



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:03 PM UTC

PDB ID : 2AX0 / pdb_00002ax0
Title : Hepatitis C Virus NS5b RNA Polymerase in complex with a covalent inhibitor (5x)
Authors : Powers, J.P.; Piper, D.E.; Li, Y.; Mayorga, V.; Anzola, J.; Chen, J.M.; Jaen, J.C.; Lee, G.; Liu, J.; Peterson, M.G.; Tonn, G.R.; Ye, Q.; Walker, N.P.; Wang, Z.
Deposited on : 2005-09-02
Resolution : 2.00 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](#) ①) 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

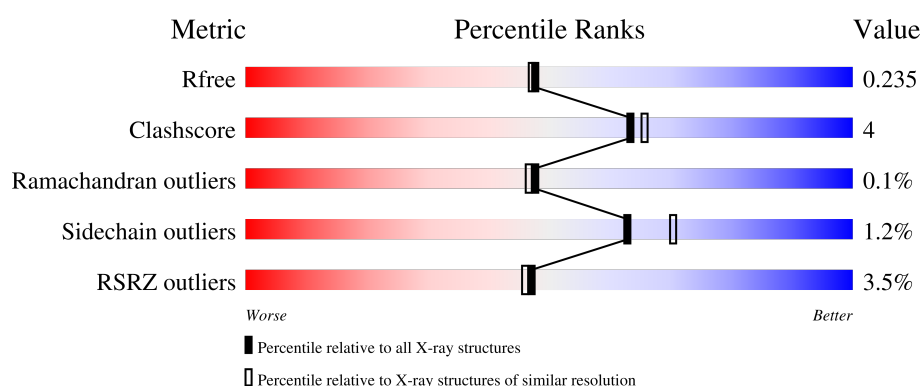
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	580	3% 83% 11% ..
1	B	580	3% 87% 8% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9595 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4315	2722	764	798	31			
1	B	557	Total	C	N	O	S	0	0	0
			4329	2730	767	801	31			

There are 42 discrepancies between the modelled and reference sequences:

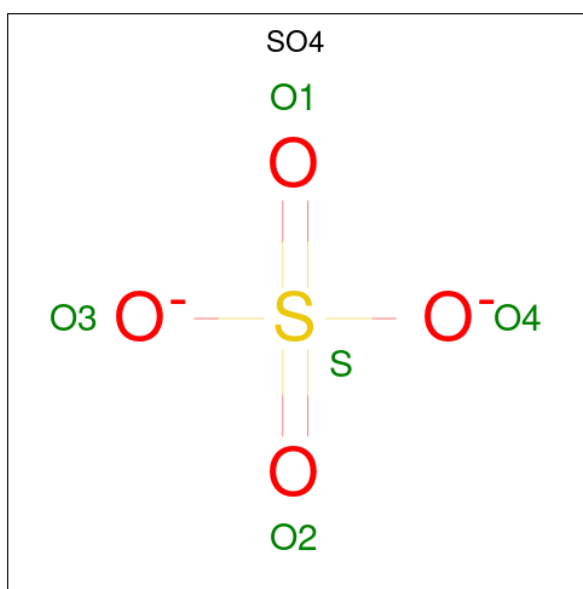
Chain	Residue	Modelled	Actual	Comment	Reference
A	499	ALA	VAL	engineered mutation	UNP P26663
A	506	ASN	SER	engineered mutation	UNP P26663
A	514	ARG	GLN	engineered mutation	UNP P26663
A	520	ILE	THR	engineered mutation	UNP P26663
A	540	ALA	PRO	engineered mutation	UNP P26663
A	543	GLY	SER	engineered mutation	UNP P26663
A	549	SER	GLY	engineered mutation	UNP P26663
A	552	THR	VAL	engineered mutation	UNP P26663
A	563	GLY	SER	engineered mutation	UNP P26663
A	564	VAL	LEU	engineered mutation	UNP P26663
A	566	HIS	ARG	engineered mutation	UNP P26663
A	571	HIS	-	expression tag	UNP P26663
A	572	HIS	-	expression tag	UNP P26663
A	573	HIS	-	expression tag	UNP P26663
A	574	HIS	-	expression tag	UNP P26663
A	575	HIS	-	expression tag	UNP P26663
A	576	HIS	-	expression tag	UNP P26663
A	577	HIS	-	expression tag	UNP P26663
A	578	HIS	-	expression tag	UNP P26663
A	579	HIS	-	expression tag	UNP P26663
A	580	HIS	-	expression tag	UNP P26663
B	499	ALA	VAL	engineered mutation	UNP P26663
B	506	ASN	SER	engineered mutation	UNP P26663
B	514	ARG	GLN	engineered mutation	UNP P26663
B	520	ILE	THR	engineered mutation	UNP P26663

