W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:41 PM GMT

PDB ID	:	4A7P
Title	:	Se-Met derivatized UgdG, UDP-glucose dehydrogenase from Sphingomonas elodea
Authors	:	Rocha, J.; Granja, A.T.; Sa-Correia, I.; Fialho, A.M.; Frazao, C.
Deposited on	:	2011-11-14
Resolution	:	3.40 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 (i) symbol.

The following versions of software and data (see references (i)) 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 3.40 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		0.501
Clashscore		9
Ramachandran outliers		1.1%
Sidechain outliers		17.4%
RSRZ outliers		44.8%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
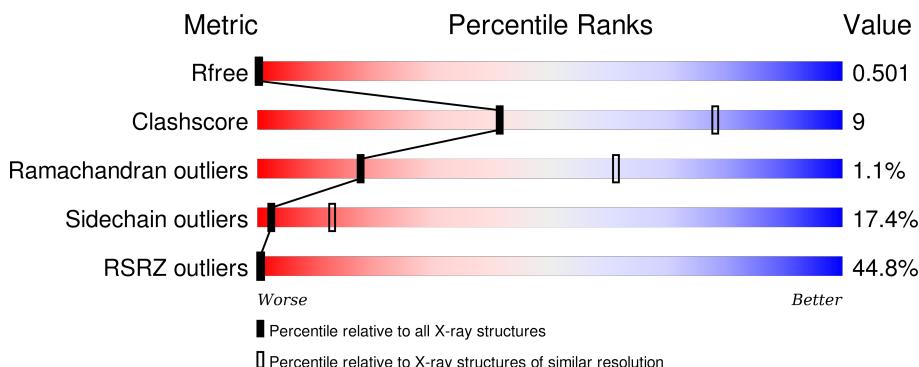
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 <=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	446	48% / 66% 25% 5% •
1	B	446	37% / 68% 23% 5% •
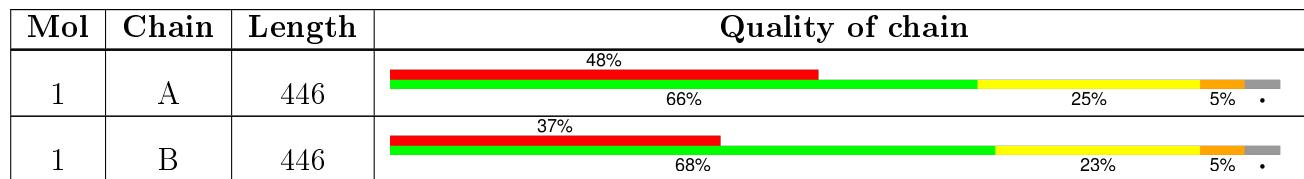
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	B	501	-	-	-	X

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6557 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 UDP-GLUCOSE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	Se	0	0	0
			3234	2035	563	623	4	9			
1	B	429	Total	C	N	O	S	Se	0	0	0
			3235	2036	563	623	4	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP A4UTT2
A	-7	HIS	-	EXPRESSION TAG	UNP A4UTT2
A	-6	HIS	-	EXPRESSION TAG	UNP A4UTT2
A	-5	HIS	-	EXPRESSION TAG	UNP A4UTT2
A	-4	HIS	-	EXPRESSION TAG	UNP A4UTT2
A	-3	HIS	-	EXPRESSION TAG	UNP A4UTT2
A	-2	GLY	-	EXPRESSION TAG	UNP A4UTT2
A	-1	SER	-	EXPRESSION TAG	UNP A4UTT2
A	1	VAL	MET	SEE REMARK 999	UNP A4UTT2
B	-8	HIS	-	EXPRESSION TAG	UNP A4UTT2
B	-7	HIS	-	EXPRESSION TAG	UNP A4UTT2
B	-6	HIS	-	EXPRESSION TAG	UNP A4UTT2
B	-5	HIS	-	EXPRESSION TAG	UNP A4UTT2
B	-4	HIS	-	EXPRESSION TAG	UNP A4UTT2
B	-3	HIS	-	EXPRESSION TAG	UNP A4UTT2
B	-2	GLY	-	EXPRESSION TAG	UNP A4UTT2
B	-1	SER	-	EXPRESSION TAG	UNP A4UTT2
B	1	VAL	MET	SEE REMARK 999	UNP A4UTT2

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

NAD
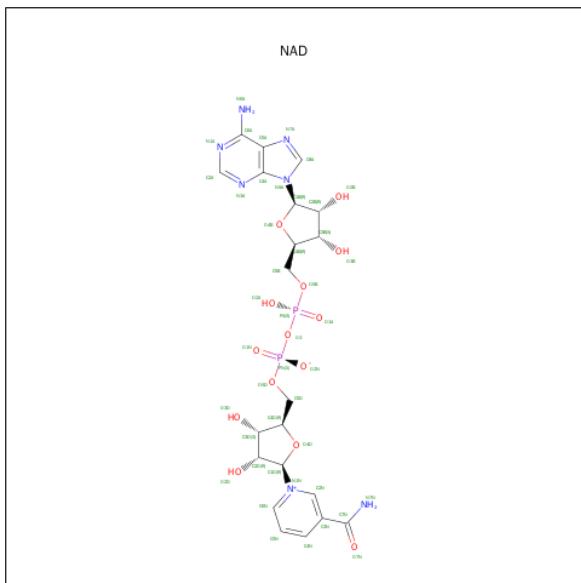
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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: UDP-GLUCOSE DEHYDROGENASE

