



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:39 PM UTC

PDB ID : 1NBO / pdb_00001nbo
Title : The dual coenzyme specificity of photosynthetic glyceraldehyde-3-phosphate dehydrogenase interpreted by the crystal structure of A4 isoform complexed with NAD
Authors : Falini, G.; Fermani, S.; Ripamonti, A.; Sabatino, P.; Sparla, F.; Pupillo, P.; Trost, P.
Deposited on : 2002-12-03
Resolution : 2.60 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](#) ①) 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

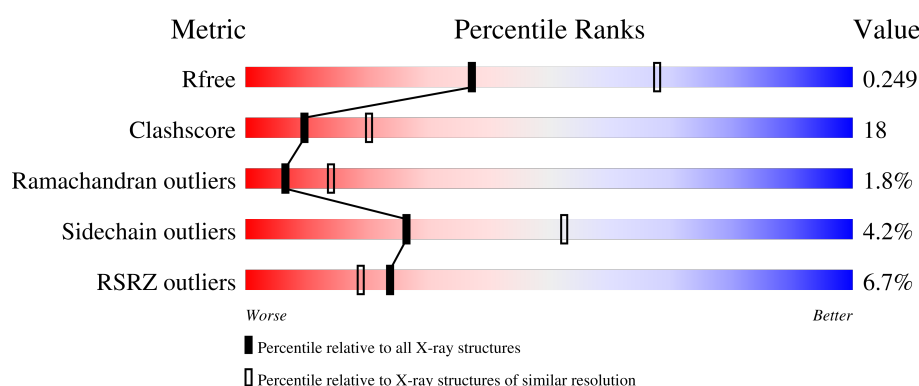
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	337	6% 66% 31% .
1	B	337	12% 65% 31% .
1	O	337	% 72% 23% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8255 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.

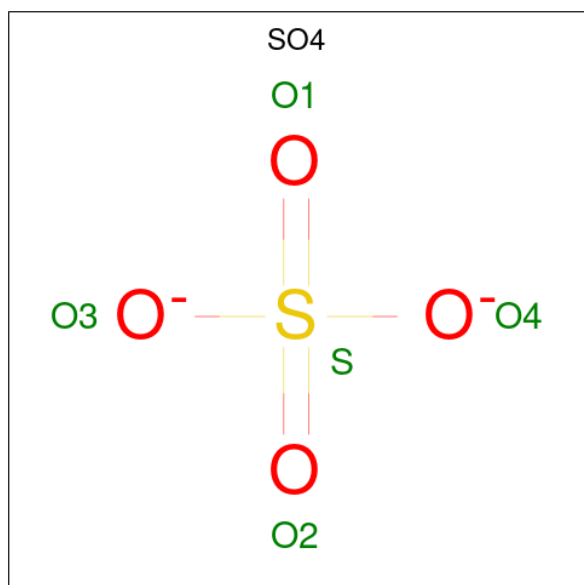
- Molecule 1 is a protein called glyceraldehyde-3-phosphate dehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	337	Total	C	N	O	S	0	8	0
			2592	1628	453	499	12			
1	A	337	Total	C	N	O	S	0	8	0
			2592	1628	453	499	12			
1	B	336	Total	C	N	O	S	0	1	0
			2540	1598	444	486	12			

There are 3 discrepancies between the modelled and reference sequences:

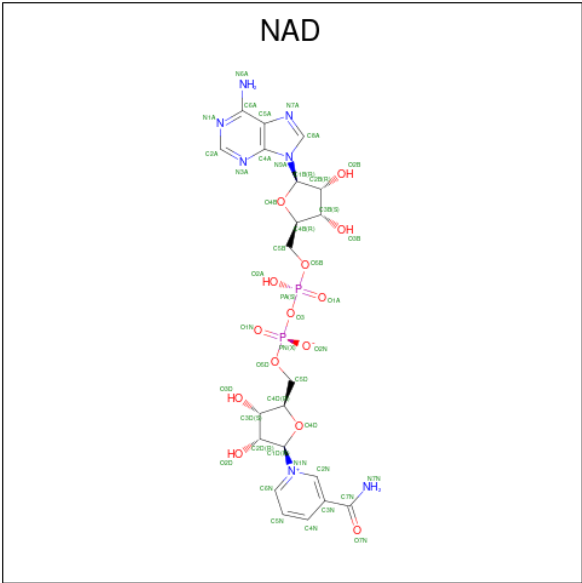
Chain	Residue	Modelled	Actual	Comment	Reference
O	334	ALA	-	cloning artifact	UNP P19866
A	334	ALA	-	cloning artifact	UNP P19866
B	334	ALA	-	cloning artifact	UNP P19866

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

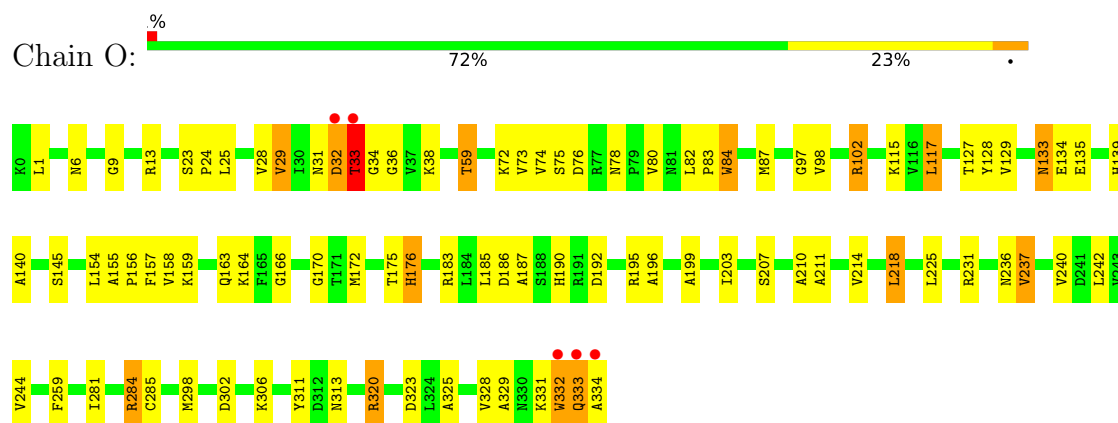
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	186	Total 186	O 186	0	0
4	A	101	Total 101	O 101	0	0
4	B	72	Total 72	O 72	0	0

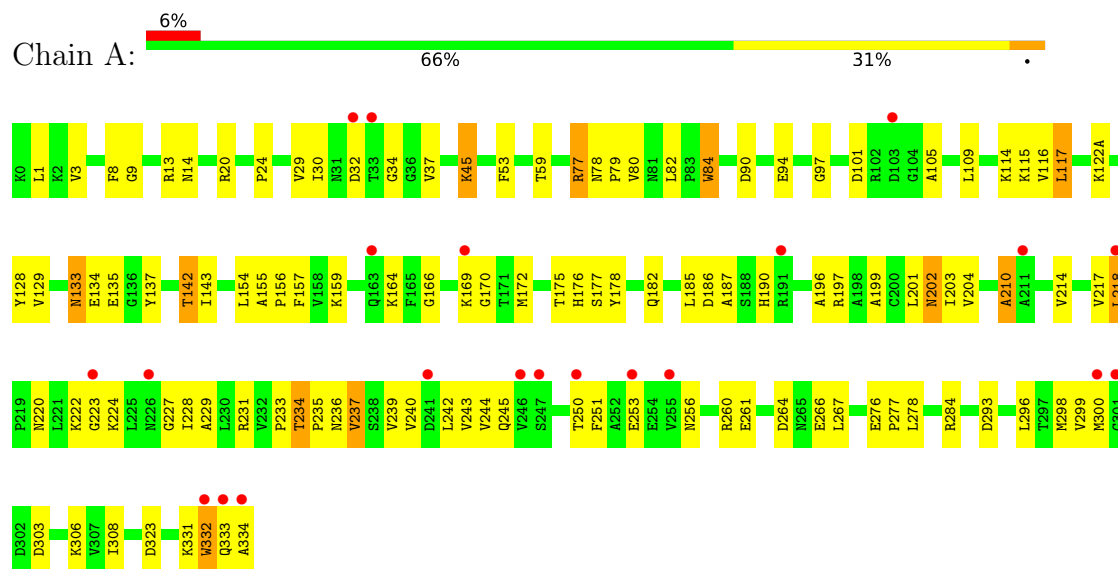
3 Residue-property plots

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 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: glyceraldehyde-3-phosphate dehydrogenase A

