Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 04:42 PM JST

PDB ID	:	5ZQ7
Title	:	SidE-Ubi-NAD
Authors	:	Wang, Y.; Gao, A.; Gao, P.
Deposited on	:	2018-04-17
Resolution	:	2.85 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:

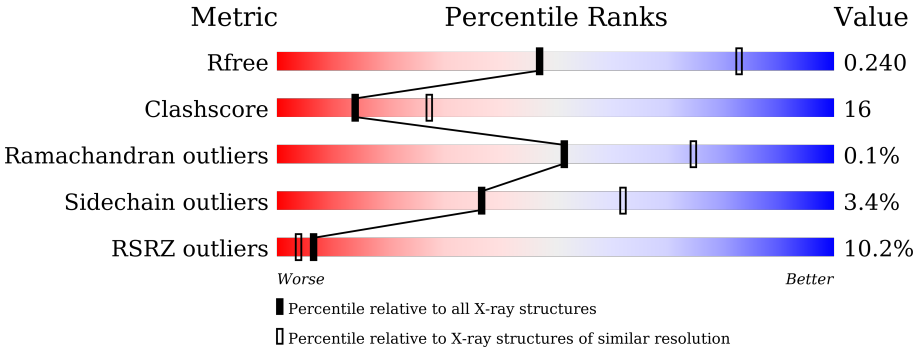
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.85 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	845	6%, 74%, 23%, • •
1	C	845	9%, 70%, 25%, • •
2	B	79	16%, 72%, 24%, •
2	D	79	46%, 54%, 41%, • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AMP	C	1102	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14508 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 SidE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	828	6606	4164	1153	1267	6	16	0	0	0
1	C	824	6578	4149	1149	1258	6	16	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MSE	-	initiating methionine	UNP Q6RCR1
A	1058	LEU	-	expression tag	UNP Q6RCR1
A	1059	GLU	-	expression tag	UNP Q6RCR1
A	1060	HIS	-	expression tag	UNP Q6RCR1
A	1061	HIS	-	expression tag	UNP Q6RCR1
A	1062	HIS	-	expression tag	UNP Q6RCR1
A	1063	HIS	-	expression tag	UNP Q6RCR1
A	1064	HIS	-	expression tag	UNP Q6RCR1
A	1065	HIS	-	expression tag	UNP Q6RCR1
C	221	MSE	-	initiating methionine	UNP Q6RCR1
C	1058	LEU	-	expression tag	UNP Q6RCR1
C	1059	GLU	-	expression tag	UNP Q6RCR1
C	1060	HIS	-	expression tag	UNP Q6RCR1
C	1061	HIS	-	expression tag	UNP Q6RCR1
C	1062	HIS	-	expression tag	UNP Q6RCR1
C	1063	HIS	-	expression tag	UNP Q6RCR1
C	1064	HIS	-	expression tag	UNP Q6RCR1
C	1065	HIS	-	expression tag	UNP Q6RCR1

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	76	595	375	102	117	1	0	0	0

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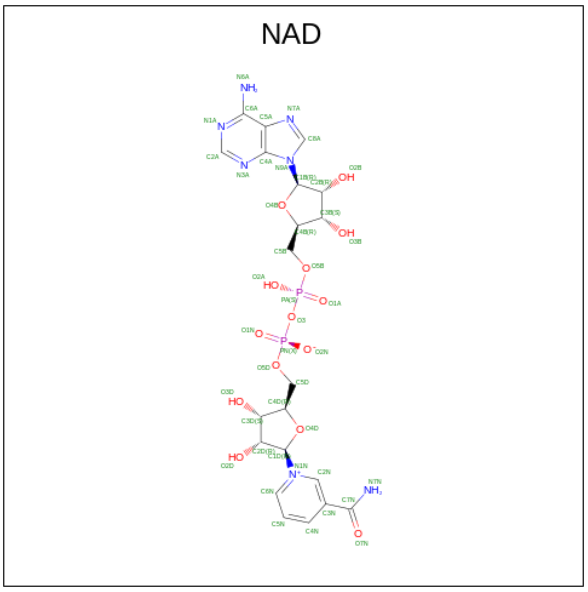
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	76	595	375	102	117	1	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

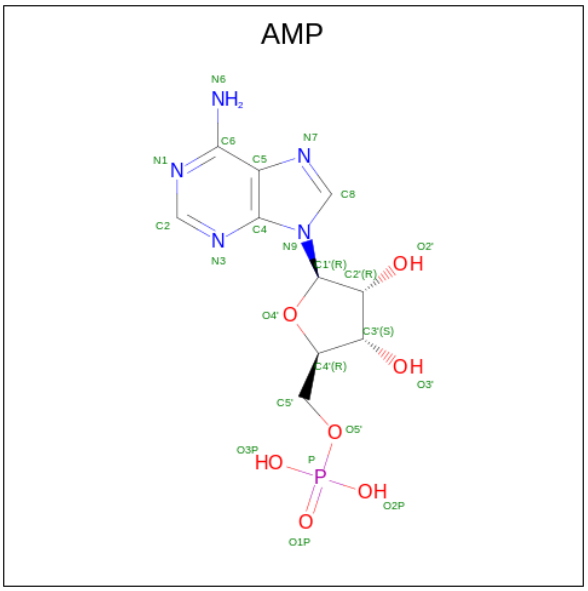
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P0CG48
B	-1	GLY	-	expression tag	UNP P0CG48
B	0	SER	-	expression tag	UNP P0CG48
B	42	ALA	ARG	engineered mutation	UNP P0CG48
D	-2	GLY	-	expression tag	UNP P0CG48
D	-1	GLY	-	expression tag	UNP P0CG48
D	0	SER	-	expression tag	UNP P0CG48
D	42	ALA	ARG	engineered mutation	UNP P0CG48

- 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
			Total	C	N	O	P		
3	A	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
3	C	1	44	21	7	14	2	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



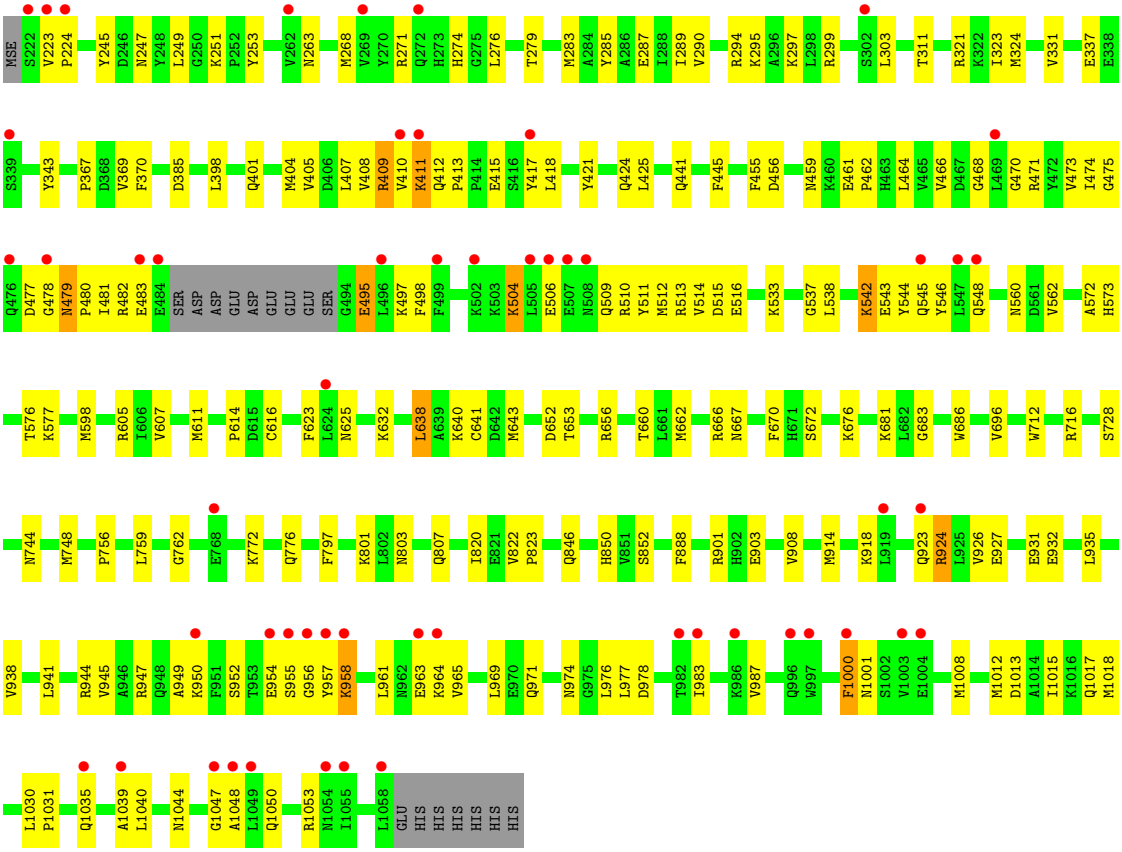
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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.

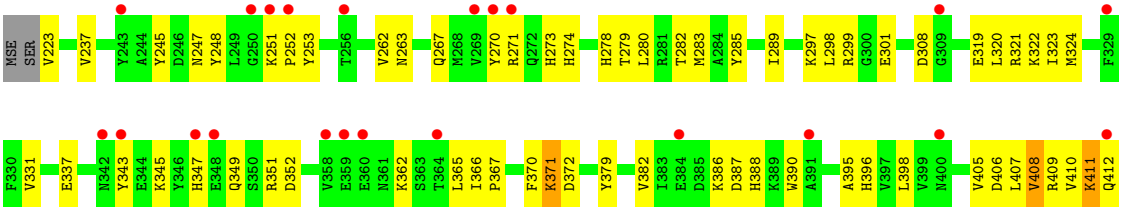
- Molecule 1: SidE

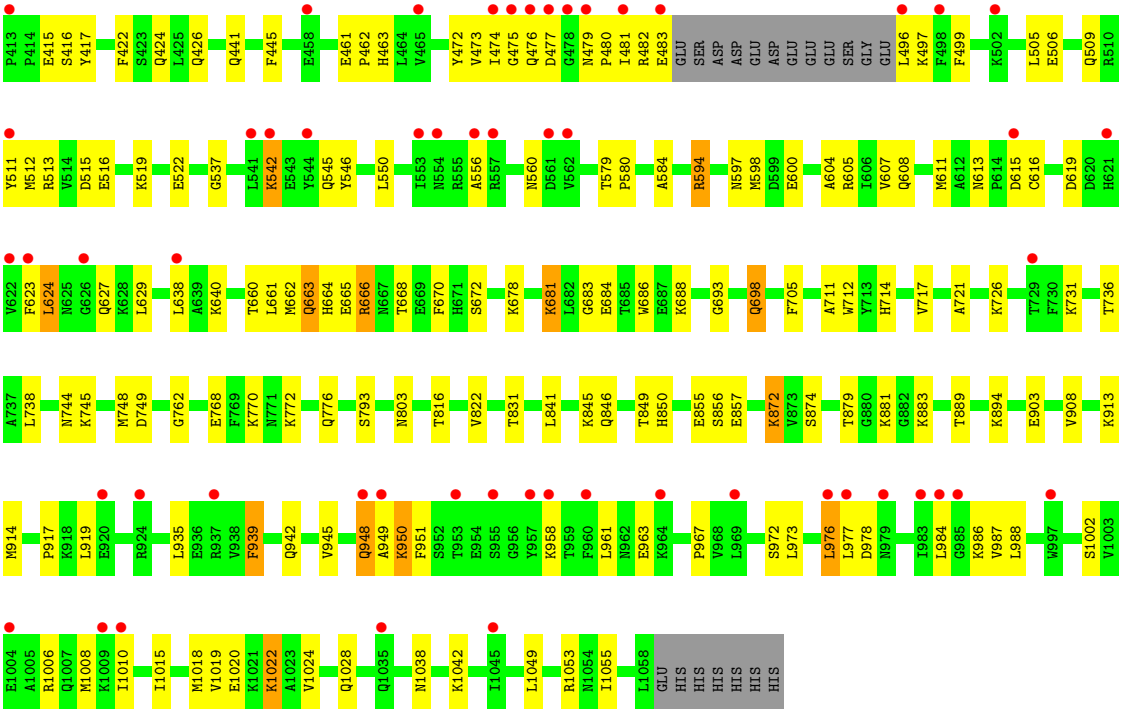
Chain A:



