Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 02:27 AM EDT

PDB ID	:	1SC6
Title	:	Crystal Structure of W139G D-3-Phosphoglycerate dehydrogenase complexed with NAD+
Authors	:	Bell, J.K.; Grant, G.A.; Banaszak, L.J.
Deposited on	:	2004-02-11
Resolution	:	2.09 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 (i) symbol.

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

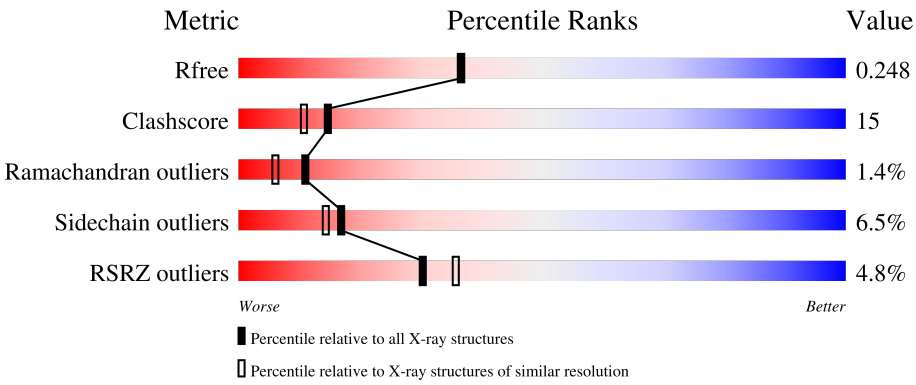
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	404	7% 65% 27% • •
1	B	404	3% 70% 22% • 5%
1	C	404	6% 66% 24% • 6%
1	D	404	2% 71% 21% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12302 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 D-3-phosphoglycerate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	390	2960	1872	517	563	8	114	1	0
1	B	385	2920	1845	512	555	8	80	1	0
1	C	378	2865	1813	501	543	8	162	1	0
1	D	384	2918	1848	508	554	8	67	1	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ALA	CYS	engineered mutation	UNP P0A9T0
A	83	ALA	CYS	engineered mutation	UNP P0A9T0
A	139	GLY	TRP	engineered mutation	UNP P0A9T0
A	175	MSE	MET	modified residue	UNP P0A9T0
A	203	MSE	MET	modified residue	UNP P0A9T0
A	220	MSE	MET	modified residue	UNP P0A9T0
A	221	MSE	MET	modified residue	UNP P0A9T0
A	229	MSE	MET	modified residue	UNP P0A9T0
A	250	ALA	CYS	engineered mutation	UNP P0A9T0
A	282	ALA	CYS	engineered mutation	UNP P0A9T0
A	341	MSE	MET	modified residue	UNP P0A9T0
A	376	MSE	MET	modified residue	UNP P0A9T0
A	397	MSE	MET	modified residue	UNP P0A9T0
B	81	ALA	CYS	engineered mutation	UNP P0A9T0
B	83	ALA	CYS	engineered mutation	UNP P0A9T0
B	139	GLY	TRP	engineered mutation	UNP P0A9T0
B	175	MSE	MET	modified residue	UNP P0A9T0
B	203	MSE	MET	modified residue	UNP P0A9T0
B	220	MSE	MET	modified residue	UNP P0A9T0
B	221	MSE	MET	modified residue	UNP P0A9T0
B	229	MSE	MET	modified residue	UNP P0A9T0

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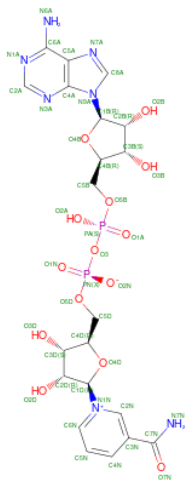
Chain	Residue	Modelled	Actual	Comment	Reference
B	250	ALA	CYS	engineered mutation	UNP P0A9T0
B	282	ALA	CYS	engineered mutation	UNP P0A9T0
B	341	MSE	MET	modified residue	UNP P0A9T0
B	376	MSE	MET	modified residue	UNP P0A9T0
B	397	MSE	MET	modified residue	UNP P0A9T0
C	81	ALA	CYS	engineered mutation	UNP P0A9T0
C	83	ALA	CYS	engineered mutation	UNP P0A9T0
C	139	GLY	TRP	engineered mutation	UNP P0A9T0
C	175	MSE	MET	modified residue	UNP P0A9T0
C	203	MSE	MET	modified residue	UNP P0A9T0
C	220	MSE	MET	modified residue	UNP P0A9T0
C	221	MSE	MET	modified residue	UNP P0A9T0
C	229	MSE	MET	modified residue	UNP P0A9T0
C	250	ALA	CYS	engineered mutation	UNP P0A9T0
C	282	ALA	CYS	engineered mutation	UNP P0A9T0
C	341	MSE	MET	modified residue	UNP P0A9T0
C	376	MSE	MET	modified residue	UNP P0A9T0
C	397	MSE	MET	modified residue	UNP P0A9T0
D	81	ALA	CYS	engineered mutation	UNP P0A9T0
D	83	ALA	CYS	engineered mutation	UNP P0A9T0
D	139	GLY	TRP	engineered mutation	UNP P0A9T0
D	175	MSE	MET	modified residue	UNP P0A9T0
D	203	MSE	MET	modified residue	UNP P0A9T0
D	220	MSE	MET	modified residue	UNP P0A9T0
D	221	MSE	MET	modified residue	UNP P0A9T0
D	229	MSE	MET	modified residue	UNP P0A9T0
D	250	ALA	CYS	engineered mutation	UNP P0A9T0
D	282	ALA	CYS	engineered mutation	UNP P0A9T0
D	341	MSE	MET	modified residue	UNP P0A9T0
D	376	MSE	MET	modified residue	UNP P0A9T0
D	397	MSE	MET	modified residue	UNP P0A9T0

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

NAD



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

- Molecule 3 is water.

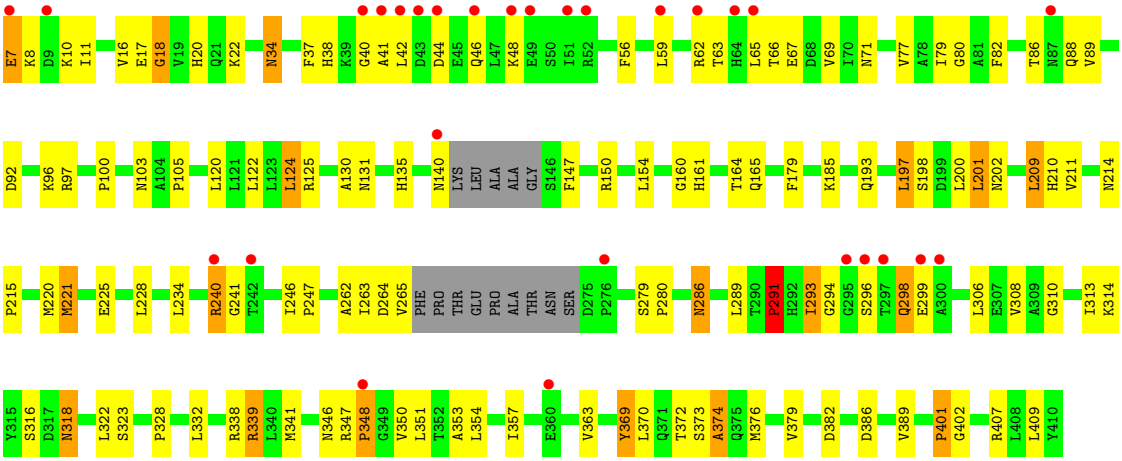
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	77	77	77	0	0
3	B	158	158	158	0	0
3	C	92	92	92	0	0
3	D	136	136	136	0	0

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.

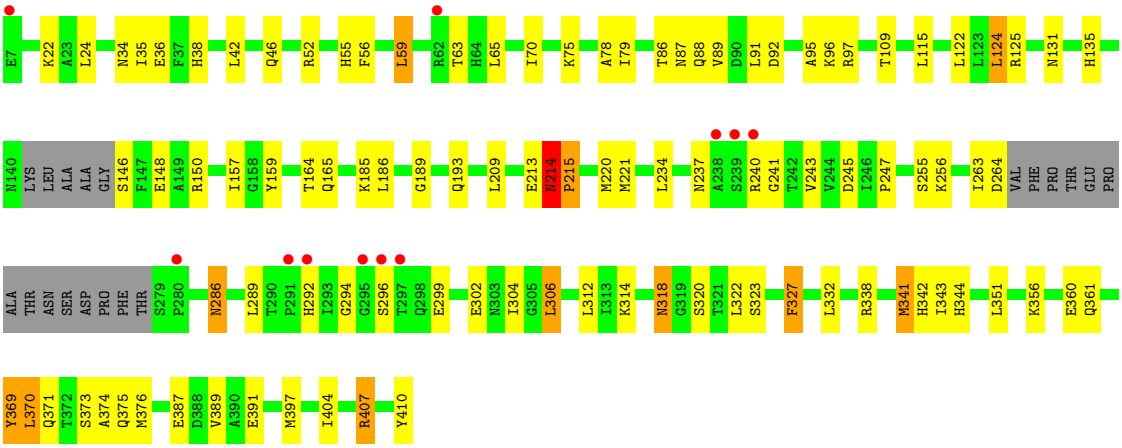
• Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain A:



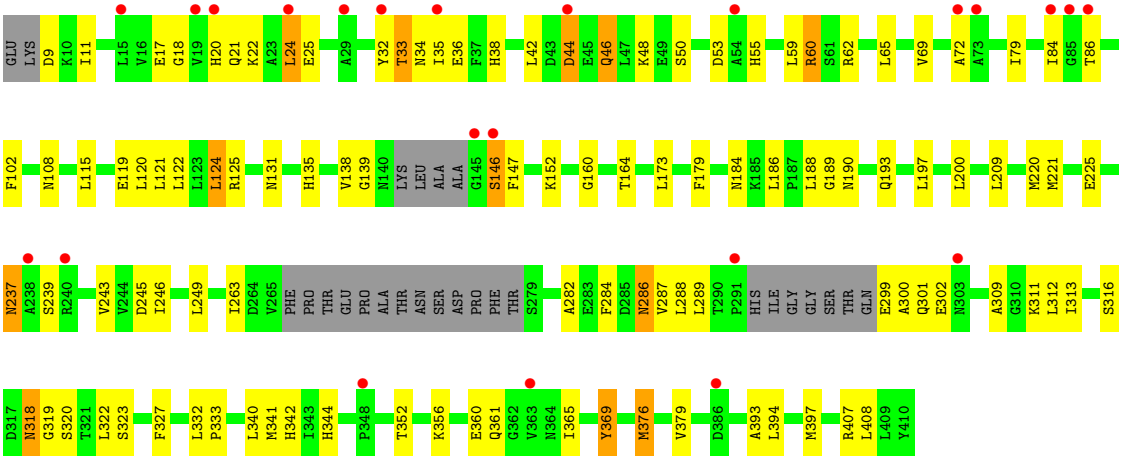
• Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain B:



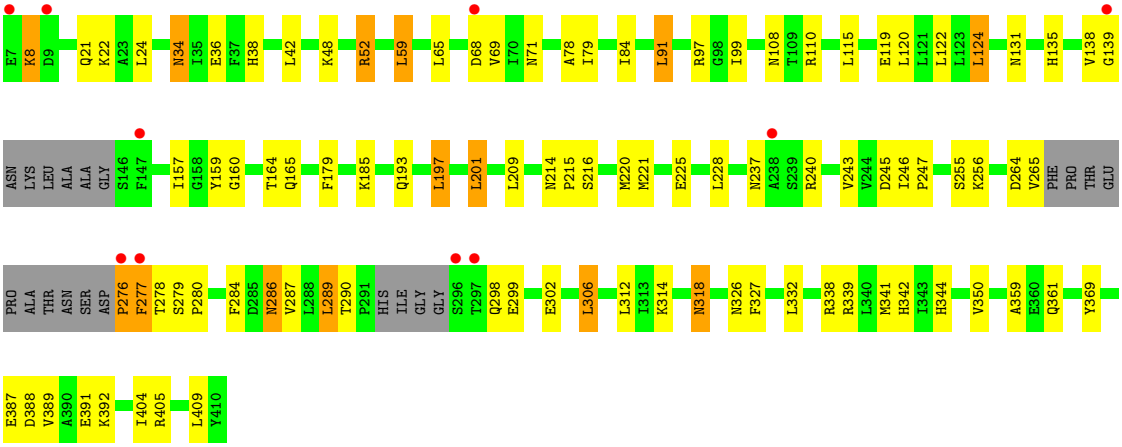
• Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain C:



- Molecule 1: D-3-phosphoglycerate dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.49Å 70.84Å 149.47Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	40.00 – 2.09 49.60 – 1.97	Depositor EDS
% Data completeness (in resolution range)	95.9 (40.00-2.09) 91.4 (49.60-1.97)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	0.76 (at 1.97Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.260 0.213 , 0.248	Depositor DCC
R_{free} test set	9325 reflections (8.91%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12302	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.37	0/2998	0.77	9/4042 (0.2%)
1	B	0.36	1/2956 (0.0%)	0.60	0/3983
1	C	0.33	0/2899	0.59	0/3906
1	D	0.37	0/2954	0.66	2/3980 (0.1%)
All	All	0.36	1/11807 (0.0%)	0.66	11/15911 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	ASN	C-N	6.61	1.46	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	MSE	CB-CG-SE	14.04	154.83	112.70
1	A	221	MSE	CG-SE-CE	-12.95	70.41	98.90
1	A	7	GLU	C-N-CA	10.66	148.36	121.70
1	A	348	PRO	CA-N-CD	-10.55	96.73	111.50
1	A	7	GLU	O-C-N	-9.05	108.22	122.70
1	D	276	PRO	CA-N-CD	-8.40	99.74	111.50
1	A	401	PRO	CA-N-CD	-7.94	100.38	111.50
1	A	291	PRO	O-C-N	-7.43	110.81	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	GLU	CA-C-N	6.22	130.89	117.20
1	A	407	ARG	CB-CA-C	-5.17	100.06	110.40
1	D	276	PRO	CA-C-N	-5.06	106.06	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	PRO	Mainchain

