



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:17 AM UTC

PDB ID : 1BXK / pdb_00001bxk
Title : DTDG-GLUCOSE 4,6-DEHYDRATASE FROM E. COLI
Authors : Thoden, J.B.; Hegeman, A.D.; Frey, P.A.; Holden, H.M.
Deposited on : 1998-10-05
Resolution : 1.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

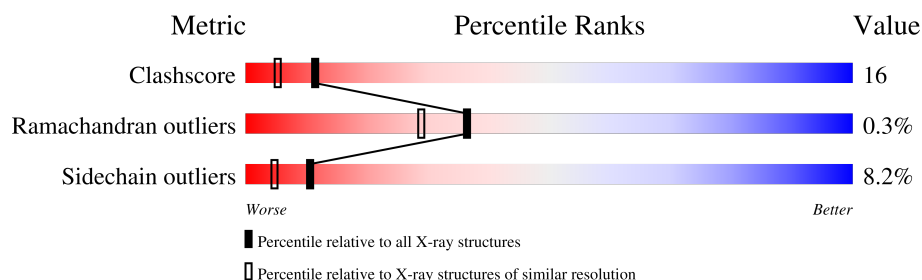
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	355	 62% 27% 6% . .
1	B	355	 64% 28% 5% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5856 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 PROTEIN (DTDP-GLUCOSE 4,6-DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	2	0
			2699	1713	459	516	11			
1	B	344	Total	C	N	O	S	0	0	0
			2710	1722	462	515	11			

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



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		

- Molecule 3 is water.

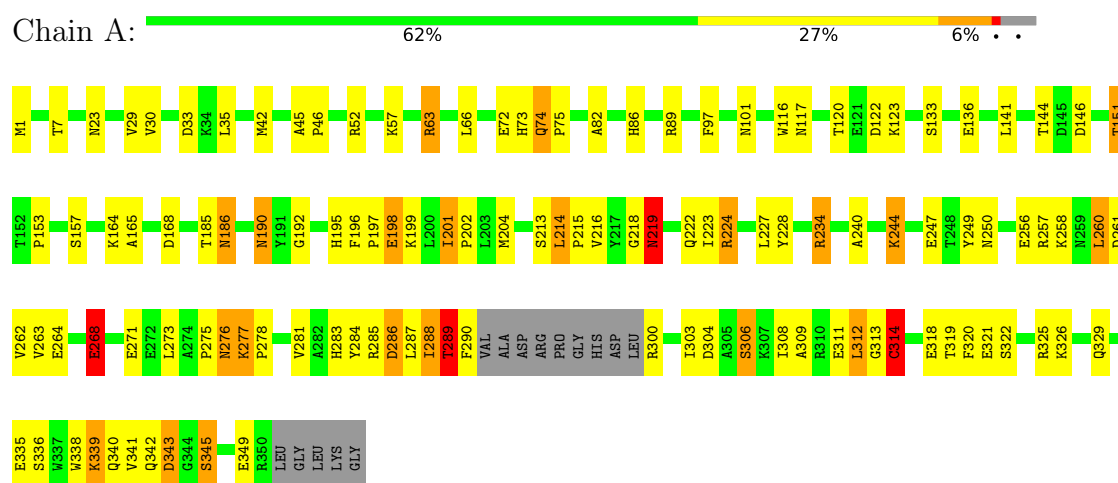
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	196	Total 196	O 196	0	0
3	B	163	Total 163	O 163	0	0

3 Residue-property plots

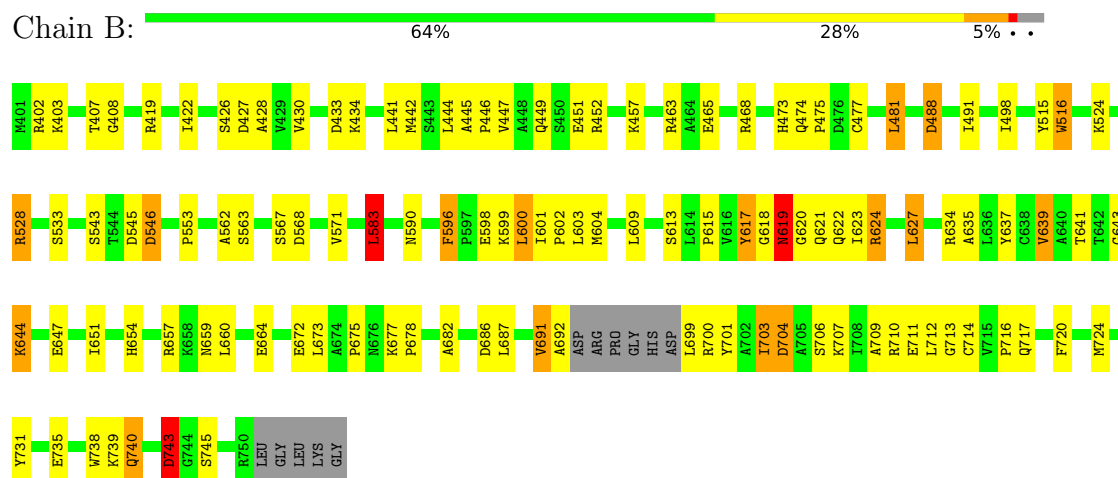
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: PROTEIN (DTDP-GLUCOSE 4,6-DEHYDRATASE)



