



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:28 PM UTC

PDB ID : 1RKX / pdb_00001rkx
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 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

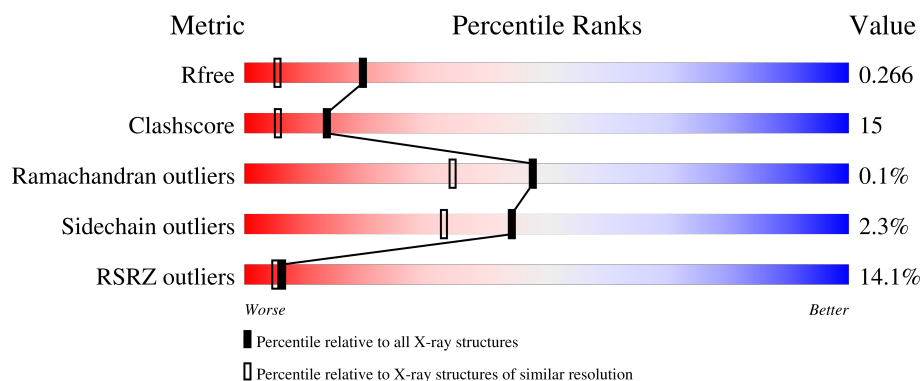
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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 $\leq 5\%$. 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	8% 75% 20% ..
1	B	357	15% 72% 23% ..
1	C	357	17% 69% 27% ..
1	D	357	16% 72% 23% ..

2 Entry composition [i](#)

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 (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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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		

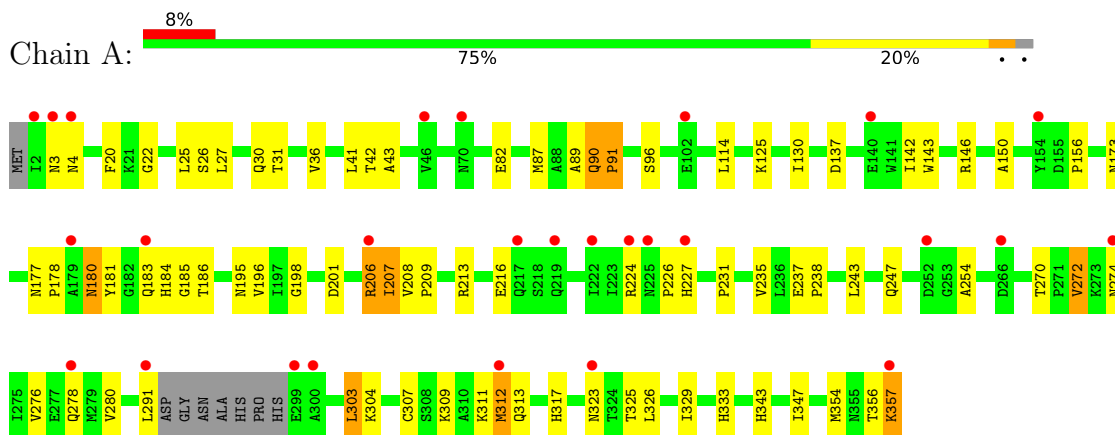
- Molecule 3 is water.

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		

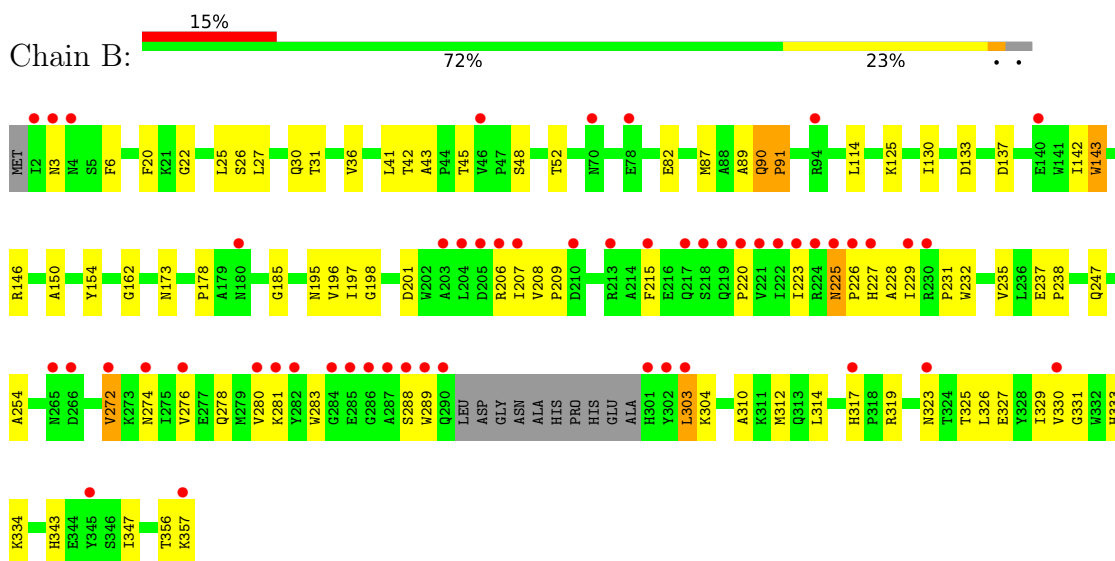
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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 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