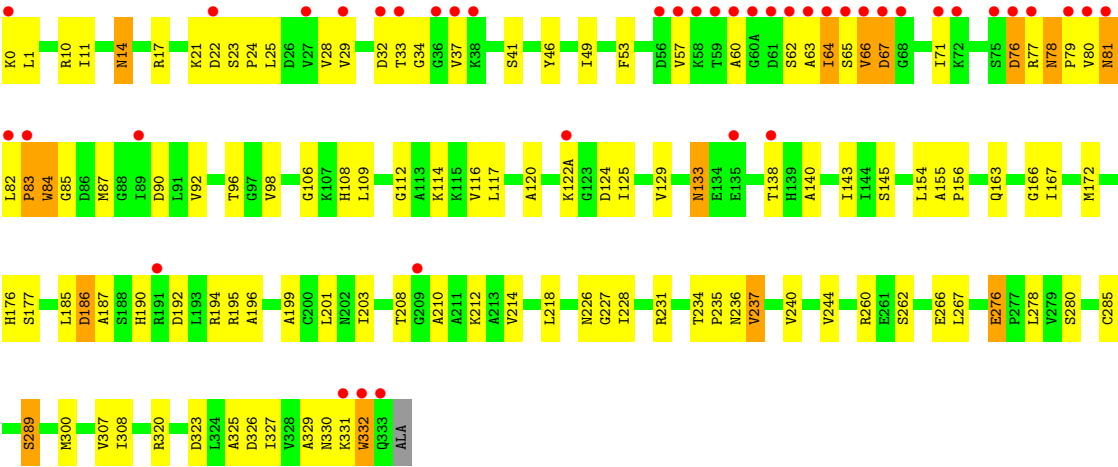


- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase A



- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase A





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	140.64Å 185.65Å 106.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.20 – 2.60 77.20 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (77.20-2.60) 99.9 (77.20-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.58 (at 2.62Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.245 0.209 , 0.249	Depositor DCC
R_{free} test set	2161 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8255	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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, SO4

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	0.37	0/2637	0.94	15/3580 (0.4%)
1	B	0.37	0/2585	0.90	7/3510 (0.2%)
1	O	0.44	0/2637	0.94	8/3580 (0.2%)
All	All	0.39	0/7859	0.93	30/10670 (0.3%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ILE	N-CA-C	-9.55	94.05	107.99
1	O	203	ILE	N-CA-C	-9.23	94.51	107.99
1	A	203	ILE	N-CA-C	-9.09	93.92	107.37
1	A	204	VAL	N-CA-C	7.23	115.34	107.60
1	B	78	ASN	CA-C-N	6.87	127.44	119.47
1	B	78	ASN	C-N-CA	6.87	127.44	119.47
1	B	199	ALA	N-CA-C	6.84	118.81	111.36
1	O	102	ARG	N-CA-C	6.33	118.18	111.28
1	A	37	VAL	N-CA-C	6.23	116.97	110.67
1	A	234	THR	CA-C-N	6.23	125.64	118.85
1	A	234	THR	C-N-CA	6.23	125.64	118.85
1	O	218	LEU	CA-C-N	5.80	126.20	119.47
1	O	218	LEU	C-N-CA	5.80	126.20	119.47
1	A	34[A]	GLY	N-CA-C	5.78	119.20	112.50
1	A	34[B]	GLY	N-CA-C	5.78	119.20	112.50
1	O	199	ALA	N-CA-C	5.72	117.51	111.28
1	B	218	LEU	CA-C-N	5.68	126.94	119.84
1	B	218	LEU	C-N-CA	5.68	126.94	119.84
1	A	202	ASN	N-CA-C	5.49	117.32	109.14
1	B	280	SER	N-CA-C	5.49	117.69	111.11
1	A	3	VAL	N-CA-C	5.44	116.42	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ASN	N-CA-C	-5.40	105.47	111.36
1	A	24	PRO	N-CA-C	-5.35	107.20	114.80
1	A	199	ALA	N-CA-C	5.34	118.02	111.82
1	A	59	THR	N-CA-C	-5.33	103.35	110.55
1	A	218	LEU	CA-C-N	5.26	125.32	119.32
1	A	218	LEU	C-N-CA	5.26	125.32	119.32
1	O	176	HIS	N-CA-C	5.11	118.14	109.76
1	O	158	VAL	N-CA-C	-5.03	105.49	110.62
1	O	175	THR	N-CA-C	-5.03	99.14	107.99

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	2592	0	2621	101	0
1	B	2540	0	2574	101	0
1	O	2592	0	2623	87	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
2	O	10	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
3	O	44	0	26	1	0
4	A	101	0	0	2	0
4	B	72	0	0	2	0
4	O	186	0	0	10	0
All	All	8255	0	7896	280	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 18.