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Chain	Residue	Modelled	Actual	Comment	Reference
B	540	ALA	PRO	engineered mutation	UNP P26663
B	543	GLY	SER	engineered mutation	UNP P26663
B	549	SER	GLY	engineered mutation	UNP P26663
B	552	THR	VAL	engineered mutation	UNP P26663
B	563	GLY	SER	engineered mutation	UNP P26663
B	564	VAL	LEU	engineered mutation	UNP P26663
B	566	HIS	ARG	engineered mutation	UNP P26663
B	571	HIS	-	expression tag	UNP P26663
B	572	HIS	-	expression tag	UNP P26663
B	573	HIS	-	expression tag	UNP P26663
B	574	HIS	-	expression tag	UNP P26663
B	575	HIS	-	expression tag	UNP P26663
B	576	HIS	-	expression tag	UNP P26663
B	577	HIS	-	expression tag	UNP P26663
B	578	HIS	-	expression tag	UNP P26663
B	579	HIS	-	expression tag	UNP P26663
B	580	HIS	-	expression tag	UNP P26663

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



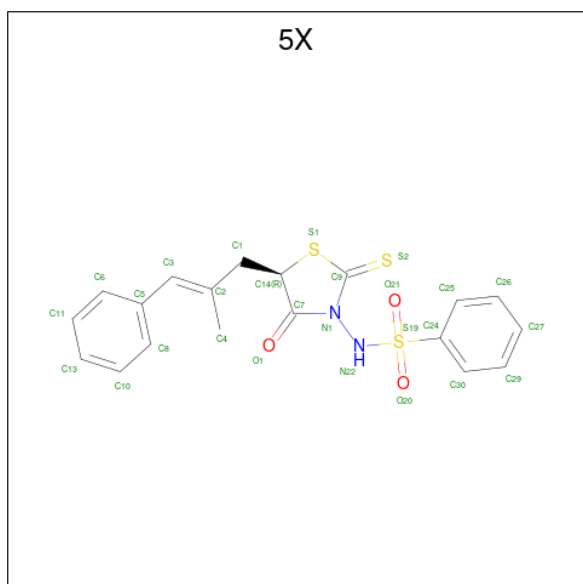
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	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		

- Molecule 3 is 5R-(2E-METHYL-3-PHENYL-ALLYL)-3-(BENZENESULFONYLAMINO)-4-OXO-2-THIONOTHIAZOLIDINE (CCD ID: 5X) (formula: C₁₉H₁₈N₂O₃S₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	19	2	3	3		
3	B	1	Total	C	N	O	S	0	0
			27	19	2	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	415	Total	O	0	0
			415	415		
4	B	447	Total	O	0	0
			447	447		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.16Å 87.31Å 163.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 92.3 (30.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.238 0.208 , 0.235	Depositor DCC
R_{free} test set	7852 reflections (9.31%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9595	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5X, SO4

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	0.39	0/4409	0.83	9/5980 (0.2%)
1	B	0.40	0/4423	0.83	6/5999 (0.1%)
All	All	0.39	0/8832	0.83	15/11979 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	VAL	N-CA-C	7.03	117.17	111.62
1	A	196	SER	N-CA-C	-6.46	100.64	110.07
1	B	11	ILE	N-CA-C	-6.03	99.61	108.54
1	B	196	SER	N-CA-C	-6.01	101.29	110.07
1	B	150	GLU	N-CA-C	-5.89	102.71	110.43
1	A	454	ILE	N-CA-C	5.86	116.92	108.48
1	A	249	ALA	N-CA-C	-5.84	104.83	111.14
1	A	261	TYR	N-CA-C	5.78	117.58	111.28
1	B	429	PHE	N-CA-C	5.42	118.11	111.82
1	A	387	ASP	N-CA-C	-5.38	101.73	109.48
1	B	175	LEU	N-CA-C	5.38	121.59	114.12
1	A	11	ILE	N-CA-C	-5.16	100.90	108.54
1	A	148	GLN	CA-C-N	5.16	125.20	119.32
1	A	148	GLN	C-N-CA	5.16	125.20	119.32
1	A	175	LEU	N-CA-C	5.14	122.01	113.89

There are no chirality outliers.