• Molecule 1: PROTEIN (DTDP-GLUCOSE 4,6-DEHYDRATASE)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.40 Å 109.20 Å 128.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	96.3 (30.00-1.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5856	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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:
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	1.15	1/2773 (0.0%)	1.64	33/3771 (0.9%)
1	B	1.84	7/2776 (0.3%)	1.63	24/3777 (0.6%)
All	All	1.53	8/5549 (0.1%)	1.63	57/7548 (0.8%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	691	VAL	CB-CG2	65.57	3.69	1.52
1	B	691	VAL	CB-CG1	38.25	2.78	1.52
1	B	457	LYS	CE-NZ	-9.98	1.19	1.49
1	B	451	GLU	CD-OE1	6.02	1.36	1.25
1	B	488	ASP	CG-OD2	5.64	1.36	1.25
1	B	672	GLU	CD-OE1	5.11	1.35	1.25
1	A	268	GLU	CD-OE2	5.11	1.35	1.25
1	B	546	ASP	CG-OD1	5.01	1.34	1.25

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	691	VAL	CA-CB-CG1	9.73	126.94	110.40
1	A	343	ASP	CB-CA-C	-9.64	95.75	110.88
1	B	528	ARG	CD-NE-CZ	-9.53	111.06	124.40
1	A	30	VAL	N-CA-CB	8.81	123.37	112.10
1	A	186	ASN	N-CA-CB	8.34	125.34	110.83
1	A	117	ASN	OD1-CG-ND2	7.66	130.26	122.60
1	A	151	THR	N-CA-CB	-7.48	99.14	110.73
1	A	74	GLN	CB-CA-C	-7.46	95.47	110.17
1	B	583	LEU	N-CA-CB	7.10	124.04	111.69
1	B	474	GLN	CB-CA-C	-6.83	105.06	111.00
1	A	117	ASN	CA-CB-CG	-6.78	105.82	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASN	N-CA-C	6.62	118.58	111.36
1	A	219	ASN	N-CA-C	-6.55	103.78	113.61
1	A	63	ARG	NE-CZ-NH2	-6.51	113.34	119.20
1	B	743	ASP	CB-CA-C	-6.47	100.72	110.88
1	B	714	CYS	N-CA-CB	6.44	120.83	110.65
1	A	73	HIS	N-CA-CB	-6.37	101.17	110.53
1	A	153	PRO	N-CA-CB	6.26	109.15	103.33
1	B	477	CYS	N-CA-CB	-5.99	100.90	111.39
1	B	553	PRO	N-CA-CB	5.97	109.01	103.39
1	B	596	PHE	CA-C-N	5.97	126.40	119.47
1	B	596	PHE	C-N-CA	5.97	126.40	119.47
1	A	116	TRP	N-CA-CB	-5.97	101.35	110.12
1	B	731	TYR	CA-CB-CG	-5.89	103.29	113.90
1	B	516	TRP	N-CA-CB	-5.83	101.55	110.12
1	A	250	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	312	LEU	N-CA-CB	5.71	118.92	110.53
1	A	288	ILE	N-CA-C	5.67	116.33	108.84
1	B	463	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	A	74	GLN	OE1-CD-NE2	5.53	128.13	122.60
1	A	196	PHE	N-CA-CB	5.52	118.65	109.98
1	B	620	GLY	N-CA-C	-5.51	106.59	115.08
1	A	289	THR	CA-CB-OG1	5.48	117.82	109.60
1	B	546	ASP	CB-CA-C	5.48	118.88	109.51
1	A	89	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	A	117	ASN	CB-CA-C	-5.40	100.63	110.63
1	B	704	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	185	THR	N-CA-CB	5.38	120.74	111.00
1	A	240	ALA	N-CA-CB	5.37	118.49	110.22
1	B	568	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	498	ILE	N-CA-CB	-5.34	103.74	110.57
1	A	52	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	A	260	LEU	N-CA-CB	5.22	117.79	110.12
1	A	86	HIS	CB-CA-C	-5.21	101.25	109.80
1	B	619	ASN	N-CA-C	-5.17	106.81	113.01
1	A	75	PRO	CA-N-CD	5.14	119.19	112.00
1	A	151	THR	OG1-CB-CG2	5.12	119.55	109.30
1	A	249	TYR	CB-CA-C	-5.11	101.97	110.14
1	B	447	VAL	CB-CA-C	-5.10	105.42	111.65
1	B	639	VAL	CA-CB-CG2	-5.10	101.73	110.40
1	B	430	VAL	CB-CA-C	5.09	117.61	110.99
1	B	562	ALA	N-CA-C	-5.09	105.74	111.28
1	A	234	ARG	N-CA-CB	-5.06	102.68	110.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	GLU	N-CA-CB	-5.06	102.66	110.20
1	A	314	CYS	N-CA-CB	5.05	118.24	110.21
1	B	644	LYS	N-CA-CB	-5.03	102.24	110.43
1	A	201	ILE	N-CA-CB	5.01	114.36	110.45