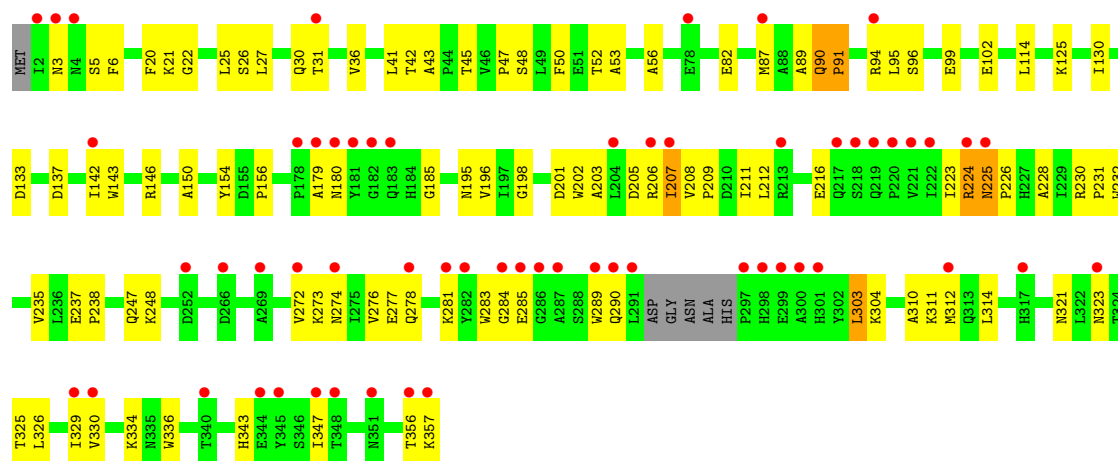


- Molecule 1: CDP-glucose-4,6-dehydratase

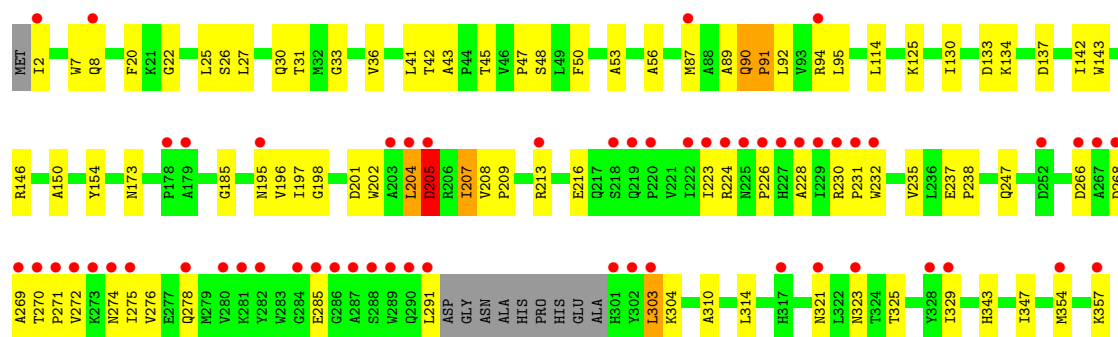
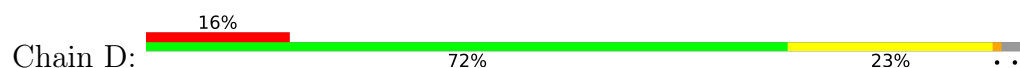


- Molecule 1: CDP-glucose-4,6-dehydratase





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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.81Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.229 , 0.266 0.229 , 0.266	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 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.38	0/2864	0.88	8/3897 (0.2%)
1	B	0.36	0/2842	0.88	11/3867 (0.3%)
1	C	0.36	0/2883	0.89	11/3923 (0.3%)
1	D	0.37	0/2850	0.89	8/3878 (0.2%)
All	All	0.37	0/11439	0.89	38/15565 (0.2%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	207	ILE	N-CA-C	8.97	119.03	110.42
1	C	207	ILE	N-CA-C	7.46	118.19	110.36
1	D	41	LEU	N-CA-C	-6.95	100.52	110.59
1	C	41	LEU	N-CA-C	-6.66	100.94	110.59
1	A	207	ILE	N-CA-C	6.62	117.11	110.23
1	B	41	LEU	N-CA-C	-6.37	101.35	110.59
1	D	150	ALA	N-CA-C	6.36	119.45	110.23
1	B	36	VAL	N-CA-C	6.34	117.72	108.53
1	A	36	VAL	N-CA-C	6.33	117.71	108.53
1	C	150	ALA	N-CA-C	6.32	119.39	110.23
1	D	36	VAL	N-CA-C	6.32	117.69	108.53
1	B	150	ALA	N-CA-C	6.29	119.35	110.23
1	C	36	VAL	N-CA-C	6.29	117.64	108.53
1	C	90	GLN	N-CA-C	-6.23	96.05	109.81
1	A	41	LEU	N-CA-C	-6.21	101.58	110.59
1	B	90	GLN	N-CA-C	-6.20	96.10	109.81
1	A	150	ALA	N-CA-C	6.19	119.20	110.23
1	A	90	GLN	N-CA-C	-6.16	96.20	109.81
1	D	90	GLN	N-CA-C	-6.04	96.45	109.81
1	C	82	GLU	N-CA-C	-5.89	106.26	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	MET	N-CA-C	5.73	117.32	111.14
1	B	82	GLU	N-CA-C	-5.61	106.60	113.50
1	C	321	ASN	N-CA-C	-5.47	103.68	110.41
1	D	133	ASP	N-CA-C	-5.47	105.86	112.54
1	B	137	ASP	N-CA-C	-5.35	101.99	109.96
1	D	137	ASP	N-CA-C	-5.30	102.07	109.96
1	A	137	ASP	N-CA-C	-5.28	102.09	109.96
1	A	82	GLU	N-CA-C	-5.28	107.01	113.50
1	C	225	ASN	CA-C-N	5.23	124.89	119.56
1	C	225	ASN	C-N-CA	5.23	124.89	119.56
1	B	143	TRP	N-CA-C	5.21	118.60	110.32
1	C	133	ASP	N-CA-C	-5.20	106.20	112.54
1	B	133	ASP	N-CA-C	-5.18	106.22	112.54
1	C	137	ASP	N-CA-C	-5.12	102.47	110.10
1	B	162	GLY	N-CA-C	-5.07	106.65	112.73
1	B	225	ASN	CA-C-N	5.05	124.84	119.28
1	B	225	ASN	C-N-CA	5.05	124.84	119.28
1	D	205	ASP	N-CA-C	-5.00	100.14	110.80

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	88	0
1	B	2763	0	2651	78	0
1	C	2802	0	2688	87	0
1	D	2771	0	2662	83	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	213	0	0	4	0
All	All	12159	0	10778	323	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 15.

