



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:49 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

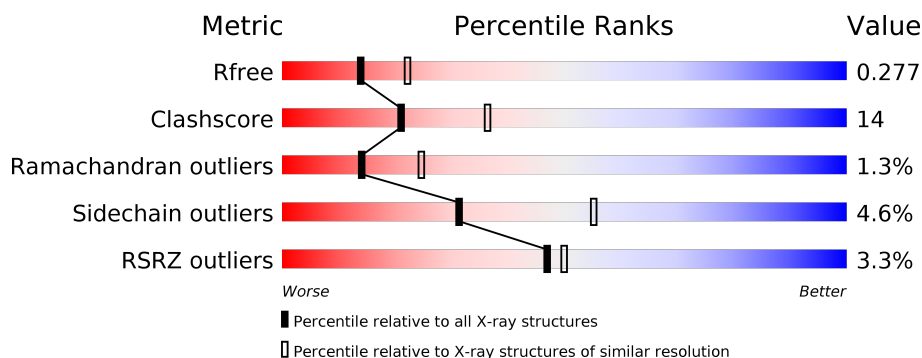
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	366	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>• •</div> </div> </div>
1	B	366	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5574 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 sinapyl alcohol dehydrogenase.

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

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	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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		

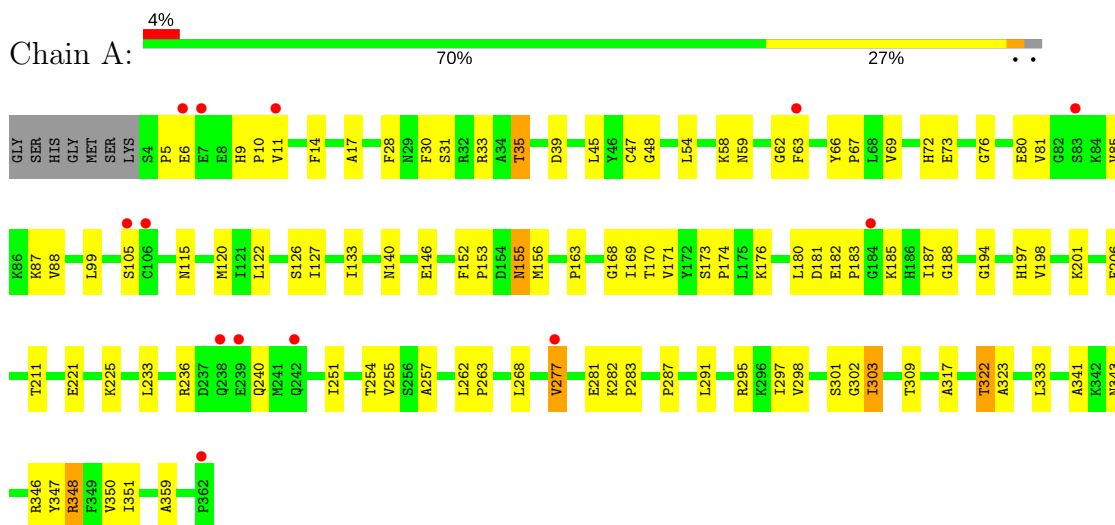
- Molecule 4 is water.