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	2699	0	2604	90	0
1	B	2710	0	2623	83	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
3	A	196	0	0	4	0
3	B	163	0	0	3	0
All	All	5856	0	5279	173	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 16.

All (173) 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:619:ASN:HB2	1:B:621:GLN:CG	1.87	1.03
1:B:619:ASN:HB2	1:B:621:GLN:HG2	1.40	1.03
1:B:442:MET:HE1	1:B:740:GLN:HE21	1.26	0.98
1:B:617:TYR:CD2	1:B:691:VAL:HG13	2.00	0.96
1:B:442:MET:CE	1:B:740:GLN:HE21	1.86	0.88
1:A:45:ALA:HB3	1:A:46:PRO:HD3	1.57	0.86
1:B:442:MET:HE1	1:B:740:GLN:NE2	1.90	0.85
1:A:234:ARG:NH2	3:A:570:HOH:O	2.11	0.84
1:A:213:SER:O	1:A:215:PRO:HD3	1.80	0.82
1:A:256:GLU:OE2	1:A:300:ARG:NH1	2.15	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASP:O	1:A:300:ARG:NH2	2.14	0.79
1:B:618:GLY:H	1:B:692:ALA:HA	1.49	0.78
1:B:617:TYR:CE2	1:B:691:VAL:HG13	2.19	0.77
1:A:285:ARG:O	1:A:288:ILE:HG13	1.84	0.76
1:A:258:LYS:O	1:A:261:ASP:HB2	1.84	0.76
1:A:219:ASN:N	1:A:219:ASN:ND2	2.32	0.75
1:B:709:ALA:O	1:B:713:GLY:HA2	1.86	0.74
1:B:619:ASN:HB2	1:B:621:GLN:HG3	1.70	0.73
1:A:260:LEU:O	1:A:263:VAL:HG12	1.88	0.73
1:A:263:VAL:HG13	1:A:264:GLU:N	2.04	0.72
1:A:308:ILE:HG12	1:A:314:CYS:SG	2.30	0.71
1:B:707:LYS:NZ	3:B:349:HOH:O	2.22	0.71
1:B:624:ARG:NH1	1:B:701:TYR:CD1	2.60	0.70
1:B:644:LYS:HD3	1:B:647:GLU:HG2	1.74	0.69
1:A:222:GLN:OE1	1:A:224:ARG:NH1	2.26	0.69
1:A:271:GLU:HG2	1:A:284:TYR:HD2	1.56	0.69
1:A:263:VAL:CG1	1:A:264:GLU:N	2.56	0.68
1:B:465:GLU:HA	1:B:465:GLU:OE1	1.93	0.67
1:A:335:GLU:O	1:A:339:LYS:HB2	1.94	0.67
1:B:444:LEU:C	1:B:446:PRO:HD2	2.20	0.67
1:B:613:SER:O	1:B:615:PRO:HD3	1.96	0.65
1:B:664:GLU:HA	1:B:664:GLU:OE1	1.96	0.65
1:A:319:THR:H	1:A:322:SER:HB3	1.62	0.64
1:B:735:GLU:HA	1:B:738:TRP:NE1	2.12	0.64
1:B:596:PHE:HB3	1:B:598:GLU:OE2	1.98	0.64
1:B:445:ALA:N	1:B:446:PRO:HD2	2.14	0.63
1:A:199:LYS:HB2	1:A:202:PRO:HG2	1.81	0.63
1:A:278:PRO:HG2	1:A:281:VAL:HG21	1.80	0.62
1:A:276:ASN:HD22	1:A:276:ASN:N	1.97	0.61
1:B:691:VAL:CG1	1:B:691:VAL:CB	2.78	0.61
1:A:325:ARG:O	1:A:329:GLN:HG3	2.01	0.60
1:A:219:ASN:N	1:A:219:ASN:HD22	1.98	0.60
1:A:218:GLY:C	1:A:219:ASN:HD22	2.09	0.60
1:B:543:SER:HB3	1:B:546:ASP:CG	2.27	0.60
1:B:599:LYS:O	1:B:603:LEU:HB2	2.02	0.60
1:A:133:SER:HB3	1:A:186:ASN:ND2	2.16	0.59
1:B:545:ASP:OD1	1:B:545:ASP:N	2.35	0.59
1:B:677:LYS:HB3	1:B:678:PRO:HD2	1.85	0.59
1:A:308:ILE:CG1	1:A:314:CYS:SG	2.91	0.58
1:A:273:LEU:C	1:A:275:PRO:HD3	2.28	0.58
1:A:304:ASP:OD1	1:A:306:SER:OG	2.23	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:LYS:HD3	1:B:647:GLU:CG	2.35	0.57
1:A:275:PRO:O	1:A:277:LYS:HD2	2.04	0.57
