Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:07 am BST

PDB ID	:	1RKX
Title	:	Crystal Structure at 1.8 Angstrom of CDP-D-glucose 4,6-dehydratase from Yersinia pseudotuberculosis
Authors	:	Vogan, E.M.; Bellamacina, C.; He, X.; Liu, H.W.; Ringe, D.; Petsko, G.A.
Deposited on	:	2003-11-23
Resolution	:	1.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

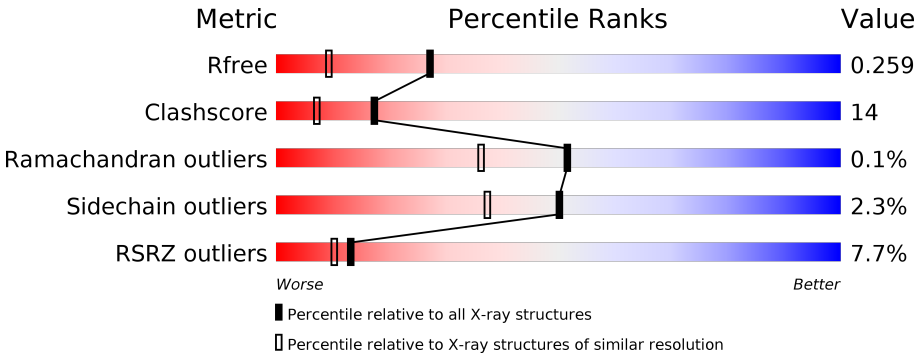
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.80 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))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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 <=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	357	3% 77% 19%
1	B	357	8% 75% 21%
1	C	357	8% 73% 24%
1	D	357	10% 75% 22%

2 Entry composition

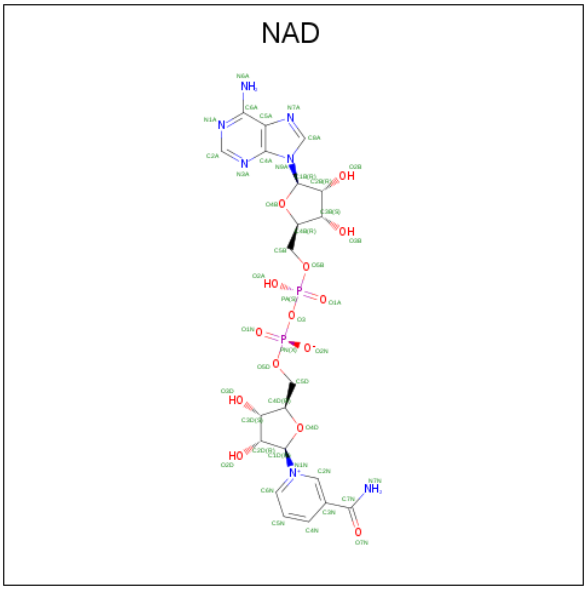
There are 3 unique types of molecules in this entry. The entry contains 12159 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CDP-glucose-4,6-dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2785	1778	477	518	12			
1	B	346	Total	C	N	O	S	0	0	0
			2763	1764	474	513	12			
1	C	351	Total	C	N	O	S	0	0	0
			2802	1789	481	520	12			
1	D	347	Total	C	N	O	S	0	0	0
			2771	1770	475	514	12			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: 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		

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

- Molecule 3 is water.

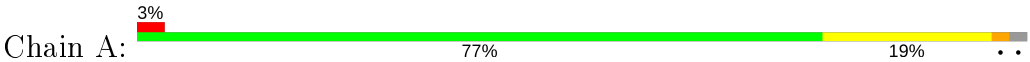
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	230	Total	O	0	0
			230	230		
3	B	205	Total	O	0	0
			205	205		
3	C	214	Total	O	0	0
			214	214		
3	D	213	Total	O	0	0
			213	213		

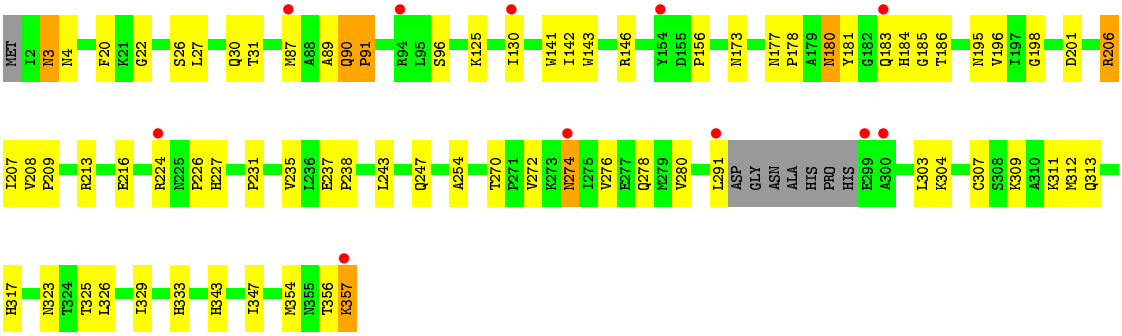
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: CDP-glucose-4,6-dehydratase

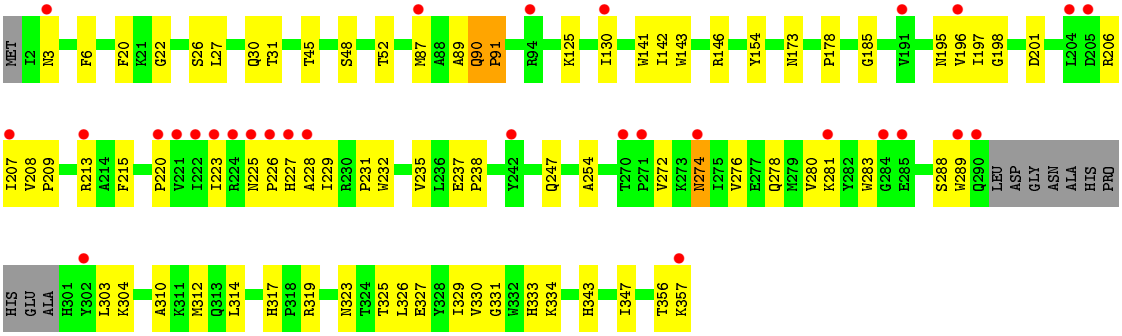
Chain A:





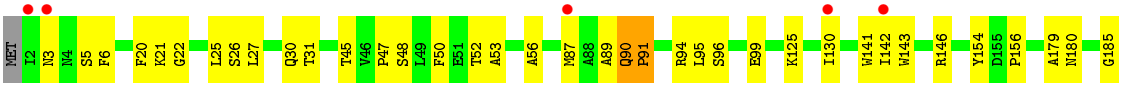
- Molecule 1: CDP-glucose-4,6-dehydratase

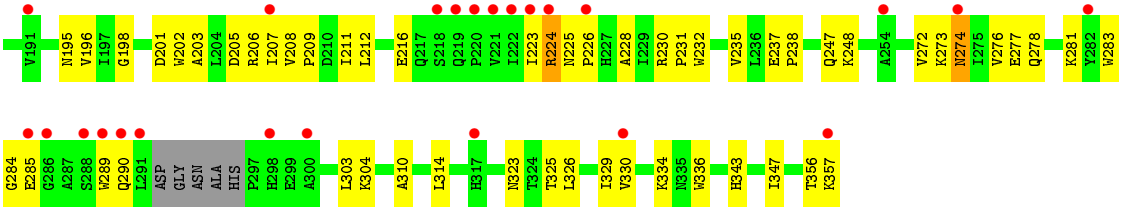
Chain B:



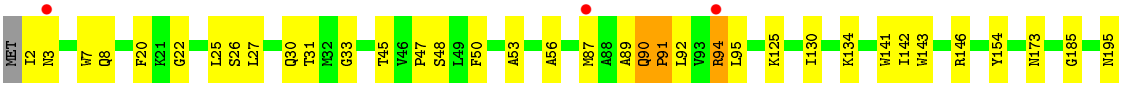
- Molecule 1: CDP-glucose-4,6-dehydratase

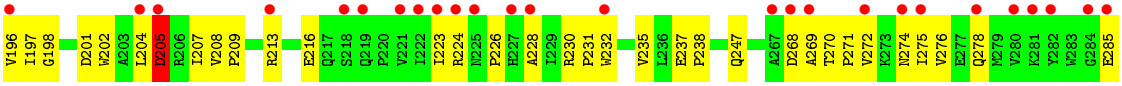
Chain C:

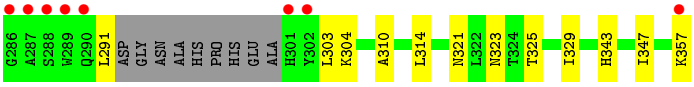




- Molecule 1: CDP-glucose-4,6-dehydratase







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.90Å 115.87Å 126.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.25 – 1.80 36.25 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (36.25-1.80) 97.6 (36.25-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 1.81Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.229 , 0.266 0.221 , 0.259	Depositor DCC
R_{free} test set	5025 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12159	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8343e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.35	0/2864	0.57	1/3897 (0.0%)
1	B	0.32	0/2842	0.57	1/3867 (0.0%)
1	C	0.33	0/2883	0.57	1/3923 (0.0%)
1	D	0.33	0/2850	0.58	1/3878 (0.0%)
All	All	0.33	0/11439	0.57	4/15565 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	90	GLN	N-CA-C	-5.54	96.05	111.00
1	B	90	GLN	N-CA-C	-5.52	96.10	111.00
1	A	90	GLN	N-CA-C	-5.48	96.20	111.00
1	D	90	GLN	N-CA-C	-5.39	96.45	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	2785	0	2673	85	0
1	B	2763	0	2651	74	0
1	C	2802	0	2688	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2771	0	2662	76	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	230	0	0	7	0
3	B	205	0	0	6	0
3	C	214	0	0	4	0
3	D	213	0	0	4	0
All	All	12159	0	10778	305	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 14.