All (280) 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:197:ARG:HH21	1:B:46:TYR:HB3	1.32	0.93
1:O:139:HIS:HE1	1:O:334:ALA:HA	1.32	0.93
1:O:6:ASN:ND2	1:O:31[A]:ASN:HD22	1.67	0.93
1:B:80:VAL:HG13	1:B:81:ASN:ND2	1.85	0.91
1:O:154:LEU:HD13	1:O:240:VAL:HG11	1.51	0.89
1:B:28:VAL:HG23	1:B:29:VAL:HG23	1.50	0.89
1:B:83:PRO:HB2	1:B:87:MET:HE2	1.53	0.89
1:B:66:VAL:HG12	1:B:67:ASP:H	1.37	0.88
1:B:33:THR:HG22	1:B:77:ARG:HG2	1.56	0.88
1:O:29[A]:VAL:HG11	1:O:87:MET:HE1	1.56	0.87
1:O:6:ASN:HD21	1:O:31[B]:ASN:HD22	1.23	0.86
1:A:197:ARG:HH21	1:B:46:TYR:CB	1.87	0.86
1:A:142:THR:HG22	1:A:143:ILE:HG13	1.58	0.83
1:B:129:VAL:H	1:B:133:ASN:HD21	1.24	0.83
1:A:170:GLY:HA3	1:A:244:VAL:HG12	1.59	0.82
1:O:6:ASN:HD21	1:O:31[A]:ASN:HD22	1.30	0.80
1:A:228:ILE:HG12	1:A:229:ALA:H	1.47	0.80
1:O:83:PRO:HG2	1:O:87:MET:HE2	1.64	0.79
1:O:29[B]:VAL:HG11	1:O:87:MET:HE1	1.63	0.79
1:O:139:HIS:CE1	1:O:334:ALA:HA	2.17	0.76
1:A:300:MET:HE3	1:A:300:MET:HA	1.68	0.75
1:A:197:ARG:NH2	1:B:46:TYR:HB3	2.01	0.75
1:O:32[B]:ASP:O	1:O:33[B]:THR:HG22	1.86	0.74
1:B:176:HIS:HB3	1:B:231:ARG:HD3	1.68	0.74
1:O:6:ASN:ND2	1:O:31[B]:ASN:HD22	1.85	0.72
1:A:201:LEU:HD21	1:B:235:PRO:HG3	1.71	0.71
1:O:78:ASN:OD1	1:O:80:VAL:HG22	1.89	0.71
1:A:90:ASP:HB3	1:A:334:ALA:HB3	1.72	0.71
1:B:80:VAL:HG13	1:B:81:ASN:HD22	1.55	0.70
1:B:138:THR:HG22	1:B:140:ALA:H	1.56	0.70
1:O:298:MET:HE2	1:O:306:LYS:HD3	1.73	0.69
1:A:332:TRP:HD1	1:A:333:GLN:H	1.39	0.69
1:A:78:ASN:CG	1:A:80:VAL:HG12	2.18	0.69
1:B:187:ALA:O	1:B:196:ALA:HB1	1.93	0.68
1:B:84:TRP:HE1	1:B:108:HIS:HD2	1.39	0.68
1:B:81:ASN:ND2	1:B:81:ASN:N	2.41	0.68
1:O:36[B]:GLY:HA3	4:O:1372:HOH:O	1.93	0.68
1:B:92:VAL:HG11	1:B:108:HIS:CD2	2.30	0.67
1:A:117:LEU:HD12	1:A:117:LEU:C	2.19	0.67
1:A:235:PRO:CG	1:B:201:LEU:HD21	2.24	0.67
1:B:167:ILE:HG23	1:B:244:VAL:CG2	2.25	0.66
1:A:228:ILE:HG12	1:A:229:ALA:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ASN:HD22	1:B:81:ASN:N	1.94	0.66
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.31	0.66
1:O:170:GLY:HA3	1:O:244:VAL:HG12	1.78	0.66
1:A:1:LEU:HD21	1:A:334:ALA:HB2	1.78	0.65
1:B:0:LYS:HD3	1:B:0:LYS:N	2.11	0.65
1:O:28:VAL:HG23	1:O:29[A]:VAL:HG22	1.78	0.65
1:O:117:LEU:C	1:O:117:LEU:HD12	2.22	0.65
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.77	0.65
1:B:154:LEU:HD13	1:B:240:VAL:HG11	1.77	0.65
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.62	0.65
1:B:212:LYS:HE3	4:B:9068:HOH:O	1.97	0.64
1:A:222:LYS:HD3	1:A:223:GLY:N	2.12	0.64
1:B:78:ASN:OD1	1:B:80:VAL:HG12	1.97	0.64
1:A:1:LEU:HD11	1:A:334:ALA:CB	2.28	0.64
1:A:331:LYS:O	1:A:332:TRP:CB	2.46	0.64
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.33	0.64
1:B:60:ALA:O	1:B:63:ALA:HB3	1.98	0.63
1:A:197:ARG:HH11	1:A:197:ARG:HG3	1.64	0.63
1:B:66:VAL:O	1:B:67:ASP:C	2.41	0.63
1:O:176:HIS:HB3	1:O:231:ARG:HD3	1.81	0.63
1:A:157:PHE:HE1	1:A:242:LEU:HD23	1.64	0.62
1:O:129:VAL:H	1:O:133:ASN:ND2	1.97	0.62
1:O:28:VAL:HG23	1:O:29[A]:VAL:CG2	2.29	0.62
1:B:129:VAL:H	1:B:133:ASN:ND2	1.96	0.62
1:A:169:LYS:HD2	1:A:224:LYS:O	2.00	0.61
1:A:235:PRO:HG2	1:B:201:LEU:HD21	1.83	0.60
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.36	0.60
1:O:129:VAL:H	1:O:133:ASN:HD21	1.48	0.60
1:B:90:ASP:OD1	1:B:114:LYS:HD2	2.02	0.60
1:O:28:VAL:HG23	1:O:29[B]:VAL:HG22	1.82	0.59
1:A:235:PRO:HG3	1:B:201:LEU:HD21	1.84	0.59
1:O:38:LYS:HE2	4:O:1399:HOH:O	2.03	0.58
1:A:266:GLU:HG3	1:A:267:LEU:HG	1.86	0.58
1:O:284:ARG:HG2	4:O:1420:HOH:O	2.02	0.58
1:O:32[B]:ASP:OD2	1:O:73:VAL:HG12	2.04	0.58
1:A:197:ARG:HG3	1:A:197:ARG:NH1	2.16	0.57
1:O:159:LYS:O	1:O:163:GLN:HG3	2.05	0.57
1:B:90:ASP:HA	1:B:114:LYS:HB2	1.86	0.57
1:B:172:MET:HG3	1:B:227:GLY:HA3	1.87	0.57
1:B:84:TRP:HE1	1:B:108:HIS:CD2	2.23	0.56
1:B:21:LYS:HG2	1:B:22:ASP:OD1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:VAL:HG13	1:B:81:ASN:HD21	1.67	0.56
1:A:331:LYS:O	1:A:332:TRP:HB2	2.05	0.56
1:B:190:HIS:HB3	1:B:196:ALA:HB2	1.88	0.56
1:A:298:MET:HE2	1:A:306:LYS:HD2	1.87	0.56
1:O:32[B]:ASP:C	1:O:33[B]:THR:HG22	2.30	0.56
1:A:276:GLU:HB3	1:A:278:LEU:HG	1.88	0.55
1:O:127:THR:HG22	1:O:145:SER:HB3	1.88	0.55
1:A:1:LEU:HD11	1:A:334:ALA:HB3	1.88	0.55
1:O:240:VAL:HG23	1:O:311:TYR:CE1	2.42	0.55
1:O:331:LYS:O	1:O:332:TRP:HB3	2.06	0.55
1:B:28:VAL:C	1:B:71:ILE:HG23	2.32	0.55
1:O:211:ALA:HB3	4:O:1402:HOH:O	2.07	0.54
1:A:210:ALA:O	1:A:214:VAL:HG23	2.07	0.54
1:A:101:ASP:HB3	1:A:122(A):LYS:HD3	1.89	0.54
1:B:29:VAL:HG11	1:B:87:MET:HE1	1.90	0.54
1:O:320:ARG:NH1	1:O:323:ASP:OD2	2.40	0.54
1:O:28:VAL:HG23	1:O:29[B]:VAL:CG2	2.35	0.54
1:B:116:VAL:HB	1:B:143:ILE:CD1	2.38	0.54
1:B:177:SER:HB2	1:B:234:THR:O	2.08	0.54
1:A:333:GLN:O	1:A:334:ALA:C	2.50	0.53
1:O:172:MET:CE	1:O:240:VAL:HG13	2.39	0.53
1:B:10:ARG:O	1:B:14:ASN:HB2	2.08	0.53
1:O:236:ASN:O	1:O:237:VAL:HB	2.08	0.53
1:A:9:GLY:O	1:A:13:ARG:HG3	2.08	0.53
1:O:157:PHE:HB2	1:O:259:PHE:CE1	2.44	0.53
1:A:8:PHE:N	1:A:32[A]:ASP:OD2	2.40	0.53
1:A:78:ASN:ND2	1:A:80:VAL:HG12	2.24	0.53
1:O:32[B]:ASP:OD2	1:O:73:VAL:CG1	2.57	0.52
1:O:139:HIS:NE2	1:O:332:TRP:CE3	2.77	0.52
1:O:320:ARG:HH11	1:O:320:ARG:HA	1.73	0.52
1:A:187:ALA:O	1:A:196:ALA:HB1	2.10	0.52
1:B:124:ASP:C	1:B:125:ILE:HD12	2.35	0.52
1:O:128:TYR:HA	1:O:133:ASN:HD21	1.75	0.52
1:B:41:SER:HB2	1:B:57:VAL:HG12	1.91	0.52
1:B:17:ARG:NH2	1:B:53:PHE:HA	2.24	0.52
1:A:78:ASN:OD1	1:A:80:VAL:HG12	2.10	0.52
1:B:37:VAL:CG2	1:B:62:SER:HA	2.39	0.52
1:B:236:ASN:O	1:B:237:VAL:HB	2.09	0.52
1:B:120:ALA:O	1:B:145:SER:HB2	2.10	0.52
1:B:167:ILE:HG23	1:B:244:VAL:HG21	1.90	0.51
1:A:332:TRP:CD1	1:A:333:GLN:H	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:154:LEU:CD1	1:O:240:VAL:HG11	2.34	0.51
1:A:20:ARG:NH2	1:A:323:ASP:OD1	2.40	0.51
1:A:251:PHE:CE2	1:A:253:GLU:HB2	2.45	0.51
1:A:114:LYS:HE3	4:A:9020:HOH:O	2.11	0.51
1:O:139:HIS:NE2	1:O:332:TRP:CZ3	2.79	0.51
1:O:32[B]:ASP:HB3	1:O:34[B]:GLY:O	2.10	0.51
1:A:45:LYS:O	1:A:45:LYS:HD3	2.10	0.50
1:B:37:VAL:HG21	1:B:62:SER:HA	1.92	0.50
1:O:25:LEU:HD11	1:O:325:ALA:HB3	1.93	0.50
1:A:157:PHE:CE1	1:A:242:LEU:HD23	2.46	0.50
1:B:1:LEU:HD22	1:B:329:ALA:HB2	1.92	0.50
1:B:323:ASP:O	1:B:327:ILE:HG13	2.12	0.50
1:O:313:ASN:HA	4:O:1438:HOH:O	2.12	0.50
1:A:29[A]:VAL:HG22	1:A:30[A]:ILE:N	2.26	0.50
1:A:190:HIS:HB3	1:A:196:ALA:HB2	1.93	0.50
1:B:276:GLU:HB3	1:B:278:LEU:HG	1.93	0.50
