



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:48 PM UTC

PDB ID : 1LA2 / pdb_00001la2
Title : Structural analysis of *Saccharomyces cerevisiae* myo-inositol phosphate synthase
Authors : Kniewel, R.; Buglino, J.A.; Shen, V.; Chadna, T.; Beckwith, A.; Lima, C.D.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYS-GXRC)
Deposited on : 2002-03-27
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

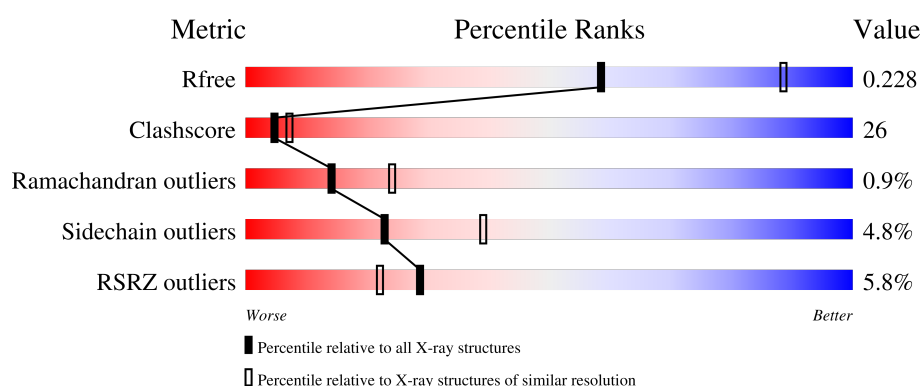
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	533	7% 54% 40% • •
1	B	533	5% 53% 40% • •
1	C	533	4% 53% 41% • •
1	D	533	5% 53% 40% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17040 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 Myo-inositol-1-phosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			
1	B	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			
1	C	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			
1	D	514	Total	C	N	O	S	Se	0	0	0
			4043	2572	677	778	6	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	SEE REMARK 999	UNP P11986
A	14	VAL	LEU	SEE REMARK 999	UNP P11986
A	?	-	PHE	SEE REMARK 999	UNP P11986
A	60	LEU	GLU	SEE REMARK 999	UNP P11986
A	69	MSE	MET	modified residue	UNP P11986
A	?	-	ALA	SEE REMARK 999	UNP P11986
A	98	GLU	LYS	SEE REMARK 999	UNP P11986
A	109	MSE	MET	modified residue	UNP P11986
A	136	MSE	MET	modified residue	UNP P11986
A	140	ASN	LYS	SEE REMARK 999	UNP P11986
A	141	ASP	HIS	SEE REMARK 999	UNP P11986