All (305) 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:3:ASN:H	1:A:247:GLN:HE22	1.15	0.93
1:A:184:HIS:HD2	1:A:186:THR:H	1.19	0.89
1:D:92:LEU:HD13	1:D:94:ARG:HH21	1.39	0.87
1:A:184:HIS:CD2	1:A:186:THR:H	1.93	0.87
1:D:94:ARG:HH12	1:D:205:ASP:CG	1.81	0.85
1:B:325:THR:O	1:B:329:ILE:HG12	1.80	0.80
1:C:94:ARG:HH22	1:C:205:ASP:CB	1.95	0.79
1:C:94:ARG:HH22	1:C:205:ASP:HB2	1.46	0.79
1:D:198:GLY:HA2	1:D:329:ILE:CD1	2.15	0.77
1:A:143:TRP:CG	1:D:146:ARG:HD2	2.19	0.76
1:B:207:ILE:HG23	1:B:208:VAL:H	1.50	0.76
1:A:198:GLY:HA2	1:A:329:ILE:CD1	2.16	0.76
1:D:198:GLY:HA2	1:D:329:ILE:HD12	1.68	0.76
1:A:198:GLY:HA2	1:A:329:ILE:HD12	1.68	0.75
1:B:198:GLY:HA2	1:B:329:ILE:HD12	1.69	0.75
1:C:198:GLY:HA2	1:C:329:ILE:CD1	2.17	0.75
1:C:198:GLY:HA2	1:C:329:ILE:HD12	1.69	0.75
1:B:198:GLY:HA2	1:B:329:ILE:CD1	2.17	0.75
1:A:180:ASN:HD22	1:A:180:ASN:H	1.37	0.73
1:A:146:ARG:HD2	1:D:143:TRP:CG	2.23	0.72
1:A:311:LYS:HE3	3:A:514:HOH:O	1.89	0.71
1:D:321:ASN:HD21	1:D:323:ASN:HB2	1.54	0.71
1:B:312:MET:HG3	1:C:142:ILE:CG2	2.21	0.71
1:D:196:VAL:HG13	1:D:235:VAL:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:HIS:CE1	1:B:357:LYS:HE3	2.26	0.70
1:A:196:VAL:HG13	1:A:235:VAL:HA	1.74	0.69
1:B:196:VAL:HG13	1:B:235:VAL:HA	1.74	0.69
1:C:196:VAL:HG13	1:C:235:VAL:HA	1.75	0.69
1:B:195:ASN:ND2	1:B:231:PRO:HG2	2.08	0.68
1:D:325:THR:O	1:D:329:ILE:HG12	1.93	0.68
1:D:226:PRO:HG2	1:D:291:LEU:HG	1.74	0.68
1:C:203:ALA:HB3	1:C:206:ARG:HD2	1.75	0.68
1:B:22:GLY:HA2	1:B:87:MET:HE3	1.76	0.67
1:C:195:ASN:ND2	1:C:231:PRO:HG2	2.09	0.67
1:A:195:ASN:ND2	1:A:231:PRO:HG2	2.09	0.67
1:A:4:ASN:HD21	1:A:354:MET:CE	2.08	0.67
1:D:195:ASN:ND2	1:D:231:PRO:HG2	2.10	0.66
1:B:317:HIS:HE1	1:B:357:LYS:HE3	1.61	0.66
1:B:146:ARG:HD3	3:B:362:HOH:O	1.94	0.66
1:A:22:GLY:HA2	1:A:87:MET:HE3	1.78	0.65
1:A:317:HIS:NE2	1:A:357:LYS:HE3	2.12	0.65
1:A:325:THR:O	1:A:329:ILE:HG12	1.97	0.65
1:B:280:VAL:HG21	1:B:289:TRP:CE3	2.32	0.65
1:B:143:TRP:CG	1:C:146:ARG:HD2	2.33	0.64
1:C:31:THR:CG2	1:C:347:ILE:HD12	2.27	0.64
1:C:89:ALA:O	1:C:91:PRO:HD3	1.97	0.64
1:D:89:ALA:O	1:D:91:PRO:HD3	1.97	0.64
1:A:89:ALA:O	1:A:91:PRO:HD3	1.97	0.64
1:D:31:THR:CG2	1:D:347:ILE:HD12	2.28	0.64
1:B:312:MET:HG3	1:C:142:ILE:HG21	1.79	0.64
1:D:92:LEU:HD13	1:D:94:ARG:NH2	2.10	0.63
1:C:343:HIS:O	1:C:347:ILE:HG12	1.98	0.63
1:A:31:THR:CG2	1:A:347:ILE:HD12	2.27	0.63
1:D:278:GLN:HE22	1:D:323:ASN:CG	2.01	0.63
1:B:142:ILE:O	1:B:304:LYS:HE2	1.99	0.63
1:B:89:ALA:O	1:B:91:PRO:HD3	1.98	0.63
1:C:22:GLY:HA2	1:C:87:MET:HE3	1.81	0.62
1:A:206:ARG:HB3	1:A:209:PRO:HD2	1.81	0.62
1:C:325:THR:O	1:C:329:ILE:HG12	1.99	0.62
1:D:22:GLY:HA2	1:D:87:MET:HE3	1.81	0.62
1:B:278:GLN:NE2	1:B:326:LEU:HD12	2.14	0.62
1:A:178:PRO:HB3	1:A:254:ALA:HB1	1.80	0.62
1:B:343:HIS:O	1:B:347:ILE:HG12	2.00	0.62
1:B:31:THR:CG2	1:B:347:ILE:HD12	2.28	0.62
1:B:227:HIS:O	1:B:229:ILE:HD12	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:VAL:HB	1:C:209:PRO:HD3	1.82	0.62
1:C:223:ILE:HD12	1:C:289:TRP:CE3	2.35	0.62
1:D:204:LEU:CD2	1:D:213:ARG:HD2	2.29	0.62
1:B:27:LEU:O	1:B:31:THR:HG23	2.00	0.61
1:A:146:ARG:HD3	3:A:368:HOH:O	1.99	0.61
1:A:343:HIS:O	1:A:347:ILE:HG12	2.01	0.61
1:C:27:LEU:O	1:C:31:THR:HG23	2.00	0.61
1:A:27:LEU:O	1:A:31:THR:HG23	2.01	0.61
1:C:146:ARG:HD3	3:C:368:HOH:O	2.01	0.61
1:C:207:ILE:O	1:C:211:ILE:HG13	2.00	0.61
1:D:27:LEU:O	1:D:31:THR:HG23	2.01	0.61
1:C:356:THR:HG22	1:C:357:LYS:HD3	1.81	0.61
1:B:207:ILE:HG23	1:B:208:VAL:N	2.14	0.61
1:D:321:ASN:ND2	1:D:323:ASN:HB2	2.17	0.60
1:B:208:VAL:HB	1:B:209:PRO:HD3	1.83	0.60
1:D:226:PRO:HA	1:D:272:VAL:CG2	2.31	0.60
1:A:96:SER:HB2	1:A:156:PRO:HB2	1.84	0.60
1:D:230:ARG:HD2	1:D:232:TRP:CZ2	2.37	0.60
1:C:207:ILE:HG13	1:C:208:VAL:N	2.17	0.59
1:C:248:LYS:HD2	1:C:314:LEU:CD2	2.33	0.59
1:D:343:HIS:O	1:D:347:ILE:HG12	2.02	0.59
1:A:3:ASN:H	1:A:247:GLN:NE2	1.94	0.58
1:A:356:THR:C	1:A:357:LYS:HG3	2.24	0.58
1:D:204:LEU:HD21	1:D:213:ARG:HD2	1.84	0.58
1:D:2:ILE:HA	1:D:247:GLN:HE22	1.69	0.58
1:C:142:ILE:O	1:C:142:ILE:HG22	2.03	0.58
1:A:356:THR:O	1:A:357:LYS:HG3	2.04	0.58
1:C:3:ASN:OD1	1:C:5:SER:HB3	2.05	0.57
1:B:226:PRO:HG2	1:B:227:HIS:ND1	2.20	0.57
1:A:207:ILE:HG23	1:A:208:VAL:N	2.19	0.57
1:A:307:CYS:HB2	3:A:514:HOH:O	2.04	0.57
1:A:278:GLN:NE2	1:A:326:LEU:HD12	2.19	0.57
1:C:207:ILE:HD11	1:C:232:TRP:CZ2	2.40	0.57
1:A:177:ASN:O	1:A:180:ASN:ND2	2.38	0.56
1:A:180:ASN:HB2	1:A:183:GLN:NE2	2.21	0.56
1:D:8:GLN:NE2	1:D:33:GLY:HA3	2.20	0.56
1:B:220:PRO:HB3	1:B:288:SER:OG	2.05	0.56
1:C:248:LYS:HD2	1:C:314:LEU:HD23	1.88	0.56
1:D:270:THR:HB	1:D:271:PRO:HD2	1.88	0.56
1:A:125:LYS:HE2	1:A:185:GLY:O	2.06	0.55
1:C:212:LEU:O	1:C:216:GLU:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLN:HE22	1:C:323:ASN:ND2	2.04	0.55
1:B:223:ILE:HG21	1:B:276:VAL:HG21	1.88	0.55
1:D:146:ARG:HD3	3:D:400:HOH:O	2.06	0.55
1:A:312:MET:HG2	3:A:535:HOH:O	2.06	0.55
1:D:204:LEU:O	1:D:205:ASP:HB2	2.07	0.55
1:C:31:THR:HG22	1:C:347:ILE:HD12	1.89	0.55
1:C:274:ASN:O	1:C:278:GLN:HG3	2.07	0.54
1:D:31:THR:HG22	1:D:347:ILE:HD12	1.89	0.54
1:A:142:ILE:O	1:A:304:LYS:HE2	2.07	0.54
1:D:125:LYS:HE2	1:D:185:GLY:O	2.07	0.54
1:B:125:LYS:HE2	1:B:185:GLY:O	2.08	0.54
1:D:198:GLY:CA	1:D:329:ILE:HD12	2.37	0.54
1:C:223:ILE:HD11	1:C:276:VAL:HG21	1.90	0.53
1:B:331:GLY:HA3	3:B:524:HOH:O	2.09	0.53
1:C:125:LYS:HE2	1:C:185:GLY:O	2.08	0.53
1:A:274:ASN:O	1:A:278:GLN:HG3	2.08	0.53
1:B:280:VAL:HG21	1:B:289:TRP:HE3	1.72	0.53
1:C:330:VAL:O	1:C:334:LYS:HG2	2.08	0.53
1:A:278:GLN:NE2	1:A:323:ASN:OD1	2.41	0.53
1:D:47:PRO:HG2	1:D:202:TRP:CE2	2.43	0.53
1:A:184:HIS:HD2	1:A:186:THR:N	1.99	0.53
1:C:323:ASN:N	1:C:323:ASN:HD22	2.05	0.53
1:B:226:PRO:HA	1:B:272:VAL:CG2	2.39	0.53
1:A:226:PRO:HA	1:A:272:VAL:CG2	2.39	0.53
1:C:231:PRO:HB3	3:C:425:HOH:O	2.08	0.53
1:A:31:THR:HG22	1:A:347:ILE:HD12	1.90	0.52
1:B:146:ARG:HD2	1:C:143:TRP:CG	2.44	0.52
1:B:225:ASN:HD22	1:B:228:ALA:CB	2.22	0.52
1:D:50:PHE:CZ	1:D:56:ALA:HB2	2.45	0.52
1:B:31:THR:HG22	1:B:347:ILE:HD12	1.90	0.52
1:C:198:GLY:CA	1:C:329:ILE:HD12	2.39	0.52
1:C:278:GLN:NE2	1:C:326:LEU:HD12	2.25	0.51
1:B:198:GLY:CA	1:B:329:ILE:HD12	2.38	0.51
1:A:357:LYS:HG2	3:A:539:HOH:O	2.09	0.51
1:C:22:GLY:HA2	1:C:87:MET:CE	2.40	0.51
1:A:198:GLY:CA	1:A:329:ILE:HD12	2.39	0.50
1:A:208:VAL:HB	1:A:209:PRO:HD3	1.93	0.50
1:C:96:SER:HB2	1:C:156:PRO:HB2	1.93	0.50
1:A:143:TRP:CD2	1:D:146:ARG:HD2	2.45	0.50
1:D:22:GLY:HA2	1:D:87:MET:CE	2.41	0.50
1:B:323:ASN:O	1:B:327:GLU:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASN:N	1:A:247:GLN:HE22	1.96	0.50
1:B:276:VAL:O	1:B:280:VAL:HG23	2.11	0.50
1:A:4:ASN:HD21	1:A:354:MET:HE3	1.76	0.50
1:B:178:PRO:HB3	1:B:254:ALA:HB1	1.94	0.49
1:D:224:ARG:O	1:D:226:PRO:HD3	2.12	0.49
1:A:181:TYR:HA	1:A:184:HIS:CE1	2.47	0.49
1:B:317:HIS:HE1	1:B:357:LYS:CE	2.24	0.49
1:A:333:HIS:HD2	3:A:410:HOH:O	1.95	0.49