There are no planarity outliers.

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	4315	0	4335	40	0
1	B	4329	0	4348	27	0
2	A	15	0	0	0	0
2	B	20	0	0	0	0
3	A	27	0	17	3	0
3	B	27	0	17	2	0
4	A	415	0	0	5	0
4	B	447	0	0	0	0
All	All	9595	0	8717	69	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 (69) 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)
3:B:1002:5X:H8	3:B:1002:5X:H41	1.62	0.81
3:A:1001:5X:H41	3:A:1001:5X:H8	1.67	0.76
1:A:83:LEU:HB2	1:A:173:MET:HA	1.67	0.76
1:B:336:LEU:HD22	1:B:356:PRO:HG3	1.73	0.71
1:A:197:PRO:HB2	4:A:1164:HOH:O	1.95	0.67
1:B:446:GLN:HE22	1:B:451:CYS:HB2	1.60	0.67
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.81	0.63
1:B:83:LEU:HB2	1:B:173:MET:HA	1.81	0.62
1:B:280:ARG:HD2	1:B:291:ASN:OD1	1.99	0.62
1:A:336:LEU:HD22	1:A:356:PRO:HG3	1.82	0.59
1:A:152:GLY:O	1:B:44:SER:HA	2.03	0.59
1:B:241:GLN:OE1	1:B:250:ARG:HG3	2.02	0.59
1:A:18:GLU:HB3	1:A:401:ARG:NH2	2.18	0.59
1:B:150:GLU:C	1:B:152:GLY:H	2.11	0.58
1:B:233:ILE:HD13	1:B:262:ILE:HA	1.88	0.54
1:A:160:ILE:HD12	1:A:282:SER:OG	2.07	0.54
1:B:346:TYR:O	1:B:347:SER:HB3	2.10	0.52
1:A:81:LYS:HE3	1:A:82:LEU:O	2.09	0.52
1:A:375:ASP:O	1:A:475:HIS:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.93	0.51
1:A:233:ILE:HD13	1:A:261:TYR:O	2.11	0.51
3:B:1002:5X:H43	3:B:1002:5X:S1	2.51	0.50
1:A:184:GLN:C	1:A:184:GLN:HE21	2.19	0.50
1:A:455:GLU:HB3	4:A:1225:HOH:O	2.10	0.50
1:A:445:CYS:SG	1:A:454:ILE:HD12	2.52	0.50
1:A:486:ALA:O	1:A:490:ARG:HG3	2.12	0.50
1:A:488:CYS:HB2	4:A:1357:HOH:O	2.11	0.49
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.95	0.48
1:A:462:ILE:O	1:A:466:LEU:HG	2.14	0.48
1:B:151:LYS:O	1:B:151:LYS:HG2	2.13	0.48
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.95	0.48
1:A:197:PRO:HB3	3:A:1001:5X:H13	1.97	0.46
1:A:308:LEU:HB2	1:A:311:CYS:SG	2.56	0.46
1:A:38:TYR:CZ	1:A:154:ARG:HG3	2.51	0.46
1:B:150:GLU:C	1:B:152:GLY:N	2.74	0.45
1:B:462:ILE:O	1:B:466:LEU:HG	2.17	0.45
1:A:86:GLU:H	1:A:86:GLU:CD	2.25	0.45
1:B:150:GLU:OE2	1:B:152:GLY:HA3	2.16	0.45
1:A:7:THR:HG21	1:A:273:ASN:ND2	2.32	0.45
1:A:220:ASP:HB2	4:A:1390:HOH:O	2.17	0.45
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.57	0.45
1:A:319:ASP:CG	1:A:366:CYS:H	2.25	0.45
1:A:346:TYR:O	1:A:347:SER:HB3	2.17	0.44
3:A:1001:5X:S1	3:A:1001:5X:H43	2.58	0.44
1:B:115:ALA:O	1:B:119:ILE:HG13	2.17	0.44
1:A:466:LEU:HD22	1:A:551:PHE:HE1	1.83	0.43
1:A:151:LYS:O	1:A:151:LYS:HG2	2.19	0.43
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.58	0.43
1:B:78:VAL:HG21	1:B:182:LEU:HD12	2.00	0.43
1:A:249:ALA:O	1:A:253:ILE:HG13	2.18	0.43
1:A:50:LYS:HD2	1:B:152:GLY:HA3	2.02	0.42
1:B:390:THR:HB	1:B:391:PRO:HD3	1.99	0.42
1:B:149:PRO:HG2	1:B:150:GLU:H	1.84	0.42
1:B:38:TYR:CE1	1:B:154:ARG:HB3	2.54	0.42
1:B:308:LEU:HB2	1:B:311:CYS:SG	2.60	0.42
1:A:506:ASN:HD21	1:A:510:ARG:HH11	1.68	0.42
1:B:361:GLU:OE1	1:B:372:VAL:HG23	2.20	0.42
1:B:93:PRO:HG3	1:B:561:TYR:HB2	2.02	0.41
1:A:485:VAL:O	1:A:489:LEU:HG	2.21	0.41
1:B:485:VAL:O	1:B:489:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:OE2	1:A:408:TRP:HD1	2.02	0.41
1:A:219:TYR:HB3	1:A:320:LEU:HD23	2.02	0.41
1:B:455:GLU:HA	1:B:456:PRO:HD2	1.96	0.41
1:A:93:PRO:HG3	1:A:561:TYR:HB2	2.04	0.40
1:A:112:SER:O	1:A:116:VAL:HG23	2.22	0.40
1:A:198:GLY:N	4:A:1164:HOH:O	2.54	0.40
1:A:118:HIS:O	1:A:122:VAL:HG23	2.22	0.40
1:A:155:LYS:HA	1:A:156:PRO:HD3	1.97	0.40
1:A:160:ILE:HA	1:A:282:SER:OG	2.22	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	550/580 (95%)	541 (98%)	9 (2%)	0	100	100
1	B	553/580 (95%)	546 (99%)	6 (1%)	1 (0%)	43	42
All	All	1103/1160 (95%)	1087 (98%)	15 (1%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	LYS

