



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:20 AM EDT

PDB ID : 2HJH / pdb_00002hjh
Title : Crystal Structure of the Sir2 deacetylase
Authors : Hall, B.E.; Ellenberger, T.E.
Deposited on : 2006-06-30
Resolution : 1.85 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

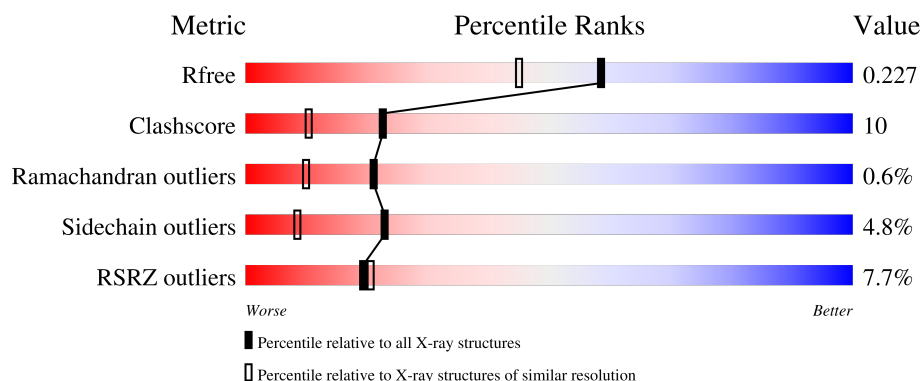
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	354	
1	B	354	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5747 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.

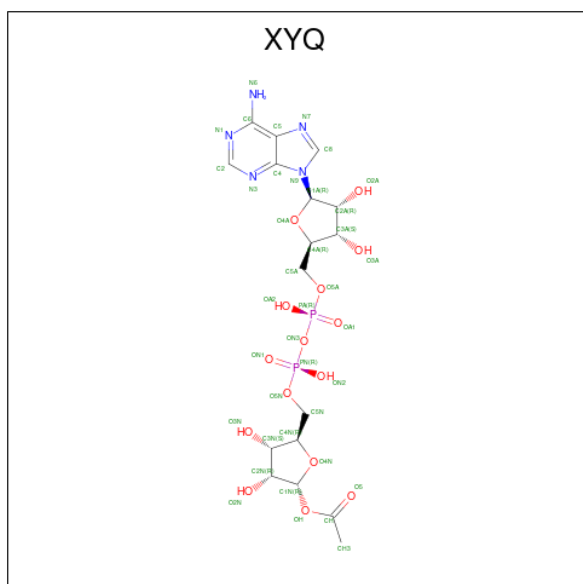
- Molecule 1 is a protein called NAD-dependent histone deacetylase SIR2.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	Se		0	1	0
			2595	1679	439	460	11	6				
1	B	326	Total	C	N	O	S	Se		0	0	0
			2539	1638	431	452	11	7				

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

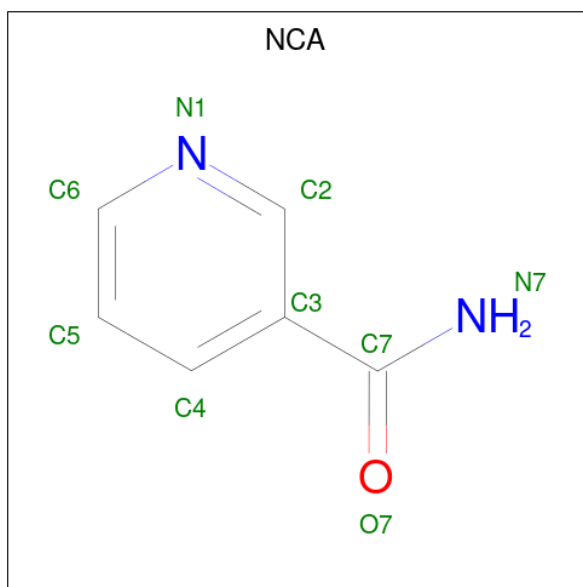
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (2R,3R,4S,5R)-5-({[(R)-{[(R)-{(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHOXY}(HYDROXY)PHOSPHORYL]OXY}(HYDROXY)PHOSPHORYL]OXY}METHYL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL ACETATE (CCD ID: XYQ) (formula: C₁₇H₂₅N₅O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			38	17	5	14	2		
3	B	1	Total	C	N	O	P	0	0
			38	17	5	14	2		

- Molecule 4 is NICOTINAMIDE (CCD ID: NCA) (formula: C₆H₆N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	6	2	1		
4	B	1	Total	C	N	O	0	0
			9	6	2	1		