1:C:226:PRO:HA	1:C:272:VAL:CG2	2.42	0.49
1:C:95:LEU:HD11	1:C:99:GLU:OE2	2.13	0.49
1:A:146:ARG:HD2	1:D:143:TRP:CD2	2.47	0.49
1:D:208:VAL:HB	1:D:209:PRO:HD3	1.95	0.49
1:A:180:ASN:H	1:A:180:ASN:ND2	2.08	0.49
1:B:226:PRO:HA	1:B:272:VAL:HG22	1.94	0.49
1:B:3:ASN:CG	1:B:247:GLN:HE22	2.16	0.48
1:B:26:SER:O	1:B:30:GLN:HG3	2.13	0.48
1:C:225:ASN:HD22	1:C:228:ALA:HB2	1.78	0.48
1:B:173:ASN:HB3	1:D:154:TYR:CE1	2.49	0.48
1:A:226:PRO:HA	1:A:272:VAL:HG22	1.96	0.48
1:A:357:LYS:OXT	1:A:357:LYS:HE2	2.12	0.48
1:B:207:ILE:HG21	1:B:232:TRP:CH2	2.48	0.48
1:B:312:MET:HG3	1:C:142:ILE:HG23	1.93	0.48
1:C:179:ALA:C	1:C:180:ASN:HD22	2.17	0.48
1:A:26:SER:O	1:A:30:GLN:HG3	2.14	0.48
1:A:356:THR:HG22	1:A:357:LYS:CG	2.44	0.48
1:D:26:SER:O	1:D:30:GLN:HG3	2.14	0.48
1:D:197:ILE:HG21	1:D:208:VAL:HG21	1.94	0.48
1:B:22:GLY:HA2	1:B:87:MET:CE	2.42	0.47
1:B:330:VAL:HG12	1:B:334:LYS:HE2	1.95	0.47
1:A:224:ARG:HG2	1:A:224:ARG:HH11	1.80	0.47
1:A:276:VAL:O	1:A:280:VAL:HG23	2.13	0.47
1:A:213:ARG:O	1:A:216:GLU:HG2	2.14	0.47
1:A:303:LEU:HD13	1:A:304:LYS:N	2.29	0.47
1:D:213:ARG:O	1:D:216:GLU:HG2	2.15	0.47
1:A:22:GLY:HA2	1:A:87:MET:CE	2.43	0.47
1:C:225:ASN:ND2	1:C:228:ALA:HB2	2.29	0.47
1:B:356:THR:HG22	1:B:357:LYS:HG3	1.96	0.47
1:D:134:LYS:HD2	3:D:541:HOH:O	2.13	0.47
1:D:207:ILE:HG23	1:D:208:VAL:N	2.30	0.47
1:B:154:TYR:CE1	1:D:173:ASN:HB3	2.50	0.47
1:D:303:LEU:HD13	1:D:304:LYS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:PRO:HA	1:C:272:VAL:HG23	1.98	0.46
1:B:125:LYS:HA	1:B:125:LYS:HE2	1.97	0.46
1:B:303:LEU:HD13	1:B:304:LYS:N	2.30	0.46
1:A:226:PRO:HG3	1:A:291:LEU:HD11	1.96	0.46
1:C:26:SER:O	1:C:30:GLN:HG3	2.15	0.46
1:C:283:TRP:HE3	1:C:330:VAL:HG13	1.81	0.46
1:A:226:PRO:HG2	1:A:227:HIS:ND1	2.31	0.46
1:A:356:THR:HG22	1:A:357:LYS:HG3	1.97	0.46
1:A:317:HIS:CE1	1:A:357:LYS:HE3	2.51	0.46
1:B:229:ILE:HD11	3:B:546:HOH:O	2.14	0.46
1:A:180:ASN:ND2	1:A:180:ASN:N	2.64	0.46
1:B:356:THR:O	1:B:357:LYS:HB2	2.16	0.46
1:C:25:LEU:HD23	1:C:87:MET:HE2	1.98	0.46
1:D:228:ALA:O	1:D:272:VAL:HG13	2.15	0.46
1:A:20:PHE:CE1	1:A:201:ASP:HB2	2.51	0.46
1:C:50:PHE:CZ	1:C:56:ALA:HB2	2.51	0.46
1:D:47:PRO:HG2	1:D:202:TRP:CD2	2.50	0.46
1:A:125:LYS:HE2	1:A:125:LYS:HA	1.97	0.46
1:A:309:LYS:HG3	1:A:313:GLN:NE2	2.30	0.46
1:C:20:PHE:CE1	1:C:201:ASP:HB2	2.50	0.46
1:D:20:PHE:CE1	1:D:201:ASP:HB2	2.51	0.46
1:C:47:PRO:HG2	1:C:202:TRP:CD2	2.51	0.45
1:C:303:LEU:HD13	1:C:304:LYS:N	2.30	0.45
1:D:94:ARG:NH1	1:D:205:ASP:OD2	2.45	0.45
1:C:130:ILE:HD12	1:C:130:ILE:N	2.32	0.45
1:C:45:THR:O	1:C:48:SER:HB3	2.15	0.45
1:C:52:THR:HG22	3:C:486:HOH:O	2.16	0.45
1:A:196:VAL:CG1	1:A:235:VAL:HA	2.43	0.45
1:B:20:PHE:CE1	1:B:201:ASP:HB2	2.51	0.45
1:C:277:GLU:O	1:C:281:LYS:HG3	2.15	0.45
1:D:125:LYS:HA	1:D:125:LYS:HE2	1.97	0.45
1:A:206:ARG:HG2	3:A:537:HOH:O	2.17	0.45
1:D:275:ILE:H	1:D:275:ILE:HD12	1.82	0.45
1:A:177:ASN:O	1:A:184:HIS:HE1	2.00	0.44
1:A:3:ASN:HD22	1:A:3:ASN:C	2.19	0.44
1:D:204:LEU:HD22	1:D:213:ARG:HD2	1.97	0.44
1:A:125:LYS:CE	1:A:185:GLY:O	2.66	0.44
1:B:52:THR:HG22	3:B:553:HOH:O	2.16	0.44
1:D:7:TRP:HE1	1:D:247:GLN:NE2	2.15	0.44
1:C:289:TRP:O	1:C:290:GLN:NE2	2.51	0.44
1:C:142:ILE:O	1:C:304:LYS:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:VAL:CG1	1:D:235:VAL:HA	2.43	0.44
1:B:6:PHE:CD2	1:B:247:GLN:HG3	2.53	0.44
1:B:333:HIS:HD2	3:B:467:HOH:O	2.00	0.44
1:A:216:GLU:OE2	1:A:333:HIS:HE1	2.01	0.44
1:B:319:ARG:HD3	1:B:357:LYS:NZ	2.33	0.44
1:B:196:VAL:CG1	1:B:235:VAL:HA	2.44	0.44
1:D:130:ILE:HD12	1:D:130:ILE:N	2.33	0.44
1:A:243:LEU:O	1:A:247:GLN:HG3	2.19	0.43
1:C:47:PRO:HG2	1:C:202:TRP:CE2	2.53	0.43
1:D:94:ARG:HD2	1:D:94:ARG:C	2.38	0.43
1:A:173:ASN:HB3	1:C:154:TYR:CE1	2.52	0.43
1:B:281:LYS:HG3	3:B:504:HOH:O	2.18	0.43
1:C:125:LYS:HA	1:C:125:LYS:HE2	1.98	0.43
1:B:195:ASN:HD22	1:B:231:PRO:HG2	1.81	0.43
1:B:319:ARG:HD3	1:B:357:LYS:HZ2	1.83	0.43
1:B:274:ASN:O	1:B:278:GLN:HG3	2.19	0.43
1:C:283:TRP:CE3	1:C:330:VAL:HG13	2.53	0.43
1:D:195:ASN:HD22	1:D:231:PRO:HG2	1.82	0.43
1:B:130:ILE:HD12	1:B:130:ILE:N	2.33	0.43
1:C:237:GLU:HB2	1:C:238:PRO:CD	2.49	0.43
1:D:25:LEU:HD23	1:D:87:MET:HE2	2.01	0.43
1:B:197:ILE:HG21	1:B:208:VAL:HG21	2.00	0.42
1:B:310:ALA:O	1:B:314:LEU:HB2	2.18	0.42
1:C:310:ALA:O	1:C:314:LEU:HB2	2.19	0.42
1:A:207:ILE:HG23	1:A:208:VAL:H	1.81	0.42
1:C:196:VAL:CG1	1:C:235:VAL:HA	2.45	0.42
1:D:268:ASP:O	1:D:270:THR:HG23	2.19	0.42
1:C:224:ARG:NH1	1:C:224:ARG:HG2	2.34	0.42
1:D:291:LEU:HD23	1:D:291:LEU:C	2.40	0.42
1:D:94:ARG:HD2	1:D:95:LEU:N	2.34	0.42
1:B:125:LYS:CE	1:B:185:GLY:O	2.67	0.42
1:B:206:ARG:HB3	1:B:209:PRO:HD2	2.02	0.42
1:B:237:GLU:HB2	1:B:238:PRO:CD	2.49	0.42
1:D:223:ILE:CD1	1:D:276:VAL:HG21	2.49	0.42
1:A:180:ASN:HD22	1:A:180:ASN:N	2.00	0.42
1:A:178:PRO:CB	1:A:254:ALA:HB1	2.49	0.42
1:D:237:GLU:HB2	1:D:238:PRO:CD	2.50	0.42
1:C:216:GLU:OE2	1:C:336:TRP:HZ3	2.02	0.42
1:A:143:TRP:CE2	1:D:146:ARG:HB3	2.54	0.42
1:A:237:GLU:HB2	1:A:238:PRO:CD	2.50	0.42
1:C:6:PHE:CD2	1:C:247:GLN:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ILE:HD11	1:D:276:VAL:HG21	2.02	0.42
1:A:195:ASN:HD22	1:A:231:PRO:HG2	1.83	0.42
1:A:130:ILE:N	1:A:130:ILE:HD12	2.34	0.42
1:A:270:THR:CG2	1:A:274:ASN:HB3	2.50	0.42
1:D:53:ALA:O	1:D:343:HIS:HD2	2.02	0.42
1:D:269:ALA:HB2	3:D:528:HOH:O	2.18	0.41
1:D:125:LYS:CE	1:D:185:GLY:O	2.68	0.41
1:A:4:ASN:HD21	1:A:354:MET:HE1	1.86	0.41
1:A:304:LYS:HE3	3:D:383:HOH:O	2.19	0.41
1:D:94:ARG:HG3	1:D:94:ARG:HH11	1.86	0.41
1:D:310:ALA:O	1:D:314:LEU:HB2	2.21	0.41
1:D:45:THR:O	1:D:48:SER:HB3	2.20	0.41
1:B:215:PHE:HB3	1:B:283:TRP:CE2	2.55	0.41
1:B:45:THR:O	1:B:48:SER:HB3	2.20	0.41
1:C:228:ALA:O	1:C:272:VAL:HG13	2.21	0.41
1:C:284:GLY:O	1:C:285:GLU:C	2.59	0.41
1:C:356:THR:O	1:C:357:LYS:HB2	2.20	0.41
1:C:53:ALA:O	1:C:343:HIS:HD2	2.03	0.41
1:D:275:ILE:N	1:D:275:ILE:HD12	2.35	0.41
1:B:356:THR:O	1:B:357:LYS:CB	2.68	0.41
1:C:125:LYS:CE	1:C:185:GLY:O	2.68	0.41
1:C:21:LYS:NZ	3:C:494:HOH:O	2.54	0.41
1:D:142:ILE:O	1:D:304:LYS:HE2	2.20	0.41
1:C:225:ASN:HA	1:C:226:PRO:HD2	1.93	0.41
1:C:278:GLN:NE2	1:C:323:ASN:ND2	2.68	0.41
1:B:278:GLN:NE2	1:B:323:ASN:OD1	2.54	0.41
1:D:226:PRO:O	1:D:272:VAL:HG22	2.21	0.40
1:C:230:ARG:HB2	1:C:232:TRP:CE2	2.56	0.40
1:A:356:THR:O	1:A:357:LYS:OXT	2.39	0.40
1:B:207:ILE:HG21	1:B:232:TRP:CZ2	2.56	0.40
1:C:195:ASN:HD22	1:C:231:PRO:HG2	1.83	0.40
1:B:228:ALA:O	1:B:272:VAL:HG13	2.22	0.40
1:C:273:LYS:O	1:C:277:GLU:HG3	2.21	0.40
1:C:223:ILE:CD1	1:C:276:VAL:HG21	2.52	0.40
1:D:20:PHE:CD1	1:D:201:ASP:HB2	2.57	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	345/357 (97%)	339 (98%)	6 (2%)	0	100	100
1	B	342/357 (96%)	335 (98%)	7 (2%)	0	100	100
1	C	347/357 (97%)	341 (98%)	6 (2%)	0	100	100
1	D	343/357 (96%)	332 (97%)	10 (3%)	1 (0%)	41	27
All	All	1377/1428 (96%)	1347 (98%)	29 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	205	ASP

