



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:41 AM GMT

PDB ID : 2NVD
Title : Human Aldose Reductase complexed with novel naphtho[1,2-d]isothiazole acetic acid derivative (2)
Authors : Steuber, H.; Heine, A.; Klebe, G.
Deposited on : 2006-11-12
Resolution : 1.55 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

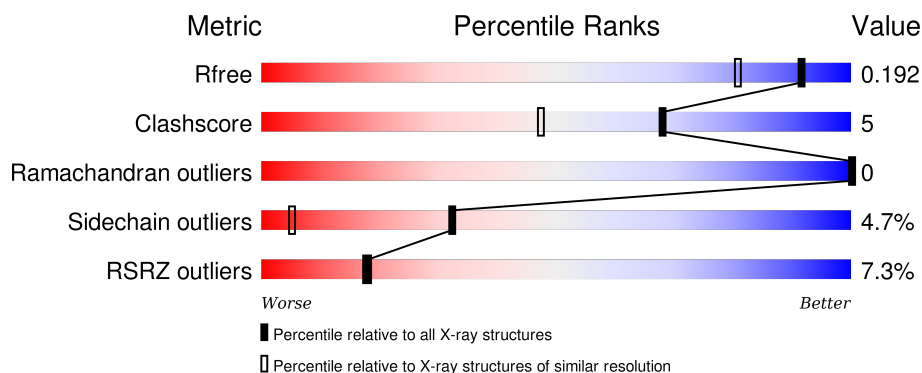
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	91344	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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. 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	316	<div> <div>7%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2906 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 Aldose reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2575	1653	431	478	13	0	15	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ILE	LEU	SEE REMARK 999	UNP P15121

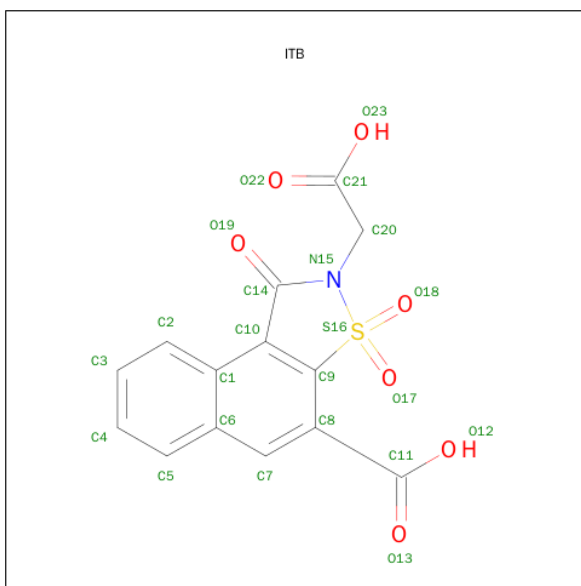
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is 2-(CARBOXYMETHYL)-1-OXO-1,2-DIHYDRONAPHTHO[1,2-D]ISOTHIAZOLE-4-CARBOXYLIC ACID 3,3-DIOXIDE (three-letter code: ITB) (formula:

C₁₄H₉NO₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			23	14	1	7	1		
3	A	1	Total	C	N	O	S	0	0
			23	14	1	7	1		
3	A	1	Total	C	N	O	S	0	0
			23	14	1	7	1		

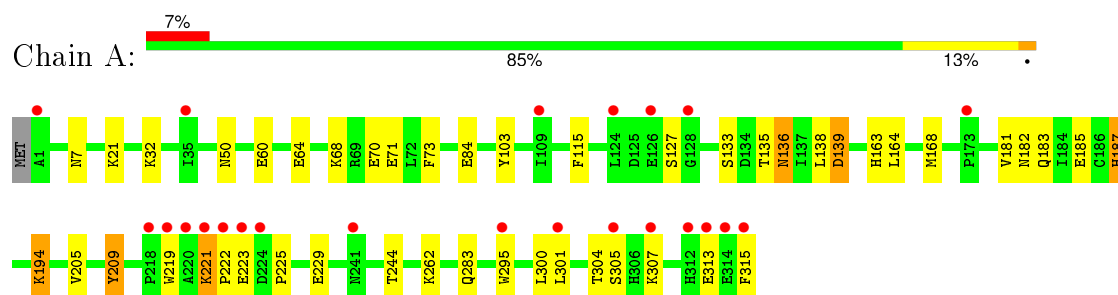
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	214	Total	O	0	0
			214	214		