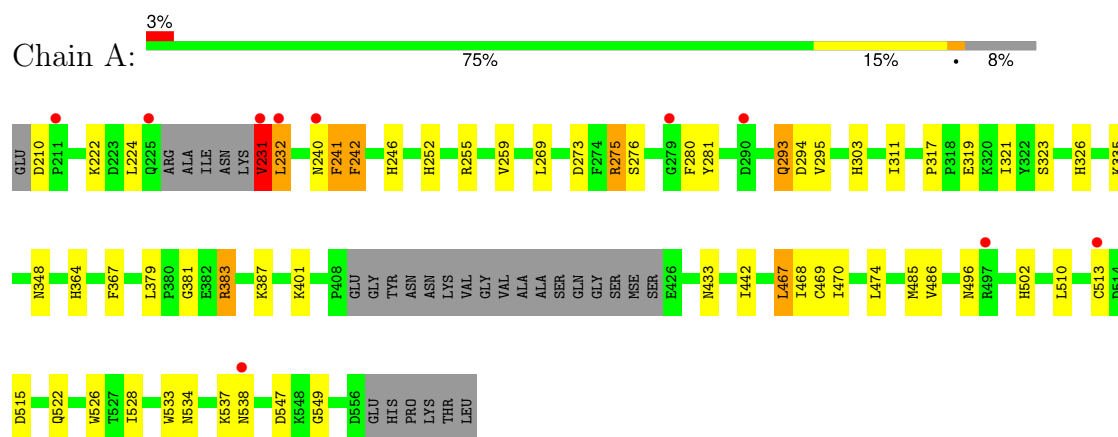
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	310	Total	O	0	0
			310	310		
5	B	207	Total	O	0	0
			207	207		

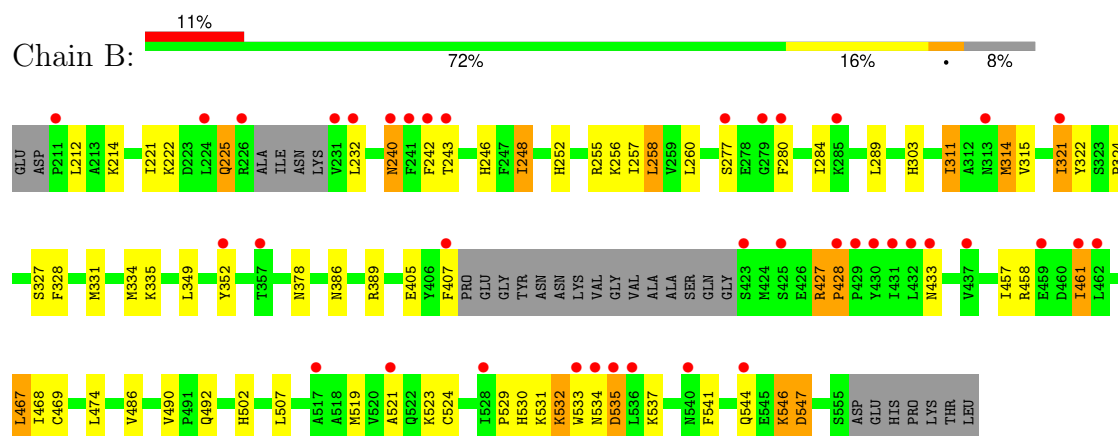
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NAD-dependent histone deacetylase SIR2



• Molecule 1: NAD-dependent histone deacetylase SIR2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.35Å 89.57Å 94.51Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.85) 96.0 (30.00-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.171 , 0.215 0.187 , 0.227	Depositor DCC
R_{free} test set	3497 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5747	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.94% 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: NCA, XYQ, ZN

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	1.39	7/2656 (0.3%)	1.18	4/3591 (0.1%)
1	B	1.28	8/2593 (0.3%)	1.14	7/3507 (0.2%)
All	All	1.34	15/5249 (0.3%)	1.16	11/7098 (0.2%)

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
1	B	0	2
All	All	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	MSE	SE-CE	12.06	2.31	1.95
1	B	315	VAL	CA-CB	8.48	1.66	1.54
1	A	295	VAL	CA-C	6.31	1.62	1.52
1	B	433	ASN	C-O	-5.52	1.16	1.24
1	A	442	ILE	N-CA	-5.50	1.40	1.46
1	B	428	PRO	C-O	-5.46	1.18	1.24
1	A	528	ILE	C-O	-5.43	1.17	1.24
1	B	427	ARG	C-O	-5.38	1.17	1.24
1	A	295	VAL	CA-CB	-5.34	1.45	1.54
1	B	255	ARG	CA-CB	5.33	1.61	1.54
1	B	257	ILE	C-O	5.33	1.30	1.24
1	A	474	LEU	C-O	5.29	1.30	1.23
1	A	255	ARG	NE-CZ	5.23	1.38	1.33
1	A	486	VAL	CA-CB	5.18	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	492	GLN	C-O	5.05	1.29	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	PRO	CA-C-O	-6.88	115.29	120.73
1	B	490	VAL	N-CA-C	6.78	114.46	108.63
1	B	327	SER	N-CA-C	5.91	118.50	111.71
1	B	328	PHE	N-CA-C	-5.89	104.98	111.82
1	B	248	ILE	N-CA-C	5.70	115.89	110.42
1	B	225	GLN	N-CA-C	-5.67	105.00	111.07
1	A	317	PRO	N-CA-CB	-5.57	100.33	103.22
1	B	221	ILE	O-C-N	-5.45	116.30	122.94
1	A	275	ARG	N-CA-C	5.29	119.71	112.88
1	B	222	LYS	N-CA-C	5.26	118.20	110.30
1	A	533	TRP	N-CA-C	5.22	117.38	111.11

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	VAL	Peptide
1	B	225	GLN	Peptide
1	B	533	TRP	Peptide

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	2595	0	2602	51	1
1	B	2539	0	2502	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	38	0	20	7	0
3	B	38	0	20	1	0
4	A	9	0	6	1	0
4	B	9	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	310	0	0	13	1
5	B	207	0	0	9	1
All	All	5747	0	5156	109	2

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 10.