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	293/299 (98%)	285 (97%)	8 (3%)	44	31
1	B	291/299 (97%)	286 (98%)	5 (2%)	60	51
1	C	295/299 (99%)	290 (98%)	5 (2%)	60	51
1	D	292/299 (98%)	283 (97%)	9 (3%)	40	25
All	All	1171/1196 (98%)	1144 (98%)	27 (2%)	50	37

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	90	GLN
1	A	91	PRO
1	A	141	TRP
1	A	180	ASN
1	A	206	ARG
1	A	274	ASN
1	A	357	LYS
1	B	90	GLN
1	B	91	PRO
1	B	141	TRP
1	B	213	ARG
1	B	274	ASN
1	C	90	GLN
1	C	91	PRO
1	C	141	TRP
1	C	224	ARG
1	C	274	ASN
1	D	3	ASN
1	D	90	GLN
1	D	91	PRO
1	D	94	ARG
1	D	141	TRP
1	D	205	ASP
1	D	274	ASN
1	D	285	GLU
1	D	357	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	ASN
1	A	30	GLN
1	A	173	ASN
1	A	180	ASN
1	A	183	GLN
1	A	184	HIS
1	A	195	ASN
1	A	233	GLN
1	A	247	GLN
1	A	261	ASN
1	A	274	ASN

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Mol	Chain	Res	Type
1	A	278	GLN
1	A	313	GLN
1	A	333	HIS
1	A	343	HIS
1	A	352	ASN
1	B	30	GLN
1	B	173	ASN
1	B	195	ASN
1	B	233	GLN
1	B	261	ASN
1	B	274	ASN
1	B	278	GLN
1	B	313	GLN
1	B	333	HIS
1	B	335	ASN
1	B	352	ASN
1	C	4	ASN
1	C	30	GLN
1	C	173	ASN
1	C	180	ASN
1	C	195	ASN
1	C	217	GLN
1	C	225	ASN
1	C	227	HIS
1	C	233	GLN
1	C	261	ASN
1	C	274	ASN
1	C	278	GLN
1	C	290	GLN
1	C	323	ASN
1	C	352	ASN
1	D	3	ASN
1	D	30	GLN
1	D	173	ASN
1	D	183	GLN
1	D	195	ASN
1	D	233	GLN
1	D	247	GLN
1	D	261	ASN
1	D	278	GLN
1	D	313	GLN
1	D	333	HIS

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Mol	Chain	Res	Type
1	D	335	ASN
1	D	352	ASN

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

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	A	360	-	42,48,48	2.17	9 (21%)	50,73,73	1.75	8 (16%)
2	NAD	C	360	-	42,48,48	2.20	7 (16%)	50,73,73	1.81	8 (16%)
2	NAD	B	360	-	42,48,48	2.21	9 (21%)	50,73,73	1.77	8 (16%)
2	NAD	D	360	-	42,48,48	2.17	8 (19%)	50,73,73	1.77	7 (14%)