5.2 Too-close contacts (i)

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	2960	0	3001	105	0
1	B	2920	0	2966	89	0
1	C	2865	0	2914	108	0
1	D	2918	0	2968	72	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	2	0
2	D	44	0	26	0	0
3	A	77	0	0	1	0
3	B	158	0	0	4	0
3	C	92	0	0	1	0
3	D	136	0	0	1	0
All	All	12302	0	11953	348	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 (348) 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:327:PHE:CD2	1:C:376:MSE:HE1	1.82	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:PHE:CE2	1:C:376:MSE:SE	2.62	1.03
1:B:109:THR:HG21	1:B:165[B]:GLN:HE21	1.24	0.99
1:B:214:ASN:C	1:B:214:ASN:HD22	1.71	0.94
1:B:109:THR:CG2	1:B:165[B]:GLN:NE2	2.29	0.94
1:D:361:GLN:HE22	1:D:389:VAL:HG13	1.33	0.93
1:A:328:PRO:HD3	1:A:376:MSE:HE3	1.52	0.92
1:A:347:ARG:HD3	1:A:402:GLY:HA3	1.49	0.92
1:A:86:THR:HA	1:A:88:GLN:HE22	1.34	0.90
1:C:289:LEU:H	1:D:131:ASN:HD22	1.23	0.85
1:A:185:LYS:H	1:A:193:GLN:HE22	1.25	0.85
1:A:214:ASN:HB2	1:A:215:PRO:HD2	1.59	0.84
1:A:318:ASN:HB2	1:A:339:ARG:HH21	1.42	0.83
1:B:109:THR:HG21	1:B:165[B]:GLN:NE2	1.91	0.83
1:C:22:LYS:HA	1:C:25:GLU:HG3	1.61	0.82
1:D:214:ASN:HB2	1:D:215:PRO:HD2	1.62	0.82
1:B:95:ALA:O	1:B:376:MSE:HE1	1.80	0.82
1:B:109:THR:HG22	1:B:165[B]:GLN:NE2	1.95	0.82
1:C:21:GLN:O	1:C:25:GLU:HG2	1.80	0.81
1:A:210:HIS:HA	1:A:240:ARG:HH22	1.45	0.81
1:B:109:THR:CG2	1:B:165[B]:GLN:HE21	1.92	0.81
1:C:60:ARG:HB3	1:C:60:ARG:HH21	1.45	0.81
1:B:286:ASN:H	1:B:286:ASN:HD22	1.28	0.80
1:B:361:GLN:HG3	1:B:389:VAL:HG13	1.62	0.79
1:C:22:LYS:HA	1:C:25:GLU:CG	2.12	0.79
1:B:88:GLN:HE21	1:B:89:VAL:HG23	1.49	0.78
1:B:86:THR:HA	1:B:88:GLN:HE22	1.49	0.78
1:C:286:ASN:HD22	1:C:286:ASN:H	1.30	0.77
1:C:289:LEU:H	1:D:131:ASN:ND2	1.82	0.77
1:A:88:GLN:HE21	1:A:89:VAL:HG23	1.50	0.77
1:A:210:HIS:HA	1:A:240:ARG:NH2	2.00	0.76
1:A:122:LEU:HD12	1:B:122:LEU:HD12	1.68	0.76
1:B:42:LEU:HB3	1:B:46:GLN:HB2	1.68	0.75
1:A:42:LEU:HD23	1:A:46:GLN:HG3	1.69	0.74
1:A:286:ASN:H	1:A:286:ASN:HD22	1.34	0.74
1:B:125:ARG:HE	1:B:146:SER:HB3	1.53	0.73
1:C:237:ASN:HD21	1:C:239:SER:HB2	1.54	0.73
1:C:122:LEU:HD12	1:D:122:LEU:HD12	1.69	0.73
1:A:197:LEU:HD22	1:A:201:LEU:HD22	1.68	0.73
1:A:103:ASN:O	1:A:105:PRO:HD3	1.88	0.73
1:D:286:ASN:H	1:D:286:ASN:HD22	1.34	0.73
1:C:327:PHE:CD2	1:C:376:MSE:CE	2.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:PHE:HE2	1:C:376:MSE:SE	2.21	0.72
1:C:131:ASN:HD22	1:D:289:LEU:H	1.35	0.71
1:C:131:ASN:ND2	1:D:289:LEU:H	1.87	0.71
1:C:125:ARG:HA	1:C:146:SER:HA	1.71	0.71
1:A:289:LEU:H	1:B:131:ASN:HD22	1.38	0.71
1:C:318:ASN:C	1:C:318:ASN:HD22	1.94	0.70
1:B:214:ASN:C	1:B:214:ASN:ND2	2.45	0.70
1:B:22:LYS:HB3	1:B:306:LEU:HD13	1.73	0.70
1:B:341:MSE:SE	1:B:407:ARG:HG2	2.42	0.70
1:A:347:ARG:HD3	1:A:402:GLY:CA	2.21	0.69
1:C:327:PHE:CE2	1:C:376:MSE:HE1	2.27	0.68
1:A:67:GLU:HG2	1:A:71:ASN:HD21	1.59	0.68
1:B:22:LYS:HB3	1:B:306:LEU:CD1	2.23	0.67
1:D:185:LYS:H	1:D:193:GLN:HE22	1.41	0.67
1:D:342:HIS:HD2	1:D:344:HIS:ND1	1.91	0.67
1:A:165[A]:GLN:HE22	1:C:189:GLY:H	1.41	0.67
1:A:59:LEU:HD23	1:A:59:LEU:H	1.59	0.67
1:B:22:LYS:HG3	1:B:302:GLU:HG3	1.77	0.67
1:A:131:ASN:HD22	1:B:289:LEU:H	1.41	0.66
1:B:356:LYS:O	1:B:360:GLU:HG3	1.95	0.66
1:D:240:ARG:HB2	1:D:264:ASP:OD2	1.96	0.66
1:D:214:ASN:OD1	1:D:216:SER:HB3	1.96	0.66
1:A:220:MSE:O	1:A:225:GLU:HG2	1.96	0.65
1:C:60:ARG:HE	1:C:301:GLN:HE22	1.44	0.65
1:C:309:ALA:O	1:C:313:ILE:HG22	1.97	0.65
1:C:327:PHE:CE2	1:C:376:MSE:CE	2.80	0.65
1:A:318:ASN:HB2	1:A:339:ARG:NH2	2.12	0.64
1:C:286:ASN:HD22	1:C:286:ASN:N	1.94	0.64
1:D:361:GLN:HE22	1:D:389:VAL:CG1	2.08	0.64
1:D:388:ASP:O	1:D:392:LYS:HG3	1.98	0.64
1:D:197:LEU:O	1:D:201:LEU:HD22	1.98	0.63
1:B:286:ASN:HD22	1:B:286:ASN:N	1.91	0.63
1:C:131:ASN:HD21	1:C:135:HIS:HE1	1.46	0.63
1:B:70:ILE:O	1:B:97:ARG:NH2	2.31	0.63
1:A:67:GLU:HG2	1:A:71:ASN:ND2	2.13	0.63
1:A:131:ASN:ND2	1:B:289:LEU:H	1.96	0.62
1:C:108:ASN:HD21	2:C:2103:NAD:H4N	1.64	0.62
1:C:356:LYS:O	1:C:360:GLU:HG3	2.00	0.62
1:A:210:HIS:CA	1:A:240:ARG:HH22	2.13	0.61
1:D:404:ILE:HG22	1:D:405:ARG:HG3	1.80	0.61
1:B:220:MSE:HG2	1:B:243:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:VAL:HG12	1:C:289:LEU:HD12	1.83	0.61
1:A:209:LEU:HB3	1:A:240:ARG:HH12	1.64	0.61
1:D:197:LEU:HD22	1:D:201:LEU:HD22	1.82	0.61
1:A:88:GLN:CD	1:A:88:GLN:H	2.04	0.61
1:B:36:GLU:OE1	1:B:38:HIS:HE1	1.83	0.61
1:B:376:MSE:HE2	1:B:404:ILE:CD1	2.30	0.61
1:C:147:PHE:HB3	1:C:152:LYS:NZ	2.15	0.61
1:A:44:ASP:O	1:A:48:LYS:HG3	2.00	0.61
1:C:20:HIS:HD2	1:C:21:GLN:H	1.49	0.61
1:A:211:VAL:HG22	1:A:240:ARG:NH1	2.16	0.60
1:A:17:GLU:OE2	1:A:62:ARG:N	2.35	0.60
1:D:48:LYS:HE3	1:D:69:VAL:HG22	1.83	0.60
1:B:185:LYS:H	1:B:193:GLN:HE22	1.50	0.60
1:A:130:ALA:CB	1:A:140:ASN:HD21	2.16	0.59
1:A:322:LEU:O	1:A:323:SER:HB2	2.03	0.59
1:A:165[B]:GLN:NE2	1:C:188:LEU:CD2	2.65	0.59
1:B:314:LYS:HD2	3:B:1886:HOH:O	2.02	0.59
1:A:71:ASN:HA	1:A:97:ARG:NH2	2.17	0.59
1:A:351:LEU:HD23	1:C:365:ILE:HD12	1.85	0.59
1:C:286:ASN:H	1:C:286:ASN:ND2	2.01	0.59
1:B:286:ASN:H	1:B:286:ASN:ND2	2.00	0.58
1:A:65:LEU:HD23	1:A:79:ILE:HD13	1.86	0.58
1:B:24:LEU:CD1	1:B:35:ILE:HG21	2.33	0.58
1:A:86:THR:CA	1:A:88:GLN:HE22	2.11	0.58
1:A:339:ARG:HD3	1:A:382:ASP:OD2	2.02	0.58
1:C:36:GLU:OE1	1:C:38:HIS:HE1	1.87	0.58
1:C:287:VAL:HG12	1:C:289:LEU:CD1	2.33	0.58
1:C:220:MSE:HG2	1:C:243:VAL:HG13	1.84	0.57
1:C:249:LEU:CD2	1:C:263:ILE:HD11	2.35	0.57
1:B:88:GLN:H	1:B:88:GLN:CD	2.08	0.57
1:C:131:ASN:HD21	1:C:135:HIS:CE1	2.22	0.57
1:C:17:GLU:OE1	1:C:60:ARG:HB2	2.05	0.57
1:D:48:LYS:HE2	1:D:69:VAL:HA	1.87	0.56
1:B:263:ILE:HG12	1:B:264:ASP:N	2.20	0.56
1:C:38:HIS:CD2	1:C:42:LEU:HD21	2.39	0.56
1:D:220:MSE:HG2	1:D:243:VAL:HG13	1.86	0.56
1:A:289:LEU:H	1:B:131:ASN:ND2	2.03	0.56
1:D:286:ASN:HD22	1:D:286:ASN:N	1.97	0.56
1:A:86:THR:HA	1:A:88:GLN:NE2	2.14	0.56
1:D:197:LEU:HD13	1:D:201:LEU:HD21	1.87	0.56
1:C:289:LEU:HD13	1:D:135:HIS:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LYS:HA	1:C:25:GLU:HG2	1.87	0.56
1:C:342:HIS:HD2	1:C:344:HIS:ND1	2.04	0.56
1:A:165[B]:GLN:NE2	1:C:188:LEU:HD23	2.22	0.55
1:A:120:LEU:O	1:A:124:LEU:HB2	2.05	0.55
1:A:286:ASN:HD22	1:A:286:ASN:N	1.99	0.55
1:D:97:ARG:O	1:D:405:ARG:HD2	2.07	0.55
1:C:108:ASN:ND2	2:C:2103:NAD:H4N	2.22	0.55
1:D:84:ILE:HD11	1:D:108:ASN:ND2	2.22	0.55
1:B:59:LEU:HD23	1:B:59:LEU:H	1.71	0.54
1:C:209:LEU:HD11	1:C:221:MSE:HG3	1.88	0.54
1:D:59:LEU:HD13	1:D:59:LEU:N	2.22	0.54
1:D:318:ASN:C	1:D:318:ASN:HD22	2.11	0.54
1:A:131:ASN:HD21	1:A:135:HIS:HE1	1.56	0.54
1:D:65:LEU:HD23	1:D:79:ILE:HD13	1.90	0.54
1:B:263:ILE:CG1	1:B:264:ASP:N	2.70	0.54
1:B:338:ARG:HD3	1:B:410:TYR:OXT	2.08	0.54
1:D:286:ASN:H	1:D:286:ASN:ND2	2.05	0.53
1:C:318:ASN:ND2	1:C:320:SER:H	2.05	0.53
1:B:65:LEU:HD23	1:B:79:ILE:HD13	1.88	0.53
1:A:160:GLY:O	1:A:164:THR:HG23	2.09	0.53
1:B:150:ARG:HG3	1:C:190:ASN:OD1	2.08	0.53
1:C:20:HIS:ND1	1:C:302:GLU:HA	2.23	0.53
1:A:353:ALA:O	1:A:357:ILE:HG13	2.08	0.53
1:B:92:ASP:O	1:B:96:LYS:HG2	2.09	0.53
1:A:161:HIS:O	1:A:165[B]:GLN:HG3	2.08	0.53
1:B:296:SER:HB3	1:B:304:ILE:HD11	1.89	0.53
1:D:131:ASN:HD21	1:D:135:HIS:HE1	1.57	0.53
1:C:33:THR:O	1:C:34:ASN:HB3	2.09	0.53
1:D:22:LYS:HB3	1:D:306:LEU:HD13	1.91	0.53
1:D:34:ASN:C	1:D:34:ASN:HD22	2.12	0.53
1:B:214:ASN:HB2	1:B:215:PRO:HD2	1.89	0.52
1:A:59:LEU:HD23	1:A:59:LEU:N	2.23	0.52
1:A:264:ASP:OD2	1:A:293:ILE:HD12	2.08	0.52
1:A:299:GLU:OE1	1:B:148:GLU:HB2	2.09	0.52
1:A:350:VAL:O	1:A:354:LEU:HD23	2.10	0.52
1:B:327:PHE:HZ	1:B:343:ILE:HD13	1.73	0.52
1:D:84:ILE:HD11	1:D:108:ASN:HD22	1.74	0.52
1:C:60:ARG:HB3	1:C:60:ARG:NH2	2.20	0.52
1:D:179:PHE:CZ	1:D:193:GLN:HB2	2.45	0.52
1:C:69:VAL:O	1:C:72:ALA:HB3	2.10	0.52
1:A:286:ASN:H	1:A:286:ASN:ND2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ARG:NE	1:B:146:SER:HB3	2.23	0.52
1:A:77:VAL:O	1:A:100:PRO:HD2	2.09	0.51
1:A:370:LEU:HD23	1:A:379:VAL:HB	1.92	0.51
1:B:124:LEU:HD13	1:B:234:LEU:CD1	2.40	0.51
1:C:65:LEU:HD23	1:C:79:ILE:HD13	1.93	0.51