- Molecule 1: SidE

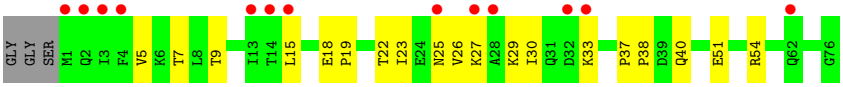
Chain C:





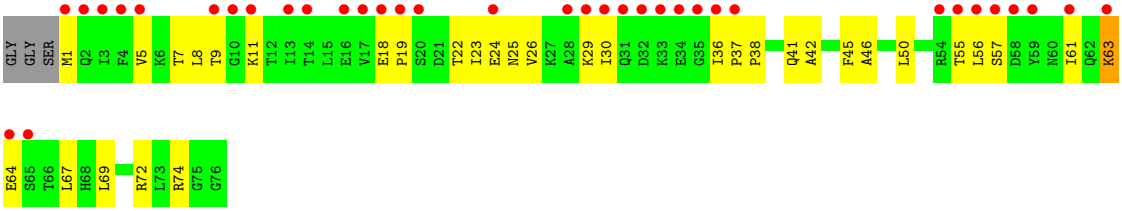
- Molecule 2: Ubiquitin

Chain B:



- Molecule 2: Ubiquitin

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.41Å 129.38Å 192.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 2.85 48.94 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.94-2.85) 99.8 (48.94-2.85)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.192 , 0.239 0.198 , 0.240	Depositor DCC
R_{free} test set	2847 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14508	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: AMP, 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	0/6720	0.58	0/9053
1	C	0.48	0/6692	0.59	0/9016
2	B	0.39	0/601	0.61	0/809
2	D	0.40	0/601	0.75	0/809
All	All	0.43	0/14614	0.60	0/19687

There are no bond length outliers.

There are no bond angle outliers.

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	6606	0	6542	184	0
1	C	6578	0	6522	235	0
2	B	595	0	621	12	0
2	D	595	0	621	33	0
3	A	44	0	26	0	0
3	C	44	0	26	3	0
4	A	23	0	12	1	0
4	C	23	0	12	7	0
All	All	14508	0	14382	454	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 16.