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	360	-	-	6/26/62/62	0/5/5/5
2	NAD	C	360	-	-	5/26/62/62	0/5/5/5
2	NAD	B	360	-	-	6/26/62/62	0/5/5/5
2	NAD	D	360	-	-	5/26/62/62	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	360	NAD	C4N-C3N	7.57	1.52	1.39
2	A	360	NAD	C4N-C3N	7.39	1.51	1.39
2	C	360	NAD	C4N-C3N	7.25	1.51	1.39
2	C	360	NAD	C2N-C3N	7.15	1.50	1.39
2	D	360	NAD	C4N-C3N	7.13	1.51	1.39
2	D	360	NAD	C2N-C3N	7.10	1.50	1.39
2	B	360	NAD	C2N-C3N	6.94	1.49	1.39
2	A	360	NAD	C2N-C3N	6.84	1.49	1.39
2	C	360	NAD	C5N-C4N	5.25	1.50	1.38
2	B	360	NAD	C5N-C4N	5.07	1.49	1.38
2	C	360	NAD	C2N-N1N	5.00	1.41	1.35
2	A	360	NAD	C5N-C4N	4.98	1.49	1.38
2	D	360	NAD	C2N-N1N	4.92	1.41	1.35
2	A	360	NAD	C2N-N1N	4.76	1.40	1.35
2	D	360	NAD	C5N-C4N	4.76	1.48	1.38
2	B	360	NAD	C2N-N1N	4.76	1.40	1.35
2	B	360	NAD	C6N-N1N	3.33	1.43	1.35
2	A	360	NAD	C6N-N1N	3.28	1.43	1.35
2	C	360	NAD	C6N-N1N	3.25	1.43	1.35
2	D	360	NAD	C6N-N1N	3.13	1.43	1.35
2	C	360	NAD	C6N-C5N	-2.94	1.32	1.38
2	D	360	NAD	C6N-C5N	-2.87	1.32	1.38
2	B	360	NAD	C6N-C5N	-2.74	1.32	1.38
2	A	360	NAD	C6N-C5N	-2.59	1.32	1.38
2	D	360	NAD	C2D-C1D	-2.44	1.50	1.53
2	A	360	NAD	C2A-N1A	2.39	1.38	1.33
2	B	360	NAD	C2D-C1D	-2.36	1.50	1.53
2	B	360	NAD	C2A-N1A	2.33	1.38	1.33
2	D	360	NAD	C2A-N1A	2.24	1.38	1.33
2	B	360	NAD	C3N-C7N	-2.11	1.47	1.50
2	C	360	NAD	C2A-N1A	2.07	1.37	1.33
2	A	360	NAD	C2B-C1B	-2.06	1.50	1.53
2	A	360	NAD	C2D-C1D	-2.05	1.50	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	360	NAD	C5N-C4N-C3N	-6.27	112.93	120.34
2	A	360	NAD	C5N-C4N-C3N	-6.25	112.95	120.34
2	C	360	NAD	C5N-C4N-C3N	-6.18	113.03	120.34
2	D	360	NAD	C5N-C4N-C3N	-6.13	113.09	120.34
2	C	360	NAD	C3N-C7N-N7N	4.82	123.53	117.75
2	D	360	NAD	C3N-C7N-N7N	4.56	123.22	117.75
2	B	360	NAD	C3N-C7N-N7N	4.55	123.21	117.75
2	A	360	NAD	C3N-C7N-N7N	4.34	122.96	117.75
2	D	360	NAD	C6N-C5N-C4N	4.26	125.63	119.44
2	C	360	NAD	C6N-C5N-C4N	4.25	125.62	119.44
2	A	360	NAD	C6N-C5N-C4N	4.23	125.58	119.44
2	B	360	NAD	C6N-C5N-C4N	4.22	125.58	119.44
2	C	360	NAD	C5A-C6A-N6A	3.91	126.29	120.35
2	D	360	NAD	C5A-C6A-N6A	3.86	126.22	120.35
2	A	360	NAD	C5A-C6A-N6A	3.72	126.01	120.35
2	B	360	NAD	C5A-C6A-N6A	3.71	125.99	120.35
2	C	360	NAD	O4B-C1B-C2B	-3.49	101.83	106.93
2	B	360	NAD	C6N-N1N-C2N	-3.38	118.90	121.97
2	A	360	NAD	C6N-N1N-C2N	-3.31	118.96	121.97
2	D	360	NAD	C6N-N1N-C2N	-3.29	118.97	121.97
2	C	360	NAD	C6N-N1N-C2N	-3.29	118.98	121.97
2	D	360	NAD	O4B-C1B-C2B	-2.84	102.78	106.93
2	A	360	NAD	O4B-C1B-C2B	-2.72	102.94	106.93
2	B	360	NAD	O4B-C1B-C2B	-2.70	102.98	106.93
2	C	360	NAD	O7N-C7N-C3N	-2.47	116.67	119.63
2	D	360	NAD	O7N-C7N-C3N	-2.44	116.71	119.63
2	B	360	NAD	O7N-C7N-C3N	-2.38	116.79	119.63
2	A	360	NAD	O7N-C7N-C3N	-2.17	117.04	119.63
2	B	360	NAD	O4B-C4B-C5B	-2.13	102.36	109.37
2	C	360	NAD	O4B-C4B-C5B	-2.11	102.44	109.37
2	A	360	NAD	O4B-C4B-C5B	-2.09	102.50	109.37

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	360	NAD	C5D-O5D-PN-O1N
2	A	360	NAD	C5D-O5D-PN-O2N
2	C	360	NAD	C5D-O5D-PN-O1N
2	C	360	NAD	C5D-O5D-PN-O2N
2	B	360	NAD	C5D-O5D-PN-O1N

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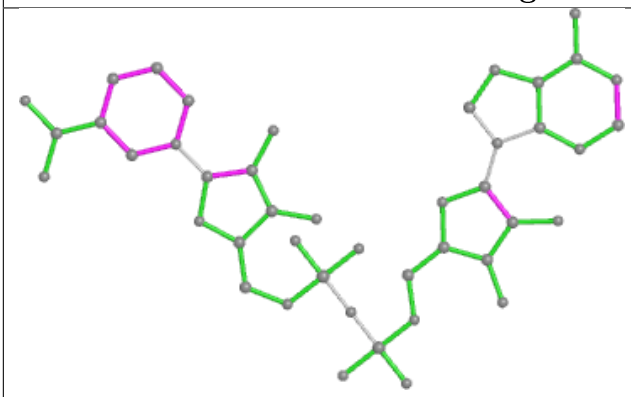
Mol	Chain	Res	Type	Atoms
2	B	360	NAD	C5D-O5D-PN-O2N
2	D	360	NAD	C5D-O5D-PN-O1N
2	D	360	NAD	C5D-O5D-PN-O2N
2	C	360	NAD	PA-O3-PN-O2N
2	D	360	NAD	PA-O3-PN-O2N
2	A	360	NAD	PA-O3-PN-O2N
2	B	360	NAD	PA-O3-PN-O2N
2	B	360	NAD	O4B-C4B-C5B-O5B
2	A	360	NAD	O4B-C4B-C5B-O5B
2	C	360	NAD	O4B-C4B-C5B-O5B
2	D	360	NAD	O4B-C4B-C5B-O5B
2	A	360	NAD	C5D-O5D-PN-O3
2	C	360	NAD	C5D-O5D-PN-O3
2	B	360	NAD	C5D-O5D-PN-O3
2	D	360	NAD	C5D-O5D-PN-O3
2	A	360	NAD	PA-O3-PN-O1N
2	B	360	NAD	PA-O3-PN-O1N

There are no ring outliers.

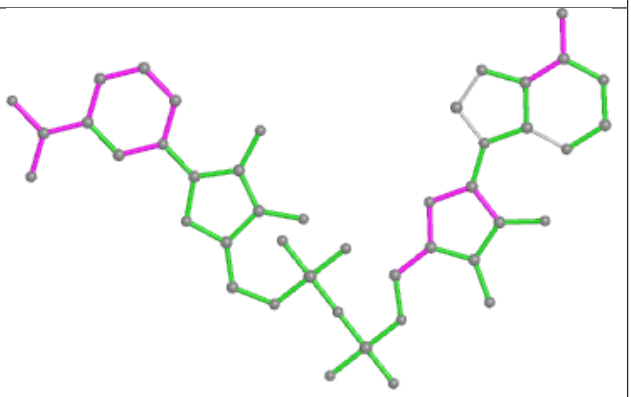
No monomer is involved in short contacts.

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 then 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.