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

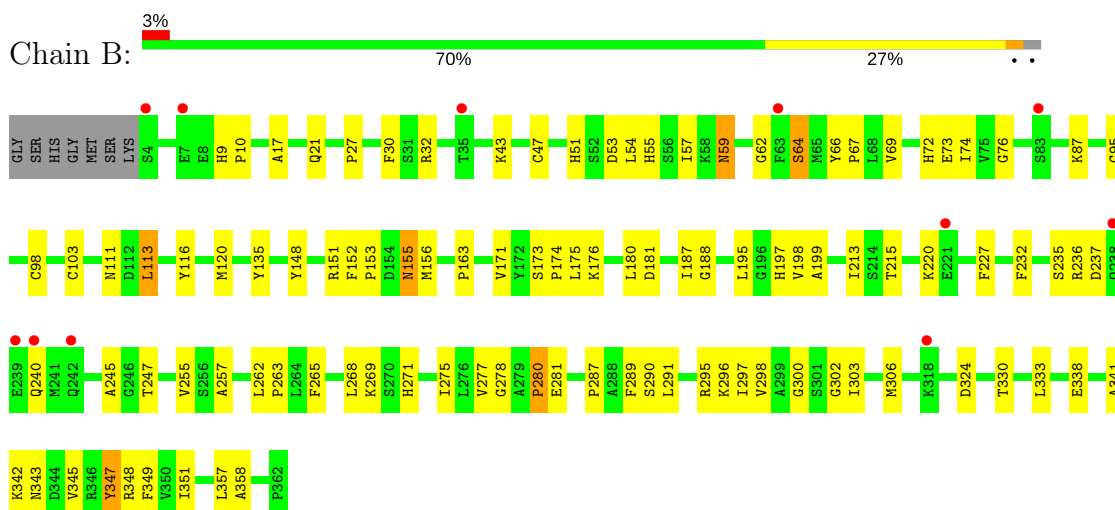
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: sinapyl alcohol dehydrogenase



- Molecule 1: sinapyl alcohol dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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 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	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

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 14.

All (150) 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: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
1:B:255:VAL:HG12	1:B:257:ALA:H	1.70	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:215:THR:HG22	1:B:235:SER:OG	2.07	0.55
1:B:291:LEU:HD21	1:B:298:VAL:CG2	2.36	0.55
1:A:5:PRO:HG2	1:A:6:GLU:OE2	2.07	0.55
1:B:9:HIS:HB3	1:B:10:PRO:HD2	1.90	0.54
1:B:271:HIS:CE1	1:B:295:ARG:HE	2.26	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: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:197:HIS:CE1	1:B:347:TYR:HB3	2.43	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:54:LEU:HD21	1:B:341:ALA:HB2	1.95	0.47
1:B:43:LYS:O	1:B:76:GLY:HA3	2.14	0.47
1:A:183:PRO:HG3	1:A:206:PHE:O	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:HB3	1:B:300:GLY:CA	2.41	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:A:194:GLY:O	1:A:198:VAL:HG23	2.16	0.46
1:B:73:GLU:OE1	1:B:348:ARG:NH1	2.49	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:A:153:PRO:HG2	1:A:156:MET:HB2	1.98	0.45
1:B:262:LEU:C	1:B:262:LEU:HD13	2.36	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:233:LEU:HD22	1:A:240:GLN:HG2	1.98	0.45
1:A:87:LYS:HG3	1:A:88:VAL:HG13	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:127:ILE:HD13	1:A:133:ILE:HD13	1.99	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:11:VAL:O	1:A:31:SER:HB2	2.16	0.44
1:A:174:PRO:HG3	1:A:301:SER:OG	2.16	0.44
1:B:277:VAL:O	3:B:600:NAP:C2N	2.63	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:HIS:CE1	1:B:198:VAL:HG23	2.54	0.42
1:B:302:GLY:HA2	3:B:600:NAP:O7N	2.19	0.42
1:A:62:GLY:O	1:A:63:PHE:HD1	2.01	0.42
1:B:227:PHE:HE2	1:B:324:ASP:OD1	2.01	0.42
1:A:251:ILE:HD12	1:A:268:LEU:CD1	2.49	0.42
1:A:282:LYS:HB3	1:A:283:PRO:CD	2.46	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:122:LEU:HB2	1:A:126:SER:HB2	2.02	0.42
1:A:155:ASN:N	1:A:155:ASN:HD22	2.10	0.42
1:A:188:GLY:HA2	1:A:211:THR:O	2.18	0.42
1:B:187:ILE:HG22	1:B:188:GLY:N	2.35	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:A:28:PHE:CE2	1:A:30:PHE:HB3	2.56	0.40
1:B:271:HIS:CE1	1:B:295:ARG:HH21	2.33	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	357/366 (98%)	333 (93%)	20 (6%)	4 (1%)	17	29
1	B	357/366 (98%)	322 (90%)	30 (8%)	5 (1%)	13	23
All	All	714/732 (98%)	655 (92%)	50 (7%)	9 (1%)	14	25

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%)	32	56
1	B	291/296 (98%)	277 (95%)	14 (5%)	30	53
All	All	582/592 (98%)	555 (95%)	27 (5%)	31	55

