Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 05:57 am GMT

PDB ID	:	2VUT
Title	:	Crystal structure of NAD-bound NmrA-AreA zinc finger complex
Authors	:	Kotaka, M.; Johnson, C.; Lamb, H.K.; Hawkins, A.R.; Ren, J.; Stammers, D.K.
Deposited on	:	2008-05-30
Resolution	:	2.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

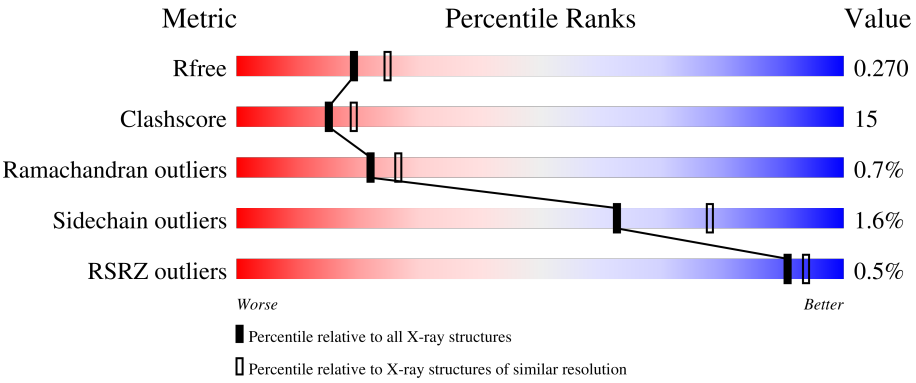
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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.



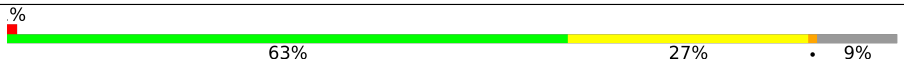
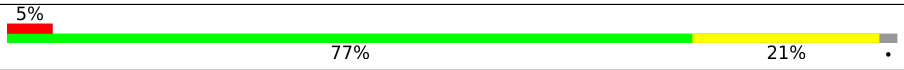
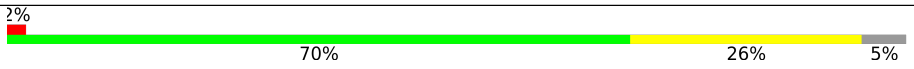
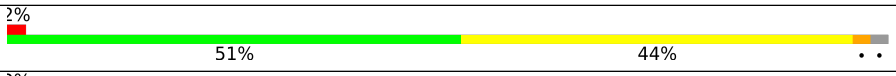
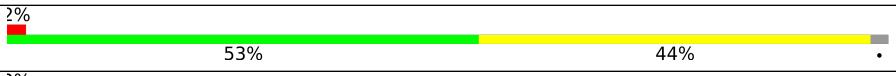
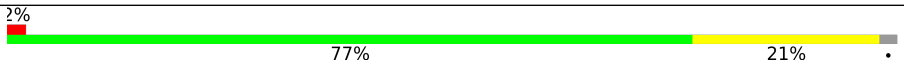
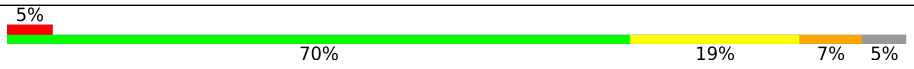
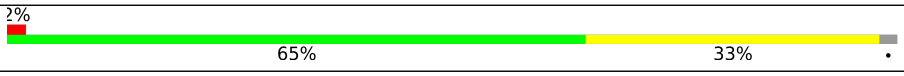
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	352	61% 29% • 10%
1	B	352	60% 30% • 9%
1	C	352	60% 30% • 10%
1	D	352	61% 29% • 9%
1	E	352	69% 20% • 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	352	
1	G	352	
1	H	352	
2	I	43	
2	J	43	
2	K	43	
2	L	43	
2	M	43	
2	N	43	
2	O	43	
2	P	43	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	C	1353	-	X	-	-
5	GOL	G	1353	-	X	-	-
5	GOL	M	1712	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25234 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 NITROGEN METABOLITE REPRESSION REGULATOR NMRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	B	320	Total	C	N	O	S	0	0	0
			2550	1648	434	460	8			
1	C	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	D	320	Total	C	N	O	S	0	0	0
			2550	1648	434	460	8			
1	E	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	F	318	Total	C	N	O	S	0	0	0
			2530	1637	428	457	8			
1	G	319	Total	C	N	O	S	0	0	0
			2541	1643	432	458	8			
1	H	319	Total	C	N	O	S	0	0	0
			2539	1642	430	459	8			

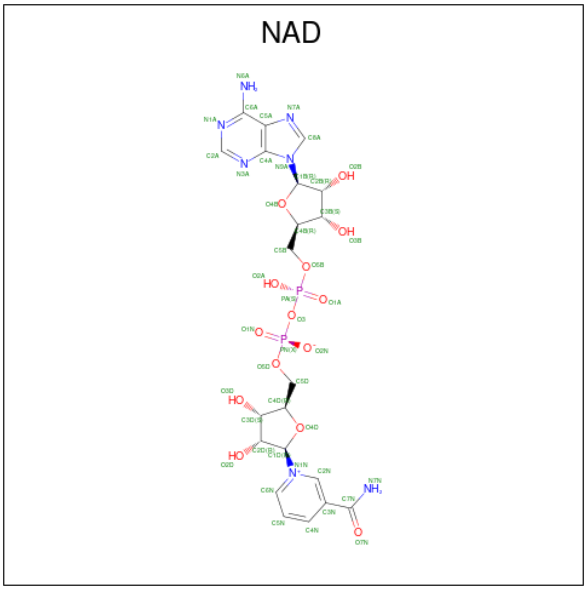
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	ARG	LEU	conflict	UNP O59919
B	238	ARG	LEU	conflict	UNP O59919
C	238	ARG	LEU	conflict	UNP O59919
D	238	ARG	LEU	conflict	UNP O59919
E	238	ARG	LEU	conflict	UNP O59919
F	238	ARG	LEU	conflict	UNP O59919
G	238	ARG	LEU	conflict	UNP O59919
H	238	ARG	LEU	conflict	UNP O59919

- Molecule 2 is a protein called NITROGEN REGULATORY PROTEIN AREA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	J	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	K	41	Total	C	N	O	S	0	0	0
			318	200	59	55	4			
2	L	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	M	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	N	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			
2	O	41	Total	C	N	O	S	0	0	0
			318	200	59	55	4			
2	P	42	Total	C	N	O	S	0	0	0
			326	206	60	56	4			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

Continued on next page...

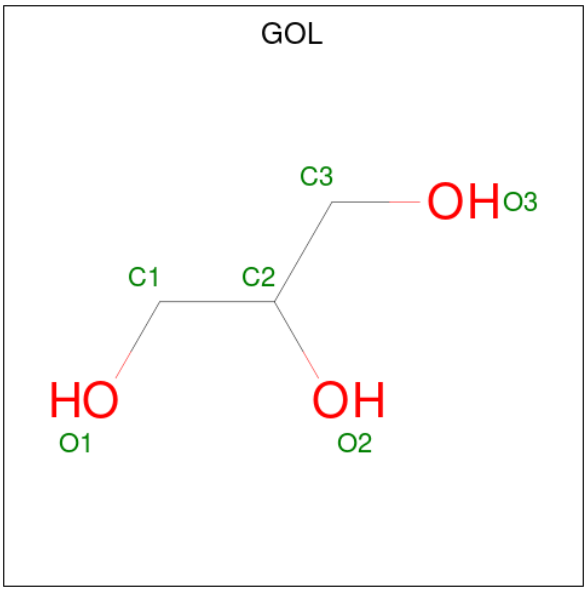
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total Zn 1 1	0	0
6	J	1	Total Zn 1 1	0	0
6	K	1	Total Zn 1 1	0	0
6	L	1	Total Zn 1 1	0	0
6	M	1	Total Zn 1 1	0	0
6	N	1	Total Zn 1 1	0	0
6	O	1	Total Zn 1 1	0	0
6	P	1	Total Zn 1 1	0	0

- Molecule 7 is water.

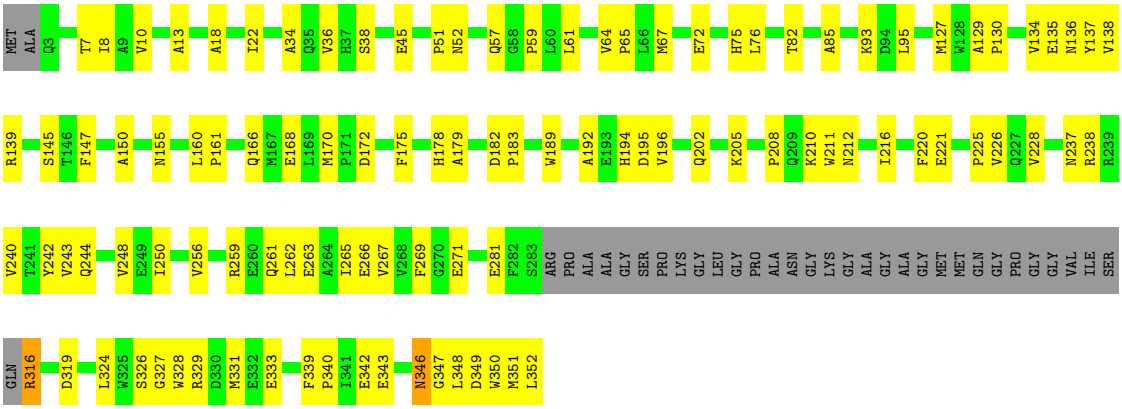
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	179	Total O 179 179	0	0
7	B	193	Total O 193 193	0	0
7	C	229	Total O 229 229	0	0
7	D	214	Total O 214 214	0	0
7	E	243	Total O 243 243	0	0
7	F	244	Total O 244 244	0	0
7	G	247	Total O 247 247	0	0
7	H	209	Total O 209 209	0	0
7	I	21	Total O 21 21	0	0
7	J	28	Total O 28 28	0	0
7	K	19	Total O 19 19	0	0
7	L	29	Total O 29 29	0	0
7	M	28	Total O 28 28	0	0
7	N	33	Total O 33 33	0	0
7	O	24	Total O 24 24	0	0
7	P	17	Total O 17 17	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.

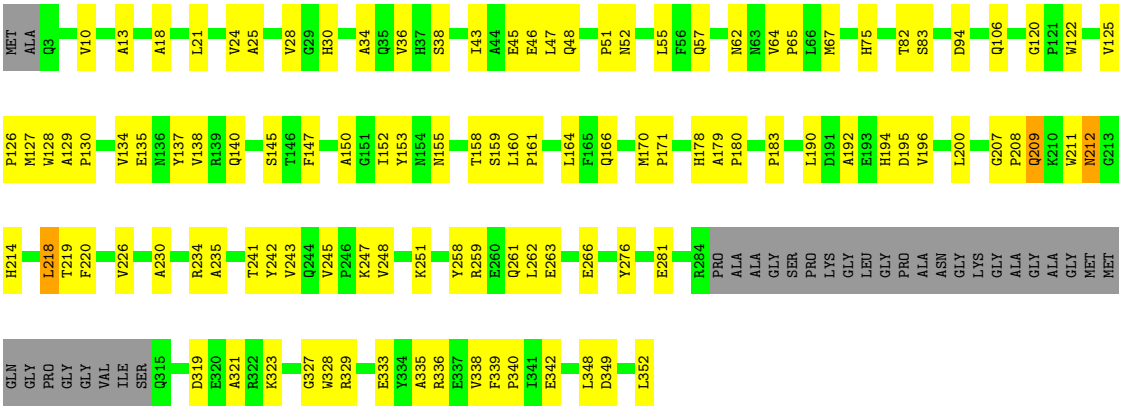
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain A:



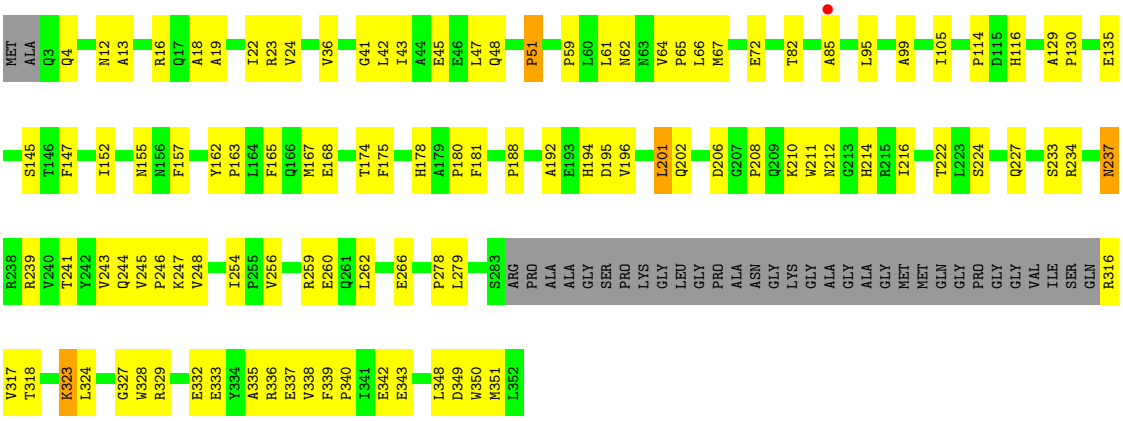
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain B:



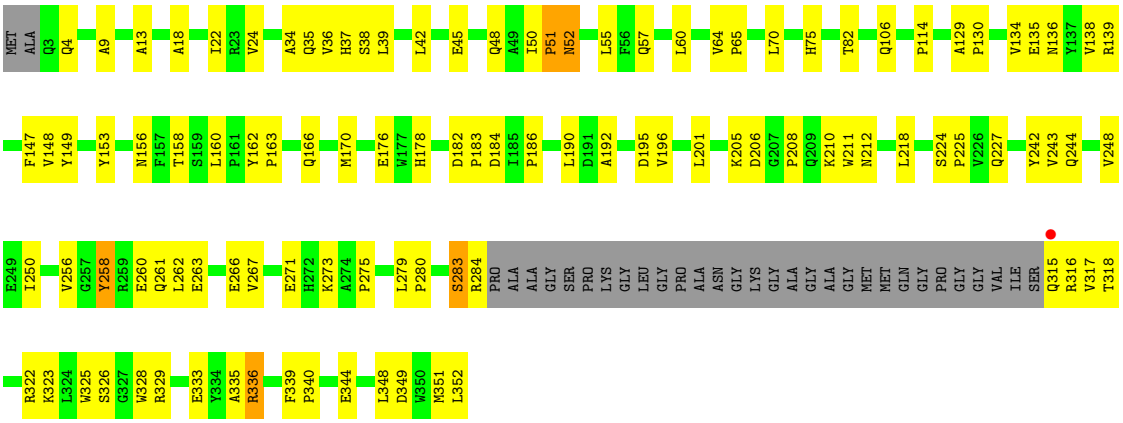
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain C:



• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain D:

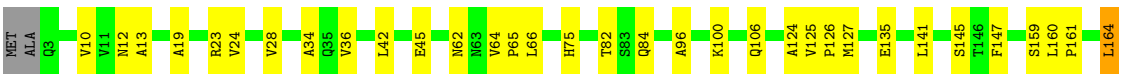


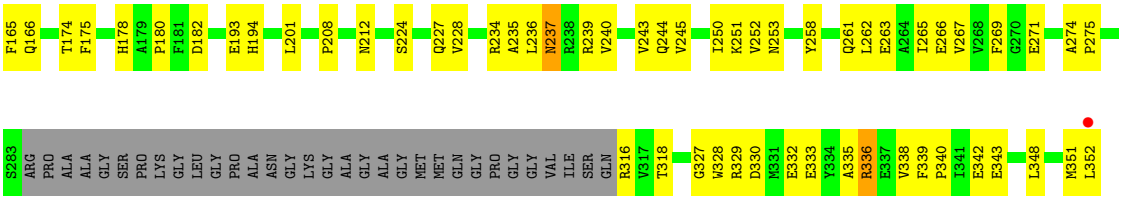
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain E:

• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

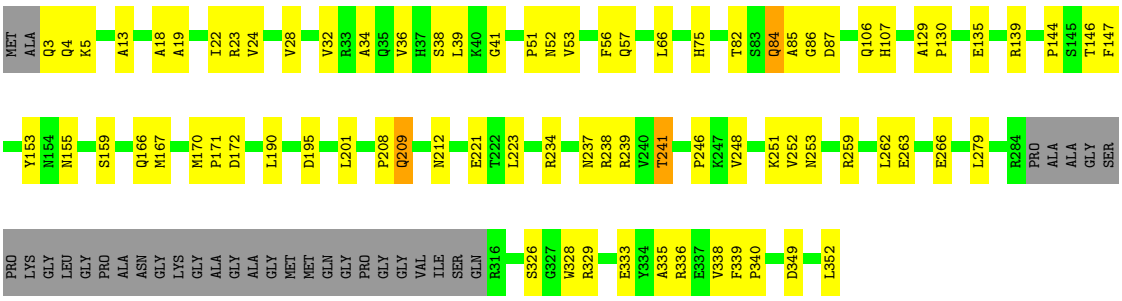
Chain F:





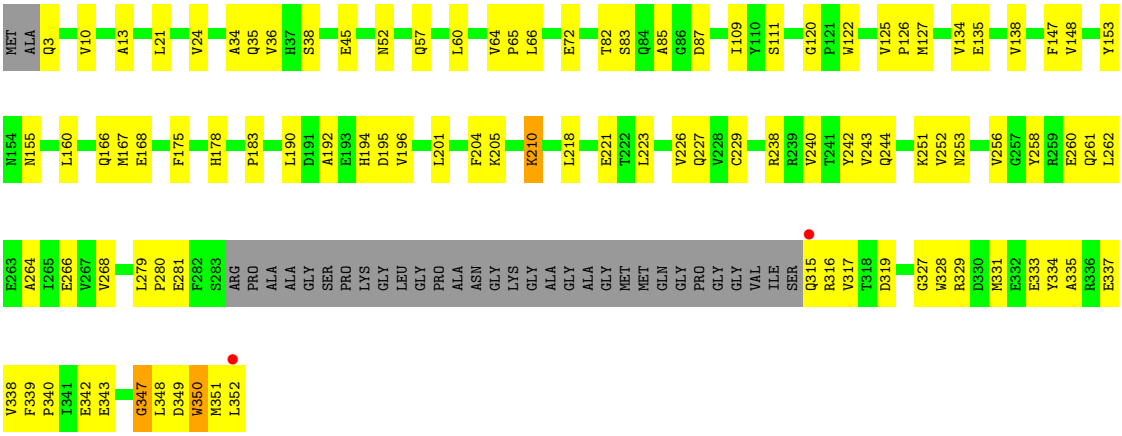
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain G:



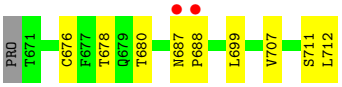
• Molecule 1: NITROGEN METABOLITE REPRESSION REGULATOR NMRA

Chain H:



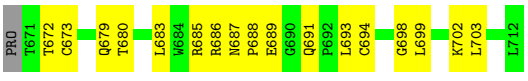
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain I:



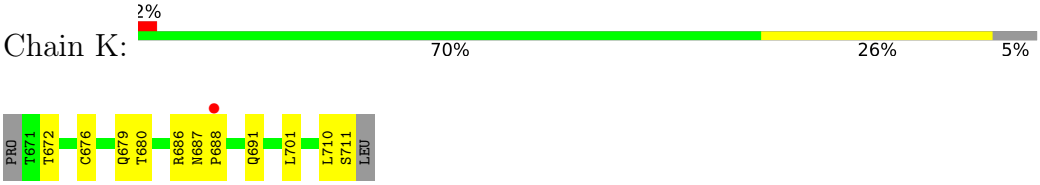
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain J:



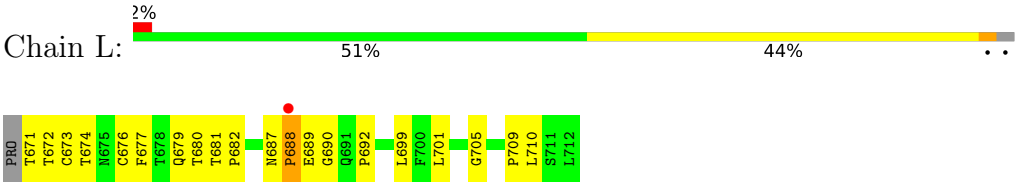
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain K:



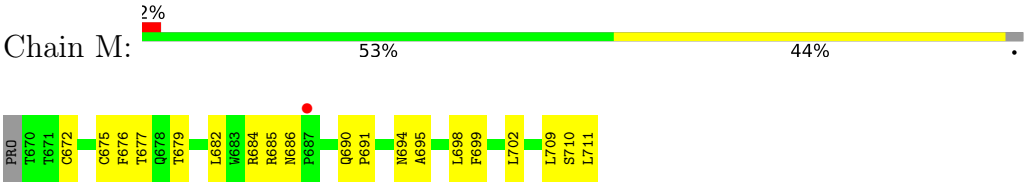
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain L:



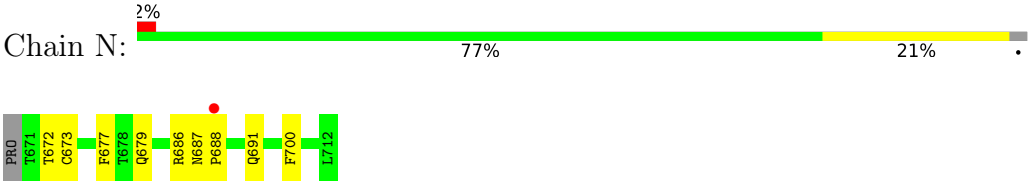
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain M:



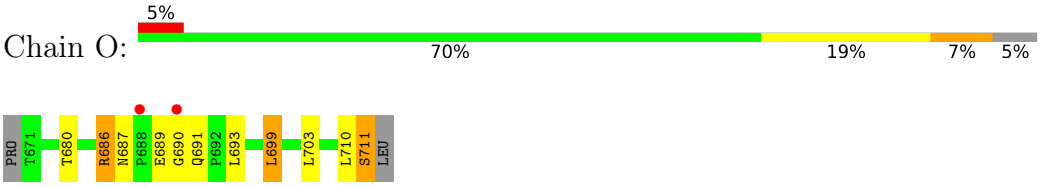
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain N:



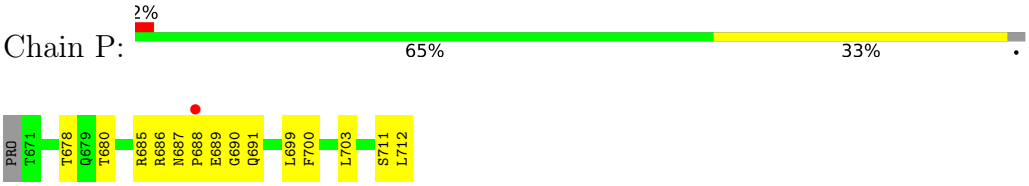
• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain O:



• Molecule 2: NITROGEN REGULATORY PROTEIN AREA

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	227.52Å 227.52Å 222.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.86 – 2.30 29.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.86-2.30) 94.7 (29.86-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.274 0.210 , 0.270	Depositor DCC
R_{free} test set	17971 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25234	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 17.86% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL, GOL, 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	0.34	0/2606	0.61	0/3557
1	B	0.33	0/2626	0.63	0/3583
1	C	0.35	0/2606	0.63	0/3557
1	D	0.34	0/2626	0.62	0/3583
1	E	0.36	0/2606	0.63	1/3557 (0.0%)
1	F	0.35	0/2606	0.63	0/3557
1	G	0.36	0/2617	0.62	0/3571
1	H	0.35	0/2615	0.61	0/3569
2	I	0.35	0/334	0.58	0/456
2	J	0.31	0/334	0.60	0/456
2	K	0.34	0/326	0.61	0/445
2	L	0.30	0/334	0.62	0/456
2	M	0.32	0/334	0.56	0/456
2	N	0.34	0/334	0.60	0/456
2	O	0.37	0/326	0.60	0/445
2	P	0.34	0/334	0.59	0/456
All	All	0.35	0/23564	0.62	1/32160 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	195	ASP	N-CA-C	5.16	124.92	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2530	0	2476	91	0
1	B	2550	0	2497	76	0
1	C	2530	0	2476	85	0
1	D	2550	0	2497	78	0
1	E	2530	0	2476	55	0
1	F	2530	0	2476	79	0
1	G	2541	0	2489	64	0
1	H	2539	0	2484	78	0
2	I	326	0	326	9	0
2	J	326	0	326	21	0
2	K	318	0	315	13	0
2	L	326	0	326	22	0
2	M	326	0	326	20	0
2	N	326	0	326	10	0
2	O	318	0	315	14	0
2	P	326	0	326	15	0
3	A	44	0	26	3	0
3	B	44	0	26	3	0
3	C	44	0	26	4	0
3	D	44	0	26	1	0
3	E	44	0	26	1	0
3	F	44	0	26	1	0
3	G	44	0	26	3	0
3	H	44	0	26	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	C	6	0	4	1	0
5	G	6	0	4	1	0
5	M	6	0	4	1	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
7	A	179	0	0	9	0
7	B	193	0	0	8	0
7	C	229	0	0	4	0
7	D	214	0	0	11	0
7	E	243	0	0	8	0
7	F	244	0	0	11	0
7	G	247	0	0	12	0
7	H	209	0	0	9	0
7	I	21	0	0	1	0
7	J	28	0	0	2	0
7	K	19	0	0	0	0
7	L	29	0	0	0	0
7	M	28	0	0	1	0
7	N	33	0	0	0	0
7	O	24	0	0	0	0
7	P	17	0	0	1	0
All	All	25234	0	22677	691	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 (691) 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)
2:M:686:ASN:HD22	2:M:690:GLN:HB2	1.19	1.04
2:P:687:ASN:HD22	2:P:691:GLN:HB2	1.17	1.01
2:J:687:ASN:HD21	2:J:691:GLN:HB2	1.28	0.98
1:H:343:GLU:HB3	1:H:348:LEU:HD12	1.42	0.96
1:E:235:ALA:HB1	1:E:336:ARG:HB2	1.46	0.95
1:C:13:ALA:HB3	1:C:36:VAL:HG12	1.48	0.93
2:J:687:ASN:ND2	2:J:691:GLN:HB2	1.87	0.90
2:N:687:ASN:HD22	2:N:691:GLN:HB2	1.35	0.89
1:A:261:GLN:HE21	1:A:265:ILE:HD11	1.37	0.88
2:N:672:THR:HG22	2:N:679:GLN:HG2	1.56	0.88
1:D:82:THR:HG22	3:D:1354:NAD:H51N	1.58	0.86
2:O:687:ASN:HD21	2:O:691:GLN:HB2	1.40	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:ASP:HA	1:F:244:GLN:NE2	1.91	0.85
1:A:13:ALA:HB3	1:A:36:VAL:HG12	1.59	0.85
1:B:38:SER:HA	1:B:57:GLN:HE21	1.40	0.84
2:L:674:THR:HG22	2:L:692:PRO:O	1.80	0.82
1:B:248:VAL:HG23	1:B:266:GLU:HG2	1.60	0.80
1:G:82:THR:HG22	3:G:1355:NAD:H51N	1.60	0.80
1:A:205:LYS:HZ2	1:A:205:LYS:HB2	1.46	0.80
2:O:710:LEU:O	2:O:711:SER:HB2	1.81	0.79
2:P:687:ASN:ND2	2:P:691:GLN:HB2	1.96	0.79
1:D:13:ALA:HB3	1:D:36:VAL:HG12	1.65	0.79
1:H:82:THR:HG22	3:H:1354:NAD:H51N	1.65	0.79
1:D:349:ASP:HB2	1:D:352:LEU:HD12	1.65	0.78
2:M:686:ASN:ND2	2:M:690:GLN:HB2	1.98	0.78
1:A:237:ASN:HA	1:B:234:ARG:HD3	1.64	0.77
1:A:82:THR:HG22	3:A:1353:NAD:H51N	1.66	0.77
1:G:259:ARG:O	1:G:263:GLU:HG3	1.83	0.77
1:B:13:ALA:HB3	1:B:36:VAL:HG12	1.65	0.77
1:F:339:PHE:HB3	1:F:340:PRO:HD3	1.67	0.77
2:J:672:THR:HG22	2:J:679:GLN:HG2	1.65	0.77
1:G:84:GLN:H	1:G:84:GLN:NE2	1.83	0.76
2:I:687:ASN:ND2	2:I:688:PRO:HD2	2.02	0.75
1:E:75:HIS:HD2	7:E:2010:HOH:O	1.70	0.75
2:K:676:CYS:HA	2:K:710:LEU:HD11	1.68	0.75
1:C:333:GLU:HG3	2:K:680:THR:HB	1.69	0.74
1:F:24:VAL:HG12	1:F:201:LEU:HD11	1.68	0.74
2:M:690:GLN:HE21	2:M:690:GLN:HA	1.52	0.74
1:E:13:ALA:HB3	1:E:36:VAL:HG12	1.70	0.74
1:B:262:LEU:O	1:B:266:GLU:HG3	1.87	0.74
1:A:135:GLU:HG3	1:A:147:PHE:CD1	2.23	0.73
5:C:1353:GOL:H11	2:K:710:LEU:HD22	1.68	0.73
1:A:175:PHE:HB2	1:A:240:VAL:HG22	1.70	0.73
1:D:50:ILE:HG22	7:D:2039:HOH:O	1.87	0.73
1:D:325:TRP:HZ3	2:L:699:LEU:HD22	1.54	0.73
1:B:333:GLU:HG3	2:J:680:THR:HB	1.70	0.72
1:F:42:LEU:HD11	7:F:2133:HOH:O	1.89	0.72
1:D:38:SER:HA	1:D:57:GLN:HE21	1.54	0.72
1:H:13:ALA:HB3	1:H:36:VAL:HG12	1.71	0.71
1:F:24:VAL:O	1:F:28:VAL:HG13	1.90	0.71
1:C:262:LEU:O	1:C:266:GLU:HG3	1.90	0.71
1:H:178:HIS:CD2	1:H:243:VAL:HB	2.26	0.71
1:D:52:ASN:N	7:D:2039:HOH:O	2.23	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:PHE:HB3	1:G:340:PRO:HD3	1.71	0.70
1:G:82:THR:HB	1:G:84:GLN:NE2	2.06	0.70
1:H:13:ALA:HB3	1:H:36:VAL:CG1	2.21	0.70
2:O:687:ASN:ND2	2:O:691:GLN:HB2	2.07	0.70
1:G:208:PRO:HG2	1:G:209:GLN:HE21	1.56	0.70
1:G:84:GLN:H	1:G:84:GLN:HE21	1.39	0.70
1:A:192:ALA:HA	1:A:196:VAL:HG23	1.72	0.69
2:M:690:GLN:HA	2:M:690:GLN:NE2	2.08	0.69
1:E:333:GLU:HG3	2:M:679:THR:HB	1.73	0.69
1:C:343:GLU:OE1	1:C:348:LEU:HD13	1.93	0.69
1:D:160:LEU:O	1:D:166:GLN:HG3	1.92	0.69
1:F:159:SER:HB2	1:F:348:LEU:HD11	1.75	0.68
1:G:171:PRO:HD2	7:G:2145:HOH:O	1.93	0.68
1:D:262:LEU:O	1:D:266:GLU:HG3	1.92	0.68
1:D:325:TRP:CZ3	2:L:699:LEU:HD22	2.27	0.68
1:E:195:ASP:OD1	1:E:328:TRP:HA	1.94	0.68
1:B:178:HIS:CD2	1:B:243:VAL:HB	2.28	0.68
1:F:13:ALA:HB3	1:F:36:VAL:HG12	1.76	0.67
1:H:178:HIS:HA	1:H:243:VAL:O	1.94	0.67
1:E:38:SER:HA	1:E:57:GLN:HE21	1.58	0.67
1:B:135:GLU:HG3	1:B:147:PHE:CD1	2.29	0.67
1:C:135:GLU:HG3	1:C:147:PHE:CD1	2.30	0.67
1:A:195:ASP:OD1	1:A:328:TRP:HA	1.95	0.67
1:A:194:HIS:HE1	1:A:327:GLY:O	1.78	0.66
1:B:183:PRO:O	1:B:226:VAL:HG23	1.94	0.66
1:B:281:GLU:HG2	7:B:2155:HOH:O	1.95	0.66
1:B:45:GLU:HG3	1:B:46:GLU:N	2.10	0.66
1:A:59:PRO:HD2	2:K:701:LEU:HD11	1.77	0.66
1:A:93:LYS:HE3	1:A:137:TYR:CD1	2.31	0.66
1:B:13:ALA:HB2	1:B:34:ALA:HB1	1.78	0.66
1:D:114:PRO:HB3	1:D:279:LEU:HD11	1.78	0.66
1:A:61:LEU:HD23	2:K:688:PRO:HB3	1.78	0.66
1:D:206:ASP:HB3	1:D:210:LYS:HD3	1.78	0.66
1:A:339:PHE:HB3	1:A:340:PRO:HD3	1.77	0.65
1:C:72:GLU:HG2	1:D:4:GLN:HE22	1.61	0.65
1:E:339:PHE:HB3	1:E:340:PRO:HD3	1.79	0.65
1:G:248:VAL:HG23	1:G:266:GLU:HG2	1.77	0.65
2:J:687:ASN:HD21	2:J:691:GLN:CB	2.07	0.65
2:L:671:THR:HG22	2:L:672:THR:H	1.59	0.65
1:D:256:VAL:O	1:D:260:GLU:HG3	1.97	0.65
1:D:333:GLU:HG3	2:L:680:THR:HB	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ARG:HD3	1:F:237:ASN:HB2	1.79	0.65
1:D:39:LEU:H	1:D:57:GLN:NE2	1.95	0.64
1:D:242:TYR:HB3	7:D:2147:HOH:O	1.97	0.64
1:A:52:ASN:N	7:A:2027:HOH:O	2.26	0.64
1:E:64:VAL:HG22	7:E:2054:HOH:O	1.98	0.64
1:A:256:VAL:HG23	7:A:2138:HOH:O	1.97	0.64
1:H:339:PHE:HB3	1:H:340:PRO:HD3	1.78	0.64
1:D:201:LEU:O	1:D:205:LYS:HG3	1.98	0.64
1:C:16:ARG:HD3	1:C:155:ASN:HD21	1.62	0.64
1:C:43:ILE:O	1:C:47:LEU:HG	1.98	0.64
1:G:335:ALA:O	1:G:340:PRO:HD3	1.97	0.64
1:D:339:PHE:HB3	1:D:340:PRO:HD3	1.80	0.64
1:B:259:ARG:O	1:B:263:GLU:HG3	1.99	0.63
1:E:192:ALA:HA	1:E:196:VAL:HG23	1.80	0.63
1:A:261:GLN:HE21	1:A:265:ILE:CD1	2.08	0.63
1:C:59:PRO:HD2	2:L:701:LEU:HD11	1.80	0.63
1:F:263:GLU:O	1:F:267:VAL:HG23	1.98	0.63
1:B:82:THR:HG22	3:B:1353:NAD:H51N	1.81	0.63
1:F:10:VAL:HG23	7:F:2080:HOH:O	1.98	0.63
1:A:134:VAL:O	1:A:138:VAL:HG23	1.98	0.63
2:P:689:GLU:OE1	2:P:691:GLN:HG3	1.99	0.63
1:G:4:GLN:HG2	7:H:2071:HOH:O	1.98	0.62
1:B:13:ALA:HB3	1:B:36:VAL:CG1	2.28	0.62
1:C:72:GLU:HG2	1:D:4:GLN:NE2	2.13	0.62
1:F:82:THR:HG22	1:F:84:GLN:H	1.64	0.62
1:C:338:VAL:HG12	1:C:342:GLU:HG3	1.82	0.62
1:B:207:GLY:HA3	1:B:209:GLN:HE21	1.63	0.62
1:D:75:HIS:HB3	1:D:106:GLN:NE2	2.14	0.62
1:E:135:GLU:HG3	1:E:147:PHE:CD1	2.35	0.62
1:A:178:HIS:CD2	1:A:243:VAL:HB	2.33	0.62
1:A:161:PRO:HA	1:A:166:GLN:NE2	2.14	0.62
1:F:19:ALA:O	1:F:23:ARG:HG3	1.99	0.62
1:G:201:LEU:HD22	7:G:2029:HOH:O	1.98	0.62
1:B:323:LYS:HE3	7:B:2084:HOH:O	2.00	0.61
1:E:24:VAL:HG12	1:E:201:LEU:HD11	1.82	0.61
2:J:686:ARG:HB3	7:J:2014:HOH:O	2.00	0.61
2:J:689:GLU:HG3	2:J:691:GLN:HG2	1.80	0.61
1:A:67:MET:HG2	1:A:95:LEU:HD23	1.81	0.61
1:D:136:ASN:ND2	7:D:2096:HOH:O	2.33	0.61
1:D:329:ARG:HG3	1:D:333:GLU:HB3	1.81	0.61
1:E:82:THR:HG22	3:E:1354:NAD:H51N	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:256:VAL:O	1:H:260:GLU:HG3	2.00	0.61
1:D:318:THR:O	1:D:322:ARG:HG3	2.01	0.61
1:A:265:ILE:HG23	1:A:269:PHE:CD2	2.36	0.60
1:C:174:THR:HG22	1:C:175:PHE:N	2.16	0.60
1:E:208:PRO:O	1:E:212:ASN:HB2	2.00	0.60
1:F:24:VAL:HG12	1:F:201:LEU:CD1	2.32	0.60
7:G:2234:HOH:O	2:O:680:THR:HG22	2.01	0.60
2:L:676:CYS:HA	2:L:710:LEU:HD11	1.83	0.60
1:A:161:PRO:HA	1:A:166:GLN:HE21	1.64	0.60
1:F:127:MET:HB2	1:F:261:GLN:NE2	2.16	0.60
2:L:687:ASN:HD22	2:L:689:GLU:HB3	1.65	0.60
1:D:48:GLN:HB3	7:D:2033:HOH:O	2.02	0.60
1:G:107:HIS:HE1	1:G:146:THR:OG1	1.85	0.60
1:C:336:ARG:HD2	2:K:680:THR:OG1	2.02	0.60
1:E:169:LEU:HD23	7:E:2116:HOH:O	2.02	0.60
1:H:135:GLU:HG3	1:H:147:PHE:CD1	2.37	0.60
1:G:52:ASN:N	7:G:2054:HOH:O	2.21	0.60
1:A:349:ASP:HA	1:A:351:MET:SD	2.43	0.59
1:B:208:PRO:HD2	1:B:209:GLN:NE2	2.18	0.59
1:C:18:ALA:O	1:C:22:ILE:HG13	2.02	0.59
1:D:248:VAL:O	1:D:250:ILE:HG13	2.00	0.59
1:A:135:GLU:HG3	1:A:147:PHE:CE1	2.36	0.59
1:D:184:ASP:O	1:D:186:PRO:HD3	2.02	0.59
1:C:224:SER:OG	1:C:227:GLN:HG3	2.02	0.59
1:D:42:LEU:O	1:D:45:GLU:HG2	2.03	0.59
1:G:208:PRO:HG2	1:G:209:GLN:NE2	2.18	0.59
1:G:239:ARG:HD3	7:G:2180:HOH:O	2.03	0.59
2:L:687:ASN:C	2:L:689:GLU:H	2.06	0.59
1:F:127:MET:HE3	1:F:258:TYR:HA	1.85	0.59
1:B:329:ARG:HG3	1:B:333:GLU:HB3	1.84	0.59
1:C:178:HIS:HA	1:C:243:VAL:O	2.02	0.59
1:H:127:MET:HE1	1:H:258:TYR:HA	1.84	0.59
1:A:220:PHE:HB2	7:A:2167:HOH:O	2.03	0.58
1:F:235:ALA:HA	1:F:336:ARG:HG3	1.84	0.58
1:G:262:LEU:O	1:G:266:GLU:HG3	2.03	0.58
1:H:13:ALA:HB2	1:H:34:ALA:HB1	1.85	0.58
1:D:13:ALA:HB3	1:D:36:VAL:CG1	2.32	0.58
1:F:62:ASN:ND2	7:F:2063:HOH:O	2.35	0.58
1:F:100:LYS:HE3	7:F:2140:HOH:O	2.02	0.58
2:M:684:ARG:HE	2:M:694:ASN:ND2	2.01	0.58
1:D:263:GLU:HA	1:D:266:GLU:OE1	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:HIS:HB3	1:D:106:GLN:HE21	1.68	0.58
1:H:160:LEU:O	1:H:166:GLN:HG3	2.04	0.58
2:L:687:ASN:OD1	2:L:688:PRO:HD2	2.04	0.58
1:G:329:ARG:HG3	1:G:333:GLU:HB3	1.85	0.58
1:A:316:ARG:HE	1:A:316:ARG:HA	1.68	0.58
1:F:13:ALA:HB2	1:F:34:ALA:HB1	1.86	0.58
1:H:195:ASP:OD1	1:H:328:TRP:HA	2.03	0.58
1:A:333:GLU:HG3	2:I:680:THR:HB	1.86	0.57
1:F:42:LEU:O	1:F:45:GLU:HG2	2.03	0.57
1:H:38:SER:HA	1:H:57:GLN:HE21	1.69	0.57
1:A:13:ALA:HB3	1:A:36:VAL:CG1	2.34	0.57
1:A:38:SER:HA	1:A:57:GLN:HE21	1.68	0.57
1:A:281:GLU:HG2	7:A:2151:HOH:O	2.04	0.57
1:G:13:ALA:HB3	1:G:36:VAL:CG1	2.33	0.57
2:I:711:SER:O	2:I:712:LEU:HB2	2.02	0.57
1:H:3:GLN:HA	7:H:2002:HOH:O	2.04	0.57
1:A:155:ASN:ND2	7:A:2096:HOH:O	2.37	0.57
1:B:134:VAL:O	1:B:138:VAL:HG23	2.03	0.57
2:N:687:ASN:ND2	2:N:691:GLN:HB2	2.13	0.57
1:A:343:GLU:OE1	1:A:348:LEU:HD13	2.04	0.57
1:D:336:ARG:HG3	7:D:2197:HOH:O	2.03	0.57
1:A:347:GLY:O	1:A:348:LEU:HG	2.05	0.57
1:B:38:SER:HA	1:B:57:GLN:NE2	2.17	0.57
1:G:13:ALA:HB2	1:G:34:ALA:HB1	1.87	0.57
2:P:711:SER:O	2:P:712:LEU:HB2	2.03	0.57
1:E:86:GLY:HA2	7:E:2064:HOH:O	2.05	0.57
1:D:224:SER:OG	1:D:227:GLN:HG3	2.05	0.57
1:F:24:VAL:HG13	2:N:700:PHE:CZ	2.39	0.57
2:O:687:ASN:OD1	2:O:689:GLU:HB3	2.05	0.57
1:D:148:VAL:HB	1:D:218:LEU:HG	1.87	0.56
2:K:672:THR:HG22	2:K:679:GLN:HG2	1.87	0.56
1:G:24:VAL:O	1:G:28:VAL:HG13	2.04	0.56
1:G:135:GLU:HG3	1:G:147:PHE:CD1	2.39	0.56
1:A:248:VAL:HG11	1:A:262:LEU:HD13	1.87	0.56
1:B:83:SER:HB3	1:B:127:MET:CE	2.36	0.56
1:E:316:ARG:HB2	7:E:2213:HOH:O	2.05	0.56
1:F:127:MET:CE	1:F:258:TYR:HA	2.35	0.56
1:F:160:LEU:O	1:F:166:GLN:HG3	2.04	0.56
1:G:38:SER:HA	1:G:57:GLN:HE21	1.69	0.56
1:D:153:TYR:HB2	1:D:156:ASN:OD1	2.05	0.56
1:F:252:VAL:HG12	1:F:253:ASN:N	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:GLN:HG3	1:H:60:LEU:HD21	1.87	0.56
1:F:82:THR:HG22	1:F:84:GLN:HG2	1.87	0.56
1:F:178:HIS:CD2	1:F:243:VAL:HB	2.41	0.56
1:G:13:ALA:HB3	1:G:36:VAL:HG12	1.85	0.56
1:G:170:MET:HB2	1:G:172:ASP:OD1	2.06	0.56
1:E:224:SER:OG	1:E:227:GLN:HG3	2.05	0.56
1:D:139:ARG:NH1	7:D:2096:HOH:O	2.38	0.56
1:E:13:ALA:HB3	1:E:36:VAL:CG1	2.36	0.56
1:F:265:ILE:HG23	1:F:269:PHE:CD2	2.40	0.56
2:M:684:ARG:HE	2:M:694:ASN:HD22	1.54	0.56
1:D:326:SER:OG	2:L:699:LEU:HD11	2.06	0.55
1:B:153:TYR:HA	1:B:190:LEU:O	2.07	0.55
2:J:687:ASN:HB3	2:J:693:LEU:CD1	2.37	0.55
1:A:166:GLN:OE1	1:A:168:GLU:HB2	2.07	0.55
1:C:195:ASP:OD1	1:C:328:TRP:HA	2.07	0.55
1:G:144:PRO:HA	1:G:212:ASN:ND2	2.21	0.55
1:H:183:PRO:O	1:H:226:VAL:HG23	2.07	0.55
1:E:64:VAL:CG2	1:E:65:PRO:HD3	2.37	0.55
1:B:338:VAL:HG12	1:B:342:GLU:HG3	1.87	0.55
1:A:72:GLU:HG2	1:C:4:GLN:NE2	2.22	0.55
5:G:1353:GOL:H11	2:O:710:LEU:HD22	1.89	0.55
1:B:52:ASN:ND2	7:B:2017:HOH:O	2.40	0.55
1:E:335:ALA:O	1:E:340:PRO:HD3	2.06	0.55
1:A:267:VAL:HG13	1:A:271:GLU:OE1	2.08	0.54
1:A:237:ASN:HA	1:B:234:ARG:CD	2.36	0.54
1:F:224:SER:OG	1:F:227:GLN:HG3	2.07	0.54
1:A:67:MET:HG2	1:A:95:LEU:CD2	2.37	0.54
1:D:317:VAL:O	1:D:317:VAL:HG22	2.06	0.54
1:A:262:LEU:O	1:A:266:GLU:HG3	2.07	0.54
1:B:160:LEU:O	1:B:166:GLN:HG3	2.07	0.54
1:B:230:ALA:O	1:B:234:ARG:HG3	2.08	0.54
1:C:23:ARG:CZ	2:K:711:SER:HB3	2.37	0.54
1:G:75:HIS:HD2	1:G:106:GLN:HE21	1.55	0.54
2:K:687:ASN:OD1	2:K:688:PRO:HD2	2.08	0.54
1:C:316:ARG:HE	1:C:317:VAL:H	1.56	0.54
1:D:37:HIS:HB2	7:D:2212:HOH:O	2.07	0.54
1:H:85:ALA:HA	3:H:1354:NAD:H61A	1.73	0.54
1:C:323:LYS:HA	1:C:323:LYS:HE2	1.89	0.54
1:E:329:ARG:CZ	1:E:338:VAL:HG21	2.39	0.54
1:A:261:GLN:NE2	1:A:265:ILE:HD11	2.15	0.53
1:H:339:PHE:O	1:H:343:GLU:HG2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:PRO:HA	7:D:2162:HOH:O	2.07	0.53
1:A:205:LYS:HB2	1:A:205:LYS:NZ	2.19	0.53
1:A:349:ASP:OD1	1:A:352:LEU:HD11	2.08	0.53
1:H:223:LEU:HA	1:H:227:GLN:NE2	2.24	0.53
1:C:206:ASP:HB3	1:C:210:LYS:HD3	1.89	0.53
1:C:256:VAL:O	1:C:260:GLU:HG3	2.09	0.53
1:D:114:PRO:HB3	1:D:279:LEU:CD1	2.38	0.53
1:F:23:ARG:NH1	7:F:2025:HOH:O	2.38	0.53
1:E:194:HIS:HE1	1:E:327:GLY:O	1.92	0.53
1:F:24:VAL:HG13	2:N:700:PHE:HZ	1.74	0.53
1:A:64:VAL:N	1:A:65:PRO:CD	2.72	0.52
1:B:43:ILE:O	1:B:47:LEU:HG	2.09	0.52
1:E:202:GLN:HG2	1:E:324:LEU:O	2.10	0.52
1:F:159:SER:HB2	1:F:348:LEU:CD1	2.39	0.52
1:F:82:THR:CG2	1:F:84:GLN:HG2	2.39	0.52
2:L:671:THR:HG22	2:L:672:THR:N	2.22	0.52
1:A:316:ARG:HB2	1:A:319:ASP:OD1	2.09	0.52
1:F:328:TRP:HZ3	1:F:330:ASP:HB3	1.73	0.52
1:C:174:THR:CG2	1:C:175:PHE:N	2.73	0.52
1:A:160:LEU:O	1:A:166:GLN:HG3	2.10	0.52
1:A:210:LYS:HE3	1:A:211:TRP:CZ2	2.44	0.52
1:F:234:ARG:HG3	7:F:2179:HOH:O	2.09	0.52
1:H:83:SER:HB3	1:H:127:MET:HG2	1.92	0.52
2:M:675:CYS:HA	2:M:709:LEU:HD11	1.92	0.52
1:A:259:ARG:O	1:A:263:GLU:HG3	2.10	0.52
1:C:245:VAL:HG12	1:C:247:LYS:H	1.75	0.52
1:F:13:ALA:HB3	1:F:36:VAL:CG1	2.40	0.52
1:F:265:ILE:HG23	1:F:269:PHE:HD2	1.75	0.52
2:J:687:ASN:HB2	2:J:688:PRO:HD2	1.92	0.52
1:B:83:SER:HB3	1:B:127:MET:HE3	1.92	0.52
1:C:82:THR:HG22	3:C:1355:NAD:H51N	1.92	0.52
1:C:233:SER:HB2	1:F:234:ARG:HG2	1.91	0.52
2:M:709:LEU:HD22	5:M:1712:GOL:H12	1.92	0.52
1:D:135:GLU:HG3	1:D:147:PHE:CD1	2.44	0.52
1:H:329:ARG:HG3	1:H:333:GLU:HB3	1.91	0.52
2:K:676:CYS:CA	2:K:710:LEU:HD11	2.40	0.52
1:D:13:ALA:HB2	1:D:34:ALA:HB1	1.92	0.51
2:N:687:ASN:HD22	2:N:691:GLN:CB	2.16	0.51
1:E:329:ARG:HG3	1:E:333:GLU:HB3	1.92	0.51
1:G:41:GLY:HA3	7:G:2041:HOH:O	2.09	0.51
1:G:159:SER:HA	1:G:167:MET:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:687:ASN:O	2:L:689:GLU:N	2.42	0.51
1:A:93:LYS:HE3	1:A:137:TYR:CE1	2.46	0.51
1:C:114:PRO:HB3	1:C:279:LEU:CD1	2.40	0.51
2:I:676:CYS:SG	2:I:678:THR:HG22	2.51	0.51
1:B:179:ALA:HB3	1:B:242:TYR:OH	2.10	0.51
1:B:247:LYS:HG3	1:B:266:GLU:OE2	2.11	0.51
1:B:45:GLU:HG3	1:B:46:GLU:H	1.74	0.51
1:H:24:VAL:HG23	2:P:700:PHE:CZ	2.45	0.51
2:M:675:CYS:SG	2:M:677:THR:HG22	2.51	0.51
1:C:114:PRO:HB3	1:C:279:LEU:HD11	1.91	0.51
1:C:145:SER:O	1:C:212:ASN:HA	2.11	0.51
1:D:315:GLN:HG2	1:D:316:ARG:N	2.26	0.51
2:J:672:THR:CG2	2:J:679:GLN:HE21	2.23	0.51
1:G:85:ALA:HA	3:G:1355:NAD:N6A	2.27	0.51
1:E:235:ALA:CB	1:E:336:ARG:HB2	2.30	0.50
1:H:210:LYS:O	1:H:210:LYS:HE2	2.12	0.50
2:P:686:ARG:HA	2:P:691:GLN:O	2.11	0.50
1:A:127:MET:HE2	7:A:2047:HOH:O	2.10	0.50
1:D:178:HIS:CD2	1:D:243:VAL:HB	2.46	0.50
1:G:19:ALA:O	1:G:23:ARG:HG3	2.12	0.50
1:G:23:ARG:NH1	7:G:2025:HOH:O	2.41	0.50
1:G:241:THR:HG23	7:G:2181:HOH:O	2.11	0.50
1:C:23:ARG:NE	2:K:711:SER:HB3	2.26	0.50
1:D:24:VAL:HA	2:L:709:PRO:HG3	1.94	0.50
1:H:262:LEU:O	1:H:266:GLU:HG2	2.10	0.50
1:H:347:GLY:O	1:H:348:LEU:HD23	2.12	0.50
2:L:699:LEU:HD23	2:L:699:LEU:O	2.11	0.50
1:B:339:PHE:N	1:B:340:PRO:HD2	2.27	0.50
1:F:75:HIS:HB3	1:F:106:GLN:NE2	2.26	0.50