All (454) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LYS:HB3	1:A:417:TYR:CE2	1.38	1.58
1:C:475:GLY:CA	1:C:509:GLN:HG2	1.43	1.42
1:C:473:VAL:HG23	1:C:481:ILE:CD1	1.47	1.42
1:C:475:GLY:HA2	1:C:509:GLN:CG	1.59	1.32
1:A:411:LYS:HB2	1:A:417:TYR:CD2	1.66	1.29
1:A:411:LYS:CB	1:A:417:TYR:CE2	2.14	1.28
1:C:949:ALA:HB2	1:C:961:LEU:CD1	1.67	1.23
1:A:411:LYS:CB	1:A:417:TYR:CD2	2.24	1.20
1:A:247:ASN:O	1:A:251:LYS:HD2	1.40	1.18
1:A:954:GLU:OE1	1:A:1000:PHE:HA	1.41	1.17
1:C:473:VAL:CG2	1:C:481:ILE:HD13	1.76	1.14
1:C:949:ALA:HB2	1:C:961:LEU:HD12	1.29	1.13
1:C:949:ALA:CB	1:C:961:LEU:HD12	1.80	1.12
1:C:472:TYR:CE2	1:C:496:LEU:HD23	1.87	1.10
1:C:424:GLN:NE2	4:C:1102:AMP:HN62	1.50	1.09
1:C:1006:ARG:O	1:C:1010:ILE:HD12	1.52	1.07
1:C:973:LEU:HD13	1:C:977:LEU:HD12	1.38	1.06
1:A:411:LYS:HD3	1:A:417:TYR:CZ	1.89	1.05
1:C:424:GLN:HE21	4:C:1102:AMP:N6	1.54	1.05
1:C:473:VAL:HG23	1:C:481:ILE:HD13	1.06	1.04
1:A:412:GLN:HG3	1:A:413:PRO:HA	1.40	1.04
1:C:415:GLU:OE2	1:C:415:GLU:N	1.89	1.04
1:C:473:VAL:HG23	1:C:481:ILE:HD12	1.36	1.02
1:C:474:ILE:HG22	1:C:480:PRO:HA	1.40	1.02
1:C:474:ILE:HG22	1:C:480:PRO:CA	1.90	1.00
1:C:973:LEU:HD13	1:C:977:LEU:CD1	1.92	1.00
1:A:483:GLU:HG2	1:A:497:LYS:HB2	1.45	0.99
1:C:405:VAL:O	1:C:408:VAL:HG12	1.62	0.98
1:C:949:ALA:HB2	1:C:961:LEU:HD11	1.44	0.98
1:A:954:GLU:OE2	1:A:1000:PHE:HB3	1.61	0.98
1:C:409:ARG:HG3	1:C:410:VAL:H	1.26	0.98
1:C:411:LYS:HB3	1:C:417:TYR:CE2	2.01	0.95
1:C:474:ILE:CG2	1:C:480:PRO:HA	1.98	0.94
4:C:1102:AMP:H8	4:C:1102:AMP:H5'2	1.32	0.94
1:C:473:VAL:CG2	1:C:481:ILE:CD1	2.40	0.93
1:A:410:VAL:HG13	1:A:411:LYS:HG2	1.50	0.93
1:A:411:LYS:HB3	1:A:417:TYR:HE2	1.28	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LYS:HE2	1:A:504:LYS:HA	1.52	0.91
1:A:504:LYS:HA	1:A:504:LYS:CE	2.01	0.90
1:A:409:ARG:HG2	1:A:445:PHE:CZ	2.07	0.89
1:C:362:LYS:O	1:C:366:ILE:HG22	1.74	0.88
2:D:1:MET:HG3	2:D:63:LYS:HB3	1.57	0.87
4:C:1102:AMP:H5'2	4:C:1102:AMP:C8	2.09	0.87
1:C:542:LYS:HA	1:C:542:LYS:CE	2.03	0.87
1:C:1006:ARG:O	1:C:1010:ILE:CD1	2.23	0.87
1:A:954:GLU:HB2	1:A:957:TYR:HB2	1.57	0.86
1:C:408:VAL:CG1	1:C:441:GLN:HE22	1.88	0.86
1:C:408:VAL:HG13	1:C:441:GLN:HE22	1.41	0.85
1:C:474:ILE:HG22	1:C:479:ASN:O	1.75	0.85
1:A:411:LYS:CD	1:A:417:TYR:CZ	2.59	0.84
1:A:405:VAL:O	1:A:408:VAL:HG23	1.77	0.84
1:C:474:ILE:HG22	1:C:479:ASN:C	1.97	0.84
1:C:949:ALA:HA	1:C:958:LYS:HZ1	1.41	0.83
1:C:223:VAL:HG22	1:C:297:LYS:HD3	1.60	0.83
1:A:410:VAL:CG1	1:A:411:LYS:HG2	2.09	0.82
2:D:5:VAL:HG12	2:D:67:LEU:HB2	1.60	0.82
1:C:945:VAL:O	1:C:949:ALA:CB	2.28	0.82
1:C:474:ILE:HG22	1:C:480:PRO:N	1.94	0.81
1:C:248:TYR:O	1:C:251:LYS:HB2	1.81	0.81
1:C:386:LYS:HD2	1:C:386:LYS:O	1.81	0.80
1:A:954:GLU:CD	1:A:1000:PHE:HA	2.02	0.80
1:C:424:GLN:HE21	4:C:1102:AMP:HN62	0.80	0.79
1:A:274:HIS:HB3	1:A:331:VAL:HG11	1.64	0.78
1:C:475:GLY:CA	1:C:509:GLN:CG	2.37	0.77
1:C:409:ARG:HG3	1:C:410:VAL:N	1.99	0.77
1:C:542:LYS:HA	1:C:542:LYS:HE2	1.64	0.77
1:C:973:LEU:CD1	1:C:977:LEU:CD1	2.61	0.77
2:D:7:THR:HG22	2:D:9:THR:H	1.49	0.77
1:C:973:LEU:CD1	1:C:977:LEU:HD11	2.14	0.77
1:C:613:ASN:HD21	1:C:615:ASP:HB2	1.49	0.76
1:C:408:VAL:CG1	1:C:441:GLN:NE2	2.48	0.76
1:C:475:GLY:HA3	1:C:509:GLN:HG2	1.62	0.76
1:A:482:ARG:HG3	1:A:495:GLU:H	1.49	0.76
1:C:762:GLY:H	3:C:1101:NAD:H72N	1.34	0.76
1:A:641:CYS:HB2	1:A:643:MSE:HE3	1.67	0.76
1:C:279:THR:HG22	1:C:283:MSE:HE2	1.65	0.75
1:C:472:TYR:CZ	1:C:496:LEU:HD23	2.21	0.75
1:C:474:ILE:N	1:C:481:ILE:HD12	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:ARG:HA	1:C:1053:ARG:HA	1.68	0.75
1:C:366:ILE:HG13	1:C:367:PRO:HA	1.69	0.75
1:C:409:ARG:HB3	1:C:445:PHE:CE2	2.22	0.74
1:A:274:HIS:ND1	1:A:337:GLU:OE2	2.20	0.74
1:A:475:GLY:HA2	1:A:509:GLN:HG2	1.70	0.74
2:D:19:PRO:HB3	2:D:57:SER:HB2	1.69	0.74
1:C:850:HIS:ND1	1:C:856:SER:HA	2.03	0.73
1:A:744:ASN:O	1:A:748:MSE:HG3	1.88	0.72
1:A:409:ARG:HG2	1:A:445:PHE:HZ	1.55	0.71
1:C:473:VAL:C	1:C:481:ILE:HD12	2.10	0.71
1:C:949:ALA:CA	1:C:958:LYS:HZ1	2.03	0.71
1:C:945:VAL:O	1:C:949:ALA:HB3	1.92	0.70
1:A:404:MSE:O	1:A:407:LEU:HB2	1.91	0.70
1:A:1053:ARG:HH11	1:C:1055:ILE:HB	1.56	0.69
1:C:472:TYR:CE2	1:C:496:LEU:CD2	2.73	0.69
1:C:409:ARG:HB3	1:C:445:PHE:CZ	2.27	0.69
1:C:475:GLY:HA2	1:C:509:GLN:HG2	0.70	0.69
1:A:478:GLY:C	1:A:479:ASN:ND2	2.45	0.69
1:C:505:LEU:HD22	1:C:506:GLU:HG2	1.73	0.69
2:B:7:THR:HG22	2:B:9:THR:H	1.59	0.69
1:C:879:THR:HG21	1:C:883:LYS:HE2	1.75	0.69
2:D:22:THR:HA	2:D:55:THR:HA	1.75	0.68
1:A:513:ARG:HB2	1:A:515:ASP:OD1	1.93	0.68
1:A:954:GLU:OE2	1:A:1000:PHE:CB	2.39	0.68
2:D:23:ILE:HD13	2:D:50:LEU:HB3	1.74	0.68
1:C:949:ALA:CB	1:C:961:LEU:CD1	2.48	0.68
2:D:45:PHE:HB2	2:D:67:LEU:HD22	1.76	0.67
1:C:474:ILE:CG2	1:C:480:PRO:CA	2.66	0.67
1:C:664:HIS:O	1:C:664:HIS:ND1	2.27	0.67
1:C:973:LEU:HD11	1:C:977:LEU:HD11	1.75	0.67
1:C:411:LYS:HB3	1:C:417:TYR:CD2	2.29	0.67
1:C:949:ALA:HB1	1:C:961:LEU:HD12	1.72	0.67
1:A:411:LYS:HD3	1:A:417:TYR:OH	1.95	0.66
1:A:477:ASP:OD2	1:A:479:ASN:ND2	2.28	0.65
1:A:1030:LEU:HD13	1:C:919:LEU:HD21	1.78	0.65
1:C:917:PRO:HB2	1:C:919:LEU:HG	1.76	0.65
1:C:474:ILE:CG2	1:C:479:ASN:O	2.45	0.65
1:A:424:GLN:HE21	4:A:1102:AMP:HN62	1.45	0.64
1:C:408:VAL:O	1:C:408:VAL:HG22	1.95	0.64
1:C:366:ILE:HD11	1:C:372:ASP:HA	1.77	0.64
1:C:482:ARG:HD3	1:C:496:LEU:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:ARG:NH2	1:C:600:GLU:OE2	2.30	0.64
1:A:224:PRO:O	1:A:294:ARG:NH2	2.29	0.63
1:A:455:PHE:O	1:A:533:LYS:HG2	1.97	0.63
1:C:945:VAL:O	1:C:949:ALA:HB2	1.97	0.63
2:D:30:ILE:HG22	2:D:36:ILE:HG21	1.79	0.63
1:C:472:TYR:CD2	1:C:496:LEU:HD23	2.31	0.63
1:C:745:LYS:NZ	1:C:749:ASP:OD2	2.31	0.63
1:C:351:ARG:NH1	1:C:352:ASP:OD1	2.32	0.63
1:C:424:GLN:NE2	4:C:1102:AMP:N6	2.26	0.63
1:C:319:GLU:O	1:C:323:ILE:HG12	1.98	0.62
1:A:947:ARG:O	1:A:950:LYS:HG2	1.98	0.62
1:A:977:LEU:HD21	1:C:598:MSE:HE1	1.82	0.62
1:A:776:GLN:HB3	1:A:803:ASN:HB3	1.82	0.62
1:A:1013:ASP:O	1:A:1017:GLN:HG3	1.99	0.61
1:C:472:TYR:CD2	1:C:496:LEU:CD2	2.83	0.61
2:D:63:LYS:O	2:D:64:GLU:HB2	2.00	0.61
2:D:41:GLN:HB3	2:D:69:LEU:HD11	1.83	0.61
1:A:504:LYS:HE2	1:A:504:LYS:CA	2.26	0.61
2:B:22:THR:HG23	2:B:25:ASN:H	1.65	0.61
1:C:627:GLN:HG3	1:C:913:LYS:HB2	1.81	0.61
1:A:598:MSE:HE3	1:A:908:VAL:HG21	1.83	0.60
1:C:512:MSE:HG3	1:C:516:GLU:HG3	1.83	0.60
1:C:343:TYR:HE2	1:C:388:HIS:NE2	2.00	0.60
1:A:506:GLU:HB2	1:A:509:GLN:OE1	2.01	0.60
1:C:411:LYS:CB	1:C:417:TYR:CD2	2.85	0.60
1:C:988:LEU:HD11	1:C:1020:GLU:HB2	1.84	0.60
1:A:483:GLU:CG	1:A:497:LYS:HB2	2.27	0.59
1:A:935:LEU:HD11	1:A:976:LEU:HB3	1.84	0.59
1:C:515:ASP:O	1:C:519:LYS:HG3	2.02	0.59
1:A:290:VAL:O	1:A:294:ARG:HG3	2.03	0.59
1:A:411:LYS:HD3	1:A:417:TYR:CE2	2.38	0.59
1:A:407:LEU:O	1:A:410:VAL:HG12	2.03	0.59
1:A:483:GLU:HG2	1:A:497:LYS:CB	2.27	0.59
1:C:762:GLY:N	3:C:1101:NAD:H72N	2.01	0.59
1:C:973:LEU:O	1:C:977:LEU:HD12	2.03	0.59
1:A:632:LYS:O	1:A:632:LYS:HG3	2.02	0.58
1:A:473:VAL:HG23	1:A:481:ILE:HD12	1.84	0.58
1:C:542:LYS:HB2	1:C:545:GLN:OE1	2.03	0.58
1:C:409:ARG:CG	1:C:410:VAL:H	2.09	0.58
1:C:248:TYR:O	1:C:271:ARG:NH2	2.36	0.58
1:C:660:THR:O	1:C:663:GLN:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:TYR:O	1:A:289:ILE:HG13	2.04	0.57
1:A:945:VAL:O	1:A:949:ALA:HB2	2.05	0.57
1:A:474:ILE:HD13	1:A:510:ARG:HH21	1.70	0.57
1:A:223:VAL:HG22	1:A:297:LYS:HD3	1.87	0.57
1:C:386:LYS:HD2	1:C:386:LYS:C	2.25	0.57
1:C:672:SER:HB2	1:C:712:TRP:HA	1.87	0.57
1:A:409:ARG:HB3	1:A:445:PHE:CE2	2.39	0.57
1:A:625:ASN:HB2	1:A:914:MSE:HG2	1.86	0.57
1:A:672:SER:HB2	1:A:712:TRP:HA	1.87	0.57
1:C:665:GLU:OE1	1:C:731:LYS:NZ	2.36	0.57
1:C:881:LYS:HB2	1:C:883:LYS:NZ	2.20	0.57
1:A:483:GLU:OE1	1:A:483:GLU:HA	2.05	0.56
1:A:605:ARG:HH21	1:A:605:ARG:HG3	1.69	0.56
1:C:939:PHE:HD1	1:C:942:GLN:OE1	1.89	0.56
1:A:456:ASP:HA	1:A:533:LYS:HG2	1.87	0.56
1:C:1049:LEU:O	1:C:1053:ARG:HG3	2.06	0.56
1:A:923:GLN:HA	1:A:926:VAL:HG12	1.87	0.56
1:A:954:GLU:O	1:A:956:GLY:HA2	2.06	0.55
2:D:46:ALA:HB1	1:C:881:LYS:HE3	1.88	0.55
1:C:662:MSE:HG3	1:C:686:TRP:CD1	2.42	0.55
1:A:653:THR:HG22	1:A:656:ARG:HH21	1.71	0.55
1:C:367:PRO:HA	1:C:370:PHE:O	2.06	0.55
1:C:613:ASN:ND2	1:C:615:ASP:HB2	2.20	0.55
1:C:976:LEU:HD21	1:C:1019:VAL:HG22	1.88	0.55
1:A:411:LYS:HD2	1:A:417:TYR:CE1	2.42	0.55
1:A:954:GLU:CB	1:A:957:TYR:HB2	2.32	0.55
1:C:776:GLN:HB3	1:C:803:ASN:HB3	1.89	0.55
1:C:984:LEU:HA	1:C:987:VAL:HG12	1.89	0.55
1:A:343:TYR:OH	1:A:385:ASP:OD2	2.23	0.54
1:A:247:ASN:O	1:A:251:LYS:CD	2.34	0.54
2:D:56:LEU:CD1	2:D:61:ILE:HB	2.37	0.54
1:C:717:VAL:HG13	1:C:736:THR:HG23	1.88	0.54
1:A:1015:ILE:HA	1:A:1018:MSE:HE3	1.89	0.54
1:A:1031:PRO:O	1:A:1035:GLN:HG3	2.08	0.54
2:D:22:THR:HG23	2:D:25:ASN:H	1.72	0.54
1:A:251:LYS:O	1:A:271:ARG:NH1	2.41	0.54
1:A:482:ARG:HG3	1:A:495:GLU:N	2.19	0.54
1:C:616:CYS:HB2	1:C:623:PHE:O	2.07	0.54
1:A:662:MSE:HG3	1:A:686:TRP:CG	2.43	0.53
1:C:542:LYS:HE2	1:C:542:LYS:CA	2.36	0.53
1:A:974:ASN:HA	1:A:977:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:GLU:HG2	2:B:19:PRO:HD2	1.90	0.53
1:C:598:MSE:HG3	1:C:908:VAL:HG21	1.89	0.53
1:A:470:GLY:HA3	1:A:498:PHE:CE1	2.44	0.53
1:C:279:THR:O	1:C:283:MSE:HG3	2.08	0.53
1:C:280:LEU:HA	1:C:283:MSE:HE3	1.90	0.53
1:A:459:ASN:O	1:A:514:VAL:HG23	2.09	0.52
1:A:963:GLU:HG3	1:A:964:LYS:HD2	1.91	0.52
2:B:22:THR:CG2	2:B:25:ASN:H	2.22	0.52
1:C:278:HIS:O	1:C:282:THR:HG23	2.09	0.52
1:C:343:TYR:CE2	1:C:388:HIS:NE2	2.76	0.52
1:C:939:PHE:HA	1:C:942:GLN:HG2	1.91	0.52
1:C:345:LYS:O	1:C:349:GLN:HG3	2.10	0.52
1:A:846:GLN:HG3	1:A:850:HIS:NE2	2.24	0.52
1:C:945:VAL:HG13	1:C:961:LEU:HD11	1.90	0.52
2:B:5:VAL:HG21	2:B:30:ILE:HD11	1.91	0.52
1:A:287:GLU:HB2	1:A:324:MSE:HE1	1.91	0.52
1:A:983:ILE:O	1:A:987:VAL:HG13	2.09	0.52
1:C:405:VAL:O	1:C:408:VAL:CG1	2.47	0.52
1:A:418:LEU:HD12	1:A:418:LEU:O	2.09	0.52
2:D:72:ARG:NH2	1:C:855:GLU:OE1	2.38	0.52
1:C:505:LEU:HB3	1:C:509:GLN:OE1	2.09	0.51
1:C:948:GLN:HB3	1:C:1008:MSE:HE1	1.92	0.51
1:C:320:LEU:O	1:C:324:MSE:HG3	2.10	0.51
1:C:935:LEU:HD21	1:C:977:LEU:HG	1.92	0.51
1:C:323:ILE:HD12	1:C:395:ALA:HA	1.91	0.51
1:C:223:VAL:HG21	1:C:298:LEU:HG	1.92	0.51
1:C:280:LEU:HD23	1:C:283:MSE:HE3	1.92	0.51
1:C:711:ALA:HA	1:C:714:HIS:CE1	2.45	0.51
2:D:8:LEU:HD11	1:C:822:VAL:HG22	1.92	0.51
