



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:31 PM UTC

PDB ID : 3VPH / pdb_00003vph
Title : L-lactate dehydrogenase from *Thermus caldophilus* GK24 complexed with oxamate, NADH and FBP
Authors : Arai, K.; Ohno, T.; Miyanaga, A.; Fushinobu, S.; Taguchi, H.
Deposited on : 2012-03-01
Resolution : 2.00 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

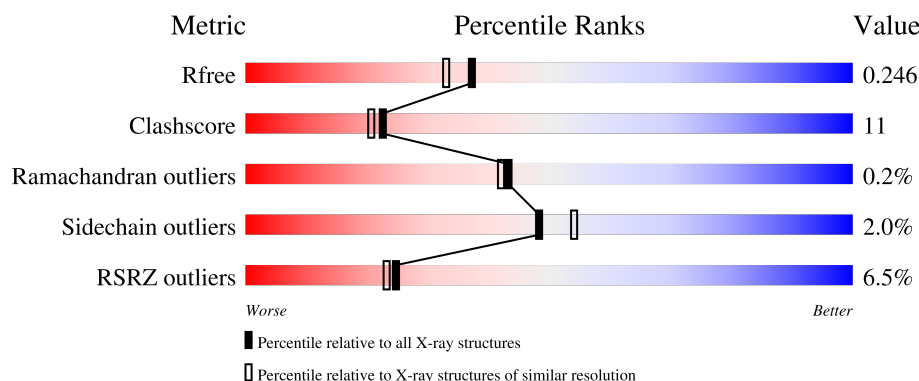
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	310	5% 84% 15% .
1	B	310	2% 84% 15% .
1	C	310	8% 78% 20% .
1	D	310	10% 77% 22% .

2 Entry composition [i](#)

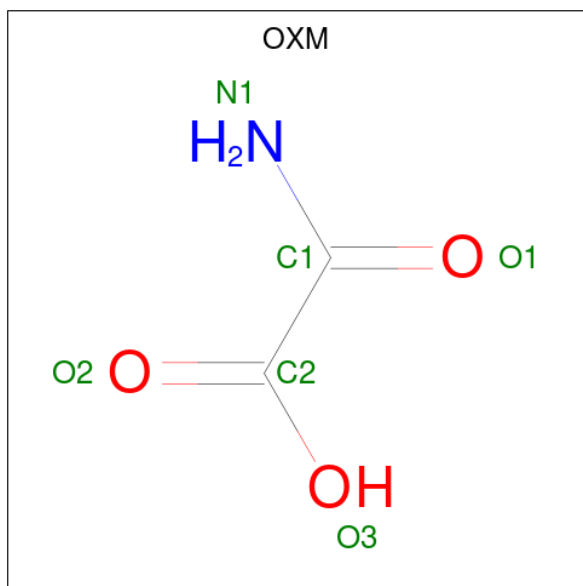
There are 6 unique types of molecules in this entry. The entry contains 9924 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2314	1466	417	428	3			
1	B	310	Total	C	N	O	S	0	0	0
			2314	1466	417	428	3			
1	C	310	Total	C	N	O	S	0	0	0
			2314	1466	417	428	3			
1	D	310	Total	C	N	O	S	0	0	0
			2314	1466	417	428	3			

- Molecule 2 is OXAMIC ACID (CCD ID: OXM) (formula: C₂H₃NO₃).



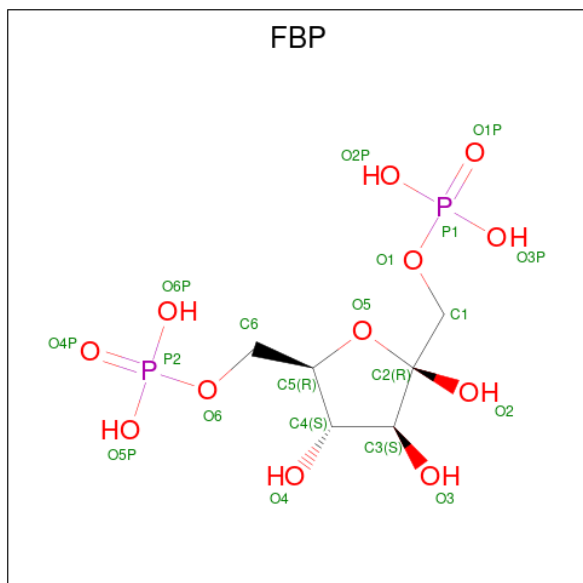
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			6	2	1	3		
2	B	1	Total	C	N	O	0	0
			6	2	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			6	2	1	3		
2	D	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 3 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



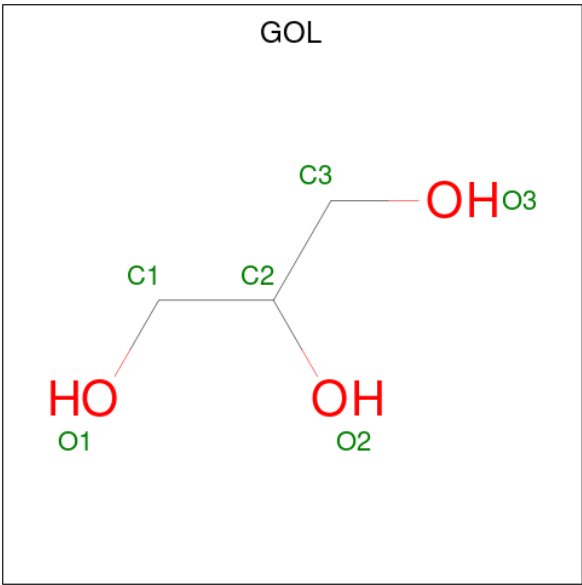
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	B	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

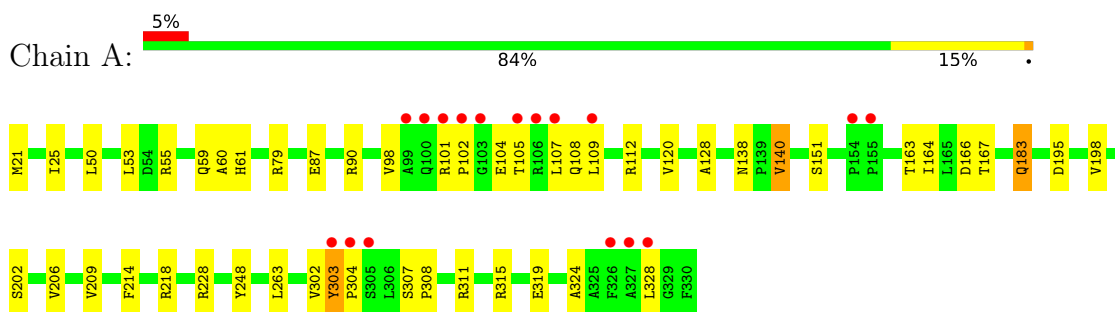
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	0
			121	121		
6	B	166	Total	O	0	0
			166	166		
6	C	80	Total	O	0	0
			80	80		
6	D	81	Total	O	0	0
			81	81		

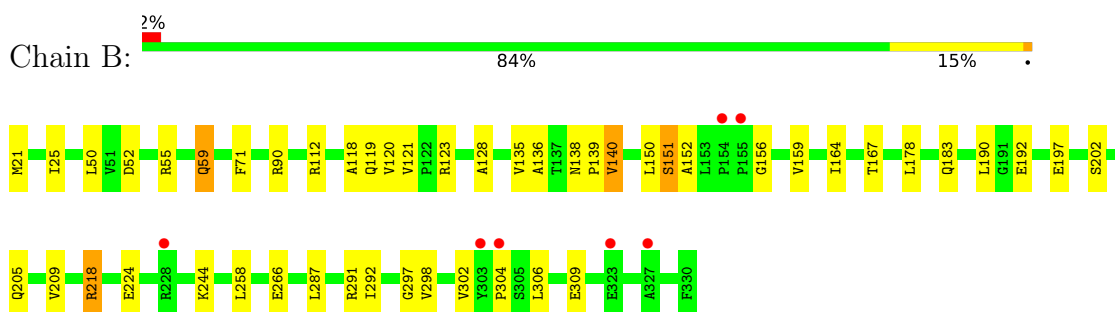
3 Residue-property plots

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.

