Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:51 AM GMT

PDB ID	:	2J3I
Title	:	CRYSTAL STRUCTURE OF ARABIDOPSIS THALIANA DOUBLE BOND REDUCTASE (AT5G16970)-BINARY COMPLEX
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Deposited on	:	2006-08-21
Resolution	:	2.80 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:

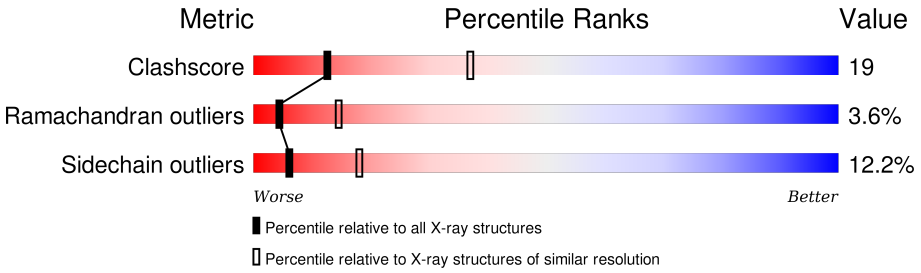
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	52% 36% 9%
1	B	345	54% 34% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5491 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.

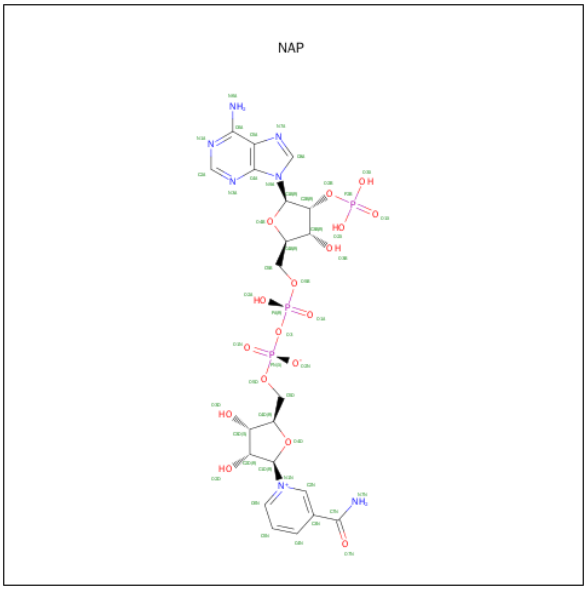
- Molecule 1 is a protein called NADP-DEPENDENT OXIDOREDUCTASE P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2623	1681	432	493	17			
1	B	345	Total	C	N	O	S	0	0	0
			2680	1717	440	506	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ASN	ILE	CONFLICT	UNP Q39172
B	1279	ASN	ILE	CONFLICT	UNP Q39172

- 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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	42	Total	O	0	0
			42	42		

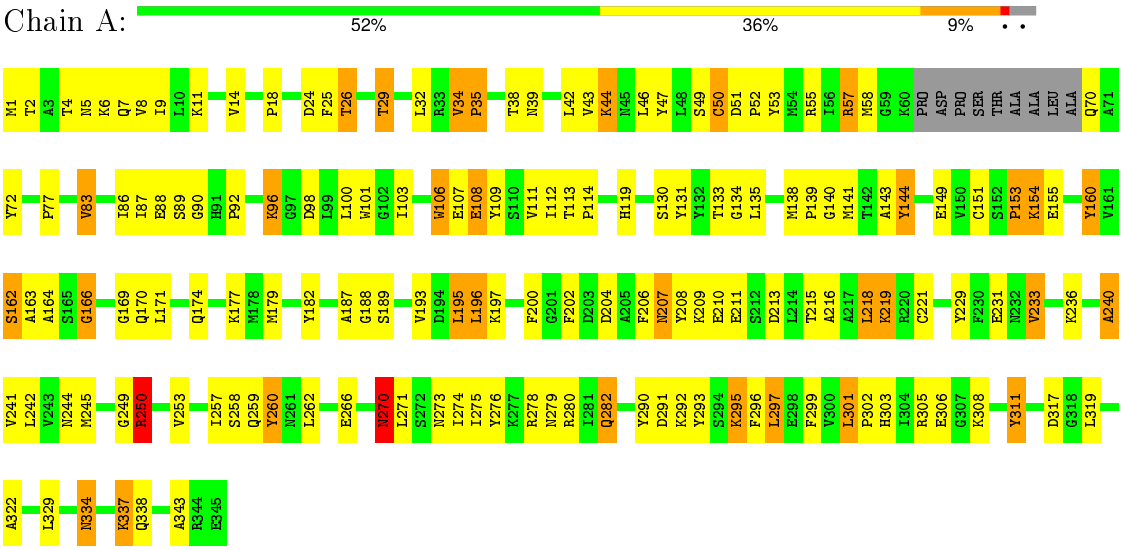
3 Residue-property plots (i)

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

Note EDS was not executed.