1:H:335:ALA:O	1:H:340:PRO:HD3	2.12	0.50
2:O:699:LEU:HD22	2:O:703:LEU:HD11	1.93	0.50
1:A:265:ILE:HG23	1:A:269:PHE:HD2	1.76	0.50
1:C:99:ALA:HB1	1:C:105:ILE:HG13	1.93	0.50
1:C:339:PHE:HB3	1:C:340:PRO:HD3	1.92	0.50
2:N:687:ASN:HB2	2:N:691:GLN:HB2	1.94	0.50
1:C:343:GLU:CD	1:C:348:LEU:HD13	2.32	0.50
2:J:687:ASN:HB3	2:J:693:LEU:HD12	1.94	0.50
1:H:10:VAL:O	1:H:34:ALA:HA	2.12	0.50
1:E:64:VAL:HG22	1:E:65:PRO:HD3	1.94	0.49
1:F:124:ALA:O	1:F:126:PRO:HD3	2.12	0.49
1:G:56:PHE:HB3	1:G:66:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:SER:OG	2:O:699:LEU:HD11	2.12	0.49
1:G:195:ASP:OD1	1:G:328:TRP:HA	2.11	0.49
1:A:189:TRP:CZ2	1:A:228:VAL:HG21	2.47	0.49
1:A:202:GLN:HG2	1:A:324:LEU:O	2.13	0.49
1:B:159:SER:OG	1:B:348:LEU:HD13	2.12	0.49
1:C:66:LEU:C	1:C:66:LEU:HD23	2.32	0.49
1:E:280:PRO:HG2	1:E:281:GLU:OE1	2.13	0.49
1:A:179:ALA:O	1:A:244:GLN:HA	2.13	0.49
2:L:673:CYS:O	2:L:677:PHE:HA	2.12	0.49
1:E:325:TRP:HA	7:E:2227:HOH:O	2.12	0.49
2:J:672:THR:HG22	2:J:679:GLN:HE21	1.76	0.49
1:A:72:GLU:HG2	1:C:4:GLN:HE22	1.77	0.49
1:F:75:HIS:HB3	1:F:106:GLN:HE21	1.78	0.49
1:D:248:VAL:HG23	1:D:266:GLU:HG2	1.95	0.49
1:D:263:GLU:O	1:D:266:GLU:HB2	2.13	0.49
1:F:328:TRP:CZ3	1:F:330:ASP:HB3	2.48	0.49
1:F:12:ASN:ND2	3:F:1354:NAD:H8A	2.28	0.48
1:H:64:VAL:CG2	1:H:65:PRO:HD3	2.42	0.48
1:C:85:ALA:HA	3:C:1355:NAD:N6A	2.28	0.48
1:C:329:ARG:HG3	1:C:333:GLU:HB3	1.95	0.48
1:E:23:ARG:NE	1:E:46:GLU:OE2	2.42	0.48
1:E:40:LYS:HB2	1:E:40:LYS:NZ	2.28	0.48
1:E:64:VAL:N	1:E:65:PRO:CD	2.76	0.48
1:A:18:ALA:O	1:A:22:ILE:HG13	2.14	0.48
1:G:252:VAL:HG22	1:G:253:ASN:N	2.27	0.48
1:H:166:GLN:HE22	1:H:251:LYS:NZ	2.11	0.48
1:H:223:LEU:HA	1:H:227:GLN:HE21	1.79	0.48
2:M:684:ARG:HG2	7:M:2014:HOH:O	2.13	0.48
1:E:75:HIS:O	1:E:76:LEU:HD23	2.14	0.48
1:C:316:ARG:HE	1:C:316:ARG:HA	1.78	0.48
1:E:182:ASP:O	1:E:225:PRO:HG2	2.13	0.48
1:A:343:GLU:HG3	1:A:350:TRP:HZ2	1.77	0.48
1:C:237:ASN:ND2	1:F:332:GLU:OE2	2.46	0.48
1:F:243:VAL:HA	7:F:2189:HOH:O	2.12	0.48
1:G:246:PRO:HG3	7:G:2189:HOH:O	2.13	0.48
2:J:687:ASN:CG	2:J:691:GLN:HB2	2.33	0.48
1:B:45:GLU:O	1:B:48:GLN:HG2	2.14	0.47
1:C:12:ASN:ND2	3:C:1355:NAD:H8A	2.28	0.47
1:E:249:GLU:HG3	7:E:2182:HOH:O	2.13	0.47
1:G:279:LEU:HD12	1:G:279:LEU:N	2.29	0.47
2:N:687:ASN:HB3	2:N:688:PRO:HD2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:PRO:HA	1:C:222:THR:HG22	1.95	0.47
1:D:195:ASP:OD1	1:D:328:TRP:HA	2.14	0.47
2:L:681:THR:OG1	2:L:682:PRO:HD2	2.15	0.47
1:A:13:ALA:HB2	1:A:34:ALA:HB1	1.96	0.47
1:D:149:TYR:O	1:D:218:LEU:N	2.45	0.47
1:H:316:ARG:NH1	7:H:2181:HOH:O	2.46	0.47
1:A:85:ALA:HA	3:A:1353:NAD:H61A	1.78	0.47
1:C:245:VAL:HG13	1:C:246:PRO:HD2	1.97	0.47
1:G:129:ALA:HB3	1:G:130:PRO:HD3	1.96	0.47
1:H:334:TYR:CD1	1:H:338:VAL:HB	2.49	0.47
2:M:710:SER:O	2:M:711:LEU:HB2	2.15	0.47
2:O:686:ARG:HA	2:O:691:GLN:O	2.15	0.47
1:C:19:ALA:O	1:C:23:ARG:HG3	2.15	0.47
1:A:45:GLU:HB2	7:A:2022:HOH:O	2.15	0.47
1:B:28:VAL:HG23	1:B:30:HIS:HD2	1.79	0.47
1:C:208:PRO:C	1:C:210:LYS:H	2.18	0.47
1:D:210:LYS:HE3	1:D:211:TRP:CZ2	2.50	0.47
1:G:82:THR:HB	1:G:84:GLN:HE22	1.80	0.47
2:M:682:LEU:HD23	2:M:694:ASN:ND2	2.30	0.47
1:A:183:PRO:HA	1:A:225:PRO:HB2	1.97	0.47
1:B:45:GLU:HB3	7:B:2031:HOH:O	2.14	0.47
1:B:129:ALA:HB3	1:B:130:PRO:HD3	1.96	0.47
1:C:201:LEU:HD11	7:C:2021:HOH:O	2.15	0.47
1:F:224:SER:O	1:F:228:VAL:HG23	2.13	0.47
1:H:85:ALA:HA	3:H:1354:NAD:N6A	2.30	0.47
1:B:194:HIS:HE1	1:B:327:GLY:O	1.98	0.47
1:D:273:LYS:HE2	7:D:2160:HOH:O	2.15	0.47
1:F:252:VAL:HG12	1:F:253:ASN:H	1.80	0.47
2:O:687:ASN:C	2:O:689:GLU:H	2.17	0.47
1:G:208:PRO:CG	1:G:209:GLN:HE21	2.24	0.47
1:H:135:GLU:HG3	1:H:147:PHE:CE1	2.50	0.47
1:H:316:ARG:HG2	1:H:317:VAL:N	2.30	0.47
1:F:193:GLU:HG2	7:F:2018:HOH:O	2.14	0.46
1:B:75:HIS:HB3	1:B:106:GLN:NE2	2.31	0.46
1:B:335:ALA:O	1:B:340:PRO:HD3	2.15	0.46
1:G:279:LEU:HD12	1:G:279:LEU:H	1.80	0.46
1:H:175:PHE:HB2	1:H:240:VAL:HG22	1.98	0.46
1:D:316:ARG:HG3	1:D:318:THR:H	1.80	0.46
1:F:343:GLU:OE1	1:F:348:LEU:HD13	2.16	0.46
2:J:673:CYS:HB2	2:J:694:CYS:HB3	1.97	0.46
1:C:61:LEU:HD23	2:L:688:PRO:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:VAL:HG22	1:H:201:LEU:HD11	1.97	0.46
2:J:683:LEU:HD23	2:J:683:LEU:C	2.35	0.46
2:P:686:ARG:NH1	2:P:690:GLY:HA2	2.31	0.46
1:A:183:PRO:HB3	1:A:242:TYR:HD2	1.80	0.46
1:C:254:ILE:HD11	1:C:259:ARG:HG2	1.97	0.46
1:D:335:ALA:O	1:D:340:PRO:HD3	2.16	0.46
1:F:161:PRO:O	1:F:252:VAL:HG23	2.15	0.46
1:A:10:VAL:O	1:A:34:ALA:HA	2.15	0.46
1:A:129:ALA:HB3	1:A:130:PRO:HD3	1.98	0.46
1:C:234:ARG:HG2	1:C:332:GLU:OE2	2.16	0.46
1:G:75:HIS:HD2	1:G:106:GLN:NE2	2.14	0.46
1:A:61:LEU:HD23	2:K:688:PRO:CB	2.46	0.46
1:A:208:PRO:O	1:A:212:ASN:HB2	2.16	0.46
1:C:41:GLY:O	1:C:45:GLU:HG3	2.15	0.46
1:E:263:GLU:O	1:E:266:GLU:HG2	2.15	0.46
1:H:66:LEU:O	1:H:66:LEU:HD12	2.16	0.46
1:D:348:LEU:H	1:D:348:LEU:HD12	1.81	0.46
1:F:329:ARG:HD2	1:F:333:GLU:HG2	1.96	0.46
1:A:139:ARG:NH1	1:G:139:ARG:HD3	2.31	0.46
1:C:48:GLN:HE21	1:D:51:PRO:HG2	1.81	0.46
1:H:64:VAL:N	1:H:65:PRO:CD	2.78	0.46
7:H:2045:HOH:O	2:P:712:LEU:HA	2.16	0.46
1:C:67:MET:HG2	1:C:95:LEU:HD23	1.97	0.45
1:F:180:PRO:HA	1:F:245:VAL:O	2.16	0.45
1:G:170:MET:HB3	7:G:2145:HOH:O	2.16	0.45
2:M:685:ARG:HA	2:M:690:GLN:O	2.16	0.45
2:M:690:GLN:HE21	2:M:690:GLN:CA	2.19	0.45
1:B:245:VAL:O	1:B:245:VAL:HG23	2.15	0.45
1:D:183:PRO:O	1:D:225:PRO:HD2	2.16	0.45
1:H:134:VAL:O	1:H:138:VAL:HG23	2.16	0.45
1:H:201:LEU:O	1:H:205:LYS:HB2	2.16	0.45
1:F:339:PHE:HB3	1:F:340:PRO:CD	2.44	0.45
1:H:238:ARG:NH2	7:H:2156:HOH:O	2.48	0.45
1:A:168:GLU:HG2	1:A:170:MET:CE	2.46	0.45
1:B:67:MET:SD	1:B:94:ASP:HB3	2.57	0.45
1:B:195:ASP:OD1	1:B:328:TRP:HA	2.17	0.45
1:C:116:HIS:NE2	1:C:278:PRO:HD3	2.32	0.45
1:D:35:GLN:HG3	1:D:60:LEU:HD21	1.99	0.45
1:F:262:LEU:O	1:F:266:GLU:HG2	2.16	0.45
1:H:52:ASN:ND2	7:H:2050:HOH:O	2.49	0.45
1:H:351:MET:HG2	1:H:352:LEU:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:TYR:HA	1:C:163:PRO:HD3	1.84	0.45
1:E:109:ILE:HD12	1:E:204:PHE:CZ	2.51	0.45
1:H:45:GLU:HA	7:H:2047:HOH:O	2.16	0.45
2:P:685:ARG:HD3	7:P:2010:HOH:O	2.16	0.45
1:A:183:PRO:HB3	1:A:242:TYR:CD2	2.52	0.45
1:C:335:ALA:O	1:C:340:PRO:HD3	2.16	0.45
1:E:24:VAL:HG12	1:E:201:LEU:CD1	2.46	0.45
1:H:21:LEU:O	1:H:24:VAL:HG12	2.15	0.45
1:H:127:MET:CE	1:H:261:GLN:HB2	2.47	0.45
2:J:672:THR:HG23	7:J:2005:HOH:O	2.17	0.45
2:P:699:LEU:O	2:P:703:LEU:HG	2.16	0.45
1:E:24:VAL:HG13	2:M:699:PHE:CZ	2.51	0.45
1:G:239:ARG:HG3	7:G:2183:HOH:O	2.17	0.45
2:I:687:ASN:ND2	2:I:688:PRO:CD	2.78	0.45
1:H:35:GLN:HG3	1:H:60:LEU:CD2	2.47	0.45
1:D:323:LYS:HE3	7:D:2128:HOH:O	2.15	0.45
1:F:96:ALA:HB1	1:F:141:LEU:HD12	1.99	0.45
1:F:261:GLN:O	1:F:265:ILE:HD12	2.17	0.45
1:H:192:ALA:HA	1:H:196:VAL:HG23	1.99	0.45
1:H:252:VAL:HG22	1:H:253:ASN:N	2.33	0.45
1:H:333:GLU:HG3	2:P:680:THR:HB	1.99	0.45
2:N:673:CYS:O	2:N:677:PHE:HA	2.17	0.45
1:E:136:ASN:ND2	7:E:2120:HOH:O	2.49	0.44
1:A:248:VAL:O	1:A:250:ILE:HD12	2.17	0.44
1:B:24:VAL:HG23	1:B:25:ALA:N	2.33	0.44
1:D:134:VAL:O	1:D:138:VAL:HG23	2.17	0.44
1:E:75:HIS:HA	1:E:104:THR:O	2.17	0.44
1:E:96:ALA:HB1	1:E:141:LEU:HD12	1.99	0.44
1:G:5:LYS:NZ	1:H:72:GLU:OE2	2.50	0.44
1:H:125:VAL:HA	1:H:126:PRO:HD2	1.78	0.44
1:B:62:ASN:HA	7:B:2045:HOH:O	2.18	0.44
1:C:64:VAL:N	1:C:65:PRO:CD	2.81	0.44
1:D:158:THR:HG21	1:D:162:TYR:HD2	1.82	0.44
1:D:315:GLN:HG2	1:D:316:ARG:H	1.81	0.44
1:F:159:SER:HB3	7:F:2145:HOH:O	2.15	0.44
1:H:153:TYR:HA	1:H:190:LEU:O	2.16	0.44
1:H:337:GLU:OE1	2:P:678:THR:HA	2.17	0.44
1:B:106:GLN:NE2	7:B:2054:HOH:O	2.51	0.44
1:B:152:ILE:HA	3:B:1353:NAD:O7N	2.17	0.44
1:D:267:VAL:O	1:D:271:GLU:HB3	2.18	0.44
1:H:229:CYS:SG	1:H:242:TYR:HB2	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ALA:HB3	1:A:242:TYR:OH	2.18	0.44
1:A:183:PRO:O	1:A:226:VAL:HG23	2.18	0.44
1:C:349:ASP:O	1:C:351:MET:N	2.51	0.44
1:D:182:ASP:O	1:D:225:PRO:HG2	2.17	0.44
1:H:343:GLU:HG3	1:H:350:TRP:HZ2	1.81	0.44
1:A:263:GLU:HA	1:A:266:GLU:OE1	2.18	0.44
1:B:150:ALA:O	3:B:1353:NAD:H5N	2.17	0.44
1:B:170:MET:HB3	1:B:171:PRO:HD2	1.98	0.44
1:F:267:VAL:O	1:F:271:GLU:HB2	2.18	0.44
1:G:144:PRO:HA	1:G:212:ASN:HD22	1.83	0.44
1:H:194:HIS:HE1	1:H:327:GLY:O	2.00	0.44
1:A:182:ASP:O	1:A:225:PRO:HG2	2.17	0.44
1:A:238:ARG:NH2	1:A:350:TRP:O	2.51	0.44
1:B:21:LEU:HB2	1:B:200:LEU:HD12	2.00	0.44
1:C:239:ARG:CZ	1:C:241:THR:HG21	2.48	0.44
2:K:686:ARG:HA	2:K:691:GLN:O	2.17	0.44
1:C:48:GLN:HG2	7:C:2038:HOH:O	2.16	0.44
1:C:114:PRO:HG3	1:C:278:PRO:HD2	2.00	0.44
1:D:9:ALA:HB1	1:D:70:LEU:HG	1.99	0.44
1:G:329:ARG:CZ	1:G:338:VAL:HG21	2.48	0.44
1:A:211:TRP:CE3	1:A:216:ILE:HD11	2.52	0.43
1:E:9:ALA:O	1:E:77:ALA:HA	2.18	0.43
1:E:144:PRO:HA	1:E:212:ASN:OD1	2.18	0.43
1:E:335:ALA:HA	1:E:339:PHE:HB2	1.99	0.43
1:C:24:VAL:HG12	1:C:201:LEU:HD23	2.01	0.43
1:D:280:PRO:HA	1:D:283:SER:HB3	2.00	0.43
1:E:19:ALA:O	1:E:23:ARG:HG3	2.18	0.43
2:P:686:ARG:HH11	2:P:690:GLY:HA2	1.82	0.43
1:A:225:PRO:HB3	1:A:242:TYR:CE1	2.53	0.43
1:B:137:TYR:O	1:B:140:GLN:HB3	2.18	0.43
2:I:687:ASN:HD22	2:I:688:PRO:HD2	1.82	0.43
1:A:150:ALA:O	3:A:1353:NAD:H5N	2.18	0.43
1:B:349:ASP:HB2	1:B:352:LEU:HD12	2.00	0.43
1:D:64:VAL:N	1:D:65:PRO:CD	2.81	0.43
1:E:39:LEU:H	1:E:57:GLN:NE2	2.16	0.43
1:F:66:LEU:C	1:F:66:LEU:HD23	2.38	0.43
1:H:126:PRO:HG2	1:H:261:GLN:HA	2.01	0.43
1:B:183:PRO:HB2	1:B:226:VAL:CG2	2.48	0.43
1:F:125:VAL:HG12	1:F:261:GLN:OE1	2.18	0.43
1:F:135:GLU:HG3	1:F:147:PHE:CE1	2.54	0.43
1:F:338:VAL:HG22	7:F:2230:HOH:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HD12	1:A:250:ILE:N	2.33	0.43
1:C:212:ASN:O	1:C:214:HIS:HD2	2.01	0.43
1:F:64:VAL:N	1:F:65:PRO:CD	2.81	0.43
1:F:135:GLU:HG3	1:F:147:PHE:CD1	2.54	0.43
1:F:166:GLN:HE22	1:F:251:LYS:NZ	2.17	0.43
2:M:690:GLN:HE21	2:M:691:PRO:HD2	1.84	0.43
1:C:66:LEU:HD12	2:L:705:GLY:O	2.19	0.43
1:B:209:GLN:HG3	7:B:2126:HOH:O	2.18	0.43
1:D:218:LEU:HD23	1:D:218:LEU:HA	1.85	0.43
1:G:39:LEU:H	1:G:57:GLN:NE2	2.17	0.43
1:G:349:ASP:HB2	1:G:352:LEU:HD12	2.01	0.43
1:A:326:SER:HB2	2:I:699:LEU:CD2	2.48	0.43
1:B:161:PRO:HB2	1:B:251:LYS:HB2	2.01	0.43
1:F:24:VAL:CG1	1:F:201:LEU:CD1	2.97	0.43
1:F:351:MET:O	1:F:352:LEU:HD23	2.19	0.43
1:C:157:PHE:HA	1:C:165:PHE:O	2.19	0.42
1:C:202:GLN:HG2	1:C:324:LEU:O	2.18	0.42
1:F:338:VAL:HG12	1:F:342:GLU:HG3	2.00	0.42
1:G:166:GLN:HE22	1:G:251:LYS:HE2	1.84	0.42
1:H:238:ARG:CZ	7:H:2156:HOH:O	2.67	0.42
1:H:280:PRO:HG2	1:H:281:GLU:OE1	2.19	0.42
2:J:699:LEU:O	2:J:703:LEU:HG	2.19	0.42
2:P:687:ASN:HB3	2:P:688:PRO:HD2	2.01	0.42
1:B:83:SER:HB3	1:B:127:MET:HE2	2.00	0.42
1:B:180:PRO:HG2	1:B:248:VAL:CG2	2.49	0.42
1:C:194:HIS:HE1	1:C:327:GLY:O	2.02	0.42
1:H:329:ARG:CZ	1:H:338:VAL:HG21	2.48	0.42
2:I:707:VAL:HA	7:I:2018:HOH:O	2.18	0.42
2:L:671:THR:O	2:L:679:GLN:HG2	2.19	0.42
2:O:686:ARG:H	2:O:686:ARG:HD2	1.84	0.42
2:P:711:SER:O	2:P:712:LEU:CB	2.66	0.42
1:B:10:VAL:HG11	1:B:18:ALA:HB1	2.01	0.42
1:C:168:GLU:O	1:C:175:PHE:HA	2.18	0.42
1:D:170:MET:HG3	1:D:176:GLU:OE2	2.20	0.42
1:G:201:LEU:HD23	1:G:201:LEU:HA	1.88	0.42
1:G:335:ALA:O	1:G:339:PHE:HB3	2.19	0.42
1:H:168:GLU:O	1:H:175:PHE:HA	2.19	0.42
1:H:338:VAL:HG12	1:H:342:GLU:HG3	2.01	0.42
1:B:120:GLY:C	1:B:122:TRP:H	2.22	0.42
1:C:180:PRO:HA	1:C:245:VAL:O	2.19	0.42
1:H:244:GLN:NE2	7:H:2161:HOH:O	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:687:ASN:C	2:L:689:GLU:N	2.72	0.42
1:A:221:GLU:OE2	1:A:331:MET:N	2.52	0.42
1:B:125:VAL:HA	1:B:126:PRO:HD2	1.78	0.42
1:C:248:VAL:N	1:C:266:GLU:OE2	2.49	0.42
1:D:18:ALA:O	1:D:22:ILE:HG13	2.20	0.42
1:G:18:ALA:O	1:G:22:ILE:HG13	2.19	0.42
1:H:127:MET:CE	1:H:258:TYR:HA	2.48	0.42
1:B:192:ALA:HA	1:B:196:VAL:HG23	2.01	0.42
1:D:129:ALA:N	1:D:130:PRO:CD	2.83	0.42
1:D:315:GLN:CG	1:D:316:ARG:H	2.32	0.42
1:E:327:GLY:O	2:M:695:ALA:HB2	2.19	0.42
1:B:158:THR:O	1:B:166:GLN:HA	2.20	0.42
1:C:239:ARG:HD2	7:C:2166:HOH:O	2.19	0.42
1:D:153:TYR:HA	1:D:190:LEU:O	2.19	0.42
1:E:252:VAL:HG22	1:E:253:ASN:N	2.35	0.42
1:B:152:ILE:HG12	1:B:276:TYR:CE2	2.54	0.42
1:C:66:LEU:HD23	1:C:66:LEU:O	2.18	0.42
1:C:211:TRP:CE3	1:C:216:ILE:HD11	2.54	0.42
1:F:10:VAL:O	1:F:34:ALA:HA	2.19	0.42
1:H:111:SER:HA	1:H:148:VAL:HG23	2.01	0.42
1:H:120:GLY:C	1:H:122:TRP:H	2.23	0.42
1:H:155:ASN:OD1	1:H:155:ASN:O	2.38	0.42
1:H:279:LEU:N	1:H:279:LEU:HD12	2.33	0.42
1:A:329:ARG:HG3	1:A:333:GLU:HB3	2.02	0.42
1:D:258:TYR:O	1:D:261:GLN:HB3	2.20	0.42
1:E:159:SER:OG	1:E:348:LEU:CD2	2.67	0.42
1:F:145:SER:O	1:F:212:ASN:HA	2.20	0.42
1:A:136:ASN:HB2	7:A:2085:HOH:O	2.20	0.42
1:B:64:VAL:HB	1:B:65:PRO:HD3	2.02	0.42
1:F:174:THR:HG22	1:F:239:ARG:HB3	2.01	0.42
1:F:208:PRO:O	1:F:212:ASN:HB2	2.19	0.42
1:F:234:ARG:CG	7:F:2179:HOH:O	2.67	0.42
2:J:686:ARG:HA	2:J:691:GLN:O	2.20	0.42
2:N:686:ARG:HA	2:N:691:GLN:O	2.20	0.42
1:A:220:PHE:CD1	1:A:220:PHE:N	2.88	0.41
1:D:192:ALA:HA	1:D:196:VAL:HG23	2.01	0.41
7:A:2029:HOH:O	1:C:51:PRO:HG2	2.19	0.41
1:B:159:SER:OG	1:B:348:LEU:CD1	2.68	0.41
1:C:178:HIS:CD2	1:C:243:VAL:HB	2.54	0.41
1:C:181:PHE:O	1:C:244:GLN:HG3	2.20	0.41
1:F:194:HIS:HE1	1:F:327:GLY:O	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:GLN:HA	7:G:2002:HOH:O	2.20	0.41
1:A:7:THR:H	1:A:75:HIS:HD2	1.67	0.41
1:B:55:LEU:HB2	7:B:2041:HOH:O	2.20	0.41
1:C:62:ASN:ND2	7:C:2044:HOH:O	2.53	0.41
1:E:10:VAL:HG12	1:E:78:PHE:HB3	2.02	0.41
1:F:274:ALA:HA	1:F:275:PRO:HD3	1.93	0.41
1:F:316:ARG:HG3	1:F:318:THR:H	1.85	0.41
1:G:86:GLY:O	1:G:87:ASP:C	2.58	0.41
1:H:221:GLU:OE2	1:H:331:MET:N	2.50	0.41
2:J:685:ARG:HD2	2:J:698:GLY:HA3	2.02	0.41
1:A:8:ILE:HG12	1:A:76:LEU:HB2	2.03	0.41
1:A:145:SER:O	1:A:212:ASN:HA	2.20	0.41
1:C:248:VAL:HG23	1:C:266:GLU:HG2	2.02	0.41
1:C:316:ARG:HA	1:C:316:ARG:NE	2.36	0.41
1:E:334:TYR:CD1	1:E:338:VAL:HB	2.55	0.41
1:F:250:ILE:HG22	1:F:252:VAL:O	2.20	0.41
1:G:209:GLN:HE21	1:G:209:GLN:H	1.68	0.41
1:H:64:VAL:HG22	1:H:65:PRO:HD3	2.02	0.41
2:I:711:SER:O	2:I:712:LEU:CB	2.67	0.41
1:B:211:TRP:O	1:B:214:HIS:HB2	2.21	0.41
1:G:32:VAL:HB	1:G:53:VAL:HG22	2.02	0.41
1:B:125:VAL:HB	1:B:128:TRP:HB2	2.03	0.41
1:H:83:SER:CB	1:H:127:MET:HG2	2.51	0.41
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.75	0.41
1:B:220:PHE:CE2	1:B:321:ALA:HB1	2.56	0.41
1:C:323:LYS:HE2	1:C:323:LYS:CA	2.50	0.41
1:D:162:TYR:HA	1:D:163:PRO:HD3	1.83	0.41
1:D:208:PRO:O	1:D:212:ASN:HB2	2.21	0.41
1:D:344:GLU:HB3	1:D:351:MET:SD	2.60	0.41
1:E:153:TYR:HA	1:E:190:LEU:O	2.21	0.41
1:F:175:PHE:HB2	1:F:240:VAL:HG22	2.03	0.41
1:G:82:THR:CG2	3:G:1355:NAD:H51N	2.41	0.41
1:G:221:GLU:HG2	1:G:223:LEU:HG	2.02	0.41
1:G:234:ARG:NH1	1:G:336:ARG:HH22	2.18	0.41
1:H:109:ILE:HD12	1:H:204:PHE:CZ	2.55	0.41
2:L:699:LEU:HD23	2:L:699:LEU:C	2.41	0.41
2:O:687:ASN:C	2:O:689:GLU:N	2.74	0.41
2:O:687:ASN:HB3	2:O:693:LEU:HD11	2.02	0.41
1:B:64:VAL:N	1:B:65:PRO:CD	2.84	0.41
1:B:258:TYR:O	1:B:261:GLN:HB3	2.20	0.41
1:C:316:ARG:HG3	1:C:318:THR:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:264:ALA:O	1:H:268:VAL:HG23	2.21	0.41
1:H:349:ASP:O	1:H:351:MET:N	2.54	0.41
2:M:698:LEU:O	2:M:702:LEU:HG	2.20	0.41
2:O:687:ASN:O	2:O:689:GLU:N	2.54	0.41
1:B:145:SER:H	1:B:212:ASN:ND2	2.18	0.40
2:J:687:ASN:HB3	2:J:693:LEU:HD11	2.02	0.40
2:J:702:LYS:HA	2:J:702:LYS:HD2	1.90	0.40
1:A:168:GLU:OE1	1:A:170:MET:HE3	2.21	0.40
1:C:152:ILE:HA	3:C:1355:NAD:O7N	2.21	0.40
1:F:164:LEU:HD23	1:F:165:PHE:CE2	2.57	0.40
1:F:335:ALA:O	1:F:340:PRO:HD3	2.20	0.40
1:B:235:ALA:HB1	1:B:336:ARG:CA	2.51	0.40
1:C:129:ALA:N	1:C:130:PRO:HD2	2.36	0.40
1:E:179:ALA:HB3	1:E:242:TYR:OH	2.21	0.40
1:A:342:GLU:O	1:A:346:ASN:HB2	2.22	0.40
1:C:239:ARG:NH2	1:C:241:THR:HG21	2.36	0.40
1:E:159:SER:OG	1:E:348:LEU:HD22	2.21	0.40
1:A:211:TRP:CZ2	1:A:324:LEU:HD21	2.56	0.40
1:C:192:ALA:HA	1:C:196:VAL:HG23	2.04	0.40
1:E:348:LEU:HD12	1:E:348:LEU:H	1.87	0.40
1:G:153:TYR:HA	1:G:190:LEU:O	2.21	0.40
1:H:315:GLN:HB2	1:H:319:ASP:OD2	2.21	0.40
2:M:672:CYS:O	2:M:676:PHE:HA	2.21	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	314/352 (89%)	295 (94%)	17 (5%)	2 (1%)	25	31
1	B	316/352 (90%)	296 (94%)	18 (6%)	2 (1%)	25	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	314/352 (89%)	299 (95%)	12 (4%)	3 (1%)	15 17
1	D	316/352 (90%)	295 (93%)	18 (6%)	3 (1%)	17 20
1	E	314/352 (89%)	295 (94%)	16 (5%)	3 (1%)	15 17
1	F	314/352 (89%)	296 (94%)	17 (5%)	1 (0%)	41 50
1	G	315/352 (90%)	294 (93%)	20 (6%)	1 (0%)	41 50
1	H	315/352 (90%)	298 (95%)	14 (4%)	3 (1%)	15 17
2	I	40/43 (93%)	36 (90%)	4 (10%)	0	100 100
2	J	40/43 (93%)	39 (98%)	1 (2%)	0	100 100
2	K	39/43 (91%)	32 (82%)	7 (18%)	0	100 100
2	L	40/43 (93%)	35 (88%)	3 (8%)	2 (5%)	2 1
2	M	40/43 (93%)	40 (100%)	0	0	100 100
2	N	40/43 (93%)	39 (98%)	1 (2%)	0	100 100
2	O	39/43 (91%)	36 (92%)	2 (5%)	1 (3%)	5 4
2	P	40/43 (93%)	39 (98%)	1 (2%)	0	100 100
All	All	2836/3160 (90%)	2664 (94%)	151 (5%)	21 (1%)	22 26

