Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 09:23 PM GMT

PDB ID	:	1YQX
Title	:	Sinapyl Alcohol Dehydrogenase at 2.5 Angstrom Resolution
Authors	:	Bomati, E.K.; Noel, J.P.
Deposited on	:	2005-02-02
Resolution	:	2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.

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

A user guide is available at http://wwpdb.org/ValidationPDFNotes.html


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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.277
Clashscore		14
Ramachandran outliers		1.3%
Sidechain outliers		4.6%
RSRZ outliers		2.1%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
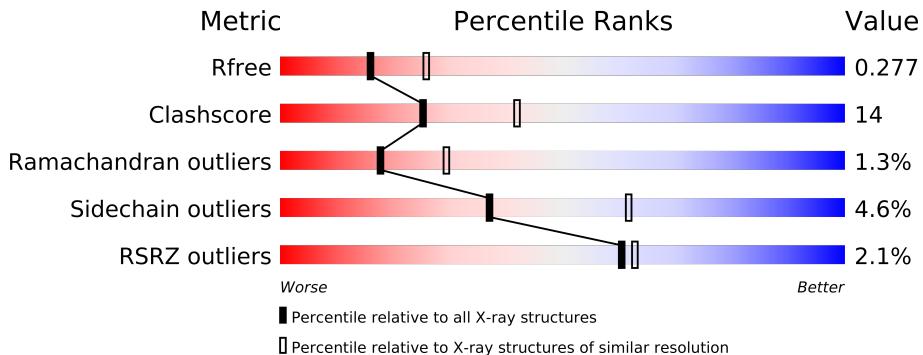
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	366	
1	B	366	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5574 atoms, of which 0 are hydrogen and 0 are deuterium.

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 sinapyl alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total 2717	C 1729	N 462	O 510	S 16	0	0	0
1	B	359	Total 2717	C 1729	N 462	O 510	S 16	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	CLONING ARTIFACT	UNP Q94G59
A	-2	SER	-	CLONING ARTIFACT	UNP Q94G59
A	-1	HIS	-	CLONING ARTIFACT	UNP Q94G59
A	0	GLY	-	CLONING ARTIFACT	UNP Q94G59
A	140	ASN	ASP	ENGINEERED	UNP Q94G59
B	-3	GLY	-	CLONING ARTIFACT	UNP Q94G59
B	-2	SER	-	CLONING ARTIFACT	UNP Q94G59
B	-1	HIS	-	CLONING ARTIFACT	UNP Q94G59
B	0	GLY	-	CLONING ARTIFACT	UNP Q94G59
B	140	ASN	ASP	ENGINEERED	UNP Q94G59

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).
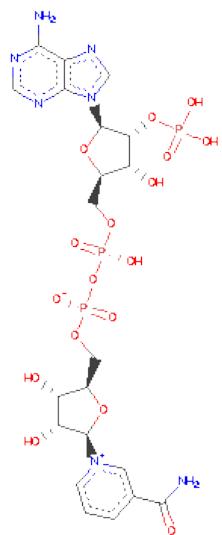
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	21	Total	O	0	0
			21	21		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: sinapyl alcohol dehydrogenase