A	158	MSE	MET	modified residue	UNP P11986
A	176	MSE	MET	modified residue	UNP P11986
A	201	ASN	GLN	SEE REMARK 999	UNP P11986
A	261	MSE	MET	modified residue	UNP P11986
A	405	MSE	MET	modified residue	UNP P11986
A	415	MSE	MET	modified residue	UNP P11986
A	423	MSE	MET	modified residue	UNP P11986
A	444	PRO	ALA	SEE REMARK 999	UNP P11986
A	452	MSE	MET	modified residue	UNP P11986
B	?	-	ARG	SEE REMARK 999	UNP P11986

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Chain	Residue	Modelled	Actual	Comment	Reference
B	14	VAL	LEU	SEE REMARK 999	UNP P11986
B	?	-	PHE	SEE REMARK 999	UNP P11986
B	60	LEU	GLU	SEE REMARK 999	UNP P11986
B	69	MSE	MET	modified residue	UNP P11986
B	?	-	ALA	SEE REMARK 999	UNP P11986
B	98	GLU	LYS	SEE REMARK 999	UNP P11986
B	109	MSE	MET	modified residue	UNP P11986
B	136	MSE	MET	modified residue	UNP P11986
B	140	ASN	LYS	SEE REMARK 999	UNP P11986
B	141	ASP	HIS	SEE REMARK 999	UNP P11986
B	158	MSE	MET	modified residue	UNP P11986
B	176	MSE	MET	modified residue	UNP P11986
B	201	ASN	GLN	SEE REMARK 999	UNP P11986
B	261	MSE	MET	modified residue	UNP P11986
B	405	MSE	MET	modified residue	UNP P11986
B	415	MSE	MET	modified residue	UNP P11986
B	423	MSE	MET	modified residue	UNP P11986
B	444	PRO	ALA	SEE REMARK 999	UNP P11986
B	452	MSE	MET	modified residue	UNP P11986
C	?	-	ARG	SEE REMARK 999	UNP P11986
C	14	VAL	LEU	SEE REMARK 999	UNP P11986
C	?	-	PHE	SEE REMARK 999	UNP P11986
C	60	LEU	GLU	SEE REMARK 999	UNP P11986