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	51	PRO
1	E	348	LEU
1	A	51	PRO
1	C	350	TRP
1	D	52	ASN
1	H	350	TRP
1	C	42	LEU
1	D	51	PRO
1	G	51	PRO
1	D	283	SER
1	E	52	ASN
1	F	164	LEU
1	H	347	GLY
2	O	690	GLY
1	B	164	LEU
1	C	51	PRO
1	H	87	ASP
2	L	688	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	690	GLY
1	A	172	ASP
1	B	51	PRO

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	266/284 (94%)	264 (99%)	2 (1%)	81 91
1	B	268/284 (94%)	261 (97%)	7 (3%)	46 63
1	C	266/284 (94%)	261 (98%)	5 (2%)	57 73
1	D	268/284 (94%)	263 (98%)	5 (2%)	57 73
1	E	266/284 (94%)	261 (98%)	5 (2%)	57 73
1	F	266/284 (94%)	263 (99%)	3 (1%)	73 86
1	G	267/284 (94%)	261 (98%)	6 (2%)	52 69
1	H	267/284 (94%)	264 (99%)	3 (1%)	73 86
2	I	38/39 (97%)	38 (100%)	0	100 100
2	J	38/39 (97%)	38 (100%)	0	100 100
2	K	37/39 (95%)	37 (100%)	0	100 100
2	L	38/39 (97%)	38 (100%)	0	100 100
2	M	38/39 (97%)	38 (100%)	0	100 100
2	N	38/39 (97%)	38 (100%)	0	100 100
2	O	37/39 (95%)	34 (92%)	3 (8%)	11 15
2	P	38/39 (97%)	38 (100%)	0	100 100
All	All	2436/2584 (94%)	2397 (98%)	39 (2%)	62 78

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	346	ASN
1	B	155	ASN
1	B	209	GLN
1	B	212	ASN
1	B	218	LEU
1	B	219	THR
1	B	241	THR
1	B	319	ASP
1	C	167	MET
1	C	201	LEU
1	C	237	ASN
1	C	323	LYS
1	C	337	GLU
1	D	55	LEU
1	D	244	GLN
1	D	258	TYR
1	D	284	ARG
1	D	336	ARG
1	E	45	GLU
1	E	51	PRO
1	E	212	ASN
1	E	237	ASN
1	E	344	GLU
1	F	236	LEU
1	F	237	ASN
1	F	336	ARG
1	G	84	GLN
1	G	155	ASN
1	G	209	GLN
1	G	237	ASN
1	G	238	ARG
1	G	241	THR
1	H	167	MET
1	H	210	LYS
1	H	218	LEU
2	O	686	ARG
2	O	699	LEU
2	O	711	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	57	GLN
1	A	62	ASN
1	A	75	HIS
1	A	178	HIS
1	A	261	GLN
1	B	3	GLN
1	B	52	ASN
1	B	57	GLN
1	B	62	ASN
1	B	106	GLN
1	B	136	ASN
1	B	166	GLN
1	B	209	GLN
1	B	212	ASN
1	C	3	GLN
1	C	4	GLN
1	C	48	GLN
1	C	62	ASN
1	C	106	GLN
1	C	136	ASN
1	C	202	GLN
1	C	237	ASN
1	C	272	HIS
1	C	346	ASN
1	D	3	GLN
1	D	4	GLN
1	D	57	GLN
1	D	106	GLN
1	D	136	ASN
1	D	166	GLN
1	D	202	GLN
1	D	244	GLN
1	D	272	HIS
1	E	52	ASN
1	E	57	GLN
1	E	62	ASN
1	E	136	ASN
1	E	237	ASN
1	F	62	ASN
1	F	136	ASN
1	F	166	GLN
1	F	178	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	237	ASN
1	F	244	GLN
1	F	253	ASN
1	F	346	ASN
1	G	3	GLN
1	G	48	GLN
1	G	52	ASN
1	G	57	GLN
1	G	75	HIS
1	G	84	GLN
1	G	107	HIS
1	G	136	ASN
1	G	166	GLN
1	G	202	GLN
1	G	209	GLN
1	G	212	ASN
1	G	244	GLN
1	G	272	HIS
1	H	4	GLN
1	H	48	GLN
1	H	52	ASN
1	H	57	GLN
1	H	62	ASN
1	H	136	ASN
1	H	166	GLN
1	H	178	HIS
1	H	227	GLN
1	H	272	HIS
1	H	346	ASN
2	I	675	ASN
2	I	687	ASN
2	J	675	ASN
2	J	679	GLN
2	K	675	ASN
2	K	679	GLN
2	L	675	ASN
2	M	674	ASN
2	M	686	ASN
2	M	690	GLN
2	M	694	ASN
2	N	675	ASN
2	N	687	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	691	GLN
2	O	679	GLN
2	P	675	ASN
2	P	687	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 15 are monoatomic - leaving 11 for Mogul analysis.

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	$\#\|Z\| > 2$
3	NAD	B	1353	-	42,48,48	3.12	14 (33%)	50,73,73	1.70	10 (20%)
5	GOL	G	1353	-	5,5,5	4.49	5 (100%)	5,5,5	5.80	3 (60%)
3	NAD	C	1355	-	42,48,48	3.13	13 (30%)	50,73,73	1.69	10 (20%)
3	NAD	E	1354	-	42,48,48	3.10	14 (33%)	50,73,73	1.72	9 (18%)
3	NAD	D	1354	-	42,48,48	3.12	13 (30%)	50,73,73	1.71	10 (20%)
3	NAD	G	1355	-	42,48,48	3.10	13 (30%)	50,73,73	1.73	9 (18%)
3	NAD	A	1353	-	42,48,48	3.13	13 (30%)	50,73,73	1.69	10 (20%)
5	GOL	M	1712	-	5,5,5	4.51	5 (100%)	5,5,5	5.78	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAD	H	1354	-	42,48,48	3.15	14 (33%)	50,73,73	1.69	10 (20%)
5	GOL	C	1353	-	5,5,5	4.54	5 (100%)	5,5,5	5.79	3 (60%)
3	NAD	F	1354	-	42,48,48	3.16	13 (30%)	50,73,73	1.72	10 (20%)

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	B	1353	-	-	6/26/62/62	0/5/5/5
5	GOL	G	1353	-	-	2/4/4/4	-
3	NAD	C	1355	-	-	6/26/62/62	0/5/5/5
3	NAD	E	1354	-	-	6/26/62/62	0/5/5/5
3	NAD	D	1354	-	-	5/26/62/62	0/5/5/5
3	NAD	G	1355	-	-	5/26/62/62	0/5/5/5
3	NAD	A	1353	-	-	6/26/62/62	0/5/5/5
5	GOL	M	1712	-	-	2/4/4/4	-
3	NAD	H	1354	-	-	5/26/62/62	0/5/5/5
5	GOL	C	1353	-	-	2/4/4/4	-
3	NAD	F	1354	-	-	5/26/62/62	0/5/5/5

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1354	NAD	C2N-N1N	11.63	1.49	1.35
3	H	1354	NAD	C2N-N1N	11.59	1.49	1.35
3	D	1354	NAD	C2N-N1N	11.48	1.48	1.35
3	B	1353	NAD	C2N-N1N	11.42	1.48	1.35
3	A	1353	NAD	C2N-N1N	11.39	1.48	1.35
3	C	1355	NAD	C2N-N1N	11.27	1.48	1.35
3	G	1355	NAD	C2N-N1N	11.13	1.48	1.35
3	E	1354	NAD	C2N-N1N	10.93	1.48	1.35
5	G	1353	GOL	C3-C2	-7.45	1.21	1.51
5	C	1353	GOL	C3-C2	-7.42	1.21	1.51
5	M	1712	GOL	C3-C2	-7.40	1.21	1.51
3	E	1354	NAD	C4N-C3N	6.75	1.50	1.39
3	H	1354	NAD	C4N-C3N	6.70	1.50	1.39
3	A	1353	NAD	O4B-C1B	6.66	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1355	NAD	O4B-C1B	6.64	1.50	1.41
3	F	1354	NAD	O4B-C1B	6.60	1.50	1.41
3	D	1354	NAD	O4B-C1B	6.55	1.50	1.41
3	G	1355	NAD	O4B-C1B	6.53	1.50	1.41
3	F	1354	NAD	C4N-C3N	6.49	1.50	1.39
3	A	1353	NAD	C4N-C3N	6.48	1.50	1.39
3	B	1353	NAD	C4N-C3N	6.47	1.50	1.39
3	C	1355	NAD	C4N-C3N	6.46	1.50	1.39
3	G	1355	NAD	C4N-C3N	6.46	1.50	1.39
3	D	1354	NAD	C4N-C3N	6.43	1.50	1.39
3	H	1354	NAD	C7N-N7N	6.32	1.45	1.33
3	B	1353	NAD	O4B-C1B	6.32	1.49	1.41
3	H	1354	NAD	O4B-C1B	6.30	1.49	1.41
3	A	1353	NAD	C7N-N7N	6.30	1.45	1.33
3	E	1354	NAD	C7N-N7N	6.24	1.44	1.33
3	E	1354	NAD	O4B-C1B	6.22	1.49	1.41
3	D	1354	NAD	C7N-N7N	6.21	1.44	1.33
3	F	1354	NAD	C7N-N7N	6.21	1.44	1.33
3	G	1355	NAD	C7N-N7N	6.21	1.44	1.33
3	C	1355	NAD	C7N-N7N	6.19	1.44	1.33
3	B	1353	NAD	C7N-N7N	6.17	1.44	1.33
3	B	1353	NAD	C2A-N1A	5.73	1.44	1.33
3	F	1354	NAD	C2A-N1A	5.72	1.44	1.33
3	A	1353	NAD	C2A-N1A	5.71	1.44	1.33
3	H	1354	NAD	C2A-N1A	5.70	1.44	1.33
3	E	1354	NAD	C2A-N1A	5.69	1.44	1.33
3	D	1354	NAD	C2A-N1A	5.68	1.44	1.33
3	C	1355	NAD	C2A-N1A	5.63	1.44	1.33
3	G	1355	NAD	C2A-N1A	5.62	1.44	1.33
3	C	1355	NAD	C8A-N7A	4.92	1.43	1.34
3	G	1355	NAD	C8A-N7A	4.91	1.43	1.34
3	D	1354	NAD	C8A-N7A	4.90	1.43	1.34
3	A	1353	NAD	C8A-N7A	4.85	1.43	1.34
3	B	1353	NAD	C8A-N7A	4.80	1.43	1.34
3	F	1354	NAD	C8A-N7A	4.74	1.43	1.34
3	E	1354	NAD	C8A-N7A	4.73	1.43	1.34
3	H	1354	NAD	C8A-N7A	4.69	1.43	1.34
5	M	1712	GOL	O1-C1	4.65	1.62	1.42
3	H	1354	NAD	C6N-C5N	4.62	1.48	1.38
5	C	1353	GOL	O1-C1	4.60	1.61	1.42
3	E	1354	NAD	C6N-C5N	4.60	1.48	1.38
3	C	1355	NAD	C6N-C5N	4.53	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1354	NAD	C6N-C5N	4.52	1.48	1.38
5	G	1353	GOL	O1-C1	4.50	1.61	1.42
3	B	1353	NAD	C6N-C5N	4.49	1.48	1.38
3	D	1354	NAD	C6N-C5N	4.45	1.48	1.38
3	A	1353	NAD	C6N-C5N	4.44	1.48	1.38
3	G	1355	NAD	C6N-C5N	4.43	1.48	1.38
3	C	1355	NAD	C6A-N1A	3.76	1.53	1.37
3	D	1354	NAD	C6A-N1A	3.72	1.53	1.37
3	F	1354	NAD	C6A-N1A	3.71	1.53	1.37
3	B	1353	NAD	C6A-N1A	3.71	1.53	1.37
3	A	1353	NAD	C6A-N1A	3.70	1.53	1.37
3	E	1354	NAD	C6A-N1A	3.70	1.53	1.37
3	H	1354	NAD	C6A-N1A	3.69	1.53	1.37
3	G	1355	NAD	C6A-N1A	3.67	1.53	1.37
3	G	1355	NAD	C5A-C4A	-3.60	1.31	1.40
3	D	1354	NAD	C5A-C4A	-3.60	1.31	1.40
3	A	1353	NAD	C5A-C4A	-3.57	1.31	1.40
3	F	1354	NAD	C5A-C4A	-3.56	1.31	1.40
3	C	1355	NAD	C5A-C4A	-3.56	1.31	1.40
3	H	1354	NAD	C5A-C4A	-3.54	1.31	1.40
3	E	1354	NAD	C5A-C4A	-3.50	1.31	1.40
3	B	1353	NAD	C5A-C4A	-3.46	1.31	1.40
5	M	1712	GOL	O3-C3	3.41	1.56	1.42
3	F	1354	NAD	O4D-C1D	3.39	1.45	1.41
5	C	1353	GOL	O3-C3	3.37	1.56	1.42
5	G	1353	GOL	O3-C3	3.30	1.56	1.42
3	H	1354	NAD	O4D-C1D	3.13	1.45	1.41
3	F	1354	NAD	C6A-N6A	3.08	1.45	1.34
3	C	1355	NAD	C6A-N6A	3.07	1.45	1.34
3	E	1354	NAD	O4D-C1D	3.06	1.45	1.41
3	B	1353	NAD	C6A-N6A	3.03	1.45	1.34
3	G	1355	NAD	C6A-N6A	3.00	1.45	1.34
3	A	1353	NAD	C6A-N6A	2.99	1.45	1.34
3	H	1354	NAD	C6A-N6A	2.98	1.44	1.34
3	E	1354	NAD	C6A-N6A	2.97	1.44	1.34
3	D	1354	NAD	C6A-N6A	2.95	1.44	1.34
3	C	1355	NAD	O4D-C1D	2.91	1.45	1.41
5	C	1353	GOL	O2-C2	-2.86	1.34	1.43
5	G	1353	GOL	C1-C2	-2.81	1.40	1.51
3	C	1355	NAD	C6A-C5A	2.70	1.53	1.43
5	C	1353	GOL	C1-C2	-2.70	1.40	1.51
3	A	1353	NAD	C6A-C5A	2.68	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1355	NAD	C6A-C5A	2.67	1.53	1.43
3	G	1355	NAD	O4D-C1D	2.66	1.44	1.41
3	C	1355	NAD	C4A-N3A	2.65	1.39	1.35
5	M	1712	GOL	C1-C2	-2.64	1.40	1.51
3	E	1354	NAD	C6A-C5A	2.60	1.53	1.43
3	D	1354	NAD	C4A-N3A	2.59	1.39	1.35
5	M	1712	GOL	O2-C2	-2.58	1.35	1.43
3	F	1354	NAD	C6A-C5A	2.58	1.52	1.43
3	D	1354	NAD	C6A-C5A	2.57	1.52	1.43
3	B	1353	NAD	C4A-N3A	2.54	1.39	1.35
3	B	1353	NAD	C6A-C5A	2.54	1.52	1.43
5	G	1353	GOL	O2-C2	-2.54	1.35	1.43
3	A	1353	NAD	C4A-N3A	2.53	1.39	1.35
3	E	1354	NAD	C4A-N3A	2.53	1.39	1.35
3	B	1353	NAD	O4D-C1D	2.53	1.44	1.41
3	H	1354	NAD	C6A-C5A	2.51	1.52	1.43
3	A	1353	NAD	O4D-C1D	2.50	1.44	1.41
3	G	1355	NAD	C4A-N3A	2.50	1.39	1.35
3	D	1354	NAD	O4D-C1D	2.47	1.44	1.41
3	F	1354	NAD	C4A-N3A	2.46	1.39	1.35
3	B	1353	NAD	C2B-C1B	2.41	1.57	1.53
3	H	1354	NAD	C4A-N3A	2.39	1.38	1.35
3	E	1354	NAD	C2B-C1B	2.28	1.57	1.53
3	H	1354	NAD	C2B-C1B	2.23	1.57	1.53