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	471/492 (96%)	466 (99%)	5 (1%)	65	73
1	B	471/492 (96%)	465 (99%)	6 (1%)	61	68
All	All	942/984 (96%)	931 (99%)	11 (1%)	63	70

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LYS
1	A	154	ARG
1	A	184	GLN
1	A	366	CYS
1	A	445	CYS
1	B	150	GLU
1	B	184	GLN
1	B	336	LEU
1	B	366	CYS
1	B	455	GLU
1	B	461	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	184	GLN
1	A	206	ASN
1	A	273	ASN
1	A	438	GLN
1	A	461	GLN
1	A	475	HIS
1	A	483	ASN
1	A	502	HIS
1	A	506	ASN
1	B	35	ASN
1	B	95	HIS
1	B	184	GLN
1	B	273	ASN
1	B	330	GLN
1	B	446	GLN

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 ⓘ

9 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	5X	B	1002	1	27,29,29	1.88	5 (18%)	32,41,41	1.25	2 (6%)
2	SO4	B	1105	-	4,4,4	0.39	0	6,6,6	0.08	0
2	SO4	A	1103	-	4,4,4	0.38	0	6,6,6	0.07	0
2	SO4	A	1101	-	4,4,4	0.34	0	6,6,6	0.08	0
3	5X	A	1001	1	27,29,29	1.93	5 (18%)	32,41,41	1.44	4 (12%)
2	SO4	B	1106	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	B	1107	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	B	1104	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	A	1102	-	4,4,4	0.37	0	6,6,6	0.07	0