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	236	ARG
1	A	277	VAL
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	238	GLN
1	B	240	GLN
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 [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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	-	44,52,52	3.56	18 (40%)	51,80,80	3.38	21 (41%)
3	NAP	B	600	-	44,52,52	3.50	17 (38%)	51,80,80	3.37	20 (39%)

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	-	-	0/27/67/67	0/5/5/5
3	NAP	B	600	-	-	0/27/67/67	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAP	O4B-C1B	-11.60	1.25	1.41
3	B	600	NAP	O4B-C1B	-11.54	1.25	1.41
3	A	500	NAP	C2D-C1D	-4.73	1.46	1.53
3	B	600	NAP	C2D-C1D	-4.06	1.47	1.53
3	A	500	NAP	PA-O1A	-3.34	1.38	1.50
3	B	600	NAP	PA-O1A	-3.06	1.39	1.50
3	B	600	NAP	C3B-C2B	-2.87	1.46	1.53
3	A	500	NAP	C3B-C2B	-2.86	1.46	1.53
3	A	500	NAP	PN-O2N	-2.03	1.44	1.55
3	B	600	NAP	C3D-C4D	2.03	1.58	1.53
3	B	600	NAP	C6N-C5N	2.61	1.44	1.38
3	A	500	NAP	C5N-C4N	2.65	1.43	1.38
3	A	500	NAP	C3D-C4D	2.81	1.60	1.53
3	B	600	NAP	C5N-C4N	3.06	1.44	1.38
3	B	600	NAP	C6N-N1N	3.17	1.43	1.35
3	A	500	NAP	C6N-C5N	3.25	1.45	1.38
3	A	500	NAP	C6N-N1N	3.37	1.44	1.35
3	A	500	NAP	O3B-C3B	4.14	1.52	1.43
3	B	600	NAP	O3B-C3B	4.20	1.52	1.43
3	A	500	NAP	C4A-N3A	4.35	1.42	1.35
3	A	500	NAP	O4D-C1D	4.39	1.47	1.41
3	B	600	NAP	O4D-C1D	4.63	1.47	1.41
3	B	600	NAP	C4N-C3N	4.90	1.47	1.39
3	B	600	NAP	C2A-N1A	5.04	1.43	1.33
3	A	500	NAP	C2A-N1A	5.19	1.43	1.33
3	A	500	NAP	C4N-C3N	5.35	1.48	1.39
3	B	600	NAP	C4A-N3A	5.36	1.43	1.35
3	B	600	NAP	C2A-N3A	5.84	1.41	1.32
3	A	500	NAP	C2A-N3A	6.16	1.42	1.32
3	B	600	NAP	P2B-O2B	6.19	1.70	1.59
3	A	500	NAP	P2B-O2B	6.45	1.70	1.59
3	B	600	NAP	C3B-C4B	6.48	1.70	1.53
3	A	500	NAP	C3B-C4B	6.58	1.70	1.53
3	A	500	NAP	O4B-C4B	8.88	1.65	1.45
3	B	600	NAP	O4B-C4B	9.00	1.65	1.45