1:B:488:ASP:HB3	3:B:314:HOH:O	2.05	0.57
1:B:583:LEU:HD12	1:B:583:LEU:N	2.21	0.56
1:B:634:ARG:NH1	3:B:264:HOH:O	2.35	0.56
1:A:45:ALA:HB3	1:A:46:PRO:CD	2.33	0.56
1:A:144:THR:HG22	1:A:144:THR:O	2.05	0.56
1:B:533:SER:O	2:B:780:NAD:H6N	2.07	0.55
1:B:743:ASP:HB3	1:B:745:SER:H	1.72	0.55
1:A:190:ASN:HA	1:A:227:LEU:O	2.07	0.54
1:A:216:VAL:CG2	1:A:288:ILE:HG23	2.37	0.54
1:A:45:ALA:N	1:A:46:PRO:HD2	2.23	0.54
1:A:276:ASN:N	1:A:276:ASN:ND2	2.55	0.54
1:A:318:GLU:OE1	1:A:322:SER:OG	2.25	0.53
1:B:673:LEU:C	1:B:675:PRO:HD3	2.33	0.53
1:B:516:TRP:O	1:B:524:LYS:HD2	2.08	0.53
1:A:57:LYS:NZ	3:A:460:HOH:O	2.41	0.53
1:B:618:GLY:H	1:B:692:ALA:CA	2.21	0.53
1:A:215:PRO:HA	1:A:289:THR:HG23	1.91	0.52
1:B:543:SER:OG	1:B:545:ASP:OD1	2.08	0.52
1:A:336:SER:O	1:A:340:GLN:HG3	2.10	0.52
1:B:428:ALA:HA	1:B:452:ARG:HB3	1.91	0.52
1:A:284:TYR:O	1:A:287:LEU:HB2	2.09	0.52
1:A:33:ASP:O	1:A:57:LYS:HA	2.10	0.51
1:B:622:GLN:HG3	1:B:699:LEU:O	2.11	0.51
1:B:682:ALA:HB3	1:B:686:ASP:OD2	2.10	0.51
1:B:590:ASN:HA	1:B:627:LEU:O	2.10	0.51
1:B:699:LEU:HB3	1:B:701:TYR:CE1	2.46	0.51
1:B:709:ALA:O	1:B:713:GLY:CA	2.58	0.51
1:A:228:TYR:CD2	1:A:318:GLU:HG3	2.46	0.51
1:B:654:HIS:CD2	1:B:716:PRO:HD2	2.45	0.51
1:B:735:GLU:HG3	1:B:738:TRP:CZ2	2.46	0.51
1:A:312:LEU:HB2	1:A:314:CYS:SG	2.51	0.50
1:B:600:LEU:C	1:B:600:LEU:HD12	2.37	0.50
1:A:213:SER:C	1:A:215:PRO:HD3	2.37	0.50
1:A:338:TRP:O	1:A:342:GLN:HG3	2.10	0.50
1:B:445:ALA:N	1:B:446:PRO:CD	2.75	0.50
1:A:45:ALA:N	1:A:46:PRO:CD	2.74	0.50
1:A:63:ARG:HG2	1:A:63:ARG:NH1	2.26	0.49
1:A:262:VAL:HG22	1:A:320:PHE:HZ	1.77	0.49
1:A:343:ASP:CB	1:A:345:SER:OG	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:ASN:CB	1:B:621:GLN:HG2	2.29	0.49
1:B:624:ARG:NH1	1:B:701:TYR:HD1	2.06	0.49
1:A:190:ASN:HD22	1:A:190:ASN:N	2.10	0.49
1:A:192:GLY:O	1:A:195:HIS:HB2	2.12	0.49
1:A:309:ALA:O	1:A:313:GLY:HA2	2.12	0.49
1:A:42:MET:HE3	1:A:349:GLU:HB3	1.95	0.48
1:A:286:ASP:N	1:A:286:ASP:OD1	2.46	0.48
1:A:343:ASP:HB3	1:A:345:SER:H	1.78	0.48
1:B:419:ARG:HD3	1:B:446:PRO:HG2	1.95	0.48
1:B:468:ARG:HH11	1:B:468:ARG:HG2	1.78	0.48
1:B:618:GLY:O	1:B:692:ALA:HB2	2.14	0.48
1:B:622:GLN:CD	1:B:624:ARG:NH1	2.71	0.48
1:A:223:ILE:CG2	1:A:224:ARG:N	2.76	0.48
1:B:407:THR:O	1:B:481:LEU:HB2	2.13	0.48
1:B:567:SER:O	1:B:571:VAL:HG23	2.14	0.48
1:A:260:LEU:HD21	1:A:264:GLU:CD	2.39	0.47
1:A:120:THR:OG1	1:A:122:ASP:OD1	2.23	0.47
1:A:268:GLU:OE1	1:A:268:GLU:HA	2.11	0.47
1:B:622:GLN:HE21	1:B:699:LEU:HB2	1.79	0.47
1:A:326:LYS:HA	1:A:329:GLN:HE21	1.80	0.47
1:B:546:ASP:O	1:B:700:ARG:NH1	2.41	0.47
1:B:475:PRO:HD2	1:B:515:TYR:CZ	2.49	0.47
1:A:216:VAL:HG21	1:A:288:ILE:HG23	1.97	0.46