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1353	GOL	O3-C3-C2	10.50	160.56	110.20
5	G	1353	GOL	O3-C3-C2	10.45	160.28	110.20
5	M	1712	GOL	O3-C3-C2	10.44	160.25	110.20
5	G	1353	GOL	O2-C2-C3	6.82	139.16	109.12
5	M	1712	GOL	O2-C2-C3	6.80	139.06	109.12
5	C	1353	GOL	O2-C2-C3	6.75	138.87	109.12
3	D	1354	NAD	N3A-C2A-N1A	-5.03	120.82	128.68
3	C	1355	NAD	N3A-C2A-N1A	-5.01	120.84	128.68
3	F	1354	NAD	N3A-C2A-N1A	-5.01	120.85	128.68
3	G	1355	NAD	N3A-C2A-N1A	-5.00	120.87	128.68
3	A	1353	NAD	N3A-C2A-N1A	-4.99	120.88	128.68
3	F	1354	NAD	O4B-C1B-C2B	-4.97	99.66	106.93
3	E	1354	NAD	O4B-C1B-C2B	-4.96	99.67	106.93
3	B	1353	NAD	N3A-C2A-N1A	-4.96	120.93	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1354	NAD	N3A-C2A-N1A	-4.95	120.94	128.68
3	E	1354	NAD	N3A-C2A-N1A	-4.94	120.96	128.68
3	G	1355	NAD	C6N-N1N-C2N	4.85	126.40	121.97
3	B	1353	NAD	O4B-C1B-C2B	-4.76	99.97	106.93
3	E	1354	NAD	O4D-C1D-C2D	-4.71	100.05	106.93
3	G	1355	NAD	O4B-C1B-C2B	-4.70	100.06	106.93
3	A	1353	NAD	C6N-N1N-C2N	4.66	126.23	121.97
3	D	1354	NAD	C6N-N1N-C2N	4.66	126.22	121.97
3	B	1353	NAD	C6N-N1N-C2N	4.61	126.17	121.97
3	E	1354	NAD	C6N-N1N-C2N	4.58	126.15	121.97
3	C	1355	NAD	C6N-N1N-C2N	4.57	126.14	121.97
3	H	1354	NAD	C6N-N1N-C2N	4.57	126.14	121.97
3	A	1353	NAD	O4B-C1B-C2B	-4.50	100.35	106.93
3	D	1354	NAD	O4B-C1B-C2B	-4.46	100.41	106.93
3	C	1355	NAD	O4B-C1B-C2B	-4.45	100.42	106.93
3	F	1354	NAD	C6N-N1N-C2N	4.39	125.98	121.97
3	H	1354	NAD	O4B-C1B-C2B	-4.32	100.62	106.93
3	D	1354	NAD	O4D-C1D-C2D	-4.24	100.72	106.93
3	H	1354	NAD	O4D-C1D-C2D	-4.22	100.76	106.93
3	G	1355	NAD	O4D-C1D-C2D	-4.21	100.77	106.93
3	F	1354	NAD	O4D-C1D-C2D	-4.17	100.83	106.93
3	B	1353	NAD	O4D-C1D-C2D	-3.95	101.15	106.93
3	C	1355	NAD	O4D-C1D-C2D	-3.94	101.16	106.93
3	D	1354	NAD	C3N-C2N-N1N	-3.80	116.71	120.43
3	G	1355	NAD	C3N-C2N-N1N	-3.80	116.71	120.43
3	A	1353	NAD	O4D-C1D-C2D	-3.66	101.57	106.93
3	H	1354	NAD	C3N-C2N-N1N	-3.58	116.93	120.43
3	E	1354	NAD	C3N-C2N-N1N	-3.57	116.94	120.43
3	B	1353	NAD	C3N-C2N-N1N	-3.56	116.94	120.43
3	F	1354	NAD	C3N-C2N-N1N	-3.56	116.95	120.43
3	A	1353	NAD	C3N-C2N-N1N	-3.55	116.96	120.43
3	C	1355	NAD	C3N-C2N-N1N	-3.47	117.04	120.43
5	G	1353	GOL	O1-C1-C2	3.41	126.54	110.20
5	C	1353	GOL	O1-C1-C2	3.36	126.31	110.20
5	M	1712	GOL	O1-C1-C2	3.31	126.05	110.20
3	F	1354	NAD	C5A-C6A-N1A	-2.91	113.75	120.35
3	A	1353	NAD	C5A-C6A-N1A	-2.89	113.81	120.35
3	H	1354	NAD	C5A-C6A-N1A	-2.89	113.81	120.35
3	B	1353	NAD	C5A-C6A-N1A	-2.88	113.83	120.35
3	C	1355	NAD	C5A-C6A-N1A	-2.87	113.85	120.35
3	D	1354	NAD	C5A-C6A-N1A	-2.86	113.86	120.35
3	G	1355	NAD	C5A-C6A-N1A	-2.85	113.89	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1354	NAD	C5A-C6A-N1A	-2.84	113.92	120.35
3	A	1353	NAD	C3N-C7N-N7N	2.67	120.95	117.75
3	B	1353	NAD	C3N-C7N-N7N	2.57	120.83	117.75
3	H	1354	NAD	C3N-C7N-N7N	2.52	120.77	117.75
3	C	1355	NAD	C3N-C7N-N7N	2.49	120.74	117.75
3	H	1354	NAD	N6A-C6A-N1A	2.48	123.73	118.57
3	F	1354	NAD	N6A-C6A-N1A	2.48	123.71	118.57
3	F	1354	NAD	C3N-C7N-N7N	2.42	120.65	117.75
3	B	1353	NAD	N6A-C6A-N1A	2.40	123.56	118.57
3	D	1354	NAD	N6A-C6A-N1A	2.39	123.53	118.57
3	E	1354	NAD	N6A-C6A-N1A	2.37	123.49	118.57
3	A	1353	NAD	N6A-C6A-N1A	2.35	123.44	118.57
3	G	1355	NAD	C3N-C7N-N7N	2.35	120.56	117.75
3	G	1355	NAD	N6A-C6A-N1A	2.34	123.43	118.57
3	D	1354	NAD	C3N-C7N-N7N	2.33	120.55	117.75
3	C	1355	NAD	N6A-C6A-N1A	2.32	123.39	118.57
3	F	1354	NAD	O7N-C7N-N7N	-2.26	119.37	122.58
3	C	1355	NAD	O7N-C7N-N7N	-2.23	119.41	122.58
3	A	1353	NAD	O7N-C7N-N7N	-2.20	119.44	122.58
3	E	1354	NAD	C3N-C7N-N7N	2.20	120.39	117.75
3	D	1354	NAD	O7N-C7N-N7N	-2.18	119.48	122.58
3	H	1354	NAD	O7N-C7N-N7N	-2.18	119.48	122.58
3	B	1353	NAD	O7N-C7N-N7N	-2.17	119.50	122.58
3	G	1355	NAD	C5N-C6N-N1N	-2.16	117.31	120.40
3	B	1353	NAD	C5N-C6N-N1N	-2.15	117.33	120.40
3	A	1353	NAD	C5N-C6N-N1N	-2.14	117.33	120.40
3	C	1355	NAD	C5N-C6N-N1N	-2.12	117.36	120.40
3	H	1354	NAD	C5N-C6N-N1N	-2.09	117.41	120.40
3	D	1354	NAD	C5N-C6N-N1N	-2.06	117.45	120.40
3	E	1354	NAD	C5N-C6N-N1N	-2.05	117.46	120.40
3	F	1354	NAD	C5N-C6N-N1N	-2.04	117.47	120.40

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1353	NAD	C5B-O5B-PA-O3
3	A	1353	NAD	O4D-C1D-N1N-C2N
3	B	1353	NAD	C5B-O5B-PA-O3
3	B	1353	NAD	O4D-C1D-N1N-C2N
3	C	1355	NAD	C5B-O5B-PA-O1A
3	C	1355	NAD	C5B-O5B-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1355	NAD	C5B-O5B-PA-O3
3	C	1355	NAD	O4D-C1D-N1N-C2N
3	D	1354	NAD	C5B-O5B-PA-O2A
3	D	1354	NAD	C5B-O5B-PA-O3
3	E	1354	NAD	C5B-O5B-PA-O3
3	E	1354	NAD	O4D-C1D-N1N-C2N
3	F	1354	NAD	C5B-O5B-PA-O1A
3	F	1354	NAD	C5B-O5B-PA-O2A
3	F	1354	NAD	C5B-O5B-PA-O3
3	G	1355	NAD	C5B-O5B-PA-O2A
3	G	1355	NAD	C5B-O5B-PA-O3
3	H	1354	NAD	C5B-O5B-PA-O3
5	C	1353	GOL	O1-C1-C2-O2
5	C	1353	GOL	C1-C2-C3-O3
5	G	1353	GOL	O1-C1-C2-C3
5	G	1353	GOL	C1-C2-C3-O3
5	M	1712	GOL	C1-C2-C3-O3
5	M	1712	GOL	O1-C1-C2-O2
3	A	1353	NAD	PA-O3-PN-O2N
3	B	1353	NAD	PA-O3-PN-O2N
3	C	1355	NAD	PA-O3-PN-O2N
3	D	1354	NAD	PA-O3-PN-O2N
3	E	1354	NAD	PA-O3-PN-O2N
3	F	1354	NAD	PA-O3-PN-O2N
3	G	1355	NAD	PA-O3-PN-O2N
3	H	1354	NAD	PA-O3-PN-O2N
3	A	1353	NAD	C5B-O5B-PA-O1A
3	A	1353	NAD	C5B-O5B-PA-O2A
3	B	1353	NAD	C5B-O5B-PA-O1A
3	B	1353	NAD	C5B-O5B-PA-O2A
3	D	1354	NAD	C5B-O5B-PA-O1A
3	E	1354	NAD	C5B-O5B-PA-O1A
3	E	1354	NAD	C5B-O5B-PA-O2A
3	G	1355	NAD	C5B-O5B-PA-O1A
3	H	1354	NAD	C5B-O5B-PA-O1A
3	H	1354	NAD	C5B-O5B-PA-O2A
3	B	1353	NAD	O4B-C4B-C5B-O5B
3	C	1355	NAD	O4B-C4B-C5B-O5B
3	D	1354	NAD	O4B-C4B-C5B-O5B
3	F	1354	NAD	O4B-C4B-C5B-O5B
3	G	1355	NAD	O4B-C4B-C5B-O5B
3	H	1354	NAD	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1353	NAD	O4B-C4B-C5B-O5B
3	E	1354	NAD	O4B-C4B-C5B-O5B

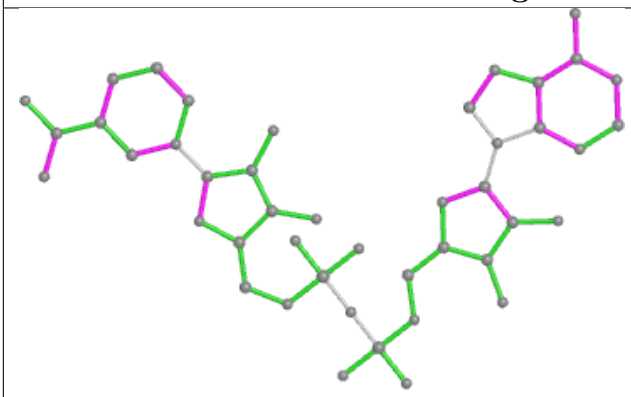
There are no ring outliers.

11 monomers are involved in 22 short contacts:

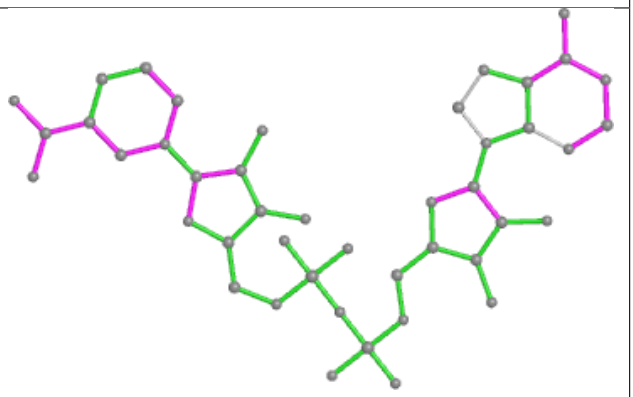
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1353	NAD	3	0
5	G	1353	GOL	1	0
3	C	1355	NAD	4	0
3	E	1354	NAD	1	0
3	D	1354	NAD	1	0
3	G	1355	NAD	3	0
3	A	1353	NAD	3	0
5	M	1712	GOL	1	0
3	H	1354	NAD	3	0
5	C	1353	GOL	1	0
3	F	1354	NAD	1	0

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 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.