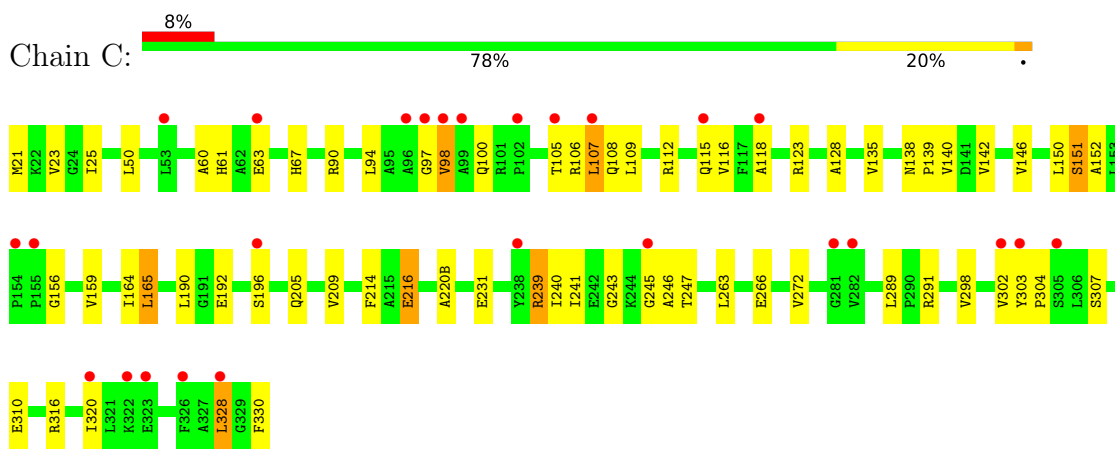
- Molecule 1: L-lactate dehydrogenase



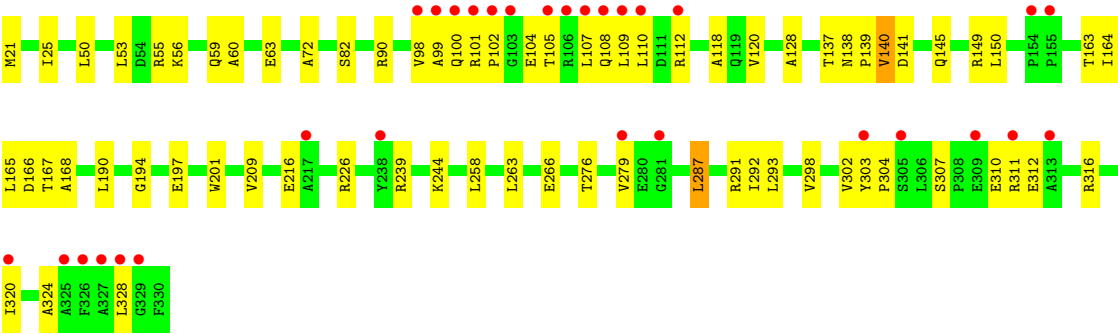
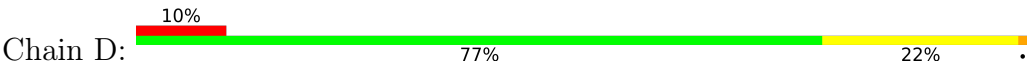
- Molecule 1: L-lactate dehydrogenase



- Molecule 1: L-lactate dehydrogenase



- Molecule 1: L-lactate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.74Å 67.84Å 147.34Å 90.00° 94.02° 90.00°	Depositor
Resolution (Å)	29.40 – 2.00 29.40 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.40-2.00) 98.6 (29.40-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.246 0.209 , 0.246	Depositor DCC
R_{free} test set	5625 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9924	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, GOL, OXM, FBP

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	0.40	0/2354	0.91	10/3202 (0.3%)
1	B	0.45	1/2354 (0.0%)	0.91	9/3202 (0.3%)
1	C	0.38	0/2354	0.86	4/3202 (0.1%)
1	D	0.36	0/2354	0.87	5/3202 (0.2%)
All	All	0.40	1/9416 (0.0%)	0.89	28/12808 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	VAL	CA-CB	5.58	1.56	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	VAL	N-CA-C	7.70	117.81	110.42
1	A	303	TYR	CA-C-N	7.00	128.59	119.84
1	A	303	TYR	C-N-CA	7.00	128.59	119.84
1	B	140	VAL	N-CA-C	6.85	118.43	110.62
1	D	120	VAL	N-CA-C	6.84	116.96	110.53
1	D	140	VAL	N-CA-C	6.59	117.28	110.36
1	A	128	ALA	CA-C-N	6.56	126.50	119.28
1	A	128	ALA	C-N-CA	6.56	126.50	119.28
1	A	140	VAL	N-CA-C	6.29	117.79	110.62
1	C	128	ALA	CA-C-N	6.17	126.06	119.28
1	C	128	ALA	C-N-CA	6.17	126.06	119.28
1	B	151	SER	N-CA-C	6.03	117.93	111.36
1	C	266	GLU	N-CA-C	5.82	117.62	111.28
1	B	120	VAL	N-CA-C	5.79	115.98	110.42
1	D	266	GLU	N-CA-C	5.79	117.59	111.28
1	A	198	VAL	N-CA-C	5.74	115.87	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ASP	N-CA-C	5.69	118.21	111.33
1	B	266	GLU	N-CA-C	5.53	117.31	111.28
1	B	202	SER	N-CA-C	5.49	117.69	111.11
1	D	128	ALA	CA-C-N	5.48	125.83	119.47
1	D	128	ALA	C-N-CA	5.48	125.83	119.47
1	B	128	ALA	CA-C-N	5.25	125.56	119.47
1	B	128	ALA	C-N-CA	5.25	125.56	119.47
1	A	202	SER	N-CA-C	5.22	117.37	111.11
1	A	151	SER	N-CA-C	5.13	117.77	111.82
1	B	135	VAL	N-CA-C	5.06	115.87	108.58
1	B	297	GLY	N-CA-C	-5.05	105.24	111.45
1	C	151	SER	N-CA-C	5.02	116.83	111.36

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	2314	0	2364	41	0
1	B	2314	0	2364	49	0
1	C	2314	0	2364	58	0
1	D	2314	0	2364	74	0
2	A	6	0	2	0	0
2	B	6	0	2	0	0
2	C	6	0	2	0	0
2	D	6	0	2	0	0
3	A	20	0	10	1	0
3	B	20	0	10	0	0
4	A	44	0	26	1	0
4	B	44	0	26	3	0
4	D	44	0	26	0	0
5	A	6	0	8	1	0
5	B	6	0	8	1	0
5	C	6	0	8	0	0
5	D	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	121	0	0	7	0
6	B	166	0	0	7	0
6	C	80	0	0	0	0
6	D	81	0	0	2	0
All	All	9924	0	9594	201	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 11.