Chain A:
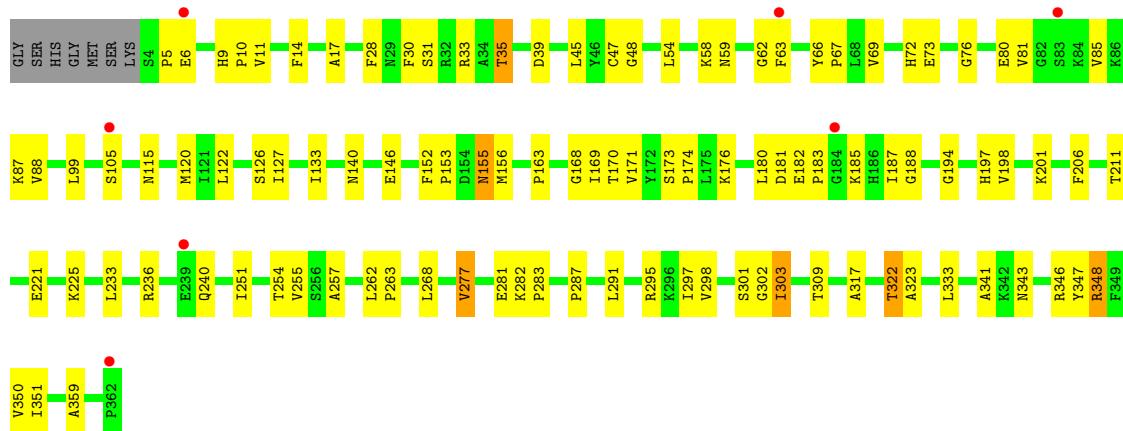
- Molecule 1: sinapyl alcohol dehydrogenase

Chain B:
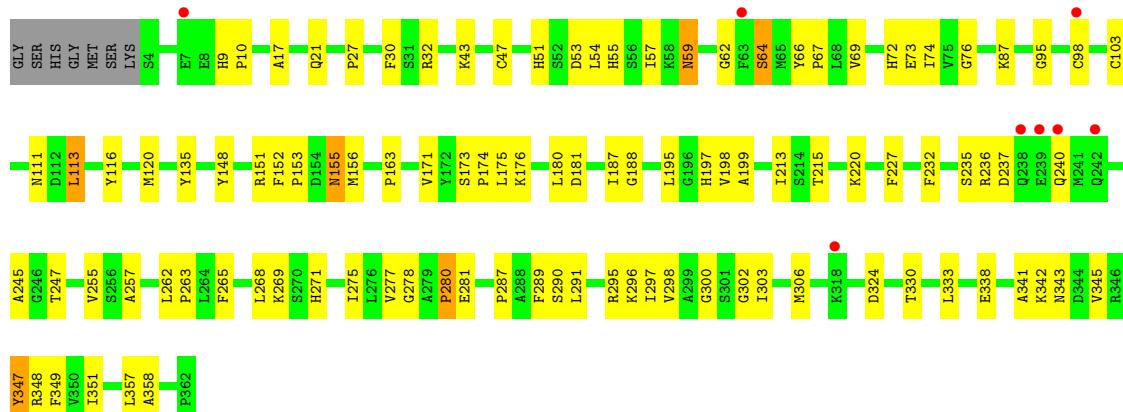
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	76.36Å 138.16Å 67.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.33 – 2.50 32.33 – 2.51	Depositor EDS
% Data completeness (in resolution range)	90.7 (32.33-2.50) 90.8 (32.33-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.278 0.211 , 0.277	Depositor DCC
R_{free} test set	2268 reflections (9.89%)	DCC
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 20.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 24756 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5574	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 13.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAP

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	0.37	0/2778	0.64	0/3760
1	B	0.38	0/2778	0.65	0/3760
All	All	0.37	0/5556	0.65	0/7520