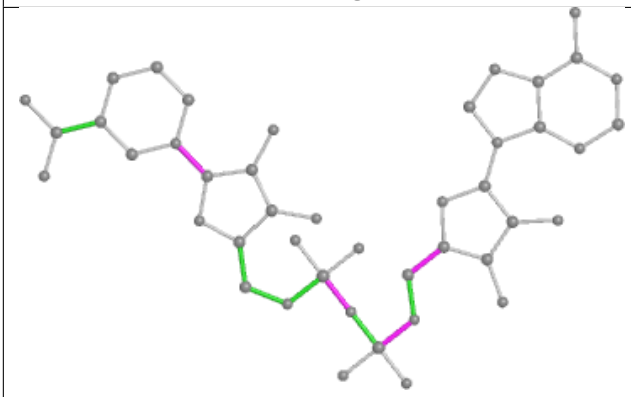
Ligand NAD B 1353



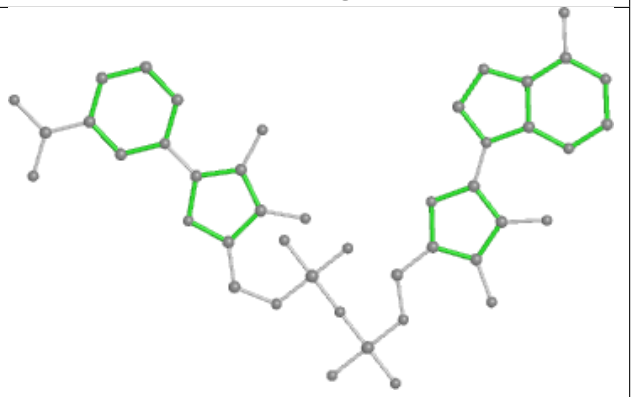
Bond lengths



Bond angles

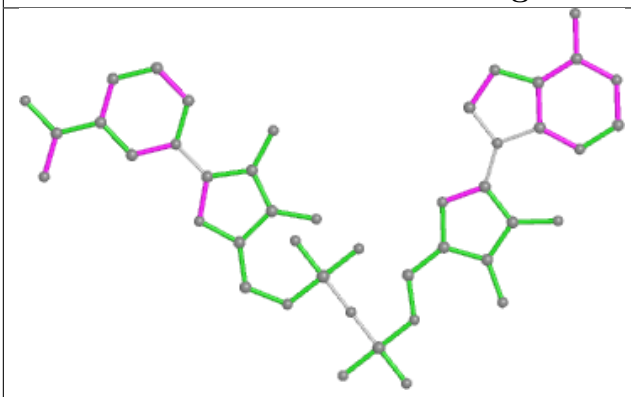


Torsions

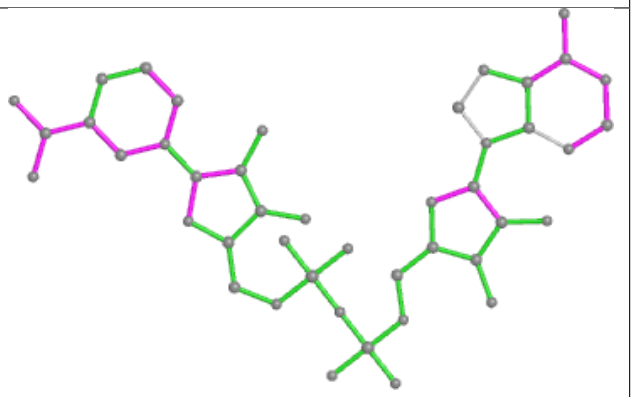


Rings

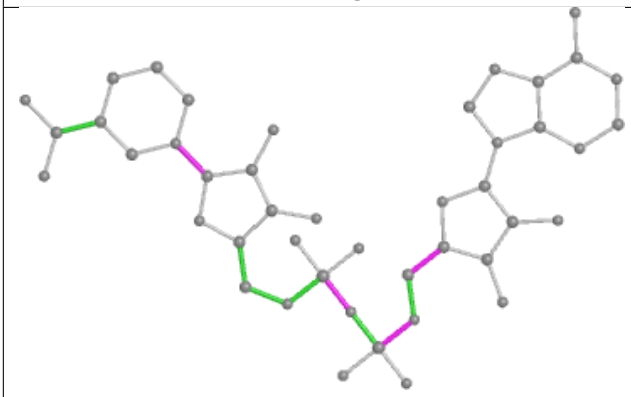
Ligand NAD C 1355



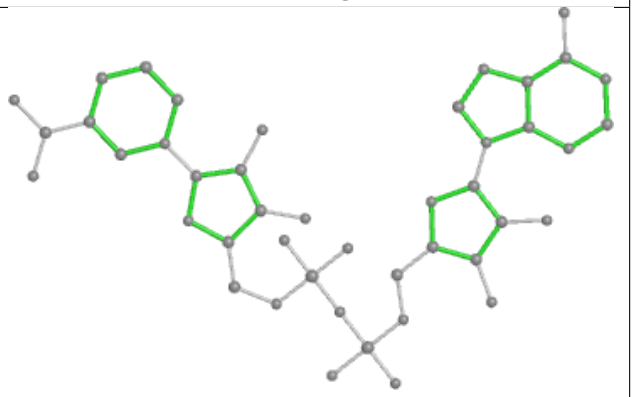
Bond lengths



Bond angles

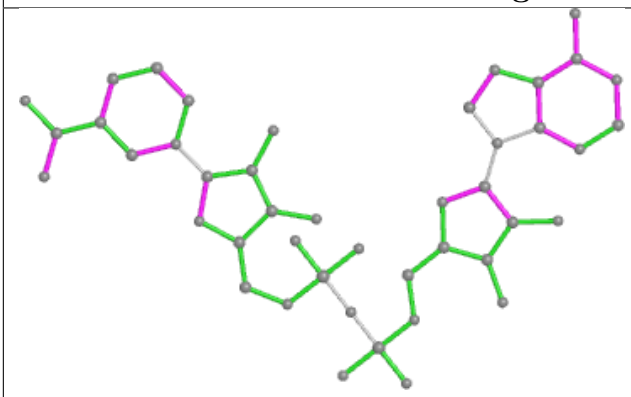


Torsions

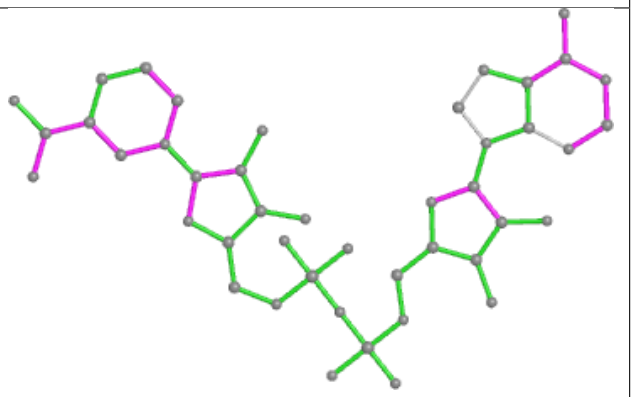


Rings

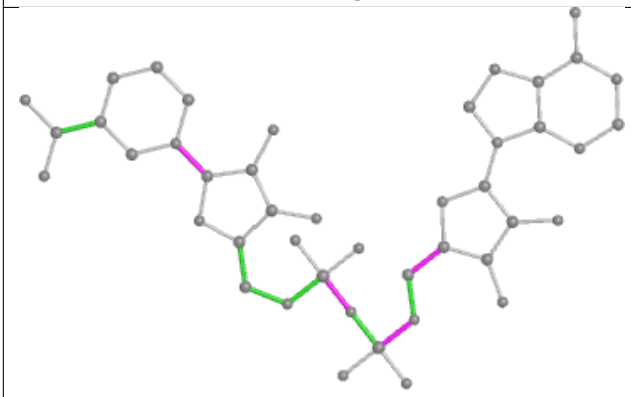
Ligand NAD E 1354



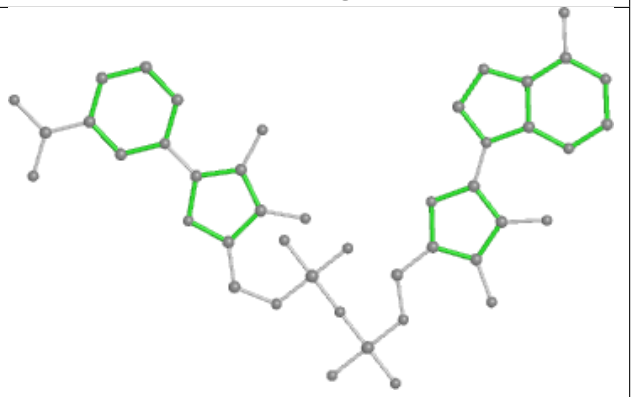
Bond lengths



Bond angles

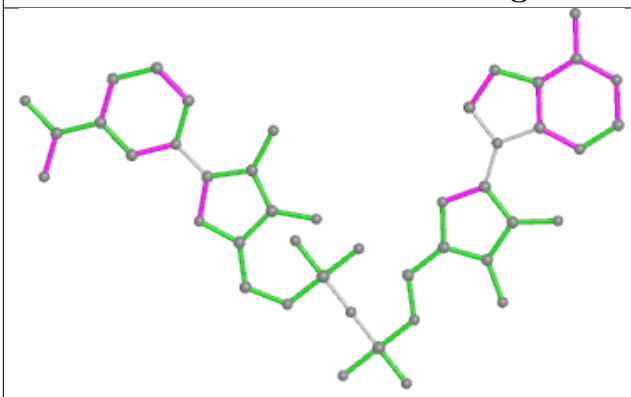


Torsions

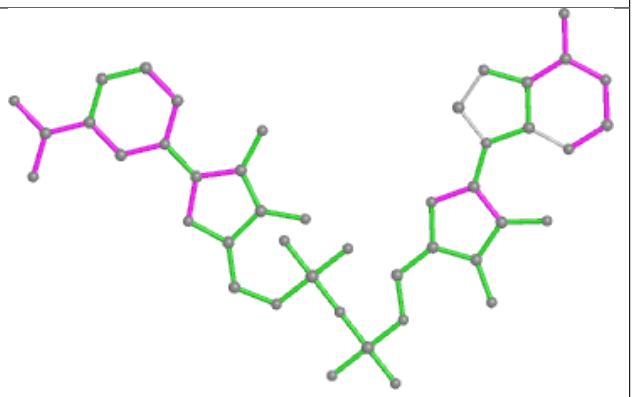


Rings

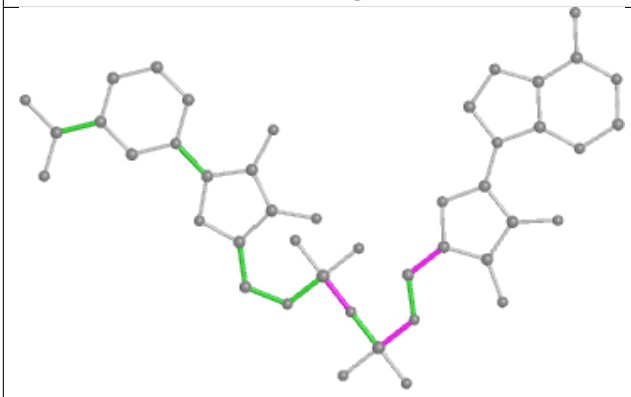
Ligand NAD D 1354



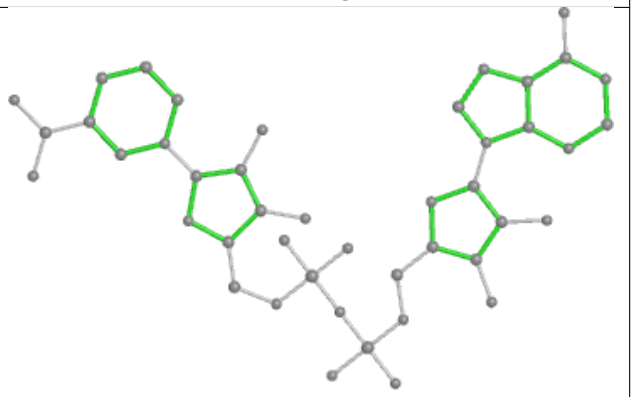
Bond lengths



Bond angles

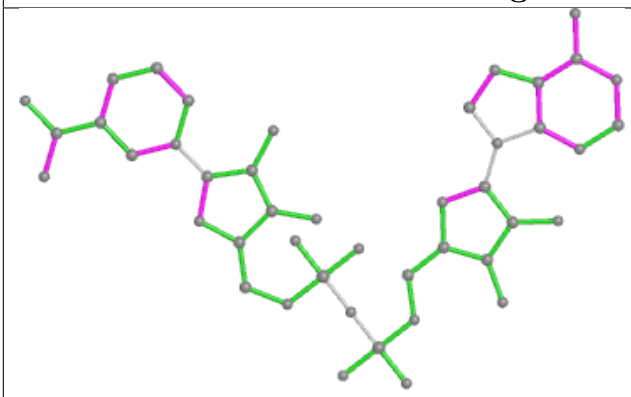


Torsions

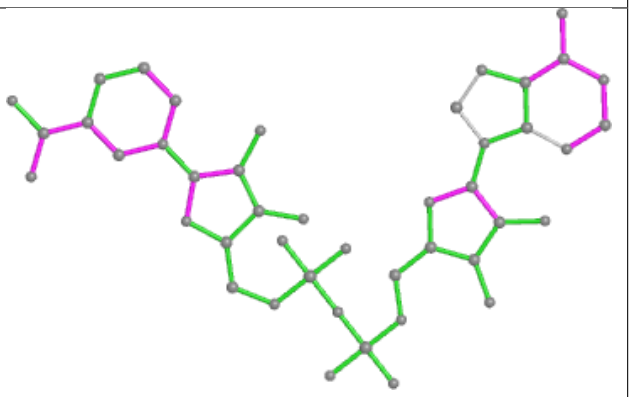


Rings

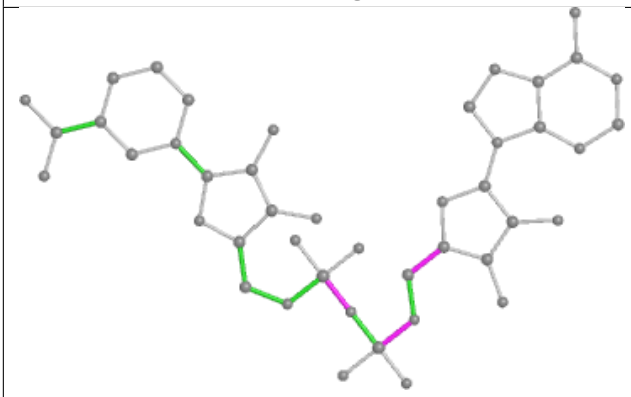
Ligand NAD G 1355



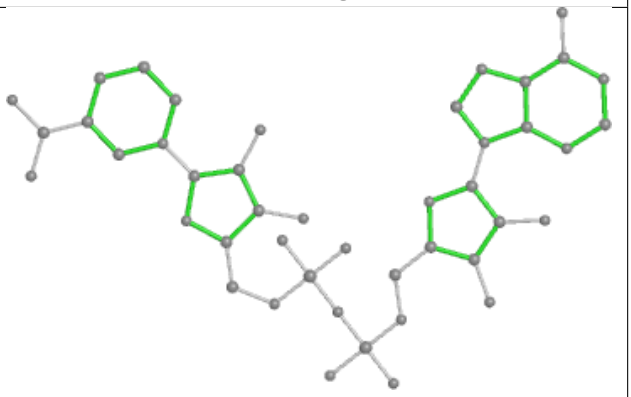
Bond lengths



Bond angles

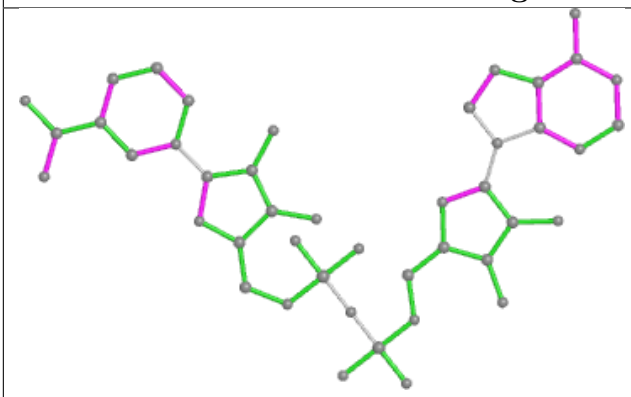


Torsions

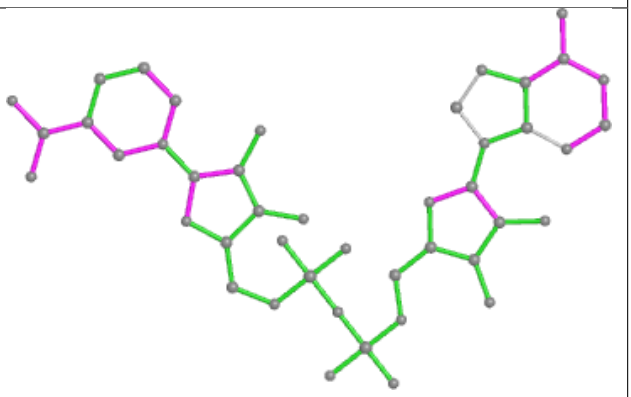


Rings

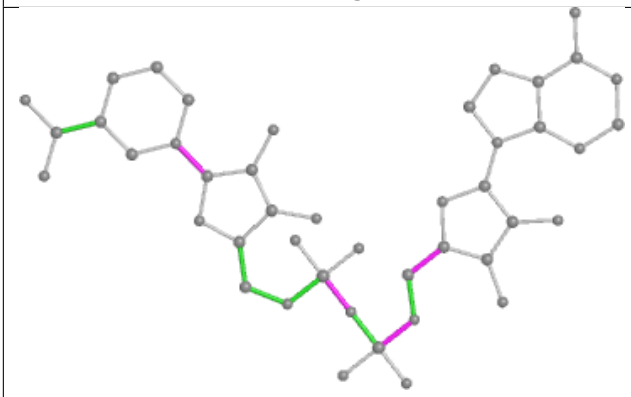
Ligand NAD A 1353



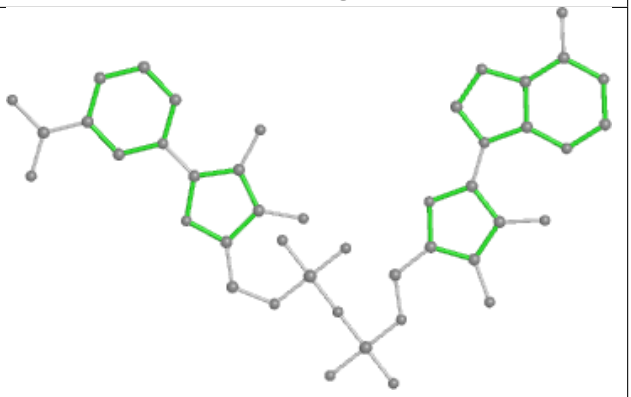
Bond lengths



Bond angles

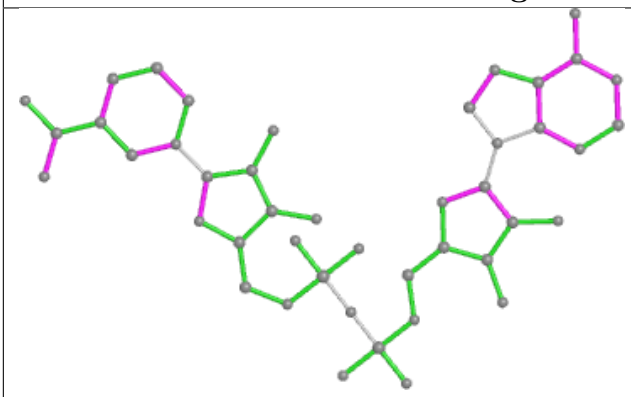


Torsions

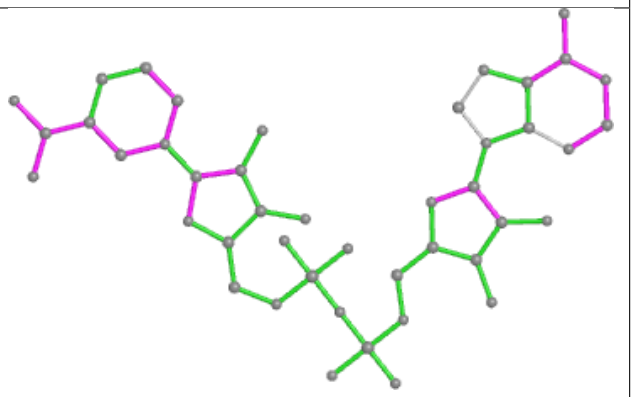


Rings

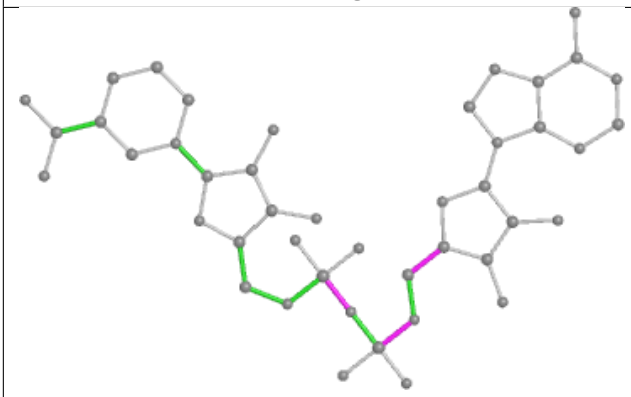
Ligand NAD H 1354



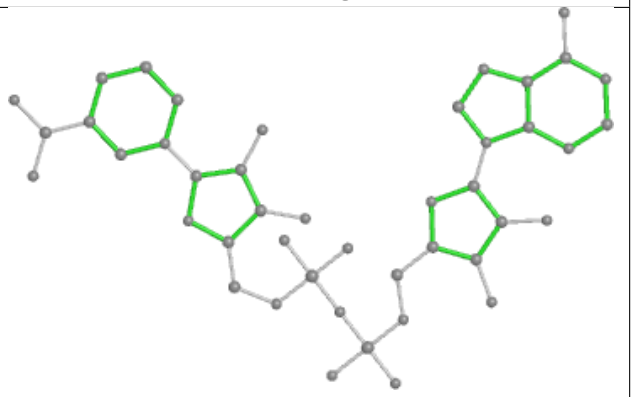
Bond lengths



Bond angles

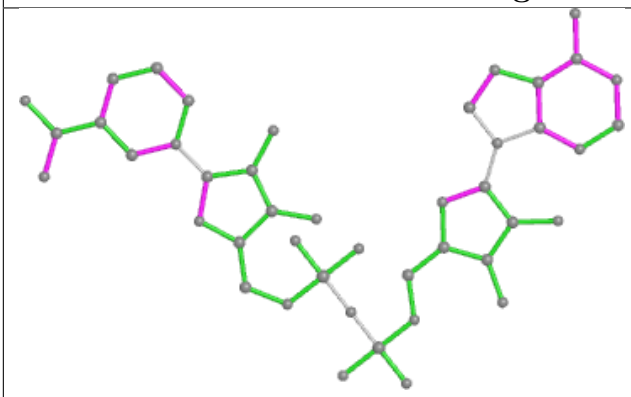


Torsions

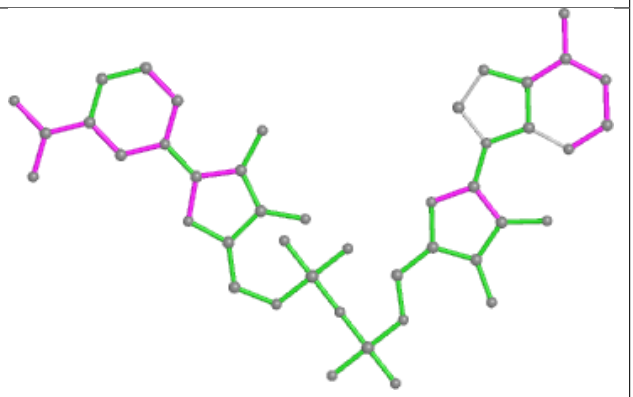


Rings

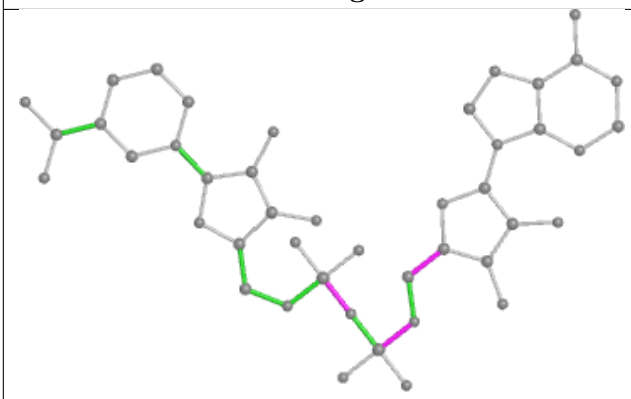
Ligand NAD F 1354



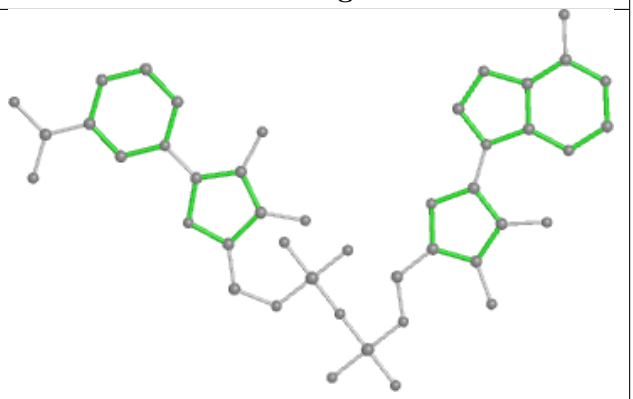
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	318/352 (90%)	-0.62	0 100 100	13, 31, 65, 88	0
1	B	320/352 (90%)	-0.55	0 100 100	12, 34, 62, 96	0
1	C	318/352 (90%)	-0.73	1 (0%) 94 96	11, 27, 49, 75	0
1	D	320/352 (90%)	-0.68	1 (0%) 94 96	15, 30, 63, 98	0
1	E	318/352 (90%)	-0.67	1 (0%) 94 96	13, 27, 56, 73	0
1	F	318/352 (90%)	-0.63	1 (0%) 94 96	10, 28, 56, 82	0
1	G	319/352 (90%)	-0.72	0 100 100	11, 27, 54, 91	0
1	H	319/352 (90%)	-0.64	2 (0%) 89 92	12, 28, 68, 92	0
2	I	42/43 (97%)	-0.25	2 (4%) 30 37	20, 39, 92, 108	0
2	J	42/43 (97%)	-0.29	0 100 100	19, 42, 88, 96	0
2	K	41/43 (95%)	-0.25	1 (2%) 59 66	14, 43, 94, 103	0
2	L	42/43 (97%)	-0.33	1 (2%) 59 66	19, 43, 96, 111	0
2	M	42/43 (97%)	-0.21	1 (2%) 59 66	16, 40, 86, 108	0
2	N	42/43 (97%)	-0.39	1 (2%) 59 66	17, 37, 80, 106	0
2	O	41/43 (95%)	-0.18	2 (4%) 29 36	21, 40, 86, 108	0
2	P	42/43 (97%)	-0.30	1 (2%) 59 66	18, 40, 90, 103	0
All	All	2884/3160 (91%)	-0.61	15 (0%) 91 94	10, 30, 66, 111	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	688	PRO	7.0
2	P	688	PRO	4.2
1	H	315	GLN	3.8
2	N	688	PRO	3.5
1	H	352	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	690	GLY	2.7
2	I	688	PRO	2.7
1	C	85	ALA	2.6
2	K	688	PRO	2.5
2	M	687	PRO	2.4
2	L	688	PRO	2.3
1	D	315	GLN	2.3
1	F	352	LEU	2.2
2	I	687	ASN	2.1
1	E	352	LEU	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	C	1353	6/6	0.88	0.15	44,55,61,62	0
5	GOL	G	1353	6/6	0.89	0.18	45,54,59,61	0
3	NAD	B	1353	44/44	0.91	0.23	60,83,116,119	0
5	GOL	M	1712	6/6	0.93	0.09	35,53,57,59	0
3	NAD	E	1354	44/44	0.94	0.20	33,77,116,120	0
3	NAD	H	1354	44/44	0.95	0.21	23,75,110,114	0
4	CL	A	1354	1/1	0.95	0.13	67,67,67,67	0
3	NAD	D	1354	44/44	0.95	0.17	41,75,119,123	0
3	NAD	A	1353	44/44	0.95	0.25	47,78,113,119	0
3	NAD	F	1354	44/44	0.95	0.23	34,75,120,127	0
3	NAD	C	1355	44/44	0.96	0.18	32,67,110,111	0
6	ZN	P	1713	1/1	0.96	0.08	36,36,36,36	0
3	NAD	G	1355	44/44	0.97	0.16	40,71,119,122	0

Continued on next page...