C	69	MSE	MET	modified residue	UNP P11986
C	?	-	ALA	SEE REMARK 999	UNP P11986
C	98	GLU	LYS	SEE REMARK 999	UNP P11986
C	109	MSE	MET	modified residue	UNP P11986
C	136	MSE	MET	modified residue	UNP P11986
C	140	ASN	LYS	SEE REMARK 999	UNP P11986
C	141	ASP	HIS	SEE REMARK 999	UNP P11986
C	158	MSE	MET	modified residue	UNP P11986
C	176	MSE	MET	modified residue	UNP P11986
C	201	ASN	GLN	SEE REMARK 999	UNP P11986
C	261	MSE	MET	modified residue	UNP P11986
C	405	MSE	MET	modified residue	UNP P11986
C	415	MSE	MET	modified residue	UNP P11986
C	423	MSE	MET	modified residue	UNP P11986
C	444	PRO	ALA	SEE REMARK 999	UNP P11986
C	452	MSE	MET	modified residue	UNP P11986
D	?	-	ARG	SEE REMARK 999	UNP P11986
D	14	VAL	LEU	SEE REMARK 999	UNP P11986
D	?	-	PHE	SEE REMARK 999	UNP P11986

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

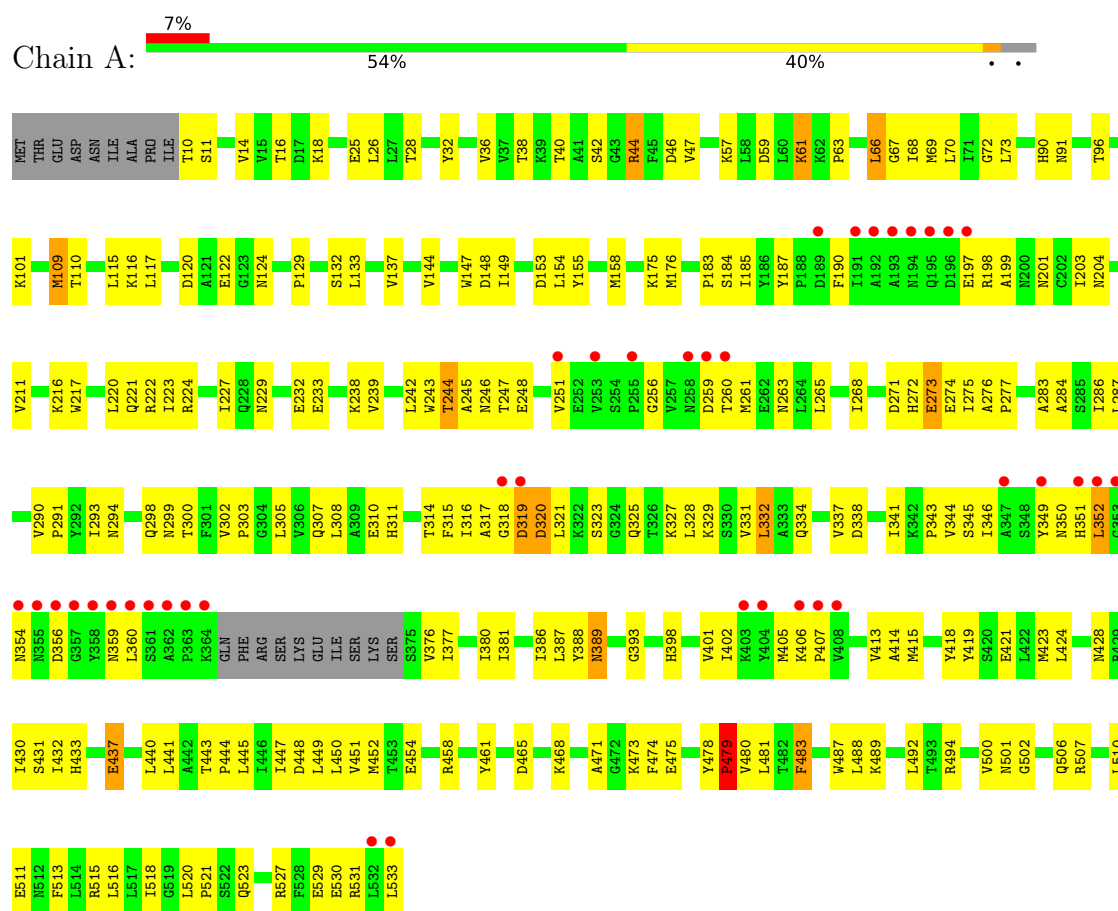
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	188	Total	O	0	0
			188	188		
3	C	194	Total	O	0	0
			194	194		
3	D	165	Total	O	0	0
			165	165		

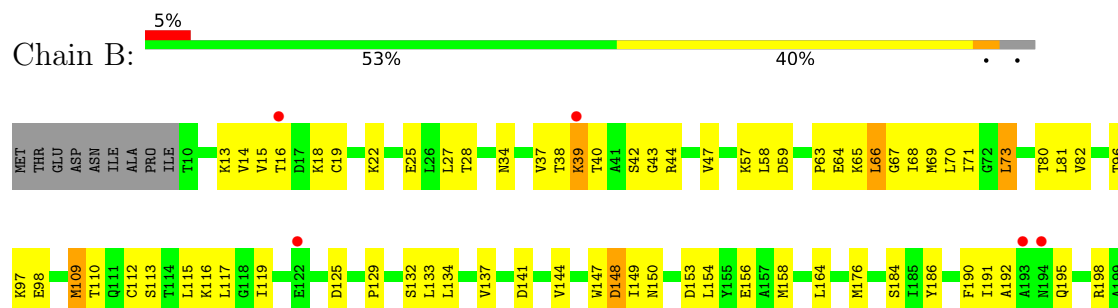
3 Residue-property plots

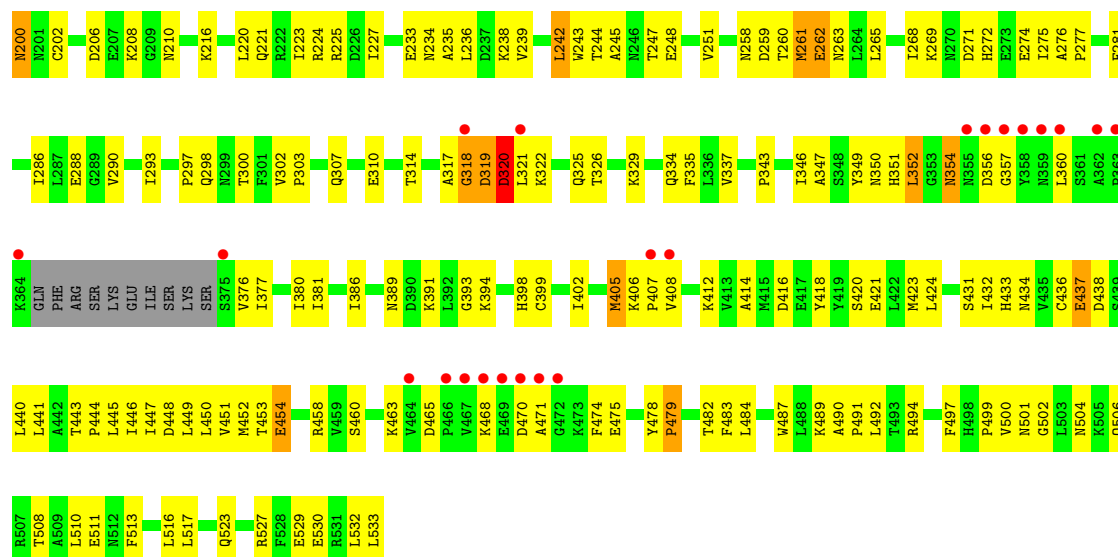
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Myo-inositol-1-phosphate synthase

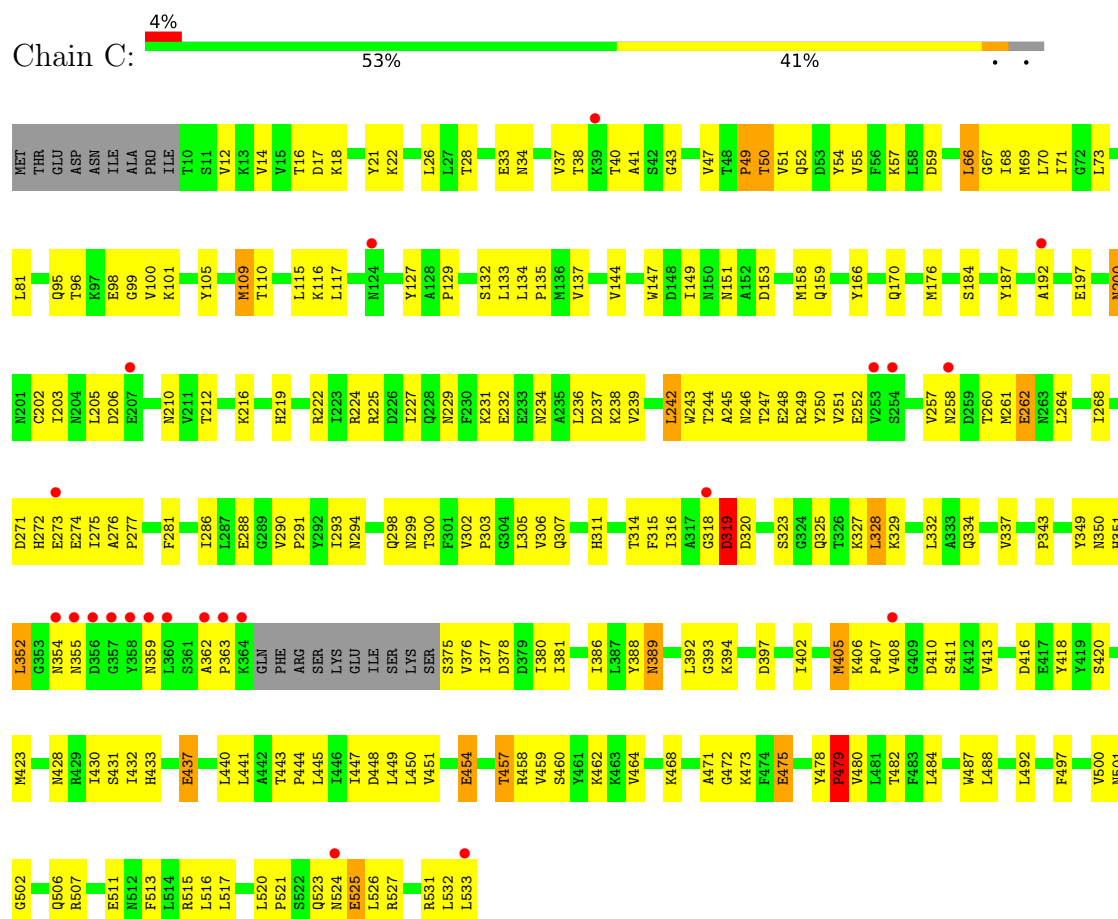


• Molecule 1: Myo-inositol-1-phosphate synthase



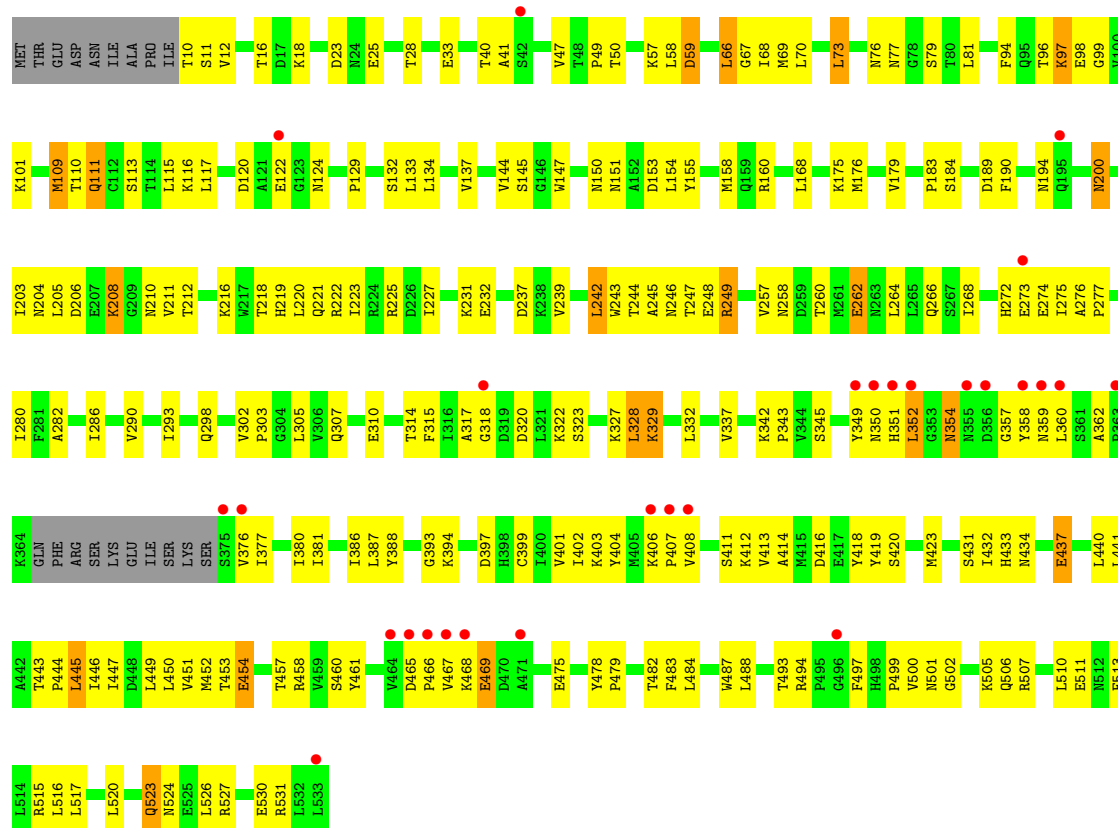


• Molecule 1: Myo-inositol-1-phosphate synthase