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2717	0	2698	71	0
1	B	2717	0	2698	80	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	48	0	25	2	0
3	B	48	0	25	5	0
4	A	19	0	0	1	0
4	B	21	0	0	2	0
All	All	5574	0	5446	150	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:500:NAP:C4B	3:A:500:NAP:O4B	1.65	1.45
3:B:600:NAP:O4B	3:B:600:NAP:C4B	1.65	1.37
1:A:14:PHE:H	1:A:140:ASN:ND2	1.60	0.98
1:A:14:PHE:H	1:A:140:ASN:HD21	1.14	0.93
1:B:155:ASN:H	1:B:155:ASN:HD22	0.94	0.92
1:B:155:ASN:HD22	1:B:155:ASN:N	1.69	0.91
1:B:155:ASN:ND2	1:B:155:ASN:H	1.71	0.86
1:A:333:LEU:HD21	1:A:351:ILE:HD11	1.63	0.79
1:B:153:PRO:HG2	1:B:156:MET:HB2	1.62	0.79
1:A:35:THR:HG21	1:A:80:GLU:OE1	1.85	0.75
1:A:282:LYS:HB3	1:A:283:PRO:HD2	1.69	0.74
1:A:155:ASN:H	1:A:155:ASN:HD22	1.34	0.73
1:B:87:LYS:HB3	1:B:151:ARG:NH1	2.06	0.70
1:A:14:PHE:N	1:A:140:ASN:ND2	2.39	0.70
1:A:281:GLU:HG3	1:A:282:LYS:HG3	1.73	0.68
1:B:87:LYS:HB3	1:B:151:ARG:HH11	1.59	0.68
1:A:291:LEU:HB3	1:B:300:GLY:HA3	1.75	0.67
1:A:35:THR:HG21	1:A:80:GLU:CD	2.13	0.67
1:A:87:LYS:HG2	1:A:146:GLU:OE1	1.95	0.66
1:A:262:LEU:HB3	1:A:263:PRO:HD3	1.77	0.66
1:A:87:LYS:HE2	1:A:146:GLU:HG2	1.78	0.65
1:B:153:PRO:HG2	1:B:156:MET:CB	2.27	0.65
1:A:14:PHE:N	1:A:140:ASN:HD21	1.93	0.64
1:B:277:VAL:O	3:B:600:NAP:H2N	1.99	0.63
1:A:155:ASN:ND2	1:A:155:ASN:H	1.98	0.62
1:B:111:ASN:O	1:B:113:LEU:HD22	1.99	0.62
1:A:17:ALA:HB2	1:A:69:VAL:HG22	1.82	0.62
1:B:338:GLU:HG2	1:B:342:LYS:HE3	1.82	0.61
1:B:347:TYR:O	1:B:348:ARG:HG2	1.99	0.61
1:A:176:LYS:HD3	1:A:181:ASP:OD1	1.99	0.61
1:B:271:HIS:HE1	1:B:295:ARG:HH21	1.48	0.60
1:B:69:VAL:HB	1:B:135:TYR:HB3	1.84	0.60
1:A:173:SER:HB3	1:A:174:PRO:HD3	1.85	0.58
1:B:291:LEU:HD21	1:B:298:VAL:HG23	1.85	0.58
1:A:169:ILE:HD13	1:A:309:THR:HA	1.86	0.58
1:B:176:LYS:HD3	1:B:181:ASP:OD1	2.03	0.57
1:B:173:SER:HB3	1:B:174:PRO:HD3	1.86	0.57
1:B:195:LEU:HD13	3:B:600:NAP:O1N	2.05	0.57
1:B:66:TYR:HB3	1:B:67:PRO:HA	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:255:VAL:HG12	1:B:257:ALA:H	1.70	0.56
1:A:221:GLU:OE2	1:A:225:LYS:HE3	2.06	0.56
1:B:17:ALA:HB2	1:B:69:VAL:HG22	1.88	0.55
1:A:99:LEU:HD11	1:A:115:ASN:HB3	1.88	0.55
1:B:236:ARG:HG2	1:B:236:ARG:HH11	1.72	0.55
1:B:291:LEU:HD21	1:B:298:VAL:CG2	2.36	0.55
1:B:215:THR:HG22	1:B:235:SER:OG	2.07	0.55
1:A:5:PRO:HG2	1:A:6:GLU:OE2	2.07	0.55
1:B:271:HIS:CE1	1:B:295:ARG:HE	2.26	0.54
1:B:9:HIS:HB3	1:B:10:PRO:HD2	1.90	0.54
1:A:262:LEU:HD13	1:A:287:PRO:HG2	1.90	0.54