All (323) 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:94:ARG:HH12	1:D:205:ASP:CG	1.81	0.87
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: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
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:278:GLN:HE22	1:D:323:ASN:CG	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ALA:HB3	1:C:206:ARG:HD2	1.75	0.68
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:A:4:ASN:HD21	1:A:354:MET:HE1	1.58	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: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:B:142:ILE:O	1:B:304:LYS:HE2	1.99	0.63
1:A:356:THR:C	1:A:357:LYS:HG3	2.24	0.63
1:B:89:ALA:O	1:B:91:PRO:HD3	1.98	0.63
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:2:ILE:HA	1:D:247:GLN:HE22	1.69	0.58
1:D:204:LEU:HD21	1:D:213:ARG:HD2	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3:ASN:CG	1:B:247:GLN:HE22	2.16	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:C:179:ALA:C	1:C:180:ASN:HD22	2.17	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:HD22	1:C:323:ASN:N	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:22:GLY:HA2	1:C:87:MET:CE	2.40	0.51
1:C:278:GLN:NE2	1:C:326:LEU:HD12	2.25	0.51
1:D:22:GLY:HA2	1:D:87:MET:CE	2.41	0.51
1:C:25:LEU:HD23	1:C:87:MET:HE2	1.93	0.51
1:B:198:GLY:CA	1:B:329:ILE:HD12	2.38	0.51
1:C:22:GLY:HA2	1:C:87:MET:HE3	1.92	0.51
1:D:22:GLY:HA2	1:D:87:MET:HE3	1.93	0.51
1:A:357:LYS:HG2	3:A:539:HOH:O	2.09	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:A:143:TRP:CD2	1:D:146:ARG:HD2	2.45	0.50
1:C:96:SER:HB2	1:C:156:PRO:HB2	1.93	0.50
1:B:323:ASN:O	1:B:327:GLU:HG3	2.10	0.50
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASN:C	1:A:3:ASN:HD22	2.19	0.49
1:A:25:LEU:HD23	1:A:87:MET:HE2	1.95	0.49
1:A:333:HIS:HD2	3:A:410:HOH:O	1.95	0.49
1:C:95:LEU:HD11	1:C:99:GLU:OE2	2.13	0.49
1:C:226:PRO:HA	1:C:272:VAL:CG2	2.42	0.49
1:A:146:ARG:HD2	1:D:143:TRP:CD2	2.47	0.49
1:B:22:GLY:HA2	1:B:87:MET:HE3	1.94	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:25:LEU:HD23	1:B:87:MET:HE2	1.95	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:A:22:GLY:HA2	1:A:87:MET:CE	2.43	0.48
1:B:22:GLY:HA2	1:B:87:MET:CE	2.42	0.48
1:B:173:ASN:HB3	1:D:154:TYR:CE1	2.49	0.48
1:A:22:GLY:HA2	1:A:87:MET:HE3	1.94	0.48
1:A:226:PRO:HA	1:A:272:VAL:HG22	1.96	0.48
1:A:357:LYS:HE2	1:A:357:LYS:OXT	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: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:94:ARG:HD2	1:D:94:ARG:C	2.38	0.48
1:D:197:ILE:HG21	1:D:208:VAL:HG21	1.94	0.48
1:D:25:LEU:HD23	1:D:87:MET:HE2	1.96	0.48
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:C:225:ASN:ND2	1:C:228:ALA:HB2	2.29	0.47
1:D:291:LEU:C	1:D:291:LEU:HD23	2.40	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
1:C:226:PRO:HA	1:C:272:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LYS:HE2	1:B:125:LYS:HA	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:317:HIS:CE1	1:A:357:LYS:HE3	2.51	0.46
1:A:356:THR:HG22	1:A:357:LYS:HG3	1.97	0.46
1:C:25:LEU:CD2	1:C:87:MET:HE2	2.46	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: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:C:284:GLY:O	1:C:285:GLU:C	2.59	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: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:C:130:ILE:N	1:C:130:ILE:HD12	2.32	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:HE2	1:D:125:LYS:HA	1.97	0.45
1:A:206:ARG:HG2	3:A:537:HOH:O	2.17	0.45
1:D:275:ILE:HD12	1:D:275:ILE:H	1.82	0.45
1:A:25:LEU:CD2	1:A:87:MET:HE2	2.47	0.45
1:A:177:ASN:O	1:A:184:HIS:HE1	2.00	0.44
1:B:25:LEU:CD2	1:B:87:MET:HE2	2.47	0.44
1:D:204:LEU:HD22	1:D:213:ARG:HD2	1.97	0.44
1:D:266:ASP:C	1:D:268:ASP:N	2.75	0.44
1:A:125:LYS:CE	1:A:185:GLY:O	2.66	0.44
1:D:25:LEU:CD2	1:D:87:MET:HE2	2.47	0.44
1:B:52:THR:HG22	3:B:553:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:HD13	1:B:303:LEU:C	2.41	0.44
1:D:7:TRP:HE1	1:D:247:GLN:NE2	2.15	0.44
1:C:142:ILE:O	1:C:304:LYS:HE2	2.17	0.44
1:C:289:TRP:O	1:C:290:GLN:NE2	2.51	0.44
1:D:196:VAL:CG1	1:D:235:VAL:HA	2.43	0.44
1:D:303:LEU:HD13	1:D:303:LEU:C	2.42	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:42:THR:O	1:D:43:ALA:C	2.60	0.44
1:D:94:ARG:C	1:D:94:ARG:CD	2.91	0.44
1:D:130:ILE:N	1:D:130:ILE:HD12	2.33	0.44
1:B:42:THR:O	1:B:43:ALA:C	2.61	0.43
1:C:42:THR:O	1:C:43:ALA:C	2.61	0.43
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:A:173:ASN:HB3	1:C:154:TYR:CE1	2.52	0.43
1:A:303:LEU:HD13	1:A:303:LEU:C	2.42	0.43
1:B:281:LYS:HG3	3:B:504:HOH:O	2.18	0.43
1:C:125:LYS:HE2	1:C:125:LYS:HA	1.98	0.43
1:B:195:ASN:HD22	1:B:231:PRO:HG2	1.81	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:C:303:LEU:HD13	1:C:303:LEU:C	2.44	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:A:42:THR:O	1:A:43:ALA:C	2.62	0.42
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:B:319:ARG:HD3	1:B:357:LYS:HZ2	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:178:PRO:CB	1:A:254:ALA:HB1	2.49	0.42
1:A:180:ASN:HD22	1:A:180:ASN:N	2.00	0.42
1:D:237:GLU:HB2	1:D:238:PRO:CD	2.50	0.42
1:A:143:TRP:CE2	1:D:146:ARG:HB3	2.54	0.42
1:C:216:GLU:OE2	1:C:336:TRP:HZ3	2.02	0.42
1:D:266:ASP:C	1:D:268:ASP:H	2.26	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
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:304:LYS:HE3	3:D:383:HOH:O	2.19	0.41
1:D:94:ARG:HH11	1:D:94:ARG:HG3	1.86	0.41
1:D:45:THR:O	1:D:48:SER:HB3	2.20	0.41
1:D:274:ASN:C	1:D:274:ASN:HD22	2.28	0.41
1:D:310:ALA:O	1:D:314:LEU:HB2	2.21	0.41
1:B:45:THR:O	1:B:48:SER:HB3	2.20	0.41
1:B:215:PHE:HB3	1:B:283:TRP:CE2	2.55	0.41
1:C:53:ALA:O	1:C:343:HIS:HD2	2.03	0.41
1:C:228:ALA:O	1:C:272:VAL:HG13	2.21	0.41
1:D:275:ILE:HD12	1:D:275:ILE:N	2.35	0.41
1:B:356:THR:O	1:B:357:LYS:CB	2.68	0.41
1:C:21:LYS:NZ	3:C:494:HOH:O	2.54	0.41
1:C:125:LYS:CE	1:C:185:GLY:O	2.68	0.41
1:C:311:LYS:HG2	1:C:312:MET:HE2	2.03	0.41
1:D:142:ILE:O	1:D:304:LYS:HE2	2.20	0.41
1:B:278:GLN:NE2	1:B:323:ASN:OD1	2.54	0.41
1:C:102:GLU:CD	1:C:102:GLU:H	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ALA:O	1:B:272:VAL:HG13	2.22	0.40
1:C:223:ILE:CD1	1:C:276:VAL:HG21	2.52	0.40
1:C:273:LYS:O	1:C:277:GLU:HG3	2.21	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 [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	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%)	36	25
All	All	1377/1428 (96%)	1347 (98%)	29 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	205	ASP

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	293/299 (98%)	285 (97%)	8 (3%)	39	27
1	B	291/299 (97%)	286 (98%)	5 (2%)	53	45
1	C	295/299 (99%)	290 (98%)	5 (2%)	53	45
1	D	292/299 (98%)	283 (97%)	9 (3%)	35	23
All	All	1171/1196 (98%)	1144 (98%)	27 (2%)	44	33

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

Mol	Chain	Res	Type
1	A	90	GLN
1	A	91	PRO
1	A	114	LEU
1	A	180	ASN
1	A	206	ARG
1	A	272	VAL
1	A	303	LEU
1	A	357	LYS
1	B	90	GLN
1	B	91	PRO
1	B	114	LEU
1	B	272	VAL
1	B	303	LEU
1	C	90	GLN
1	C	91	PRO
1	C	114	LEU
1	C	224	ARG
1	C	303	LEU
1	D	90	GLN
1	D	91	PRO
1	D	114	LEU
1	D	204	LEU
1	D	205	ASP
1	D	285	GLU
1	D	303	LEU
1	D	354	MET
1	D	357	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN

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Mol	Chain	Res	Type
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	265	ASN
1	A	274	ASN
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	233	GLN
1	B	247	GLN
1	B	261	ASN
1	B	274	ASN
1	B	278	GLN
1	B	333	HIS
1	B	343	HIS
1	B	352	ASN
1	C	4	ASN
1	C	30	GLN
1	C	173	ASN
1	C	180	ASN
1	C	183	GLN
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

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Mol	Chain	Res	Type
1	C	335	ASN
1	C	352	ASN
1	D	3	ASN
1	D	8	GLN
1	D	30	GLN
1	D	173	ASN
1	D	183	GLN
1	D	195	ASN
1	D	217	GLN
1	D	233	GLN
1	D	247	GLN
1	D	261	ASN
1	D	278	GLN
1	D	333	HIS
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 oligosaccharides 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	D	360	-	46,48,48	2.33	9 (19%)	64,73,73	1.58	6 (9%)
2	NAD	C	360	-	46,48,48	2.38	9 (19%)	64,73,73	1.60	8 (12%)
2	NAD	A	360	-	46,48,48	2.38	9 (19%)	64,73,73	1.57	8 (12%)
2	NAD	B	360	-	46,48,48	2.39	10 (21%)	64,73,73	1.59	7 (10%)

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	D	360	-	-	5/30/62/62	0/5/5/5
2	NAD	C	360	-	-	6/30/62/62	0/5/5/5
2	NAD	A	360	-	-	6/30/62/62	0/5/5/5
2	NAD	B	360	-	-	6/30/62/62	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	360	NAD	C4N-C3N	8.48	1.52	1.39
2	A	360	NAD	C4N-C3N	8.27	1.51	1.39
2	C	360	NAD	C4N-C3N	8.12	1.51	1.39
2	D	360	NAD	C4N-C3N	7.99	1.51	1.39
2	C	360	NAD	C2N-C3N	7.00	1.50	1.39
2	D	360	NAD	C2N-C3N	6.95	1.50	1.39
2	B	360	NAD	C2N-C3N	6.80	1.49	1.39
2	A	360	NAD	C2N-C3N	6.70	1.49	1.39
2	C	360	NAD	C5N-C4N	6.47	1.50	1.38
2	B	360	NAD	C5N-C4N	6.25	1.49	1.38
2	A	360	NAD	C5N-C4N	6.15	1.49	1.38
2	D	360	NAD	C5N-C4N	5.87	1.48	1.38
2	C	360	NAD	C2N-N1N	5.52	1.41	1.35
2	D	360	NAD	C2N-N1N	5.44	1.41	1.35
2	A	360	NAD	C2N-N1N	5.26	1.40	1.35
2	B	360	NAD	C2N-N1N	5.25	1.40	1.35
2	A	360	NAD	PA-O3	-4.54	1.54	1.59
2	C	360	NAD	PN-O3	4.26	1.64	1.59
2	B	360	NAD	PA-O3	-3.80	1.55	1.59
2	D	360	NAD	PN-O3	3.68	1.63	1.59
2	B	360	NAD	PN-O3	3.68	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	360	NAD	PN-O3	3.62	1.63	1.59
2	B	360	NAD	C6N-N1N	3.61	1.43	1.35
2	A	360	NAD	C6N-N1N	3.55	1.43	1.35
2	C	360	NAD	C6N-N1N	3.51	1.43	1.35
2	D	360	NAD	C6N-N1N	3.39	1.43	1.35
2	D	360	NAD	PA-O3	-3.28	1.56	1.59
2	C	360	NAD	C6N-C5N	-3.15	1.32	1.38
2	D	360	NAD	C6N-C5N	-3.06	1.32	1.38
2	B	360	NAD	C6N-C5N	-2.93	1.32	1.38
2	C	360	NAD	PA-O3	-2.79	1.56	1.59
2	A	360	NAD	C6N-C5N	-2.77	1.32	1.38
2	A	360	NAD	C2A-N1A	2.49	1.38	1.33
2	B	360	NAD	C2A-N1A	2.42	1.38	1.33
2	D	360	NAD	C2A-N1A	2.33	1.38	1.33
2	C	360	NAD	C2A-N1A	2.15	1.37	1.33
2	B	360	NAD	C3N-C7N	-2.15	1.47	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	360	NAD	C5N-C4N-C3N	-7.57	112.93	120.36
2	A	360	NAD	C5N-C4N-C3N	-7.55	112.95	120.36
2	C	360	NAD	C5N-C4N-C3N	-7.47	113.03	120.36
2	D	360	NAD	C5N-C4N-C3N	-7.40	113.09	120.36
2	C	360	NAD	C3N-C7N-N7N	4.70	123.53	117.74
2	D	360	NAD	C3N-C7N-N7N	4.45	123.22	117.74
2	B	360	NAD	C3N-C7N-N7N	4.44	123.21	117.74
2	D	360	NAD	C6N-C5N-C4N	4.29	125.63	119.45
2	C	360	NAD	C6N-C5N-C4N	4.28	125.62	119.45
2	A	360	NAD	C6N-C5N-C4N	4.25	125.58	119.45
2	B	360	NAD	C6N-C5N-C4N	4.25	125.58	119.45
2	A	360	NAD	C3N-C7N-N7N	4.24	122.96	117.74
2	B	360	NAD	C6N-N1N-C2N	-3.50	118.90	121.88
2	A	360	NAD	C6N-N1N-C2N	-3.43	118.96	121.88
2	D	360	NAD	C6N-N1N-C2N	-3.42	118.97	121.88
2	C	360	NAD	C6N-N1N-C2N	-3.41	118.98	121.88
2	B	360	NAD	O3-PN-O1N	-2.40	103.49	110.70
2	C	360	NAD	O7N-C7N-C3N	-2.39	116.67	119.60
2	D	360	NAD	O7N-C7N-C3N	-2.36	116.71	119.60
2	B	360	NAD	O7N-C7N-C3N	-2.30	116.79	119.60
2	C	360	NAD	O4B-C1B-C2B	-2.24	101.83	106.62
2	A	360	NAD	O3-PN-O1N	-2.20	104.08	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	360	NAD	O4B-C4B-C5B	-2.18	102.36	109.33
2	C	360	NAD	O4B-C4B-C5B	-2.15	102.44	109.33
2	A	360	NAD	O4B-C4B-C5B	-2.13	102.50	109.33
2	C	360	NAD	O3-PN-O1N	-2.12	104.31	110.70
2	A	360	NAD	O7N-C7N-C3N	-2.09	117.04	119.60
2	A	360	NAD	O2N-PN-O5D	2.04	116.82	107.57
2	D	360	NAD	O4B-C4B-C5B	-2.00	102.92	109.33

There are no chirality outliers.