- Molecule 1: UDP-GLUCOSE DEHYDROGENASE
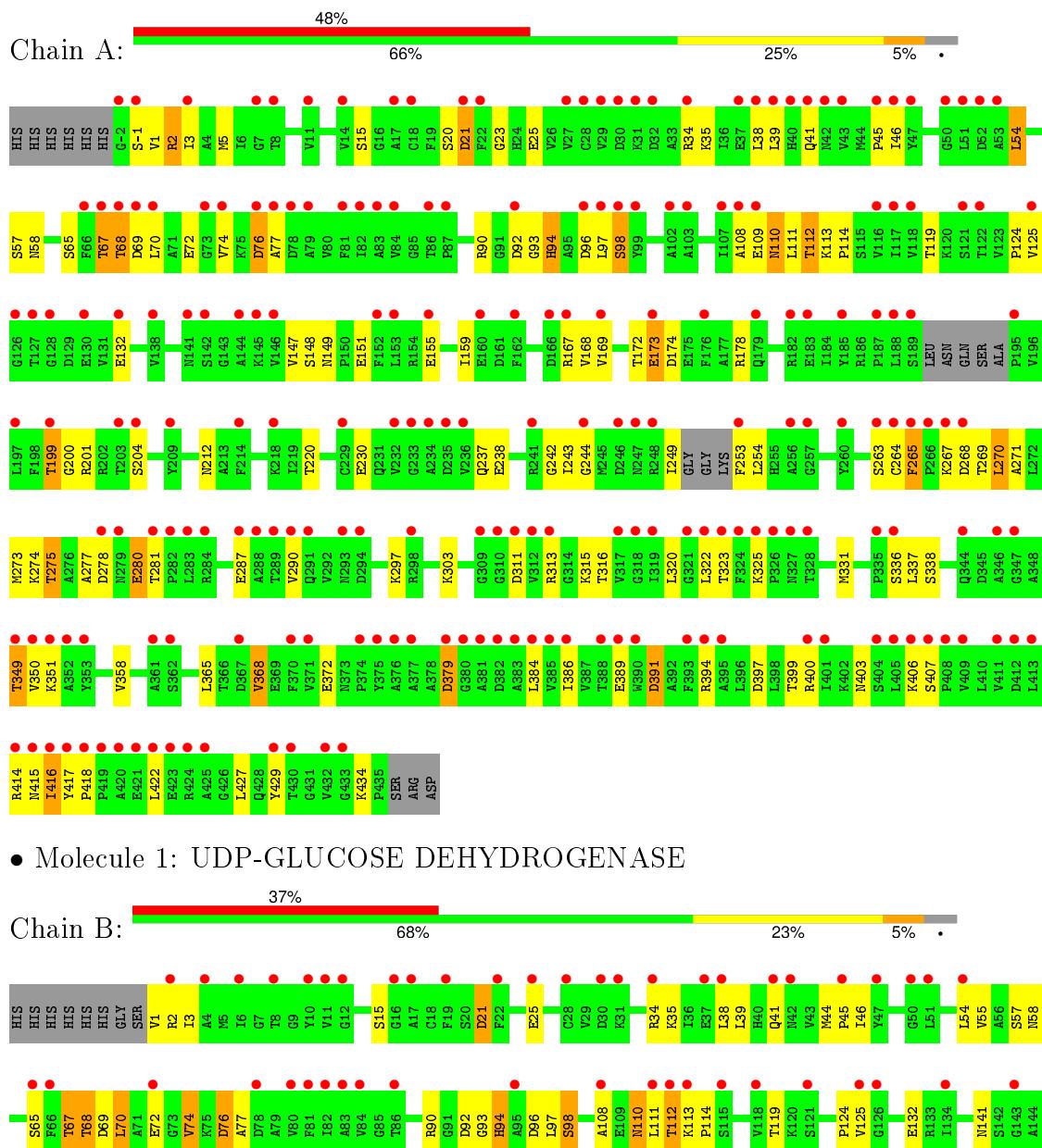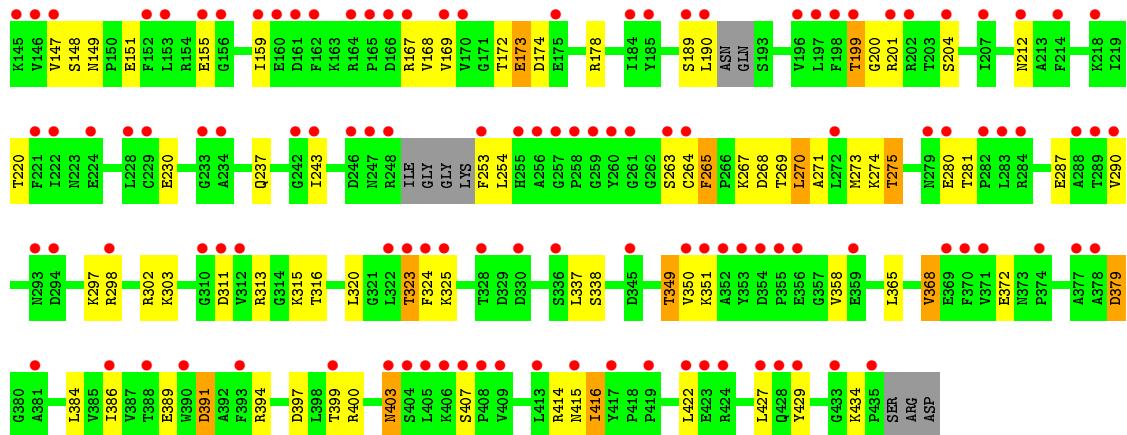
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.03Å　　109.03Å　　175.81Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	48.76　–　3.40 48.76　–　3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.76-3.40) 99.2 (48.76-3.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.63 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.230　,　(Not available) 0.484　,　　　　0.501	Depositor DCC
R_{free} test set	1014 reflections (7.22%)	DCC
Wilson B-factor (Å^2)	226.7	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 83.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.68$, $<L^2> = 0.55$	Xtriage
Outliers	31 of 15086 reflections (0.205%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6557	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.65% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: NAD