1:B:163:PRO:HB3	1:B:348:ARG:HD2	1.89	0.54
1:B:171:VAL:HG11	1:B:199:ALA:HB2	1.91	0.53
1:B:197:HIS:CE1	1:B:347:TYR:HB3	2.43	0.53
1:A:168:GLY:HA2	1:A:198:VAL:HG11	1.90	0.53
1:B:213:ILE:N	1:B:213:ILE:HD12	2.23	0.53
1:B:237:ASP:OD1	1:B:240:GLN:HB2	2.09	0.53
1:A:81:VAL:HB	1:A:85:VAL:HG21	1.89	0.53
1:B:262:LEU:HB3	1:B:263:PRO:HD3	1.91	0.52
1:B:348:ARG:NE	4:B:4014:HOH:O	2.42	0.52
1:A:297:ILE:HD12	1:A:297:ILE:C	2.31	0.51
1:A:73:GLU:CD	1:A:163:PRO:HA	2.31	0.51
1:A:33:ARG:HH21	1:A:39:ASP:CG	2.14	0.50
1:B:73:GLU:CD	1:B:163:PRO:HA	2.32	0.50
1:B:262:LEU:O	1:B:262:LEU:HD13	2.11	0.50
1:B:333:LEU:HD21	1:B:351:ILE:CD1	2.42	0.49
1:B:278:GLY:C	1:B:280:PRO:HD3	2.32	0.49
1:B:59:ASN:HD21	1:B:62:GLY:C	2.16	0.49
1:A:9:HIS:HB3	1:A:10:PRO:HD2	1.94	0.49
1:A:182:GLU:O	1:A:185:LYS:HB2	2.12	0.48
1:B:245:ALA:O	1:B:247:THR:HG23	2.12	0.48
1:A:254:THR:HA	1:A:277:VAL:HG12	1.95	0.48
1:B:262:LEU:N	1:B:263:PRO:CD	2.77	0.48
1:A:47:CYS:HA	1:A:73:GLU:O	2.13	0.48
1:B:345:VAL:HB	1:B:349:PHE:CE2	2.49	0.48
1:B:148:TYR:HA	1:B:306:MET:HE2	1.96	0.48
1:A:255:VAL:HG12	1:A:257:ALA:H	1.79	0.48
1:A:180:LEU:HB3	1:A:187:ILE:HD12	1.94	0.47
1:A:282:LYS:HE3	4:A:2010:HOH:O	2.13	0.47
1:B:43:LYS:O	1:B:76:GLY:HA3	2.14	0.47
1:B:54:LEU:HD21	1:B:341:ALA:HB2	1.95	0.47
1:A:291:LEU:HB3	1:B:300:GLY:CA	2.41	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:183:PRO:HG3	1:A:206:PHE:O	2.14	0.47
1:B:220:LYS:HA	1:B:232:PHE:CD1	2.50	0.47
1:A:295:ARG:HD3	1:B:116:TYR:OH	2.15	0.46
1:B:66:TYR:HA	1:B:67:PRO:C	2.36	0.46
1:B:32:ARG:HG2	1:B:32:ARG:HH11	1.80	0.46
1:B:174:PRO:HB3	1:B:275:ILE:HG21	1.97	0.46
1:B:47:CYS:HA	1:B:73:GLU:O	2.16	0.46
1:B:73:GLU:OE1	1:B:348:ARG:NH1	2.49	0.46
1:A:194:GLY:O	1:A:198:VAL:HG23	2.16	0.46
1:A:153:PRO:HG2	1:A:156:MET:CB	2.46	0.46
1:A:322:THR:HG23	1:A:323:ALA:N	2.31	0.45
1:B:53:ASP:O	1:B:57:ILE:HG23	2.16	0.45
1:A:171:VAL:O	1:A:174:PRO:HD2	2.16	0.45
1:B:262:LEU:C	1:B:262:LEU:HD13	2.36	0.45
1:A:153:PRO:HG2	1:A:156:MET:HB2	1.98	0.45
1:A:54:LEU:HD21	1:A:341:ALA:HB2	1.99	0.45
1:B:74:ILE:O	1:B:95:GLY:HA2	2.16	0.45
1:A:87:LYS:HG3	1:A:88:VAL:HG13	1.98	0.45
1:A:233:LEU:HD22	1:A:240:GLN:HG2	1.98	0.45
1:B:180:LEU:HB3	1:B:187:ILE:HD12	1.97	0.45
1:B:155:ASN:ND2	1:B:155:ASN:N	2.42	0.45
1:A:322:THR:CG2	1:A:323:ALA:N	2.80	0.45
1:B:265:PHE:HA	1:B:268:LEU:HD12	1.99	0.45
1:A:127:ILE:HD13	1:A:133:ILE:HD13	1.99	0.45
1:A:11:VAL:O	1:A:31:SER:HB2	2.16	0.44
1:B:277:VAL:O	3:B:600:NAP:C2N	2.63	0.44