1:A:17:GLU:HA	1:A:40:GLY:HA2	1.91	0.51
1:B:52:ARG:HB3	1:B:52:ARG:NH1	2.25	0.51
1:B:245:ASP:OD1	1:B:247:PRO:HD2	2.11	0.51
1:B:342:HIS:HD2	1:B:344:HIS:ND1	2.10	0.50
1:D:120:LEU:O	1:D:124:LEU:HB2	2.10	0.50
1:A:131:ASN:HD21	1:A:135:HIS:CE1	2.29	0.50
1:B:375:GLN:CD	1:B:375:GLN:H	2.15	0.50
1:D:240:ARG:CB	1:D:264:ASP:OD2	2.58	0.50
1:C:53:ASP:CG	1:C:53:ASP:O	2.50	0.50
1:A:373:SER:OG	1:A:374:ALA:N	2.45	0.50
1:D:339:ARG:HG2	1:D:409:LEU:HD12	1.94	0.50
1:D:255:SER:O	1:D:256:LYS:HB2	2.11	0.50
1:A:18:GLY:HA2	1:A:37:PHE:CZ	2.47	0.49
1:B:55:HIS:CD2	1:B:75:LYS:HB3	2.47	0.49
1:B:88:GLN:NE2	1:B:89:VAL:HG23	2.22	0.49
1:D:265:VAL:HG22	1:D:290:THR:O	2.12	0.49
1:B:59:LEU:HD12	1:B:63:THR:HB	1.94	0.49
1:A:16:VAL:O	1:A:17:GLU:HB2	2.13	0.49
1:B:159:TYR:CE1	1:B:164:THR:HG22	2.47	0.49
1:C:33:THR:HG22	1:C:34:ASN:H	1.78	0.49
1:C:46:GLN:NE2	1:C:50:SER:OG	2.45	0.49
1:C:20:HIS:CD2	1:C:21:GLN:N	2.81	0.49
1:D:36:GLU:OE1	1:D:38:HIS:HE1	1.96	0.49
1:B:370:LEU:HD22	1:B:371:GLN:N	2.28	0.49
1:D:209:LEU:HD11	1:D:221:MSE:HG3	1.95	0.49
1:A:124:LEU:HD13	1:A:234:LEU:CD1	2.43	0.48
1:B:59:LEU:HD23	1:B:59:LEU:N	2.27	0.48
1:C:138:VAL:HG12	1:C:139:GLY:N	2.28	0.48
1:D:157:ILE:HB	1:D:209:LEU:HD23	1.95	0.48
1:D:246:ILE:HB	1:D:247:PRO:HD3	1.95	0.48
1:A:11:ILE:O	1:A:34:ASN:HB3	2.14	0.48
1:A:279:SER:OG	1:A:280:PRO:HD3	2.12	0.48
1:C:135:HIS:CE1	1:D:289:LEU:HD22	2.48	0.48
1:B:318:ASN:ND2	1:B:320:SER:H	2.11	0.48
1:B:255:SER:O	1:B:256:LYS:HB2	2.14	0.48
1:B:263:ILE:CG1	1:B:264:ASP:H	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:SER:O	1:A:202:ASN:ND2	2.47	0.48
1:A:363:VAL:CG2	1:A:389:VAL:HG11	2.44	0.48
1:C:22:LYS:HD2	1:C:22:LYS:N	2.29	0.47
1:B:373:SER:O	1:B:374:ALA:HB3	2.14	0.47
1:D:287:VAL:HG12	1:D:289:LEU:HD13	1.96	0.47
1:C:245:ASP:HA	3:C:2024:HOH:O	2.13	0.47
1:B:131:ASN:HD21	1:B:135:HIS:HE1	1.62	0.47
1:A:209:LEU:HB3	1:A:240:ARG:NH1	2.29	0.47
1:D:52:ARG:NH1	1:D:52:ARG:HB3	2.30	0.47
1:A:313:ILE:HG22	1:A:314:LYS:HE2	1.96	0.47
1:C:316:SER:HA	1:C:407:ARG:HH22	1.80	0.47
1:A:246:ILE:HB	1:A:247:PRO:HD3	1.96	0.47
1:B:189:GLY:H	1:D:165[A]:GLN:HE22	1.62	0.47
1:D:245:ASP:OD1	1:D:247:PRO:HD2	2.14	0.47
1:A:211:VAL:H	1:A:240:ARG:CZ	2.28	0.47
1:B:131:ASN:HD21	1:B:135:HIS:CE1	2.32	0.47
1:C:340:LEU:HD13	1:C:397:MSE:SE	2.65	0.47
1:A:124:LEU:HD13	1:A:234:LEU:HD12	1.97	0.46
1:A:66:THR:OG1	1:A:69:VAL:HG23	2.15	0.46
1:A:332:LEU:HD13	1:A:369:TYR:HB2	1.97	0.46
1:C:20:HIS:CE1	1:C:22:LYS:HD3	2.50	0.46
1:C:322:LEU:O	1:C:323:SER:HB2	2.15	0.46
1:C:352:THR:CG2	1:C:356:LYS:HE2	2.46	0.46
1:C:11:ILE:HG23	1:C:55:HIS:CD2	2.50	0.46
1:C:20:HIS:CD2	1:C:21:GLN:H	2.29	0.46
1:C:179:PHE:CZ	1:C:193:GLN:HB2	2.50	0.46
1:B:387:GLU:O	1:B:391:GLU:HG3	2.16	0.46
1:C:237:ASN:ND2	1:C:239:SER:HB2	2.27	0.46
1:A:318:ASN:C	1:A:409:LEU:HD13	2.35	0.46
1:C:318:ASN:HD22	1:C:319:GLY:N	2.13	0.46
1:B:213:GLU:O	1:B:214:ASN:HB3	2.14	0.46
1:A:200:LEU:C	1:A:200:LEU:HD23	2.36	0.46
1:A:339:ARG:HG2	1:A:409:LEU:HD12	1.98	0.46
1:A:130:ALA:HB2	1:A:140:ASN:HD21	1.79	0.45
1:A:179:PHE:CZ	1:A:193:GLN:HB2	2.51	0.45
1:D:91:LEU:HG	1:D:326:ASN:HB3	1.99	0.45
1:D:220:MSE:O	1:D:225:GLU:HG2	2.16	0.45
1:A:346:ASN:ND2	1:A:372:THR:HB	2.32	0.45
1:B:342:HIS:HE1	1:B:397:MSE:O	1.98	0.45
1:D:38:HIS:CG	1:D:42:LEU:HD11	2.52	0.45
1:C:318:ASN:C	1:C:318:ASN:ND2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ILE:N	1:C:246:ILE:HD12	2.32	0.45
1:C:284:PHE:HB3	1:C:286:ASN:ND2	2.32	0.45
1:A:209:LEU:C	1:A:240:ARG:HH22	2.20	0.45
1:B:318:ASN:HD22	1:B:318:ASN:C	2.21	0.45
1:C:352:THR:O	1:C:356:LYS:HG3	2.17	0.45
1:D:21:GLN:NE2	3:D:2052:HOH:O	2.50	0.45
1:D:387:GLU:O	1:D:391:GLU:HG3	2.17	0.45
1:C:361:GLN:HE22	1:C:393:ALA:HA	1.82	0.44
1:D:115:LEU:O	1:D:119:GLU:HG3	2.17	0.44
1:B:87:ASN:HA	3:B:1998:HOH:O	2.17	0.44
1:C:115:LEU:O	1:C:119:GLU:HG3	2.17	0.44
1:C:282:ALA:O	1:D:135:HIS:HD2	2.00	0.44
1:B:22:LYS:HG3	1:B:302:GLU:CG	2.46	0.44
1:B:124:LEU:HD13	1:B:234:LEU:HD11	2.00	0.44
1:B:376:MSE:HE2	1:B:404:ILE:HD12	1.98	0.44
1:D:284:PHE:HB3	1:D:286:ASN:ND2	2.32	0.44
1:A:82:PHE:HB3	3:A:1902:HOH:O	2.16	0.44
1:D:265:VAL:HG12	1:D:278:THR:HG21	2.00	0.44
1:B:318:ASN:HD22	1:B:320:SER:H	1.65	0.44
1:B:332:LEU:HD13	1:B:369:TYR:HB2	2.00	0.44
1:C:20:HIS:NE2	1:C:22:LYS:HD3	2.33	0.44
1:C:131:ASN:ND2	1:C:135:HIS:CE1	2.85	0.44
1:A:59:LEU:HD23	1:A:80:GLY:O	2.18	0.43
1:A:147:PHE:HB3	1:B:299:GLU:OE1	2.18	0.43
1:A:7:GLU:CD	1:A:7:GLU:N	2.71	0.43
1:B:286:ASN:N	1:B:286:ASN:ND2	2.62	0.43
1:C:33:THR:O	1:C:34:ASN:CB	2.65	0.43
1:D:159:TYR:CE1	1:D:164:THR:HG22	2.52	0.43
1:A:82:PHE:HA	1:A:308:VAL:HG21	2.01	0.43
1:A:88:GLN:CD	1:A:88:GLN:N	2.69	0.43
1:A:41:ALA:C	1:A:42:LEU:HD12	2.38	0.43
1:A:211:VAL:H	1:A:240:ARG:NH1	2.16	0.43
1:D:359:ALA:C	1:D:361:GLN:H	2.20	0.43
1:C:22:LYS:N	1:C:22:LYS:CD	2.81	0.43
1:B:209:LEU:HD11	1:B:221:MSE:HG3	2.00	0.43
1:A:20:HIS:ND1	1:A:22:LYS:HB2	2.34	0.43
1:C:300:ALA:C	1:C:302:GLU:N	2.72	0.43
1:C:225:GLU:H	1:C:225:GLU:CD	2.21	0.43
1:C:332:LEU:HA	1:C:333:PRO:HD3	1.88	0.43
1:A:125:ARG:HH12	1:B:115:LEU:HB2	1.84	0.43
1:C:60:ARG:HE	1:C:301:GLN:NE2	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:LYS:HD3	1:D:314:LYS:HA	1.77	0.43
1:B:59:LEU:N	1:B:59:LEU:CD2	2.81	0.43
1:D:138:VAL:HG12	1:D:139:GLY:N	2.34	0.43
1:D:197:LEU:HD13	1:D:201:LEU:CD2	2.49	0.43
1:A:370:LEU:C	1:A:370:LEU:HD13	2.40	0.42
1:B:157:ILE:HB	1:B:209:LEU:HD23	2.00	0.42
1:D:131:ASN:HD21	1:D:135:HIS:CE1	2.37	0.42
1:B:322:LEU:O	1:B:323:SER:HB2	2.18	0.42
1:C:288:LEU:C	1:C:289:LEU:HD12	2.39	0.42
1:D:78:ALA:HA	1:D:99:ILE:HG23	2.01	0.42
1:A:122:LEU:HD12	1:B:122:LEU:CD1	2.45	0.42
1:C:62:ARG:HH21	1:C:62:ARG:HG2	1.84	0.42
1:C:200:LEU:HD13	1:C:200:LEU:C	2.39	0.42
1:A:346:ASN:HD21	1:A:372:THR:HB	1.85	0.42
1:C:25:GLU:HG2	1:C:25:GLU:H	1.67	0.42
1:C:120:LEU:O	1:C:124:LEU:HB2	2.20	0.42
1:C:121:LEU:HD23	1:C:121:LEU:HA	1.90	0.42
1:A:56:PHE:CZ	1:A:316:SER:HB2	2.54	0.42
1:C:102:PHE:CD1	1:C:311:LYS:HB3	2.55	0.42
1:D:160:GLY:O	1:D:164:THR:HG23	2.20	0.42
1:A:92:ASP:O	1:A:96:LYS:HG2	2.20	0.41
1:C:44:ASP:O	1:C:48:LYS:HG3	2.20	0.41
1:C:246:ILE:N	1:C:246:ILE:CD1	2.83	0.41
1:A:310:GLY:O	1:A:314:LYS:HG2	2.20	0.41
1:C:173:LEU:O	1:D:110:ARG:NH2	2.53	0.41
1:C:327:PHE:HD2	1:C:376:MSE:HE1	1.68	0.41
1:C:394:LEU:HD22	1:C:408:LEU:HB2	2.02	0.41
1:D:344:HIS:CG	1:D:350:VAL:HG11	2.55	0.41
1:A:262:ALA:O	1:A:263:ILE:HD13	2.21	0.41
1:B:65:LEU:HD12	1:B:65:LEU:HA	1.90	0.41
1:D:22:LYS:HD2	1:D:302:GLU:HG3	2.02	0.41
1:D:279:SER:N	1:D:280:PRO:CD	2.83	0.41
1:A:306:LEU:HB3	1:C:184:ASN:ND2	2.36	0.41
1:C:220:MSE:O	1:C:225:GLU:HG2	2.19	0.41
1:A:265:VAL:O	1:A:291:PRO:HA	2.21	0.41
1:B:125:ARG:NH1	3:B:1852:HOH:O	2.46	0.41
1:C:24:LEU:CD1	1:C:35:ILE:HG21	2.50	0.41
1:C:318:ASN:HD22	1:C:320:SER:H	1.67	0.41
1:A:306:LEU:HB3	1:C:184:ASN:HD21	1.85	0.41
1:A:350:VAL:O	1:A:354:LEU:CD2	2.69	0.41
1:C:65:LEU:CD2	1:C:79:ILE:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ASN:OD1	1:D:97:ARG:HD2	2.20	0.41
1:A:38:HIS:CD2	1:A:42:LEU:HD11	2.56	0.41
1:A:351:LEU:HD12	1:A:351:LEU:HA	1.91	0.41
1:B:86:THR:HA	1:B:88:GLN:NE2	2.26	0.41
1:A:279:SER:N	1:A:280:PRO:CD	2.84	0.41
1:C:299:GLU:C	1:C:301:GLN:H	2.23	0.41
1:D:298:GLN:HG3	1:D:299:GLU:N	2.36	0.40
1:A:350:VAL:HG13	1:A:351:LEU:N	2.37	0.40
1:B:55:HIS:HD2	1:B:75:LYS:HB3	1.84	0.40
1:B:97:ARG:NH1	3:B:1880:HOH:O	2.54	0.40
1:C:160:GLY:O	1:C:164:THR:HG23	2.22	0.40
1:A:63:THR:O	1:A:88:GLN:HB2	2.21	0.40
1:B:56:PHE:CE1	1:B:78:ALA:HB3	2.56	0.40
1:C:24:LEU:HD13	1:C:35:ILE:HG21	2.03	0.40
1:C:407:ARG:CG	1:C:408:LEU:N	2.84	0.40
1:A:42:LEU:HD23	1:A:46:GLN:CG	2.47	0.40
1:B:125:ARG:HA	1:B:146:SER:HA	2.04	0.40
1:C:369:TYR:O	1:C:379:VAL:HA	2.22	0.40
1:D:91:LEU:HD12	1:D:91:LEU:HA	1.93	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	385/404 (95%)	354 (92%)	20 (5%)	11 (3%)	4 1
1	B	380/404 (94%)	361 (95%)	15 (4%)	4 (1%)	14 9
1	C	371/404 (92%)	345 (93%)	22 (6%)	4 (1%)	14 9
1	D	377/404 (93%)	361 (96%)	14 (4%)	2 (0%)	29 26
All	All	1513/1616 (94%)	1421 (94%)	71 (5%)	21 (1%)	11 6