All (23) torsion outliers are listed below:

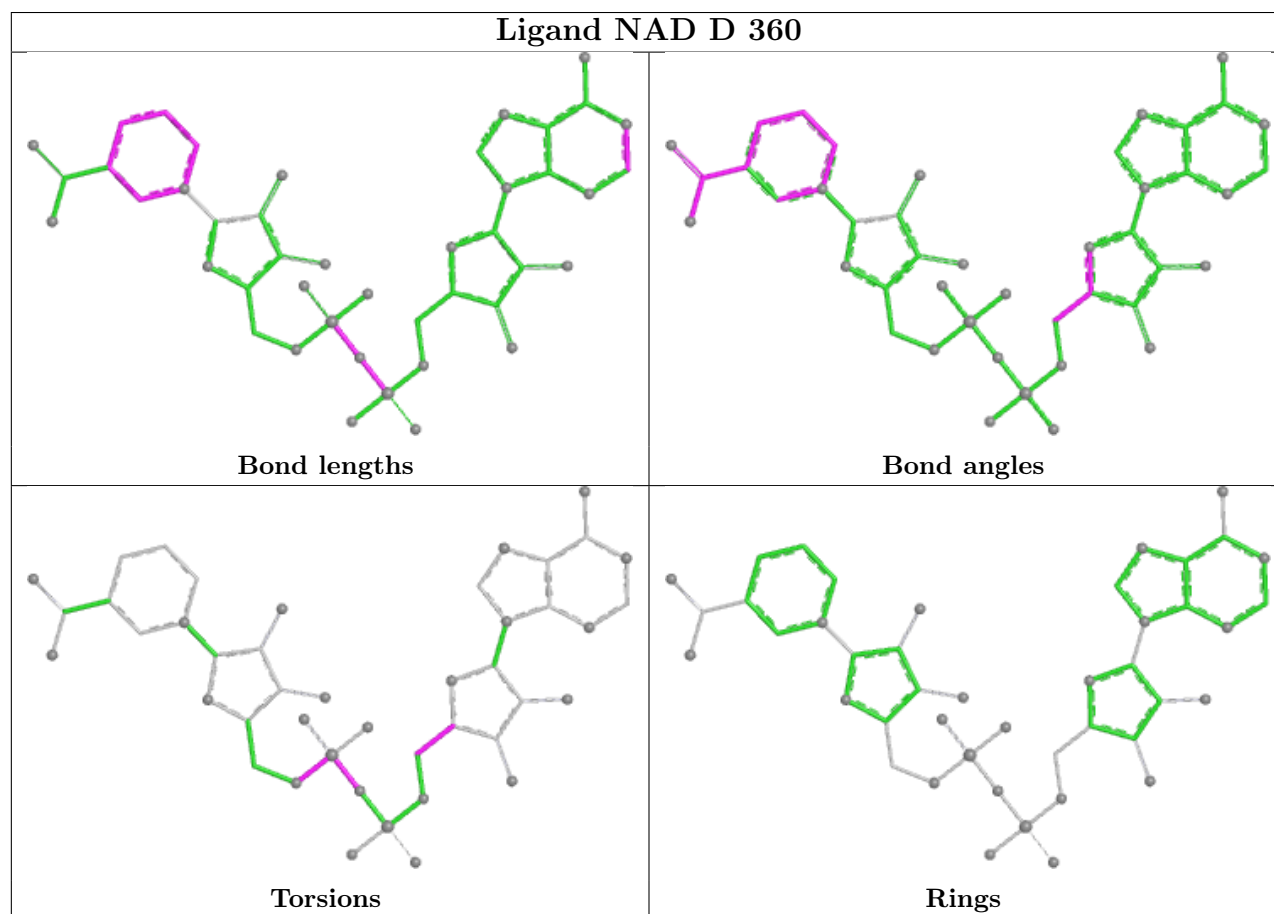
Mol	Chain	Res	Type	Atoms
2	A	360	NAD	C5D-O5D-PN-O3
2	A	360	NAD	C5D-O5D-PN-O1N
2	A	360	NAD	C5D-O5D-PN-O2N
2	B	360	NAD	C5D-O5D-PN-O3
2	B	360	NAD	C5D-O5D-PN-O1N
2	B	360	NAD	C5D-O5D-PN-O2N
2	C	360	NAD	C5D-O5D-PN-O3
2	C	360	NAD	C5D-O5D-PN-O1N
2	C	360	NAD	C5D-O5D-PN-O2N
2	D	360	NAD	C5D-O5D-PN-O3
2	D	360	NAD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

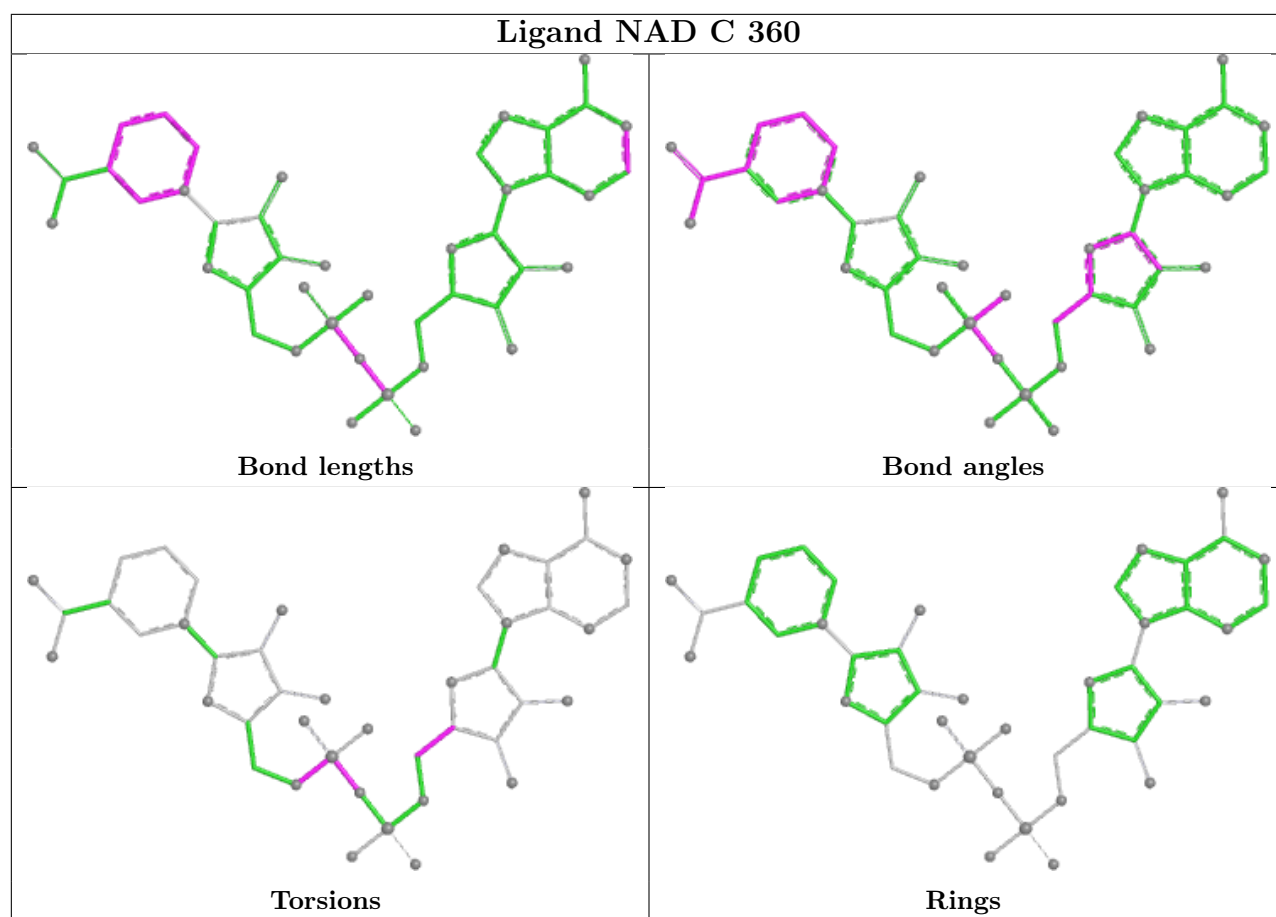
There are no ring outliers.