• Molecule 1: Myo-inositol-1-phosphate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.69Å 187.35Å 98.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.65 19.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.96-2.65) 99.1 (19.96-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.83 (at 2.56Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.224 , 0.280 0.227 , 0.228	Depositor DCC
R_{free} test set	4706 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17040	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2470e-03.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.29	0/4112	0.75	3/5561 (0.1%)
1	B	0.29	0/4112	0.76	2/5561 (0.0%)
1	C	0.29	0/4112	0.76	2/5561 (0.0%)
1	D	0.28	0/4112	0.75	1/5561 (0.0%)
All	All	0.29	0/16448	0.76	8/22244 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	GLY	N-CA-C	6.64	119.08	110.45
1	C	144	VAL	N-CA-C	5.70	117.20	108.71
1	A	72	GLY	N-CA-C	-5.60	105.90	115.08
1	C	237	ASP	N-CA-C	-5.53	106.46	113.43
1	B	144	VAL	N-CA-C	5.30	116.92	108.87
1	A	198	ARG	N-CA-C	-5.29	106.33	112.89
1	A	144	VAL	N-CA-C	5.08	116.58	108.87
1	D	144	VAL	N-CA-C	5.04	116.53	108.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4043	0	4038	221	0
1	B	4043	0	4038	219	0
1	C	4043	0	4038	223	0
1	D	4043	0	4038	234	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	2	0
3	A	145	0	0	6	0
3	B	188	0	0	5	0
3	C	194	0	0	11	0
3	D	165	0	0	10	0
All	All	17040	0	16256	836	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 26.