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 ($\text{RSRZ} > 2$). 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: Aldose reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.39Å 66.64Å 47.14Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	30.00 – 1.55 22.21 – 1.55	Depositor EDS
% Data completeness (in resolution range)	80.6 (30.00-1.55) 93.9 (22.21-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 1.55Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.130 , 0.200 0.140 , 0.192	Depositor DCC
R_{free} test set	2085 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.3	EDS
Estimated twinning fraction	0.000 for -l,k,h 0.027 for -h,-k,l 0.018 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41678 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2906	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NAP, ITB

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	0.51	0/2688	1.19	12/3649 (0.3%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	TYR	CA-CB-CG	8.95	130.40	113.40
1	A	283	GLN	CG-CD-OE1	8.46	138.52	121.60
1	A	209	TYR	CB-CG-CD1	7.40	125.44	121.00
1	A	307	LYS	C-N-CA	5.94	136.54	121.70
1	A	115	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	A	283	GLN	CB-CG-CD	5.67	126.33	111.60
1	A	64	GLU	OE1-CD-OE2	-5.51	116.68	123.30
1	A	139	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	73	PHE	CB-CG-CD1	-5.30	117.09	120.80
1	A	103	TYR	CB-CG-CD1	5.28	124.17	121.00
1	A	187	HIS	ND1-CG-CD2	-5.21	98.71	106.00
1	A	103	TYR	CB-CG-CD2	-5.07	117.96	121.00

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	2575	0	2583	24	0
2	A	48	0	25	3	0
3	A	69	0	21	2	0
4	A	214	0	0	4	0
All	All	2906	0	2629	25	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 5.

All (25) 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:A:70:GLU:HB3	3:A:800:ITB:O22	1.92	0.69
1:A:194:LYS:HD3	4:A:1217:HOH:O	1.94	0.68
1:A:221:LYS:HB3	1:A:223:GLU:OE1	2.00	0.60
1:A:185:GLU:OE2	1:A:187:HIS:HE1	1.86	0.59
1:A:244[B]:THR:HG22	4:A:1082:HOH:O	2.09	0.52
1:A:181:VAL:HA	1:A:205:VAL:O	2.10	0.52
1:A:68:LYS:HE2	1:A:71:GLU:OE2	2.11	0.51
1:A:84[B]:GLU:OE2	1:A:133:SER:OG	2.29	0.50
1:A:70:GLU:HG3	4:A:1186:HOH:O	2.11	0.50
1:A:219:TRP:O	1:A:221:LYS:HE3	2.14	0.48
1:A:229:GLU:HA	1:A:229:GLU:OE2	2.12	0.48
1:A:222:PRO:HG2	1:A:223:GLU:OE2	2.17	0.44
1:A:301:LEU:O	1:A:304:THR:HG23	2.18	0.43
1:A:183:GLN:OE1	2:A:500:NAP:H2N	2.18	0.43
1:A:225:PRO:HG2	1:A:295:TRP:CE2	2.54	0.42
1:A:262:LYS:O	2:A:500:NAP:H8A	2.19	0.42
1:A:32:LYS:HE2	1:A:60:GLU:OE1	2.20	0.42
1:A:163[A]:HIS:ND1	1:A:315:PHE:O	2.49	0.42
1:A:223:GLU:CD	1:A:223:GLU:H	2.22	0.42
1:A:164[B]:LEU:HD12	4:A:1175:HOH:O	2.19	0.42
2:A:500:NAP:C5N	3:A:600:ITB:H7	2.50	0.42
1:A:219:TRP:O	1:A:221:LYS:HG3	2.22	0.40
1:A:136[A]:ASN:HD21	1:A:139:ASP:CG	2.25	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	328/316 (104%)	326 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/281 (105%)	279 (95%)	15 (5%)	29	4