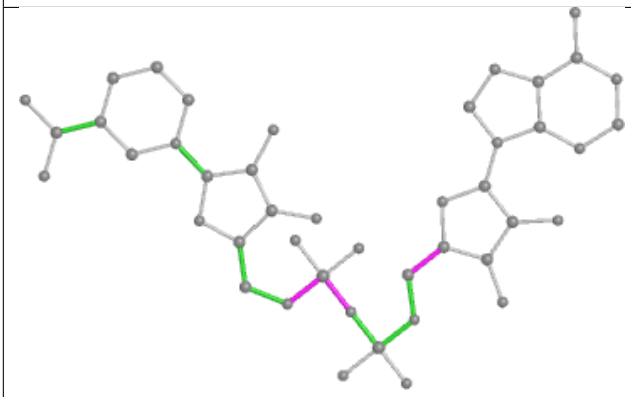
Ligand NAD A 360



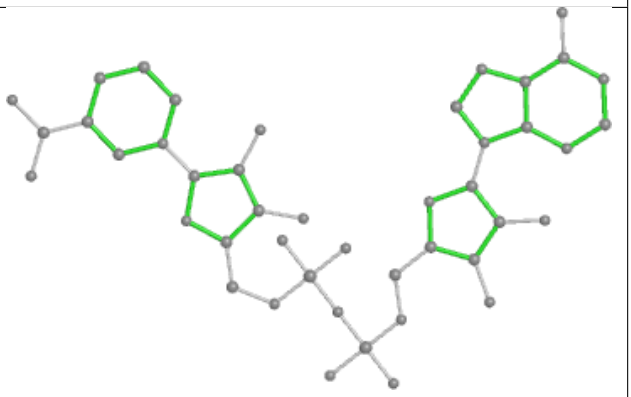
Bond lengths



Bond angles

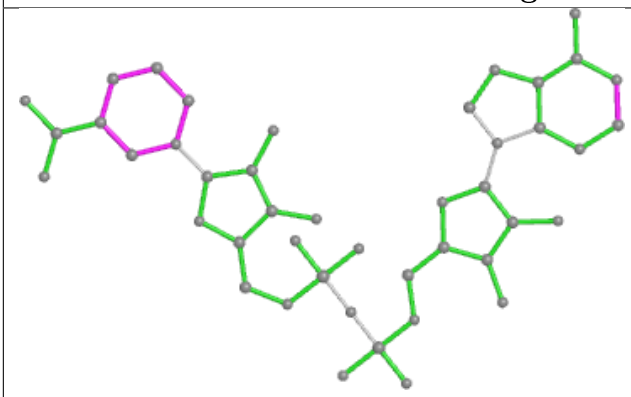


Torsions

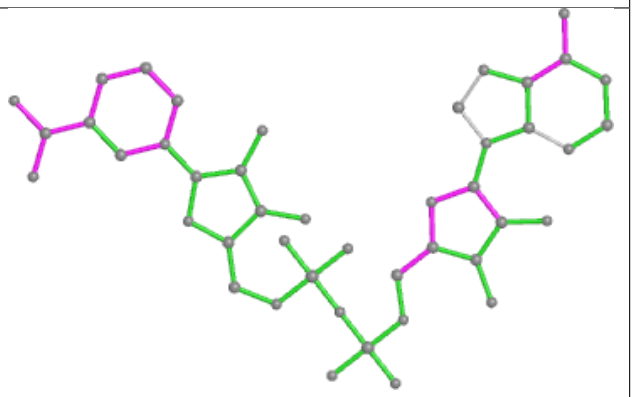


Rings

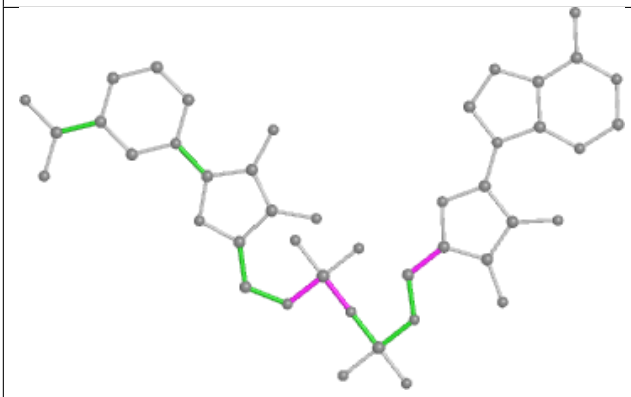
Ligand NAD C 360



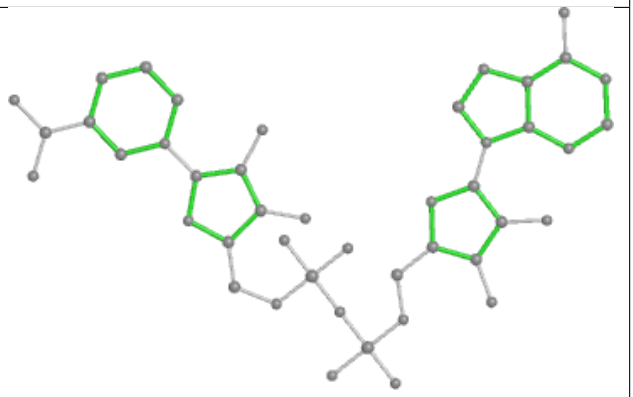
Bond lengths



Bond angles

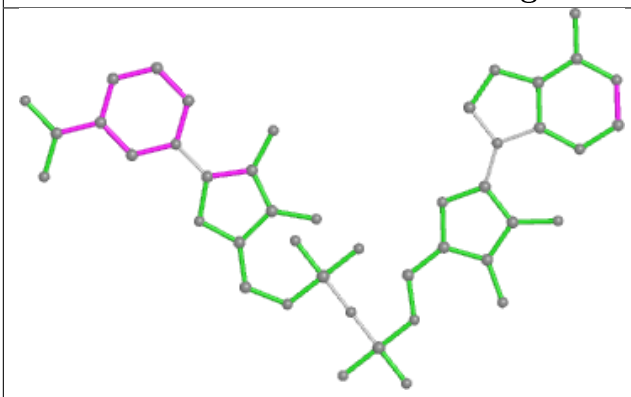


Torsions

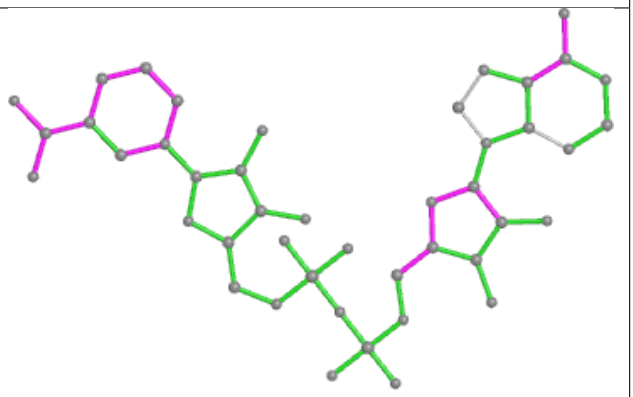


Rings

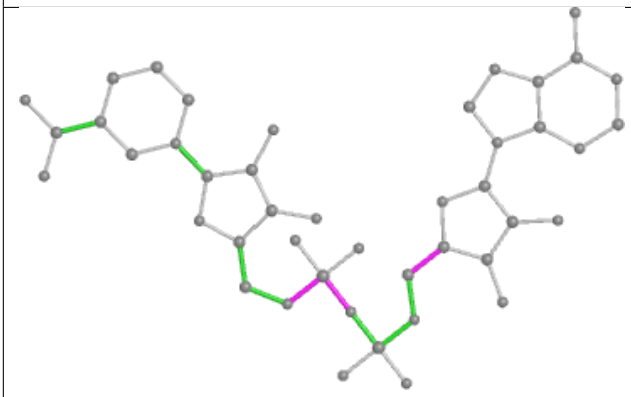
Ligand NAD B 360



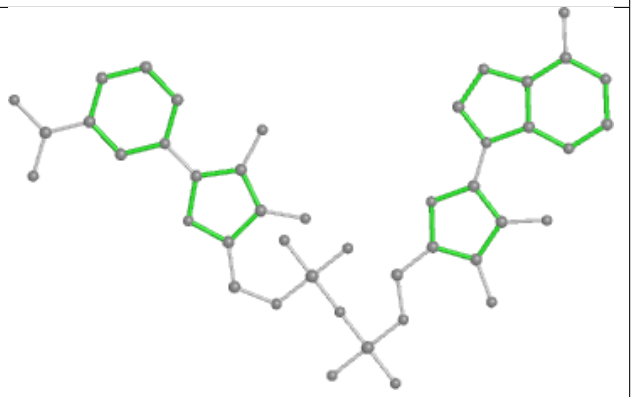
Bond lengths



Bond angles

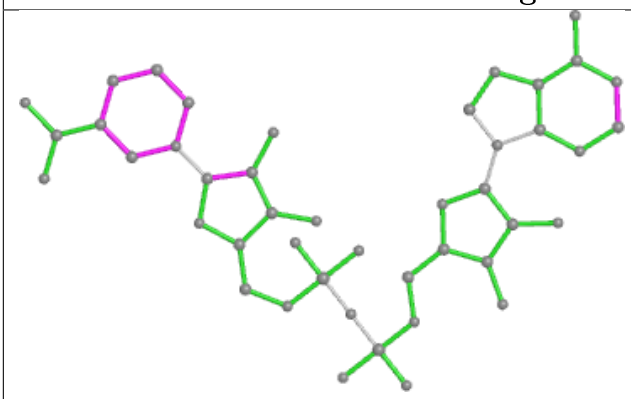


Torsions

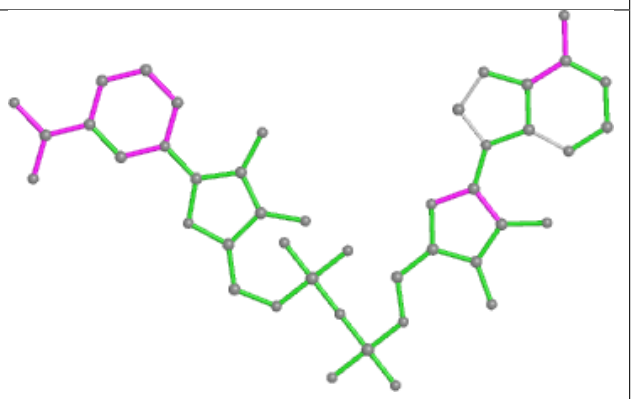


Rings

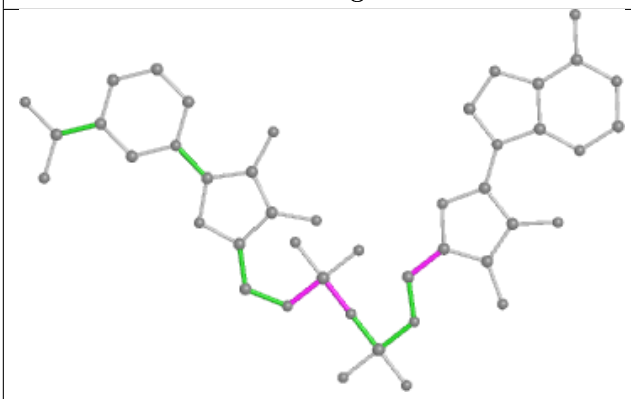
Ligand NAD D 360



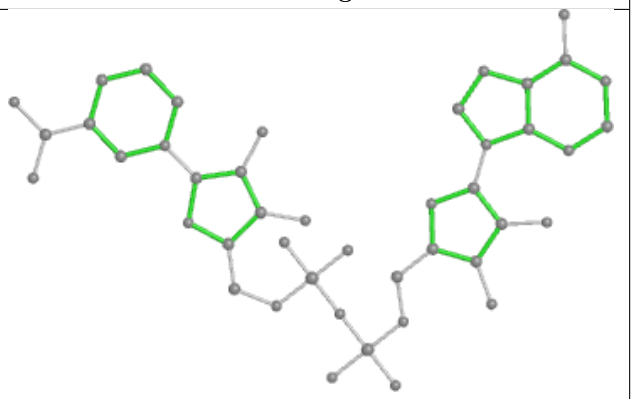
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	349/357 (97%)	0.21	11 (3%)	47	41	11, 20, 47, 64	0
1	B	346/357 (96%)	0.46	30 (8%)	10	8	12, 23, 60, 81	0
1	C	351/357 (98%)	0.53	29 (8%)	11	8	11, 25, 52, 82	0
1	D	347/357 (97%)	0.43	37 (10%)	6	4	12, 22, 54, 82	0
All	All	1393/1428 (97%)	0.41	107 (7%)	13	10	11, 22, 54, 82	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	ILE	8.8
1	B	223	ILE	8.2
1	B	224	ARG	7.8
1	B	289	TRP	6.5
1	A	300	ALA	6.0
1	D	357	LYS	5.9
1	B	225	ASN	5.9
1	C	222	ILE	5.5
1	C	2	ILE	5.2
1	D	301	HIS	5.0
1	D	204	LEU	4.9
1	D	289	TRP	4.8
1	C	357	LYS	4.6
1	B	357	LYS	4.5
1	C	3	ASN	4.3
1	D	302	TYR	4.3
1	C	286	GLY	4.0
1	B	227	HIS	4.0
1	D	227	HIS	3.9
1	D	285	GLU	3.8
1	C	298	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	285	GLU	3.8
1	D	267	ALA	3.8
1	D	269	ALA	3.8
1	D	274	ASN	3.8
1	B	220	PRO	3.6
1	C	289	TRP	3.6
1	C	290	GLN	3.6
1	D	232	TRP	3.5