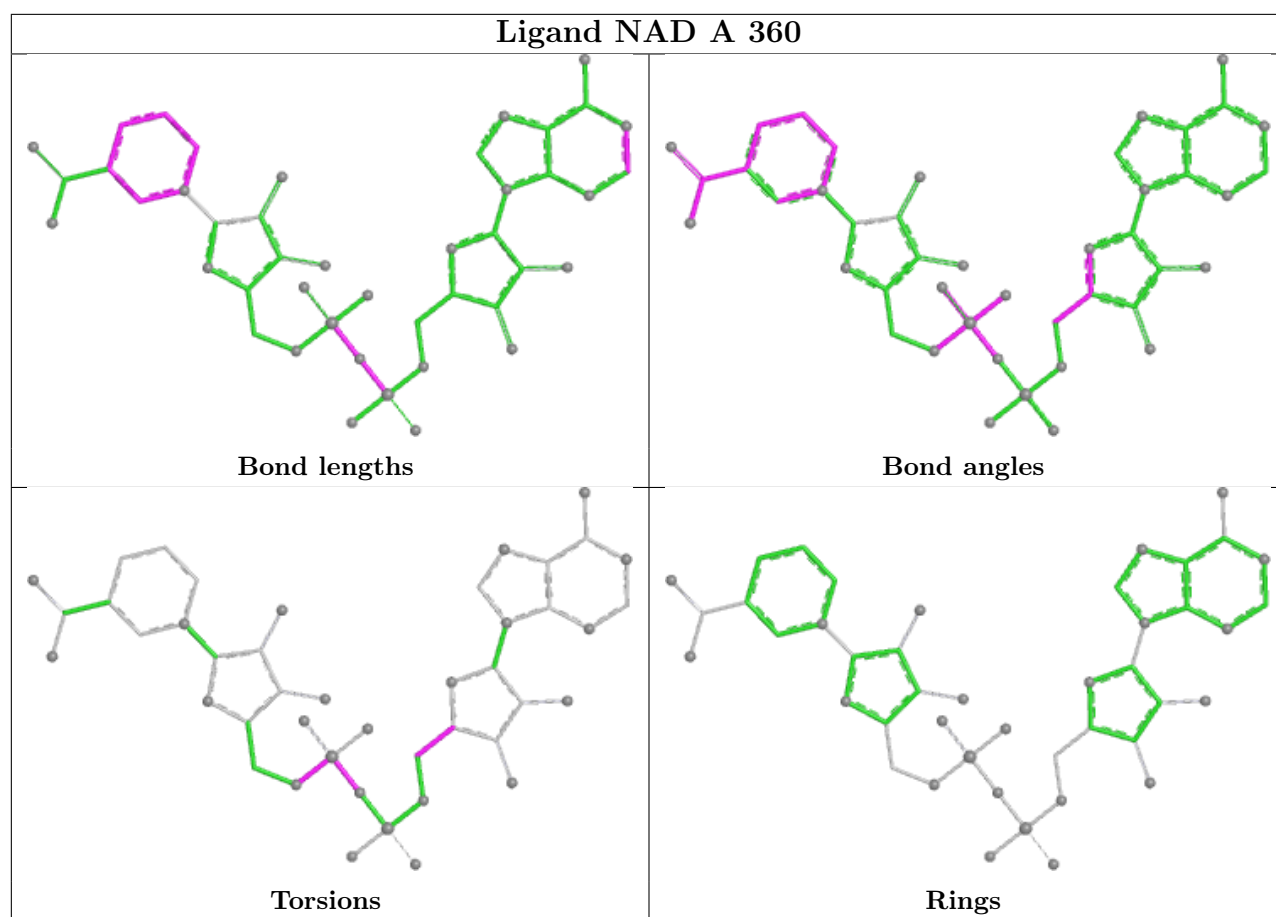
No monomer is involved in short contacts.