2:D:22:THR:HG22	2:D:25:ASN:OD1	2.10	0.51
1:C:462:PRO:HA	1:C:513:ARG:HA	1.93	0.51
1:A:411:LYS:CD	1:A:417:TYR:CE1	2.94	0.51
1:A:641:CYS:CB	1:A:643:MSE:HE3	2.36	0.51
1:A:820:ILE:O	1:A:823:PRO:HD2	2.11	0.51
1:A:245:TYR:OH	1:A:560:ASN:OD1	2.24	0.50
1:A:412:GLN:HG3	1:A:413:PRO:CA	2.28	0.50
1:A:822:VAL:HB	1:A:823:PRO:HD3	1.94	0.50
1:A:249:LEU:O	1:A:271:ARG:HD2	2.11	0.50
2:D:56:LEU:HD11	2:D:61:ILE:HB	1.91	0.50
1:C:262:VAL:HG12	1:C:263:ASN:H	1.76	0.50
1:C:237:VAL:HG21	1:C:324:MSE:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:ARG:HB3	1:C:445:PHE:HE2	1.75	0.50
1:C:474:ILE:HA	1:C:480:PRO:HA	1.93	0.50
1:A:479:ASN:ND2	1:A:479:ASN:N	2.59	0.50
1:A:969:LEU:HD11	1:A:1012:MSE:HE1	1.94	0.50
1:A:797:PHE:CE1	1:A:801:LYS:HD2	2.46	0.50
1:C:285:TYR:O	1:C:289:ILE:HG13	2.11	0.50
1:A:938:VAL:HG22	1:A:1015:ILE:HD12	1.92	0.50
1:A:956:GLY:O	1:A:1000:PHE:HE1	1.94	0.50
1:C:416:SER:OG	1:C:463:HIS:ND1	2.37	0.49
1:C:607:VAL:O	1:C:611:MSE:HG2	2.11	0.49
1:A:263:ASN:OD1	1:A:268:MSE:HG2	2.11	0.49
1:A:473:VAL:HG12	1:A:511:TYR:HD1	1.76	0.49
1:C:237:VAL:HG23	1:C:321:ARG:HG3	1.93	0.49
1:A:367:PRO:HA	1:A:370:PHE:O	2.12	0.49
1:A:949:ALA:O	1:A:958:LYS:HD3	2.13	0.49
1:A:961:LEU:HA	1:A:965:VAL:HG22	1.93	0.49
1:C:846:GLN:HG3	1:C:850:HIS:NE2	2.26	0.49
2:D:25:ASN:O	2:D:29:LYS:HD3	2.12	0.49
1:C:1024:VAL:HA	1:C:1028:GLN:HE21	1.76	0.49
1:C:252:PRO:HG3	1:C:270:TYR:CE1	2.47	0.49
1:C:537:GLY:HA2	1:C:546:TYR:CZ	2.47	0.49
1:C:1010:ILE:HD12	1:C:1010:ILE:H	1.78	0.49
1:A:478:GLY:C	1:A:479:ASN:HD22	2.16	0.49
1:A:401:GLN:O	1:A:405:VAL:HG23	2.12	0.49
1:A:545:GLN:HA	1:A:548:GLN:HB2	1.95	0.49
1:C:1002:SER:O	1:C:1006:ARG:HG2	2.13	0.49
1:A:954:GLU:OE2	1:A:1000:PHE:CA	2.61	0.49
1:C:624:LEU:HD23	1:C:914:MSE:SE	2.63	0.49
1:C:772:LYS:O	1:C:776:GLN:HG3	2.13	0.49
1:C:976:LEU:HD13	1:C:984:LEU:HD21	1.94	0.48
1:A:573:HIS:CE1	1:A:577:LYS:HE2	2.48	0.48
1:C:274:HIS:HB3	1:C:331:VAL:HG21	1.95	0.48
1:C:624:LEU:CD2	1:C:914:MSE:SE	3.12	0.48
1:A:666:ARG:HA	1:A:683:GLY:HA3	1.95	0.48
2:D:19:PRO:CB	2:D:57:SER:HB2	2.41	0.48
2:D:22:THR:CG2	2:D:24:GLU:HB2	2.44	0.48
2:B:15:LEU:HD23	2:B:33:LYS:NZ	2.29	0.48
1:C:366:ILE:HG13	1:C:367:PRO:CA	2.41	0.48
1:A:409:ARG:CG	1:A:445:PHE:CZ	2.90	0.48
1:C:666:ARG:HA	1:C:683:GLY:HA3	1.95	0.48
1:C:745:LYS:HA	1:C:748:MSE:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:ASP:HB3	1:A:696:VAL:HG11	1.95	0.47
1:A:418:LEU:HD23	1:A:455:PHE:CD2	2.49	0.47
1:C:407:LEU:C	1:C:409:ARG:H	2.15	0.47
1:C:475:GLY:HA3	1:C:509:GLN:HE21	1.79	0.47
1:A:410:VAL:CG1	1:A:411:LYS:CE	2.91	0.47
1:A:479:ASN:N	1:A:479:ASN:HD22	2.12	0.47
1:A:978:ASP:OD1	1:C:605:ARG:NH2	2.46	0.47
1:A:1040:LEU:HG	1:A:1048:ALA:CB	2.45	0.47
1:A:542:LYS:HE2	1:A:542:LYS:HA	1.97	0.47
2:B:25:ASN:O	2:B:29:LYS:HG3	2.14	0.47
1:C:497:LYS:HG3	1:C:499:PHE:CE1	2.49	0.47
1:A:954:GLU:O	1:A:957:TYR:N	2.47	0.47
1:A:1040:LEU:HG	1:A:1048:ALA:HB2	1.97	0.47
1:C:857:GLU:OE1	3:C:1101:NAD:O2D	2.31	0.47
1:A:415:GLU:H	1:A:415:GLU:CD	2.17	0.47
2:D:36:ILE:HG23	2:D:41:GLN:NE2	2.29	0.47
1:A:515:ASP:OD1	1:A:516:GLU:N	2.48	0.47
1:C:279:THR:O	1:C:282:THR:OG1	2.22	0.47
1:A:482:ARG:CG	1:A:495:GLU:H	2.21	0.47
1:A:410:VAL:CG1	1:A:411:LYS:HE2	2.45	0.46
1:C:474:ILE:HG23	1:C:480:PRO:HA	1.93	0.46
1:C:948:GLN:HG3	1:C:948:GLN:O	2.15	0.46
1:A:468:GLY:O	1:A:498:PHE:HZ	1.99	0.46
1:A:542:LYS:HA	1:A:542:LYS:CE	2.46	0.46
1:C:881:LYS:HB2	1:C:883:LYS:HZ2	1.78	0.46
1:A:407:LEU:HD23	1:A:407:LEU:HA	1.80	0.46
1:A:957:TYR:O	1:A:961:LEU:HG	2.15	0.46
1:C:351:ARG:HG2	1:C:351:ARG:HH11	1.80	0.46
2:B:23:ILE:O	2:B:27:LYS:HG3	2.15	0.46
1:C:390:TRP:CZ2	4:C:1102:AMP:H2'	2.51	0.46
1:C:461:GLU:HG3	1:C:462:PRO:HD2	1.98	0.46
1:A:640:LYS:NZ	1:A:903:GLU:OE2	2.48	0.46
1:C:343:TYR:HE1	1:C:347:HIS:CE1	2.34	0.46
1:C:474:ILE:HD12	1:C:475:GLY:N	2.30	0.46
1:A:249:LEU:O	1:A:271:ARG:CD	2.63	0.46
1:A:756:PRO:HG2	1:A:759:LEU:HD21	1.97	0.46
1:A:954:GLU:HB2	1:A:957:TYR:CB	2.35	0.46
1:C:410:VAL:HG13	1:C:411:LYS:N	2.30	0.46
1:C:816:THR:O	1:C:857:GLU:HA	2.16	0.46
1:A:474:ILE:N	1:A:510:ARG:O	2.41	0.46
1:C:744:ASN:HB3	1:C:748:MSE:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:748:MSE:HA	1:C:845:LYS:HD2	1.98	0.46
2:D:1:MET:HE1	2:D:56:LEU:HD21	1.98	0.46
1:C:473:VAL:HG12	1:C:511:TYR:HD1	1.81	0.46
1:A:480:PRO:HB3	1:A:512:MSE:HE3	1.98	0.45
1:C:604:ALA:O	1:C:608:GLN:HG3	2.16	0.45
1:A:954:GLU:CD	1:A:1000:PHE:CA	2.82	0.45
1:C:949:ALA:C	1:C:958:LYS:HZ1	2.20	0.45
1:A:407:LEU:CD1	1:A:421:TYR:OH	2.64	0.45
1:C:693:GLY:O	1:C:698:GLN:HG2	2.16	0.45
1:C:945:VAL:HG13	1:C:961:LEU:CD1	2.47	0.45
1:A:762:GLY:HA3	1:A:823:PRO:HB3	1.99	0.45
2:B:22:THR:O	2:B:26:VAL:HG23	2.17	0.45
1:C:343:TYR:HE2	1:C:388:HIS:CE1	2.34	0.45
1:C:474:ILE:CA	1:C:481:ILE:HD12	2.46	0.45
1:A:405:VAL:O	1:A:408:VAL:CG2	2.59	0.45
1:C:422:PHE:O	1:C:426:GLN:HB2	2.16	0.45
1:A:417:TYR:CD1	1:A:466:VAL:HG21	2.51	0.45
1:C:474:ILE:CB	1:C:479:ASN:O	2.65	0.45
1:A:473:VAL:HG23	1:A:481:ILE:CD1	2.47	0.45
2:B:37:PRO:HG2	2:B:40:GLN:HG3	1.99	0.45
1:C:629:LEU:HD11	1:C:914:MSE:HE1	1.99	0.45
1:C:768:GLU:CD	1:C:768:GLU:H	2.18	0.45
1:A:944:ARG:HG2	1:A:1008:MSE:HE1	1.98	0.44
1:C:770:LYS:HD2	1:C:831:THR:OG1	2.18	0.44
1:A:245:TYR:HA	1:A:249:LEU:HB2	1.99	0.44
1:C:872:LYS:HE2	1:C:889:THR:OG1	2.17	0.44
1:A:924:ARG:HA	1:A:927:GLU:HG2	2.00	0.44
1:C:273:HIS:HB2	1:C:337:GLU:OE1	2.17	0.44
1:A:279:THR:O	1:A:283:MSE:HG3	2.17	0.44
1:A:676:LYS:HD3	1:A:676:LYS:N	2.32	0.44
1:A:772:LYS:O	1:A:776:GLN:HG3	2.18	0.44
1:C:245:TYR:CE1	1:C:560:ASN:HA	2.53	0.44
1:C:472:TYR:CD2	1:C:496:LEU:HD21	2.53	0.44
1:C:950:LYS:HD3	1:C:950:LYS:HA	1.59	0.44
1:A:932:GLU:OE2	1:C:913:LYS:HD3	2.17	0.44
1:C:482:ARG:HD2	1:C:483:GLU:N	2.32	0.44
1:A:323:ILE:HD13	1:A:398:LEU:HD12	2.00	0.44
1:A:409:ARG:H	1:A:409:ARG:HG3	1.53	0.44
1:C:607:VAL:HG22	1:C:738:LEU:HD23	1.99	0.44
1:A:614:PRO:HG2	1:A:660:THR:HG22	2.00	0.44
1:C:480:PRO:HB3	1:C:512:MSE:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:MSE:HG3	1:A:686:TRP:CD1	2.53	0.43
1:C:1022:LYS:N	1:C:1022:LYS:HD2	2.33	0.43
1:A:515:ASP:OD1	1:A:516:GLU:HG3	2.18	0.43
1:A:607:VAL:O	1:A:611:MSE:HG2	2.18	0.43
1:A:616:CYS:HB2	1:A:623:PHE:O	2.19	0.43
2:D:42:ALA:O	2:D:69:LEU:HD12	2.18	0.43
1:C:522:GLU:H	1:C:522:GLU:HG3	1.61	0.43
1:C:537:GLY:HA2	1:C:546:TYR:CE2	2.53	0.43
2:B:37:PRO:HA	2:B:38:PRO:HD3	1.93	0.43
1:C:1018:MSE:HE2	1:C:1018:MSE:HB3	1.93	0.43
1:A:474:ILE:HD12	1:A:512:MSE:HA	2.00	0.43
1:A:497:LYS:HD2	1:A:498:PHE:H	1.82	0.43
1:A:941:LEU:HD12	1:A:941:LEU:HA	1.81	0.43
1:A:955:SER:HA	1:A:956:GLY:HA2	1.72	0.43
1:A:1039:ALA:O	1:A:1044:ASN:N	2.52	0.43
1:A:249:LEU:HA	1:A:271:ARG:HD3	1.99	0.43
2:B:23:ILE:HG12	2:B:54:ARG:O	2.18	0.43
1:C:371:LYS:HA	1:C:371:LYS:HD3	1.61	0.43
1:C:411:LYS:HB2	1:C:417:TYR:CD2	2.54	0.43
1:C:963:GLU:O	1:C:967:PRO:HG2	2.18	0.43
1:A:462:PRO:HA	1:A:513:ARG:HA	2.01	0.43
1:A:638:LEU:HD12	1:A:638:LEU:HA	1.91	0.42
1:A:276:LEU:HD11	1:A:562:VAL:HG22	2.01	0.42
1:A:295:LYS:O	1:A:299:ARG:HG3	2.20	0.42
2:D:37:PRO:HA	2:D:38:PRO:HD3	1.93	0.42
1:C:267:GLN:HB3	1:C:556:ALA:CB	2.48	0.42
1:C:638:LEU:HD13	1:C:721:ALA:HA	2.01	0.42
1:A:1047:GLY:HA2	1:A:1050:GLN:HB3	2.01	0.42
1:C:365:LEU:HD23	1:C:365:LEU:HA	1.85	0.42
1:C:579:THR:OG1	1:C:580:PRO:HD3	2.18	0.42
1:A:413:PRO:HB3	1:A:461:GLU:OE1	2.19	0.42
1:A:667:ASN:HD22	1:A:681:LYS:NZ	2.18	0.42
1:A:716:ARG:NH1	1:A:728:SER:OG	2.46	0.42
1:C:505:LEU:HD23	1:C:505:LEU:HA	1.62	0.42
1:C:668:THR:HG23	1:C:731:LYS:HD3	2.01	0.42
2:D:74:ARG:O	1:C:849:THR:HG23	2.20	0.42
1:A:538:LEU:HD23	1:A:538:LEU:HA	1.91	0.42
1:C:986:LYS:HA	1:C:986:LYS:HD3	1.53	0.42
1:A:407:LEU:HD13	1:A:421:TYR:OH	2.20	0.42
2:D:11:LYS:HE3	2:D:11:LYS:HB3	1.90	0.42
2:D:41:GLN:CB	2:D:69:LEU:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ASP:O	1:C:409:ARG:HG2	2.19	0.42
1:C:1038:ASN:O	1:C:1042:LYS:HG3	2.20	0.42
1:A:410:VAL:HG13	1:A:411:LYS:HE2	2.02	0.41
1:C:474:ILE:C	1:C:481:ILE:HD11	2.39	0.41
1:A:303:LEU:HB2	1:A:311:THR:HG21	2.02	0.41
2:D:36:ILE:HG23	2:D:36:ILE:O	2.20	0.41
1:C:972:SER:O	1:C:976:LEU:HD22	2.21	0.41
1:C:550:LEU:HD23	1:C:550:LEU:HA	1.91	0.41
1:C:664:HIS:ND1	1:C:664:HIS:C	2.72	0.41
1:A:572:ALA:O	1:A:576:THR:HG23	2.21	0.41
1:A:971:GLN:HB3	1:A:987:VAL:HG11	2.02	0.41
2:D:7:THR:HG22	2:D:8:LEU:N	2.35	0.41
2:D:26:VAL:O	2:D:30:ILE:HG13	2.21	0.41
1:C:407:LEU:C	1:C:409:ARG:N	2.74	0.41
1:C:841:LEU:HD13	1:C:894:LYS:HB2	2.03	0.41
1:A:497:LYS:HD2	1:A:497:LYS:HA	1.51	0.41
1:C:247:ASN:C	1:C:248:TYR:CD2	2.93	0.41
1:A:542:LYS:HD3	1:A:543:GLU:H	1.86	0.41
2:D:74:ARG:HG2	1:C:705:PHE:HB2	2.02	0.41
1:C:299:ARG:NH1	1:C:301:GLU:OE2	2.54	0.41
1:A:473:VAL:HG12	1:A:511:TYR:CD1	2.56	0.41
1:C:382:VAL:HG22	1:C:396:HIS:CD2	2.56	0.41
1:A:954:GLU:OE2	1:A:1000:PHE:HA	2.20	0.41
1:C:366:ILE:HA	1:C:367:PRO:HA	1.76	0.41
1:C:398:LEU:HD23	1:C:398:LEU:HA	1.91	0.41
1:C:594:ARG:HH12	1:C:597:ASN:ND2	2.19	0.41
1:A:398:LEU:HD23	1:A:398:LEU:HA	1.86	0.40
1:A:464:LEU:HD13	1:A:471:ARG:NH1	2.35	0.40
1:C:481:ILE:HG21	1:C:499:PHE:HZ	1.85	0.40
1:C:584:ALA:HA	1:C:793:SER:HB3	2.02	0.40
1:C:883:LYS:H	1:C:883:LYS:HG3	1.75	0.40
1:A:807:GLN:NE2	1:A:807:GLN:HA	2.36	0.40
1:C:322:LYS:HD2	1:C:379:TYR:CE2	2.56	0.40
1:C:367:PRO:O	1:C:370:PHE:O	2.40	0.40
1:A:605:ARG:NH2	1:C:978:ASP:OD1	2.54	0.40
1:A:797:PHE:CZ	1:A:801:LYS:HD2	2.56	0.40
1:A:888:PHE:CD1	1:A:888:PHE:N	2.89	0.40
2:D:7:THR:CG2	2:D:8:LEU:N	2.84	0.40
1:C:681:LYS:HE3	1:C:684:GLU:OE2	2.22	0.40
1:C:744:ASN:O	1:C:748:MSE:HG3	2.21	0.40
1:C:903:GLU:O	1:C:903:GLU:HG2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:THR:HG23	2:D:24:GLU:HB2	2.04	0.40
1:C:640:LYS:NZ	1:C:903:GLU:OE2	2.54	0.40
1:A:321:ARG:HD2	1:A:369:VAL:HG13	2.03	0.40
1:A:537:GLY:HA2	1:A:546:TYR:CZ	2.57	0.40
1:A:772:LYS:HE3	1:A:772:LYS:HB2	1.71	0.40
1:C:984:LEU:HD23	1:C:1019:VAL:HG13	2.03	0.40
1:C:1015:ILE:HA	1:C:1018:MSE:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	824/845 (98%)	805 (98%)	19 (2%)	0	100	100
1	C	820/845 (97%)	794 (97%)	25 (3%)	1 (0%)	51	75
2	B	74/79 (94%)	72 (97%)	2 (3%)	0	100	100
2	D	74/79 (94%)	72 (97%)	2 (3%)	0	100	100
All	All	1792/1848 (97%)	1743 (97%)	48 (3%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	408	VAL