1	C	224	ARG	3.4
1	D	225	ASN	3.3
1	B	204	LEU	3.3
1	D	223	ILE	3.3
1	D	268	ASP	3.2
1	D	284	GLY	3.2
1	B	290	GLN	3.2
1	C	300	ALA	3.2
1	C	207	ILE	3.2
1	A	357	LYS	3.2
1	B	221	VAL	3.1
1	D	282	TYR	3.0
1	D	228	ALA	3.0
1	B	285	GLU	3.0
1	B	274	ASN	2.9
1	D	278	GLN	2.9
1	C	291	LEU	2.9
1	D	87	MET	2.9
1	D	224	ARG	2.9
1	D	281	LYS	2.9
1	D	272	VAL	2.8
1	D	286	GLY	2.8
1	B	87	MET	2.7
1	C	288	SER	2.7
1	D	205	ASP	2.7
1	B	284	GLY	2.7
1	C	274	ASN	2.6
1	C	221	VAL	2.6
1	A	130	ILE	2.6
1	C	219	GLN	2.6
1	B	196	VAL	2.5
1	D	222	ILE	2.5
1	D	275	ILE	2.5
1	D	288	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	130	ILE	2.4
1	C	330	VAL	2.4
1	B	205	ASP	2.4
1	C	282	TYR	2.4
1	D	219	GLN	2.4
1	D	287	ALA	2.4
1	C	220	PRO	2.4
1	A	183	GLN	2.3
1	B	213	ARG	2.3
1	A	274	ASN	2.3
1	B	207	ILE	2.3
1	B	281	LYS	2.3
1	C	317	HIS	2.3
1	B	94	ARG	2.3
1	A	224	ARG	2.3
1	B	242	TYR	2.2
1	A	87	MET	2.2
1	B	130	ILE	2.2
1	A	154	TYR	2.2
1	A	94	ARG	2.2
1	B	226	PRO	2.2
1	B	302	TYR	2.2
1	D	290	GLN	2.2
1	D	196	VAL	2.2
1	C	223	ILE	2.2
1	C	218	SER	2.2
1	D	221	VAL	2.2
1	C	226	PRO	2.1
1	C	142	ILE	2.1
1	C	254	ALA	2.1
1	A	299	GLU	2.1
1	B	270	THR	2.1
1	D	280	VAL	2.1
1	B	228	ALA	2.1
1	D	3	ASN	2.1
1	A	291	LEU	2.1
1	C	87	MET	2.0
1	B	3	ASN	2.0
1	B	191	VAL	2.0
1	B	271	PRO	2.0
1	D	213	ARG	2.0
1	D	218	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	191	VAL	2.0
1	D	94	ARG	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)

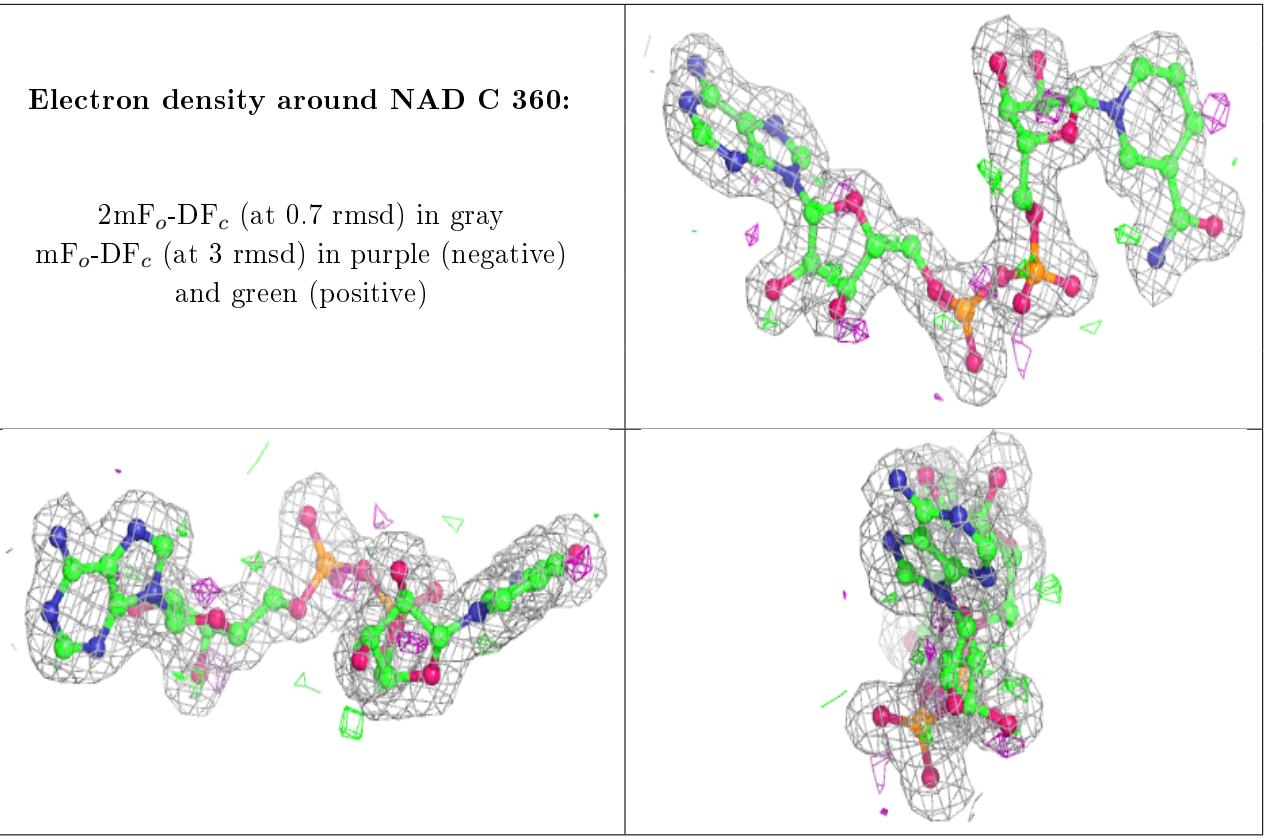
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	C	360	44/44	0.94	0.12	14,19,21,24	0
2	NAD	D	360	44/44	0.95	0.12	13,17,19,19	0
2	NAD	B	360	44/44	0.96	0.12	15,18,21,23	0
2	NAD	A	360	44/44	0.96	0.12	11,16,19,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