All (201) 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:C:21:MET:HE3	1:C:90:ARG:HD2	1.21	1.10
1:C:107:LEU:H	1:C:107:LEU:HD12	1.31	0.94
1:A:209:VAL:HG12	1:D:304:PRO:HA	1.51	0.92
1:C:21:MET:CE	1:C:90:ARG:HD2	2.07	0.83
1:D:138:ASN:HD22	1:D:140:VAL:H	1.29	0.78
1:B:190:LEU:HD11	1:B:304:PRO:HG3	1.65	0.78
1:B:304:PRO:HB2	6:B:584:HOH:O	1.87	0.74
1:A:209:VAL:CG1	1:D:304:PRO:HA	2.17	0.74
1:B:59:GLN:HE21	1:B:59:GLN:HA	1.52	0.72
1:D:21:MET:CE	1:D:90:ARG:HG3	2.20	0.71
1:D:55:ARG:NH2	1:D:82:SER:HB3	2.05	0.71
1:B:205:GLN:HG3	6:B:559:HOH:O	1.91	0.70
1:B:156:GLY:HA2	1:B:298:VAL:HG22	1.73	0.70
1:B:209:VAL:HG21	1:C:302:VAL:CG1	2.23	0.69
1:D:190:LEU:HD11	1:D:304:PRO:HG3	1.74	0.69
1:A:98:VAL:CG1	1:A:112:ARG:HH21	2.07	0.68
1:B:209:VAL:HG21	1:C:302:VAL:HG12	1.75	0.67
1:D:21:MET:HE3	1:D:90:ARG:NH1	2.09	0.67
1:C:105:THR:HG22	1:C:106:ARG:N	2.09	0.65
1:A:55:ARG:HG2	6:A:586:HOH:O	1.97	0.64
1:A:304:PRO:HA	1:D:209:VAL:HG22	1.80	0.64
1:C:107:LEU:H	1:C:107:LEU:CD1	2.09	0.64
1:B:136:ALA:O	4:B:403:NAD:H2N	1.97	0.64
1:C:138:ASN:HA	1:C:140:VAL:N	2.13	0.64
1:C:156:GLY:HA2	1:C:298:VAL:HG22	1.80	0.64
1:D:21:MET:HE3	1:D:90:ARG:HG3	1.80	0.62
1:B:21:MET:HG2	1:B:90:ARG:NH1	2.13	0.62
1:A:98:VAL:HG11	1:A:112:ARG:HE	1.65	0.62
1:B:287:LEU:O	1:B:291:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ILE:HD12	1:D:258:LEU:HD21	1.82	0.61
1:D:307:SER:OG	1:D:310:GLU:HG3	2.00	0.61
1:C:63:GLU:HG2	1:C:67:HIS:CE1	2.36	0.61
1:B:59:GLN:HA	1:B:59:GLN:NE2	2.16	0.61
1:D:291:ARG:HD3	1:D:298:VAL:HG11	1.83	0.61
1:B:178:LEU:O	1:B:218:ARG:HD3	2.00	0.60
1:D:100:GLN:OE1	1:D:104:GLU:HB3	2.01	0.60
1:D:105:THR:OG1	1:D:108:GLN:HG2	2.02	0.60
1:D:324:ALA:O	1:D:328:LEU:HD23	2.02	0.60
1:A:308:PRO:HG3	6:A:595:HOH:O	2.02	0.59
1:A:98:VAL:HG12	1:A:112:ARG:HH21	1.66	0.59
1:D:138:ASN:HA	1:D:140:VAL:N	2.17	0.59
1:C:159:VAL:HG22	1:C:298:VAL:HG13	1.85	0.59
1:B:304:PRO:HA	1:C:209:VAL:HG22	1.85	0.59
1:A:302:VAL:HG12	1:D:209:VAL:HG21	1.85	0.58
1:B:218:ARG:O	1:B:218:ARG:HG3	2.01	0.58
1:C:316:ARG:O	1:C:320:ILE:HG13	2.04	0.58
1:D:98:VAL:HG21	1:D:112:ARG:NH2	2.18	0.58
1:B:55:ARG:HG2	1:B:55:ARG:HH11	1.69	0.58
1:B:156:GLY:HA2	1:B:298:VAL:CG2	2.34	0.58
1:B:164:ILE:HD12	1:B:258:LEU:HD21	1.86	0.58
1:C:100:GLN:HB2	1:C:109:LEU:HD22	1.86	0.57
1:D:312:GLU:O	1:D:316:ARG:HG2	2.04	0.57
1:A:302:VAL:CG1	1:D:209:VAL:HG21	2.35	0.57
1:C:60:ALA:HB3	1:D:244:LYS:HG3	1.86	0.57
1:B:209:VAL:HG22	1:C:304:PRO:HA	1.87	0.56
1:A:25:ILE:HB	1:A:50:LEU:HD23	1.88	0.56
1:C:105:THR:CG2	1:C:106:ARG:N	2.69	0.56
1:D:316:ARG:HH11	1:D:316:ARG:HG3	1.70	0.56
4:A:403:NAD:H6N	6:A:512:HOH:O	2.05	0.56
1:A:104:GLU:CD	1:A:109:LEU:HG	2.30	0.56
1:D:21:MET:HE2	1:D:90:ARG:HG3	1.88	0.56
1:A:61:HIS:HA	1:B:244:LYS:HD2	1.87	0.55
1:C:21:MET:HE3	1:C:90:ARG:CD	2.14	0.55
1:D:107:LEU:HD23	1:D:107:LEU:O	2.06	0.55
1:C:302:VAL:HG12	1:C:303:TYR:N	2.22	0.55
1:A:105:THR:OG1	1:A:108:GLN:HG3	2.07	0.55
1:A:60:ALA:HB3	1:B:244:LYS:HG3	1.89	0.54
1:D:55:ARG:HH21	1:D:82:SER:HB3	1.71	0.54
1:D:316:ARG:O	1:D:320:ILE:HG13	2.07	0.54
1:B:90:ARG:NH1	6:B:525:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:LEU:HD12	1:C:330:PHE:CE1	2.43	0.54
1:A:55:ARG:HD3	6:A:523:HOH:O	2.08	0.53
1:D:56:LYS:HG2	6:D:528:HOH:O	2.07	0.53
1:D:108:GLN:O	1:D:112:ARG:HG3	2.07	0.53
1:A:138:ASN:HA	1:A:140:VAL:N	2.24	0.53
1:A:183:GLN:HB2	6:A:501:HOH:O	2.08	0.53
1:C:156:GLY:HA2	1:C:298:VAL:CG2	2.38	0.53
1:D:163:THR:HA	1:D:166:ASP:OD1	2.09	0.53
1:C:216:GLU:HG3	1:C:220(B):ALA:HB2	1.89	0.53
1:D:101:ARG:HG3	1:D:112:ARG:HH12	1.74	0.52
1:A:206:VAL:O	1:A:209:VAL:HG22	2.10	0.52
1:A:21:MET:HE1	6:A:604:HOH:O	2.09	0.52
1:B:55:ARG:HG2	1:B:55:ARG:NH1	2.24	0.52
1:D:287:LEU:C	1:D:287:LEU:HD12	2.35	0.52
1:A:183:GLN:HG3	3:A:402:FBP:O3	2.10	0.51
1:D:25:ILE:HB	1:D:50:LEU:HD23	1.93	0.51
1:C:241:ILE:HG23	1:C:245:GLY:O	2.10	0.51
1:B:138:ASN:HA	1:B:140:VAL:N	2.26	0.50
1:B:119:GLN:O	1:B:123:ARG:HD3	2.11	0.50
1:D:59:GLN:O	1:D:63:GLU:HG3	2.11	0.50
1:D:302:VAL:HG12	1:D:303:TYR:N	2.26	0.50
1:A:315:ARG:O	1:A:319:GLU:HG3	2.11	0.50
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.76	0.50
1:D:194:GLY:O	1:D:197:GLU:HG2	2.12	0.49
1:C:105:THR:CG2	1:C:106:ARG:H	2.26	0.49
1:A:307:SER:O	1:A:311:ARG:HG3	2.13	0.49
1:C:105:THR:CB	1:C:108:GLN:HE21	2.26	0.49
1:D:101:ARG:HB3	1:D:102:PRO:HD2	1.95	0.49
1:C:328:LEU:HD13	1:C:328:LEU:O	2.12	0.49
1:C:60:ALA:CB	1:D:244:LYS:HG3	2.43	0.49
1:A:163:THR:HA	1:A:166:ASP:OD1	2.13	0.49
1:B:209:VAL:HG21	1:C:302:VAL:HG11	1.95	0.48
1:A:60:ALA:CB	1:B:244:LYS:HG3	2.43	0.48
1:D:138:ASN:HA	1:D:139:PRO:C	2.38	0.48
1:A:98:VAL:HG21	1:A:112:ARG:HB3	1.96	0.48