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	5X	B	1002	1	-	1/17/35/35	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5X	A	1001	1	-	2/17/35/35	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	5X	S19-N22	5.36	1.76	1.65
3	A	1001	5X	S19-N22	5.17	1.76	1.65
3	A	1001	5X	C7-N1	-3.75	1.33	1.39
3	B	1002	5X	C7-N1	-3.64	1.33	1.39
3	A	1001	5X	C14-S1	-3.40	1.76	1.82
3	B	1002	5X	C14-S1	-2.73	1.77	1.82
3	A	1001	5X	C5-C3	2.34	1.51	1.46
3	A	1001	5X	C3-C2	2.30	1.36	1.33
3	B	1002	5X	C3-C2	2.23	1.36	1.33
3	B	1002	5X	C5-C3	2.22	1.51	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	5X	C7-C14-S1	-4.69	102.37	106.11
3	B	1002	5X	C7-C14-S1	-4.57	102.46	106.11
3	A	1001	5X	O1-C7-N1	-3.76	119.34	123.60
3	B	1002	5X	O1-C7-N1	-3.16	120.02	123.60
3	A	1001	5X	C7-N1-N22	2.22	124.81	122.74
3	A	1001	5X	C6-C5-C3	-2.11	113.96	121.22

There are no chirality outliers.

All (3) torsion outliers are listed below:

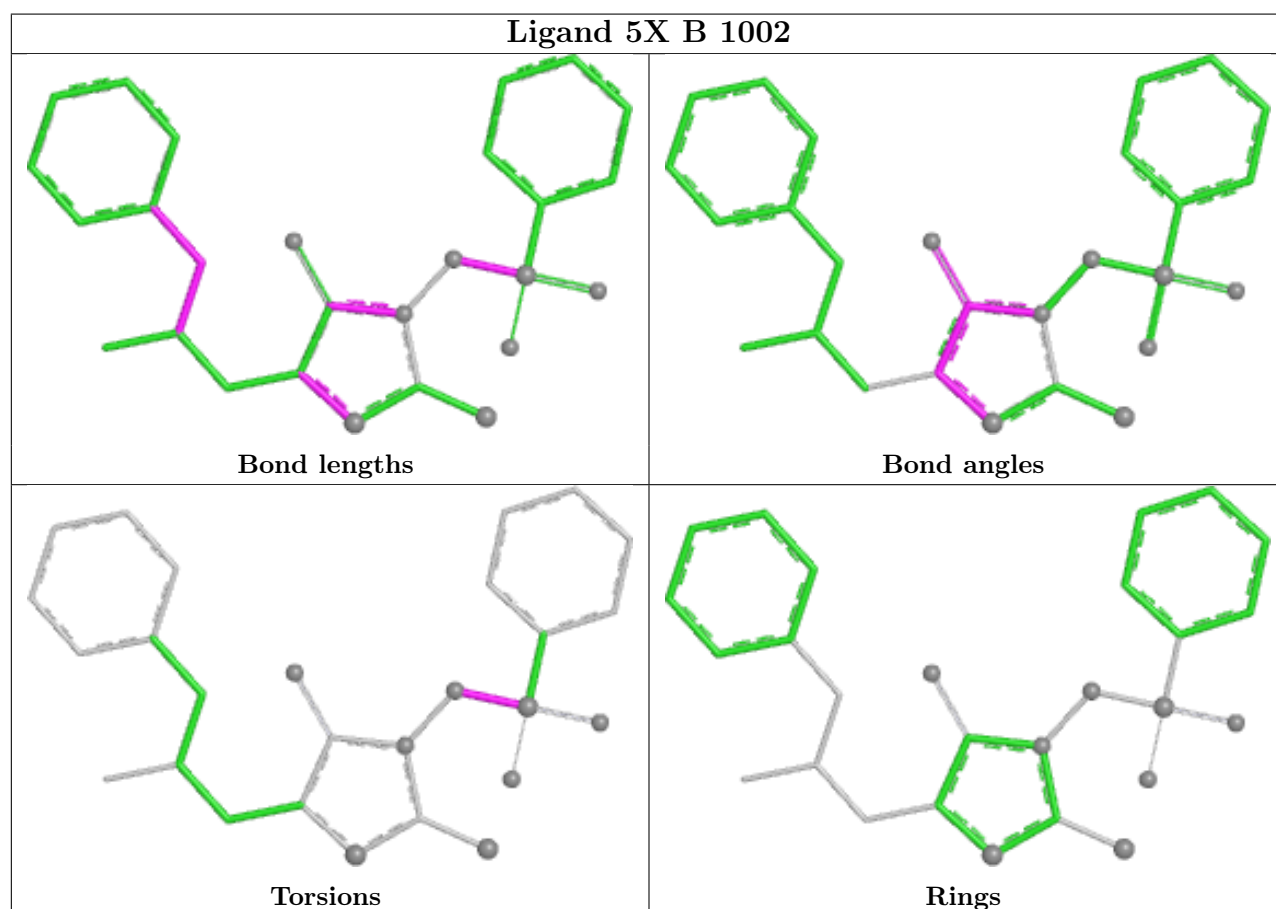
Mol	Chain	Res	Type	Atoms
3	B	1002	5X	N1-N22-S19-O20
3	A	1001	5X	N1-N22-S19-O20
3	A	1001	5X	N1-N22-S19-O21