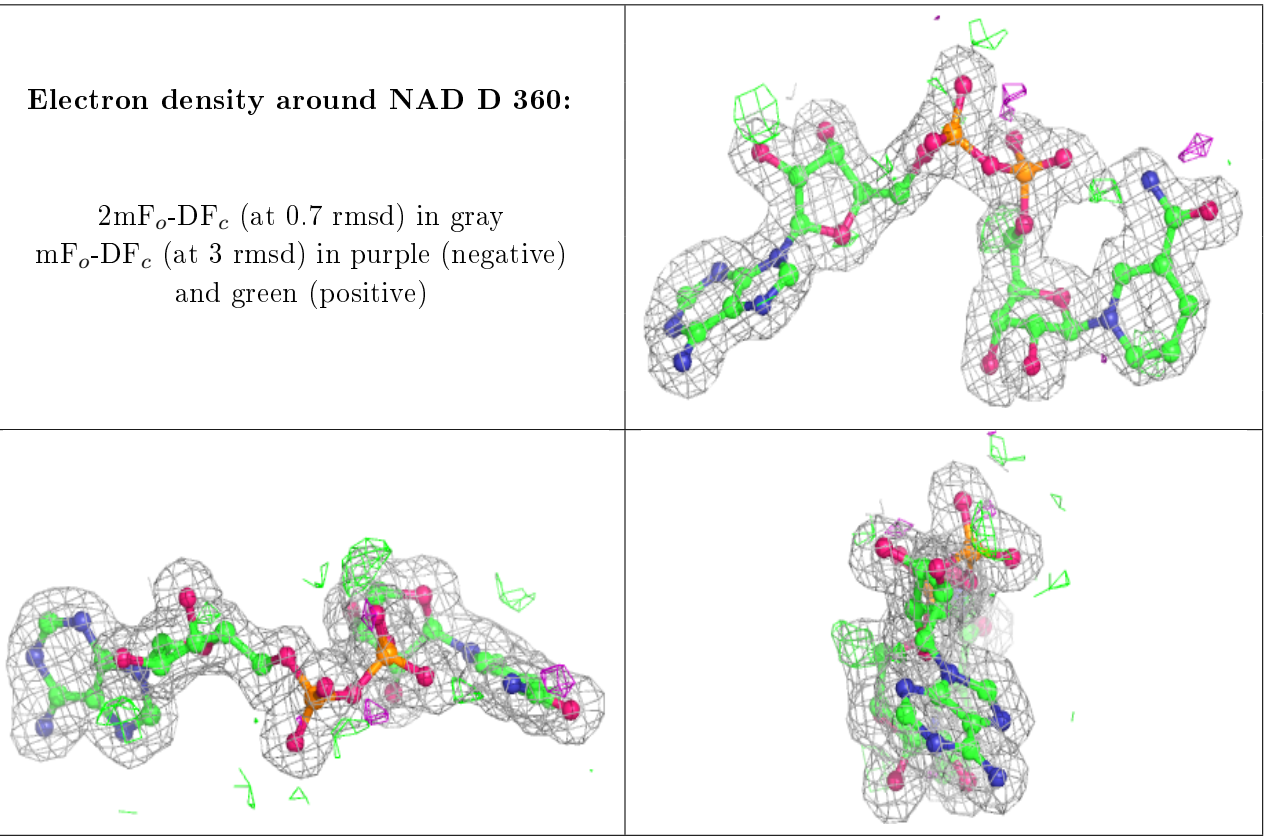
Electron density around NAD C 360:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



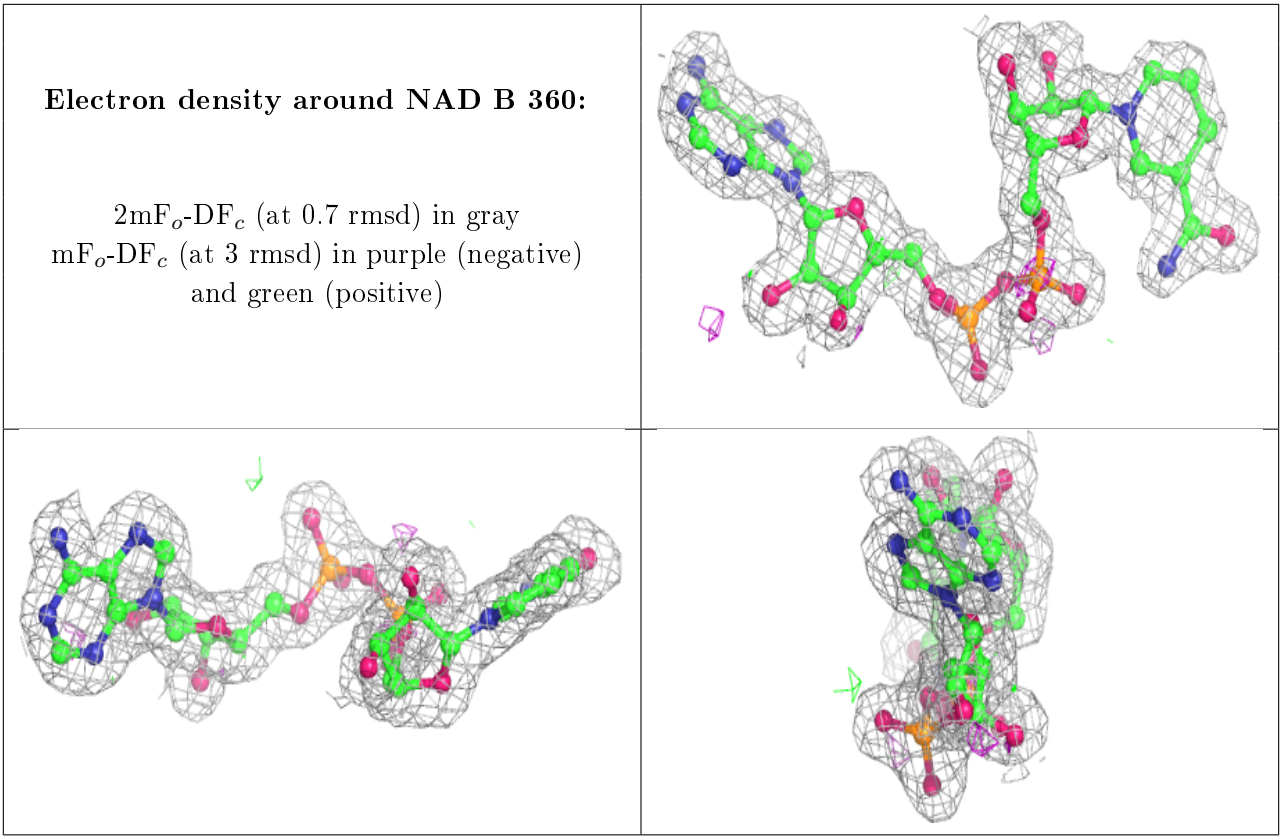
Electron density around NAD D 360:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



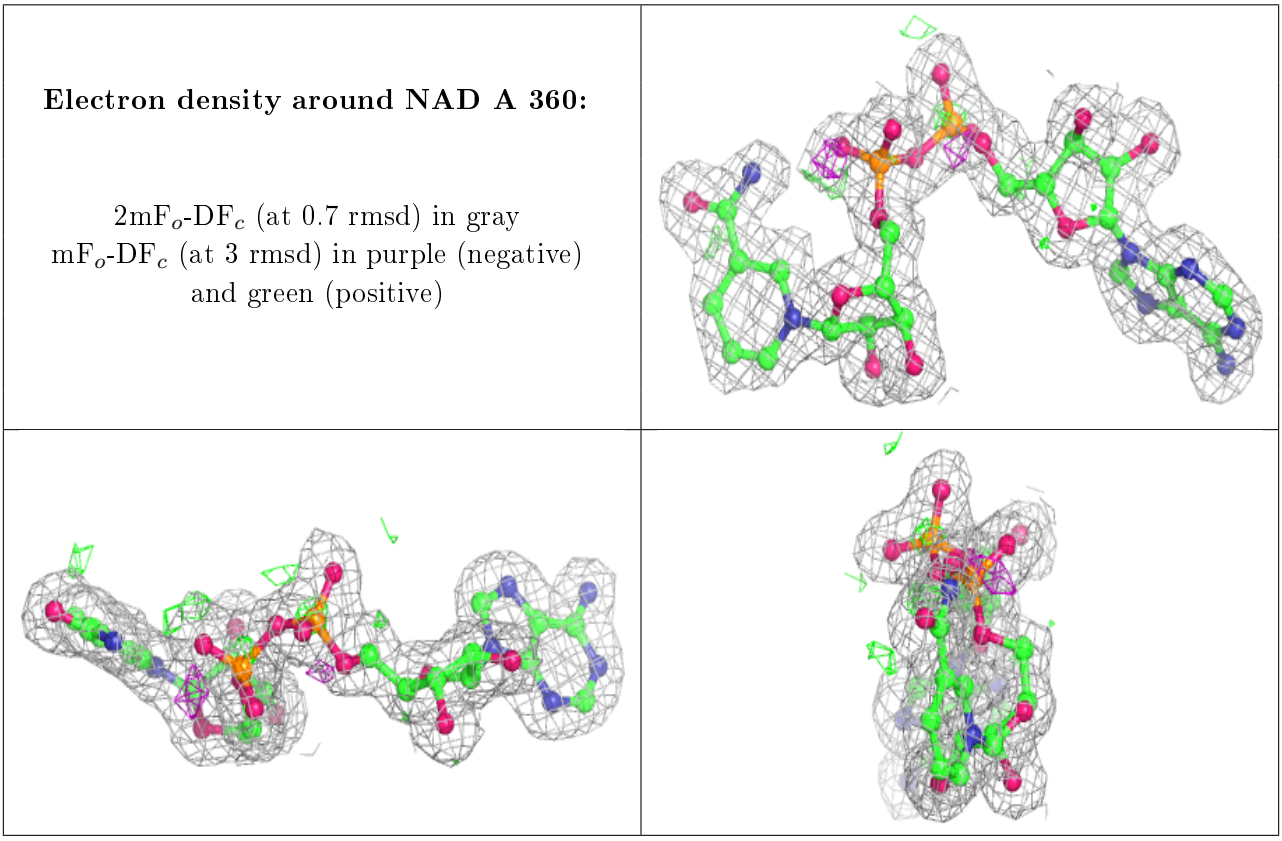
Electron density around NAD B 360:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NAD A 360:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.