1:A:174:PRO:HG3	1:A:301:SER:OG	2.16	0.44
1:A:66:TYR:HA	1:A:67:PRO:C	2.37	0.44
1:A:127:ILE:CD1	1:A:133:ILE:HD13	2.47	0.44
1:A:170:THR:OG1	1:A:303:ILE:HA	2.18	0.44
1:A:17:ALA:HB2	1:A:69:VAL:CG2	2.47	0.44
1:A:197:HIS:O	1:A:201:LYS:HG3	2.18	0.44
1:B:236:ARG:HG2	1:B:236:ARG:NH1	2.34	0.43
1:A:45:LEU:HG	1:A:76:GLY:HA2	2.00	0.43
1:B:333:LEU:HD21	1:B:351:ILE:HD11	2.00	0.43
1:A:194:GLY:HA3	1:A:348:ARG:NH1	2.32	0.43
1:B:51:HIS:HD2	1:B:55:HIS:CD2	2.36	0.43
1:A:302:GLY:HA2	3:A:500:NAP:O7N	2.19	0.43
1:B:345:VAL:O	1:B:347:TYR:N	2.45	0.43
1:B:330:THR:HG21	1:B:357:LEU:HD12	2.01	0.43
1:B:287:PRO:HG2	1:B:290:SER:OG	2.19	0.43
1:B:197:HIS:CE1	1:B:198:VAL:HG23	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:302:GLY:HA2	3:B:600:NAP:O7N	2.19	0.42
1:B:227:PHE:HE2	1:B:324:ASP:OD1	2.01	0.42
1:A:62:GLY:O	1:A:63:PHE:HD1	2.01	0.42
1:A:282:LYS:HB3	1:A:283:PRO:CD	2.46	0.42
1:A:251:ILE:HD12	1:A:268:LEU:CD1	2.49	0.42
1:A:48:GLY:HA2	1:A:350:VAL:HA	2.02	0.42
1:A:153:PRO:HG3	1:A:317:ALA:HB2	2.02	0.42
1:B:171:VAL:O	1:B:175:LEU:HG	2.20	0.42
1:B:278:GLY:O	1:B:280:PRO:HD3	2.20	0.42
1:A:155:ASN:N	1:A:155:ASN:HD22	2.10	0.42
1:B:187:ILE:HG22	1:B:188:GLY:N	2.35	0.42
1:A:188:GLY:HA2	1:A:211:THR:O	2.18	0.42
1:A:122:LEU:HB2	1:A:126:SER:HB2	2.02	0.42
1:B:227:PHE:CE2	1:B:324:ASP:OD1	2.72	0.42
1:B:297:ILE:CG2	1:B:298:VAL:N	2.83	0.41
1:B:59:ASN:CG	1:B:64:SER:HB2	2.40	0.41
1:A:33:ARG:NE	1:A:39:ASP:OD1	2.52	0.41
1:B:51:HIS:CD2	1:B:55:HIS:NE2	2.89	0.41
1:B:148:TYR:HA	1:B:306:MET:CE	2.51	0.41
1:B:269:LYS:O	1:B:296:LYS:HE2	2.20	0.41
1:A:66:TYR:HB3	1:A:67:PRO:HA	2.03	0.41
1:B:348:ARG:CZ	4:B:4014:HOH:O	2.68	0.40
1:A:302:GLY:O	1:A:303:ILE:C	2.60	0.40
1:B:220:LYS:HA	1:B:232:PHE:CE1	2.56	0.40
1:A:297:ILE:HD12	1:A:298:VAL:N	2.36	0.40
1:B:271:HIS:CE1	1:B:295:ARG:HH21	2.33	0.40
1:A:28:PHE:CE2	1:A:30:PHE:HB3	2.56	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	357/366 (98%)	333 (93%)	20 (6%)	4 (1%)	21	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	357/366 (98%)	322 (90%)	30 (8%)	5 (1%)	16	27
All	All	714/732 (98%)	655 (92%)	50 (7%)	9 (1%)	18	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	TYR
1	A	303	ILE
1	B	64	SER
1	B	303	ILE
1	B	347	TYR
1	A	105	SER
1	A	359	ALA
1	B	358	ALA
1	B	280	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	291/296 (98%)	278 (96%)	13 (4%)	38	63
1	B	291/296 (98%)	277 (95%)	14 (5%)	35	60
All	All	582/592 (98%)	555 (95%)	27 (5%)	37	62