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	291	PRO
1	A	296	SER
1	A	374	ALA
1	B	292	HIS
1	C	32	TYR
1	D	277	PHE
1	C	146	SER
1	A	34	ASN
1	A	241	GLY
1	A	293	ILE
1	A	298	GLN
1	A	240	ARG
1	A	294	GLY
1	B	241	GLY
1	D	8	LYS
1	B	215	PRO
1	C	18	GLY
1	A	18	GLY
1	B	294	GLY
1	C	84	ILE

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	312/313 (100%)	293 (94%)	19 (6%)	18	16
1	B	307/313 (98%)	289 (94%)	18 (6%)	19	17
1	C	301/313 (96%)	283 (94%)	18 (6%)	19	16
1	D	308/313 (98%)	284 (92%)	24 (8%)	12	9
All	All	1228/1252 (98%)	1149 (94%)	79 (6%)	17	14

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	124	LEU
1	A	150	ARG
1	A	154	LEU
1	A	197	LEU
1	A	201	LEU
1	A	209	LEU
1	A	221	MSE
1	A	228	LEU
1	A	286	ASN
1	A	298	GLN
1	A	318	ASN
1	A	338	ARG
1	A	339	ARG
1	A	341	MSE
1	A	348	PRO
1	A	369	TYR
1	A	386	ASP
1	A	401	PRO
1	B	34	ASN
1	B	59	LEU
1	B	91	LEU
1	B	124	LEU
1	B	186	LEU
1	B	214	ASN
1	B	237	ASN
1	B	240	ARG
1	B	286	ASN
1	B	306	LEU
1	B	312	LEU
1	B	318	ASN
1	B	327	PHE
1	B	341	MSE
1	B	351	LEU
1	B	369	TYR
1	B	370	LEU
1	B	407	ARG
1	C	9	ASP
1	C	24	LEU
1	C	33	THR
1	C	44	ASP
1	C	46	GLN
1	C	59	LEU

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Mol	Chain	Res	Type
1	C	60	ARG
1	C	86	THR
1	C	124	LEU
1	C	186	LEU
1	C	197	LEU
1	C	237	ASN
1	C	286	ASN
1	C	312	LEU
1	C	318	ASN
1	C	341	MSE
1	C	369	TYR
1	C	376	MSE
1	D	8	LYS
1	D	24	LEU
1	D	34	ASN
1	D	52	ARG
1	D	59	LEU
1	D	68	ASP
1	D	91	LEU
1	D	124	LEU
1	D	197	LEU
1	D	201	LEU
1	D	228	LEU
1	D	237	ASN
1	D	276	PRO
1	D	277	PHE
1	D	286	ASN
1	D	289	LEU
1	D	306	LEU
1	D	312	LEU
1	D	318	ASN
1	D	327	PHE
1	D	332	LEU
1	D	338	ARG
1	D	341	MSE
1	D	369	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	88	GLN

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Mol	Chain	Res	Type
1	A	131	ASN
1	A	135	HIS
1	A	140	ASN
1	A	193	GLN
1	A	202	ASN
1	A	286	ASN
1	A	301	GLN
1	A	318	ASN
1	A	335	HIS
1	A	346	ASN
1	A	355	ASN
1	A	368	GLN
1	B	34	ASN
1	B	38	HIS
1	B	87	ASN
1	B	88	GLN
1	B	131	ASN
1	B	184	ASN
1	B	193	GLN
1	B	202	ASN
1	B	214	ASN
1	B	237	ASN
1	B	257	HIS
1	B	286	ASN
1	B	318	ASN
1	B	342	HIS
1	B	355	ASN
1	B	368	GLN
1	C	38	HIS
1	C	46	GLN
1	C	55	HIS
1	C	131	ASN
1	C	135	HIS
1	C	184	ASN
1	C	237	ASN
1	C	286	ASN
1	C	318	ASN
1	C	342	HIS
1	C	355	ASN
1	C	361	GLN
1	C	368	GLN
1	D	34	ASN