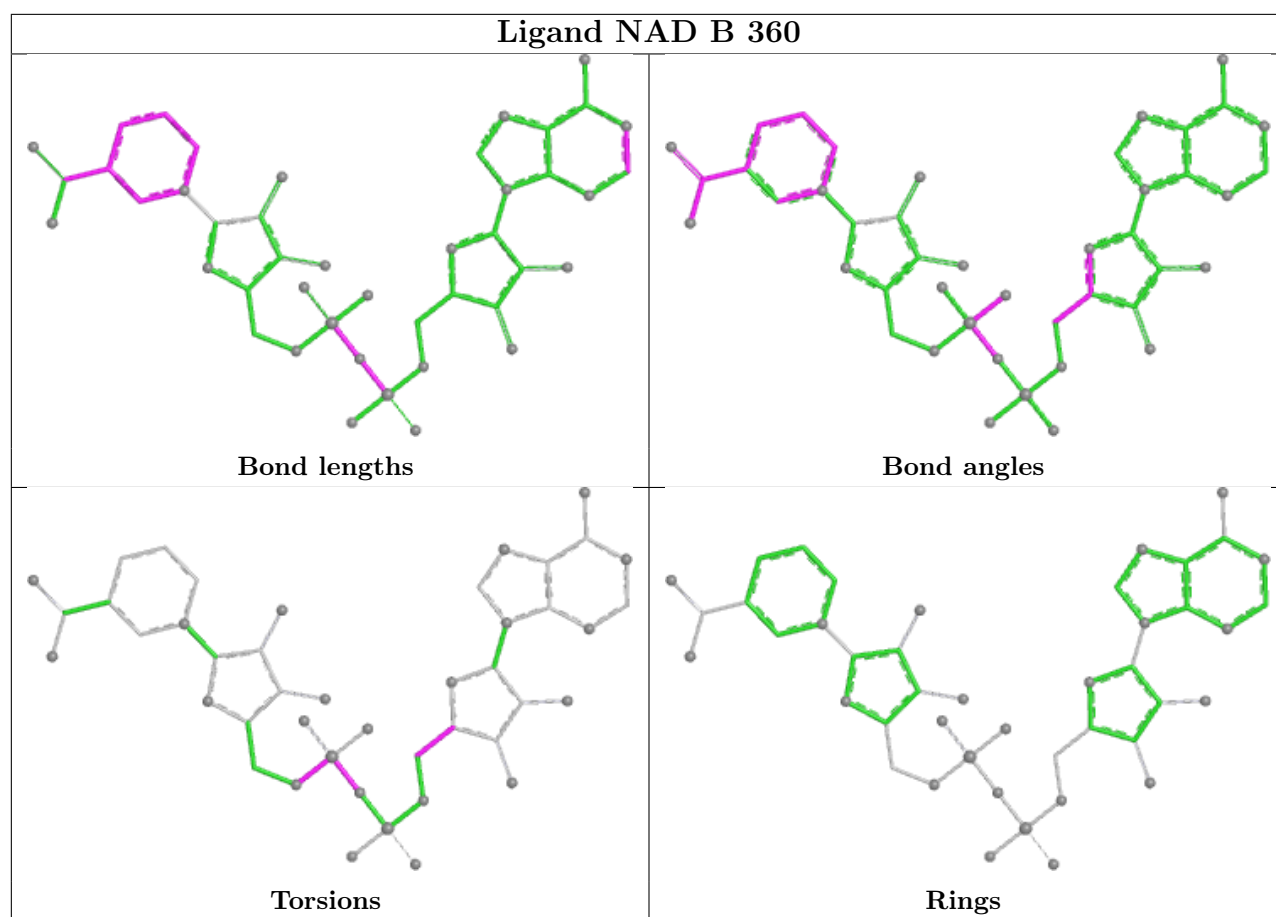
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	349/357 (97%)	0.49	27 (7%) 19 17	11, 20, 47, 64	0
1	B	346/357 (96%)	0.75	53 (15%) 5 4	12, 23, 60, 81	0
1	C	351/357 (98%)	0.99	59 (16%) 4 3	11, 25, 52, 82	0
1	D	347/357 (97%)	0.79	58 (16%) 4 3	12, 22, 54, 82	0
All	All	1393/1428 (97%)	0.75	197 (14%) 6 5	11, 22, 54, 82	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	289	TRP	7.3
1	C	2	ILE	7.0
1	D	232	TRP	6.6
1	B	223	ILE	6.1
1	D	204	LEU	5.8
1	B	222	ILE	5.7
1	A	300	ALA	5.7
1	C	207	ILE	5.2
1	B	357	LYS	5.1
1	D	302	TYR	5.1
1	C	286	GLY	4.9
1	C	298	HIS	4.9
1	B	221	VAL	4.9
1	D	289	TRP	4.9
1	C	3	ASN	4.7
1	C	357	LYS	4.6
1	D	267	ALA	4.5
1	D	301	HIS	4.4
1	D	272	VAL	4.4
1	B	266	ASP	4.4
1	D	94	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	291	LEU	4.3
1	B	204	LEU	4.3
1	B	225	ASN	4.2
1	D	269	ALA	4.1
1	A	291	LEU	4.1
1	B	286	GLY	4.1
1	D	357	LYS	4.1
1	D	266	ASP	4.0
1	D	268	ASP	4.0
1	C	222	ILE	4.0
1	C	291	LEU	4.0
1	D	227	HIS	4.0
1	D	274	ASN	4.0
1	A	266	ASP	3.9
1	A	357	LYS	3.9
1	B	224	ARG	3.8
1	B	220	PRO	3.7
1	A	102	GLU	3.7
1	C	274	ASN	3.7
1	B	290	GLN	3.7
1	D	205	ASP	3.7
1	D	223	ILE	3.6
1	C	285	GLU	3.6
1	C	4	ASN	3.6
1	C	317	HIS	3.6
1	C	330	VAL	3.6
1	D	303	LEU	3.6
1	A	140	GLU	3.5
1	C	142	ILE	3.5
1	D	222	ILE	3.5
1	B	205	ASP	3.3
1	D	280	VAL	3.3
1	B	213	ARG	3.3
1	B	207	ILE	3.2
1	C	348	THR	3.2
1	C	290	GLN	3.2
1	C	323	ASN	3.1
1	D	275	ILE	3.1
1	A	154	TYR	3.1
1	B	302	TYR	3.1
1	B	227	HIS	3.1
1	C	289	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	274	ASN	3.1
1	A	312	MET	3.1
1	B	4	ASN	3.1
1	B	285	GLU	3.1
1	B	206	ARG	3.0
1	A	46	VAL	3.0
1	D	213	ARG	3.0
1	A	2	ILE	3.0
1	D	273	LYS	3.0
1	A	179	ALA	3.0
1	C	300	ALA	3.0
1	B	301	HIS	2.9
1	C	301	HIS	2.9
1	C	221	VAL	2.9
1	D	278	GLN	2.9
1	C	329	ILE	2.9
1	C	281	LYS	2.9
1	D	282	TYR	2.9
1	D	284	GLY	2.9
1	D	285	GLU	2.9
1	B	226	PRO	2.9
1	D	228	ALA	2.9
1	B	317	HIS	2.9
1	C	299	GLU	2.9
1	B	180	ASN	2.9
1	B	219	GLN	2.9
1	A	299	GLU	2.9
1	A	183	GLN	2.8
1	C	287	ALA	2.8
1	B	330	VAL	2.8
1	C	78	GLU	2.8
1	C	179	ALA	2.8
1	D	2	ILE	2.8
1	D	224	ARG	2.8
1	C	224	ARG	2.8
1	C	178	PRO	2.8
1	C	312	MET	2.8
1	A	219	GLN	2.7
1	A	224	ARG	2.7
1	D	225	ASN	2.7
1	A	225	ASN	2.7
1	D	290	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	218	SER	2.7
1	D	229	ILE	2.7
1	D	323	ASN	2.7
1	D	286	GLY	2.6
1	D	195	ASN	2.6
1	C	340	THR	2.6
1	B	288	SER	2.6
1	B	3	ASN	2.6
1	D	219	GLN	2.6
1	A	4	ASN	2.6
1	C	297	PRO	2.6
1	B	230	ARG	2.6
1	D	230	ARG	2.6
1	A	3	ASN	2.6
1	D	321	ASN	2.6
1	D	271	PRO	2.5
1	D	354	MET	2.5
1	B	2	ILE	2.5
1	C	219	GLN	2.5
1	C	344	GLU	2.5
1	B	282	TYR	2.5
1	C	345	TYR	2.5
1	D	329	ILE	2.5
1	B	78	GLU	2.5
1	B	274	ASN	2.4
1	C	266	ASP	2.4
1	D	231	PRO	2.4
1	C	269	ALA	2.4
1	C	220	PRO	2.4
1	B	46	VAL	2.4
1	B	265	ASN	2.4
1	D	270	THR	2.4
1	C	347	ILE	2.4
1	B	287	ALA	2.4
1	C	183	GLN	2.4
1	D	317	HIS	2.4
1	B	284	GLY	2.4
1	C	272	VAL	2.4
1	D	281	LYS	2.4
1	A	252	ASP	2.3
1	C	206	ARG	2.3
1	C	278	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	203	ALA	2.3
1	C	351	ASN	2.3
1	C	252	ASP	2.3
1	C	356	THR	2.3
1	B	215	PHE	2.3
1	A	227	HIS	2.3
1	A	323	ASN	2.3
1	D	226	PRO	2.3
1	B	280	VAL	2.3
1	D	252	ASP	2.3
1	A	217	GLN	2.3
1	C	218	SER	2.3
1	D	87	MET	2.3
1	D	287	ALA	2.2
1	B	323	ASN	2.2
1	C	180	ASN	2.2
1	C	225	ASN	2.2
1	B	272	VAL	2.2
1	C	217	GLN	2.2
1	D	220	PRO	2.2
1	C	282	TYR	2.2
1	A	222	ILE	2.2
1	A	70	ASN	2.2
1	C	94	ARG	2.2
1	B	140	GLU	2.2
1	B	210	ASP	2.2
1	C	204	LEU	2.2
1	B	94	ARG	2.2
1	B	70	ASN	2.1
1	D	328	TYR	2.1
1	A	278	GLN	2.1
1	B	281	LYS	2.1
1	C	87	MET	2.1
1	B	276	VAL	2.1
1	B	303	LEU	2.1
1	D	203	ALA	2.1
1	D	218	SER	2.1
1	C	284	GLY	2.1
1	B	217	GLN	2.1
1	D	8	GLN	2.1
1	A	206	ARG	2.1
1	D	288	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	345	TYR	2.0
1	C	182	GLY	2.0
1	D	178	PRO	2.0
1	C	213	ARG	2.0
1	D	179	ALA	2.0
1	B	229	ILE	2.0
1	C	31	THR	2.0
1	C	181	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