1:A:169:LYS:NZ	1:A:224:LYS:HA	2.27	0.50
1:A:243:VAL:HG23	1:A:243:VAL:O	2.11	0.50
1:A:78:ASN:HB3	2:A:9002:SO4:O1	2.11	0.50
1:B:82:LEU:C	1:B:84:TRP:H	2.20	0.50
1:O:1:LEU:HD22	1:O:329:ALA:HB2	1.93	0.50
1:A:29[B]:VAL:HG22	1:A:30[B]:ILE:N	2.27	0.50
1:B:236:ASN:ND2	1:B:237:VAL:H	2.09	0.50
1:B:76:ASP:C	1:B:78:ASN:H	2.20	0.49
1:A:236:ASN:O	1:A:237:VAL:HB	2.11	0.49
1:A:256:ASN:O	1:A:260:ARG:HG3	2.13	0.49
1:O:32[B]:ASP:HB2	1:O:74:VAL:O	2.12	0.49
1:O:190:HIS:HB3	1:O:196:ALA:HB2	1.95	0.49
1:O:36[A]:GLY:HA3	4:O:1372:HOH:O	2.12	0.49
1:A:78:ASN:ND2	1:A:80:VAL:CG1	2.77	0.48
1:B:0:LYS:HD3	1:B:0:LYS:H3	1.77	0.48
1:O:185:LEU:O	1:O:186:ASP:C	2.56	0.48
1:A:169:LYS:HZ3	1:A:224:LYS:HA	1.78	0.48
1:B:85:GLY:CA	1:B:112:GLY:HA3	2.44	0.48
1:B:106:GLY:O	1:B:109:LEU:N	2.45	0.48
1:A:186:ASP:CG	1:A:197:ARG:HD3	2.38	0.48
1:O:210:ALA:O	1:O:214:VAL:HG23	2.14	0.48
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.96	0.48
1:B:260:ARG:HD2	4:B:9012:HOH:O	2.12	0.48
1:B:29:VAL:HG11	1:B:84:TRP:HZ3	1.79	0.48
1:O:159:LYS:HB2	1:O:218:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:HH21	1:B:46:TYR:HB2	1.73	0.47
1:B:79:PRO:HA	1:B:82:LEU:CD1	2.44	0.47
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.96	0.47
1:O:139:HIS:HE2	1:O:332:TRP:HZ3	1.63	0.47
1:A:115:LYS:NZ	1:A:137:TYR:OH	2.33	0.47
1:A:134:GLU:HG2	1:A:135:GLU:N	2.30	0.47
1:A:175:THR:OG1	1:A:239:VAL:CG1	2.63	0.47
1:B:262:SER:HB3	1:B:267:LEU:HD12	1.96	0.47
1:O:331:LYS:O	1:O:332:TRP:CB	2.63	0.47
1:A:250:THR:O	1:A:299:VAL:HG11	2.15	0.47
1:B:185:LEU:O	1:B:186:ASP:C	2.58	0.46
1:B:37:VAL:HG21	1:B:62:SER:CA	2.44	0.46
1:B:125:ILE:HD12	1:B:125:ILE:N	2.29	0.46
1:O:172:MET:HE2	1:O:240:VAL:HG13	1.97	0.46
1:B:66:VAL:HG12	1:B:67:ASP:N	2.15	0.46
1:B:116:VAL:HB	1:B:143:ILE:HD13	1.98	0.46
1:O:117:LEU:C	1:O:117:LEU:CD1	2.88	0.46
1:B:25:LEU:HD21	1:B:325:ALA:HB3	1.97	0.46
1:O:78:ASN:CG	1:O:80:VAL:HG22	2.40	0.46
1:B:64:ILE:CG2	1:B:65:SER:N	2.78	0.46
1:B:266:GLU:N	1:B:266:GLU:OE1	2.49	0.46
1:A:117:LEU:C	1:A:117:LEU:CD1	2.89	0.46
1:B:210:ALA:O	1:B:214:VAL:HG23	2.16	0.46
1:O:140:ALA:HB2	1:A:220:ASN:HA	1.97	0.46
1:O:25:LEU:HD11	1:O:325:ALA:CB	2.46	0.46
1:A:306:LYS:NZ	4:A:9068:HOH:O	2.48	0.46
1:A:178:TYR:HA	1:A:182:GLN:OE1	2.15	0.45
1:B:176:HIS:HB3	1:B:231:ARG:CD	2.43	0.45
1:A:133:ASN:C	1:A:133:ASN:ND2	2.74	0.45
1:A:129:VAL:HG23	1:A:217:VAL:HG11	1.98	0.45
1:B:0:LYS:O	1:B:0:LYS:HG2	2.16	0.45
1:A:154:LEU:HD11	1:A:172:MET:HE3	1.99	0.45
1:A:251:PHE:CD2	1:A:253:GLU:HB2	2.52	0.45
1:O:328:VAL:CG1	1:O:334:ALA:CB	2.95	0.45
1:A:332:TRP:HD1	1:A:333:GLN:N	2.12	0.45
1:A:260:ARG:O	1:A:264:ASP:OD2	2.35	0.45
1:B:320:ARG:HA	1:B:320:ARG:NE	2.32	0.45
1:B:37:VAL:HG21	1:B:63:ALA:H	1.82	0.44
1:A:293:ASP:OD1	1:A:296:LEU:HG	2.17	0.44
1:B:82:LEU:HA	1:B:83:PRO:HD3	1.79	0.44
1:O:1:LEU:HD23	1:O:25:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:32[B]:ASP:O	1:O:33[B]:THR:CG2	2.61	0.44
1:O:6:ASN:HD21	1:O:31[A]:ASN:ND2	2.00	0.44
1:O:332:TRP:O	1:O:334:ALA:N	2.51	0.44
1:O:187:ALA:O	1:O:196:ALA:HB1	2.18	0.44
1:A:45:LYS:HE2	1:A:53:PHE:O	2.18	0.44
1:A:77:ARG:O	1:A:79:PRO:HD3	2.18	0.44
1:A:300:MET:HA	1:A:300:MET:CE	2.45	0.44
1:B:212:LYS:NZ	1:B:226:ASN:OD1	2.52	0.43
1:A:243:VAL:HG12	1:A:306:LYS:HG3	2.00	0.43
1:A:298:MET:HE2	1:A:306:LYS:CD	2.48	0.43
1:O:23:SER:HA	1:O:24:PRO:HD3	1.82	0.43
1:O:102:ARG:NH2	4:O:1411:HOH:O	2.41	0.43
1:B:23:SER:HA	1:B:24:PRO:HD3	1.84	0.43
1:O:134:GLU:HG2	1:O:135:GLU:N	2.33	0.43
1:O:332:TRP:O	1:O:333:GLN:C	2.61	0.43
1:A:186:ASP:HA	1:A:196:ALA:O	2.19	0.43
1:O:242:LEU:O	1:O:306:LYS:HA	2.18	0.43
1:B:194:ARG:C	1:B:196:ALA:H	2.25	0.43
1:B:32:ASP:C	1:B:34:GLY:H	2.27	0.42
1:O:32[B]:ASP:HB2	1:O:75:SER:CB	2.49	0.42
1:O:183:ARG:HD2	4:O:1498:HOH:O	2.19	0.42
1:A:159:LYS:HB2	1:A:218:LEU:HD11	2.01	0.42
1:B:289:SER:OG	1:B:320:ARG:HD2	2.19	0.42
1:B:96:THR:OG1	1:B:98:VAL:HG22	2.18	0.42
1:B:331:LYS:O	1:B:332:TRP:O	2.38	0.42
1:O:9:GLY:O	1:O:13:ARG:HG3	2.19	0.42
1:O:32[B]:ASP:HB3	1:O:33[B]:THR:H	1.25	0.42
1:O:115:LYS:CE	1:O:334:ALA:HB1	2.50	0.42
1:A:97:GLY:HA2	3:A:5335:NAD:O3D	2.19	0.42
1:A:109:LEU:HD11	1:A:142:THR:CG2	2.49	0.42
1:A:129:VAL:H	1:A:133:ASN:ND2	2.17	0.42
1:B:307:VAL:C	1:B:308:ILE:HD12	2.45	0.42
4:O:1436:HOH:O	1:A:332:TRP:HH2	2.03	0.42
1:A:169:LYS:NZ	1:A:223:GLY:O	2.53	0.42
1:B:41:SER:N	1:B:64:ILE:HD11	2.35	0.42
1:B:82:LEU:HD13	1:B:84:TRP:CE2	2.54	0.42
1:B:129:VAL:N	1:B:133:ASN:HD21	2.05	0.42
1:A:176:HIS:O	1:A:231:ARG:HA	2.19	0.42
1:O:31[B]:ASN:OD1	1:O:32[B]:ASP:N	2.52	0.42
1:B:192:ASP:HB3	1:B:195:ARG:HB2	2.02	0.42
1:O:164:LYS:HE2	1:O:164:LYS:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ALA:HB1	1:A:116:VAL:HG11	2.02	0.41
1:A:245:GLN:HA	1:A:303:ASP:O	2.19	0.41
1:A:197:ARG:HH11	1:A:197:ARG:CG	2.29	0.41
1:A:202:ASN:O	1:A:233:PRO:HD3	2.19	0.41
1:O:32[B]:ASP:HB2	1:O:75:SER:HB2	2.02	0.41
1:B:117:LEU:C	1:B:117:LEU:HD23	2.46	0.41
1:O:29[A]:VAL:HG13	1:O:72:LYS:HB3	2.01	0.41
1:O:154:LEU:HD22	1:O:172:MET:HE3	2.02	0.41
1:B:11:ILE:HD12	3:B:6335:NAD:O4D	2.21	0.41
1:B:133:ASN:C	1:B:133:ASN:HD22	2.29	0.41
1:A:185:LEU:O	1:A:186:ASP:C	2.63	0.41
1:B:208:THR:HG22	1:B:228:ILE:HA	2.02	0.41
1:A:172:MET:SD	1:A:227:GLY:HA3	2.61	0.41
1:A:186:ASP:OD2	1:A:197:ARG:HD3	2.21	0.41
1:O:59:THR:HG23	4:O:1481:HOH:O	2.20	0.41
1:A:177:SER:HB3	1:A:234:THR:O	2.21	0.41
1:A:251:PHE:CD1	1:A:251:PHE:N	2.88	0.41
1:B:0:LYS:N	1:B:0:LYS:CD	2.82	0.41
1:B:176:HIS:O	1:B:231:ARG:HA	2.20	0.41
1:O:192:ASP:HB3	1:O:195:ARG:HB2	2.02	0.40
1:A:240:VAL:O	1:A:308:ILE:HA	2.19	0.40
1:A:332:TRP:CD1	1:A:333:GLN:N	2.89	0.40
1:B:25:LEU:HD11	1:B:326:ASP:HA	2.02	0.40
1:O:298:MET:HE2	1:O:306:LYS:CD	2.46	0.40
1:A:45:LYS:HD3	1:A:45:LYS:C	2.46	0.40
1:B:76:ASP:C	1:B:78:ASN:N	2.79	0.40
1:A:133:ASN:C	1:A:133:ASN:HD22	2.29	0.40
1:A:276:GLU:HA	1:A:277:PRO:HD3	1.92	0.40
1:B:85:GLY:HA3	1:B:112:GLY:HA3	2.02	0.40
1:O:97:GLY:HA2	3:O:1335:NAD:O3D	2.22	0.40
1:O:328:VAL:CG1	1:O:334:ALA:HB2	2.52	0.40
1:A:164:LYS:NZ	1:A:261:GLU:OE1	2.55	0.40
1:B:326:ASP:O	1:B:330:ASN:ND2	2.55	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	343/337 (102%)	312 (91%)	27 (8%)	4 (1%)	10	23
1	B	335/337 (99%)	297 (89%)	31 (9%)	7 (2%)	5	11
1	O	343/337 (102%)	316 (92%)	18 (5%)	9 (3%)	4	7
All	All	1021/1011 (101%)	925 (91%)	76 (7%)	20 (2%)	6	12