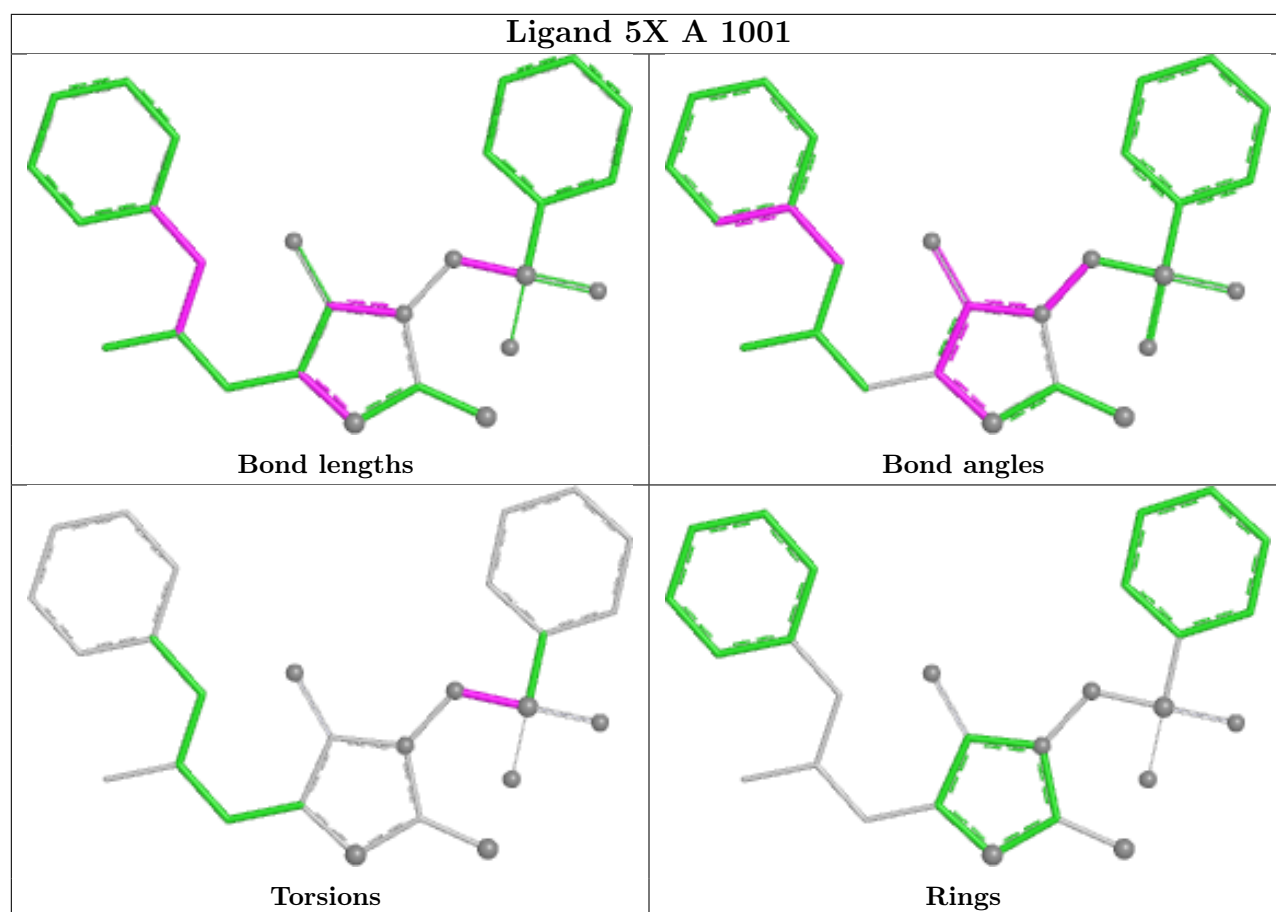
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	5X	2	0
3	A	1001	5X	3	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	554/580 (95%)	0.30	19 (3%) 48 47	18, 28, 44, 49	0
1	B	557/580 (96%)	0.19	20 (3%) 46 45	17, 27, 43, 56	0
All	All	1111/1160 (95%)	0.25	39 (3%) 47 46	17, 27, 43, 56	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	150	GLU	5.0
1	B	152	GLY	5.0
1	B	149	PRO	4.8
1	B	151	LYS	4.3
1	B	543	GLY	4.1
1	A	498	ARG	4.0
1	A	402	HIS	3.9
1	A	405	VAL	3.7
1	A	540	ALA	3.6
1	B	402	HIS	3.5
1	A	403	THR	3.3
1	A	128	GLU	3.3
1	B	148	GLN	3.3
1	A	401	ARG	2.6
1	A	483	ASN	2.6
1	B	405	VAL	2.5
1	B	14	CYS	2.5
1	A	106	LYS	2.5
1	B	403	THR	2.4
1	B	501	ARG	2.4
1	A	101	PHE	2.4
1	A	105	ALA	2.4
1	A	158	ARG	2.4
1	B	76	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	246	ALA	2.3
1	B	534	LEU	2.3
1	A	121	SER	2.3
1	B	540	ALA	2.3
1	A	110	ASN	2.2
1	B	181	THR	2.2
1	B	101	PHE	2.1
1	A	120	HIS	2.1
1	B	542	ALA	2.1
1	B	539	ILE	2.1
1	B	88	ALA	2.1
1	A	14	CYS	2.1
1	A	9	ALA	2.1
1	A	535	LYS	2.1
1	A	100	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	1102	5/5	0.73	0.19	57,58,58,58	0
2	SO4	B	1107	5/5	0.75	0.11	62,62,62,62	0
2	SO4	B	1106	5/5	0.85	0.10	64,64,64,64	0
2	SO4	A	1103	5/5	0.86	0.14	50,50,51,51	0
3	5X	A	1001	27/27	0.86	0.13	34,41,48,53	0
3	5X	B	1002	27/27	0.86	0.13	34,40,48,52	0
2	SO4	A	1101	5/5	0.94	0.10	48,48,48,48	0
2	SO4	B	1104	5/5	0.95	0.10	36,36,36,37	0