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	0.26	0/3275	0.52	0/4422
1	B	0.26	0/3276	0.52	0/4425
All	All	0.26	0/6551	0.52	0/8847

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	3234	0	3264	61	1
1	B	3235	0	3265	56	1
2	A	44	0	26	0	0
2	B	44	0	26	0	0
All	All	6557	0	6581	112	1

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 9.

All (112) 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:112:THR:OG1	1:A:113:LYS:N	2.25	0.70
1:B:112:THR:OG1	1:B:113:LYS:N	2.24	0.68
1:B:351:LYS:NZ	1:B:379:ASP:O	2.29	0.65
1:A:2:ARG:HG2	1:A:77:ALA:HA	1.80	0.64
1:A:351:LYS:NZ	1:A:379:ASP:O	2.30	0.62
1:A:391:ASP:OD1	1:A:391:ASP:N	2.32	0.62
1:A:269:THR:OG1	1:A:270:LEU:N	2.34	0.61
1:B:2:ARG:HG2	1:B:77:ALA:HA	1.81	0.61
1:B:92:ASP:OD1	1:B:93:GLY:N	2.34	0.60
1:B:365:LEU:HB3	1:B:368:VAL:HG21	1.83	0.60
1:A:92:ASP:OD1	1:A:93:GLY:N	2.34	0.59
1:A:365:LEU:HB3	1:A:368:VAL:HG21	1.83	0.59
1:B:149:ASN:ND2	1:B:169:VAL:O	2.30	0.59
1:B:269:THR:OG1	1:B:270:LEU:N	2.34	0.59
1:B:311:ASP:OD2	1:B:313:ARG:NH1	2.36	0.59
1:A:149:ASN:ND2	1:A:169:VAL:O	2.30	0.57
1:B:391:ASP:OD1	1:B:391:ASP:N	2.32	0.57
1:B:271:ALA:O	1:B:275:THR:OG1	2.23	0.57
1:B:96:ASP:OD1	1:B:98:SER:OG	2.22	0.56
1:A:96:ASP:OD1	1:A:98:SER:OG	2.24	0.56
1:A:311:ASP:OD2	1:A:313:ARG:NH1	2.39	0.55
1:A:108:ALA:HA	1:A:111:LEU:HD22	1.90	0.54
1:A:94:HIS:HB2	1:A:274:LYS:HZ2	1.72	0.54
1:A:2:ARG:HA	1:A:25:GLU:HB2	1.90	0.54
1:A:271:ALA:O	1:A:275:THR:OG1	2.24	0.54
1:B:108:ALA:HA	1:B:111:LEU:HD22	1.89	0.54
1:B:1:VAL:O	1:B:25:GLU:N	2.39	0.53
1:A:57:SER:OG	1:A:58:ASN:N	2.42	0.53
1:B:2:ARG:HA	1:B:25:GLU:HB2	1.90	0.53
1:B:57:SER:OG	1:B:58:ASN:N	2.41	0.53
1:A:69:ASP:OD1	1:A:72:GLU:N	2.38	0.53
1:A:-1:SER:HB2	1:A:23:GLY:O	2.08	0.53
1:A:273:MSE:SE	1:A:287:GLU:HA	2.59	0.53
1:A:3:ILE:N	1:A:25:GLU:O	2.39	0.52
1:B:273:MSE:SE	1:B:287:GLU:HA	2.59	0.52
1:A:67:THR:OG1	1:A:68:THR:N	2.43	0.52
1:B:237:GLN:NE2	1:B:415:ASN:HB3	2.25	0.52
1:A:278:ASP:OD2	1:B:298:ARG:NH2	2.42	0.52
1:B:67:THR:OG1	1:B:68:THR:N	2.43	0.52
1:A:237:GLN:NE2	1:A:415:ASN:HB3	2.25	0.52
1:A:267:LYS:NZ	1:A:268:ASP:OD1	2.40	0.52
1:A:94:HIS:CG	1:A:274:LYS:HG2	2.45	0.52

<div align="center">

Continued on next page...