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Mol	Chain	Res	Type
1	D	38	HIS
1	D	108	ASN
1	D	131	ASN
1	D	135	HIS
1	D	161	HIS
1	D	184	ASN
1	D	193	GLN
1	D	195	GLN
1	D	202	ASN
1	D	237	ASN
1	D	286	ASN
1	D	318	ASN
1	D	335	HIS
1	D	342	HIS
1	D	355	ASN
1	D	361	GLN
1	D	368	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	A	2101	-	42,48,48	2.17	8 (19%)	50,73,73	1.74	9 (18%)
2	NAD	C	2103	-	42,48,48	2.16	9 (21%)	50,73,73	1.75	8 (16%)
2	NAD	D	2104	-	42,48,48	2.20	9 (21%)	50,73,73	1.79	8 (16%)
2	NAD	B	2102	-	42,48,48	2.19	10 (23%)	50,73,73	1.81	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	2101	-	-	3/26/62/62	0/5/5/5
2	NAD	C	2103	-	-	3/26/62/62	0/5/5/5
2	NAD	D	2104	-	-	2/26/62/62	0/5/5/5
2	NAD	B	2102	-	-	1/26/62/62	0/5/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2104	NAD	C2N-N1N	6.62	1.43	1.35
2	A	2101	NAD	C5N-C4N	6.50	1.52	1.38
2	D	2104	NAD	C5N-C4N	6.50	1.52	1.38
2	B	2102	NAD	C5N-C4N	6.35	1.52	1.38
2	C	2103	NAD	C5N-C4N	6.33	1.52	1.38
2	C	2103	NAD	C2N-N1N	6.24	1.42	1.35
2	A	2101	NAD	C2N-N1N	6.22	1.42	1.35
2	B	2102	NAD	C2N-N1N	6.19	1.42	1.35
2	B	2102	NAD	C2N-C3N	5.82	1.48	1.39
2	C	2103	NAD	C2N-C3N	5.72	1.47	1.39
2	A	2101	NAD	C2N-C3N	5.68	1.47	1.39
2	A	2101	NAD	C4N-C3N	5.68	1.49	1.39
2	B	2102	NAD	C4N-C3N	5.67	1.49	1.39
2	C	2103	NAD	C4N-C3N	5.65	1.49	1.39
2	D	2104	NAD	C2N-C3N	5.65	1.47	1.39
2	D	2104	NAD	C4N-C3N	5.61	1.48	1.39
2	B	2102	NAD	C6N-N1N	3.71	1.44	1.35
2	A	2101	NAD	C6N-N1N	3.69	1.44	1.35
2	D	2104	NAD	C6N-N1N	3.61	1.44	1.35
2	C	2103	NAD	C6N-N1N	3.60	1.44	1.35
2	A	2101	NAD	O4B-C1B	-2.86	1.37	1.41
2	C	2103	NAD	C7N-N7N	2.72	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2102	NAD	O4B-C1B	-2.72	1.37	1.41
2	B	2102	NAD	C7N-N7N	2.61	1.38	1.33
2	D	2104	NAD	C7N-N7N	2.52	1.37	1.33
2	C	2103	NAD	C2A-N1A	2.44	1.38	1.33
2	D	2104	NAD	C2A-N1A	2.38	1.38	1.33
2	A	2101	NAD	C2A-N1A	2.36	1.38	1.33
2	D	2104	NAD	O4B-C1B	-2.33	1.37	1.41
2	C	2103	NAD	O4B-C1B	-2.31	1.37	1.41
2	B	2102	NAD	C2A-N1A	2.31	1.38	1.33
2	A	2101	NAD	C7N-N7N	2.17	1.37	1.33
2	B	2102	NAD	C2D-C1D	-2.11	1.50	1.53
2	C	2103	NAD	C6N-C5N	-2.05	1.34	1.38
2	D	2104	NAD	C6N-C5N	-2.04	1.34	1.38
2	B	2102	NAD	C6N-C5N	-2.02	1.34	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2104	NAD	C3N-C7N-N7N	6.00	124.95	117.75
2	B	2102	NAD	C3N-C7N-N7N	5.99	124.94	117.75
2	D	2104	NAD	O7N-C7N-C3N	-5.70	112.81	119.63
2	C	2103	NAD	C3N-C7N-N7N	5.68	124.57	117.75
2	B	2102	NAD	O7N-C7N-C3N	-5.64	112.88	119.63
2	A	2101	NAD	C3N-C7N-N7N	5.55	124.41	117.75
2	C	2103	NAD	O7N-C7N-C3N	-5.49	113.06	119.63
2	A	2101	NAD	O7N-C7N-C3N	-5.40	113.17	119.63
2	B	2102	NAD	C6N-N1N-C2N	-4.62	117.76	121.97
2	D	2104	NAD	O4B-C1B-C2B	-4.46	100.41	106.93
2	A	2101	NAD	C6N-N1N-C2N	-4.39	117.97	121.97
2	D	2104	NAD	C6N-N1N-C2N	-4.39	117.97	121.97
2	C	2103	NAD	O4B-C1B-C2B	-4.31	100.62	106.93
2	C	2103	NAD	C6N-N1N-C2N	-4.29	118.06	121.97
2	B	2102	NAD	O4B-C1B-C2B	-4.20	100.79	106.93
2	A	2101	NAD	O4B-C1B-C2B	-3.91	101.22	106.93
2	B	2102	NAD	C5N-C4N-C3N	-3.48	116.23	120.34
2	A	2101	NAD	C5N-C4N-C3N	-3.40	116.31	120.34
2	D	2104	NAD	C5N-C4N-C3N	-3.27	116.47	120.34
2	C	2103	NAD	C5N-C4N-C3N	-3.18	116.58	120.34
2	B	2102	NAD	C5N-C6N-N1N	2.99	124.69	120.40
2	A	2101	NAD	C5N-C6N-N1N	2.95	124.63	120.40
2	D	2104	NAD	C5N-C6N-N1N	2.95	124.63	120.40
2	C	2103	NAD	C5N-C6N-N1N	2.90	124.56	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2104	NAD	C5A-C6A-N6A	2.82	124.64	120.35
2	B	2102	NAD	C5A-C6A-N6A	2.80	124.61	120.35
2	A	2101	NAD	C5A-C6A-N6A	2.69	124.44	120.35
2	C	2103	NAD	C5A-C6A-N6A	2.69	124.44	120.35
2	B	2102	NAD	C4A-C5A-N7A	2.26	111.75	109.40
2	A	2101	NAD	C4A-C5A-N7A	2.25	111.75	109.40
2	C	2103	NAD	C4A-C5A-N7A	2.19	111.68	109.40
2	A	2101	NAD	O5B-C5B-C4B	-2.17	101.52	108.99
2	D	2104	NAD	C4A-C5A-N7A	2.16	111.65	109.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2103	NAD	O4D-C4D-C5D-O5D
2	D	2104	NAD	PN-O3-PA-O1A
2	A	2101	NAD	O4B-C4B-C5B-O5B
2	B	2102	NAD	O4B-C4B-C5B-O5B
2	C	2103	NAD	O4B-C4B-C5B-O5B
2	D	2104	NAD	O4B-C4B-C5B-O5B
2	A	2101	NAD	O4D-C4D-C5D-O5D
2	C	2103	NAD	C3D-C4D-C5D-O5D
2	A	2101	NAD	C3D-C4D-C5D-O5D

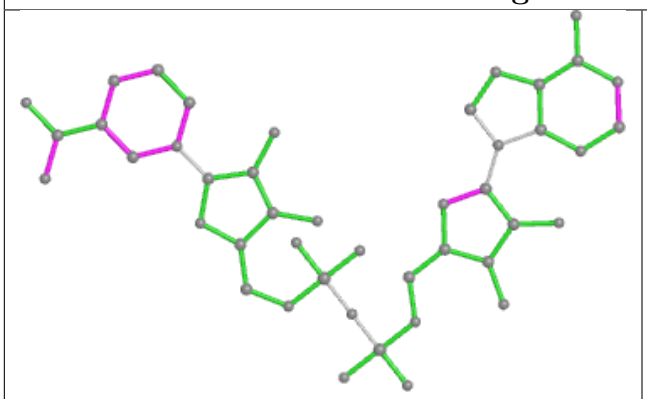
There are no ring outliers.

1 monomer is involved in 2 short contacts:

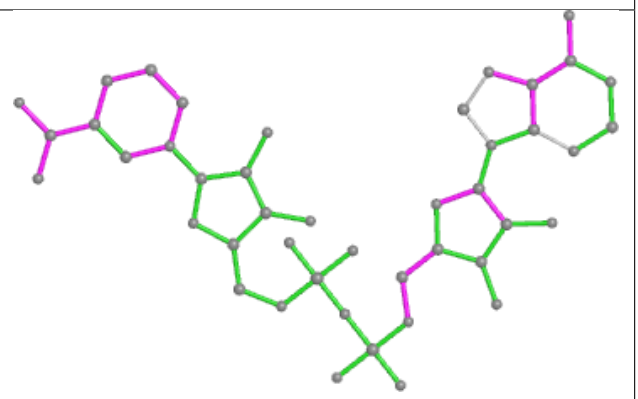
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2103	NAD	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