1:C:112:ARG:O	1:C:116:VAL:HG23	2.13	0.48
1:C:241:ILE:HG12	1:C:246:ALA:HA	1.95	0.48
1:B:52:ASP:OD1	4:B:403:NAD:H1B	2.13	0.48
1:C:190:LEU:HD11	1:C:304:PRO:HG3	1.95	0.48
1:D:201:TRP:CZ3	1:D:226:ARG:HG2	2.48	0.48
1:C:61:HIS:ND1	1:D:244:LYS:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:THR:HG22	5:A:404:GOL:H11	1.97	0.47
1:A:21:MET:SD	1:A:90:ARG:NH1	2.87	0.47
1:D:168:ALA:HB2	5:D:403:GOL:H12	1.97	0.47
1:D:258:LEU:HD22	1:D:293:LEU:CD2	2.45	0.47
1:A:183:GLN:NE2	1:A:183:GLN:HA	2.30	0.47
1:B:167:THR:HG22	5:B:404:GOL:H11	1.96	0.47
1:B:192:GLU:O	1:B:197:GLU:HB3	2.15	0.47
1:C:107:LEU:HD12	1:C:107:LEU:N	2.12	0.46
1:B:21:MET:HE1	6:B:586:HOH:O	2.15	0.46
1:B:292:ILE:N	1:B:292:ILE:HD12	2.30	0.46
1:D:137:THR:O	1:D:140:VAL:HA	2.15	0.46
1:D:307:SER:O	1:D:311:ARG:HG3	2.15	0.46
1:B:224:GLU:H	1:B:224:GLU:CD	2.24	0.46
1:B:118:ALA:HA	1:B:150:LEU:HD13	1.97	0.46
1:B:309:GLU:CD	1:B:309:GLU:H	2.22	0.46
1:C:328:LEU:HD12	1:C:330:PHE:CD1	2.50	0.46
1:D:276:THR:HG21	1:D:279:VAL:HG22	1.98	0.46
1:B:25:ILE:HB	1:B:50:LEU:HD23	1.98	0.46
1:B:304:PRO:HA	1:C:209:VAL:CG2	2.45	0.46
1:C:118:ALA:HA	1:C:150:LEU:HD13	1.97	0.46
1:C:190:LEU:HD11	1:C:304:PRO:CG	2.46	0.46
1:D:21:MET:HE3	1:D:90:ARG:CZ	2.45	0.46
1:C:272:VAL:HG23	1:C:291:ARG:HD2	1.97	0.45
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.82	0.45
1:A:101:ARG:HB3	1:A:102:PRO:HD2	1.98	0.45
1:B:183:GLN:HA	1:B:183:GLN:OE1	2.17	0.45
4:B:403:NAD:H6N	6:B:541:HOH:O	2.16	0.45
1:C:123:ARG:HH11	1:C:123:ARG:HG3	1.81	0.45
1:D:21:MET:HE2	1:D:263:LEU:HD22	1.98	0.45
1:A:183:GLN:NE2	1:A:183:GLN:CA	2.78	0.45
1:D:100:GLN:HA	1:D:100:GLN:NE2	2.32	0.45
1:D:292:ILE:HD12	1:D:292:ILE:N	2.31	0.45
1:A:214:PHE:CE1	1:D:302:VAL:HG21	2.52	0.44
1:A:304:PRO:HA	1:D:209:VAL:CG2	2.45	0.44
1:C:138:ASN:HA	1:C:139:PRO:C	2.42	0.44
1:D:98:VAL:HG22	1:D:99:ALA:N	2.33	0.44
1:A:59:GLN:NE2	1:A:59:GLN:HA	2.32	0.44
1:A:98:VAL:HG11	1:A:112:ARG:HH21	1.80	0.44
1:C:105:THR:HB	1:C:108:GLN:HE21	1.82	0.44
1:B:304:PRO:O	1:B:306:LEU:HG	2.18	0.44
1:C:94:LEU:HD12	1:C:135:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:VAL:O	1:C:146:VAL:HG23	2.18	0.43
1:C:243:GLY:HA3	1:D:60:ALA:HB2	2.00	0.43
1:D:239:ARG:HH11	1:D:239:ARG:HG2	1.82	0.43
1:B:209:VAL:CG2	1:C:304:PRO:HA	2.48	0.43
1:D:118:ALA:HA	1:D:150:LEU:HD13	2.01	0.43
1:A:324:ALA:O	1:A:328:LEU:HD23	2.19	0.43
1:D:104:GLU:CD	1:D:112:ARG:HH11	2.27	0.43
1:D:279:VAL:HG11	1:D:287:LEU:HD21	2.00	0.43
1:C:25:ILE:HB	1:C:50:LEU:HD23	2.01	0.42
1:B:21:MET:HG2	1:B:90:ARG:CZ	2.48	0.42
1:B:287:LEU:C	1:B:287:LEU:HD12	2.45	0.42
1:C:105:THR:HB	1:C:108:GLN:HG3	2.00	0.42
1:D:98:VAL:HG21	1:D:112:ARG:HH21	1.83	0.42
1:D:164:ILE:CD1	1:D:258:LEU:HD21	2.50	0.42
1:C:289:LEU:O	1:C:291:ARG:HG3	2.20	0.42
1:D:145:GLN:O	1:D:149:ARG:HG2	2.19	0.42
1:B:302:VAL:HG11	1:C:214:PHE:CD1	2.54	0.42
1:D:140:VAL:HG13	1:D:141:ASP:N	2.34	0.42
1:C:231:GLU:HG2	1:C:239:ARG:HH12	1.84	0.42
1:D:110:LEU:HD13	1:D:139:PRO:HD2	2.02	0.42
1:A:104:GLU:OE2	1:A:112:ARG:NH1	2.53	0.41
1:B:112:ARG:HD2	6:B:570:HOH:O	2.20	0.41
1:C:192:GLU:OE1	1:C:196:SER:HB3	2.20	0.41
1:C:164:ILE:HG23	1:C:165:LEU:N	2.35	0.41
1:D:100:GLN:NE2	1:D:109:LEU:HD11	2.35	0.41
1:D:316:ARG:HG3	1:D:316:ARG:NH1	2.33	0.41
1:D:104:GLU:OE1	1:D:112:ARG:NH1	2.49	0.41
1:A:79:ARG:NH1	6:A:550:HOH:O	2.50	0.41
1:B:138:ASN:HA	1:B:139:PRO:C	2.46	0.41
1:D:72:ALA:HB3	6:D:510:HOH:O	2.20	0.41
1:B:224:GLU:CD	1:B:224:GLU:N	2.79	0.41
1:C:151:SER:O	1:C:152:ALA:HB3	2.21	0.41
1:D:190:LEU:HD11	1:D:304:PRO:CG	2.45	0.41
1:B:159:VAL:HG22	1:B:298:VAL:HG13	2.02	0.41
1:C:164:ILE:CG2	1:C:165:LEU:N	2.84	0.41
1:A:303:TYR:HA	1:A:304:PRO:HD2	1.81	0.40
1:B:59:GLN:NE2	6:B:569:HOH:O	2.54	0.40
1:C:240:ILE:CG2	1:C:247:THR:HG22	2.51	0.40
1:D:104:GLU:HG2	1:D:105:THR:N	2.37	0.40
1:D:302:VAL:CG1	1:D:303:TYR:N	2.84	0.40
1:B:151:SER:O	1:B:152:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:VAL:CG2	1:D:112:ARG:NH2	2.84	0.40
1:C:23:VAL:CG2	1:C:263:LEU:HD11	2.52	0.40
1:C:97:GLY:O	1:C:98:VAL:C	2.64	0.40
1:C:307:SER:OG	1:C:310:GLU:HG3	2.21	0.40
1:D:100:GLN:HE21	1:D:109:LEU:HD11	1.86	0.40
1:A:164:ILE:HG12	1:B:71:PHE:CE1	2.56	0.40
1:D:104:GLU:HG2	1:D:108:GLN:HB2	2.04	0.40
1:D:167:THR:HG22	5:D:403:GOL:H11	2.04	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	308/310 (99%)	297 (96%)	10 (3%)	1 (0%)	36	35
1	B	308/310 (99%)	300 (97%)	8 (3%)	0	100	100
1	C	308/310 (99%)	295 (96%)	12 (4%)	1 (0%)	36	35
1	D	308/310 (99%)	295 (96%)	13 (4%)	0	100	100
All	All	1232/1240 (99%)	1187 (96%)	43 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	98	VAL
1	A	248	TYR