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	ASP
1	B	332	TRP
1	O	32[A]	ASP
1	O	32[B]	ASP
1	O	33[A]	THR
1	O	33[B]	THR
1	O	237	VAL
1	O	333	GLN
1	A	332	TRP
1	A	237	VAL
1	B	237	VAL
1	A	210	ALA
1	B	83	PRO
1	O	302	ASP
1	O	332	TRP
1	A	166	GLY
1	B	66	VAL
1	B	186	ASP
1	O	166	GLY
1	B	166	GLY

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	285/279 (102%)	277 (97%)	8 (3%)	38	66
1	B	280/279 (100%)	267 (95%)	13 (5%)	24	49
1	O	285/279 (102%)	269 (94%)	16 (6%)	19	40
All	All	850/837 (102%)	813 (96%)	37 (4%)	26	50

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	29[A]	VAL
1	O	29[B]	VAL
1	O	33[A]	THR
1	O	33[B]	THR
1	O	59	THR
1	O	76	ASP
1	O	84	TRP
1	O	98	VAL
1	O	117	LEU
1	O	133	ASN
1	O	207	SER
1	O	225	LEU
1	O	281	ILE
1	O	284	ARG
1	O	285	CYS
1	O	320	ARG
1	A	45	LYS
1	A	77	ARG
1	A	84	TRP
1	A	94	GLU
1	A	117	LEU
1	A	133	ASN
1	A	142	THR
1	A	284	ARG
1	B	14	ASN
1	B	49	ILE

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Mol	Chain	Res	Type
1	B	64	ILE
1	B	76	ASP
1	B	81	ASN
1	B	84	TRP
1	B	122(A)	LYS
1	B	133	ASN
1	B	163	GLN
1	B	276	GLU
1	B	285	CYS
1	B	289	SER
1	B	300	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	6	ASN
1	O	39	GLN
1	O	81	ASN
1	O	133	ASN
1	O	220	ASN
1	O	256	ASN
1	O	265	ASN
1	O	330	ASN
1	A	78	ASN
1	A	81	ASN
1	A	133	ASN
1	A	139	HIS
1	A	152	ASN
1	A	256	ASN
1	A	330	ASN
1	B	81	ASN
1	B	133	ASN
1	B	139	HIS
1	B	152	ASN
1	B	202	ASN
1	B	236	ASN
1	B	256	ASN
1	B	330	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 ⓘ