All (836) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:MSE:HE3	1:D:444:PRO:HG3	1.27	1.11
1:A:437:GLU:HG3	1:A:440:LEU:HD12	1.29	1.09
1:D:437:GLU:HG3	1:D:440:LEU:HD12	1.35	1.08
1:A:129:PRO:HG2	1:A:132:SER:HB3	1.45	0.96
1:D:96:THR:HG23	1:D:98:GLU:H	1.34	0.93
1:B:73:LEU:HD22	1:B:154:LEU:HD21	1.50	0.92
1:D:69:MSE:HE2	1:D:239:VAL:HG11	1.52	0.92
1:D:242:LEU:HD22	1:D:293:ILE:HB	1.50	0.90
1:C:69:MSE:HE1	1:C:227:ILE:HG12	1.51	0.90
1:C:437:GLU:HG3	1:C:440:LEU:HD12	1.52	0.89
1:B:69:MSE:HE2	1:B:239:VAL:HG11	1.53	0.88
1:C:16:THR:HG22	1:C:18:LYS:H	1.39	0.88
1:A:492:LEU:HD23	1:A:492:LEU:H	1.39	0.87
1:A:73:LEU:HD13	1:A:154:LEU:HD21	1.56	0.87
1:B:69:MSE:HE1	1:B:227:ILE:HG12	1.57	0.87
1:B:437:GLU:HG3	1:B:440:LEU:HD12	1.57	0.86
1:B:70:LEU:HD11	1:B:81:LEU:HD13	1.56	0.86
1:D:16:THR:HG22	1:D:18:LYS:H	1.41	0.85
1:B:109:MSE:O	1:B:113:SER:HB3	1.78	0.84
1:D:69:MSE:HE1	1:D:227:ILE:HG12	1.59	0.83
1:B:129:PRO:HG2	1:B:132:SER:HB3	1.62	0.82
1:C:96:THR:HG22	1:C:99:GLY:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:MSE:HG2	1:A:424:LEU:HG	1.62	0.81
1:B:376:VAL:HG22	1:B:501:ASN:HB3	1.61	0.81
1:B:40:THR:HG22	1:B:42:SER:H	1.43	0.80
1:A:44:ARG:HE	1:B:13:LYS:HD2	1.46	0.80
1:A:69:MSE:HE1	1:A:227:ILE:HG12	1.60	0.80
1:D:96:THR:HG22	1:D:99:GLY:O	1.80	0.80
1:B:321:LEU:HG	1:B:445:LEU:HD22	1.61	0.80
1:C:376:VAL:HG22	1:C:501:ASN:HB3	1.64	0.79
1:D:524:ASN:HD22	1:D:526:LEU:H	1.31	0.79
1:D:110:THR:HG21	1:D:451:VAL:HG11	1.64	0.79
1:D:70:LEU:HD11	1:D:81:LEU:HD22	1.65	0.78
1:A:183:PRO:HA	1:A:201:ASN:OD1	1.84	0.78
1:C:129:PRO:HB3	1:D:386:ILE:HD11	1.67	0.76
1:A:345:SER:HB3	1:A:419:TYR:HB3	1.66	0.76
1:B:39:LYS:H	1:B:39:LYS:HD2	1.50	0.76
1:A:16:THR:HG22	1:A:18:LYS:H	1.51	0.76
1:B:242:LEU:HD22	1:B:293:ILE:HB	1.69	0.75
1:C:261:MSE:HE1	1:C:311:HIS:HB2	1.69	0.75
1:C:129:PRO:HG2	1:C:132:SER:HB3	1.68	0.75
1:D:73:LEU:HD22	1:D:154:LEU:HD11	1.69	0.74
1:D:129:PRO:HG2	1:D:132:SER:HB3	1.69	0.74
1:D:218:THR:HA	1:D:221:GLN:HE21	1.51	0.74
1:C:96:THR:HG23	1:C:98:GLU:H	1.51	0.74
1:B:59:ASP:HB3	1:B:458:ARG:HB3	1.70	0.74
1:C:318:GLY:O	1:C:319:ASP:HB2	1.87	0.74
1:D:293:ILE:HG23	1:D:317:ALA:HB3	1.68	0.74
1:D:352:LEU:HD11	1:D:360:LEU:HD12	1.70	0.74
1:C:316:ILE:HD11	1:C:480:VAL:HG22	1.70	0.74
1:B:423:MSE:HG2	1:B:424:LEU:HG	1.70	0.73
1:C:492:LEU:HD23	1:C:492:LEU:H	1.54	0.73
1:A:433:HIS:HB3	1:B:431:SER:HB2	1.69	0.73
1:B:248:GLU:OE2	1:B:277:PRO:HG2	1.89	0.73
1:B:443:THR:HB	1:B:444:PRO:HD3	1.70	0.73