1:B:635:ALA:O	1:B:639:VAL:HG23	2.15	0.46
1:A:97:PHE:O	1:A:101:ASN:HB2	2.15	0.46
1:A:7:THR:HG1	1:A:82:ALA:H	1.62	0.46
1:A:201:ILE:N	1:A:202:PRO:CD	2.79	0.46
1:B:546:ASP:OD1	1:B:546:ASP:N	2.26	0.46
1:B:660:LEU:O	1:B:664:GLU:HG2	2.16	0.46
1:A:290:PHE:N	1:A:290:PHE:CD1	2.84	0.45
1:B:427:ASP:O	1:B:452:ARG:HD2	2.16	0.45
1:B:637:TYR:CZ	1:B:641:THR:HG21	2.52	0.45
1:A:136:GLU:HA	3:A:562:HOH:O	2.16	0.45
1:A:343:ASP:HB3	1:A:345:SER:OG	2.16	0.45
1:B:675:PRO:O	1:B:677:LYS:HG3	2.16	0.45
1:B:618:GLY:HA2	1:B:692:ALA:HB1	1.99	0.45
1:A:262:VAL:HG22	1:A:320:PHE:CZ	2.52	0.45
1:B:720:PHE:O	1:B:724:MET:HG2	2.17	0.45
1:A:197:PRO:CD	1:A:341:VAL:HG11	2.47	0.44
1:A:283:HIS:HB2	1:A:286:ASP:OD2	2.17	0.44
1:A:35:LEU:HD12	1:A:57:LYS:HD2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:ILE:CG2	1:B:704:ASP:N	2.79	0.44
1:B:654:HIS:HD2	1:B:716:PRO:HD2	1.83	0.44
1:A:141:LEU:HD13	1:A:146:ASP:O	2.16	0.44
1:B:615:PRO:CB	1:B:691:VAL:HG12	2.48	0.44
1:A:263:VAL:CG1	1:A:264:GLU:H	2.28	0.44
1:A:321:GLU:H	1:A:321:GLU:CD	2.24	0.44
1:B:419:ARG:CD	1:B:446:PRO:HG2	2.47	0.44
1:A:42:MET:CG	1:A:349:GLU:HG3	2.49	0.43
1:B:711:GLU:C	1:B:712:LEU:HD23	2.42	0.43
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.82	0.43
1:A:164:LYS:HE3	3:A:412:HOH:O	2.17	0.43
1:B:687:LEU:HD23	1:B:687:LEU:HA	1.72	0.43
1:A:216:VAL:HG23	1:A:288:ILE:HG23	1.99	0.43
1:B:609:LEU:HA	1:B:609:LEU:HD23	1.79	0.43
1:B:613:SER:C	1:B:615:PRO:HD3	2.45	0.42
1:B:639:VAL:O	1:B:643:GLY:HA3	2.19	0.42
1:B:468:ARG:HG2	1:B:468:ARG:NH1	2.34	0.42
1:B:403:LYS:HE3	1:B:473:HIS:O	2.19	0.42
1:A:244:LYS:HB3	1:A:247:GLU:CG	2.50	0.42
1:A:335:GLU:HA	1:A:338:TRP:NE1	2.35	0.42
1:B:651:ILE:HG21	1:B:651:ILE:HD13	1.85	0.41
1:B:710:ARG:HH11	1:B:710:ARG:HD2	1.64	0.41
1:B:441:LEU:HD23	1:B:441:LEU:HA	1.90	0.41
1:A:275:PRO:O	1:A:277:LYS:HE3	2.20	0.41
1:A:285:ARG:C	1:A:287:LEU:H	2.27	0.41
1:B:619:ASN:CB	1:B:621:GLN:HG3	2.47	0.41
1:A:146:ASP:OD1	1:A:146:ASP:N	2.34	0.41
1:A:201:ILE:N	1:A:202:PRO:HD2	2.36	0.41
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.78	0.41
1:A:260:LEU:O	1:A:264:GLU:HB2	2.20	0.41
1:A:319:THR:O	1:A:320:PHE:C	2.63	0.41
1:B:604:MET:HE1	1:B:615:PRO:O	2.20	0.40
1:B:408:GLY:HA2	1:B:433:ASP:OD2	2.21	0.40
1:B:601:ILE:HB	1:B:602:PRO:HD3	2.03	0.40
1:B:603:LEU:HA	1:B:603:LEU:HD12	1.82	0.40
1:A:165:ALA:O	1:A:168:ASP:HB2	2.21	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	339/355 (96%)	318 (94%)	20 (6%)	1 (0%)	36	29
1	B	340/355 (96%)	320 (94%)	19 (6%)	1 (0%)	36	29
All	All	679/710 (96%)	638 (94%)	39 (6%)	2 (0%)	36	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	600	LEU
1	A	214	LEU