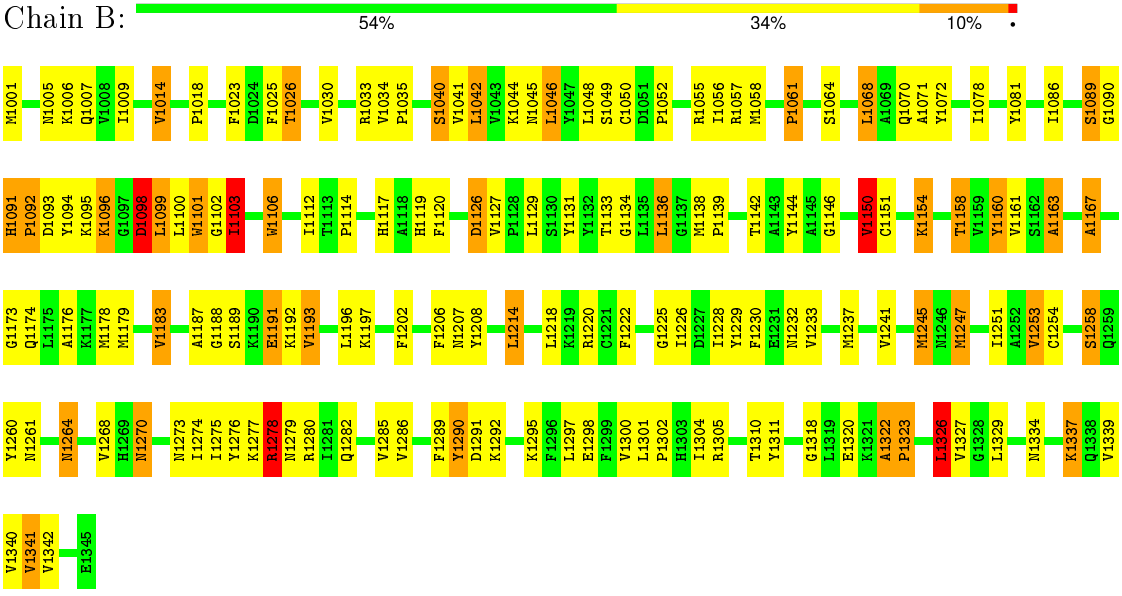
• Molecule 1: NADP-DEPENDENT OXIDOREDUCTASE P1

Chain A:



• Molecule 1: NADP-DEPENDENT OXIDOREDUCTASE P1

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.15Å 122.66Å 147.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.9 (15.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5491	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.81	0/2681	1.62	44/3625 (1.2%)
1	B	0.80	0/2740	1.59	33/3708 (0.9%)
All	All	0.81	0/5421	1.60	77/7333 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1057	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	101	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	A	305	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	1106	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	A	50	CYS	CA-C-N	-8.39	98.74	117.20
1	B	1055	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	57	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	101	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	B	1106	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	A	101	TRP	CG-CD2-CE3	7.57	140.71	133.90
1	B	1247	MET	CG-SD-CE	-7.54	88.14	100.20
1	A	106	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	B	1160	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	A	101	TRP	CB-CG-CD1	-7.33	117.48	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	TYR	CB-CG-CD1	-7.32	116.61	121.00
1	A	280	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	245	MET	CG-SD-CE	-7.23	88.64	100.20
1	B	1101	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	B	1055	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	B	1101	TRP	CD1-CG-CD2	7.21	112.07	106.30
1	A	106	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	250	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	101	TRP	CA-CB-CG	7.06	127.12	113.70
1	B	1253	VAL	CA-C-N	-6.80	102.24	117.20
1	A	219	LYS	CB-CG-CD	6.65	128.88	111.60
1	A	163	ALA	N-CA-C	-6.60	93.18	111.00
1	B	1103	ILE	CA-C-N	-6.57	102.75	117.20
1	A	260	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	B	1290	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	B	1341	VAL	CA-CB-CG1	-6.35	101.38	110.90
1	B	1183	VAL	CB-CA-C	-6.34	99.35	111.40
1	A	44	LYS	CA-CB-CG	6.23	127.11	113.40
1	A	50	CYS	O-C-N	6.06	132.39	122.70
1	A	208	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	A	2	THR	CA-C-N	-5.89	104.25	117.20
1	A	166	GLY	CA-C-N	-5.87	104.29	117.20
1	B	1206	PHE	CA-C-N	-5.80	104.43	117.20
1	B	1318	GLY	CA-C-N	-5.79	104.46	117.20
1	A	34	VAL	N-CA-C	5.78	126.60	111.00
1	A	162	SER	N-CA-C	5.71	126.43	111.00
1	B	1280	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	1057	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	278	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	1061	PRO	N-CA-C	5.59	126.64	112.10
1	B	1179	MET	CA-CB-CG	5.57	122.77	113.30
1	B	1260	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	A	34	VAL	CA-CB-CG2	-5.53	102.61	110.90
1	B	1014	VAL	CA-CB-CG2	-5.52	102.62	110.90
1	B	1086	ILE	CG1-CB-CG2	-5.51	99.28	111.40
1	A	270	ASN	N-CA-C	5.51	125.87	111.00
1	A	211	GLU	CA-C-N	-5.43	105.25	117.20
1	A	153	PRO	CA-C-N	-5.41	105.31	117.20
1	B	1072	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	1163	ALA	CA-C-N	-5.38	105.37	117.20
1	A	51	ASP	CA-CB-CG	5.31	125.08	113.40
1	A	219	LYS	CA-CB-CG	5.30	125.07	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1150	VAL	CA-C-N	5.27	128.80	117.20
1	B	1326	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	236	LYS	CA-CB-CG	5.24	124.92	113.40
1	B	1278	ARG	N-CA-C	5.23	125.12	111.00
1	B	1253	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	A	144	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	B	1042	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	278	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	1233	VAL	N-CA-C	5.17	124.95	111.00
1	B	1098	ASP	N-CA-C	5.14	124.87	111.00
1	A	160	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	218	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	219	LYS	CG-CD-CE	5.12	127.26	111.90
1	A	305	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	182	TYR	N-CA-C	-5.08	97.27	111.00
1	A	233	VAL	CA-C-N	5.07	126.33	116.20
1	A	14	VAL	CG1-CB-CG2	-5.06	102.81	110.90
1	A	240	ALA	CA-C-N	-5.05	106.09	117.20
1	A	108	GLU	CA-CB-CG	5.05	124.50	113.40
1	A	311	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	B	1099	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1322	ALA	Peptide

5.2 Too-close contacts (i)

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	2623	0	2594	98	0
1	B	2680	0	2643	112	0
2	A	48	0	25	5	0
2	B	48	0	25	11	0
3	A	50	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	0	0	1	0
All	All	5491	0	5287	206	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 19.