All (109) 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:314:MSE:SE	1:B:314:MSE:CE	2.31	1.28
1:B:407:PHE:C	5:B:1398:HOH:O	2.04	0.98
1:B:378:ASN:HB3	5:B:1422:HOH:O	1.72	0.88
1:B:546:LYS:O	1:B:547:ASP:HB2	1.73	0.87
1:A:467:LEU:HD21	1:A:469:CYS:SG	2.15	0.86
1:B:427:ARG:HB3	1:B:428:PRO:HD2	1.58	0.86
1:B:530:HIS:HD2	1:B:532:LYS:H	1.22	0.84
1:A:485:MSE:HE1	1:B:212:LEU:HD11	1.62	0.81
1:A:383:ARG:NH1	5:A:1527:HOH:O	2.14	0.79
1:B:534:ASN:O	1:B:535:ASP:CB	2.34	0.75
1:B:467:LEU:HD21	1:B:469:CYS:SG	2.27	0.73
1:B:242:PHE:O	1:B:507:LEU:HD13	1.90	0.72
1:B:519:MSE:HG3	1:B:541:PHE:CD1	2.24	0.72
1:A:348:ASN:ND2	5:A:1509:HOH:O	2.23	0.71
1:A:280:PHE:HB2	4:A:900:NCA:H6	1.72	0.70
1:B:467:LEU:C	1:B:467:LEU:HD23	2.17	0.70
1:B:240:ASN:N	1:B:240:ASN:ND2	2.44	0.66
1:A:241:PHE:HA	1:A:246:HIS:CD2	2.30	0.66
1:A:231:VAL:HG22	1:A:232:LEU:HA	1.78	0.66
1:B:519:MSE:HG3	1:B:541:PHE:CG	2.32	0.65
1:B:240:ASN:ND2	1:B:240:ASN:H	1.93	0.65
1:A:467:LEU:C	1:A:467:LEU:HD23	2.22	0.64
1:B:546:LYS:O	1:B:547:ASP:CB	2.45	0.64
1:A:515:ASP:OD2	5:A:1500:HOH:O	2.16	0.63
1:A:210:ASP:N	5:A:1395:HOH:O	2.32	0.61
1:B:335:LYS:NZ	5:B:1242:HOH:O	2.31	0.61
1:B:427:ARG:HB3	1:B:428:PRO:CD	2.30	0.60
1:A:242:PHE:H	1:A:246:HIS:HD2	1.50	0.60
1:A:513:CYS:HG	3:A:1222:XYQ:C2	2.15	0.59
1:A:326:HIS:HE1	5:A:1231:HOH:O	1.85	0.59
1:B:240:ASN:N	1:B:240:ASN:HD22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:GLN:HE21	1:A:537:LYS:HA	1.69	0.58
1:A:240:ASN:O	1:A:241:PHE:HB2	2.04	0.57
4:B:901:NCA:H5	5:B:1289:HOH:O	2.04	0.57
1:A:513:CYS:SG	3:A:1222:XYQ:N1	2.71	0.57
1:B:457:ILE:HG13	1:B:461:ILE:HD13	1.87	0.56
1:B:386:ASN:ND2	1:B:389:ARG:HH11	2.04	0.56
1:A:323:SER:H	1:A:326:HIS:HD2	1.53	0.56
1:A:252:HIS:HE1	5:A:1342:HOH:O	1.87	0.56
1:A:485:MSE:CE	1:B:212:LEU:HD11	2.33	0.56
1:A:275:ARG:HG3	5:A:1371:HOH:O	2.06	0.56
1:B:386:ASN:HD22	1:B:389:ARG:HH11	1.54	0.56
1:A:513:CYS:SG	3:A:1222:XYQ:C2	2.94	0.55
1:A:242:PHE:O	1:A:549:GLY:HA2	2.07	0.55
3:B:1222:XYQ:CH3	5:B:1268:HOH:O	2.54	0.54
1:A:534:ASN:HA	1:A:537:LYS:HE3	1.89	0.54
1:B:519:MSE:HE3	1:B:523:LYS:CE	2.38	0.53
1:B:352:TYR:C	5:B:1371:HOH:O	2.51	0.52
1:B:311:ILE:C	1:B:311:ILE:HD12	2.35	0.52
1:B:530:HIS:CD2	1:B:532:LYS:H	2.14	0.52
1:B:519:MSE:HE3	1:B:523:LYS:HD2	1.93	0.51
1:B:322:TYR:CE2	5:B:1371:HOH:O	2.63	0.50
1:A:383:ARG:HH11	1:A:383:ARG:HG3	1.77	0.50
1:B:242:PHE:CE2	1:B:246:HIS:HE1	2.30	0.50
1:A:367:PHE:O	1:A:381:GLY:HA3	2.11	0.50