11 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	SO4	B	9001	-	4,4,4	0.41	0	6,6,6	0.07	0
2	SO4	A	5338	-	4,4,4	0.33	0	6,6,6	0.10	0
3	NAD	B	6335	-	46,48,48	1.71	9 (19%)	64,73,73	1.76	13 (20%)
2	SO4	B	6339	-	4,4,4	0.32	0	6,6,6	0.10	0
3	NAD	A	5335	-	46,48,48	1.64	9 (19%)	64,73,73	1.80	14 (21%)
3	NAD	O	1335	-	46,48,48	1.86	9 (19%)	64,73,73	1.75	10 (15%)
2	SO4	A	9002	-	4,4,4	0.34	0	6,6,6	0.10	0
2	SO4	O	1338	-	4,4,4	0.41	0	6,6,6	0.07	0
2	SO4	A	5339	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	B	6338	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	O	1339	-	4,4,4	0.46	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	5335	-	-	10/30/62/62	0/5/5/5
3	NAD	O	1335	-	-	5/30/62/62	0/5/5/5
3	NAD	B	6335	-	-	10/30/62/62	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1335	NAD	C3N-C7N	4.77	1.57	1.50
3	B	6335	NAD	C3N-C7N	4.58	1.57	1.50
3	A	5335	NAD	C3N-C7N	4.52	1.57	1.50
3	O	1335	NAD	PA-O3	-4.40	1.54	1.59
3	B	6335	NAD	C6N-N1N	4.29	1.45	1.35
3	B	6335	NAD	C2N-N1N	4.26	1.39	1.35
3	O	1335	NAD	PN-O3	-4.18	1.55	1.59
3	A	5335	NAD	C6N-N1N	4.08	1.44	1.35
3	O	1335	NAD	C6N-N1N	4.07	1.44	1.35
3	O	1335	NAD	C4N-C3N	3.88	1.45	1.39
3	O	1335	NAD	C2N-N1N	3.73	1.39	1.35
3	A	5335	NAD	C2N-N1N	3.38	1.38	1.35
3	B	6335	NAD	C4N-C3N	3.34	1.44	1.39
3	A	5335	NAD	C4N-C3N	3.28	1.44	1.39
3	B	6335	NAD	PN-O3	-3.17	1.56	1.59
3	A	5335	NAD	PN-O3	-3.07	1.56	1.59
3	A	5335	NAD	PA-O3	-3.00	1.56	1.59
3	O	1335	NAD	C4A-N3A	2.81	1.39	1.34
3	B	6335	NAD	PA-O3	-2.69	1.56	1.59
3	A	5335	NAD	C4A-N3A	2.42	1.38	1.34
3	B	6335	NAD	C4A-N3A	2.39	1.38	1.34
3	O	1335	NAD	C5N-C4N	2.38	1.43	1.38
3	O	1335	NAD	O4D-C1D	2.34	1.44	1.40
3	B	6335	NAD	C5N-C4N	2.22	1.42	1.38
3	B	6335	NAD	O5B-C5B	2.07	1.52	1.44
3	A	5335	NAD	C5N-C4N	2.03	1.42	1.38
3	A	5335	NAD	C2A-N1A	2.01	1.37	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6335	NAD	C5N-C6N-N1N	-5.63	112.70	120.38
3	A	5335	NAD	C5N-C6N-N1N	-5.55	112.81	120.38
3	O	1335	NAD	C5N-C6N-N1N	-5.53	112.83	120.38
3	O	1335	NAD	C6N-N1N-C2N	5.40	126.47	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5335	NAD	C6N-N1N-C2N	5.40	126.47	121.88
3	B	6335	NAD	C6N-N1N-C2N	5.24	126.34	121.88
3	A	5335	NAD	C3N-C7N-N7N	4.10	122.79	117.74
3	B	6335	NAD	C6N-C5N-C4N	4.07	125.31	119.45
3	O	1335	NAD	C6N-C5N-C4N	3.99	125.21	119.45
3	A	5335	NAD	C6N-C5N-C4N	3.93	125.12	119.45
3	A	5335	NAD	C4N-C3N-C7N	-3.78	110.76	121.06
3	O	1335	NAD	C5N-C4N-C3N	-3.73	116.70	120.36
3	B	6335	NAD	C4N-C3N-C7N	-3.73	110.90	121.06
3	O	1335	NAD	C4N-C3N-C7N	-3.65	111.13	121.06
3	A	5335	NAD	C5N-C4N-C3N	-3.56	116.87	120.36
3	B	6335	NAD	C5N-C4N-C3N	-3.41	117.02	120.36
3	O	1335	NAD	C3N-C7N-N7N	3.39	121.92	117.74
3	B	6335	NAD	C3N-C7N-N7N	3.03	121.47	117.74
3	A	5335	NAD	O7N-C7N-C3N	-2.85	116.11	119.60
3	A	5335	NAD	C2N-C3N-C7N	2.85	127.69	119.46
3	B	6335	NAD	C2N-C3N-C7N	2.83	127.64	119.46
3	A	5335	NAD	C2N-C3N-C4N	2.83	121.55	118.26
3	O	1335	NAD	C2N-C3N-C7N	2.80	127.53	119.46
3	B	6335	NAD	C2N-C3N-C4N	2.75	121.46	118.26
3	B	6335	NAD	O3D-C3D-C4D	-2.72	103.26	111.08
3	O	1335	NAD	C2N-C3N-C4N	2.64	121.33	118.26
3	B	6335	NAD	O2A-PA-O3	2.59	114.28	107.27
3	B	6335	NAD	C6N-N1N-C1D	-2.52	114.78	119.73
3	O	1335	NAD	O3D-C3D-C4D	-2.49	103.92	111.08
3	A	5335	NAD	O3D-C3D-C4D	-2.49	103.93	111.08
3	B	6335	NAD	C4D-O4D-C1D	2.47	112.19	109.92
3	A	5335	NAD	C6N-N1N-C1D	-2.43	114.96	119.73
3	O	1335	NAD	C6N-N1N-C1D	-2.41	115.00	119.73
3	A	5335	NAD	O5B-C5B-C4B	-2.21	101.45	108.99
3	A	5335	NAD	C4D-O4D-C1D	2.13	111.87	109.92
3	A	5335	NAD	O2A-PA-O3	2.10	112.95	107.27
3	B	6335	NAD	O3-PN-O1N	-2.09	104.42	110.70

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	1335	NAD	O4D-C1D-N1N-C2N
3	O	1335	NAD	O4D-C1D-N1N-C6N
3	A	5335	NAD	O4D-C1D-N1N-C2N
3	B	6335	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	B	6335	NAD	O4D-C1D-N1N-C6N
3	B	6335	NAD	C2D-C1D-N1N-C2N
3	B	6335	NAD	C2D-C1D-N1N-C6N
3	B	6335	NAD	O4B-C4B-C5B-O5B
3	A	5335	NAD	O4B-C4B-C5B-O5B
3	B	6335	NAD	C3B-C4B-C5B-O5B
3	B	6335	NAD	C2B-C1B-N9A-C8A
3	A	5335	NAD	C5B-O5B-PA-O2A
3	A	5335	NAD	C5B-O5B-PA-O3
3	B	6335	NAD	C5B-O5B-PA-O2A
3	B	6335	NAD	C5B-O5B-PA-O3
3	O	1335	NAD	C2D-C1D-N1N-C2N
3	O	1335	NAD	C2D-C1D-N1N-C6N
3	A	5335	NAD	O4D-C1D-N1N-C6N
3	A	5335	NAD	C2N-C3N-C7N-N7N
3	A	5335	NAD	PA-O3-PN-O2N
3	B	6335	NAD	PA-O3-PN-O2N
3	A	5335	NAD	C2N-C3N-C7N-O7N
3	O	1335	NAD	O4B-C4B-C5B-O5B
3	A	5335	NAD	C3B-C4B-C5B-O5B
3	A	5335	NAD	PA-O3-PN-O1N

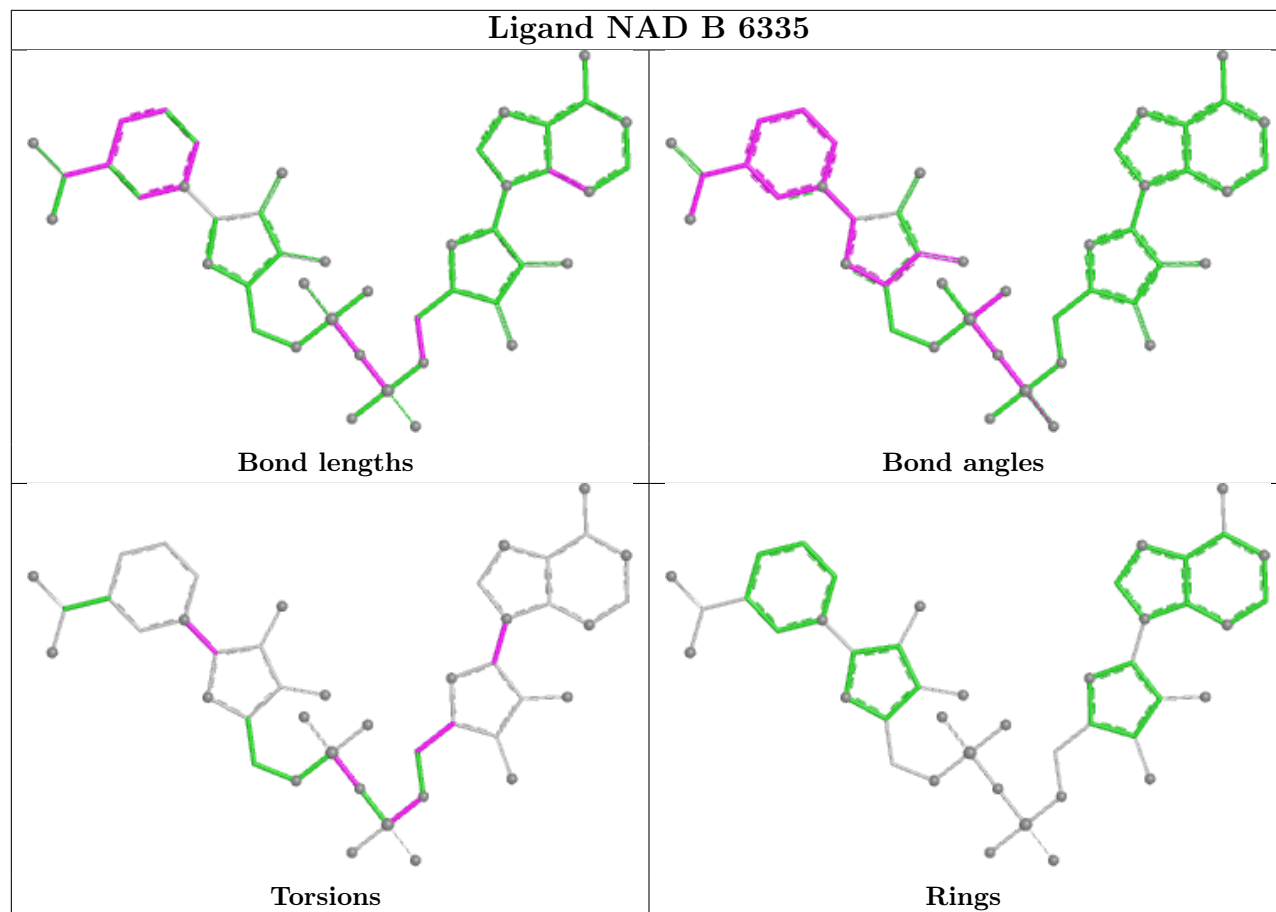
There are no ring outliers.