</div>

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLU:OE1	1:A:201:ARG:NH2	2.43	0.51
1:B:94:HIS:HB2	1:B:274:LYS:HZ2	1.75	0.51
1:A:244:GLY:HA2	1:A:249:ILE:HG21	1.92	0.51
1:B:391:ASP:HA	1:B:394:ARG:HG3	1.93	0.51
1:B:132:GLU:OE1	1:B:201:ARG:NH2	2.42	0.51
1:A:1:VAL:O	1:A:25:GLU:N	2.39	0.51
1:B:397:ASP:OD1	1:B:400:ARG:N	2.43	0.51
1:B:94:HIS:CG	1:B:274:LYS:HG2	2.47	0.50
1:A:397:ASP:OD1	1:A:400:ARG:N	2.43	0.50
1:A:39:LEU:HD21	1:A:45:PRO:HD3	1.94	0.49
1:A:391:ASP:HA	1:A:394:ARG:HG3	1.94	0.49
1:B:3:ILE:N	1:B:25:GLU:O	2.39	0.49
1:A:422:LEU:HD12	1:A:427:LEU:HD12	1.95	0.49
1:B:39:LEU:HD21	1:B:45:PRO:HD3	1.94	0.49
1:B:422:LEU:HD12	1:B:427:LEU:HD12	1.95	0.49
1:A:278:ASP:OD1	1:B:298:ARG:NE	2.44	0.48
1:B:267:LYS:NZ	1:B:268:ASP:OD1	2.40	0.48
1:A:237:GLN:HE21	1:A:415:ASN:HB3	1.79	0.48
1:A:21:ASP:OD1	1:A:58:ASN:ND2	2.46	0.47
1:A:34:ARG:HD2	1:A:34:ARG:HA	1.64	0.46
1:A:20:SER:OG	1:A:58:ASN:ND2	2.36	0.46
1:B:237:GLN:HE21	1:B:415:ASN:HB3	1.80	0.46
1:A:199:THR:OG1	1:A:200:GLY:O	2.34	0.45
1:B:199:THR:OG1	1:B:200:GLY:O	2.34	0.45
1:B:21:ASP:OD1	1:B:58:ASN:ND2	2.45	0.45
1:A:97:LEU:HD11	1:A:124:PRO:HG2	1.99	0.45
1:A:422:LEU:O	1:A:427:LEU:N	2.46	0.45
1:B:155:GLU:O	1:B:325:LYS:NZ	2.44	0.45
1:B:386:ILE:HG21	1:B:416:ILE:HD11	1.97	0.45
1:A:320:LEU:HG	1:A:384:LEU:HD11	1.99	0.44
1:A:386:ILE:HG21	1:A:416:ILE:HD11	1.98	0.44
1:B:69:ASP:OD1	1:B:72:GLU:N	2.37	0.44
1:B:320:LEU:HG	1:B:384:LEU:HD11	1.98	0.44
1:A:-1:SER:O	1:A:-1:SER:OG	2.34	0.44
1:A:97:LEU:HD21	1:A:124:PRO:HD2	1.98	0.44
1:B:97:LEU:HD11	1:B:124:PRO:HG2	1.99	0.44
1:B:172:THR:OG1	1:B:173:GLU:N	2.51	0.44
1:A:172:THR:OG1	1:A:173:GLU:N	2.51	0.44
1:B:97:LEU:HD21	1:B:124:PRO:HD2	1.98	0.43
1:B:422:LEU:O	1:B:427:LEU:N	2.45	0.43
1:A:172:THR:O	1:A:178:ARG:NH2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD22	1:A:54:LEU:HA	1.77	0.43
1:A:277:ALA:O	1:B:302:ARG:NH1	2.51	0.43
1:B:172:THR:O	1:B:178:ARG:NH2	2.52	0.43
1:A:331:MSE:HB3	1:A:331:MSE:HE3	1.89	0.43
1:B:315:LYS:HD3	1:B:315:LYS:HA	1.79	0.43
1:B:110:ASN:N	1:B:110:ASN:OD1	2.51	0.43
1:B:434:LYS:HA	1:B:434:LYS:HD3	1.83	0.43
1:B:34:ARG:HA	1:B:34:ARG:HD2	1.65	0.43
1:B:389:GLU:HG2	1:B:414:ARG:HD2	2.00	0.42
1:A:278:ASP:HA	1:B:302:ARG:HD3	2.00	0.42
1:A:315:LYS:O	1:A:349:THR:OG1	2.37	0.42
1:A:389:GLU:HG2	1:A:414:ARG:HD2	2.01	0.42
1:A:417:TYR:HA	1:A:418:PRO:HD2	1.93	0.42
1:A:155:GLU:O	1:A:325:LYS:NZ	2.44	0.42
1:A:230:GLU:CD	1:A:303:LYS:HZ1	2.23	0.42
1:A:280:GLU:OE2	1:B:302:ARG:NH2	2.44	0.41
1:A:76:ASP:HA	1:A:113:LYS:HG2	2.02	0.41
1:B:403:ASN:OD1	1:B:403:ASN:N	2.52	0.41
1:A:110:ASN:OD1	1:A:110:ASN:N	2.53	0.41
1:B:230:GLU:CD	1:B:303:LYS:HZ3	2.23	0.41
1:B:44:MSE:HE1	1:B:55:VAL:HG11	2.03	0.41
1:B:70:LEU:HD23	1:B:74:VAL:HG21	2.03	0.41
1:B:76:ASP:HA	1:B:113:LYS:HG2	2.02	0.41
1:A:434:LYS:HD3	1:A:434:LYS:HA	1.82	0.40
1:B:315:LYS:O	1:B:349:THR:OG1	2.37	0.40
1:A:322:LEU:O	1:A:336:SER:OG	2.28	0.40
1:B:323:THR:OG1	1:B:324:PHE:N	2.54	0.40
1:A:5:MSE:HB2	1:A:5:MSE:HE2	1.94	0.40
1:A:238:GLU:O	1:A:242:GLY:N	2.51	0.40