3:A:1222:XYQ:CH3	5:A:1322:HOH:O	2.59	0.50
1:A:335:LYS:HZ2	1:A:526:TRP:CG	2.30	0.49
1:A:281:TYR:CZ	1:A:293:GLN:HG3	2.47	0.49
1:B:467:LEU:C	1:B:467:LEU:CD2	2.84	0.49
1:B:467:LEU:HD23	1:B:468:ILE:N	2.27	0.49
1:A:273:ASP:OD2	1:A:276:SER:OG	2.30	0.49
1:B:457:ILE:O	1:B:461:ILE:HB	2.13	0.48
1:A:246:HIS:HE1	5:A:1393:HOH:O	1.95	0.48
1:A:513:CYS:HG	3:A:1222:XYQ:C6	2.23	0.48
1:A:467:LEU:HD23	1:A:468:ILE:N	2.29	0.48
1:B:248:ILE:HD13	1:B:523:LYS:HB3	1.96	0.48
1:A:293:GLN:NE2	5:A:1478:HOH:O	2.45	0.48
1:B:252:HIS:NE2	5:B:1387:HOH:O	2.14	0.47
1:B:474:LEU:O	1:B:502:HIS:HE1	1.98	0.47
1:A:259:VAL:CG1	1:A:470[B]:ILE:HD12	2.45	0.47
1:A:231:VAL:HG22	1:A:232:LEU:CA	2.44	0.46
1:A:496:ASN:O	1:A:510:LEU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:HIS:HD2	5:A:1391:HOH:O	1.98	0.45
1:A:335:LYS:NZ	1:A:526:TRP:CG	2.85	0.45
1:A:275:ARG:NE	3:A:1222:XYQ:OA1	2.49	0.45
1:A:502:HIS:CD2	5:A:1391:HOH:O	2.70	0.45
1:B:280:PHE:CB	4:B:901:NCA:O7	2.65	0.44
1:B:386:ASN:ND2	1:B:389:ARG:NH1	2.65	0.44
1:B:243:THR:O	1:B:507:LEU:HD22	2.17	0.44
1:B:232:LEU:N	1:B:232:LEU:CD1	2.81	0.44
1:A:222:LYS:HE3	1:A:364:HIS:CE1	2.54	0.43
1:A:269:LEU:HB3	1:A:321:ILE:HD12	2.01	0.43
1:B:519:MSE:HE3	1:B:523:LYS:CD	2.48	0.43
1:B:331:MSE:HA	1:B:334:MSE:HE3	1.99	0.43
3:A:1222:XYQ:CH3	5:A:1479:HOH:O	2.65	0.43
1:B:334:MSE:HE1	1:B:529:PRO:HG3	1.99	0.43
1:B:530:HIS:CD2	1:B:531:LYS:N	2.86	0.43
1:A:311:ILE:HD12	1:A:311:ILE:C	2.43	0.43
1:B:243:THR:OG1	1:B:246:HIS:CG	2.72	0.43
1:A:534:ASN:OD1	1:A:537:LYS:HE3	2.18	0.43
1:B:519:MSE:HE3	1:B:523:LYS:HE2	2.01	0.42
1:A:224:LEU:HD13	1:A:293:GLN:OE1	2.19	0.42
1:B:474:LEU:O	1:B:502:HIS:CE1	2.72	0.42
1:B:242:PHE:CD2	1:B:242:PHE:N	2.88	0.42
1:A:485:MSE:HG2	1:B:214:LYS:HB3	2.02	0.42
1:B:260:LEU:C	1:B:260:LEU:HD23	2.45	0.42
1:B:322:TYR:N	1:B:322:TYR:CD2	2.88	0.42
1:A:281:TYR:OH	1:A:293:GLN:HG3	2.20	0.41
1:A:242:PHE:N	1:A:246:HIS:HD2	2.17	0.41
1:A:259:VAL:HG13	1:A:470[B]:ILE:HD12	2.02	0.41
1:A:303:HIS:O	1:A:433:ASN:HB2	2.20	0.41
1:B:427:ARG:CB	1:B:428:PRO:CD	2.91	0.41
1:B:256:LYS:NZ	5:B:1339:HOH:O	2.53	0.41
1:A:224:LEU:HD22	1:A:293:GLN:OE1	2.20	0.41
1:B:284:ILE:CG2	1:B:289:LEU:HD22	2.51	0.41
1:A:467:LEU:C	1:A:467:LEU:CD2	2.93	0.40
1:B:258:LEU:HD12	1:B:258:LEU:HA	1.87	0.40
1:B:521:ALA:O	1:B:524:CYS:HB2	2.21	0.40
1:B:321:ILE:O	1:B:349:LEU:HD22	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASP:OD2	5:B:1410:HOH:O[1_655]	2.14	0.06
5:A:1377:HOH:O	5:A:1448:HOH:O[2_647]	2.19	0.01