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	287/296 (97%)	262 (91%)	25 (9%)	9	4
1	B	287/296 (97%)	264 (92%)	23 (8%)	11	5
All	All	574/592 (97%)	526 (92%)	48 (8%)	10	4

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	29	VAL
1	A	74	GLN
1	A	123	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	151	THR
1	A	157	SER
1	A	190	ASN
1	A	198[A]	GLU
1	A	198[B]	GLU
1	A	204	MET
1	A	214	LEU
1	A	219	ASN
1	A	224	ARG
1	A	244	LYS
1	A	257	ARG
1	A	268	GLU
1	A	276	ASN
1	A	277	LYS
1	A	286	ASP
1	A	289	THR
1	A	303	ILE
1	A	306	SER
1	A	314	CYS
1	A	339	LYS
1	A	345	SER
1	B	402	ARG
1	B	422	ILE
1	B	426	SER
1	B	434	LYS
1	B	449	GLN
1	B	481	LEU
1	B	491	ILE
1	B	528	ARG
1	B	563	SER
1	B	583	LEU
1	B	617	TYR
1	B	619	ASN
1	B	623	ILE
1	B	624	ARG
1	B	627	LEU
1	B	657	ARG
1	B	659	ASN
1	B	703	ILE
1	B	706	SER
1	B	717	GLN
1	B	739	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	740	GLN
1	B	743	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	186	ASN
1	A	190	ASN
1	A	207	ASN
1	A	219	ASN
1	A	221	GLN
1	A	259	ASN
1	A	276	ASN
1	A	329	GLN
1	B	486	HIS
1	B	607	ASN
1	B	621	GLN
1	B	622	GLN
1	B	654	HIS
1	B	679	HIS
1	B	683	HIS
1	B	740	GLN
1	B	742	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	380	-	46,48,48	1.43	5 (10%)	64,73,73	2.31	15 (23%)
2	NAD	B	780	-	46,48,48	1.96	10 (21%)	64,73,73	2.00	15 (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	380	-	-	2/30/62/62	0/5/5/5
2	NAD	B	780	-	-	2/30/62/62	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	780	NAD	PN-O3	6.66	1.66	1.59
2	A	380	NAD	PN-O3	4.97	1.64	1.59
2	B	780	NAD	C4N-C3N	4.79	1.46	1.39
2	B	780	NAD	PA-O3	-4.61	1.54	1.59
2	B	780	NAD	C2N-N1N	3.70	1.39	1.35
2	A	380	NAD	C4N-C3N	3.37	1.44	1.39
2	A	380	NAD	C2A-N1A	3.04	1.39	1.33
2	B	780	NAD	C6N-N1N	2.81	1.41	1.35
2	B	780	NAD	C3N-C7N	2.80	1.54	1.50
2	B	780	NAD	C5N-C4N	2.67	1.43	1.38
2	B	780	NAD	O7N-C7N	-2.56	1.19	1.24
2	A	380	NAD	PA-O2A	-2.39	1.44	1.55
2	B	780	NAD	PN-O2N	-2.36	1.44	1.55
2	A	380	NAD	O7N-C7N	-2.32	1.19	1.24
2	B	780	NAD	O2D-C2D	2.14	1.48	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	380	NAD	C5N-C4N-C3N	-8.47	112.04	120.36
2	A	380	NAD	C3N-C7N-N7N	-6.20	110.10	117.74
2	B	780	NAD	C5N-C6N-N1N	-5.74	112.56	120.38
2	A	380	NAD	C2N-C3N-C4N	5.73	124.93	118.26
2	A	380	NAD	C4N-C3N-C7N	-5.70	105.54	121.06
2	B	780	NAD	C5N-C4N-C3N	-5.48	114.98	120.36
2	B	780	NAD	C6N-N1N-C2N	5.35	126.42	121.88
2	A	380	NAD	C6N-N1N-C2N	4.69	125.87	121.88
2	B	780	NAD	C6N-C5N-C4N	4.58	126.05	119.45
2	B	780	NAD	C4N-C3N-C7N	-4.38	109.12	121.06
2	A	380	NAD	C6N-C5N-C4N	4.36	125.74	119.45
2	A	380	NAD	O7N-C7N-C3N	4.19	124.72	119.60
2	A	380	NAD	C5N-C6N-N1N	-3.61	115.46	120.38
2	B	780	NAD	C2N-N1N-C1D	-3.52	111.35	119.13
2	B	780	NAD	C2N-C3N-C7N	3.46	129.45	119.46
2	B	780	NAD	O2A-PA-O3	3.44	116.58	107.27
2	A	380	NAD	C2N-C3N-C7N	3.43	129.35	119.46
2	B	780	NAD	O7N-C7N-C3N	3.32	123.66	119.60
2	B	780	NAD	O3-PN-O1N	-2.98	101.74	110.70
2	A	380	NAD	O4B-C1B-C2B	-2.73	100.77	106.62
2	B	780	NAD	O5D-C5D-C4D	-2.73	99.70	108.99
2	B	780	NAD	C2N-C3N-C4N	2.58	121.26	118.26
2	A	380	NAD	C5A-C6A-N6A	2.49	129.45	123.29
2	B	780	NAD	C4D-O4D-C1D	2.48	112.19	109.92
2	A	380	NAD	N3A-C2A-N1A	2.43	132.26	128.58
2	A	380	NAD	C2N-N1N-C1D	-2.39	113.87	119.13
2	A	380	NAD	C4B-O4B-C1B	2.20	114.33	109.47
2	B	780	NAD	PN-O5D-C5D	-2.15	109.05	121.35
2	A	380	NAD	O3D-C3D-C4D	2.12	117.17	111.08
2	B	780	NAD	O2N-PN-O3	2.02	112.74	107.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