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	719/719 (100%)	698 (97%)	21 (3%)	42	67
1	C	716/719 (100%)	687 (96%)	29 (4%)	30	56
2	B	67/68 (98%)	66 (98%)	1 (2%)	65	82
2	D	67/68 (98%)	65 (97%)	2 (3%)	41	65
All	All	1569/1574 (100%)	1516 (97%)	53 (3%)	37	62

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	TYR
1	A	409	ARG
1	A	411	LYS
1	A	425	LEU
1	A	441	GLN
1	A	479	ASN
1	A	495	GLU
1	A	504	LYS
1	A	542	LYS
1	A	544	TYR
1	A	638	LEU
1	A	670	PHE
1	A	852	SER
1	A	901	ARG
1	A	918	LYS
1	A	924	ARG
1	A	931	GLU
1	A	952	SER
1	A	958	LYS
1	A	1000	PHE
1	A	1001	ASN
2	B	51	GLU
2	D	18	GLU
2	D	63	LYS
1	C	253	TYR
1	C	308	ASP
1	C	371	LYS
1	C	387	ASP
1	C	411	LYS
1	C	412	GLN

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Mol	Chain	Res	Type
1	C	476	GLN
1	C	477	ASP
1	C	542	LYS
1	C	594	ARG
1	C	619	ASP
1	C	624	LEU
1	C	661	LEU
1	C	663	GLN
1	C	666	ARG
1	C	670	PHE
1	C	678	LYS
1	C	681	LYS
1	C	688	LYS
1	C	698	GLN
1	C	726	LYS
1	C	872	LYS
1	C	874	SER
1	C	939	PHE
1	C	948	GLN
1	C	950	LYS
1	C	951	PHE
1	C	976	LEU
1	C	1022	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	GLN
1	A	479	ASN
1	A	625	ASN
1	A	667	ASN
1	A	915	GLN
1	A	1028	GLN
1	C	342	ASN
1	C	347	HIS
1	C	424	GLN
1	C	441	GLN
1	C	476	GLN
1	C	613	ASN
1	C	621	HIS
1	C	799	GLN
1	C	948	GLN

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Mol	Chain	Res	Type
1	C	1028	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	$\#\|Z\| > 2$
4	AMP	C	1102	-	22,25,25	1.38	2 (9%)	25,38,38	1.81	10 (40%)
3	NAD	A	1101	-	42,48,48	2.27	10 (23%)	50,73,73	1.68	10 (20%)
4	AMP	A	1102	-	22,25,25	1.57	5 (22%)	25,38,38	2.06	9 (36%)
3	NAD	C	1101	-	42,48,48	2.27	9 (21%)	50,73,73	1.94	11 (22%)

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
4	AMP	C	1102	-	-	2/6/26/26	0/3/3/3
3	NAD	A	1101	-	-	1/26/62/62	0/5/5/5
4	AMP	A	1102	-	-	0/6/26/26	0/3/3/3
3	NAD	C	1101	-	-	6/26/62/62	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	NAD	C3N-C7N	-7.20	1.39	1.50
3	A	1101	NAD	O7N-C7N	6.60	1.36	1.24
3	C	1101	NAD	C3N-C7N	-6.54	1.40	1.50
3	C	1101	NAD	O7N-C7N	6.29	1.36	1.24
3	C	1101	NAD	C2N-N1N	6.26	1.42	1.35
3	C	1101	NAD	C2A-N3A	5.04	1.40	1.32
3	A	1101	NAD	C2N-N1N	4.92	1.41	1.35
3	A	1101	NAD	C2A-N3A	4.62	1.39	1.32
3	A	1101	NAD	O4B-C1B	3.67	1.46	1.41
4	A	1102	AMP	C4-N3	-3.51	1.30	1.35
3	A	1101	NAD	O4D-C1D	3.46	1.45	1.41
3	C	1101	NAD	O4B-C1B	3.23	1.45	1.41
3	C	1101	NAD	C2A-N1A	3.23	1.39	1.33
3	A	1101	NAD	C2A-N1A	3.16	1.39	1.33
4	C	1102	AMP	C2'-C1'	-2.97	1.49	1.53
4	A	1102	AMP	C2'-C1'	-2.92	1.49	1.53
3	C	1101	NAD	O4D-C1D	2.83	1.45	1.41
3	A	1101	NAD	C6A-C5A	-2.67	1.33	1.43
3	A	1101	NAD	C5A-C4A	-2.60	1.34	1.40
3	C	1101	NAD	C5A-C4A	-2.58	1.34	1.40
3	C	1101	NAD	C6A-C5A	-2.40	1.34	1.43
4	A	1102	AMP	C2'-C3'	-2.38	1.46	1.53
3	A	1101	NAD	C6N-N1N	2.35	1.41	1.35
4	A	1102	AMP	C5-N7	-2.32	1.31	1.39
4	A	1102	AMP	P-O2P	-2.24	1.46	1.54
4	C	1102	AMP	C4-N3	-2.22	1.32	1.35