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	320/354 (90%)	308 (96%)	10 (3%)	2 (1%)	21	10
1	B	320/354 (90%)	312 (98%)	6 (2%)	2 (1%)	21	10
All	All	640/708 (90%)	620 (97%)	16 (2%)	4 (1%)	21	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	535	ASP
1	A	241	PHE
1	A	242	PHE
1	B	547	ASP

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	291/313 (93%)	280 (96%)	11 (4%)	29	14
1	B	277/313 (88%)	261 (94%)	16 (6%)	18	6
All	All	568/626 (91%)	541 (95%)	27 (5%)	23	8

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	VAL
1	A	232	LEU
1	A	293	GLN
1	A	319	GLU
1	A	379	LEU
1	A	383	ARG
1	A	387	LYS
1	A	401	LYS
1	A	467	LEU
1	A	538	ASN
1	A	547	ASP
1	B	240	ASN
1	B	258	LEU
1	B	277	SER
1	B	303	HIS
1	B	311	ILE
1	B	321	ILE
1	B	324	PRO
1	B	405	GLU
1	B	458	ARG
1	B	461	ILE
1	B	467	LEU
1	B	486	VAL
1	B	532	LYS
1	B	537	LYS
1	B	544	GLN
1	B	546	LYS

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	246	HIS
1	A	313	ASN
1	A	326	HIS
1	A	348	ASN
1	A	378	ASN
1	A	496	ASN
1	A	502	HIS
1	A	522	GLN
1	B	240	ASN
1	B	252	HIS

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Mol	Chain	Res	Type
1	B	310	ASN
1	B	341	ASN
1	B	386	ASN
1	B	496	ASN
1	B	502	HIS
1	B	530	HIS

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 6 ligands modelled in this entry, 2 are 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	NCA	B	901	-	9,9,9	0.53	0	11,11,11	1.42	2 (18%)
4	NCA	A	900	-	9,9,9	1.18	1 (11%)	11,11,11	1.98	3 (27%)
3	XYQ	B	1222	1	41,41,42	1.46	7 (17%)	59,62,64	2.95	24 (40%)
3	XYQ	A	1222	1	41,41,42	1.65	8 (19%)	59,62,64	2.88	22 (37%)

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	NCA	B	901	-	-	4/4/4/4	0/1/1/1
4	NCA	A	900	-	-	0/4/4/4	0/1/1/1
3	XYQ	B	1222	1	-	6/25/57/58	0/4/4/4
3	XYQ	A	1222	1	-	5/25/57/58	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1222	XYQ	C4-N3	4.61	1.43	1.34
3	B	1222	XYQ	C4-N3	4.44	1.42	1.34
3	B	1222	XYQ	OH-C1N	3.91	1.46	1.40
3	A	1222	XYQ	C8-N7	3.30	1.38	1.31
3	A	1222	XYQ	C5-N7	-2.95	1.33	1.39
3	B	1222	XYQ	C8-N7	2.93	1.37	1.31
3	A	1222	XYQ	C4-N9	-2.85	1.31	1.37
3	B	1222	XYQ	C5-C4	-2.84	1.34	1.39
3	A	1222	XYQ	PA-ON3	2.72	1.62	1.59
3	A	1222	XYQ	OH-C1N	2.65	1.44	1.40
3	B	1222	XYQ	C4-N9	-2.59	1.32	1.37
3	A	1222	XYQ	PN-ON3	2.53	1.62	1.59
3	B	1222	XYQ	C5-N7	-2.42	1.34	1.39
3	B	1222	XYQ	O4N-C4N	-2.31	1.39	1.45
3	A	1222	XYQ	C5-C4	-2.08	1.35	1.39