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	232/232 (100%)	226 (97%)	6 (3%)	40	44
1	B	232/232 (100%)	230 (99%)	2 (1%)	70	78
1	C	232/232 (100%)	225 (97%)	7 (3%)	36	38
1	D	232/232 (100%)	228 (98%)	4 (2%)	53	60
All	All	928/928 (100%)	909 (98%)	19 (2%)	48	54

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	87	GLU
1	A	107	LEU
1	A	183	GLN
1	A	218	ARG
1	A	263	LEU
1	B	59	GLN
1	B	218	ARG
1	C	107	LEU
1	C	115	GLN
1	C	165	LEU
1	C	205	GLN
1	C	216	GLU
1	C	239	ARG
1	C	328	LEU
1	D	53	LEU
1	D	165	LEU
1	D	216	GLU
1	D	287	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	115	GLN
1	A	183	GLN
1	A	205	GLN

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Mol	Chain	Res	Type
1	B	59	GLN
1	B	100	GLN
1	B	115	GLN
1	B	183	GLN
1	B	205	GLN
1	C	108	GLN
1	C	119	GLN
1	C	145	GLN
1	D	100	GLN
1	D	138	ASN
1	D	205	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	OXM	B	401	-	5,5,5	3.87	1 (20%)	2,6,6	1.60	0
3	FBP	A	402	-	18,20,20	0.98	0	21,32,32	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAD	A	403	-	46,48,48	1.98	15 (32%)	64,73,73	2.58	15 (23%)
5	GOL	B	404	-	5,5,5	0.53	0	5,5,5	0.24	0
4	NAD	B	403	-	46,48,48	1.97	17 (36%)	64,73,73	2.61	16 (25%)
2	OXM	D	401	-	5,5,5	4.14	1 (20%)	2,6,6	1.41	0
5	GOL	D	403	-	5,5,5	0.48	0	5,5,5	0.18	0
3	FBP	B	402	-	18,20,20	0.99	0	21,32,32	0.82	0
4	NAD	D	402	-	46,48,48	2.01	15 (32%)	64,73,73	2.59	13 (20%)
5	GOL	A	404	-	5,5,5	0.53	0	5,5,5	0.23	0
2	OXM	C	401	-	5,5,5	3.13	1 (20%)	2,6,6	1.77	0
5	GOL	C	402	-	5,5,5	0.56	0	5,5,5	0.22	0
2	OXM	A	401	-	5,5,5	3.95	1 (20%)	2,6,6	1.56	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
2	OXM	B	401	-	-	4/4/4/4	-
3	FBP	A	402	-	-	0/13/32/32	0/1/1/1
4	NAD	A	403	-	-	8/30/62/62	0/5/5/5
5	GOL	B	404	-	-	4/4/4/4	-
4	NAD	B	403	-	-	8/30/62/62	0/5/5/5
2	OXM	D	401	-	-	4/4/4/4	-
5	GOL	D	403	-	-	2/4/4/4	-
3	FBP	B	402	-	-	0/13/32/32	0/1/1/1
4	NAD	D	402	-	-	8/30/62/62	0/5/5/5
5	GOL	A	404	-	-	3/4/4/4	-
2	OXM	C	401	-	-	1/4/4/4	-
5	GOL	C	402	-	-	2/4/4/4	-
2	OXM	A	401	-	-	4/4/4/4	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	OXM	C1-C2	-8.91	1.44	1.55
2	A	401	OXM	C1-C2	-8.47	1.45	1.55
2	B	401	OXM	C1-C2	-8.35	1.45	1.55
2	C	401	OXM	C1-C2	-6.51	1.47	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	402	NAD	C2N-N1N	5.51	1.41	1.35
4	A	403	NAD	C2N-N1N	5.33	1.40	1.35
4	B	403	NAD	C2N-N1N	4.62	1.40	1.35
4	A	403	NAD	C5A-C4A	-3.80	1.32	1.39
4	D	402	NAD	C5A-C4A	-3.70	1.32	1.39
4	D	402	NAD	C6N-N1N	3.65	1.43	1.35
4	B	403	NAD	C6N-N1N	3.65	1.43	1.35
4	A	403	NAD	C5A-N7A	-3.58	1.32	1.39
4	B	403	NAD	C5A-C4A	-3.58	1.32	1.39
4	B	403	NAD	C5A-N7A	-3.54	1.32	1.39
4	B	403	NAD	C1B-N9A	3.53	1.56	1.46
4	D	402	NAD	C5A-N7A	-3.52	1.32	1.39
4	D	402	NAD	C8A-N7A	3.42	1.38	1.31
4	A	403	NAD	PA-O3	3.37	1.63	1.59
4	A	403	NAD	C6N-N1N	3.36	1.43	1.35
4	D	402	NAD	O4D-C1D	3.29	1.45	1.40
4	B	403	NAD	O4D-C1D	3.24	1.45	1.40
4	D	402	NAD	C2A-N3A	3.24	1.39	1.33
4	A	403	NAD	O4D-C1D	3.19	1.45	1.40
4	A	403	NAD	C8A-N7A	3.17	1.37	1.31
4	B	403	NAD	C8A-N7A	3.15	1.37	1.31
4	B	403	NAD	C2A-N1A	3.11	1.39	1.33
4	B	403	NAD	C2A-N3A	3.08	1.39	1.33
4	D	402	NAD	C1B-N9A	3.06	1.54	1.46
4	D	402	NAD	C2A-N1A	3.03	1.39	1.33
4	A	403	NAD	C2A-N1A	3.01	1.39	1.33
4	A	403	NAD	C2A-N3A	2.86	1.39	1.33
4	A	403	NAD	C1B-N9A	2.67	1.53	1.46
4	D	402	NAD	C5N-C4N	2.52	1.43	1.38
4	D	402	NAD	C4A-N3A	2.51	1.39	1.34
4	B	403	NAD	C4A-N3A	2.48	1.39	1.34
4	B	403	NAD	C5N-C4N	2.43	1.43	1.38
4	B	403	NAD	O3D-C3D	2.35	1.48	1.43
4	A	403	NAD	C5N-C4N	2.30	1.42	1.38
4	D	402	NAD	C4N-C3N	2.25	1.42	1.39
4	A	403	NAD	C4A-N3A	2.23	1.38	1.34
4	D	402	NAD	O3D-C3D	2.23	1.48	1.43
4	A	403	NAD	C4N-C3N	2.22	1.42	1.39
4	D	402	NAD	C6N-C5N	2.17	1.43	1.38
4	B	403	NAD	O4B-C4B	2.15	1.49	1.45
4	B	403	NAD	C4N-C3N	2.10	1.42	1.39
4	B	403	NAD	C6N-C5N	2.09	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	NAD	PA-O3	2.04	1.61	1.59
4	A	403	NAD	O3B-C3B	2.04	1.48	1.43
4	D	402	NAD	O4B-C4B	2.03	1.49	1.45
4	A	403	NAD	C6N-C5N	2.02	1.42	1.38
4	B	403	NAD	O4B-C1B	2.01	1.46	1.42

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	NAD	O3-PA-O1A	-9.44	82.31	110.70
4	D	402	NAD	O2A-PA-O3	-9.31	82.10	107.27
4	B	403	NAD	O3-PA-O1A	-9.21	82.99	110.70
4	A	403	NAD	O2A-PA-O3	-9.20	82.42	107.27
4	B	403	NAD	O2A-PA-O3	-9.19	82.44	107.27
4	A	403	NAD	O3-PA-O1A	-9.16	83.14	110.70
4	B	403	NAD	C5A-C4A-N3A	-6.22	118.15	126.72
4	A	403	NAD	C5A-C4A-N3A	-6.01	118.44	126.72
4	D	402	NAD	C5A-C4A-N3A	-5.92	118.56	126.72
4	A	403	NAD	N3A-C2A-N1A	-5.78	119.83	128.58
4	D	402	NAD	N3A-C2A-N1A	-5.73	119.90	128.58
4	B	403	NAD	N3A-C2A-N1A	-5.68	119.99	128.58
4	B	403	NAD	C6A-C5A-N7A	-5.26	121.95	132.09
4	B	403	NAD	C6A-C5A-C4A	5.20	124.27	117.18
4	A	403	NAD	C6A-C5A-N7A	-5.18	122.10	132.09
4	A	403	NAD	C6A-C5A-C4A	5.18	124.25	117.18
4	D	402	NAD	C6A-C5A-N7A	-5.07	122.31	132.09
4	D	402	NAD	C6A-C5A-C4A	5.06	124.09	117.18
4	B	403	NAD	N3A-C4A-N9A	4.86	135.44	127.17
4	A	403	NAD	N3A-C4A-N9A	4.70	135.17	127.17
4	B	403	NAD	C4D-O4D-C1D	-4.67	105.65	109.92
4	D	402	NAD	N3A-C4A-N9A	4.51	134.84	127.17
4	A	403	NAD	N9A-C8A-N7A	-4.29	107.85	113.94
4	D	402	NAD	C4D-O4D-C1D	-4.29	106.00	109.92
4	D	402	NAD	N9A-C8A-N7A	-4.26	107.89	113.94
4	A	403	NAD	C4D-O4D-C1D	-3.95	106.31	109.92
4	B	403	NAD	N9A-C8A-N7A	-3.95	108.33	113.94
4	B	403	NAD	C2A-N3A-C4A	3.47	120.32	111.83
4	A	403	NAD	C2A-N3A-C4A	3.41	120.16	111.83
4	D	402	NAD	C2A-N3A-C4A	3.34	119.99	111.83
4	A	403	NAD	O2A-PA-O1A	2.88	125.86	112.44
4	D	402	NAD	O2A-PA-O1A	2.83	125.59	112.44
4	B	403	NAD	C4A-C5A-N7A	2.80	113.78	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	NAD	C4A-C5A-N7A	2.69	113.66	110.58
4	B	403	NAD	O2A-PA-O1A	2.66	124.81	112.44
4	D	402	NAD	C4A-C5A-N7A	2.64	113.60	110.58
4	B	403	NAD	C3N-C7N-N7N	-2.37	114.81	117.74
4	A	403	NAD	C6N-N1N-C2N	-2.33	119.89	121.88
4	A	403	NAD	C3N-C7N-N7N	-2.17	115.06	117.74
4	B	403	NAD	C6N-N1N-C1D	2.14	123.93	119.73
4	B	403	NAD	C6N-N1N-C2N	-2.12	120.07	121.88
4	A	403	NAD	O4B-C1B-N9A	2.07	112.06	108.09
4	D	402	NAD	C6N-N1N-C2N	-2.04	120.14	121.88
4	B	403	NAD	O2A-PA-O5B	2.01	116.69	107.57