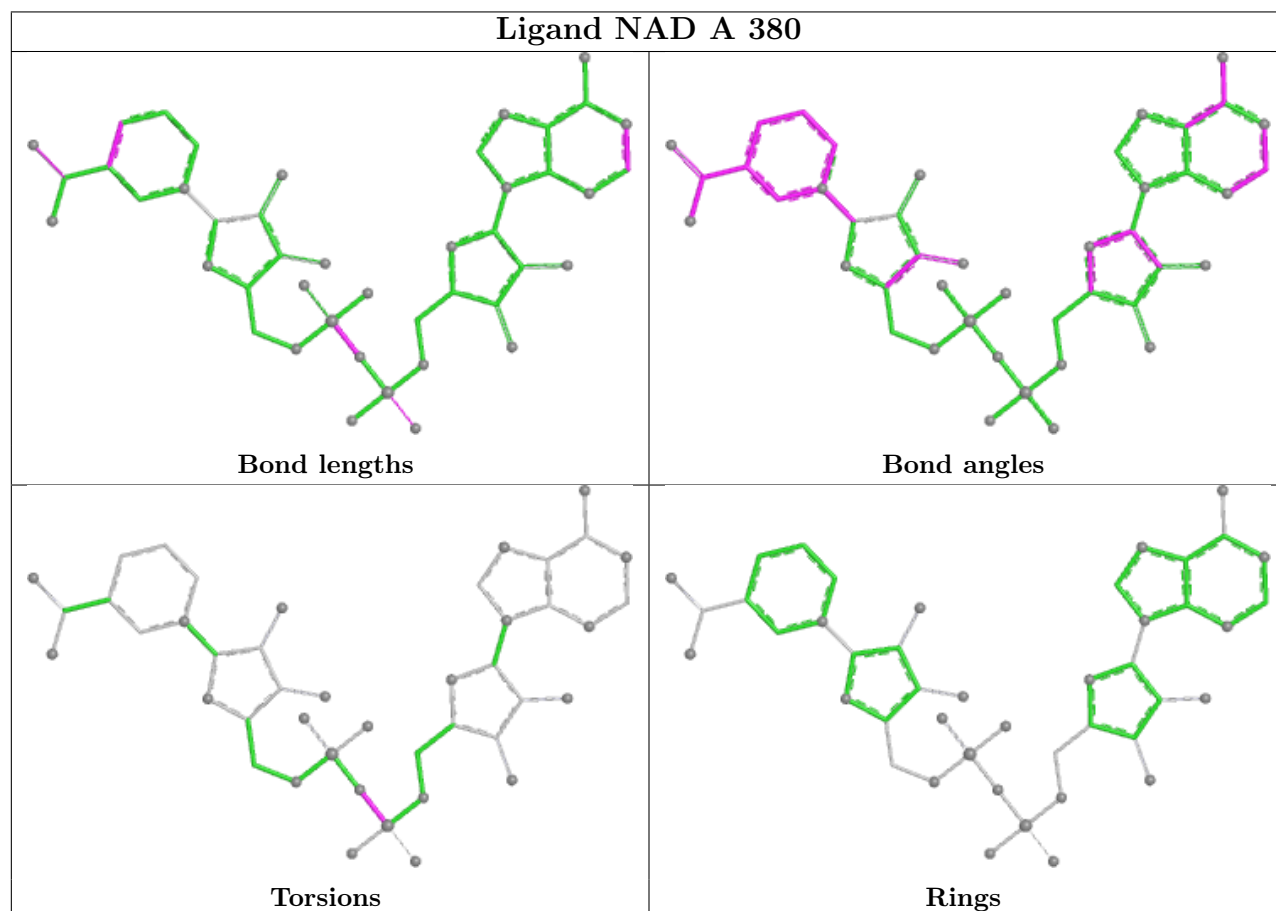
Mol	Chain	Res	Type	Atoms
2	A	380	NAD	PN-O3-PA-O2A
2	B	780	NAD	PN-O3-PA-O2A
2	B	780	NAD	PN-O3-PA-O1A
2	A	380	NAD	PN-O3-PA-O1A