4	A	900	NCA	C3-C7	2.00	1.53	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1222	XYQ	O4N-C1N-OH	-15.24	95.22	111.95
3	A	1222	XYQ	O4N-C1N-OH	-14.53	96.01	111.95
3	A	1222	XYQ	N1-C2-N3	-7.48	117.25	128.58
3	B	1222	XYQ	N1-C2-N3	-5.69	119.97	128.58
3	B	1222	XYQ	O4N-C1N-C2N	4.93	111.25	104.98
4	A	900	NCA	C3-C7-N7	4.85	123.71	117.74
3	B	1222	XYQ	C5-C4-N9	4.80	111.04	105.81
3	B	1222	XYQ	N9-C8-N7	-4.64	107.35	113.94
3	A	1222	XYQ	C5-C6-N6	-4.21	112.87	123.29
3	A	1222	XYQ	C2A-C1A-N9	4.11	123.51	113.30
3	A	1222	XYQ	O4N-C1N-C2N	3.83	109.85	104.98
3	A	1222	XYQ	N9-C8-N7	-3.73	108.64	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1222	XYQ	C4-C5-N7	-3.68	106.38	110.58
3	B	1222	XYQ	C5-C4-N3	-3.60	121.77	126.72
3	A	1222	XYQ	N6-C6-N1	3.48	126.12	118.38
3	A	1222	XYQ	O3A-C3A-C4A	-3.46	101.14	111.08
3	A	1222	XYQ	C2-N1-C6	3.41	124.33	118.73
3	A	1222	XYQ	C5-C4-N9	3.31	109.42	105.81
3	B	1222	XYQ	O3N-C3N-C4N	-3.23	101.80	111.08
3	B	1222	XYQ	C2A-C1A-N9	3.10	121.01	113.30
3	B	1222	XYQ	OH-CH-CH3	3.05	120.98	109.74
3	A	1222	XYQ	C5-C4-N3	-2.99	122.60	126.72
3	B	1222	XYQ	C5-N7-C8	2.96	108.10	103.45
3	B	1222	XYQ	O3A-C3A-C2A	-2.93	102.43	111.82
3	B	1222	XYQ	C5-C6-N6	-2.78	116.40	123.29
3	B	1222	XYQ	C2-N3-C4	2.76	118.58	111.83
3	A	1222	XYQ	C2A-C3A-C4A	2.70	107.82	102.61
3	B	1222	XYQ	C6-C5-N7	2.69	137.27	132.09
4	A	900	NCA	O7-C7-C3	-2.65	116.35	119.60
3	B	1222	XYQ	O3A-C3A-C4A	-2.61	103.57	111.08
4	B	901	NCA	C6-N1-C2	2.60	121.41	116.85
3	A	1222	XYQ	C2-N3-C4	2.58	118.12	111.83
3	A	1222	XYQ	C5N-C4N-C3N	-2.56	105.99	115.21
3	A	1222	XYQ	ON2-PN-ON1	2.49	124.00	112.44
3	A	1222	XYQ	O3N-C3N-C4N	-2.40	104.18	111.08
3	B	1222	XYQ	C2A-C3A-C4A	2.36	107.17	102.61
3	A	1222	XYQ	OH-CH-CH3	2.36	118.43	109.74
3	A	1222	XYQ	OH-C1N-C2N	-2.32	104.11	107.81
3	B	1222	XYQ	C4-N9-C1A	-2.31	121.22	126.63
3	B	1222	XYQ	O4N-C4N-C3N	2.31	109.73	105.15
3	B	1222	XYQ	O5A-PA-OA1	-2.26	99.99	108.94
3	A	1222	XYQ	C5A-C4A-C3A	-2.26	107.09	115.21
3	A	1222	XYQ	OA2-PA-ON3	-2.25	101.19	107.27
3	B	1222	XYQ	O2N-C2N-C1N	2.20	118.02	111.82
3	A	1222	XYQ	O2N-C2N-C1N	2.20	118.00	111.82
3	A	1222	XYQ	C2N-C3N-C4N	2.19	106.85	102.61
3	B	1222	XYQ	O4N-C4N-C5N	-2.16	102.41	109.33
4	A	900	NCA	C6-N1-C2	2.08	120.50	116.85
3	B	1222	XYQ	C1A-N9-C8	2.07	131.70	127.09
4	B	901	NCA	C3-C2-N1	-2.03	120.49	123.50
3	B	1222	XYQ	C5N-C4N-C3N	-2.01	107.98	115.21