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1101	NAD	N3A-C2A-N1A	-6.91	117.88	128.68
3	C	1101	NAD	N3A-C2A-N1A	-6.49	118.54	128.68
3	C	1101	NAD	O5B-PA-O1A	-5.89	86.04	109.07
4	A	1102	AMP	O3'-C3'-C2'	-4.78	96.37	111.82
3	C	1101	NAD	O2A-PA-O5B	-4.31	87.74	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1102	AMP	O2'-C2'-C3'	-4.04	98.75	111.82
4	C	1102	AMP	C3'-C2'-C1'	4.04	107.06	100.98
4	A	1102	AMP	C3'-C2'-C1'	3.97	106.95	100.98
3	C	1101	NAD	PN-O3-PA	-3.81	119.77	132.83
3	C	1101	NAD	C6N-N1N-C2N	-3.45	118.83	121.97
3	A	1101	NAD	C6N-N1N-C2N	-2.95	119.29	121.97
4	C	1102	AMP	O2P-P-O5'	-2.84	99.18	106.73
3	A	1101	NAD	C2B-C3B-C4B	-2.82	97.17	102.64
4	C	1102	AMP	N3-C2-N1	-2.80	124.30	128.68
3	A	1101	NAD	C2D-C3D-C4D	-2.69	97.42	102.64
3	A	1101	NAD	O7N-C7N-C3N	-2.68	116.42	119.63
3	A	1101	NAD	C5A-C6A-N6A	-2.68	116.28	120.35
4	C	1102	AMP	C4-C5-N7	-2.58	106.71	109.40
4	C	1102	AMP	O3P-P-O5'	-2.55	99.94	106.73
3	C	1101	NAD	O4D-C4D-C5D	-2.53	101.06	109.37
4	A	1102	AMP	C5'-C4'-C3'	-2.48	105.88	115.18
3	A	1101	NAD	O7N-C7N-N7N	2.47	126.08	122.58
3	A	1101	NAD	PN-O3-PA	-2.38	124.66	132.83
4	A	1102	AMP	N3-C2-N1	-2.37	124.97	128.68
4	C	1102	AMP	O3P-P-O2P	2.37	116.68	107.64
3	A	1101	NAD	O4B-C4B-C3B	-2.36	100.44	105.11
3	C	1101	NAD	O4D-C1D-C2D	-2.30	103.57	106.93
3	A	1101	NAD	C1B-N9A-C4A	-2.30	122.61	126.64
3	C	1101	NAD	C2B-C3B-C4B	-2.27	98.23	102.64
4	C	1102	AMP	P-O5'-C5'	-2.25	112.09	118.30
4	C	1102	AMP	C5'-C4'-C3'	-2.22	106.88	115.18
4	A	1102	AMP	O3P-P-O5'	-2.14	101.05	106.73
4	A	1102	AMP	C4-C5-N7	-2.10	107.21	109.40
3	C	1101	NAD	O2A-PA-O1A	2.09	122.57	112.24
3	C	1101	NAD	C5A-C6A-N6A	-2.04	117.25	120.35
4	C	1102	AMP	O3P-P-O1P	2.01	118.56	110.68
3	C	1101	NAD	C4A-C5A-N7A	-2.01	107.30	109.40
4	A	1102	AMP	P-O5'-C5'	-2.01	112.77	118.30
4	A	1102	AMP	O2P-P-O5'	-2.00	101.41	106.73
4	C	1102	AMP	C2'-C3'-C4'	2.00	106.53	102.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1101	NAD	C5B-O5B-PA-O1A
3	C	1101	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
3	C	1101	NAD	O4B-C4B-C5B-O5B
3	C	1101	NAD	C3B-C4B-C5B-O5B
4	C	1102	AMP	C3'-C4'-C5'-O5'
4	C	1102	AMP	O4'-C4'-C5'-O5'
3	C	1101	NAD	C3D-C4D-C5D-O5D
3	A	1101	NAD	C5B-O5B-PA-O1A
3	C	1101	NAD	C5B-O5B-PA-O2A

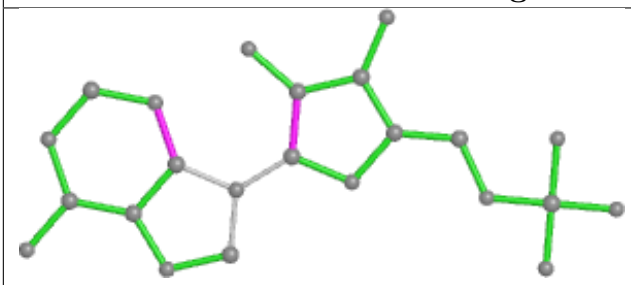
There are no ring outliers.

3 monomers are involved in 11 short contacts:

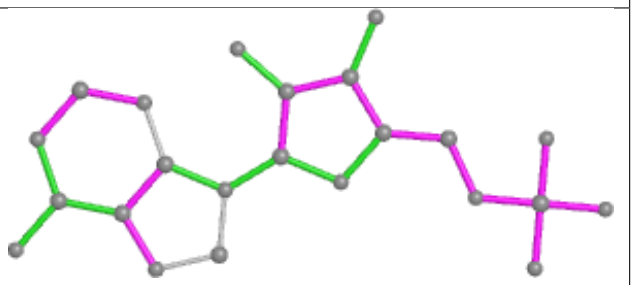
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1102	AMP	7	0
4	A	1102	AMP	1	0
3	C	1101	NAD	3	0

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.