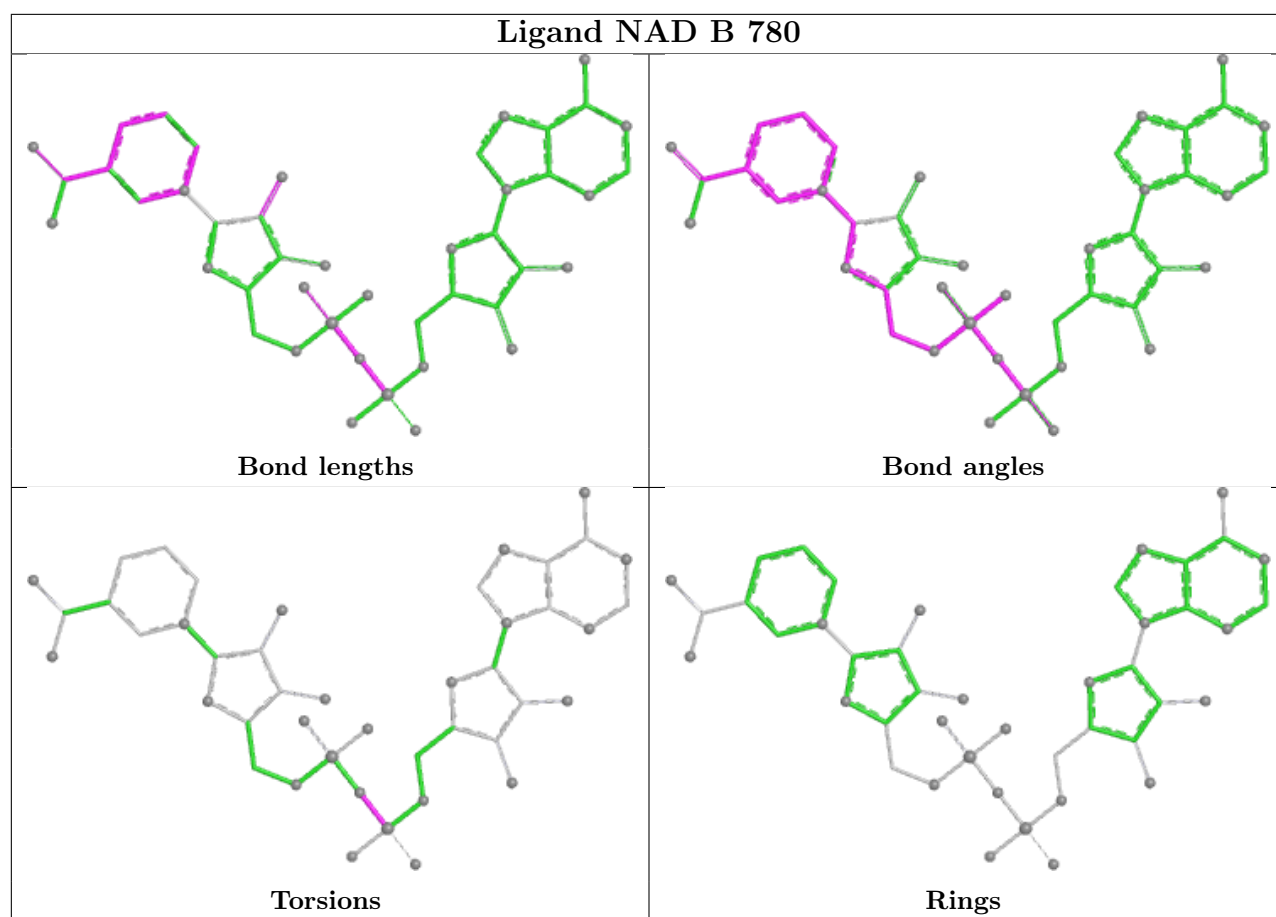
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	780	NAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.