All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1188:GLY:H	2:B:351:NAP:P2B	1.81	1.02
1:B:1208:TYR:HE1	2:B:351:NAP:O3X	1.47	0.95
1:B:1189:SER:HB3	1:B:1192:LYS:HB2	1.59	0.84
1:A:207:ASN:HD22	1:A:209:LYS:H	1.28	0.81
1:A:52:PRO:HB2	2:A:350:NAP:H3D	1.63	0.78
1:A:50:CYS:HB2	1:A:338:GLN:HB3	1.63	0.78
1:B:1208:TYR:CE1	2:B:351:NAP:O3X	2.37	0.77
1:A:229:TYR:CE2	1:A:231:GLU:HG2	2.21	0.76
1:B:1114:PRO:HA	1:B:1119:HIS:HD2	1.50	0.74
1:B:1158:THR:HG21	1:B:1225:GLY:O	1.88	0.74
1:B:1099:LEU:HD21	1:B:1129:LEU:HD21	1.70	0.74
1:A:229:TYR:CD2	1:A:241:VAL:HG11	2.25	0.72
1:B:1285:VAL:HA	2:B:351:NAP:H72N	1.56	0.71
1:A:213:ASP:HB2	1:A:216:ALA:HB3	1.71	0.71
1:B:1188:GLY:N	2:B:351:NAP:P2B	2.63	0.71
1:A:34:VAL:HA	1:A:88:GLU:HB3	1.72	0.70
1:B:1218:LEU:HD23	1:B:1226:ILE:HD11	1.74	0.70
1:B:1264:ASN:H	1:B:1264:ASN:HD22	1.40	0.67
1:A:282:GLN:HE22	1:B:1278:ARG:NH2	1.93	0.66
1:B:1056:ILE:HD11	1:B:1068:LEU:HG	1.78	0.66
1:A:329:LEU:HA	1:A:334:ASN:OD1	1.96	0.66
1:B:1187:ALA:O	1:B:1207:ASN:HA	1.96	0.66
1:A:207:ASN:ND2	1:A:209:LYS:H	1.96	0.64
1:B:1114:PRO:HA	1:B:1119:HIS:CD2	2.31	0.63
1:B:1134:GLY:HA3	1:B:1311:TYR:OH	1.99	0.63
1:A:188:GLY:N	2:A:350:NAP:O1X	2.31	0.63
1:A:160:TYR:HD2	1:A:229:TYR:CD1	2.17	0.62
1:A:49:SER:HB2	1:A:133:THR:HB	1.79	0.62
1:A:219:LYS:HD2	1:A:244:ASN:ND2	2.13	0.62
1:B:1117:HIS:HD2	1:B:1290:TYR:HB2	1.65	0.62
1:A:53:TYR:HD1	1:A:57:ARG:HG3	1.66	0.61
1:B:1144:TYR:OH	1:B:1295:LYS:HE3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:HB2	1:A:87:ILE:HD11	1.84	0.59
1:B:1187:ALA:HB1	2:B:351:NAP:O2X	2.02	0.59
1:B:1167:ALA:HB2	1:B:1337:LYS:HD2	1.85	0.59
1:B:1006:LYS:HG2	1:B:1007:GLN:N	2.16	0.59
1:A:9:ILE:HA	1:A:77:PRO:HA	1.86	0.58
1:A:46:LEU:HB2	1:A:47:TYR:HD2	1.69	0.57
1:A:7:GLN:HB3	1:A:107:GLU:HG2	1.86	0.57
1:B:1158:THR:HG23	1:B:1222:PHE:CD2	2.39	0.57
1:B:1329:LEU:HA	1:B:1334:ASN:HD22	1.70	0.57
1:A:270:ASN:H	1:A:270:ASN:HD22	1.52	0.57
1:B:1277:LYS:HE3	1:B:1279:ASN:HD21	1.69	0.57
1:B:1006:LYS:HG2	1:B:1007:GLN:H	1.69	0.57
1:B:1270:ASN:ND2	1:B:1270:ASN:H	2.02	0.57
1:A:153:PRO:HB2	1:A:179:MET:SD	2.44	0.57
1:B:1106:TRP:CH2	1:B:1326:LEU:HD23	2.40	0.57
1:A:250:ARG:N	1:A:250:ARG:HE	2.03	0.56
1:A:249:GLY:HA2	1:A:250:ARG:HH21	1.69	0.56
1:A:170:GLN:O	1:A:174:GLN:HG3	2.04	0.56
1:A:5:ASN:HD21	1:A:108:GLU:H	1.52	0.56
1:B:1329:LEU:HA	1:B:1334:ASN:ND2	2.20	0.56
1:A:103:ILE:O	1:A:119:HIS:HE1	1.89	0.56
1:B:1049:SER:HB2	1:B:1133:THR:HB	1.87	0.56
1:B:1052:PRO:HB2	2:B:351:NAP:H3D	1.89	0.55
1:A:250:ARG:HE	1:A:250:ARG:H	1.55	0.55
1:A:47:TYR:HB2	1:A:83:VAL:HG13	1.87	0.55
1:B:1146:GLY:O	1:B:1150:VAL:HB	2.06	0.55
1:A:138:MET:C	1:A:138:MET:SD	2.86	0.55
1:B:1160:TYR:HB2	1:B:1222:PHE:CZ	2.42	0.54
1:A:52:PRO:CB	2:A:350:NAP:H3D	2.37	0.54
1:B:1052:PRO:HB2	2:B:351:NAP:C3D	2.38	0.54
1:B:1273:ASN:HA	1:B:1276:TYR:CD1	2.43	0.54
1:B:1040:SER:O	1:B:1090:GLY:HA3	2.07	0.54
1:A:200:PHE:HB2	1:A:202:PHE:CE2	2.42	0.54
1:B:1161:VAL:HG23	1:B:1230:PHE:HB3	1.90	0.53
1:A:86:ILE:HG12	1:A:98:ASP:O	2.08	0.53
1:A:52:PRO:HB2	2:A:350:NAP:C3D	2.38	0.53
1:B:1050:CYS:HB3	1:B:1329:LEU:HD11	1.91	0.53
1:B:1174:GLN:HE22	1:B:1310:THR:H	1.56	0.53