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	21	LYS
1	A	50	ASN
1	A	127	SER
1	A	136[A]	ASN
1	A	136[B]	ASN
1	A	138	LEU
1	A	182	ASN
1	A	194	LYS
1	A	209	TYR
1	A	221	LYS
1	A	300	LEU
1	A	305[A]	SER

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Mol	Chain	Res	Type
1	A	305[B]	SER
1	A	313	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	50	ASN
1	A	182	ASN
1	A	187	HIS
1	A	283	GLN

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAP	A	500	-	42,52,52	1.36	8 (19%)	54,80,80	1.72	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ITB	A	600	-	18,25,25	3.13	5 (27%)	27,39,39	5.04	16 (59%)
3	ITB	A	700	-	18,25,25	3.49	5 (27%)	27,39,39	3.11	12 (44%)
3	ITB	A	800	-	18,25,25	3.58	6 (33%)	27,39,39	2.80	10 (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
2	NAP	A	500	-	-	0/27/67/67	0/5/5/5
3	ITB	A	600	-	-	0/1/28/28	0/3/3/3
3	ITB	A	700	-	-	0/1/28/28	0/3/3/3
3	ITB	A	800	-	-	0/1/28/28	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	ITB	S16-N15	-13.64	1.52	1.67
3	A	700	ITB	S16-N15	-13.47	1.52	1.67
3	A	600	ITB	S16-N15	-11.65	1.54	1.67
3	A	600	ITB	C14-N15	-2.83	1.35	1.39
3	A	700	ITB	C10-C1	-2.81	1.38	1.43
3	A	700	ITB	C14-N15	-2.76	1.35	1.39
3	A	800	ITB	C20-N15	-2.69	1.44	1.48
2	A	500	NAP	C8A-N7A	-2.57	1.29	1.34
3	A	800	ITB	C14-N15	-2.55	1.35	1.39
3	A	600	ITB	C10-C1	-2.48	1.39	1.43
3	A	600	ITB	C7-C6	-2.18	1.37	1.42
3	A	800	ITB	C10-C1	-2.07	1.40	1.43
3	A	700	ITB	C20-N15	-2.04	1.45	1.48
2	A	500	NAP	PA-O2A	-2.01	1.46	1.54
3	A	600	ITB	O18-S16	2.03	1.46	1.43
3	A	700	ITB	O17-S16	2.04	1.46	1.43
2	A	500	NAP	C3B-C2B	2.07	1.57	1.53
2	A	500	NAP	C4N-C3N	2.23	1.43	1.39
3	A	800	ITB	C7-C8	2.32	1.41	1.37
2	A	500	NAP	C2A-N1A	2.37	1.38	1.33
3	A	800	ITB	O18-S16	2.41	1.46	1.43
2	A	500	NAP	C6N-N1N	2.44	1.42	1.35
2	A	500	NAP	O4D-C1D	2.77	1.44	1.41
2	A	500	NAP	C2A-N3A	3.02	1.37	1.32

