Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:21 PM GMT

PDB ID	:	1ADC
Title	:	CRYSTALLOGRAPHIC STUDIES OF ISOSTERIC NAD ANALOGUES BOUND TO ALCOHOL DEHYDROGENASE: SPECIFICITY AND SUBSTRATE BINDING IN TWO TERNARY COMPLEXES
Authors	:	Li, H.; Hallows, W.A.; Punzi, J.S.; Pankiewicz, K.W.; Watanabe, K.A.; Goldstein, B.M.
Deposited on	:	1993-12-13
Resolution	:	2.70 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:

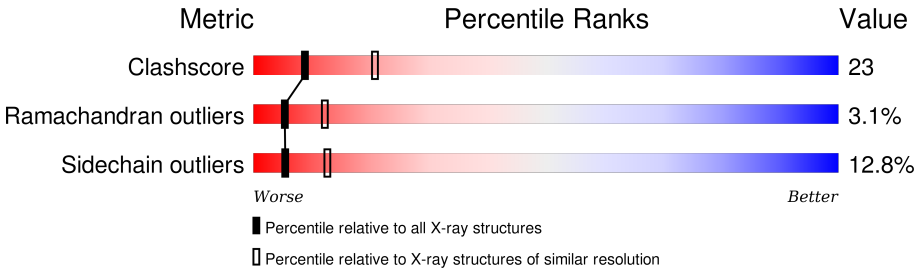
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	374	57% 36% 7%
1	B	374	50% 43% 7%

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
4	EOH	A	378	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7009 atoms, of which 1306 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.

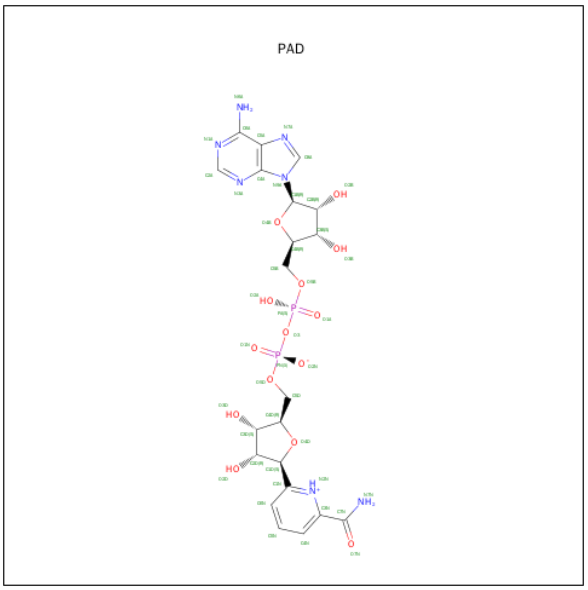
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	374	Total	C	H	N	O	S	0	0	0
			3391	1769	607	472	520	23			
1	B	374	Total	C	H	N	O	S	0	0	0
			3392	1769	607	472	521	23			

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

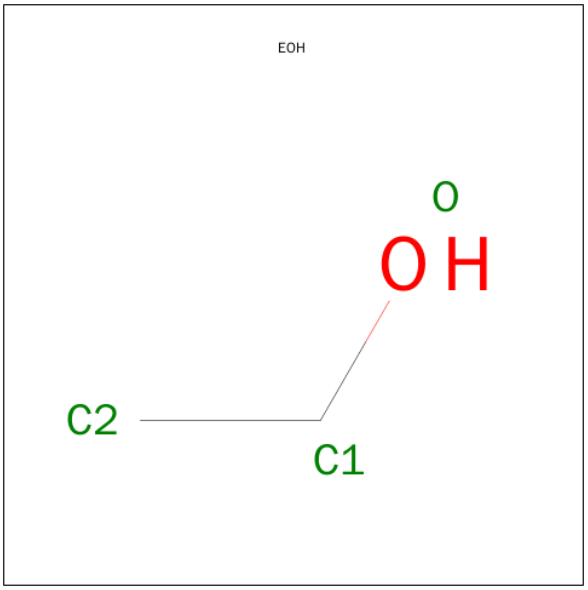
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 5-BETA-D-RIBOFURANOSYLPICOLINAMIDE ADENINE-DINUCLEOTIDE (three-letter code: PAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			52	21	8	7	14	2		
3	B	1	Total	C	H	N	O	P	0	0
			52	21	8	7	14	2		

- Molecule 4 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			5	2	2	1		
4	B	1	Total	C	H	O	0	0
			5	2	2	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	28	Total	H	O	0	0
			84	56	28		
5	B	8	Total	H	O	0	0
			24	16	8		