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

Mol	Chain	Res	Type
1	A	35	THR
1	A	58	LYS
1	A	59	ASN
1	A	72	HIS
1	A	120	MET
1	A	152	PHE
1	A	155	ASN
1	A	236	ARG
1	A	277	VAL

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Mol	Chain	Res	Type
1	A	322	THR
1	A	343	ASN
1	A	346	ARG
1	A	348	ARG
1	B	21	GLN
1	B	27	PRO
1	B	30	PHE
1	B	59	ASN
1	B	72	HIS
1	B	98	CYS
1	B	103	CYS
1	B	113	LEU
1	B	120	MET
1	B	152	PHE
1	B	155	ASN
1	B	281	GLU
1	B	289	PHE
1	B	343	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	29	ASN
1	A	59	ASN
1	A	111	ASN
1	A	129	HIS
1	A	155	ASN
1	A	226	ASN
1	A	240	GLN
1	A	242	GLN
1	A	343	ASN
1	A	355	ASN
1	B	9	HIS
1	B	21	GLN
1	B	29	ASN
1	B	51	HIS
1	B	59	ASN
1	B	111	ASN
1	B	155	ASN
1	B	238	GLN
1	B	240	GLN

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Mol	Chain	Res	Type
1	B	242	GLN
1	B	271	HIS
1	B	319	HIS
1	B	320	ASN
1	B	343	ASN
1	B	355	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	#$|Z| > 2$
3	NAP	A	500	-	52,52,52	3.20	19 (36%)	80,80,80	3.18	28 (35%)
3	NAP	B	600	-	52,52,52	3.14	19 (36%)	80,80,80	3.21	29 (36%)