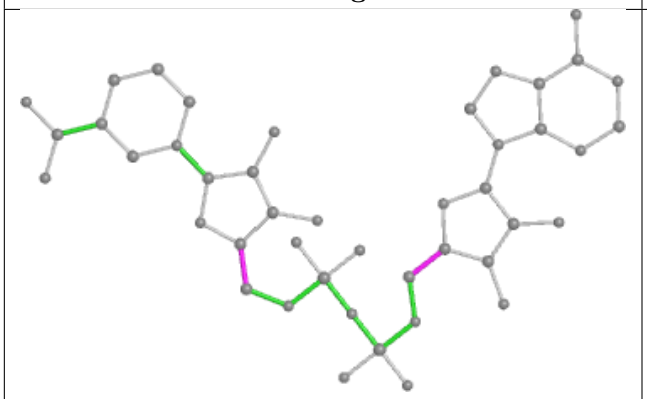
Ligand NAD A 2101



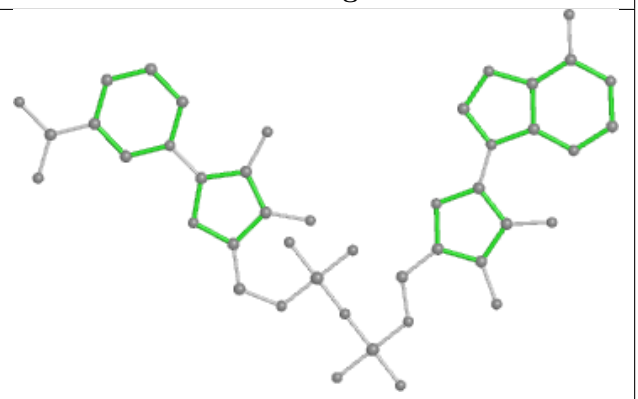
Bond lengths



Bond angles

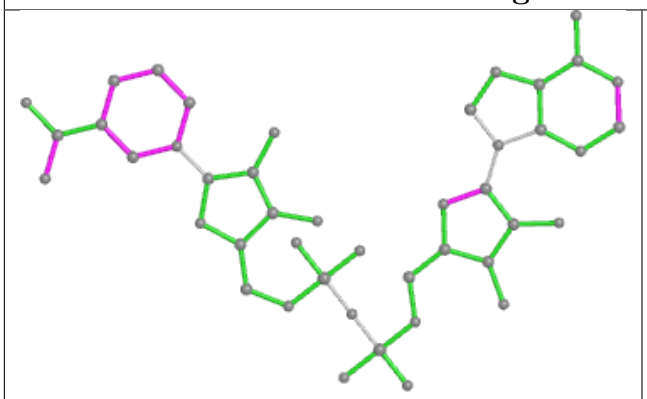


Torsions

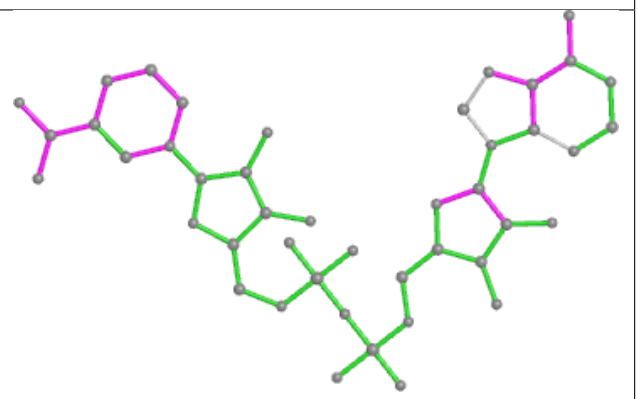


Rings

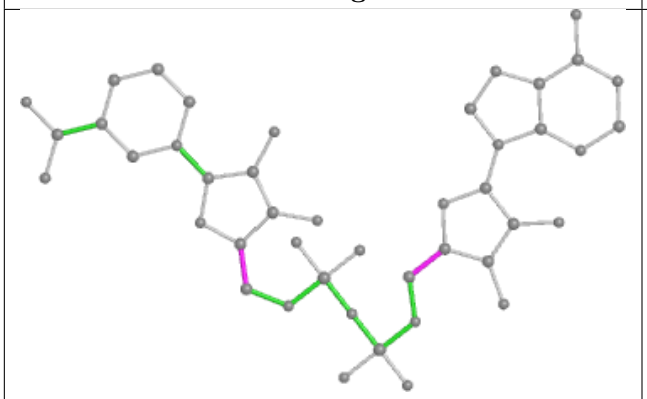
Ligand NAD C 2103



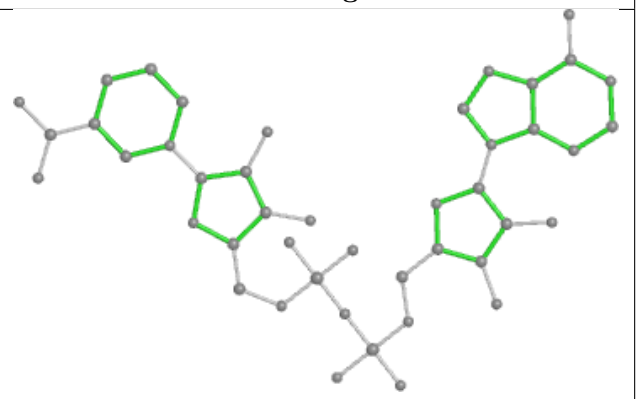
Bond lengths



Bond angles

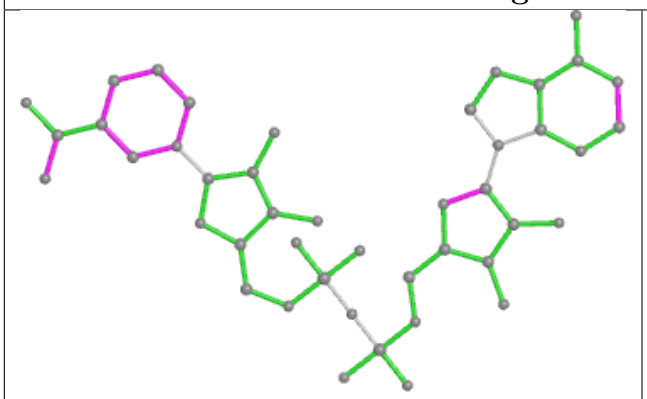


Torsions

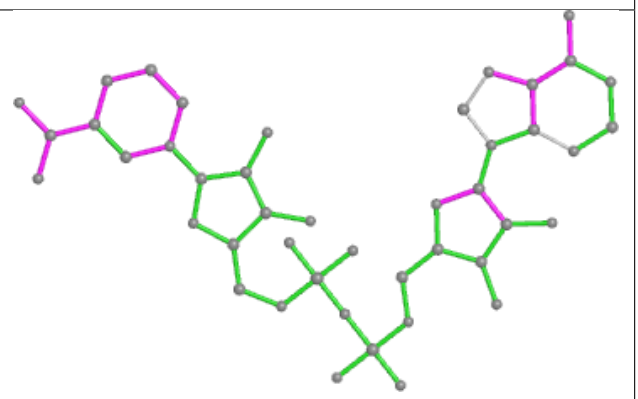


Rings

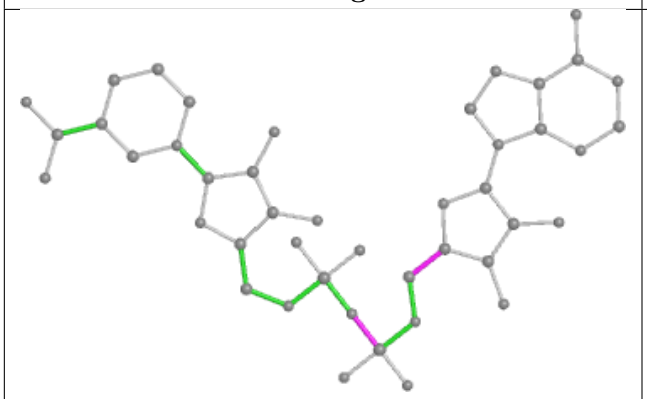
Ligand NAD D 2104



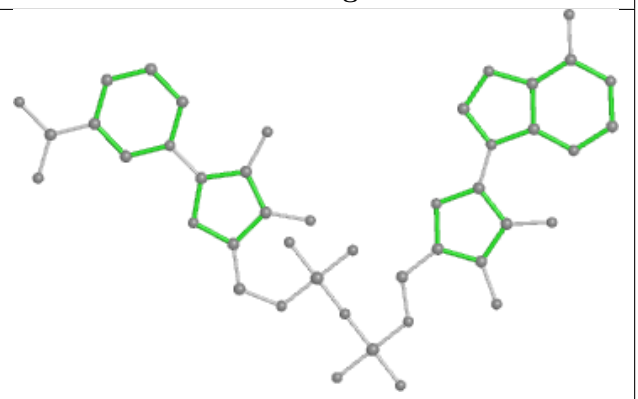
Bond lengths



Bond angles

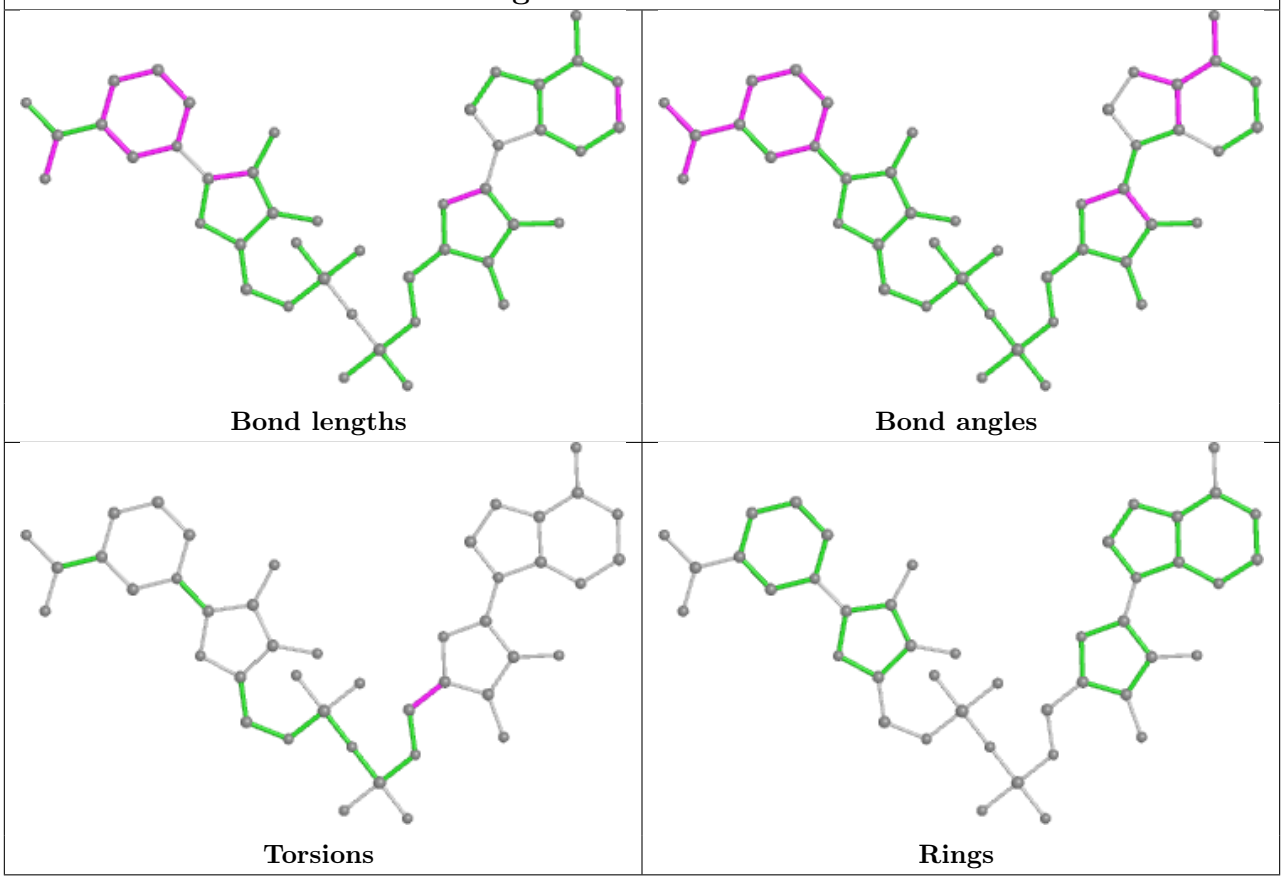


Torsions



Rings

Ligand NAD B 2102



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	382/404 (94%)	0.36	28 (7%)	15	19	12, 40, 64, 73	36 (9%)
1	B	375/404 (92%)	0.01	11 (2%)	51	57	11, 30, 55, 74	20 (5%)
1	C	368/404 (91%)	0.39	23 (6%)	20	24	12, 40, 65, 73	39 (10%)
1	D	376/404 (93%)	0.04	10 (2%)	54	60	10, 32, 54, 73	22 (5%)
All	All	1501/1616 (92%)	0.20	72 (4%)	30	36	10, 35, 62, 74	117 (7%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	HIS	15.4
1	A	296	SER	7.5
1	C	86	THR	6.9
1	C	84	ILE	5.6
1	A	41	ALA	5.0
1	D	276	PRO	4.9
1	A	295	GLY	4.4
1	C	240	ARG	4.3
1	A	240	ARG	4.2
1	C	35	ILE	3.8
1	D	277	PHE	3.7
1	A	300	ALA	3.7
1	B	7	GLU	3.6
1	C	73	ALA	3.4
1	D	139	GLY	3.4
1	B	296	SER	3.4
1	A	276	PRO	3.2
1	C	72	ALA	3.2
1	C	85	GLY	3.1
1	C	19	VAL	3.1
1	A	43	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	360	GLU	3.0
1	B	240	ARG	2.9
1	B	295	GLY	2.9
1	D	296	SER	2.9
1	A	64	HIS	2.9
1	B	280	PRO	2.9
1	A	7	GLU	2.8
1	B	291	PRO	2.7
1	B	297	THR	2.7
1	B	62	ARG	2.7
1	B	239	SER	2.6
1	C	348	PRO	2.6
1	A	242	THR	2.6
1	C	145	GLY	2.6
1	C	44	ASP	2.5
1	C	32	TYR	2.5
1	C	303	ASN	2.5
1	A	140	ASN	2.5