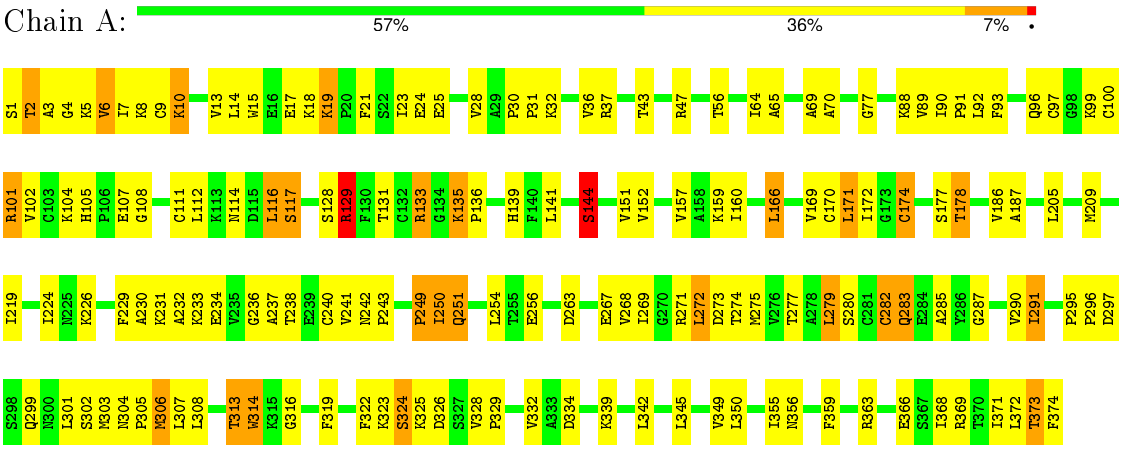
3 Residue-property plots (i)

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.

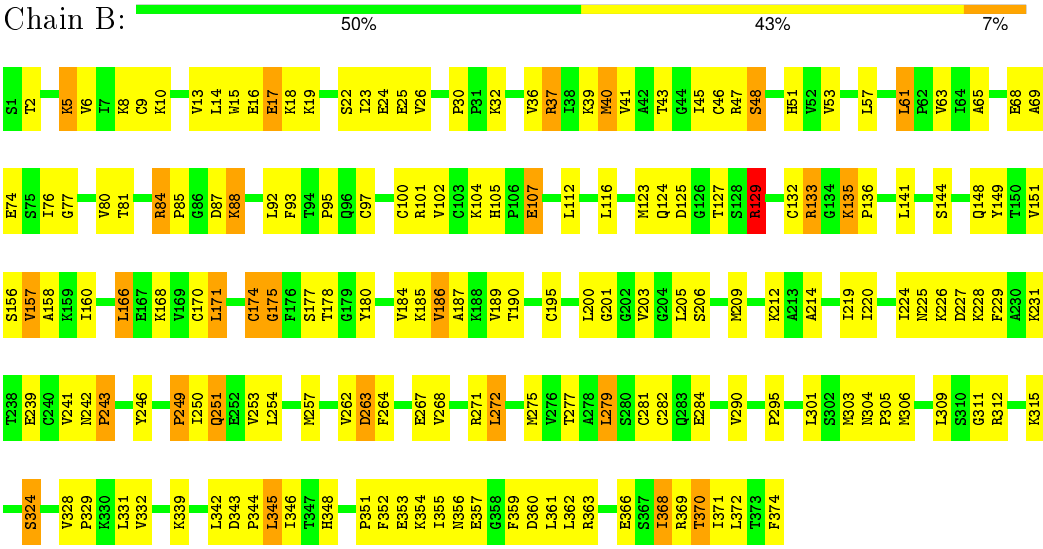
- Molecule 1: ALCOHOL DEHYDROGENASE

Chain A:



- Molecule 1: ALCOHOL DEHYDROGENASE

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 1	Depositor
Cell constants a, b, c, α, β, γ	51.90Å 44.80Å 93.00Å 103.10° 87.80° 70.40°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7009	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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: ZN, EOH, PAD

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	0.55	0/2836	0.79	1/3834 (0.0%)
1	B	0.54	0/2837	0.81	0/3834
All	All	0.54	0/5673	0.80	1/7668 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	ARG	N-CA-C	-6.04	94.70	111.00

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	2784	607	2850	120	0
1	B	2785	607	2848	155	0
2	A	2	0	0	1	0
2	B	2	0	0	0	0
3	A	44	8	26	3	0
3	B	44	8	26	3	0
4	A	3	2	6	2	0
4	B	3	2	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	56	0	4	0
5	B	8	16	0	0	0
All	All	5703	1306	5761	267	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 23.