There are no chirality outliers.

All (15) torsion outliers are listed below:

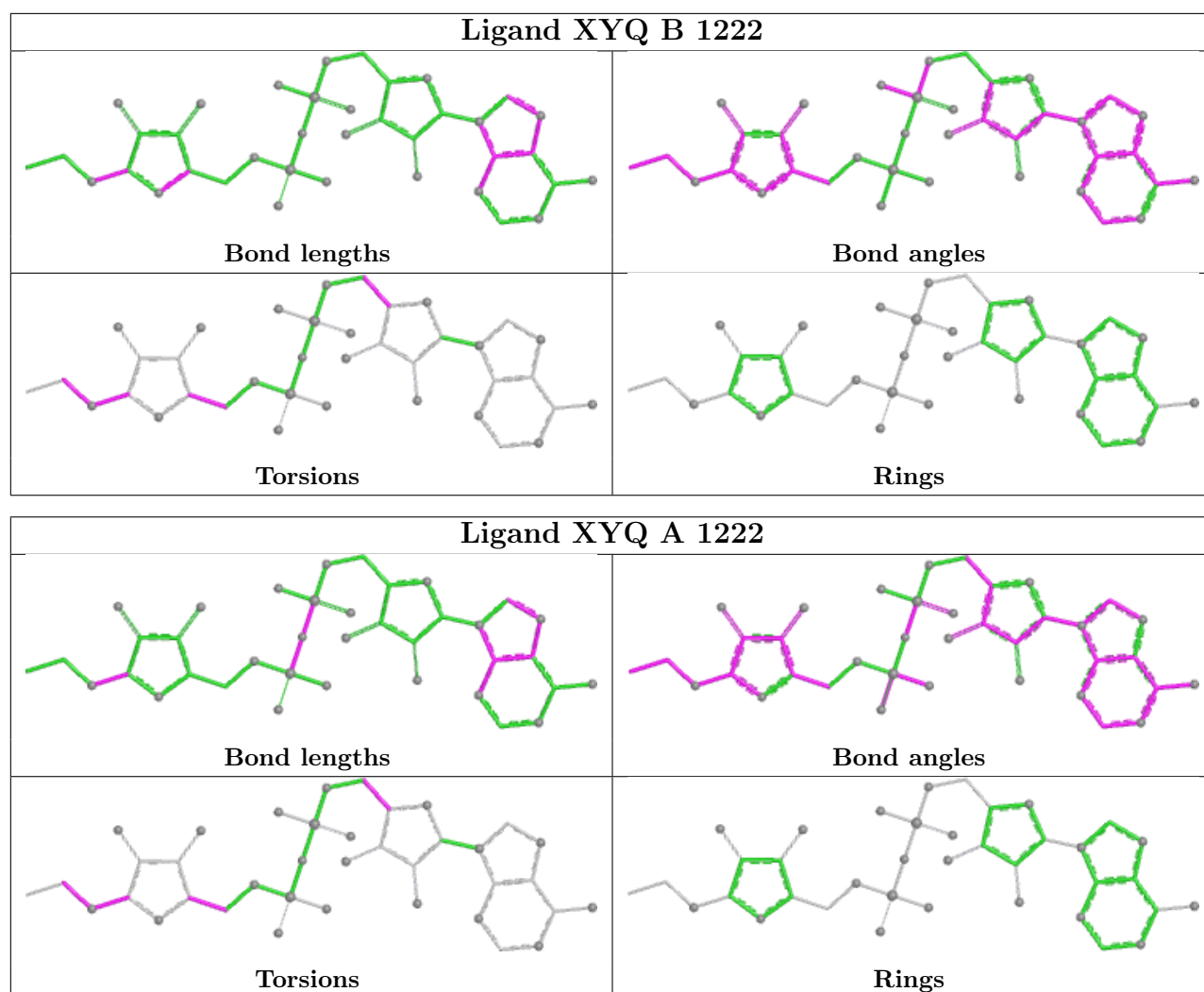
Mol	Chain	Res	Type	Atoms
3	A	1222	XYQ	CH3-CH-OH-C1N
3	A	1222	XYQ	C2N-C1N-OH-CH
3	A	1222	XYQ	O4N-C1N-OH-CH
3	B	1222	XYQ	CH3-CH-OH-C1N
3	B	1222	XYQ	C2N-C1N-OH-CH
3	B	1222	XYQ	O4N-C1N-OH-CH
4	B	901	NCA	C2-C3-C7-O7
4	B	901	NCA	C2-C3-C7-N7
4	B	901	NCA	C4-C3-C7-O7
4	B	901	NCA	C4-C3-C7-N7
3	B	1222	XYQ	O4N-C4N-C5N-O5N
3	B	1222	XYQ	C3N-C4N-C5N-O5N
3	A	1222	XYQ	O4N-C4N-C5N-O5N
3	A	1222	XYQ	O4A-C4A-C5A-O5A
3	B	1222	XYQ	O4A-C4A-C5A-O5A

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	901	NCA	2	0
4	A	900	NCA	1	0
3	B	1222	XYQ	1	0
3	A	1222	XYQ	7	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	484:ASN	C	485:MSE	N	1.19

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	319/354 (90%)	0.06	10 (3%) 51 55	9, 24, 43, 66	4 (1%)
1	B	319/354 (90%)	0.93	39 (12%) 8 8	21, 34, 49, 62	0
All	All	638/708 (90%)	0.50	49 (7%) 19 20	9, 30, 48, 66	4 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	ASN	7.0
1	B	243	THR	5.6
1	A	497	ARG	5.5
1	B	242	PHE	5.5
1	B	430	TYR	5.3
1	A	231	VAL	5.0
1	B	429	PRO	4.3
1	B	536	LEU	4.0
1	A	513	CYS	4.0
1	B	280	PHE	4.0
1	B	352	TYR	3.9
1	A	232	LEU	3.8
1	B	521	ALA	3.8
1	B	224	LEU	3.7
1	B	231	VAL	3.5
1	A	211	PRO	3.3
1	B	232	LEU	3.2
1	B	211	PRO	3.2
1	B	535	ASP	3.1
1	B	462	LEU	3.1
1	B	279	GLY	3.1
1	B	226	ARG	3.0
1	B	425	SER	2.9
1	B	240	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	431	ILE	2.8
1	B	423	SER	2.7
1	B	528	ILE	2.7
1	B	277	SER	2.6
1	B	544	GLN	2.5
1	B	407	PHE	2.5
1	A	225	GLN	2.4
1	A	240	ASN	2.4
1	A	279	GLY	2.4
1	B	534	ASN	2.4
1	B	321	ILE	2.3
1	B	461	ILE	2.3
1	B	533	TRP	2.3
1	B	357	THR	2.3
1	B	432	LEU	2.3
1	B	459	GLU	2.2
1	B	428	PRO	2.2
1	B	433	ASN	2.2
1	B	313	ASN	2.1
1	B	437	VAL	2.1
1	B	540	ASN	2.1
1	A	290	ASP	2.1
1	B	241	PHE	2.0
1	B	285	LYS	2.0
1	B	517	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