1:D:115:LEU:HD22	1:D:511:GLU:HG2	1.70	0.73
1:C:151:ASN:H	1:C:200:ASN:HD21	1.37	0.72
1:C:389:ASN:ND2	1:C:392:LEU:H	1.87	0.72
1:D:343:PRO:HA	1:D:420:SER:HA	1.69	0.72
1:C:441:LEU:O	1:C:445:LEU:HD13	1.88	0.72
1:D:445:LEU:HG	1:D:487:TRP:HD1	1.55	0.71
1:B:262:GLU:CD	1:B:262:GLU:H	1.97	0.71
1:C:433:HIS:HB3	1:D:431:SER:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HD21	1:A:133:LEU:HD21	1.71	0.71
1:B:399:CYS:SG	1:C:405:MSE:HE1	2.31	0.71
1:C:511:GLU:O	1:C:515:ARG:HG3	1.91	0.71
1:D:109:MSE:O	1:D:113:SER:HB3	1.90	0.70
1:C:117:LEU:HD21	1:C:133:LEU:HD21	1.74	0.70
1:D:248:GLU:OE2	1:D:277:PRO:HG2	1.92	0.70
1:A:117:LEU:HD21	1:A:133:LEU:CD2	2.23	0.69
1:B:349:TYR:C	1:B:350:ASN:HD22	2.00	0.69
1:D:441:LEU:C	1:D:444:PRO:HD2	2.17	0.69
1:C:302:VAL:HB	1:C:303:PRO:HD2	1.75	0.68
1:C:386:ILE:HD11	1:D:129:PRO:HB3	1.76	0.68
1:D:502:GLY:O	1:D:506:GLN:HG3	1.94	0.68
1:C:68:ILE:HG12	1:C:450:LEU:HD13	1.75	0.68
1:A:69:MSE:HE2	1:A:239:VAL:HG11	1.77	0.67
1:C:147:TRP:HB3	1:C:184:SER:HB2	1.76	0.67
1:C:22:LYS:HD2	1:C:22:LYS:O	1.95	0.67
1:A:239:VAL:O	1:A:290:VAL:HG13	1.93	0.67
1:A:533:LEU:HD23	1:B:463:LYS:NZ	2.09	0.67
1:A:349:TYR:C	1:A:350:ASN:HD22	2.04	0.66
1:B:116:LYS:HD3	1:B:523:GLN:HE22	1.60	0.66
1:B:153:ASP:OD2	1:B:156:GLU:HG3	1.94	0.66
1:C:329:LYS:HA	1:C:418:TYR:OH	1.96	0.66
1:A:259:ASP:HA	1:A:303:PRO:HG2	1.76	0.66
1:C:248:GLU:OE2	1:C:277:PRO:HG2	1.96	0.66
1:A:478:TYR:CE2	1:A:494:ARG:HG2	2.31	0.65
1:C:437:GLU:HG3	1:C:440:LEU:CD1	2.25	0.65
1:B:234:ASN:O	1:B:236:LEU:N	2.29	0.65
1:D:79:SER:HA	1:D:154:LEU:HD12	1.79	0.65
1:B:334:GLN:HE21	1:B:380:ILE:HG12	1.60	0.65
1:C:22:LYS:HD2	1:C:22:LYS:C	2.21	0.65
1:D:345:SER:HB3	1:D:419:TYR:HB3	1.79	0.65
1:B:445:LEU:HG	1:B:487:TRP:HD1	1.61	0.65
1:C:527:ARG:NH2	1:D:500:VAL:HG11	2.11	0.65
1:A:511:GLU:O	1:A:515:ARG:HG3	1.96	0.65
1:C:251:VAL:HG21	1:C:274:GLU:O	1.97	0.65
1:B:405:MSE:HE3	1:C:397:ASP:HB3	1.79	0.64
1:C:262:GLU:CD	1:C:262:GLU:H	2.03	0.64
1:D:262:GLU:CD	1:D:262:GLU:H	2.04	0.64
1:A:334:GLN:HE21	1:A:380:ILE:HG12	1.62	0.64
1:B:96:THR:HG22	1:B:98:GLU:H	1.62	0.64
1:A:70:LEU:CD2	1:A:242:LEU:HB3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ILE:HG12	1:D:450:LEU:HD13	1.78	0.64
1:C:328:LEU:HD21	1:D:332:LEU:HD21	1.79	0.64
1:C:257:VAL:HG11	1:C:272:HIS:CD2	2.32	0.64
1:D:96:THR:HG21	1:D:101:LYS:HE3	1.80	0.64
1:C:239:VAL:O	1:C:290:VAL:HG13	1.96	0.63
1:A:445:LEU:HG	1:A:487:TRP:HD1	1.64	0.63
1:B:318:GLY:O	1:B:319:ASP:HB2	1.99	0.63