All (267) 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:105:HIS:HD2	1:B:107:GLU:H	1.10	0.93
1:B:251:GLN:HG3	1:B:277:THR:HG23	1.50	0.92
1:B:47:ARG:HD3	3:B:377:PAD:O1A	1.71	0.90
1:B:187:ALA:HB2	1:B:290:VAL:HG21	1.56	0.86
1:B:224:ILE:HA	1:B:242:ASN:ND2	1.94	0.83
1:B:105:HIS:CD2	1:B:107:GLU:H	1.97	0.82
1:A:114:ASN:HD22	1:A:116:LEU:H	1.28	0.82
1:B:129:ARG:HG2	1:B:151:VAL:HG11	1.61	0.82
1:A:9:CYS:O	1:A:25:GLU:HA	1.79	0.81
1:A:272:LEU:HG	1:A:301:LEU:HB3	1.64	0.80
1:B:5:LYS:HE2	1:B:6:VAL:HG23	1.64	0.78
1:B:249:PRO:HB3	1:B:251:GLN:HE22	1.49	0.78
1:A:169:VAL:HG13	1:A:172:ILE:HD12	1.67	0.76
1:B:153:ASP:HB2	1:B:155:ILE:HG22	1.67	0.76
1:B:180:TYR:O	1:B:184:VAL:HG12	1.85	0.75
1:A:92:LEU:HD13	1:A:324:SER:HB3	1.67	0.74
1:A:70:ALA:HB1	1:A:166:LEU:HD22	1.67	0.74
1:B:129:ARG:HG2	1:B:151:VAL:CG1	2.18	0.73
1:A:43:THR:HG23	1:A:374:PHE:HE1	1.53	0.72
1:A:5:LYS:HD2	1:A:30:PRO:HG3	1.72	0.71
1:A:100:CYS:O	1:A:104:LYS:HG2	1.91	0.70
1:B:68:GLU:OE2	1:B:171:LEU:HD12	1.91	0.70
1:B:231:LYS:HE3	1:B:344:PRO:O	1.92	0.69
1:B:105:HIS:HD2	1:B:107:GLU:N	1.89	0.69
1:A:251:GLN:HG3	1:A:277:THR:HG23	1.74	0.69
1:A:187:ALA:HB2	1:A:290:VAL:HG21	1.75	0.69
1:B:178:THR:HG21	3:B:377:PAD:H4N	1.73	0.68
1:A:43:THR:HG22	1:A:69:ALA:HB2	1.73	0.68
1:A:64:ILE:O	1:A:144:SER:HB3	1.92	0.68
1:B:160:ILE:HG13	1:B:332:VAL:HG21	1.76	0.68
1:A:5:LYS:NZ	1:A:6:VAL:HG23	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:PRO:HD2	1:B:354:LYS:HD2	1.76	0.67
1:A:93:PHE:CE2	4:A:378:EOH:H22	2.30	0.66
1:B:97:CYS:HB3	1:B:155:ILE:HD11	1.78	0.66
1:B:5:LYS:HA	1:B:30:PRO:HG3	1.77	0.65
1:A:111:CYS:HG	2:A:376:ZN:ZN	1.08	0.65
1:B:93:PHE:HB2	1:B:141:LEU:HD23	1.79	0.64
1:B:203:VAL:HG22	3:B:377:PAD:O2N	1.96	0.64
1:A:313:THR:HB	1:B:315:LYS:HG2	1.79	0.64
1:B:263:ASP:HB3	1:B:264:PHE:CD1	2.33	0.64
1:B:359:PHE:O	1:B:363:ARG:HG3	1.97	0.64
1:A:313:THR:HG21	5:A:401:HOH:O	1.98	0.64
1:A:89:VAL:HG12	1:A:159:LYS:HA	1.82	0.62
1:A:282:CYS:SG	1:A:287:GLY:HA3	2.40	0.62
1:B:36:VAL:O	1:B:151:VAL:HA	1.98	0.62
1:B:250:ILE:HG13	1:B:254:LEU:HD12	1.82	0.61
1:A:178:THR:HG21	3:A:377:PAD:H4N	1.82	0.61
1:A:174:CYS:O	1:A:178:THR:HG23	2.00	0.61
1:B:195:CYS:HA	1:B:264:PHE:O	1.99	0.61
1:B:5:LYS:CA	1:B:30:PRO:HG3	2.31	0.61
1:B:324:SER:O	1:B:328:VAL:HG22	2.00	0.61
1:B:203:VAL:HG23	1:B:268:VAL:CG2	2.31	0.60
1:B:346:ILE:HG12	1:B:371:ILE:HD11	1.83	0.60
1:A:373:THR:HG21	5:A:403:HOH:O	2.02	0.60
1:A:231:LYS:O	1:A:234:GLU:HB3	2.02	0.60
1:B:133:ARG:HD2	1:B:133:ARG:N	2.17	0.60
1:A:43:THR:HG22	1:A:69:ALA:CB	2.32	0.59
1:B:102:VAL:HG23	1:B:112:LEU:HD12	1.84	0.59
1:A:233:LYS:HA	1:A:237:ALA:HB3	1.85	0.59
1:B:10:LYS:HA	1:B:24:GLU:O	2.03	0.59
1:A:5:LYS:HA	1:A:30:PRO:HG3	1.85	0.59
1:B:241:VAL:HG13	1:B:246:TYR:CE2	2.37	0.59
1:B:69:ALA:HA	1:B:170:CYS:HB2	1.86	0.58
1:B:328:VAL:HG23	1:B:329:PRO:HD3	1.84	0.58
1:A:283:GLN:HE22	1:A:285:ALA:HB3	1.69	0.58
1:B:225:ASN:HD21	1:B:227:ASP:HB2	1.68	0.58
1:A:250:ILE:HD12	1:A:254:LEU:CD2	2.34	0.58
