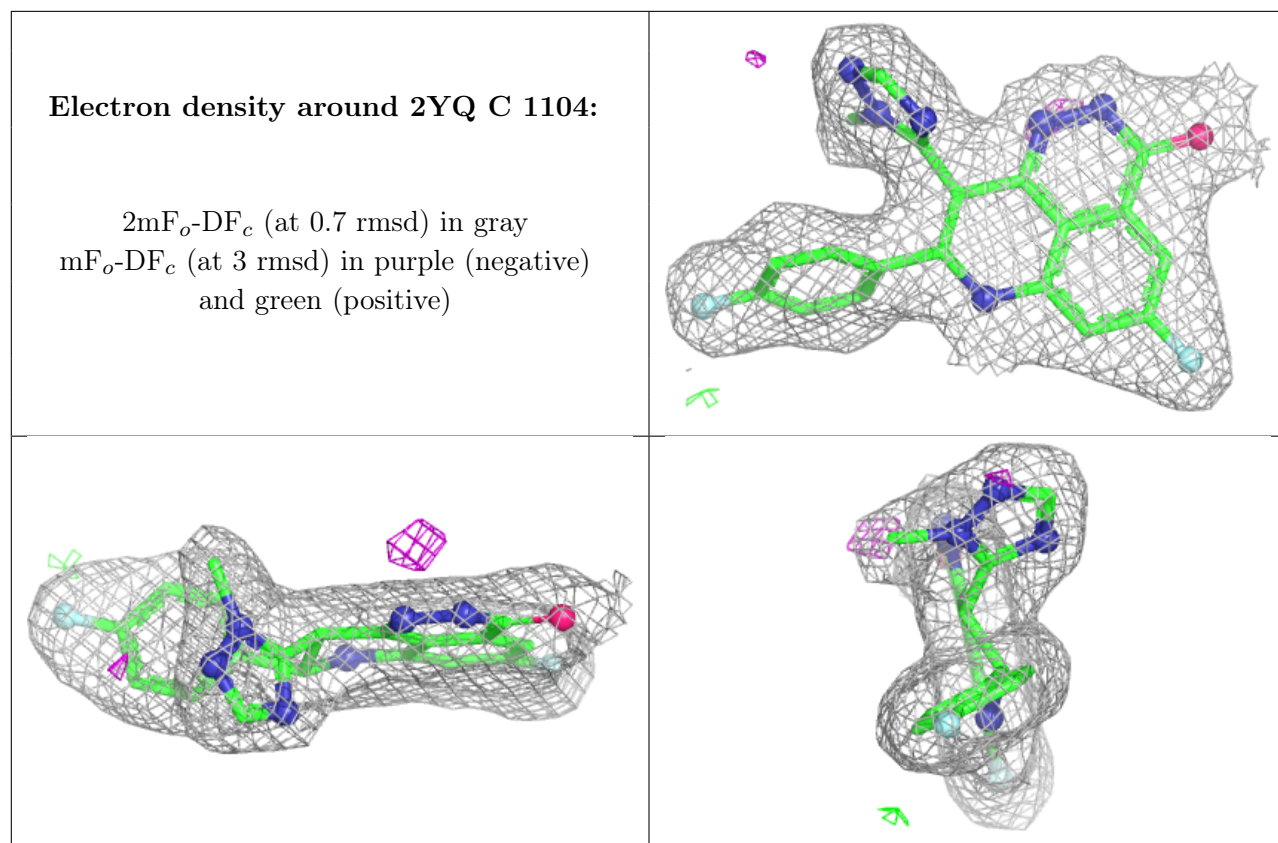
Electron density around 2YQ D 1104:

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

**Electron density around 2YQ A 1105:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.