1:B:1214:LEU:HD11	1:B:1237:MET:SD	2.48	0.53
1:B:1273:ASN:HA	1:B:1276:TYR:HD1	1.73	0.53
1:A:273:ASN:HD21	1:B:1064:SER:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1095:LYS:O	1:B:1098:ASP:HB2	2.09	0.53
1:B:1014:VAL:HG21	1:B:1058:MET:HE2	1.91	0.52
1:B:1133:THR:O	1:B:1337:LYS:HD3	2.10	0.52
1:A:187:ALA:HB3	1:A:193:VAL:HG22	1.90	0.52
1:A:297:LEU:O	1:A:301:LEU:HB2	2.10	0.52
1:B:1151:CYS:HB3	1:B:1228:ILE:HG23	1.91	0.52
1:B:1270:ASN:HD22	1:B:1270:ASN:H	1.56	0.52
1:B:1247:MET:HG2	1:B:1277:LYS:HB2	1.91	0.52
1:A:53:TYR:CD1	1:A:57:ARG:HG3	2.45	0.51
1:A:135:LEU:O	1:A:140:GLY:HA3	2.10	0.51
1:A:231:GLU:HG3	1:A:253:VAL:HG22	1.92	0.51
1:B:1033:ARG:HD3	1:B:1034:VAL:H	1.75	0.51
1:B:1100:LEU:HD21	1:B:1112:ILE:HD11	1.93	0.51
1:A:38:THR:HG23	1:A:39:ASN:H	1.75	0.50
1:B:1101:TRP:NE1	1:B:1120:PHE:HB2	2.26	0.50
1:B:1117:HIS:CD2	1:B:1290:TYR:HB2	2.44	0.50
1:A:219:LYS:HA	1:A:244:ASN:HD21	1.76	0.50
1:B:1264:ASN:ND2	1:B:1264:ASN:H	2.08	0.50
1:B:1174:GLN:HE22	1:B:1310:THR:N	2.09	0.50
1:A:4:THR:HA	1:A:29:THR:HA	1.93	0.50
1:A:83:VAL:HG12	1:A:133:THR:HG23	1.94	0.50
1:B:1091:HIS:CE1	1:B:1093:ASP:H	2.29	0.50
1:A:5:ASN:ND2	1:A:109:TYR:H	2.08	0.49
1:B:1014:VAL:HG21	1:B:1058:MET:CE	2.42	0.49
1:B:1138:MET:HG2	1:B:1290:TYR:OH	2.13	0.49
1:A:164:ALA:HA	1:A:169:GLY:HA3	1.95	0.49
1:B:1264:ASN:ND2	1:B:1264:ASN:N	2.61	0.49
1:A:114:PRO:HA	1:A:119:HIS:CD2	2.48	0.49
1:B:1023:PHE:HD2	1:B:1078:ILE:HD11	1.78	0.48
1:A:6:LYS:NZ	1:A:25:PHE:HB3	2.28	0.48
1:B:1264:ASN:HD22	1:B:1264:ASN:N	2.10	0.48
1:B:1329:LEU:HD23	1:B:1334:ASN:ND2	2.28	0.48
1:B:1158:THR:CG2	1:B:1226:ILE:HA	2.42	0.48
1:A:215:THR:HA	1:A:240:ALA:HB1	1.96	0.48
1:B:1163:ALA:HB3	1:B:1232:ASN:HB2	1.94	0.48
1:B:1131:TYR:HB3	1:B:1136:LEU:HD22	1.95	0.48
1:B:1103:ILE:H	1:B:1119:HIS:CE1	2.32	0.48
1:A:337:LYS:HZ3	1:A:337:LYS:HA	1.77	0.48
1:B:1154:LYS:NZ	1:B:1154:LYS:HA	2.29	0.48
1:B:1091:HIS:CD2	1:B:1094:TYR:HD1	2.32	0.47
1:A:162:SER:HB3	1:A:229:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:N	1:A:270:ASN:HD22	2.11	0.47
1:A:89:SER:H	1:A:96:LYS:HG2	1.78	0.47
1:A:42:LEU:HG	1:A:111:VAL:HG22	1.95	0.47
1:A:275:ILE:CG1	1:B:1253:VAL:HG12	2.45	0.47
1:A:200:PHE:HB2	1:A:202:PHE:HE2	1.78	0.47
1:A:233:VAL:HG23	1:A:258:SER:HB3	1.96	0.47
1:A:43:VAL:HG12	1:A:86:ILE:HA	1.96	0.47
1:B:1095:LYS:HA	3:B:2015:HOH:O	2.14	0.47
1:A:206:PHE:CD2	1:A:221:CYS:SG	3.02	0.47
1:A:141:MET:SD	1:A:293:TYR:HA	2.55	0.47
1:A:187:ALA:O	1:A:207:ASN:HA	2.14	0.47
2:B:351:NAP:H6N	2:B:351:NAP:H51N	1.97	0.46
1:A:6:LYS:CE	1:A:25:PHE:HB3	2.45	0.46
1:B:1048:LEU:HD22	1:B:1342:VAL:HG21	1.97	0.46
1:A:295:LYS:HE3	3:A:2045:HOH:O	2.15	0.46
1:B:1045:ASN:O	1:B:1342:VAL:HB	2.15	0.46
1:B:1189:SER:OG	1:B:1191:GLU:HG3	2.16	0.46
1:A:273:ASN:HD21	1:B:1064:SER:CB	2.28	0.46
1:A:219:LYS:HD2	1:A:244:ASN:CG	2.37	0.46
1:B:1094:TYR:CE2	1:B:1100:LEU:HD23	2.50	0.46
1:B:1158:THR:HG21	1:B:1226:ILE:HA	1.98	0.46
1:A:189:SER:O	1:A:193:VAL:HG23	2.16	0.45
1:A:144:TYR:HE1	1:A:299:PHE:CD2	2.33	0.45
1:A:5:ASN:HD21	1:A:109:TYR:H	1.63	0.45
1:B:1300:VAL:HG22	1:B:1304:ILE:HD11	1.97	0.45
1:B:1160:TYR:CE2	1:B:1218:LEU:HD21	2.52	0.45
1:A:302:PRO:O	1:A:306:GLU:HB2	2.16	0.45