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	NAP	O4B-C4B-C3B	-10.69	83.91	105.17
3	B	600	NAP	O4B-C4B-C3B	-10.64	84.02	105.17
3	B	600	NAP	N3A-C2A-N1A	-7.37	122.44	128.86
3	A	500	NAP	N3A-C2A-N1A	-6.64	123.07	128.86
3	A	500	NAP	O5D-PN-O1N	-5.01	89.02	109.25
3	A	500	NAP	O3B-C3B-C4B	-4.77	97.14	111.09
3	B	600	NAP	O3B-C3B-C4B	-4.76	97.18	111.09
3	B	600	NAP	O5D-PN-O1N	-4.54	90.94	109.25
3	B	600	NAP	O2N-PN-O5D	-4.47	87.02	108.14
3	A	500	NAP	O2N-PN-O5D	-4.08	88.88	108.14
3	A	500	NAP	O3B-C3B-C2B	-3.82	100.31	111.18
3	B	600	NAP	O3B-C3B-C2B	-3.78	100.43	111.18
3	B	600	NAP	O5B-C5B-C4B	-3.41	96.92	109.00
3	A	500	NAP	O5B-C5B-C4B	-3.37	97.04	109.00
3	B	600	NAP	C1B-N9A-C4A	-3.13	121.22	126.64
3	B	600	NAP	C3B-C2B-C1B	-3.07	96.74	102.75
3	A	500	NAP	C3B-C2B-C1B	-3.05	96.79	102.75
3	A	500	NAP	C1B-N9A-C4A	-2.94	121.56	126.64
3	A	500	NAP	C5N-C4N-C3N	-2.75	117.11	120.35
3	B	600	NAP	C5N-C4N-C3N	-2.51	117.39	120.35
3	B	600	NAP	O2B-C2B-C1B	-2.30	101.47	110.06
3	A	500	NAP	O2B-C2B-C1B	-2.28	101.57	110.06
3	B	600	NAP	O7N-C7N-C3N	-2.04	117.24	119.62
3	A	500	NAP	O7N-C7N-C3N	-2.03	117.25	119.62
3	A	500	NAP	C5N-C6N-N1N	-2.00	117.32	120.40
3	B	600	NAP	C3N-C7N-N7N	2.14	120.21	117.77
3	B	600	NAP	O3X-P2B-O2X	2.17	116.37	107.61
3	A	500	NAP	C3N-C7N-N7N	2.17	120.25	117.77
3	A	500	NAP	O3X-P2B-O2X	2.21	116.52	107.61
3	A	500	NAP	O2N-PN-O1N	2.39	124.66	112.28
3	A	500	NAP	O2A-PA-O1A	2.51	125.28	112.28
3	B	600	NAP	O2N-PN-O1N	2.55	125.49	112.28
3	B	600	NAP	O2A-PA-O1A	2.60	125.74	112.28
3	B	600	NAP	C2N-C3N-C4N	2.67	121.31	118.26
3	A	500	NAP	C2N-C3N-C4N	3.14	121.84	118.26
3	A	500	NAP	C5A-C6A-N6A	3.38	127.36	120.47
3	B	600	NAP	C5A-C6A-N6A	3.38	127.36	120.47
3	A	500	NAP	C2B-C3B-C4B	4.20	111.51	101.95
3	B	600	NAP	C2B-C3B-C4B	4.27	111.66	101.95
3	B	600	NAP	C4B-O4B-C1B	13.96	124.63	109.77
3	A	500	NAP	C4B-O4B-C1B	14.23	124.92	109.77



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	NAP	2	0
3	B	600	NAP	5	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	359/366 (98%)	0.14	13 (3%) 43 45	16, 31, 49, 58	0
1	B	359/366 (98%)	0.32	11 (3%) 49 52	20, 33, 51, 69	0
All	All	718/732 (98%)	0.23	24 (3%) 47 50	16, 32, 50, 69	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	PRO	5.1
1	B	63	PHE	3.5
1	B	239	GLU	3.2
1	B	242	GLN	3.0
1	B	238	GLN	3.0
1	B	7	GLU	2.9
1	A	63	PHE	2.7
1	A	239	GLU	2.5
1	A	83	SER	2.4
1	B	240	GLN	2.4
1	B	4	SER	2.4
1	A	106	CYS	2.4
1	A	184	GLY	2.4
1	B	221	GLU	2.4
1	A	242	GLN	2.3
1	B	35	THR	2.3
1	A	11	VAL	2.2
1	B	83	SER	2.2
1	A	6	GLU	2.1
1	A	105	SER	2.1
1	B	318	LYS	2.1
1	A	277	VAL	2.0
1	A	7	GLU	2.0
1	A	238	GLN	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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAP	A	500	48/48	0.95	0.13	-0.81	6,18,24,28	0
3	NAP	B	600	48/48	0.94	0.14	-0.87	13,25,29,29	0
2	ZN	B	3000	1/1	0.99	0.07	-1.61	32,32,32,32	0
2	ZN	B	4000	1/1	0.99	0.14	-2.07	29,29,29,29	0
2	ZN	A	2000	1/1	0.96	0.06	-2.24	43,43,43,43	0
2	ZN	A	1000	1/1	0.99	0.13	-	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.