All (1) 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:406:LYS:NZ	1:B:141:ASN:OD1[7_467]	2.13	0.07

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	423/446 (95%)	381 (90%)	38 (9%)	4 (1%)	21	65
1	B	423/446 (95%)	382 (90%)	36 (8%)	5 (1%)	16	59
All	All	846/892 (95%)	763 (90%)	74 (9%)	9 (1%)	17	61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASP
1	B	379	ASP
1	B	189	SER
1	A	114	PRO
1	B	114	PRO
1	B	358	VAL
1	A	265	PHE
1	A	358	VAL
1	B	265	PHE

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	341/346 (99%)	281 (82%)	60 (18%)	2	12
1	B	341/346 (99%)	282 (83%)	59 (17%)	2	13
All	All	682/692 (99%)	563 (83%)	119 (17%)	2	13

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	15	SER
1	A	21	ASP
1	A	35	LYS
1	A	38	LEU
1	A	41	GLN
1	A	46	ILE
1	A	54	LEU
1	A	65	SER
1	A	67	THR
1	A	68	THR
1	A	70	LEU
1	A	74	VAL
1	A	76	ASP
1	A	90	ARG
1	A	94	HIS
1	A	98	SER
1	A	109	GLU
1	A	110	ASN
1	A	112	THR
1	A	119	THR
1	A	125	VAL
1	A	147	VAL
1	A	148	SER
1	A	151	GLU
1	A	159	ILE
1	A	167	ARG
1	A	168	VAL
1	A	173	GLU
1	A	174	ASP
1	A	199	THR
1	A	204	SER
1	A	212	ASN
1	A	220	THR
1	A	243	ILE
1	A	253	PHE
1	A	254	LEU
1	A	263	SER
1	A	264	CYS
1	A	265	PHE
1	A	270	LEU
1	A	275	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	280	GLU
1	A	281	THR
1	A	290	VAL
1	A	297	LYS
1	A	316	THR
1	A	323	THR
1	A	337	LEU
1	A	338	SER
1	A	349	THR
1	A	350	VAL
1	A	368	VAL
1	A	372	GLU
1	A	391	ASP
1	A	399	THR
1	A	403	ASN
1	A	407	SER
1	A	416	ILE
1	A	429	TYR
1	B	15	SER
1	B	21	ASP
1	B	35	LYS
1	B	38	LEU
1	B	41	GLN
1	B	46	ILE
1	B	54	LEU
1	B	65	SER
1	B	67	THR
1	B	68	THR
1	B	70	LEU
1	B	74	VAL
1	B	76	ASP
1	B	90	ARG
1	B	94	HIS
1	B	98	SER
1	B	110	ASN
1	B	112	THR
1	B	119	THR
1	B	125	VAL
1	B	147	VAL
1	B	148	SER
1	B	151	GLU
1	B	159	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	167	ARG
1	B	168	VAL
1	B	173	GLU
1	B	174	ASP
1	B	190	LEU
1	B	199	THR
1	B	204	SER
1	B	212	ASN
1	B	220	THR
1	B	243	ILE
1	B	253	PHE
1	B	254	LEU
1	B	263	SER
1	B	264	CYS
1	B	265	PHE
1	B	270	LEU
1	B	275	THR
1	B	280	GLU
1	B	281	THR
1	B	290	VAL
1	B	297	LYS
1	B	316	THR
1	B	323	THR
1	B	337	LEU
1	B	338	SER
1	B	349	THR
1	B	350	VAL
1	B	368	VAL
1	B	372	GLU
1	B	391	ASP
1	B	399	THR
1	B	403	ASN
1	B	407	SER
1	B	416	ILE
1	B	429	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

2 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	NAD	A	501	-	38,48,48	1.59	7 (18%)	47,73,73	2.28	11 (23%)
2	NAD	B	501	-	38,48,48	1.59	7 (18%)	47,73,73	2.30	11 (23%)