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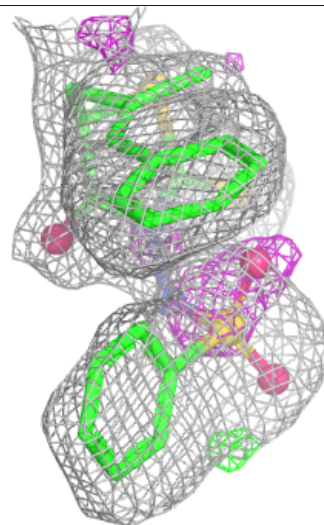
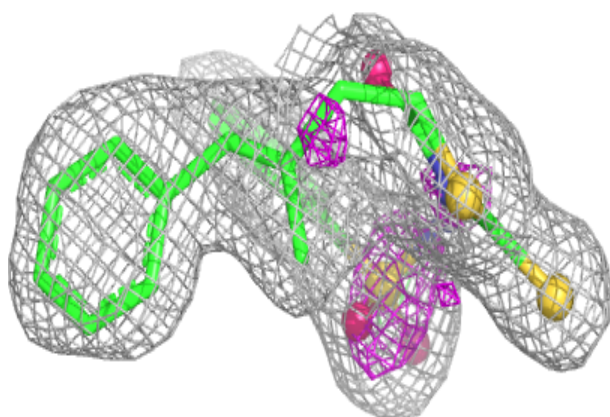
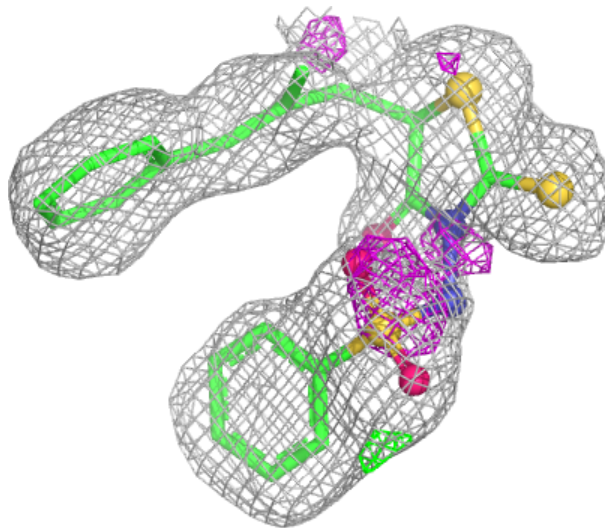
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	1105	5/5	0.97	0.07	32,32,32,32	0