1	C	24	LEU	2.4
1	B	238	ALA	2.3
1	A	9	ASP	2.3
1	C	15	LEU	2.3
1	D	7	GLU	2.3
1	A	42	LEU	2.3
1	C	363	VAL	2.3
1	A	51	ILE	2.3
1	C	146	SER	2.2
1	A	48	LYS	2.2
1	D	297	THR	2.2
1	C	291	PRO	2.2
1	A	348	PRO	2.2
1	D	68	ASP	2.2
1	A	297	THR	2.2
1	C	238	ALA	2.2
1	C	54	ALA	2.2
1	A	299	GLU	2.1
1	A	59	LEU	2.1
1	C	386	ASP	2.1
1	A	52	ARG	2.1
1	A	65	LEU	2.1
1	D	9	ASP	2.1
1	C	29	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	238	ALA	2.0
1	D	147	PHE	2.0
1	A	46	GLN	2.0
1	A	49	GLU	2.0
1	A	87	ASN	2.0
1	C	20	HIS	2.0
1	A	62	ARG	2.0
1	A	40	GLY	2.0
1	A	44	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

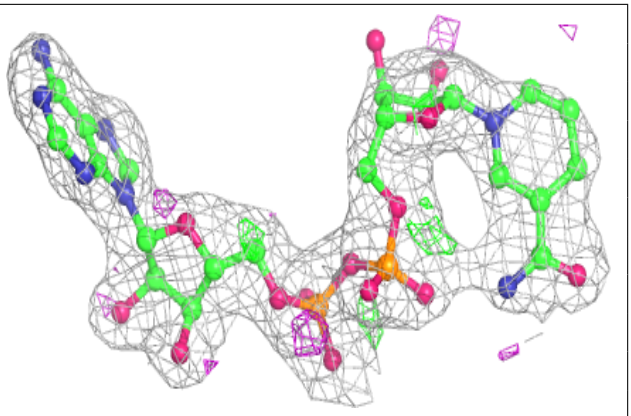
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

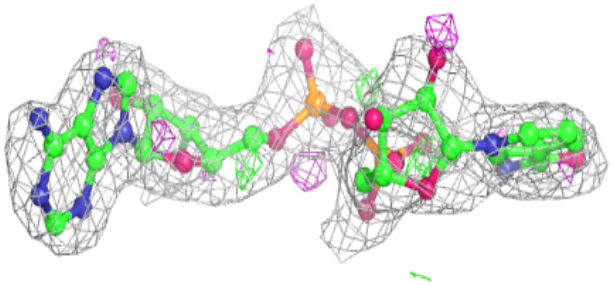
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	A	2101	44/44	0.94	0.13	29,38,47,49	1
2	NAD	C	2103	44/44	0.95	0.14	26,36,46,48	1
2	NAD	B	2102	44/44	0.96	0.14	17,24,45,47	1
2	NAD	D	2104	44/44	0.97	0.13	22,28,39,42	1

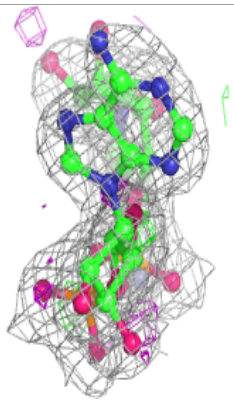
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 2101:

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

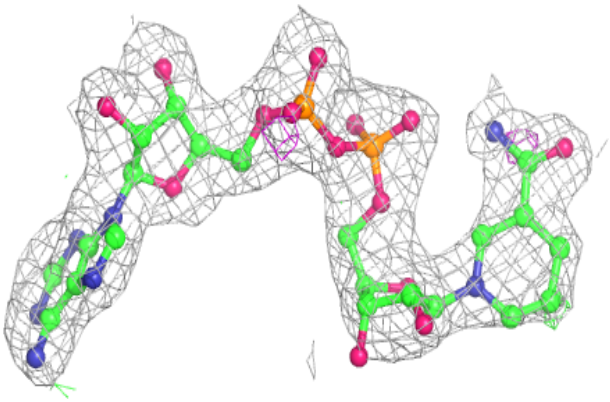


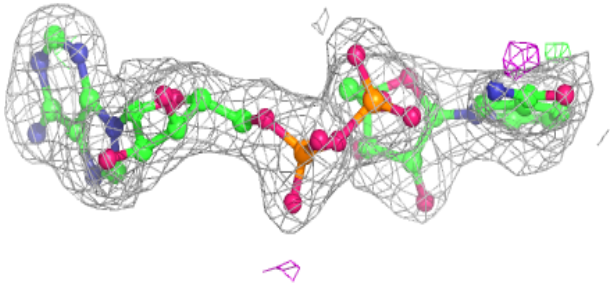


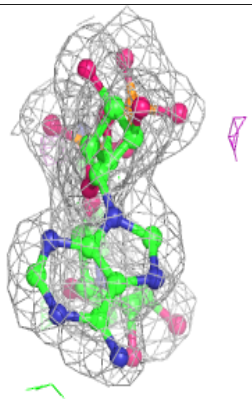


Electron density around NAD C 2103:

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

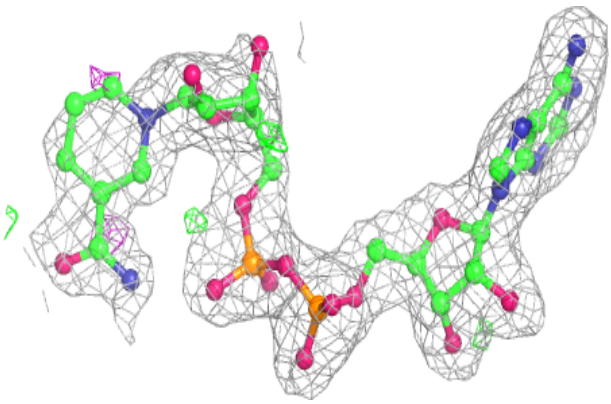


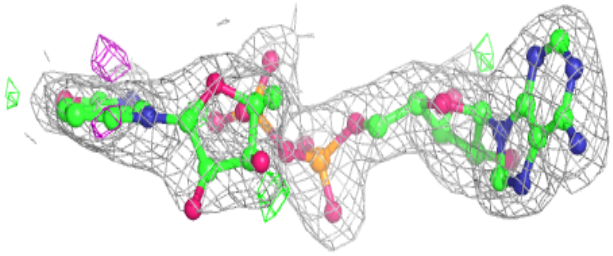




Electron density around NAD B 2102:

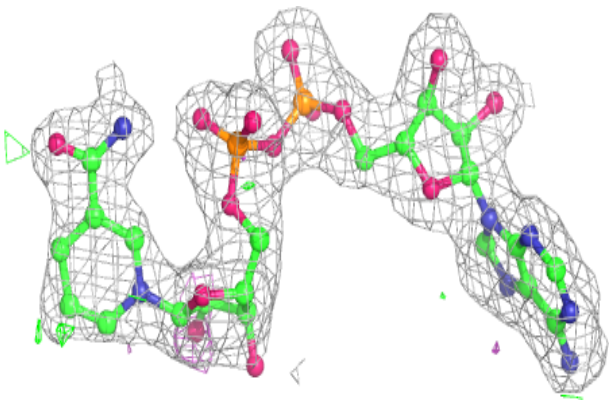
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

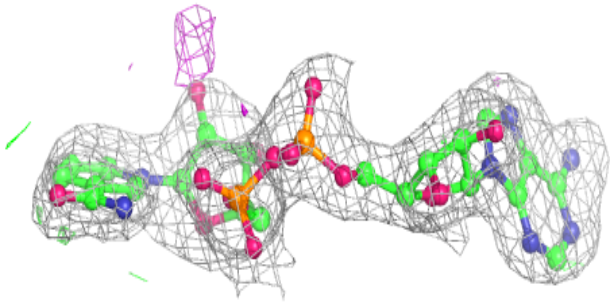


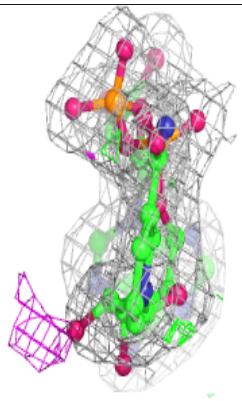


Electron density around NAD D 2104:

$2mF_o$-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.