1:B:132:CYS:O	1:B:133:ARG:HB2	2.04	0.57
1:A:269:ILE:HG22	1:A:271:ARG:HG3	1.85	0.57
1:A:295:PRO:HD2	1:B:309:LEU:CD1	2.34	0.57
1:B:267:GLU:HG3	1:B:275:MET:HA	1.85	0.57
1:B:61:LEU:HD12	1:B:63:VAL:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:HIS:CE1	1:A:107:GLU:HB3	2.38	0.57
1:B:282:CYS:O	1:B:312:ARG:NH1	2.38	0.57
1:A:295:PRO:HD2	1:B:309:LEU:HD11	1.86	0.57
1:B:348:HIS:HB2	1:B:370:THR:HB	1.87	0.57
1:A:28:VAL:O	1:A:37:ARG:NH2	2.37	0.57
1:B:174:CYS:O	1:B:178:THR:HG23	2.05	0.57
1:A:4:GLY:O	1:A:5:LYS:HG2	2.05	0.57
1:B:16:GLU:HB2	1:B:19:LYS:HG3	1.87	0.56
1:A:209:MET:HE3	1:A:345:LEU:HD21	1.86	0.56
1:B:88:LYS:HG2	1:B:166:LEU:HD11	1.88	0.56
1:B:5:LYS:HA	1:B:30:PRO:CG	2.35	0.56
1:B:45:ILE:HD13	1:B:359:PHE:CD1	2.40	0.56
1:B:76:ILE:HD13	1:B:85:PRO:HG3	1.86	0.56
1:A:301:LEU:O	1:A:301:LEU:HD12	2.05	0.56
1:B:152:VAL:HG21	1:B:157:VAL:HG23	1.88	0.56
1:A:170:CYS:SG	1:A:371:ILE:CD1	2.94	0.56
1:B:225:ASN:HD22	1:B:228:LYS:HG2	1.70	0.56
1:A:229:PHE:HB3	1:A:233:LYS:NZ	2.21	0.55
1:B:359:PHE:HB3	1:B:363:ARG:HH21	1.72	0.55
1:B:241:VAL:HG13	1:B:246:TYR:HE2	1.71	0.55
5:A:401:HOH:O	1:B:315:LYS:HE2	2.07	0.55
1:B:17:GLU:H	1:B:17:GLU:CD	2.10	0.55
1:A:187:ALA:HB2	1:A:290:VAL:CG2	2.36	0.55
1:A:100:CYS:HB2	1:A:112:LEU:HD23	1.89	0.54
1:B:343:ASP:HB2	1:B:344:PRO:HD3	1.90	0.54
1:A:328:VAL:HB	1:A:329:PRO:HD3	1.89	0.53
1:B:187:ALA:HB2	1:B:290:VAL:CG2	2.31	0.53
1:B:206:SER:O	1:B:209:MET:HB2	2.09	0.53
1:A:178:THR:HG22	1:A:319:PHE:HA	1.89	0.53
1:A:229:PHE:HB3	1:A:233:LYS:HZ2	1.73	0.53
1:A:31:PRO:HD3	1:A:37:ARG:HB2	1.90	0.53
1:B:102:VAL:HG23	1:B:112:LEU:CD1	2.38	0.53
1:A:308:LEU:O	1:B:316:GLY:HA3	2.09	0.53
1:B:97:CYS:HA	1:B:155:ILE:HG13	1.92	0.52
1:B:219:ILE:HB	1:B:237:ALA:HA	1.91	0.52
1:B:328:VAL:HG23	1:B:329:PRO:CD	2.39	0.52
1:A:108:GLY:O	1:A:323:LYS:NZ	2.42	0.52
1:A:97:CYS:SG	1:A:111:CYS:SG	3.07	0.52
1:A:250:ILE:HD12	1:A:254:LEU:HD21	1.92	0.52
1:B:73:VAL:HG11	1:B:76:ILE:HD11	1.91	0.52
1:A:229:PHE:O	1:A:233:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLY:O	1:B:205:LEU:HG	2.10	0.52
1:B:253:VAL:O	1:B:257:MET:HG3	2.09	0.52
1:B:32:LYS:O	1:B:77:GLY:HA3	2.10	0.52
1:B:220:ILE:HG21	1:B:254:LEU:HD21	1.93	0.51
1:B:73:VAL:HG11	1:B:76:ILE:CD1	2.40	0.51
1:A:279:LEU:HD13	1:A:307:LEU:HD23	1.92	0.51
1:B:8:LYS:HA	1:B:26:VAL:O	2.10	0.51
1:A:229:PHE:CD1	1:A:240:CYS:HB3	2.46	0.51
1:A:23:ILE:HD11	1:A:355:ILE:HG22	1.93	0.51
1:B:345:LEU:O	1:B:369:ARG:HB2	2.11	0.51
1:A:90:ILE:HD12	1:A:328:VAL:CG1	2.41	0.51
1:A:209:MET:CE	1:A:345:LEU:HD21	2.40	0.51
1:B:43:THR:OG1	1:B:374:PHE:HE2	1.94	0.51
1:B:5:LYS:C	1:B:30:PRO:HG3	2.32	0.50
1:A:32:LYS:O	1:A:77:GLY:HA3	2.11	0.50
1:B:368:ILE:HG22	1:B:369:ARG:N	2.27	0.50
1:B:17:GLU:HB3	1:B:53:VAL:O	2.12	0.50
1:A:328:VAL:O	1:A:332:VAL:HG23	2.11	0.50
1:B:158:ALA:O	1:B:160:ILE:HD13	2.11	0.50
1:B:51:HIS:HB3	1:B:57:LEU:HB2	1.94	0.50
1:A:114:ASN:ND2	1:A:116:LEU:H	2.04	0.50
1:B:5:LYS:HE2	1:B:6:VAL:H	1.77	0.50