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	OXM	N1-C1-C2-O2
2	A	401	OXM	N1-C1-C2-O3
2	A	401	OXM	O1-C1-C2-O2
2	A	401	OXM	O1-C1-C2-O3
2	B	401	OXM	N1-C1-C2-O2
2	B	401	OXM	N1-C1-C2-O3
2	B	401	OXM	O1-C1-C2-O3
2	C	401	OXM	O1-C1-C2-O3
2	D	401	OXM	N1-C1-C2-O2
2	D	401	OXM	N1-C1-C2-O3
2	D	401	OXM	O1-C1-C2-O2
2	D	401	OXM	O1-C1-C2-O3
4	A	403	NAD	C5B-O5B-PA-O3
4	A	403	NAD	O4D-C1D-N1N-C2N
4	A	403	NAD	O4D-C1D-N1N-C6N
4	A	403	NAD	C2D-C1D-N1N-C2N
4	A	403	NAD	C2D-C1D-N1N-C6N
4	B	403	NAD	C5B-O5B-PA-O3
4	B	403	NAD	O4D-C1D-N1N-C2N
4	B	403	NAD	O4D-C1D-N1N-C6N
4	B	403	NAD	C2D-C1D-N1N-C2N
4	B	403	NAD	C2D-C1D-N1N-C6N
4	D	402	NAD	C5B-O5B-PA-O3
4	D	402	NAD	O4D-C1D-N1N-C2N
4	D	402	NAD	O4D-C1D-N1N-C6N
4	D	402	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
4	D	402	NAD	C2D-C1D-N1N-C6N
5	A	404	GOL	O1-C1-C2-O2
5	A	404	GOL	O1-C1-C2-C3
5	B	404	GOL	O1-C1-C2-C3
5	B	404	GOL	C1-C2-C3-O3
5	C	402	GOL	O1-C1-C2-C3
4	B	403	NAD	O4B-C4B-C5B-O5B
5	D	403	GOL	O1-C1-C2-C3
5	B	404	GOL	O1-C1-C2-O2
5	C	402	GOL	O1-C1-C2-O2
4	A	403	NAD	O4B-C4B-C5B-O5B
4	A	403	NAD	C3B-C4B-C5B-O5B
2	B	401	OXM	O1-C1-C2-O2
4	B	403	NAD	C3B-C4B-C5B-O5B
4	D	402	NAD	O4B-C4B-C5B-O5B
4	D	402	NAD	C3B-C4B-C5B-O5B
5	B	404	GOL	O2-C2-C3-O3
5	A	404	GOL	O2-C2-C3-O3
5	D	403	GOL	O1-C1-C2-O2
4	B	403	NAD	C4B-C5B-O5B-PA
4	A	403	NAD	C4B-C5B-O5B-PA
4	D	402	NAD	C4B-C5B-O5B-PA

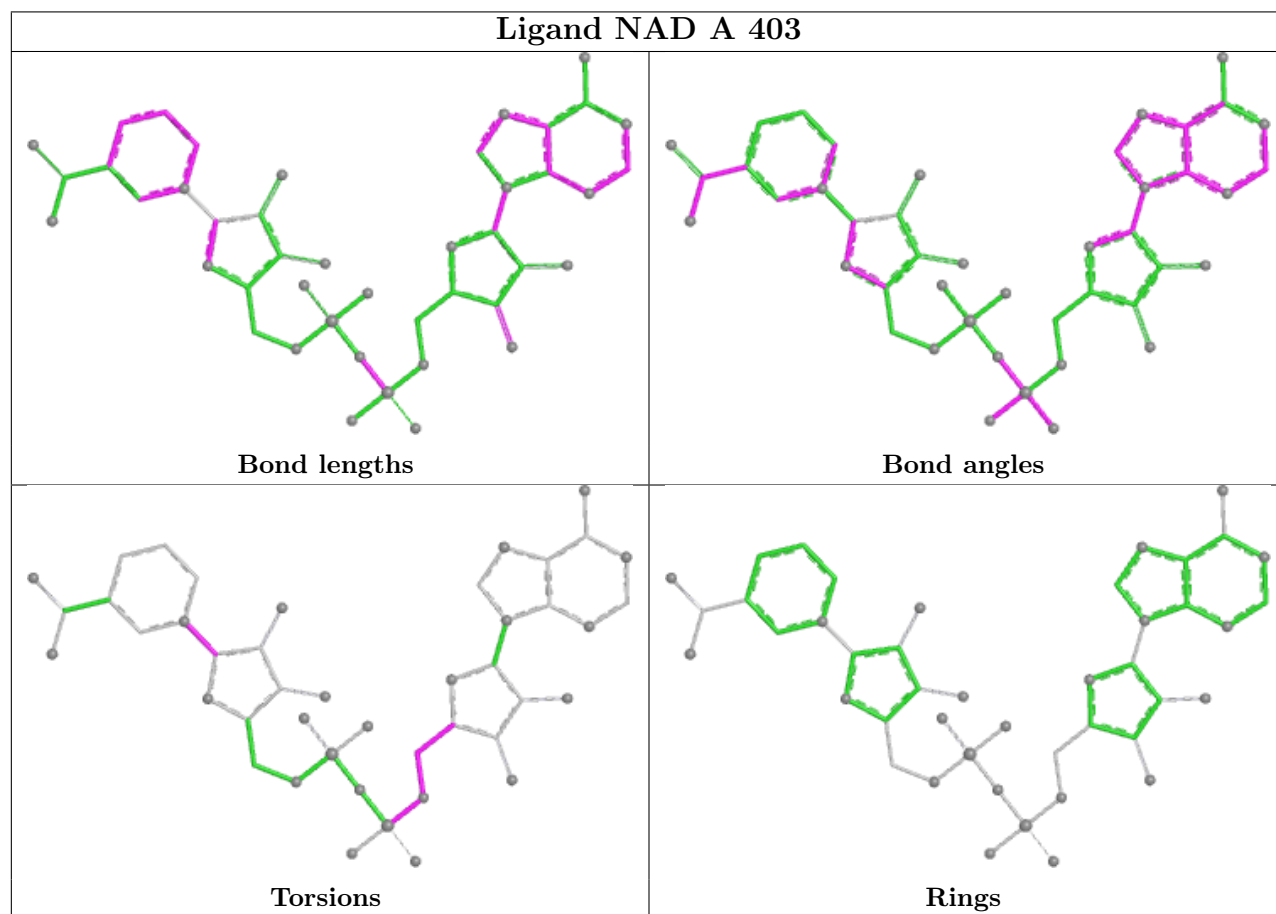
There are no ring outliers.