1:D:77:ASN:HB2	1:D:244:THR:HG21	1.81	0.63
1:D:337:VAL:HG21	1:D:380:ILE:HG22	1.79	0.63
1:A:149:ILE:O	1:A:199:ALA:HA	1.98	0.63
1:D:208:LYS:HE3	1:D:208:LYS:H	1.64	0.63
1:A:61:LYS:NZ	1:A:61:LYS:HB3	2.14	0.63
1:A:261:MSE:HE3	1:A:307:GLN:HG2	1.81	0.63
1:C:59:ASP:HB3	1:C:458:ARG:HB3	1.80	0.63
1:C:95:GLN:NE2	1:C:100:VAL:HG22	2.13	0.63
1:D:70:LEU:HD11	1:D:81:LEU:CD2	2.29	0.63
1:A:129:PRO:HG2	1:A:132:SER:CB	2.26	0.62
1:A:203:ILE:HD13	1:A:222:ARG:HG2	1.81	0.62
1:A:406:LYS:N	1:A:407:PRO:HD2	2.13	0.62
1:B:437:GLU:CG	1:B:440:LEU:HD12	2.28	0.62
1:D:116:LYS:HD3	1:D:523:GLN:HE22	1.64	0.62
1:D:511:GLU:O	1:D:515:ARG:HG3	1.99	0.62
1:B:186:TYR:HE1	1:B:191:ILE:HD11	1.64	0.62
1:B:337:VAL:HG21	1:B:380:ILE:CG2	2.30	0.62
1:C:478:TYR:CD1	1:C:479:PRO:HD2	2.34	0.62
1:C:531:ARG:HG2	1:D:482:THR:OG1	1.99	0.62
1:A:70:LEU:HD23	1:A:242:LEU:HB3	1.81	0.62
1:A:533:LEU:HD23	1:B:463:LYS:HZ1	1.65	0.62
1:D:246:ASN:HB3	1:D:359:ASN:ND2	2.15	0.62
1:A:224:ARG:NH1	1:A:287:LEU:HB3	2.15	0.61
1:C:332:LEU:HD21	1:D:328:LEU:HD21	1.82	0.61
1:D:40:THR:HG22	1:D:41:ALA:N	2.14	0.61
1:D:414:ALA:HB3	1:D:434:ASN:HB3	1.81	0.61
1:D:59:ASP:O	1:D:458:ARG:HD2	2.00	0.61
1:D:318:GLY:O	1:D:488:LEU:HD13	2.00	0.61
1:B:57:LYS:HB3	1:B:460:SER:OG	2.00	0.61
1:D:478:TYR:CE2	1:D:494:ARG:HB3	2.36	0.61
1:A:351:HIS:CE1	1:A:413:VAL:HB	2.36	0.61
1:A:445:LEU:HD21	1:A:487:TRP:HB3	1.82	0.61
1:D:40:THR:HG22	1:D:41:ALA:H	1.64	0.61
1:B:16:THR:HG22	1:B:18:LYS:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LEU:HD22	1:C:293:ILE:HB	1.81	0.61
1:C:441:LEU:C	1:C:444:PRO:HD2	2.25	0.61
1:D:239:VAL:O	1:D:290:VAL:HG13	2.00	0.61
1:B:239:VAL:O	1:B:290:VAL:HG13	2.00	0.61
1:A:449:LEU:HD21	1:A:487:TRP:HB2	1.82	0.60
1:D:160:ARG:HD2	3:D:987:HOH:O	2.01	0.60
1:D:329:LYS:HD3	1:D:416:ASP:OD2	2.01	0.60
1:A:116:LYS:HB3	1:A:523:GLN:NE2	2.16	0.60
1:A:246:ASN:HD22	1:A:359:ASN:HB2	1.66	0.60
1:A:352:LEU:HD22	1:A:354:ASN:ND2	2.17	0.60
1:D:57:LYS:HB3	1:D:460:SER:OG	2.02	0.60
1:A:203:ILE:HD11	3:A:902:HOH:O	2.01	0.60
1:C:431:SER:HB2	1:D:433:HIS:HB3	1.82	0.60
1:C:525:GLU:HG3	1:D:505:LYS:HB3	1.82	0.60
1:C:300:THR:O	1:C:305:LEU:HD12	2.01	0.60
1:C:449:LEU:HD21	1:C:487:TRP:HB2	1.84	0.60
1:D:272:HIS:CE1	1:D:274:GLU:HG3	2.37	0.60
1:A:38:THR:OG1	1:A:46:ASP:HB2	2.01	0.60
1:D:151:ASN:H	1:D:200:ASN:HD21	1.48	0.60
1:C:225:ARG:NH1	1:C:229:ASN:HB2	2.17	0.60
1:A:261:MSE:HE1	1:A:311:HIS:HB2	1.84	0.60
1:C:129:PRO:HG2	1:C:132:SER:CB	2.32	0.60