1:A:305:PRO:HG2	1:B:295:PRO:HG3	1.94	0.49
1:B:73:VAL:HB	1:B:85:PRO:HA	1.92	0.49
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.12	0.49
1:B:279:LEU:CD2	1:B:312:ARG:HD2	2.42	0.49
1:A:21:PHE:H	1:A:356:ASN:HD21	1.58	0.49
1:A:30:PRO:HA	1:A:37:ARG:NH1	2.28	0.49
1:A:283:GLN:HG3	1:B:101:ARG:NH2	2.28	0.49
1:A:171:LEU:HD11	1:A:369:ARG:HG3	1.94	0.49
1:B:206:SER:HA	1:B:209:MET:HG3	1.94	0.48
1:B:100:CYS:O	1:B:104:LYS:HG2	2.13	0.48
1:B:22:SER:O	1:B:24:GLU:HG3	2.14	0.48
1:B:73:VAL:HG23	1:B:87:ASP:O	2.11	0.48
1:B:18:LYS:NZ	1:B:18:LYS:HB3	2.28	0.48
1:B:272:LEU:O	1:B:275:MET:HB2	2.12	0.48
1:A:230:ALA:O	1:A:234:GLU:HB2	2.14	0.48
1:B:361:LEU:HD13	1:B:366:GLU:HG3	1.96	0.48
1:B:268:VAL:O	1:B:268:VAL:HG22	2.14	0.48
1:B:14:LEU:HD12	1:B:61:LEU:HD11	1.96	0.48
1:B:39:LYS:HG3	1:B:149:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ILE:HG23	1:B:356:ASN:H	1.79	0.48
1:A:8:LYS:NZ	1:A:25:GLU:HG2	2.29	0.48
1:A:96:GLN:HG2	1:A:96:GLN:O	2.14	0.47
1:B:224:ILE:HA	1:B:242:ASN:HD21	1.74	0.47
1:B:46:CYS:SG	1:B:48:SER:OG	2.68	0.47
1:B:279:LEU:HD22	1:B:312:ARG:HD2	1.95	0.47
1:B:41:VAL:HG23	1:B:71:GLY:HA2	1.96	0.47
1:B:205:LEU:O	1:B:209:MET:HG3	2.15	0.47
1:A:350:LEU:HD12	1:A:350:LEU:N	2.30	0.47
1:B:37:ARG:HB3	1:B:74:GLU:OE1	2.15	0.47
1:B:153:ASP:CB	1:B:155:ILE:HG22	2.38	0.47
1:B:61:LEU:CD1	1:B:63:VAL:HG12	2.45	0.47
1:A:269:ILE:CG2	1:A:271:ARG:HG3	2.45	0.47
1:B:5:LYS:O	1:B:37:ARG:NH2	2.48	0.47
1:B:250:ILE:HG13	1:B:254:LEU:CD1	2.45	0.47
1:A:6:VAL:N	1:A:30:PRO:HD3	2.30	0.46
1:A:250:ILE:HG23	1:A:254:LEU:CD2	2.45	0.46
1:A:275:MET:SD	1:A:291:ILE:HD12	2.55	0.46
1:B:37:ARG:CG	1:B:37:ARG:HH11	2.27	0.46
1:B:5:LYS:HG3	1:B:6:VAL:H	1.81	0.46
1:B:284:GLU:HA	1:B:312:ARG:NH1	2.31	0.46
1:A:334:ASP:O	1:A:339:LYS:HB2	2.15	0.46
1:A:10:LYS:HA	1:A:24:GLU:O	2.16	0.46
1:A:88:LYS:HB3	1:A:166:LEU:HD21	1.98	0.46
1:A:250:ILE:HG23	1:A:254:LEU:HD23	1.98	0.46
1:A:302:SER:HA	1:B:301:LEU:O	2.16	0.46
1:A:345:LEU:O	1:A:369:ARG:HB2	2.16	0.46
1:B:178:THR:HG22	1:B:319:PHE:HA	1.98	0.46
1:A:135:LYS:HA	1:A:136:PRO:HD3	1.79	0.45
1:A:13:VAL:HG11	1:A:15:TRP:CE2	2.51	0.45
1:A:47:ARG:HB3	3:A:377:PAD:H3D	1.98	0.45
1:A:56:THR:HG23	1:A:296:PRO:HA	1.97	0.45
1:B:186:VAL:CG2	1:B:187:ALA:N	2.79	0.45
1:B:301:LEU:C	1:B:301:LEU:HD12	2.36	0.45
1:A:18:LYS:O	1:A:19:LYS:HD2	2.17	0.45
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.78	0.45
1:B:189:VAL:O	1:B:214:ALA:HB1	2.17	0.45
1:B:92:LEU:HD21	1:B:328:VAL:HG21	1.99	0.45
1:A:114:ASN:HD21	1:A:117:SER:H	1.64	0.44
1:B:355:ILE:HG23	1:B:356:ASN:N	2.31	0.44
1:B:155:ILE:HG23	1:B:156:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:GLU:O	1:B:361:LEU:HD23	2.18	0.44
1:A:101:ARG:HD2	1:A:101:ARG:HA	1.75	0.44
1:A:256:GLU:HG3	5:A:395:HOH:O	2.18	0.44
1:B:92:LEU:HD13	1:B:324:SER:HB2	1.99	0.44
1:B:37:ARG:NH1	1:B:74:GLU:OE1	2.50	0.44
1:B:135:LYS:HA	1:B:136:PRO:HD3	1.71	0.44
1:B:37:ARG:HG2	1:B:74:GLU:OE1	2.18	0.44
1:A:177:SER:O	1:A:322:PHE:HE2	2.01	0.44