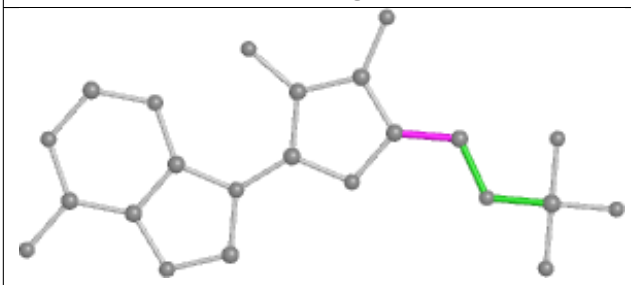
Ligand AMP C 1102



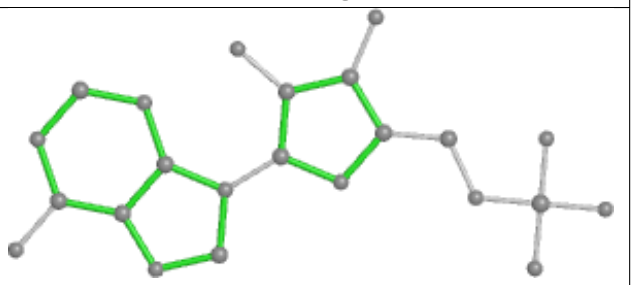
Bond lengths



Bond angles

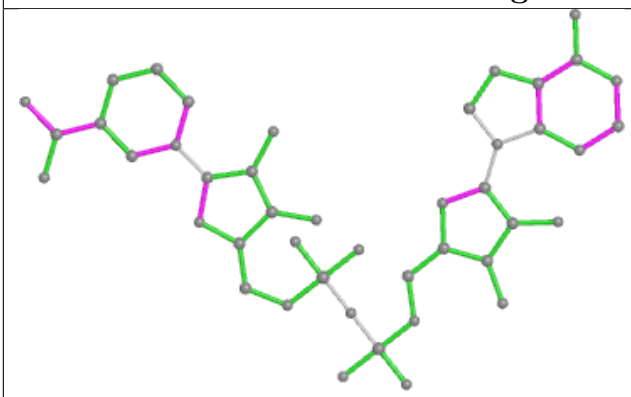


Torsions

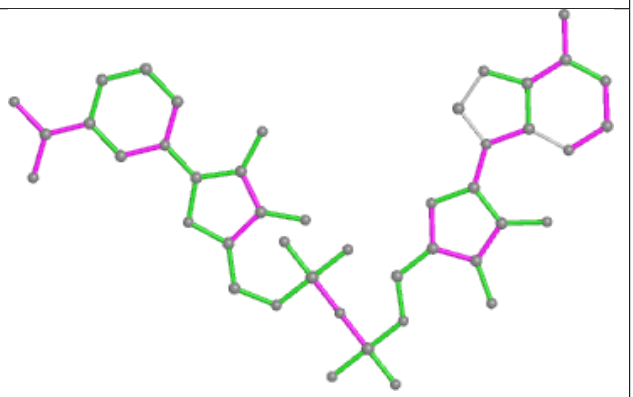


Rings

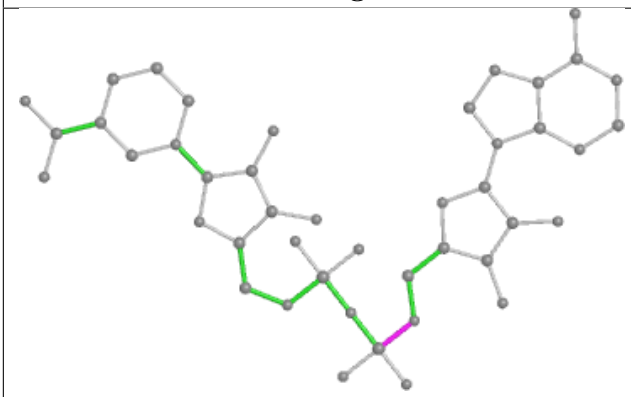
Ligand NAD A 1101



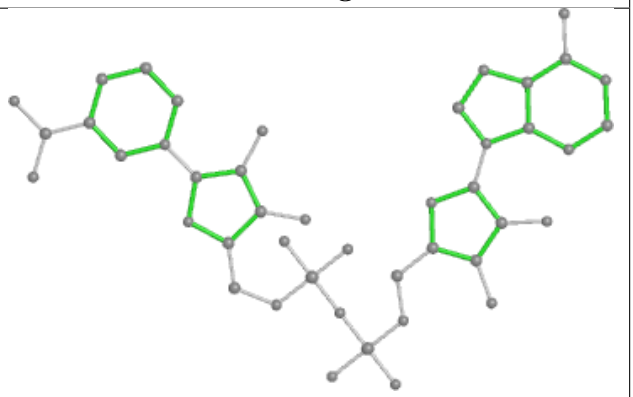
Bond lengths



Bond angles

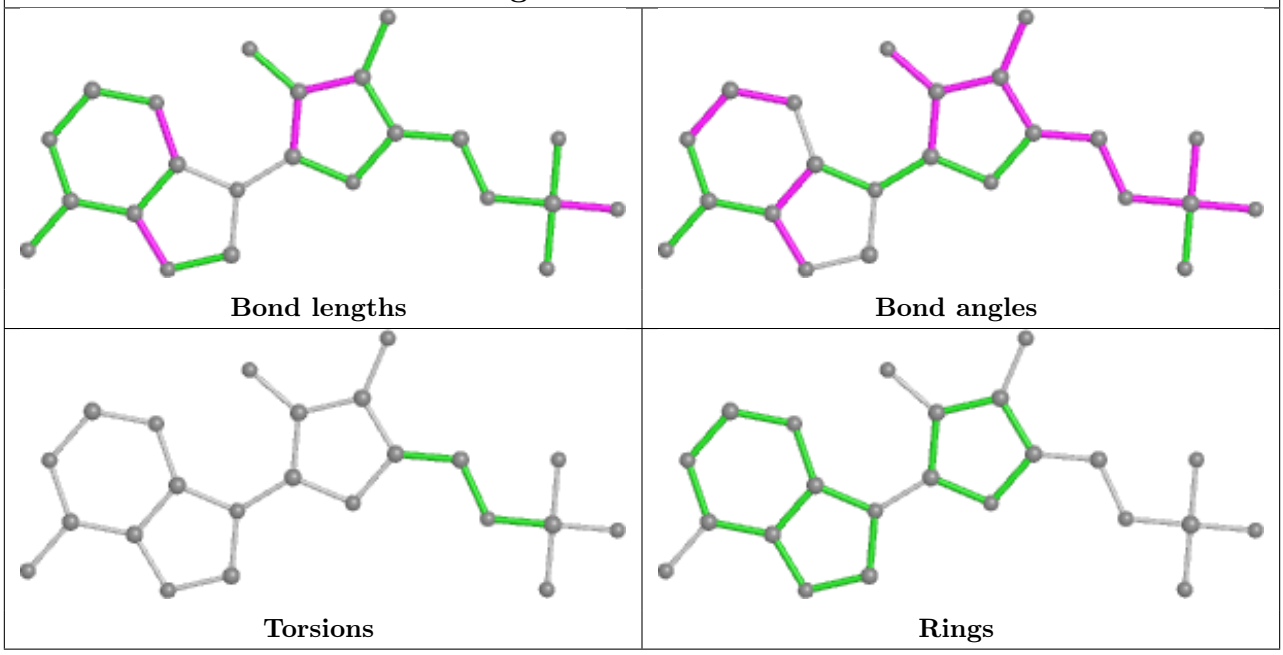


Torsions

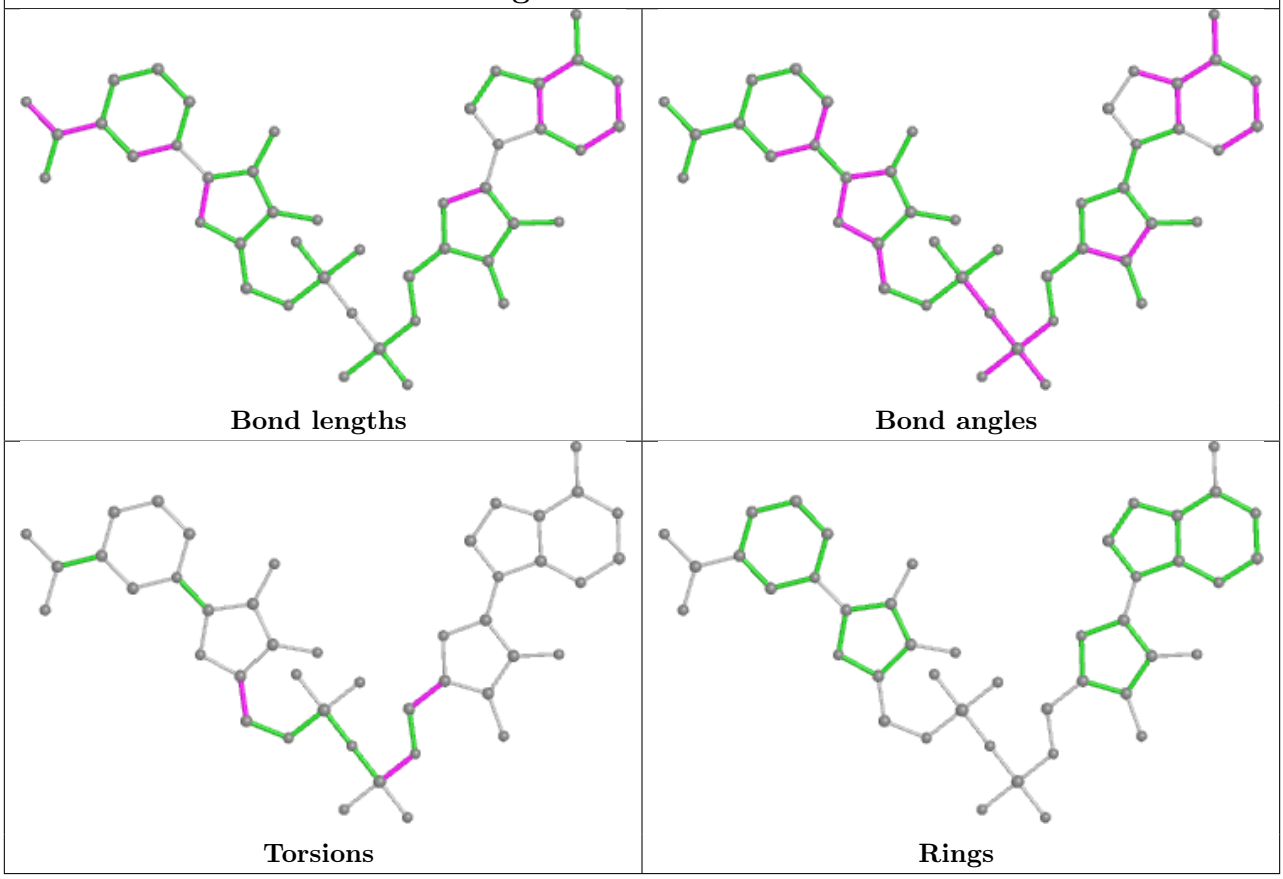


Rings

Ligand AMP A 1102



Ligand NAD C 1101



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	812/845 (96%)	0.33	54 (6%)	17	12	24, 46, 104, 142	0
1	C	808/845 (95%)	0.54	77 (9%)	8	4	26, 66, 111, 158	0
2	B	76/79 (96%)	0.96	13 (17%)	1	1	34, 59, 83, 93	0
2	D	76/79 (96%)	2.30	36 (47%)	0	0	61, 119, 144, 157	0
All	All	1772/1848 (95%)	0.54	180 (10%)	6	4	24, 58, 115, 158	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	955	SER	10.6
2	D	32	ASP	9.1
2	D	13	ILE	8.1
1	A	1000	PHE	7.6
2	D	19	PRO	7.6
1	A	957	TYR	7.3
2	D	57	SER	7.1
2	D	59	TYR	6.9
1	C	544	TYR	6.5
1	A	223	VAL	6.1
2	D	28	ALA	5.5
1	C	475	GLY	5.4
1	A	956	GLY	5.2
1	C	979	ASN	5.2
2	D	35	GLY	5.1
2	B	1	MET	5.1
1	C	957	TYR	5.1
2	D	31	GLN	5.1
1	C	384	GLU	5.0
2	D	3	ILE	4.7
1	A	222	SER	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	63	LYS	4.7
2	D	4	PHE	4.6
2	D	14	THR	4.5
2	D	64	GLU	4.5
2	D	33	LYS	4.5
1	A	545	GLN	4.4
2	D	54	ARG	4.4
1	C	977	LEU	4.3
1	A	1004	GLU	4.3
2	D	58	ASP	4.3
1	A	411	LYS	4.3
2	D	2	GLN	4.2
1	C	554	ASN	4.2
2	D	55	THR	4.2
2	B	14	THR	4.2
2	D	18	GLU	4.1
2	D	1	MET	4.0
1	C	949	ALA	3.9
2	D	36	ILE	3.9
1	C	343	TYR	3.8
1	C	948	GLN	3.8
2	B	25	ASN	3.8
1	C	1010	ILE	3.7
1	A	1047	GLY	3.7
2	B	2	GLN	3.7
1	A	508	ASN	3.6
1	A	1049	LEU	3.6
1	C	413	PRO	3.6
1	C	615	ASP	3.6
1	A	1054	ASN	3.6
1	A	339	SER	3.6
2	B	62	GLN	3.5
1	C	476	GLN	3.5
1	C	483	GLU	3.4
1	C	269	VAL	3.4
1	C	412	GLN	3.4
1	C	984	LEU	3.3
1	C	553	ILE	3.3
1	C	960	PHE	3.3
1	A	496	LEU	3.3
1	A	476	GLN	3.3
1	A	262	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	498	PHE	3.2
2	D	29	LYS	3.2
1	C	626	GLY	3.2
1	A	1003	VAL	3.1
1	C	271	ARG	3.1
1	C	342	ASN	3.0
1	A	1048	ALA	3.0
1	C	481	ILE	3.0
1	C	556	ALA	2.9
1	C	479	ASN	2.9
1	A	547	LEU	2.9
1	A	1039	ALA	2.9
2	B	28	ALA	2.9
1	C	511	TYR	2.9
1	A	923	GLN	2.9
1	A	499	PHE	2.9
1	C	976	LEU	2.9
1	A	963	GLU	2.8
2	D	34	GLU	2.8
2	D	30	ILE	2.8
1	A	410	VAL	2.8
2	D	20	SER	2.8
2	D	5	VAL	2.8
1	A	469	LEU	2.8
1	C	465	VAL	2.8
1	C	478	GLY	2.7
1	A	484	GLU	2.7
1	A	768	GLU	2.7
1	A	507	GLU	2.7
1	A	997	TRP	2.7
2	D	65	SER	2.7
1	C	243	TYR	2.7
2	D	56	LEU	2.7
1	C	955	SER	2.7
1	A	483	GLU	2.6
1	A	958	LYS	2.6
2	D	17	VAL	2.6
1	C	964	LYS	2.6
1	C	562	VAL	2.6
2	D	16	GLU	2.6
2	D	9	THR	2.6
1	C	496	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	964	LYS	2.6
2	B	15	LEU	2.6
1	A	506	GLU	2.6
1	C	953	THR	2.5
1	C	1009	LYS	2.5
1	C	958	LYS	2.5
1	C	329	PHE	2.5
2	B	4	PHE	2.5
1	C	360	GLU	2.5
1	A	302	SER	2.5
1	A	417	TYR	2.5
2	D	61	ILE	2.5
1	C	997	TRP	2.4
1	C	256	THR	2.4
1	C	623	PHE	2.4
1	C	937	ARG	2.4
1	A	224	PRO	2.4
2	D	37	PRO	2.4
2	B	27	LYS	2.4
1	A	1035	GLN	2.4
1	C	621	HIS	2.4
1	C	502	LYS	2.4
1	A	505	LEU	2.4
1	C	541	LEU	2.4
1	C	557	ARG	2.3
1	A	983	ILE	2.3
2	B	3	ILE	2.3
1	C	1045	ILE	2.3
2	B	33	LYS	2.3
1	C	270	TYR	2.3
1	C	924	ARG	2.3
1	A	1055	ILE	2.3
1	A	548	GLN	2.3
1	A	950	LYS	2.2
1	C	251	LYS	2.2
1	A	478	GLY	2.2
1	C	250	GLY	2.2
1	C	347	HIS	2.2
1	C	985	GLY	2.2
1	A	982	THR	2.2
2	B	32	ASP	2.2
1	C	622	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	252	PRO	2.2
1	C	969	LEU	2.2
1	A	996	GLN	2.2
1	C	477	ASP	2.2
1	C	561	ASP	2.1
1	C	638	LEU	2.1
1	A	954	GLU	2.1
1	C	359	GLU	2.1
1	C	474	ILE	2.1
1	C	920	GLU	2.1
1	C	364	THR	2.1
1	C	391	ALA	2.1
1	C	983	ILE	2.1
1	A	986	LYS	2.1
1	A	269	VAL	2.1
1	A	272	GLN	2.1
1	C	542	LYS	2.1
1	C	729	THR	2.1
1	C	309	GLY	2.1
1	C	348	GLU	2.1
1	C	458	GLU	2.1
2	D	10	GLY	2.1
2	D	24	GLU	2.1
1	C	400	ASN	2.1
1	A	1058	LEU	2.0
1	C	1004	GLU	2.0
2	D	11	LYS	2.0
1	A	624	LEU	2.0
1	A	919	LEU	2.0
1	C	1035	GLN	2.0
1	A	502	LYS	2.0
2	B	13	ILE	2.0
1	C	358	VAL	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)

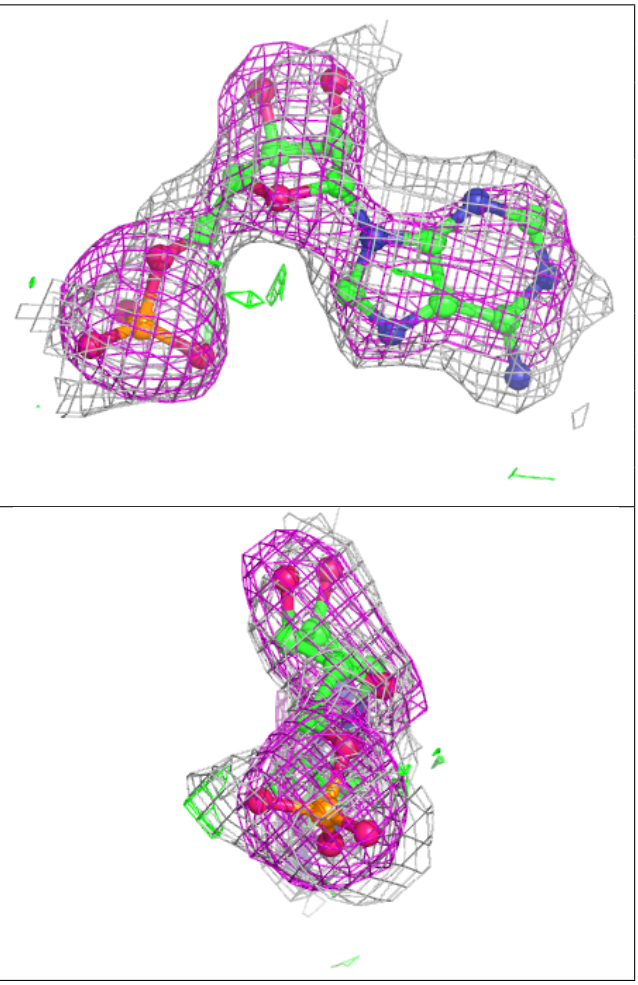
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	AMP	A	1102	23/23	0.88	0.34	20,20,20,20	0
4	AMP	C	1102	23/23	0.90	0.43	20,20,20,20	0
3	NAD	A	1101	44/44	0.97	0.19	21,32,40,48	0
3	NAD	C	1101	44/44	0.97	0.19	28,42,50,51	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.