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	NAD	A	501	-	-	0/22/62/62	0/5/5/5
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O3D-C3D	-2.15	1.37	1.43
2	A	501	NAD	C2B-C3B	-2.15	1.47	1.53
2	B	501	NAD	C2B-C3B	-2.12	1.47	1.53
2	A	501	NAD	O3D-C3D	-2.11	1.37	1.43
2	A	501	NAD	O2B-C2B	-2.05	1.38	1.43
2	B	501	NAD	O2B-C2B	-2.05	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	C6N-N1N	2.29	1.41	1.35
2	A	501	NAD	C6N-N1N	2.31	1.41	1.35
2	B	501	NAD	C2A-N3A	2.89	1.37	1.32
2	A	501	NAD	C2A-N3A	2.91	1.37	1.32
2	B	501	NAD	C6A-N6A	3.07	1.44	1.34
2	A	501	NAD	C6A-N6A	3.08	1.44	1.34
2	A	501	NAD	C7N-N7N	5.55	1.44	1.33
2	B	501	NAD	C7N-N7N	5.59	1.44	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NAD	N3A-C2A-N1A	-11.74	119.91	128.89
2	A	501	NAD	N3A-C2A-N1A	-11.61	120.00	128.89
2	A	501	NAD	PN-O3-PA	-4.73	119.43	132.73
2	B	501	NAD	PN-O3-PA	-4.71	119.50	132.73
2	A	501	NAD	C4B-O4B-C1B	-3.98	105.34	109.72
2	B	501	NAD	C4B-O4B-C1B	-3.92	105.41	109.72
2	B	501	NAD	C4A-C5A-N7A	-2.57	107.11	109.48
2	A	501	NAD	C4A-C5A-N7A	-2.46	107.22	109.48
2	B	501	NAD	O7N-C7N-N7N	-2.38	119.24	122.59
2	A	501	NAD	O7N-C7N-N7N	-2.31	119.35	122.59
2	B	501	NAD	O2N-PN-O1N	-2.07	101.28	112.53
2	A	501	NAD	O2N-PN-O1N	-2.07	101.31	112.53
2	A	501	NAD	O3-PA-O5B	2.14	108.61	102.94
2	B	501	NAD	O3-PA-O5B	2.15	108.63	102.94
2	B	501	NAD	O4B-C4B-C3B	2.23	109.64	105.15
2	A	501	NAD	O4B-C4B-C3B	2.26	109.71	105.15
2	B	501	NAD	O3-PN-O5D	2.54	109.67	102.94
2	A	501	NAD	O3-PN-O5D	2.54	109.68	102.94
2	B	501	NAD	O4D-C1D-N1N	2.69	111.08	108.13
2	A	501	NAD	O4D-C1D-N1N	2.71	111.11	108.13
2	A	501	NAD	C3N-C7N-N7N	3.59	121.74	117.82
2	B	501	NAD	C3N-C7N-N7N	3.63	121.79	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	420/446 (94%)	2.85	212 (50%)	0	0	79, 127, 170, 216	0
1	B	420/446 (94%)	2.14	164 (39%)	0	1	79, 127, 169, 215	0
All	All	840/892 (94%)	2.50	376 (44%)	0	0	79, 127, 170, 216	0