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	ITB	O19-C14-C10	-12.18	117.28	129.25
3	A	600	ITB	C9-C10-C14	-9.96	105.42	111.57
3	A	700	ITB	O19-C14-C10	-9.21	120.19	129.25
3	A	800	ITB	C9-C10-C14	-7.11	107.18	111.57
3	A	700	ITB	C9-C10-C14	-6.89	107.31	111.57
3	A	800	ITB	O19-C14-C10	-6.79	122.58	129.25
2	A	500	NAP	C3N-C7N-N7N	-5.62	111.67	117.82
3	A	600	ITB	O18-S16-N15	-4.69	106.64	109.88
3	A	600	ITB	C7-C8-C9	-4.47	111.33	118.10
3	A	600	ITB	C7-C6-C1	-4.31	114.09	119.18
2	A	500	NAP	O4D-C1D-N1N	-4.21	103.50	108.13
3	A	600	ITB	C4-C5-C6	-3.55	114.74	120.44
2	A	500	NAP	C3N-C2N-N1N	-3.37	116.47	120.36
3	A	600	ITB	C9-S16-N15	-2.66	91.62	92.61
3	A	700	ITB	C3-C2-C1	-2.51	117.33	120.88
3	A	700	ITB	O17-S16-N15	-2.23	108.34	109.88
3	A	800	ITB	O18-S16-C9	-2.17	108.45	111.11
2	A	500	NAP	C5N-C4N-C3N	-2.09	117.70	120.33
2	A	500	NAP	C5N-C6N-N1N	-2.03	116.96	120.47
2	A	500	NAP	O3D-C3D-C4D	2.10	117.36	111.05
2	A	500	NAP	O3X-P2B-O2X	2.13	115.50	107.38
3	A	700	ITB	O19-C14-N15	2.18	126.61	123.07
3	A	600	ITB	O17-S16-O18	2.35	119.73	116.20
3	A	800	ITB	O17-S16-O18	2.37	119.76	116.20
3	A	700	ITB	C10-C14-N15	2.40	111.08	108.72
3	A	700	ITB	O17-S16-O18	2.50	119.95	116.20
3	A	800	ITB	C14-N15-S16	2.67	116.44	115.07
3	A	700	ITB	C2-C1-C6	3.07	121.93	117.91
3	A	800	ITB	O18-S16-N15	3.11	112.03	109.88
2	A	500	NAP	C4B-O4B-C1B	3.20	113.24	109.72
3	A	600	ITB	C10-C14-N15	3.23	111.90	108.72
3	A	800	ITB	C10-C14-N15	3.30	111.97	108.72
2	A	500	NAP	C2N-C3N-C4N	3.56	122.25	118.29
3	A	700	ITB	C14-N15-S16	3.76	117.00	115.07
3	A	700	ITB	C10-C9-S16	4.28	109.62	106.83
3	A	700	ITB	C9-C10-C1	4.34	121.79	117.65
3	A	600	ITB	C5-C6-C1	4.48	125.18	119.10
3	A	600	ITB	O19-C14-N15	4.51	130.38	123.07
3	A	800	ITB	C9-C10-C1	4.53	121.97	117.65
3	A	800	ITB	C10-C9-S16	4.55	109.80	106.83
3	A	700	ITB	C9-S16-N15	4.55	94.30	92.61
3	A	800	ITB	C9-S16-N15	4.76	94.37	92.61

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	600	ITB	C14-N15-S16	5.89	118.08	115.07
3	A	600	ITB	C8-C7-C6	7.03	132.68	121.85
3	A	600	ITB	O17-S16-N15	7.05	114.75	109.88
3	A	600	ITB	C9-C10-C1	8.47	125.72	117.65
3	A	600	ITB	C10-C9-S16	9.20	112.83	106.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAP	3	0
3	A	600	ITB	1	0
3	A	800	ITB	1	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, 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	315/316 (99%)	0.50	23 (7%) 18 18	7, 13, 34, 67	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	TRP	9.1
1	A	314	GLU	7.1
1	A	222	PRO	6.8
1	A	1	ALA	6.6
1	A	221	LYS	6.1
1	A	315	PHE	5.2
1	A	313	GLU	4.0
1	A	301	LEU	3.3
1	A	126	GLU	3.2
1	A	220	ALA	3.2
1	A	223	GLU	3.2
1	A	312	HIS	3.1
1	A	241	ASN	3.1
1	A	295	TRP	2.8
1	A	124	LEU	2.7
1	A	173	PRO	2.7
1	A	305[A]	SER	2.6
1	A	307	LYS	2.6
1	A	35	ILE	2.6
1	A	224	ASP	2.5
1	A	218	PRO	2.4
1	A	128	GLY	2.2
1	A	109	ILE	2.2

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ITB	A	700	23/23	0.94	0.21	1.39	18,25,32,41	0
3	ITB	A	600	23/23	0.94	0.12	0.88	11,15,30,32	0
2	NAP	A	500	48/48	0.97	0.07	-1.20	6,9,13,15	0
3	ITB	A	800	23/23	0.90	0.27	-	24,34,41,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.