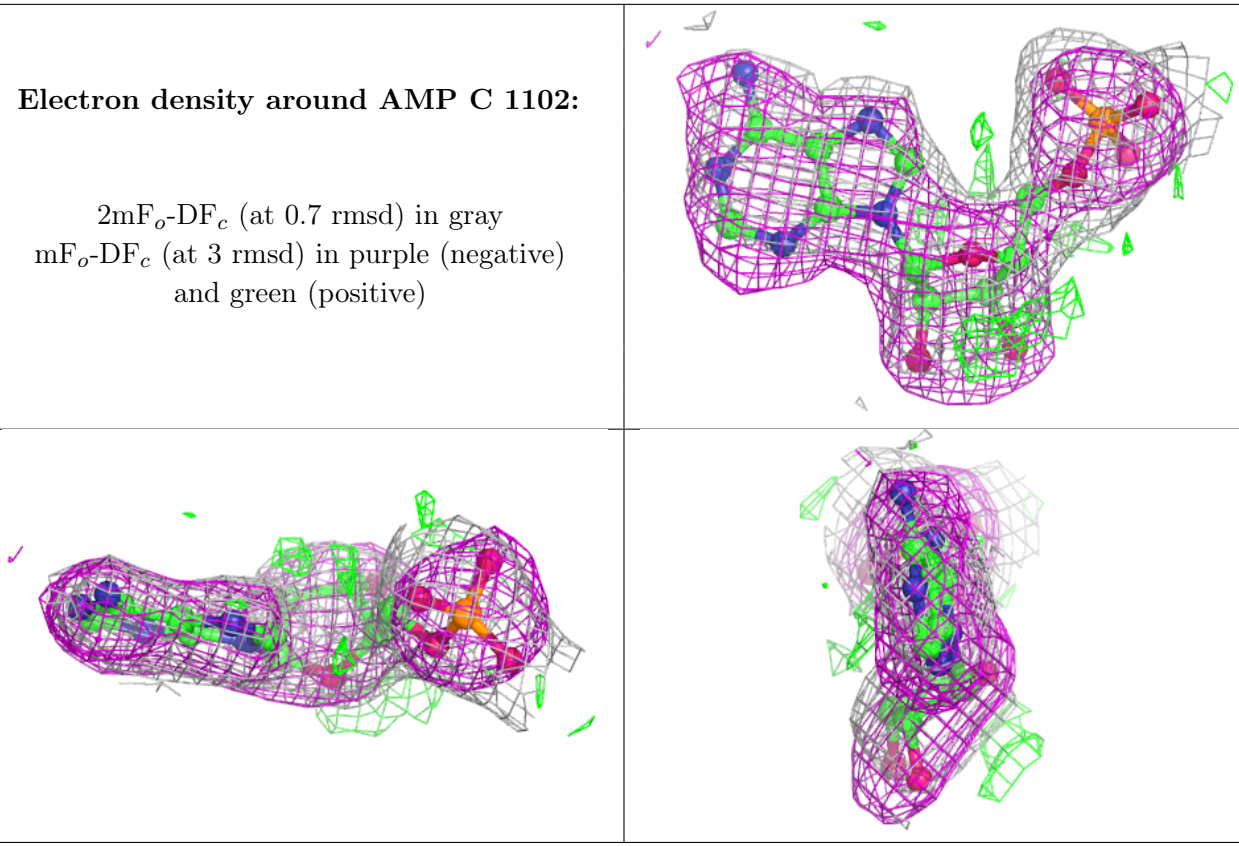
Electron density around AMP A 1102:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



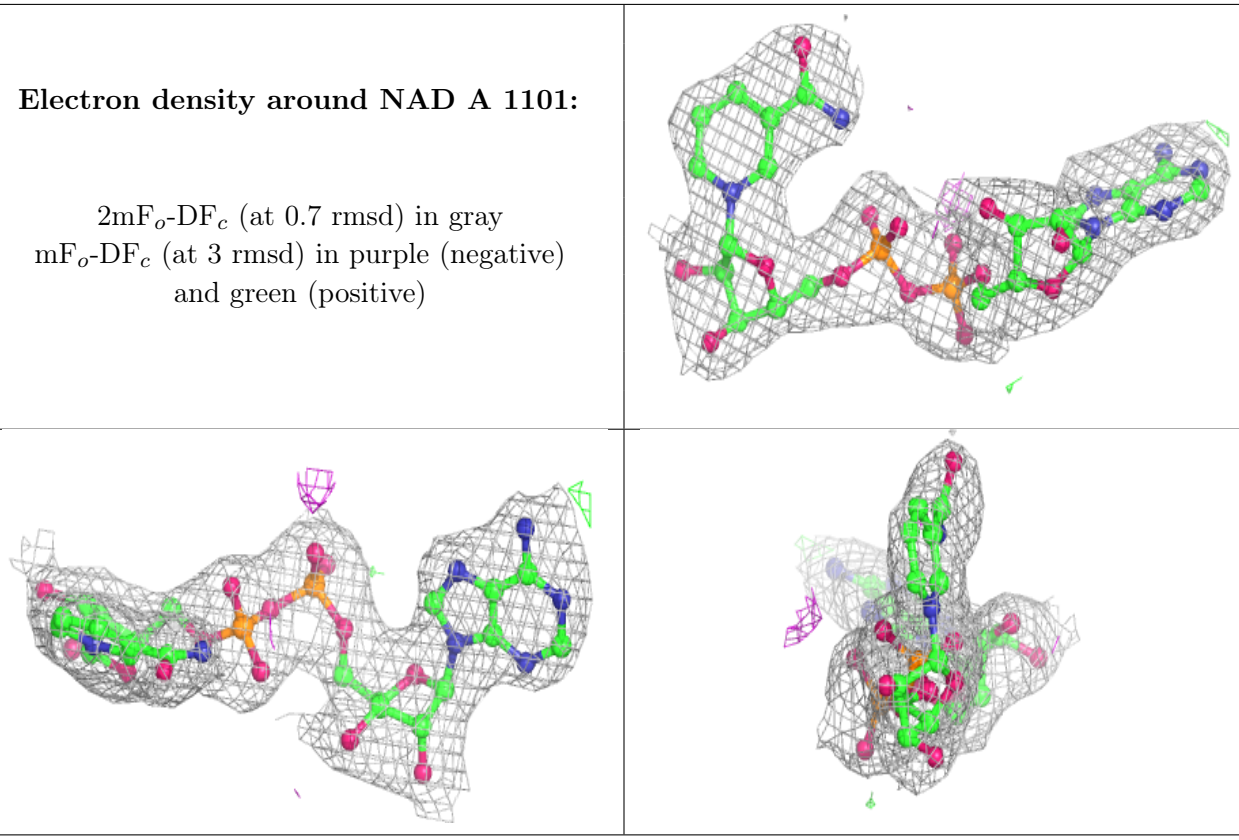
Electron density around AMP C 1102:

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



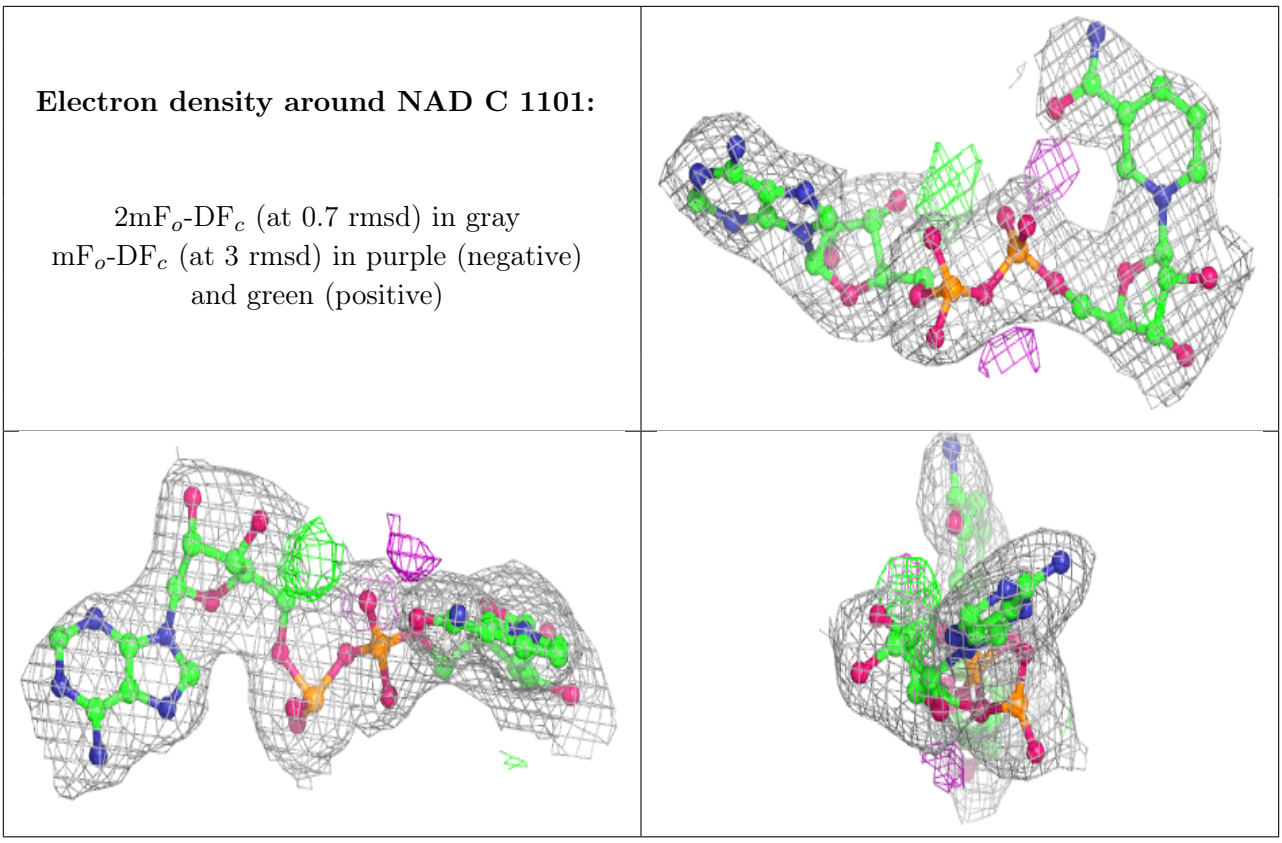
Electron density around NAD A 1101:

$2mF_o$-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 1101:

$2mF_o$-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.