All (376) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	ALA	26.8
1	A	28	CYS	22.4
1	B	165	PRO	18.6
1	A	327	ASN	16.9
1	B	423	GLU	16.4
1	A	351	LYS	13.2
1	A	82	ILE	13.1
1	A	325	LYS	13.0
1	A	247	ASN	12.1
1	A	166	ASP	11.6
1	B	86	THR	11.6
1	A	324	PHE	11.0
1	B	311	ASP	10.6
1	B	155	GLU	10.5
1	A	39	LEU	10.4
1	A	419	PRO	10.1
1	B	330	ASP	9.9
1	A	38	LEU	9.9
1	B	37	GLU	9.8
1	B	351	LYS	9.8
1	B	377	ALA	9.5
1	B	22	PHE	9.3
1	A	68	THR	9.2
1	A	41	GLN	9.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	352	ALA	9.0
1	A	380	GLY	8.9
1	A	189	SER	8.8
1	A	310	GLY	8.8
1	A	282	PRO	8.8
1	B	407	SER	8.7
1	B	408	PRO	8.7
1	B	370	PHE	8.6
1	B	66	PHE	8.6
1	A	204	SER	8.5
1	A	379	ASP	8.5
1	B	242	GLY	8.4
1	A	385	VAL	8.3
1	A	375	TYR	8.2
1	A	50	GLY	8.2
1	A	416	ILE	8.2
1	B	312	VAL	8.1
1	A	31	LYS	7.9
1	A	209	TYR	7.7
1	A	322	LEU	7.7
1	B	405	LEU	7.6
1	A	98	SER	7.5
1	A	46	ILE	7.4
1	B	422	LEU	7.4
1	A	234	ALA	7.4
1	B	406	LYS	7.4
1	A	326	PRO	7.3
1	A	34	ARG	7.2
1	B	234	ALA	7.2
1	B	409	VAL	7.2
1	A	404	SER	7.2
1	A	352	ALA	7.1
1	A	425	ALA	7.1
1	A	29	VAL	7.1
1	A	328	THR	7.1
1	B	111	LEU	7.1
1	A	350	VAL	7.1
1	A	395	ALA	7.0
1	A	185	TYR	6.9
1	B	156	GLY	6.9
1	B	82	ILE	6.8
1	A	52	ASP	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	167	ARG	6.7
1	A	141	ASN	6.7
1	B	28	CYS	6.7
1	B	161	ASP	6.7
1	B	233	GLY	6.6
1	A	67	THR	6.5
1	B	169	VAL	6.5
1	A	393	PHE	6.3
1	B	378	ALA	6.3
1	A	167	ARG	6.3
1	A	374	PRO	6.3
1	B	190	LEU	6.3
1	A	412	ASP	6.3
1	B	8	THR	6.2
1	A	182	ARG	6.1
1	A	176	PHE	6.1
1	B	121	SER	6.1
1	A	394	ARG	6.0
1	A	69	ASP	6.0
1	A	78	ASP	6.0
1	A	102	ALA	5.9
1	A	371	VAL	5.9
1	A	21	ASP	5.7
1	B	310	GLY	5.7
1	A	422	LEU	5.7
1	B	17	ALA	5.7
1	B	10	TYR	5.7
1	A	336	SER	5.6
1	A	-1	SER	5.6
1	A	145	LYS	5.6
1	B	170	VAL	5.5
1	B	47	TYR	5.4
1	B	201	ARG	5.4
1	A	22	PHE	5.4
1	A	260	TYR	5.4
1	A	127	THR	5.4
1	B	355	PRO	5.3
1	B	81	PHE	5.3
1	B	324	PHE	5.3
1	A	155	GLU	5.2
1	A	311	ASP	5.2
1	A	138	VAL	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	427	LEU	5.2
1	A	42	ASN	5.1
1	A	142	SER	5.1
1	A	73	GLY	5.1
1	A	51	LEU	5.1
1	B	4	ALA	5.1
1	A	323	THR	5.0
1	B	424	ARG	5.0
1	A	424	ARG	5.0
1	A	126	GLY	5.0
1	B	199	THR	5.0
1	A	408	PRO	4.9
1	B	166	ASP	4.9
1	A	27	VAL	4.9
1	A	76	ASP	4.9
1	A	384	LEU	4.8
1	A	53	ALA	4.8
1	B	325	LYS	4.8
1	B	259	GLY	4.7
1	B	189	SER	4.7
1	A	18	CYS	4.7
1	A	433	GLY	4.7
1	A	128	GLY	4.7
1	B	404	SER	4.6
1	A	386	ILE	4.6
1	B	80	VAL	4.6
1	A	203	THR	4.6
1	A	421	GLU	4.6
1	B	145	LYS	4.6
1	A	146	VAL	4.6
1	B	162	PHE	4.6
1	A	244	GLY	4.5
1	A	246	ASP	4.5
1	B	279	ASN	4.5
1	A	-2	GLY	4.5
1	A	32	ASP	4.4
1	A	268	ASP	4.4
1	A	97	LEU	4.4
1	B	247	ASN	4.4
1	A	99	TYR	4.4
1	B	399	THR	4.4
1	A	74	VAL	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	146	VAL	4.3
1	A	173	GLU	4.3
1	A	96	ASP	4.3
1	B	164	ARG	4.3
1	A	66	PHE	4.3
1	A	287	GLU	4.3
1	B	415	ASN	4.3
1	A	418	PRO	4.2
1	B	42	ASN	4.2
1	B	429	TYR	4.2
1	A	45	PRO	4.1
1	B	323	THR	4.1
1	A	411	VAL	4.1
1	A	179	GLN	4.1
1	A	81	PHE	4.1
1	A	125	VAL	4.1
1	A	264	CYS	4.1
1	A	107	ILE	4.1
1	A	40	HIS	4.0
1	B	356	GLU	4.0
1	B	374	PRO	4.0
1	A	236	VAL	4.0
1	B	298	ARG	4.0
1	B	255	HIS	4.0
1	A	79	ALA	4.0
1	A	87	PRO	4.0
1	A	109	GLU	4.0
1	A	108	ALA	3.9
1	A	291	GLN	3.9
1	B	428	GLN	3.9
1	B	25	GLU	3.9
1	B	354	ASP	3.9
1	B	72	GLU	3.9
1	B	419	PRO	3.8
1	B	95	ALA	3.8
1	A	381	ALA	3.8
1	A	407	SER	3.8
1	B	11	VAL	3.8
1	A	253	PHE	3.8
1	A	317	VAL	3.8
1	A	313	ARG	3.8
1	A	118	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	409	VAL	3.7
1	B	403	ASN	3.7