1:A:47:TYR:HB2	1:A:83:VAL:CG1	2.46	0.45
1:A:44:LYS:HD3	1:A:109:TYR:HE2	1.82	0.45
1:A:270:ASN:H	1:A:270:ASN:ND2	2.14	0.45
1:B:1251:ILE:HG22	1:B:1253:VAL:HG23	1.98	0.45
1:A:260:TYR:HE1	2:A:350:NAP:HO2N	1.63	0.45
1:B:1117:HIS:HB3	1:B:1290:TYR:HD1	1.81	0.45
1:B:1229:TYR:CG	1:B:1241:VAL:HG11	2.51	0.45
1:A:259:GLN:HE22	1:A:266:GLU:HB2	1.82	0.45
1:A:32:LEU:HD13	1:A:87:ILE:HG21	1.99	0.45
1:A:44:LYS:NZ	1:A:343:ALA:HB1	2.32	0.44
1:B:1322:ALA:HB2	1:B:1340:VAL:HG11	1.98	0.44
1:A:271:LEU:HD12	1:B:1268:VAL:HG21	2.00	0.44
1:A:154:LYS:HE2	1:A:155:GLU:N	2.33	0.44
1:A:143:ALA:HB3	1:A:171:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:CYS:O	1:A:250:ARG:HD2	2.17	0.44
1:B:1035:PRO:HG2	1:B:1042:LEU:N	2.32	0.44
1:B:1023:PHE:CD2	1:B:1078:ILE:HD11	2.53	0.44
1:A:8:VAL:CG2	1:A:319:LEU:HB3	2.48	0.44
1:B:1292:LYS:HB3	1:B:1295:LYS:HE2	2.00	0.44
1:B:1081:TYR:HA	1:B:1102:GLY:O	2.17	0.44
1:A:292:LYS:HE3	3:A:2043:HOH:O	2.18	0.44
1:A:52:PRO:HG3	1:A:329:LEU:HD13	1.99	0.44
1:A:274:ILE:HG22	1:A:279:ASN:OD1	2.18	0.43
1:B:1273:ASN:HB3	1:B:1277:LYS:HE2	2.00	0.43
1:B:1034:VAL:HA	1:B:1035:PRO:HD3	1.75	0.43
1:B:1005:ASN:HB3	1:B:1030:VAL:HG23	2.00	0.43
1:B:1041:VAL:HG12	1:B:1089:SER:O	2.18	0.43
1:B:1161:VAL:HG11	1:B:1202:PHE:HE1	1.84	0.43
1:B:1142:THR:CG2	1:B:1254:CYS:SG	3.06	0.43
1:B:1189:SER:O	1:B:1193:VAL:HG12	2.18	0.43
1:A:253:VAL:HG12	1:B:1275:ILE:HG22	2.01	0.43
1:B:1187:ALA:HA	2:B:351:NAP:O3X	2.19	0.43
1:B:1009:ILE:O	1:B:1023:PHE:HA	2.19	0.43
1:A:11:LYS:HD3	1:A:24:ASP:HB2	2.00	0.43
1:A:334:ASN:O	1:A:334:ASN:ND2	2.52	0.43
1:A:42:LEU:HD23	1:A:43:VAL:N	2.34	0.42
1:B:1018:PRO:HB2	1:B:1327:VAL:HG22	2.00	0.42
2:B:351:NAP:H4B	2:B:351:NAP:O1A	2.18	0.42
1:B:1139:PRO:HB2	1:B:1167:ALA:HB1	2.01	0.42
1:B:1226:ILE:HG22	1:B:1228:ILE:O	2.20	0.42
1:B:1044:LYS:O	1:B:1046:LEU:HD13	2.20	0.42
1:B:1275:ILE:HG13	1:B:1276:TYR:N	2.34	0.41
1:B:1048:LEU:HD22	1:B:1342:VAL:CG2	2.50	0.41
1:A:18:PRO:HD3	1:A:55:ARG:HD3	2.01	0.41
1:A:197:LYS:HB3	1:A:197:LYS:HE3	1.73	0.41
1:B:1096:LYS:HD3	1:B:1096:LYS:H	1.84	0.41
1:A:112:ILE:HG13	1:A:112:ILE:O	2.20	0.41
1:B:1173:GLY:HA3	1:B:1202:PHE:CZ	2.55	0.41
1:B:1339:VAL:HG12	1:B:1340:VAL:N	2.36	0.41
1:A:303:HIS:HB3	1:A:308:LYS:HB3	2.02	0.41
1:B:1056:ILE:HD11	1:B:1068:LEU:CG	2.49	0.41
1:B:1297:LEU:O	1:B:1301:LEU:HB2	2.20	0.41
1:B:1245:MET:SD	1:B:1279:ASN:OD1	2.79	0.41
1:A:293:TYR:O	1:A:296:PHE:HB3	2.21	0.41
1:B:1025:PHE:CZ	1:B:1320:GLU:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1295:LYS:O	1:B:1298:GLU:HB3	2.21	0.41
1:A:141:MET:HG2	1:A:290:TYR:CD1	2.56	0.41
1:B:1049:SER:HB3	1:B:1081:TYR:O	2.21	0.40
1:A:166:GLY:O	1:A:170:GLN:HG2	2.20	0.40
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.93	0.40
1:A:1:MET:HB3	1:A:32:LEU:CD1	2.51	0.40
1:A:8:VAL:HB	1:A:106:TRP:HE3	1.86	0.40
1:B:1274:ILE:HG21	1:B:1274:ILE:HD13	1.86	0.40
1:B:1297:LEU:HD23	1:B:1297:LEU:HA	1.83	0.40
1:A:7:GLN:HG2	1:A:26:THR:O	2.22	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	332/345 (96%)	274 (82%)	51 (15%)	7 (2%)	9 29
1	B	341/345 (99%)	282 (83%)	42 (12%)	17 (5%)	3 8
All	All	673/690 (98%)	556 (83%)	93 (14%)	24 (4%)	4 14