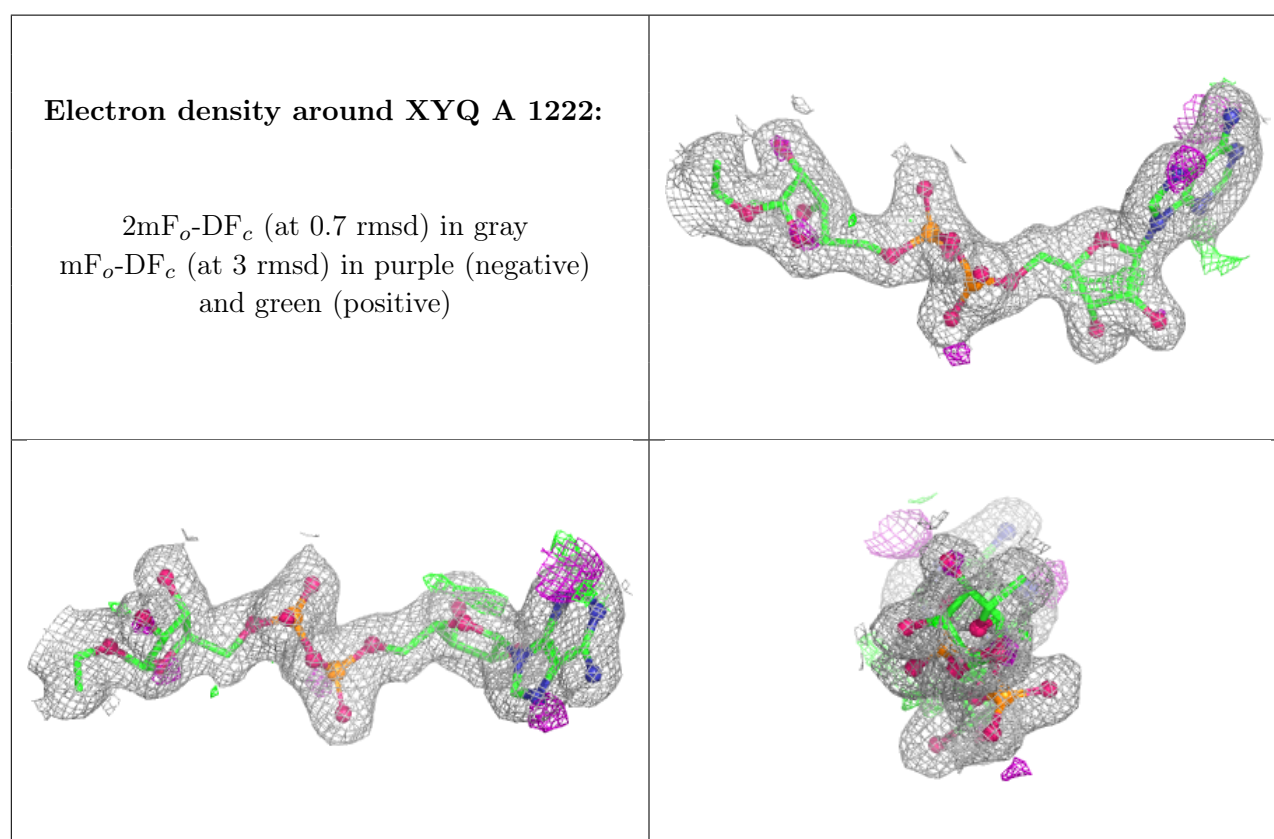
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

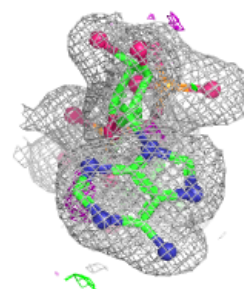
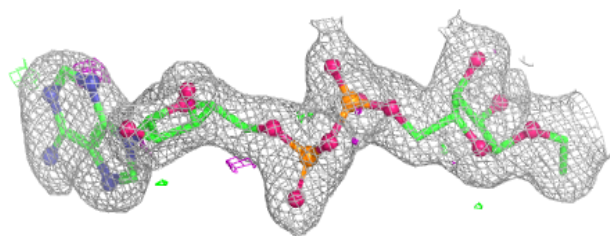
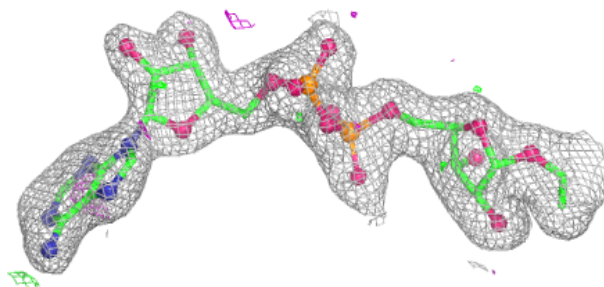
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NCA	A	900	9/9	0.67	0.27	81,83,86,86	0
4	NCA	B	901	9/9	0.81	0.61	124,125,126,126	9
3	XYQ	A	1222	38/39	0.97	0.06	17,21,25,25	0
3	XYQ	B	1222	38/39	0.97	0.07	20,29,37,38	0
2	ZN	B	800	1/1	0.99	0.02	31,31,31,31	0
2	ZN	A	800	1/1	1.00	0.02	32,32,32,32	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 XYQ B 1222:

$2mF_o-DF_c$ (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.