1:B:10:LYS:HB2	1:B:148:GLN:OE1	2.18	0.44
1:B:76:ILE:HG23	1:B:80:VAL:HB	1.99	0.44
1:B:242:ASN:HD22	1:B:243:PRO:HD2	1.83	0.44
1:A:169:VAL:HG12	1:A:169:VAL:O	2.18	0.44
1:B:37:ARG:CB	1:B:37:ARG:HH11	2.31	0.44
1:A:92:LEU:HD21	1:A:328:VAL:HG21	2.00	0.43
1:A:43:THR:HG23	1:A:374:PHE:CE1	2.42	0.43
1:B:45:ILE:HD11	1:B:372:LEU:HD11	1.99	0.43
1:A:349:VAL:HA	1:A:371:ILE:O	2.18	0.43
1:A:2:THR:O	1:A:3:ALA:HB2	2.18	0.43
1:A:93:PHE:CD2	4:A:378:EOH:H22	2.53	0.43
1:A:219:ILE:HD12	1:A:236:GLY:O	2.19	0.43
1:A:5:LYS:HZ3	1:A:6:VAL:HG23	1.84	0.43
1:A:316:GLY:O	1:B:311:GLY:HA2	2.19	0.43
1:A:160:ILE:HD11	1:A:166:LEU:CD2	2.48	0.43
1:A:5:LYS:HA	1:A:5:LYS:HD2	1.88	0.43
1:A:350:LEU:O	1:A:372:LEU:HA	2.19	0.43
1:B:177:SER:OG	1:B:331:LEU:HD13	2.19	0.43
1:B:368:ILE:HG22	1:B:369:ARG:H	1.84	0.43
1:A:359:PHE:O	1:A:363:ARG:HG3	2.19	0.43
1:B:249:PRO:HB3	1:B:251:GLN:NE2	2.25	0.43
1:B:212:LYS:HG2	1:B:212:LYS:O	2.19	0.43
1:B:304:ASN:HA	1:B:305:PRO:HD2	1.91	0.43
1:B:262:VAL:HG12	1:B:264:PHE:N	2.34	0.42
1:A:139:HIS:CD2	1:A:139:HIS:N	2.87	0.42
1:A:90:ILE:HG22	1:A:91:PRO:O	2.19	0.42
1:A:267:GLU:HG3	1:A:275:MET:HA	2.01	0.42
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.80	0.42
1:B:229:PHE:O	1:B:232:ALA:HB3	2.20	0.42
1:B:186:VAL:HG11	1:B:317:ALA:CB	2.50	0.42
1:B:13:VAL:HG11	1:B:15:TRP:CE2	2.54	0.42
1:B:175:GLY:HA2	1:B:203:VAL:HG12	2.02	0.42
1:A:366:GLU:HA	1:A:366:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LYS:HD3	1:B:231:LYS:HA	1.88	0.41
1:B:116:LEU:O	1:B:116:LEU:HD12	2.20	0.41
1:A:36:VAL:O	1:A:151:VAL:HA	2.19	0.41
1:A:93:PHE:HB2	1:A:141:LEU:HD13	2.02	0.41
1:B:262:VAL:HG12	1:B:263:ASP:N	2.35	0.41
1:A:129:ARG:HB2	1:A:139:HIS:CE1	2.56	0.41
1:A:304:ASN:OD1	1:A:306:MET:HB2	2.19	0.41
1:A:268:VAL:HG12	3:A:377:PAD:H51N	2.01	0.41
1:A:128:SER:O	1:A:129:ARG:NE	2.49	0.41
1:B:351:PRO:O	1:B:352:PHE:C	2.59	0.41
1:B:9:CYS:O	1:B:25:GLU:HA	2.21	0.41
1:A:8:LYS:HZ1	1:A:25:GLU:HG2	1.86	0.41
1:B:40:MET:CE	1:B:40:MET:HA	2.51	0.41
1:A:224:ILE:HA	1:A:242:ASN:ND2	2.35	0.41
1:A:102:VAL:HG23	1:A:112:LEU:CD2	2.51	0.41
1:A:205:LEU:HD22	1:A:232:ALA:HA	2.03	0.41
1:B:81:THR:HA	1:B:84:ARG:NH2	2.35	0.41
1:B:88:LYS:HG2	1:B:166:LEU:HD21	2.03	0.41
1:A:279:LEU:HG	1:A:314:TRP:CE2	2.56	0.41
1:B:175:GLY:O	1:B:203:VAL:HG12	2.22	0.40
1:A:349:VAL:O	1:A:349:VAL:HG12	2.21	0.40
1:B:186:VAL:CG2	1:B:290:VAL:HG11	2.50	0.40
1:A:92:LEU:CD2	1:A:328:VAL:HG21	2.52	0.40
1:B:76:ILE:HD13	1:B:85:PRO:CG	2.50	0.40
1:A:152:VAL:HG21	1:A:157:VAL:HB	2.03	0.40
1:A:157:VAL:O	1:A:325:LYS:HE3	2.20	0.40
1:B:93:PHE:CB	1:B:141:LEU:HD23	2.49	0.40
1:B:123:MET:HB2	1:B:127:THR:O	2.21	0.40
1:B:224:ILE:HA	1:B:242:ASN:HD22	1.80	0.40
1:A:7:ILE:HG13	1:A:37:ARG:NH2	2.36	0.40
1:B:369:ARG:HA	1:B:369:ARG:HD3	1.93	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	372/374 (100%)	325 (87%)	35 (9%)	12 (3%)	5 12
1	B	372/374 (100%)	321 (86%)	40 (11%)	11 (3%)	5 13
All	All	744/748 (100%)	646 (87%)	75 (10%)	23 (3%)	5 12