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	PRO
1	A	96	LYS
1	A	270	ASN
1	B	1089	SER
1	B	1270	ASN
1	B	1278	ARG
1	A	134	GLY
1	B	1026	THR

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Mol	Chain	Res	Type
1	B	1071	ALA
1	B	1126	ASP
1	B	1167	ALA
1	B	1258	SER
1	B	1305	ARG
1	B	1098	ASP
1	A	196	LEU
1	A	322	ALA
1	B	1176	ALA
1	B	1323	PRO
1	A	90	GLY
1	B	1070	GLN
1	B	1092	PRO
1	B	1061	PRO
1	B	1286	VAL
1	B	1150	VAL

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	283/289 (98%)	247 (87%)	36 (13%)	5 16
1	B	289/289 (100%)	255 (88%)	34 (12%)	6 19
All	All	572/578 (99%)	502 (88%)	70 (12%)	6 18

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	29	THR
1	A	35	PRO
1	A	58	MET
1	A	70	GLN
1	A	72	TYR
1	A	83	VAL

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Mol	Chain	Res	Type
1	A	92	PRO
1	A	100	LEU
1	A	113	THR
1	A	130	SER
1	A	139	PRO
1	A	149	GLU
1	A	154	LYS
1	A	177	LYS
1	A	195	LEU
1	A	196	LEU
1	A	204	ASP
1	A	207	ASN
1	A	210	GLU
1	A	218	LEU
1	A	242	LEU
1	A	250	ARG
1	A	257	ILE
1	A	262	LEU
1	A	270	ASN
1	A	276	TYR
1	A	282	GLN
1	A	291	ASP
1	A	295	LYS
1	A	297	LEU
1	A	301	LEU
1	A	311	TYR
1	A	317	ASP
1	A	334	ASN
1	A	337	LYS
1	B	1001	MET
1	B	1026	THR
1	B	1040	SER
1	B	1046	LEU
1	B	1068	LEU
1	B	1091	HIS
1	B	1092	PRO
1	B	1096	LYS
1	B	1103	ILE
1	B	1126	ASP
1	B	1127	VAL
1	B	1136	LEU
1	B	1154	LYS