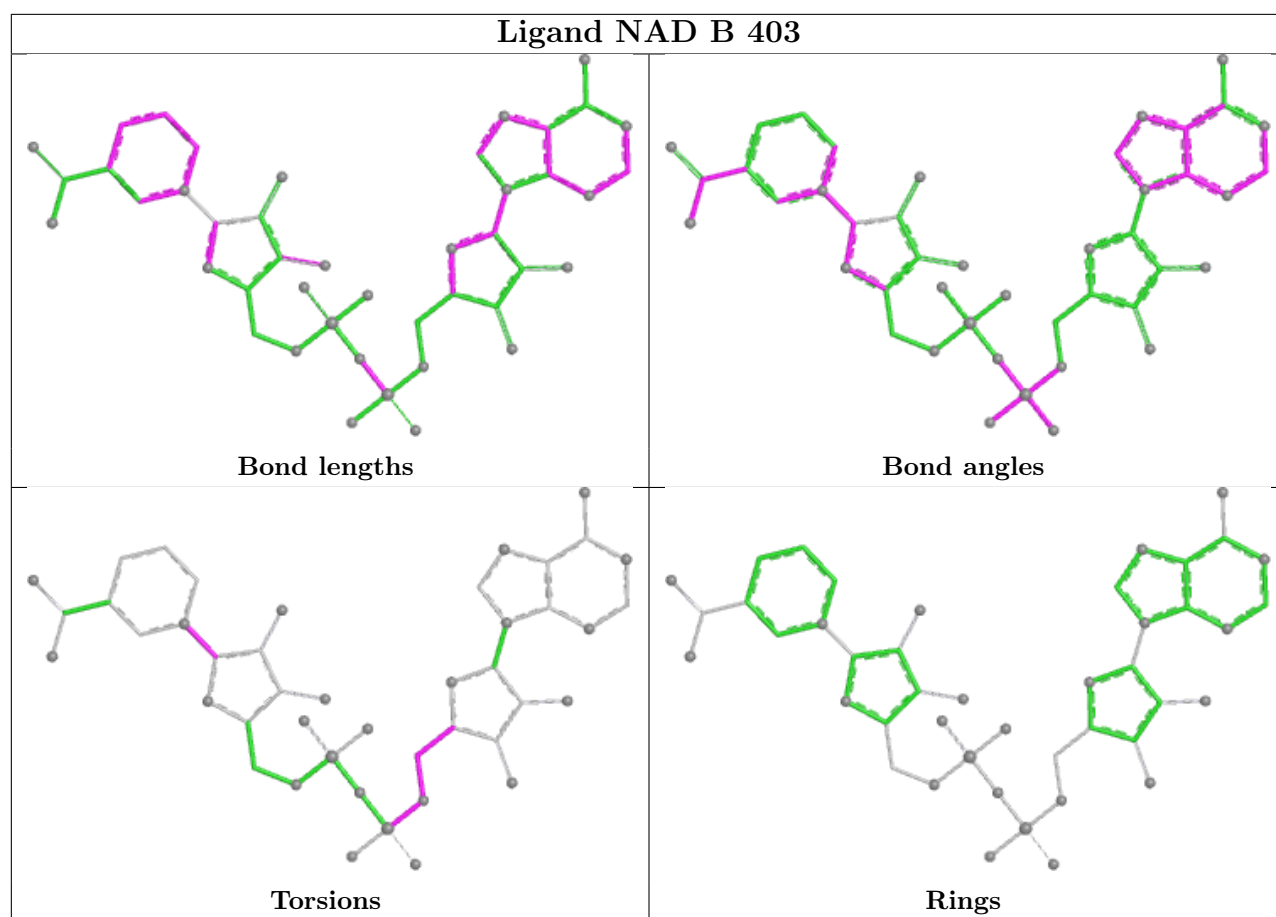
6 monomers are involved in 9 short contacts:

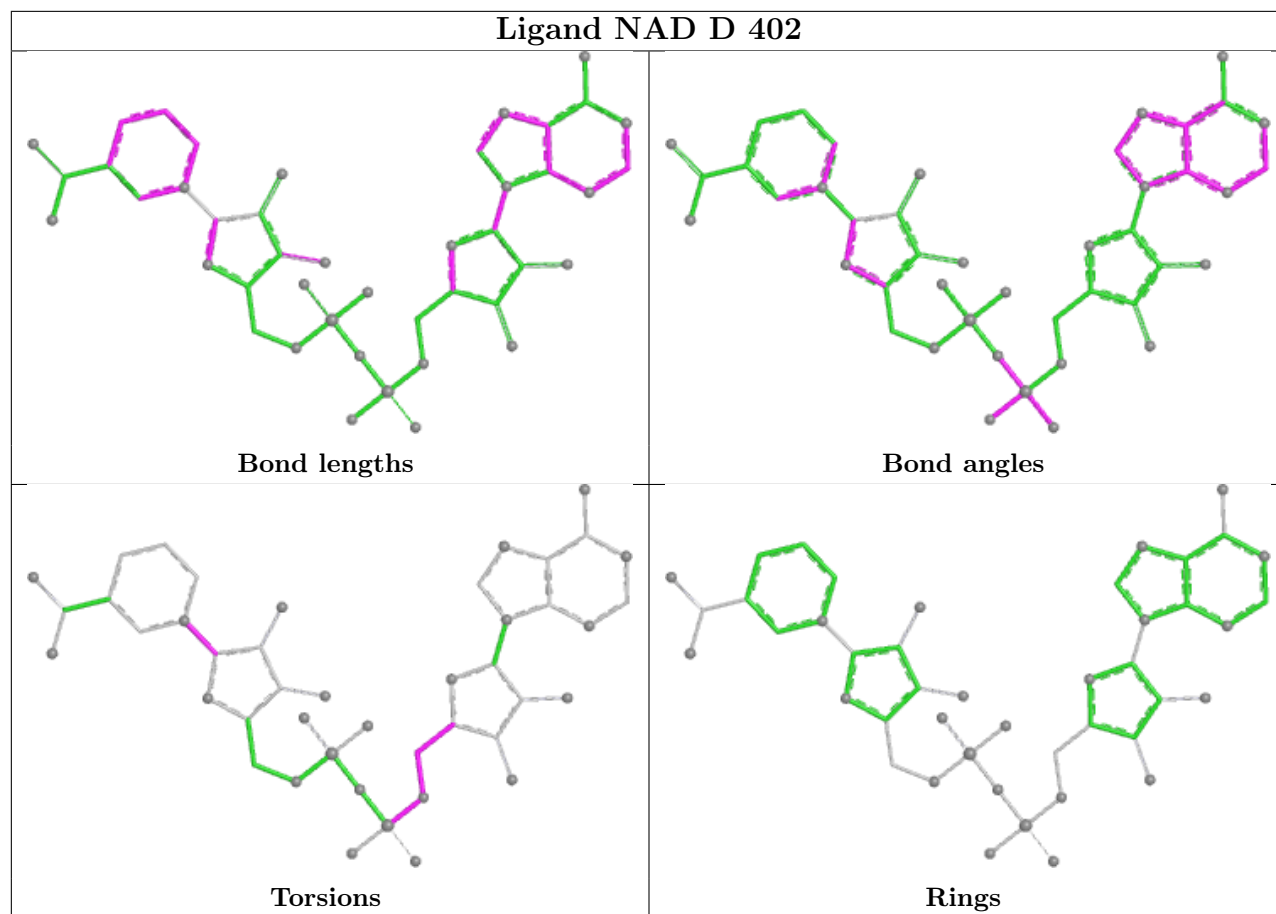
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	FBP	1	0
4	A	403	NAD	1	0
5	B	404	GOL	1	0
4	B	403	NAD	3	0
5	D	403	GOL	2	0
5	A	404	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	310/310 (100%)	0.01	17 (5%) 30 29	15, 28, 54, 93	0
1	B	310/310 (100%)	-0.18	7 (2%) 61 60	15, 26, 46, 56	0
1	C	310/310 (100%)	0.54	26 (8%) 17 15	22, 36, 60, 78	0
1	D	310/310 (100%)	0.60	30 (9%) 13 12	22, 36, 65, 109	0
All	All	1240/1240 (100%)	0.24	80 (6%) 25 23	15, 31, 59, 109	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	PRO	6.9
1	D	107	LEU	6.0
1	C	98	VAL	5.9
1	D	109	LEU	5.3
1	C	99	ALA	4.8
1	C	97	GLY	4.8
1	B	303	TYR	4.4
1	B	154	PRO	4.3
1	D	101	ARG	4.2
1	D	155	PRO	4.0
1	D	154	PRO	3.9
1	A	328	LEU	3.8
1	B	304	PRO	3.8
1	A	102	PRO	3.8
1	C	282	VAL	3.7
1	A	305	SER	3.5
1	D	328	LEU	3.4
1	C	323	GLU	3.3
1	D	303	TYR	3.3
1	D	110	LEU	3.3
1	D	105	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	303	TYR	3.2
1	D	99	ALA	3.2
1	B	155	PRO	3.2
1	C	53	LEU	3.2
1	D	103	GLY	3.0
1	D	108	GLN	3.0
1	A	99	ALA	2.9
1	C	107	LEU	2.9
1	A	107	LEU	2.8
1	C	155	PRO	2.8
1	A	109	LEU	2.8
1	A	326	PHE	2.8
1	D	100	GLN	2.8
1	D	309	GLU	2.8
1	C	328	LEU	2.7
1	C	154	PRO	2.7
1	D	217	ALA	2.7
1	A	103	GLY	2.7
1	A	101	ARG	2.7
1	D	329	GLY	2.7
1	D	326	PHE	2.6
1	A	155	PRO	2.6
1	A	303	TYR	2.6
1	D	279	VAL	2.6
1	D	311	ARG	2.6
1	C	196	SER	2.6
1	C	302	VAL	2.6
1	C	326	PHE	2.6
1	C	245	GLY	2.5
1	D	320	ILE	2.5
1	D	281	GLY	2.4
1	A	105	THR	2.4
1	C	96	ALA	2.4
1	D	313	ALA	2.4
1	A	100	GLN	2.4
1	C	102	PRO	2.4
1	C	320	ILE	2.4
1	A	154	PRO	2.4
1	B	327	ALA	2.3
1	D	98	VAL	2.3
1	D	106	ARG	2.3
1	B	323	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	228	ARG	2.3
1	C	305	SER	2.3
1	C	105	THR	2.3
1	A	106	ARG	2.2
1	A	304	PRO	2.2
1	D	238	TYR	2.2
1	C	118	ALA	2.2
1	C	115	GLN	2.1
1	C	238	TYR	2.1
1	C	281	GLY	2.1
1	D	305	SER	2.1
1	A	327	ALA	2.1
1	C	63	GLU	2.0
1	D	325	ALA	2.1
1	D	327	ALA	2.0
1	D	112	ARG	2.0
1	C	322	LYS	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(Å ²)	Q<0.9
2	OXM	C	401	6/6	0.82	0.13	29,33,46,46	0
2	OXM	B	401	6/6	0.83	0.12	24,27,32,39	0
2	OXM	D	401	6/6	0.84	0.13	29,35,40,41	0
4	NAD	B	403	44/44	0.85	0.13	26,50,59,64	0
2	OXM	A	401	6/6	0.87	0.12	23,30,43,43	0
5	GOL	D	403	6/6	0.88	0.14	35,42,49,50	0