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	THR
1	A	2	THR
1	A	166	LEU
1	A	174	CYS
1	A	297	ASP
1	A	324	SER
1	B	174	CYS
1	A	144	SER
1	B	65	ALA
1	B	166	LEU
1	A	65	ALA
1	A	368	ILE
1	B	368	ILE
1	B	129	ARG
1	B	144	SER
1	A	129	ARG
1	B	175	GLY
1	B	324	SER
1	A	186	VAL
1	A	6	VAL
1	B	95	PRO
1	A	249	PRO
1	B	236	GLY

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	308/308 (100%)	269 (87%)	39 (13%)	5 13
1	B	308/308 (100%)	268 (87%)	40 (13%)	5 12
All	All	616/616 (100%)	537 (87%)	79 (13%)	5 12

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	10	LYS
1	A	14	LEU
1	A	17	GLU
1	A	19	LYS
1	A	99	LYS
1	A	101	ARG
1	A	116	LEU
1	A	117	SER
1	A	129	ARG
1	A	131	THR
1	A	133	ARG
1	A	135	LYS
1	A	144	SER
1	A	171	LEU
1	A	178	THR
1	A	226	LYS
1	A	238	THR
1	A	241	VAL
1	A	243	PRO
1	A	249	PRO
1	A	250	ILE
1	A	251	GLN
1	A	263	ASP
1	A	272	LEU
1	A	273	ASP
1	A	279	LEU
1	A	280	SER
1	A	282	CYS
1	A	283	GLN
1	A	291	ILE
1	A	299	GLN
1	A	303	MET
1	A	306	MET
1	A	313	THR