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Mol	Chain	Res	Type
1	B	1158	THR
1	B	1178	MET
1	B	1183	VAL
1	B	1191	GLU
1	B	1193	VAL
1	B	1196	LEU
1	B	1197	LYS
1	B	1214	LEU
1	B	1220	ARG
1	B	1245	MET
1	B	1258	SER
1	B	1261	ASN
1	B	1264	ASN
1	B	1282	GLN
1	B	1289	PHE
1	B	1291	ASP
1	B	1302	PRO
1	B	1323	PRO
1	B	1326	LEU
1	B	1337	LYS
1	B	1341	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	70	GLN
1	A	79	GLN
1	A	119	HIS
1	A	207	ASN
1	A	232	ASN
1	A	244	ASN
1	A	270	ASN
1	A	273	ASN
1	A	282	GLN
1	B	1117	HIS
1	B	1119	HIS
1	B	1124	HIS
1	B	1170	GLN
1	B	1174	GLN
1	B	1264	ASN
1	B	1270	ASN

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Mol	Chain	Res	Type
1	B	1279	ASN
1	B	1334	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)

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	NAP	A	350	-	42,52,52	1.34	6 (14%)	54,80,80	2.46	13 (24%)
2	NAP	B	351	1	42,52,52	1.19	3 (7%)	54,80,80	2.40	9 (16%)

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	350	-	-	0/27/67/67	0/5/5/5
2	NAP	B	351	1	-	0/27/67/67	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	351	NAP	C6N-N1N	2.02	1.40	1.35
2	A	350	NAP	C5D-C4D	2.17	1.58	1.51
2	B	351	NAP	C3N-C7N	2.28	1.54	1.50
2	A	350	NAP	C6N-N1N	2.35	1.41	1.35
2	A	350	NAP	C3N-C7N	2.62	1.54	1.50
2	A	350	NAP	O4B-C1B	2.88	1.44	1.41
2	A	350	NAP	PN-O5D	2.97	1.72	1.59
2	A	350	NAP	O4D-C1D	3.62	1.45	1.41
2	B	351	NAP	O4D-C1D	4.35	1.46	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	351	NAP	N3A-C2A-N1A	-9.08	121.94	128.89
2	A	350	NAP	N3A-C2A-N1A	-8.73	122.21	128.89
2	A	350	NAP	O4D-C4D-C3D	-4.65	95.77	105.15
2	B	351	NAP	O4D-C4D-C3D	-3.65	97.79	105.15
2	A	350	NAP	C3N-C7N-N7N	-2.23	115.37	117.82
2	A	350	NAP	C4B-O4B-C1B	-2.17	107.33	109.72
2	A	350	NAP	O2B-P2B-O1X	-2.14	101.77	107.11
2	B	351	NAP	C3N-C7N-N7N	-2.00	115.62	117.82
2	A	350	NAP	O5B-C5B-C4B	2.00	116.51	109.12
2	A	350	NAP	O7N-C7N-C3N	2.22	122.00	119.59
2	B	351	NAP	PN-O3-PA	2.85	140.72	132.73
2	A	350	NAP	O3-PA-O5B	3.19	111.40	102.94
2	A	350	NAP	C4A-C5A-N7A	3.56	112.75	109.48
2	B	351	NAP	C4A-C5A-N7A	3.56	112.76	109.48
2	A	350	NAP	O4D-C4D-C5D	3.71	122.58	109.32
2	B	351	NAP	O5D-C5D-C4D	3.77	123.00	109.12
2	B	351	NAP	O3-PN-O5D	4.87	115.86	102.94
2	A	350	NAP	O5D-C5D-C4D	6.19	131.93	109.12
2	A	350	NAP	O3-PN-O5D	6.59	120.43	102.94
2	B	351	NAP	P2B-O2B-C2B	7.31	139.09	121.56
2	B	351	NAP	O4D-C1D-N1N	7.56	116.44	108.13
2	A	350	NAP	O4D-C1D-N1N	7.98	116.89	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	NAP	5	0
2	B	351	NAP	11	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.