4 monomers are involved in 4 short contacts:

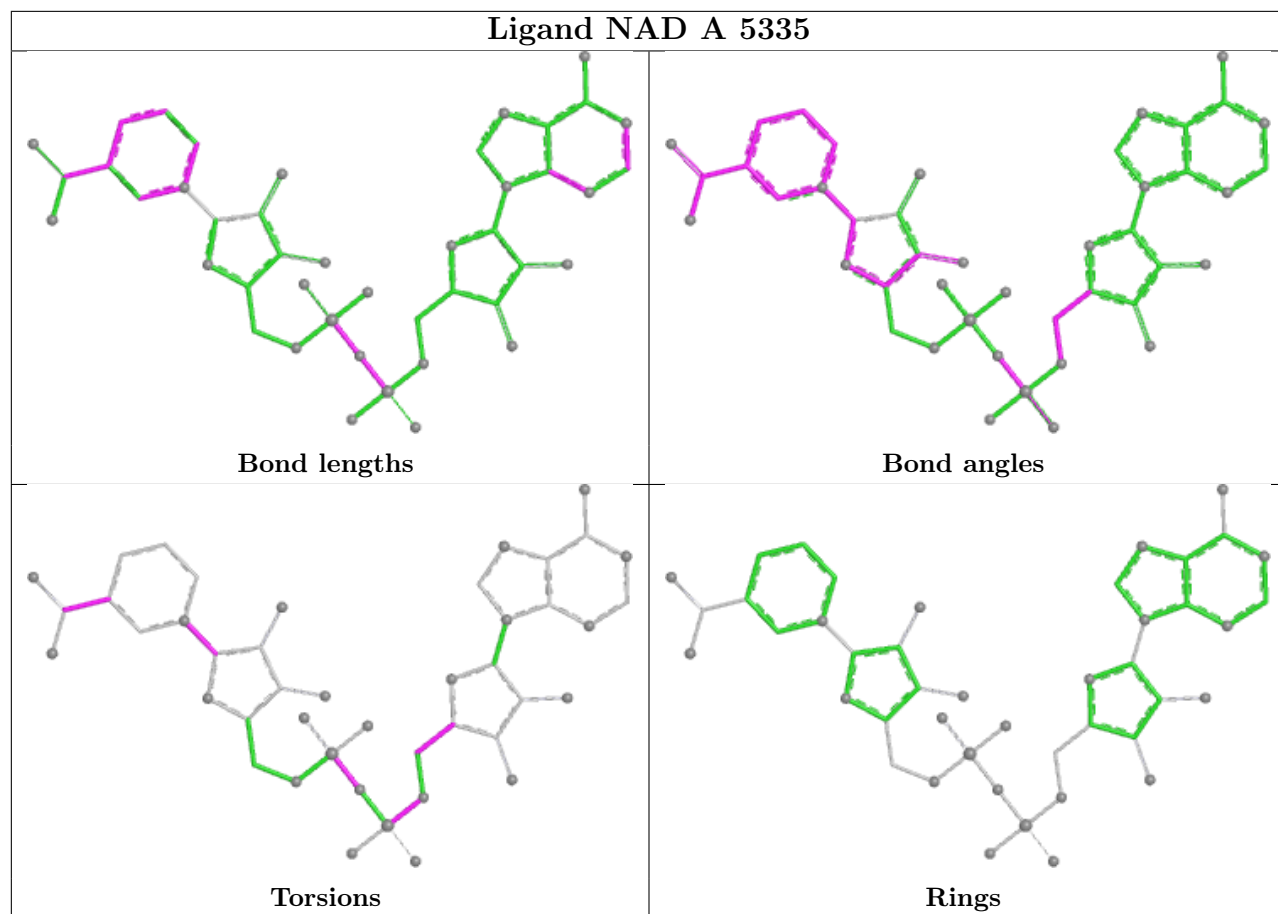
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	6335	NAD	1	0
3	A	5335	NAD	1	0
3	O	1335	NAD	1	0
2	A	9002	SO4	1	0

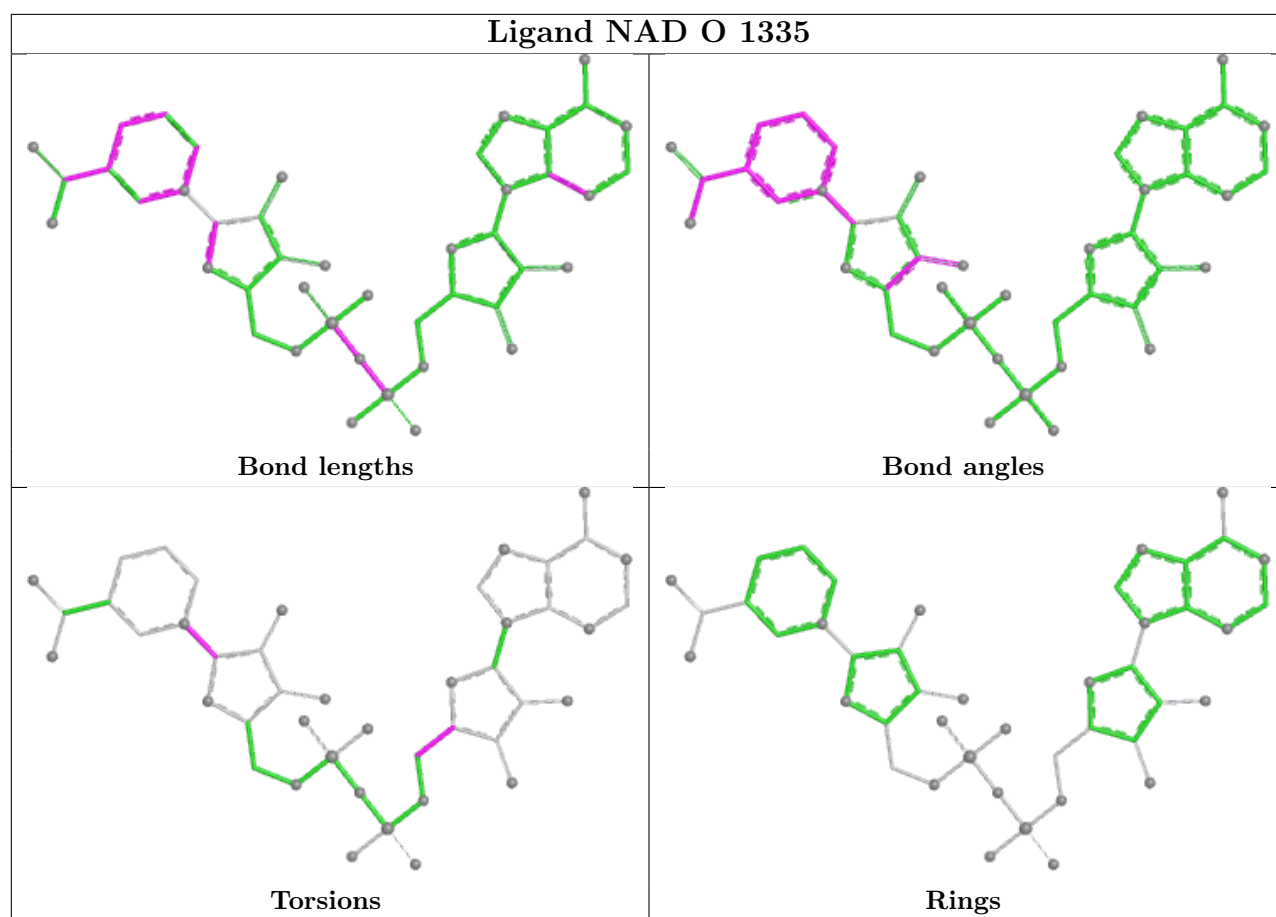
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand NAD A 5335