1	A	429	TYR	3.7
1	B	282	PRO	3.7
1	B	390	TRP	3.7
1	B	83	ALA	3.7
1	B	336	SER	3.6
1	A	389	GLU	3.6
1	A	383	ALA	3.6
1	B	388	THR	3.6
1	A	417	TYR	3.6
1	A	121	SER	3.6
1	A	7	GLY	3.5
1	B	30	ASP	3.5
1	A	152	PHE	3.5
1	A	309	GLY	3.5
1	A	14	VAL	3.5
1	B	196	VAL	3.5
1	A	8	THR	3.5
1	A	362	SER	3.5
1	B	381	ALA	3.4
1	B	113	LYS	3.4
1	A	84	VAL	3.4
1	A	335	PRO	3.4
1	A	130	GLU	3.4
1	B	19	PHE	3.4
1	B	294	ASP	3.4
1	B	108	ALA	3.4
1	A	241	ARG	3.4
1	B	197	LEU	3.4
1	A	132	GLU	3.4
1	A	37	GLU	3.3
1	A	406	LYS	3.3
1	A	432	VAL	3.3
1	B	125	VAL	3.3
1	A	423	GLU	3.3
1	B	118	VAL	3.3
1	A	376	ALA	3.3
1	A	415	ASN	3.3
1	B	246	ASP	3.3
1	A	248	ARG	3.2
1	A	312	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	319	ILE	3.2
1	A	43	VAL	3.2
1	A	116	VAL	3.2
1	B	214	PHE	3.2
1	B	184	ILE	3.2
1	A	3	ILE	3.2
1	A	162	PHE	3.1
1	B	371	VAL	3.1
1	A	382	ASP	3.1
1	A	298	ARG	3.1
1	B	359	GLU	3.1
1	B	290	VAL	3.1
1	A	265	PHE	3.1
1	A	195	PRO	3.1
1	A	278	ASP	3.1
1	A	370	PHE	3.1
1	B	16	GLY	3.0
1	A	347	GLY	3.0
1	B	115	SER	3.0
1	A	70	LEU	3.0
1	B	41	GLN	3.0
1	B	12	GLY	3.0
1	B	386	ILE	3.0
1	A	279	ASN	3.0
1	A	263	SER	3.0
1	A	235	ASP	3.0
1	A	321	GLY	3.0
1	B	51	LEU	3.0
1	B	263	SER	3.0
1	B	258	PRO	3.0
1	A	183	GLU	3.0
1	B	212	ASN	2.9
1	A	361	ALA	2.9
1	B	289	THR	2.9
1	B	38	LEU	2.9
1	A	281	THR	2.9
1	B	31	LYS	2.9
1	A	188	LEU	2.9
1	B	34	ARG	2.9
1	A	160	GLU	2.9
1	A	233	GLY	2.9
1	A	405	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	11	VAL	2.9
1	A	256	ALA	2.8
1	A	289	THR	2.8
1	A	290	VAL	2.8
1	B	147	VAL	2.8
1	B	126	GLY	2.8
1	A	257	GLY	2.8
1	A	197	LEU	2.8
1	B	175	GLU	2.8
1	A	122	THR	2.8
1	A	413	LEU	2.7
1	B	284	ARG	2.7
1	B	350	VAL	2.7
1	B	202	ARG	2.7
1	B	435	PRO	2.7
1	B	293	ASN	2.7
1	B	84	VAL	2.7
1	A	30	ASP	2.6
1	A	103	ALA	2.6
1	B	260	TYR	2.6
1	B	283	LEU	2.6
1	A	266	PRO	2.6
1	B	369	GLU	2.6
1	A	353	TYR	2.6
1	B	433	GLY	2.6
1	A	349	THR	2.6
1	B	264	CYS	2.6
1	B	204	SER	2.6
1	B	185	TYR	2.6
1	B	417	TYR	2.6
1	A	346	ALA	2.6
1	A	293	ASN	2.6
1	B	393	PHE	2.6
1	A	153	LEU	2.6
1	B	152	PHE	2.6
1	B	353	TYR	2.5
1	A	47	TYR	2.5
1	A	144	ALA	2.5
1	A	420	ALA	2.5
1	A	284	ARG	2.5
1	A	400	ARG	2.5
1	A	414	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	169	VAL	2.5
1	B	143	GLY	2.4
1	A	401	ILE	2.4
1	B	228	LEU	2.4
1	A	214	PHE	2.4
1	B	6	ILE	2.4
1	B	261	GLY	2.4
1	A	367	ASP	2.4
1	B	345	ASP	2.4
1	B	272	LEU	2.4
1	B	229	CYS	2.3
1	B	248	ARG	2.3
1	B	54	LEU	2.3
1	A	199	THR	2.3
1	B	253	PHE	2.3
1	A	390	TRP	2.3
1	A	218	LYS	2.3
1	B	221	PHE	2.3
1	A	344	GLN	2.3
1	B	322	LEU	2.3
1	A	86	THR	2.3
1	B	112	THR	2.3
1	A	17	ALA	2.2
1	A	77	ALA	2.2
1	A	388	THR	2.2
1	B	159	ILE	2.2
1	A	92	ASP	2.2
1	A	117	ILE	2.2
1	B	207	ILE	2.2
1	A	229	CYS	2.2
1	A	430	THR	2.2
1	B	160	GLU	2.2
1	B	65	SER	2.2
1	A	294	ASP	2.2
1	B	198	PHE	2.2
1	B	288	ALA	2.1
1	B	45	PRO	2.1
1	A	377	ALA	2.1
1	B	257	GLY	2.1
1	B	224	GLU	2.1
1	B	2	ARG	2.1
1	A	267	LYS	2.1

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	413	LEU	2.1
1	A	187	PRO	2.1
1	B	218	LYS	2.1
1	B	50	GLY	2.1
1	B	134	ILE	2.0
1	B	78	ASP	2.0
1	B	328	THR	2.0
1	B	280	GLU	2.0
1	A	232	VAL	2.0
1	B	243	ILE	2.0
1	A	283	LEU	2.0
1	B	222	ILE	2.0
1	B	256	ALA	2.0
1	A	318	GLY	2.0
1	A	288	ALA	2.0
1	B	153	LEU	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, 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($Å^2$)	Q<0.9
2	NAD	B	501	44/44	0.51	0.41	-0.31	88,110,146,336	0
2	NAD	A	501	44/44	0.54	0.34	-0.56	96,111,144,336	0

6.5 Other polymers (i)

There are no such residues in this entry.