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Mol	Chain	Res	Type
1	A	314	TRP
1	A	326	ASP
1	A	342	LEU
1	A	373	THR
1	B	5	LYS
1	B	17	GLU
1	B	23	ILE
1	B	37	ARG
1	B	40	MET
1	B	48	SER
1	B	61	LEU
1	B	84	ARG
1	B	88	LYS
1	B	107	GLU
1	B	124	GLN
1	B	125	ASP
1	B	129	ARG
1	B	133	ARG
1	B	135	LYS
1	B	157	VAL
1	B	168	LYS
1	B	171	LEU
1	B	185	LYS
1	B	186	VAL
1	B	190	THR
1	B	226	LYS
1	B	239	GLU
1	B	243	PRO
1	B	249	PRO
1	B	251	GLN
1	B	263	ASP
1	B	271	ARG
1	B	272	LEU
1	B	279	LEU
1	B	281	CYS
1	B	303	MET
1	B	306	MET
1	B	339	LYS
1	B	342	LEU
1	B	345	LEU
1	B	353	GLU
1	B	360	ASP

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Mol	Chain	Res	Type
1	B	362	LEU
1	B	370	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	259	ASN
1	A	283	GLN
1	A	300	ASN
1	A	356	ASN
1	B	105	HIS
1	B	138	HIS
1	B	225	ASN
1	B	242	ASN
1	B	251	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	PAD	A	377	-	41,48,48	1.40	4 (9%)	49,73,73	2.14	14 (28%)
4	EOH	A	378	2	2,2,2	0.80	0	1,1,1	0.27	0
3	PAD	B	377	-	41,48,48	1.69	7 (17%)	49,73,73	2.21	13 (26%)
4	EOH	B	378	2	2,2,2	1.01	0	1,1,1	0.12	0

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	PAD	A	377	-	-	0/26/62/62	0/5/5/5
4	EOH	A	378	2	-	0/0/0/0	0/0/0/0
3	PAD	B	377	-	-	0/26/62/62	0/5/5/5
4	EOH	B	378	2	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	377	PAD	C1N-C1D	-5.72	1.46	1.51
3	B	377	PAD	C1N-C1D	-4.18	1.48	1.51
3	B	377	PAD	C2D-C1D	-3.09	1.51	1.53
3	B	377	PAD	C3D-C4D	-2.60	1.46	1.53
3	B	377	PAD	C5A-C4A	-2.10	1.35	1.40
3	A	377	PAD	C5A-N7A	-2.02	1.32	1.39
3	A	377	PAD	C3N-N2N	2.95	1.38	1.34
3	A	377	PAD	C1N-N2N	3.09	1.38	1.34
3	B	377	PAD	C3N-C7N	3.31	1.56	1.51
3	B	377	PAD	C1N-N2N	4.60	1.40	1.34
3	B	377	PAD	C3N-N2N	5.71	1.43	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	377	PAD	N3A-C2A-N1A	-7.31	123.30	128.89
3	A	377	PAD	N3A-C2A-N1A	-6.81	123.68	128.89
3	B	377	PAD	C6N-C1N-N2N	-5.16	117.08	122.50
3	A	377	PAD	C3N-C7N-N7N	-4.81	111.49	116.21
3	B	377	PAD	O4D-C1D-C2D	-4.42	100.21	104.73
3	B	377	PAD	C4N-C3N-N2N	-3.98	118.15	122.90
3	A	377	PAD	PN-O3-PA	-3.28	123.51	132.73
3	A	377	PAD	C4B-O4B-C1B	-3.18	106.22	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	377	PAD	O5D-PN-O1N	-3.07	97.72	109.62
3	A	377	PAD	C6N-C1N-N2N	-2.27	120.11	122.50
3	A	377	PAD	C1B-N9A-C4A	-2.11	123.75	126.94
3	A	377	PAD	O3D-C3D-C4D	-2.01	105.01	111.05
3	A	377	PAD	C2B-C1B-N9A	2.03	117.39	114.29
3	B	377	PAD	O2A-PA-O1A	2.05	123.64	112.53
3	A	377	PAD	O2N-PN-O3	2.11	114.69	105.09
3	A	377	PAD	O5B-C5B-C4B	2.27	117.49	109.12
3	B	377	PAD	C3D-C2D-C1D	2.40	104.58	101.79
3	B	377	PAD	O2N-PN-O3	2.46	116.27	105.09
3	B	377	PAD	O5D-C5D-C4D	2.74	119.21	109.12
3	B	377	PAD	N6A-C6A-N1A	3.08	125.81	119.20
3	B	377	PAD	O4D-C4D-C5D	3.16	120.62	109.32
3	B	377	PAD	C3N-N2N-C1N	3.28	121.90	118.72
3	A	377	PAD	O7N-C7N-C3N	4.05	123.41	119.67
3	B	377	PAD	C4A-C5A-N7A	4.19	113.33	109.48
3	B	377	PAD	C4D-O4D-C1D	4.36	114.03	109.58
3	A	377	PAD	C4A-C5A-N7A	4.48	113.60	109.48
3	A	377	PAD	C4N-C3N-C7N	4.78	123.20	119.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	377	PAD	3	0
4	A	378	EOH	2	0
3	B	377	PAD	3	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.