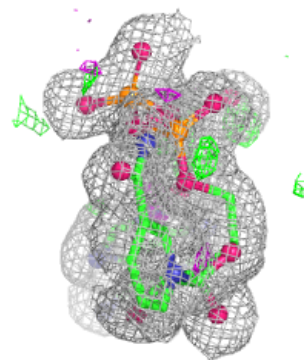
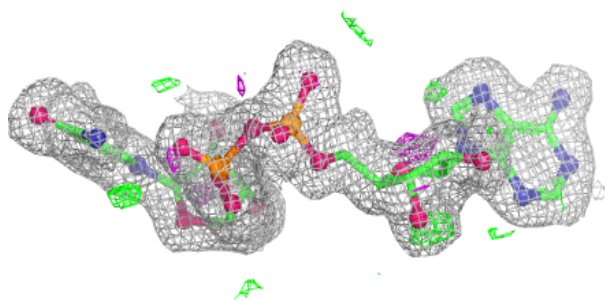
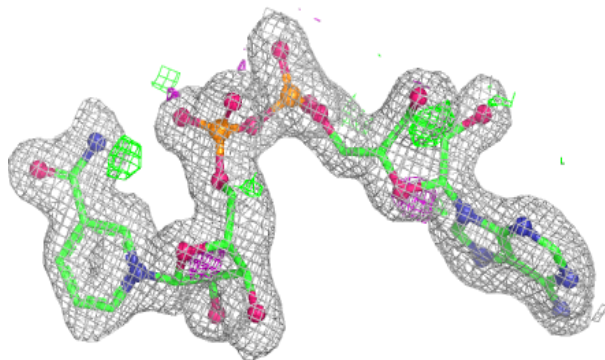
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	C	360	44/44	0.94	0.08	14,19,21,24	0
2	NAD	D	360	44/44	0.95	0.07	13,17,19,19	0
2	NAD	A	360	44/44	0.96	0.07	11,16,19,23	0
2	NAD	B	360	44/44	0.96	0.07	15,18,21,23	0

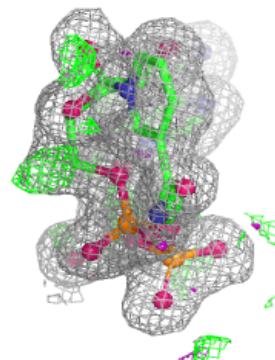
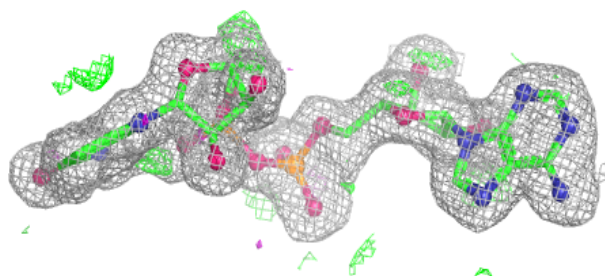
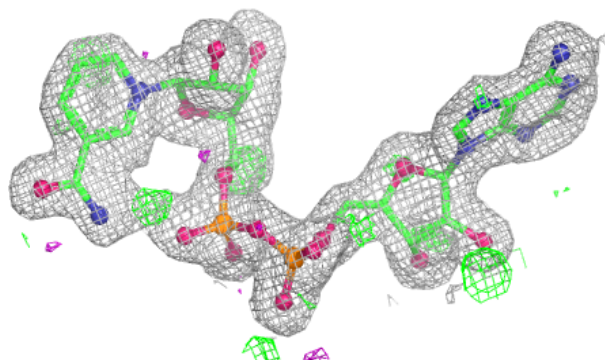
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

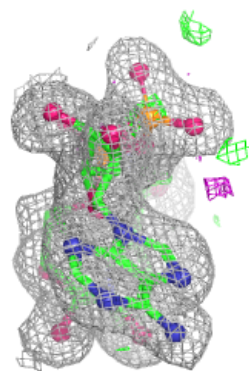
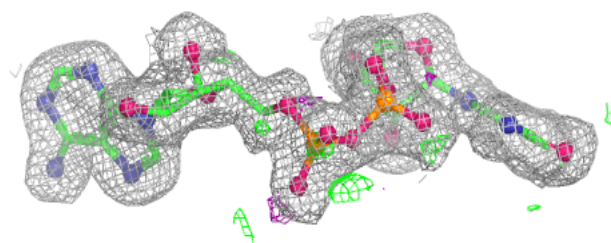
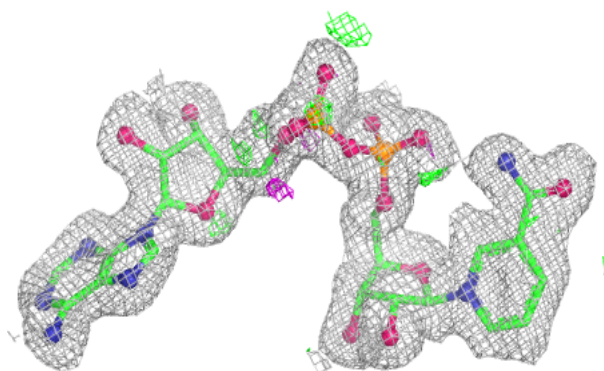
**Electron density around NAD D 360:**

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

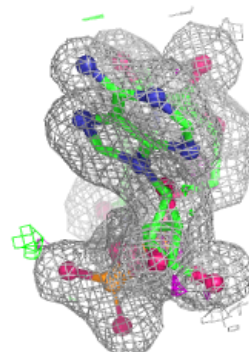
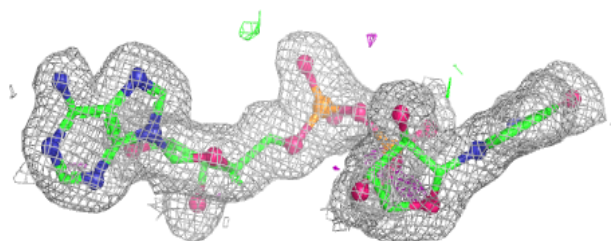
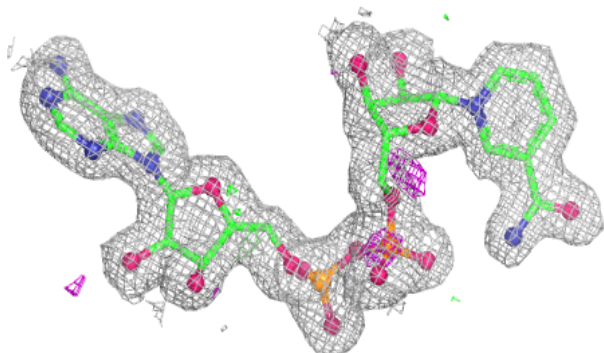


Electron density around NAD A 360:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.