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	NAP	A	500	-	-	0/35/67/67	0/3/5/5
3	NAP	B	600	-	-	0/35/67/67	0/3/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAP	O4B-C1B	-10.47	1.25	1.41
3	B	600	NAP	O4B-C1B	-10.42	1.25	1.41
3	B	600	NAP	O4B-C4B	8.69	1.65	1.45
3	A	500	NAP	O4B-C4B	8.58	1.65	1.45
3	A	500	NAP	C3B-C4B	6.25	1.70	1.53
3	B	600	NAP	C3B-C4B	6.16	1.70	1.53
3	A	500	NAP	C2N-N1N	6.00	1.43	1.35
3	B	600	NAP	C2N-N1N	5.87	1.42	1.35
3	A	500	NAP	C2A-N3A	5.19	1.42	1.32
3	A	500	NAP	C2D-C1D	-5.16	1.46	1.53
3	B	600	NAP	C4A-N3A	5.13	1.43	1.35
3	A	500	NAP	C4N-C3N	5.10	1.48	1.39
3	A	500	NAP	C2A-N1A	4.96	1.43	1.33
3	B	600	NAP	C2A-N3A	4.91	1.41	1.32
3	B	600	NAP	C2A-N1A	4.82	1.43	1.33
3	B	600	NAP	C2B-C1B	4.70	1.61	1.52
3	B	600	NAP	C4N-C3N	4.67	1.47	1.39
3	A	500	NAP	C2B-C1B	4.64	1.61	1.52
3	B	600	NAP	C2D-C1D	-4.40	1.47	1.53
3	A	500	NAP	C4A-N3A	4.16	1.42	1.35
3	B	600	NAP	O4D-C1D	4.11	1.47	1.41
3	B	600	NAP	O3B-C3B	4.00	1.52	1.43
3	A	500	NAP	O3B-C3B	3.94	1.52	1.43
3	A	500	NAP	O4D-C1D	3.89	1.47	1.41
3	A	500	NAP	P2B-O2B	3.56	1.70	1.59
3	A	500	NAP	PA-O1A	-3.43	1.38	1.51
3	B	600	NAP	P2B-O2B	3.41	1.70	1.59
3	B	600	NAP	PA-O1A	-3.15	1.39	1.51
3	A	500	NAP	C6N-C5N	3.08	1.45	1.38
3	A	500	NAP	C6N-N1N	3.07	1.44	1.35
3	B	600	NAP	C6N-N1N	2.89	1.43	1.35
3	B	600	NAP	C3B-C2B	-2.75	1.46	1.53
3	A	500	NAP	C3B-C2B	-2.74	1.46	1.53
3	B	600	NAP	C8A-N9A	2.68	1.40	1.36
3	A	500	NAP	C3D-C4D	2.67	1.60	1.53
3	B	600	NAP	C6N-C5N	2.48	1.44	1.38
3	B	600	NAP	C5N-C4N	2.47	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAP	C5N-C4N	2.14	1.43	1.39