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.

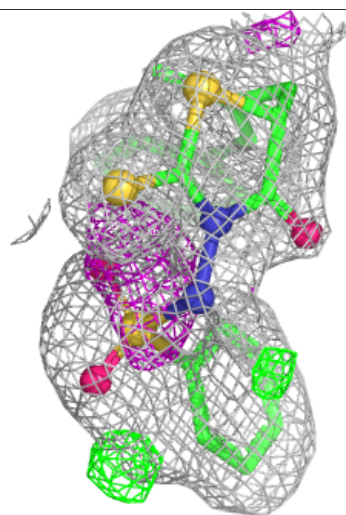
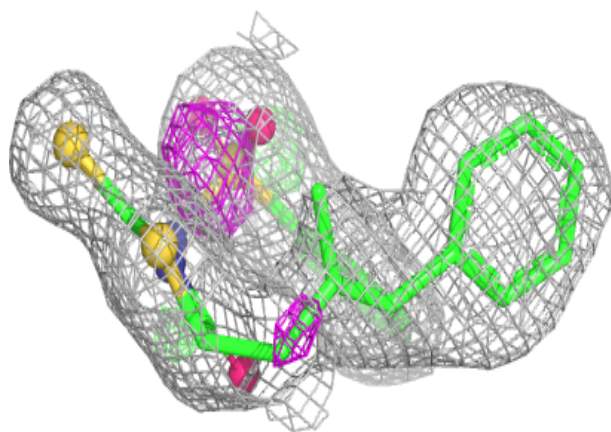
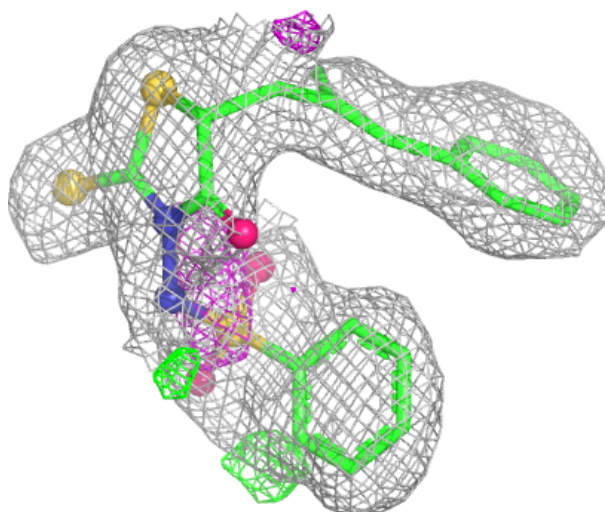
Electron density around 5X A 1001:

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



Electron density around 5X B 1002:

$2mF_o-DF_c$ (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.