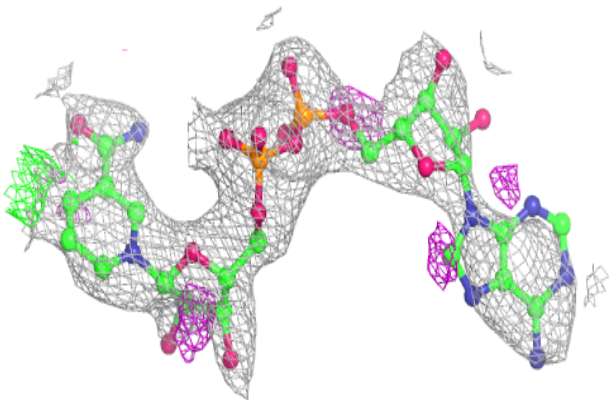
Continued from previous page...

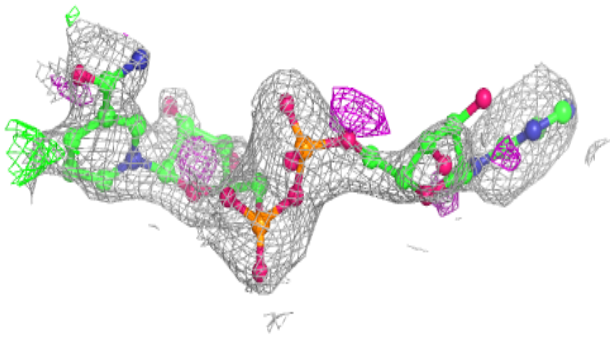
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ZN	O	1712	1/1	0.97	0.10	33,33,33,33	0
4	CL	D	1353	1/1	0.97	0.07	62,62,62,62	0
4	CL	H	1353	1/1	0.98	0.06	51,51,51,51	0
6	ZN	M	1713	1/1	0.98	0.11	27,27,27,27	0
4	CL	C	1354	1/1	0.98	0.09	55,55,55,55	0
4	CL	G	1354	1/1	0.98	0.07	48,48,48,48	0
4	CL	F	1353	1/1	0.99	0.09	62,62,62,62	0
4	CL	E	1353	1/1	0.99	0.12	63,63,63,63	0
6	ZN	I	1713	1/1	0.99	0.09	32,32,32,32	0
6	ZN	J	1713	1/1	1.00	0.08	38,38,38,38	0
6	ZN	N	1713	1/1	1.00	0.10	31,31,31,31	0
6	ZN	K	1712	1/1	1.00	0.09	27,27,27,27	0
6	ZN	L	1713	1/1	1.00	0.09	31,31,31,31	0

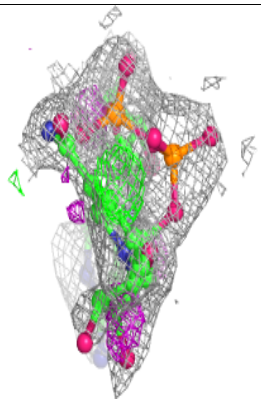
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 1353:

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

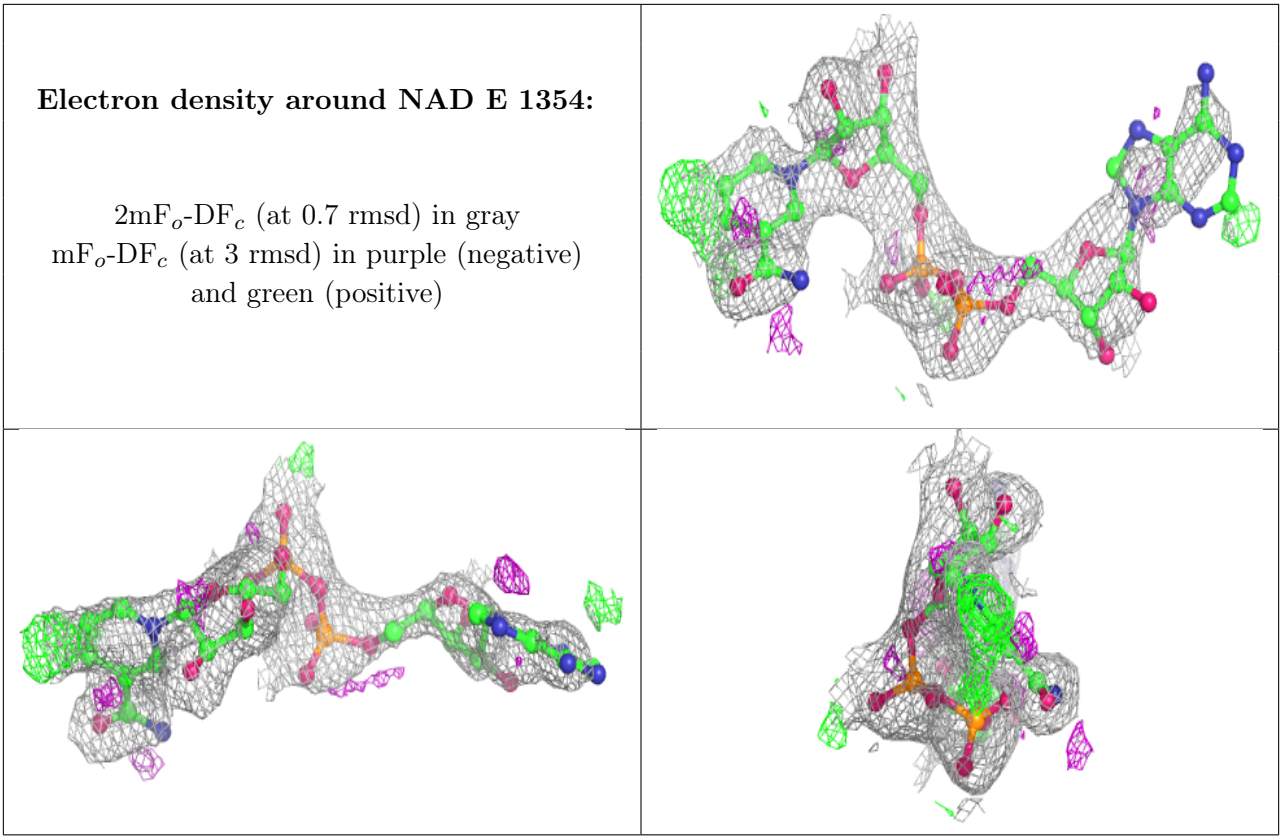






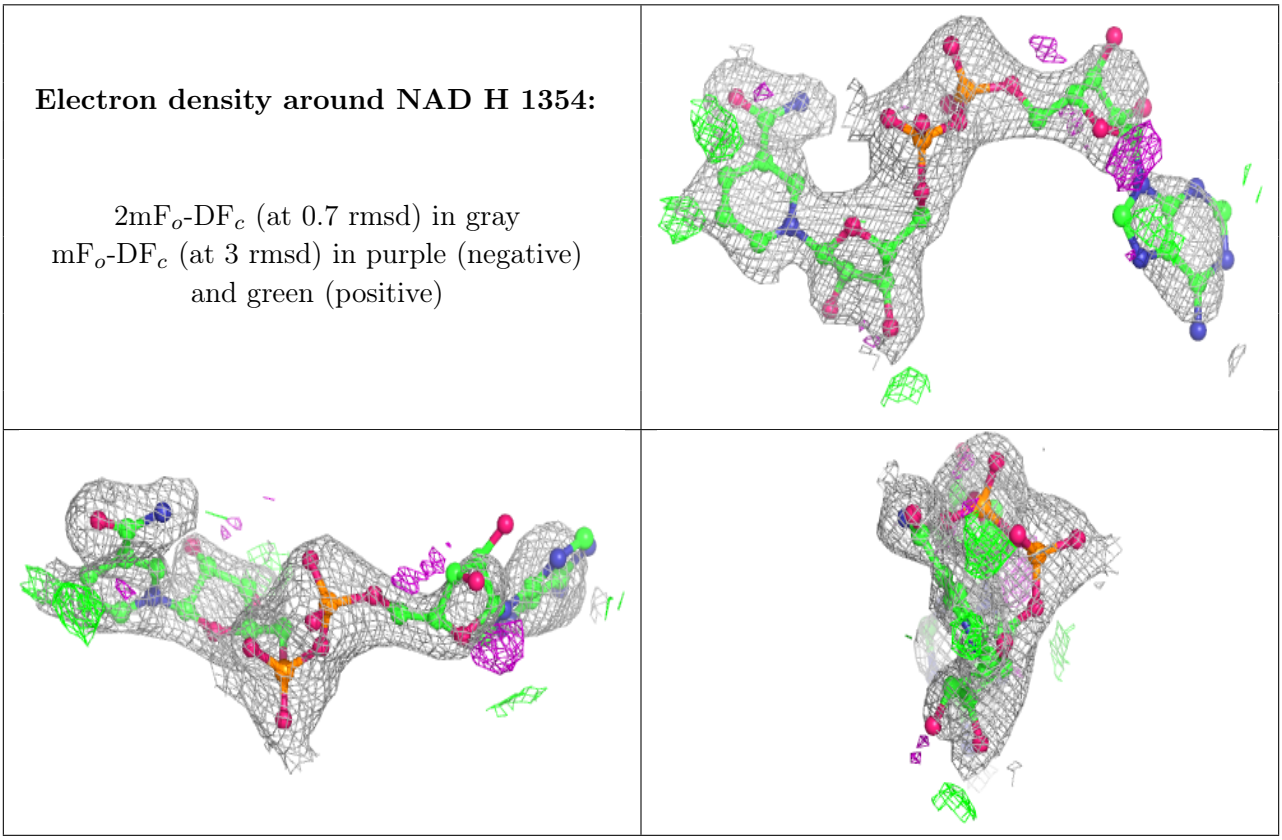
Electron density around NAD E 1354:

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



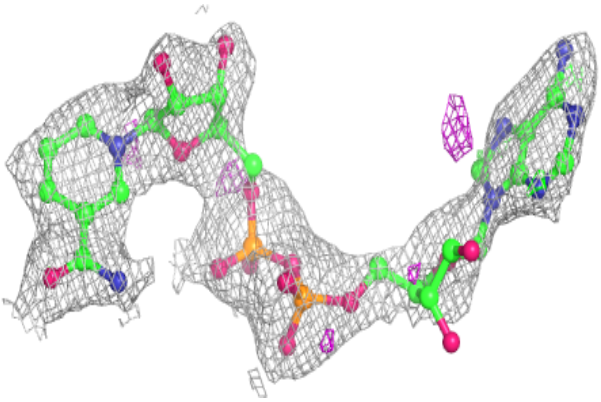
Electron density around NAD H 1354:

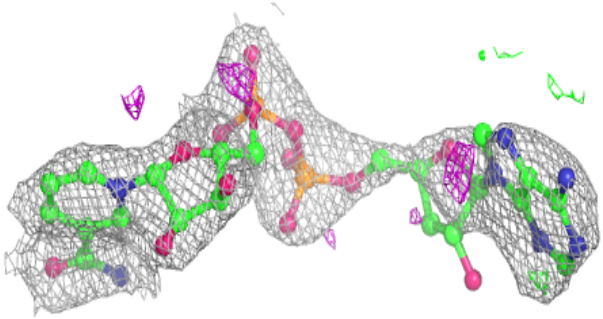
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

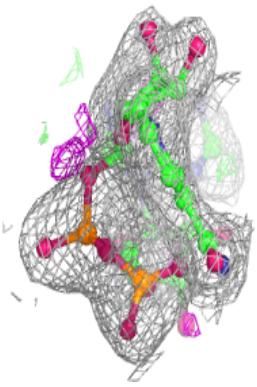


Electron density around NAD D 1354:

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

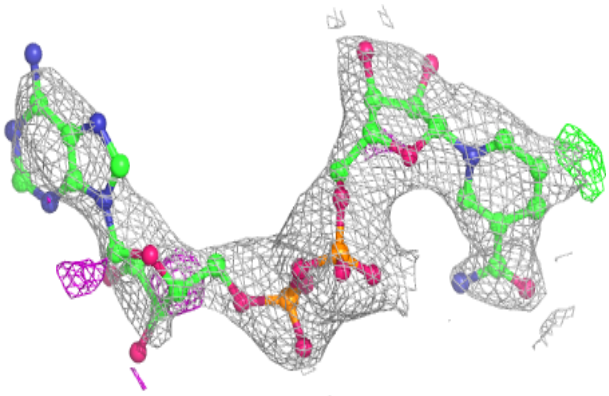


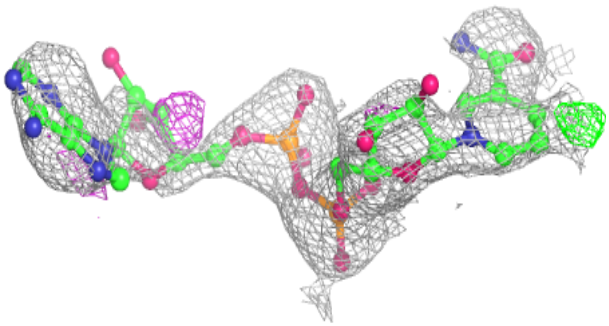


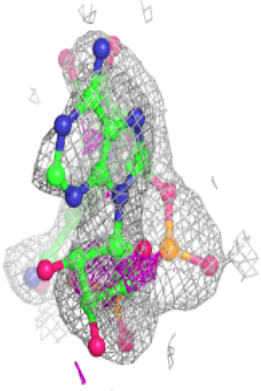


Electron density around NAD A 1353:

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

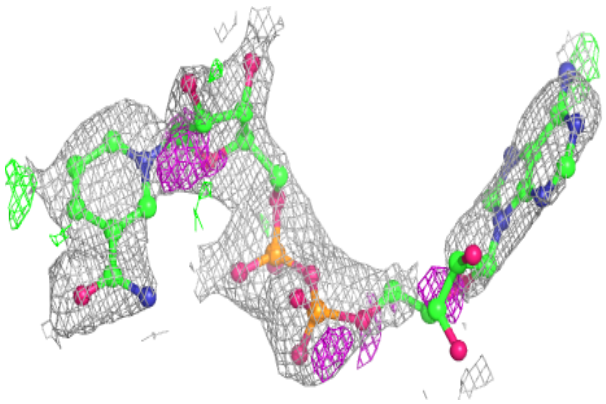


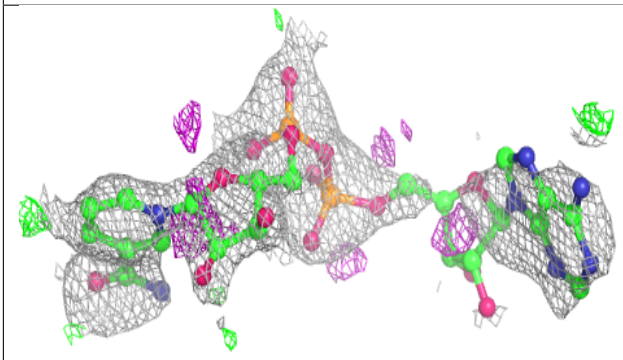


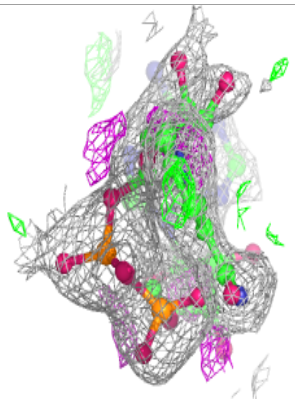


Electron density around NAD F 1354:

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

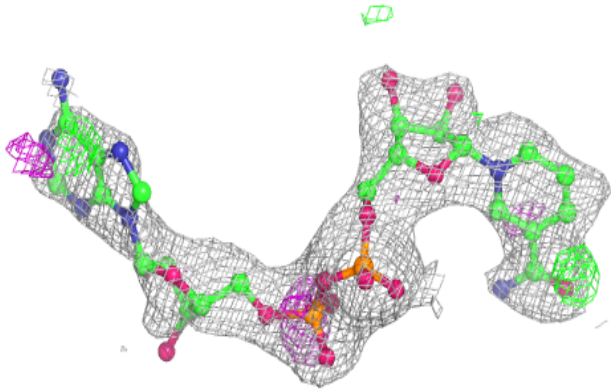


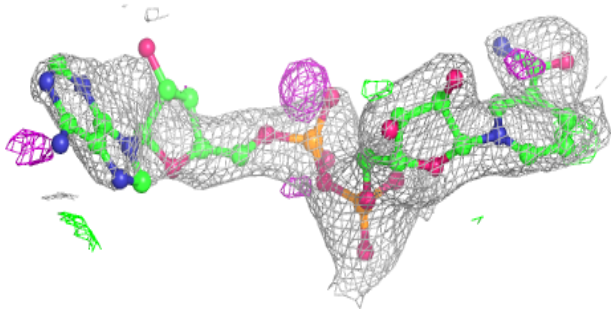


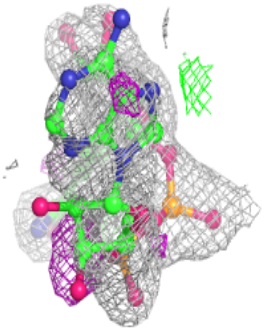


Electron density around NAD C 1355:

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

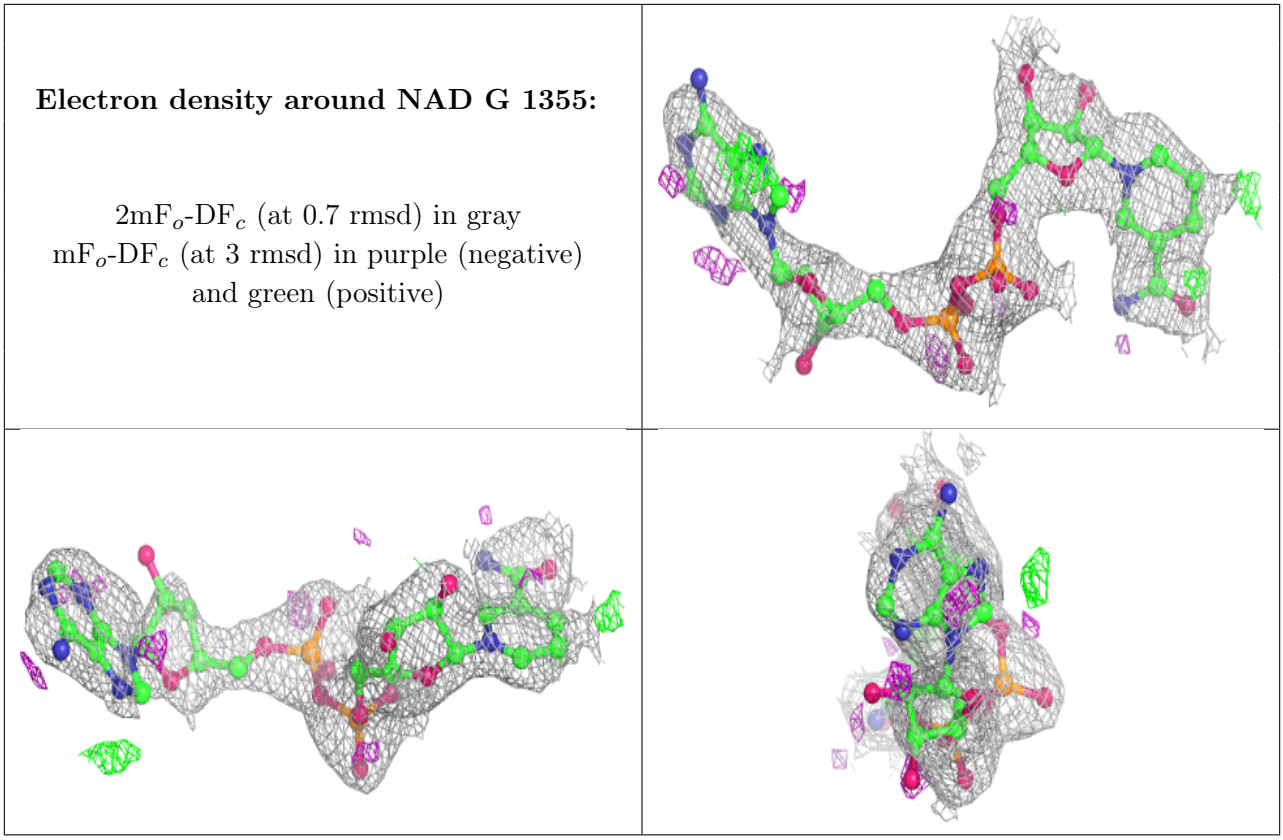






Electron density around NAD G 1355:

$2mF_o$-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.