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	NAP	C4B-O4B-C1B	13.96	124.92	109.75
3	B	600	NAP	C4B-O4B-C1B	13.70	124.63	109.75
3	B	600	NAP	O4B-C1B-N9A	12.93	120.47	108.44
3	A	500	NAP	O4B-C1B-N9A	12.50	120.07	108.44
3	A	500	NAP	O4B-C4B-C3B	-10.49	83.91	105.17
3	B	600	NAP	O4B-C4B-C3B	-10.43	84.02	105.17
3	B	600	NAP	N3A-C2A-N1A	-7.50	122.44	128.71
3	A	500	NAP	N3A-C2A-N1A	-6.74	123.07	128.71
3	A	500	NAP	O3-PN-O1N	5.20	121.24	108.83
3	B	600	NAP	O2N-PN-O5D	-5.13	87.02	108.19
3	B	600	NAP	O3-PN-O1N	5.03	120.84	108.83
3	A	500	NAP	O3B-C3B-C4B	-4.73	97.14	111.08
3	B	600	NAP	O3B-C3B-C4B	-4.72	97.18	111.08
3	A	500	NAP	O2N-PN-O5D	-4.67	88.88	108.19
3	A	500	NAP	O5D-PN-O1N	-4.62	89.02	108.61
3	B	600	NAP	O4D-C1D-N1N	-4.27	103.58	107.95
3	B	600	NAP	O5D-PN-O1N	-4.16	90.94	108.61
3	B	600	NAP	C2B-C3B-C4B	4.09	111.66	101.94
3	A	500	NAP	C2B-C3B-C4B	4.03	111.51	101.94
3	A	500	NAP	O4D-C1D-N1N	-3.77	104.10	107.95
3	A	500	NAP	O3B-C3B-C2B	-3.70	100.31	111.20
3	B	600	NAP	O3B-C3B-C2B	-3.66	100.43	111.20
3	B	600	NAP	C2D-C1D-N1N	3.30	119.45	113.86
3	B	600	NAP	O5B-C5B-C4B	-3.27	96.92	108.94
3	A	500	NAP	O5B-C5B-C4B	-3.24	97.04	108.94
3	B	600	NAP	O3-PN-O5D	-3.20	88.54	101.36
3	B	600	NAP	C1B-N9A-C4A	-3.13	121.22	126.64
3	A	500	NAP	C2N-C3N-C4N	3.12	121.84	118.31
3	A	500	NAP	C2D-C1D-N1N	3.09	119.09	113.86
3	B	600	NAP	C3B-C2B-C1B	-3.08	96.74	102.73
3	A	500	NAP	C3B-C2B-C1B	-3.05	96.79	102.73
3	A	500	NAP	O3-PN-O5D	-3.05	89.15	101.36
3	A	500	NAP	C1B-N9A-C4A	-2.94	121.56	126.64
3	A	500	NAP	C5A-C6A-N6A	2.94	127.36	120.72
3	B	600	NAP	C5A-C6A-N6A	2.94	127.36	120.72
3	A	500	NAP	O4B-C1B-C2B	-2.80	104.33	106.95
3	B	600	NAP	C2N-C3N-C4N	2.64	121.31	118.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	600	NAP	O4B-C1B-C2B	-2.59	104.52	106.95
3	B	600	NAP	C8A-N9A-C1B	2.53	131.37	126.38
3	A	500	NAP	C8A-N9A-C1B	2.49	131.28	126.38
3	A	500	NAP	C5N-C4N-C3N	-2.47	117.11	120.32
3	A	500	NAP	N3A-C4A-N9A	2.44	129.83	125.43
3	B	600	NAP	O2A-PA-O1A	2.42	125.74	112.21
3	B	600	NAP	O2B-C2B-C1B	-2.40	101.47	110.36
3	A	500	NAP	O2B-C2B-C1B	-2.37	101.57	110.36
3	A	500	NAP	O2A-PA-O1A	2.34	125.28	112.21
3	A	500	NAP	O3X-P2B-O2X	2.29	116.52	107.61
3	B	600	NAP	N6A-C6A-N1A	-2.26	114.93	119.36
3	B	600	NAP	C5N-C4N-C3N	-2.25	117.39	120.32
3	B	600	NAP	O3X-P2B-O2X	2.25	116.37	107.61
3	B	600	NAP	O2N-PN-O1N	2.25	125.49	118.72
3	A	500	NAP	C3N-C7N-N7N	2.18	120.25	117.77
3	B	600	NAP	C3N-C7N-N7N	2.15	120.21	117.77
3	B	600	NAP	N3A-C4A-N9A	2.14	129.30	125.43
3	A	500	NAP	N6A-C6A-N1A	-2.10	115.25	119.36
3	B	600	NAP	O7N-C7N-C3N	-2.07	117.24	119.58
3	A	500	NAP	O7N-C7N-C3N	-2.07	117.25	119.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	359/366 (98%)	0.05	7 (1%)	64	66	16, 31, 49, 58	0
1	B	359/366 (98%)	0.18	8 (2%)	59	61	20, 33, 51, 69	0
All	All	718/732 (98%)	0.11	15 (2%)	60	63	16, 32, 50, 69	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	PRO	4.8
1	B	63	PHE	2.7
1	B	239	GLU	2.6
1	B	238	GLN	2.6
1	B	242	GLN	2.4
1	A	184	GLY	2.4
1	A	63	PHE	2.4
1	B	240	GLN	2.4
1	A	83	SER	2.3
1	B	318	LYS	2.3
1	B	7	GLU	2.2
1	B	98	CYS	2.1
1	A	105	SER	2.1
1	A	6	GLU	2.1
1	A	239	GLU	2.1

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 carbohydrates in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAP	A	500	48/48	0.13	-0.51	6,18,24,28	0
3	NAP	B	600	48/48	0.14	-0.93	13,25,29,29	0
2	ZN	B	3000	1/1	0.07	-1.30	32,32,32,32	0
2	ZN	A	2000	1/1	0.07	-1.74	43,43,43,43	0
2	ZN	B	4000	1/1	0.13	-1.83	29,29,29,29	0
2	ZN	A	1000	1/1	0.10	-2.02	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.