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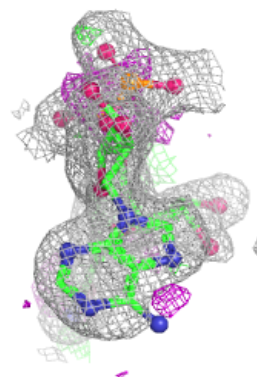
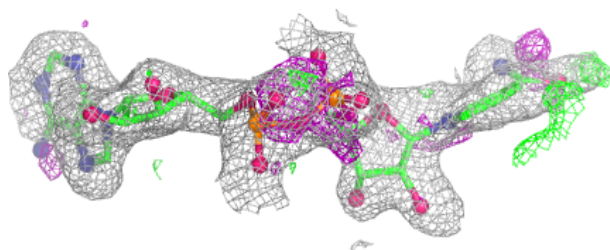
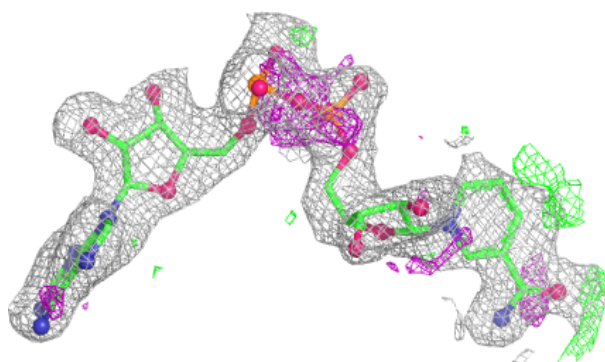
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	C	402	6/6	0.91	0.11	28,33,37,38	0
4	NAD	D	402	44/44	0.91	0.11	30,46,59,61	0
5	GOL	B	404	6/6	0.93	0.08	21,31,32,40	0
3	FBP	A	402	20/20	0.93	0.11	27,43,51,52	0
3	FBP	B	402	20/20	0.93	0.11	32,43,56,64	0
5	GOL	A	404	6/6	0.94	0.08	26,33,33,37	0
4	NAD	A	403	44/44	0.96	0.07	18,29,38,40	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.

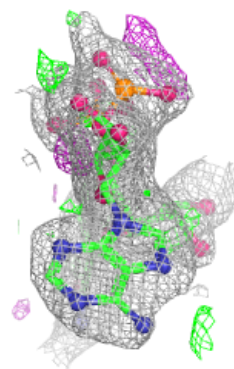
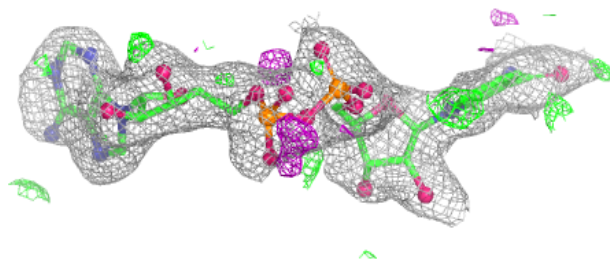
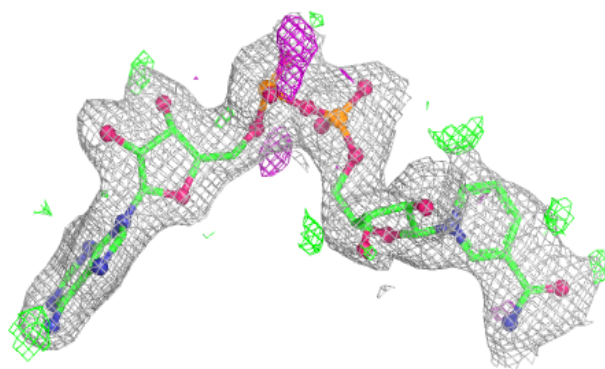
Electron density around NAD B 403:

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

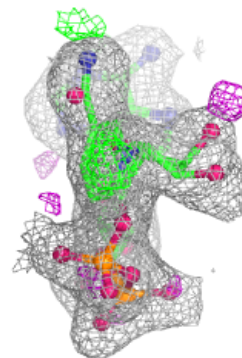
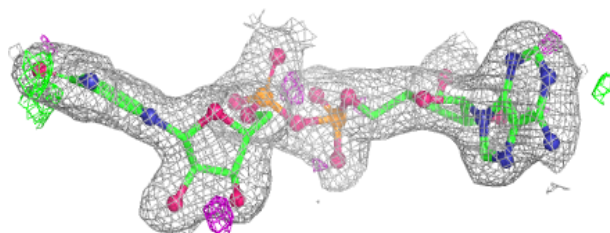
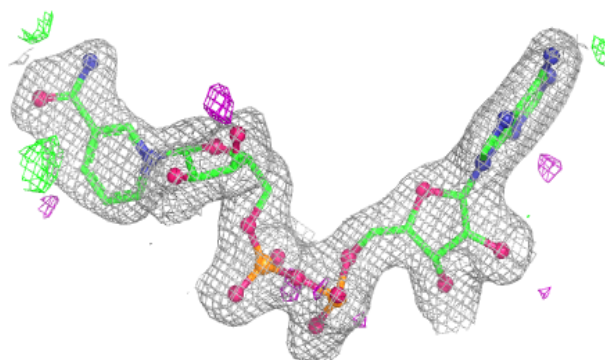


Electron density around NAD D 402:

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

**Electron density around NAD A 403:**

$2mF_o-DF_c$ (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.