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	337/337 (100%)	0.54	21 (6%) 26 21	12, 36, 58, 67	8 (2%)
1	B	336/337 (99%)	0.64	42 (12%) 8 6	16, 39, 79, 95	1 (0%)
1	O	337/337 (100%)	-0.37	5 (1%) 72 68	7, 18, 36, 66	8 (2%)
All	All	1010/1011 (99%)	0.27	68 (6%) 24 19	7, 31, 69, 95	17 (1%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ALA	8.9
1	B	62	SER	6.1
1	O	332	TRP	5.0
1	A	333	GLN	4.7
1	B	332	TRP	4.6
1	A	332	TRP	4.6
1	B	63	ALA	4.4
1	O	32[A]	ASP	4.3
1	B	333	GLN	4.2
1	B	60	ALA	3.8
1	B	66	VAL	3.7
1	B	59	THR	3.6
1	B	72	LYS	3.3
1	B	65	SER	3.3
1	O	334	ALA	3.3
1	B	61	ASP	3.1
1	B	82	LEU	3.1
1	B	64	ILE	3.1
1	A	32[A]	ASP	3.0
1	O	333	GLN	3.0
1	B	0	LYS	2.9
1	B	29	VAL	2.8
1	B	37	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	138	THR	2.7
1	B	135	GLU	2.7
1	B	83	PRO	2.7
1	B	89	ILE	2.7
1	A	246	VAL	2.7
1	B	56	ASP	2.7
1	A	163	GLN	2.5
1	B	27	VAL	2.5
1	B	76	ASP	2.5
1	A	250	THR	2.5
1	A	253	GLU	2.4
1	B	60(A)	GLY	2.4
1	B	58	LYS	2.4
1	B	75	SER	2.4
1	B	57	VAL	2.4
1	A	226	ASN	2.3
1	B	68	GLY	2.3
1	B	22	ASP	2.3
1	B	32	ASP	2.3
1	O	33[A]	THR	2.3
1	A	33[A]	THR	2.3
1	A	247	SER	2.3
1	B	331	LYS	2.2
1	B	71	ILE	2.2
1	B	77	ARG	2.2
1	B	79	PRO	2.2
1	B	191	ARG	2.2
1	B	67	ASP	2.2
1	A	300	MET	2.2
1	A	255	VAL	2.2
1	B	38	LYS	2.1
1	A	241	ASP	2.1
1	A	211	ALA	2.1
1	B	33	THR	2.1
1	A	218	LEU	2.1
1	B	209	GLY	2.1
1	B	122(A)	LYS	2.0
1	A	223	GLY	2.0
1	A	301	GLY	2.0
1	B	36	GLY	2.0
1	B	80	VAL	2.0
1	A	191	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	103	ASP	2.0
1	A	169	LYS	2.0
1	B	81	ASN	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](#)

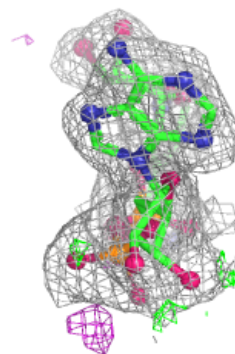
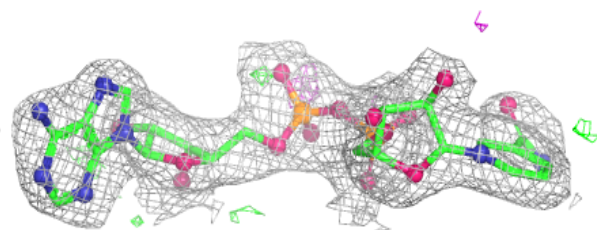
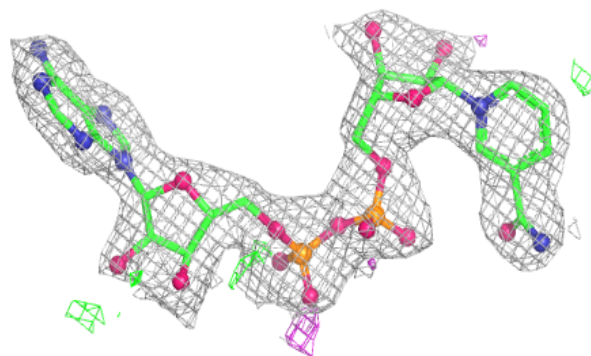
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	B	6339	5/5	0.62	0.28	56,57,58,59	5
2	SO4	A	5339	5/5	0.63	0.28	66,68,69,69	5
2	SO4	A	9002	5/5	0.78	0.24	65,65,66,66	5
2	SO4	O	1339	5/5	0.85	0.16	52,53,55,55	0
2	SO4	A	5338	5/5	0.89	0.18	48,48,50,50	5
2	SO4	B	6338	5/5	0.92	0.14	51,52,53,53	5
2	SO4	B	9001	5/5	0.92	0.12	60,61,62,62	0
3	NAD	A	5335	44/44	0.92	0.11	37,44,47,48	0
3	NAD	B	6335	44/44	0.92	0.11	40,46,57,58	0
2	SO4	O	1338	5/5	0.97	0.08	40,41,42,43	0
3	NAD	O	1335	44/44	0.98	0.06	15,20,22,25	0

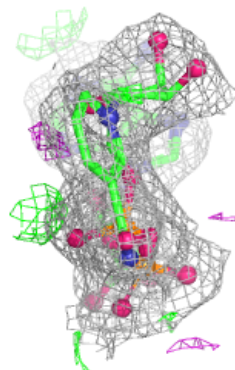
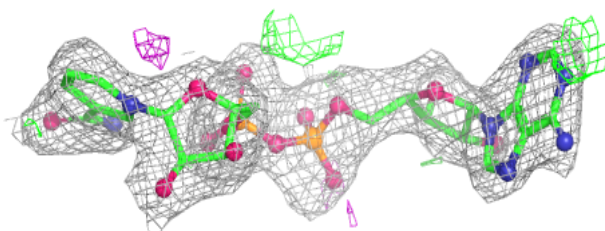
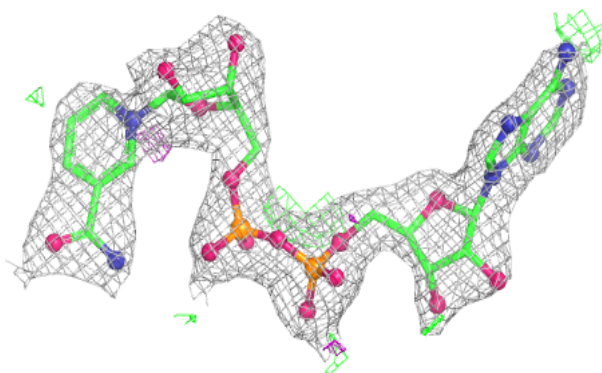
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 5335:

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

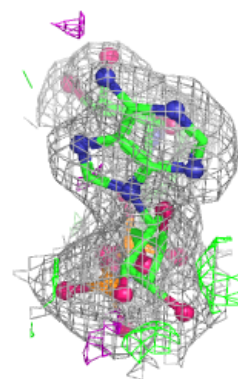
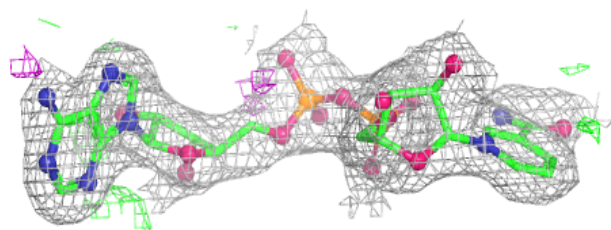
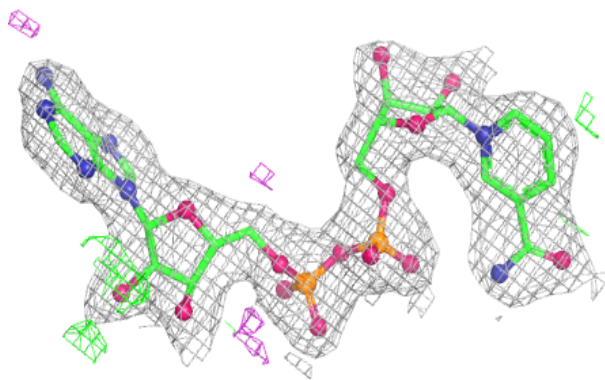
**Electron density around NAD B 6335:**

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



Electron density around NAD O 1335:

$2mF_o-DF_c$ (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.