1:A:73:LEU:CD1	1:A:154:LEU:HD21	2.30	0.59
1:A:337:VAL:HG21	1:A:380:ILE:CG2	2.31	0.59
1:C:109:MSE:HG3	1:C:110:THR:N	2.16	0.59
1:C:473:LYS:HE3	1:C:475:GLU:OE1	2.02	0.59
1:D:116:LYS:HD3	1:D:523:GLN:NE2	2.16	0.59
1:A:327:LYS:O	1:A:331:VAL:HG23	2.02	0.59
1:C:247:THR:HA	1:C:298:GLN:HE21	1.66	0.59
1:D:342:LYS:HB2	1:D:387:LEU:HD22	1.83	0.59
1:D:443:THR:HB	1:D:444:PRO:HD3	1.83	0.59
1:B:117:LEU:HD21	1:B:133:LEU:CD2	2.33	0.59
1:A:318:GLY:O	1:A:319:ASP:HB2	2.03	0.59
1:A:377:ILE:O	1:A:381:ILE:HG13	2.03	0.59
1:C:389:ASN:HD22	1:C:392:LEU:H	1.51	0.59
1:A:341:ILE:O	1:A:343:PRO:HD3	2.03	0.59
1:B:195:GLN:HE21	1:B:195:GLN:HA	1.66	0.59
1:B:247:THR:HA	1:B:298:GLN:HE21	1.67	0.58
1:B:478:TYR:CD1	1:B:479:PRO:HD2	2.37	0.58
1:B:129:PRO:HG2	1:B:132:SER:CB	2.32	0.58
1:A:437:GLU:HG3	1:A:440:LEU:CD1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ARG:HD2	1:C:288:GLU:OE2	2.03	0.58
1:B:208:LYS:N	1:B:208:LYS:HD2	2.18	0.58
1:C:323:SER:O	1:C:327:LYS:HG3	2.03	0.58
1:D:247:THR:HA	1:D:298:GLN:HE21	1.68	0.58
1:B:343:PRO:HA	1:B:420:SER:HA	1.86	0.58
1:A:443:THR:HB	1:A:444:PRO:HD3	1.84	0.58
1:A:527:ARG:HB2	1:A:531:ARG:NH1	2.17	0.58
1:D:469:GLU:H	1:D:469:GLU:CD	2.11	0.58
1:D:515:ARG:NH1	1:D:523:GLN:HG2	2.19	0.58
1:D:150:ASN:HA	1:D:200:ASN:ND2	2.19	0.58
1:A:197:GLU:CD	1:A:197:GLU:H	2.12	0.57
1:C:349:TYR:C	1:C:350:ASN:HD22	2.12	0.57
1:A:527:ARG:NE	1:B:500:VAL:HG21	2.19	0.57
1:C:318:GLY:HA2	1:C:488:LEU:HD22	1.85	0.57
1:C:458:ARG:NH1	1:C:458:ARG:HB2	2.19	0.57
1:C:516:LEU:C	1:C:516:LEU:HD12	2.29	0.57
1:B:195:GLN:HE22	1:B:198:ARG:HD3	1.68	0.57
1:D:204:ASN:ND2	1:D:211:VAL:HG13	2.19	0.57
1:A:10:THR:HA	1:B:43:GLY:O	2.05	0.57
1:A:221:GLN:HG2	3:A:966:HOH:O	2.03	0.57
1:C:49:PRO:HG2	1:D:16:THR:OG1	2.04	0.57
1:C:272:HIS:HB3	1:C:275:ILE:HD13	1.84	0.57
1:D:449:LEU:HD21	1:D:487:TRP:HB2	1.86	0.57
1:A:26:LEU:O	1:A:57:LYS:HA	2.05	0.57
1:A:387:LEU:HD21	1:B:112:CYS:HB3	1.86	0.57
1:B:502:GLY:O	1:B:506:GLN:HG3	2.04	0.57
1:B:69:MSE:HE1	1:B:227:ILE:CG1	2.34	0.57
1:C:238:LYS:HE3	1:C:457:THR:HG21	1.87	0.57
1:A:109:MSE:HG3	1:A:110:THR:N	2.19	0.57
1:A:129:PRO:HB3	1:B:386:ILE:HD11	1.86	0.57
1:C:343:PRO:HA	1:C:420:SER:HA	1.87	0.57
1:C:443:THR:HB	1:C:444:PRO:HD3	1.86	0.57
1:C:502:GLY:O	1:C:506:GLN:HG3	2.05	0.57
1:A:405:MSE:HE1	1:D:399:CYS:SG	2.44	0.57
1:B:406:LYS:N	1:B:407:PRO:HD2	2.19	0.57
1:B:70:LEU:HD23	1:B:242:LEU:HB3	1.87	0.56
1:B:208:LYS:HD2	1:B:208:LYS:H	1.69	0.56
1:C:261:MSE:HE3	1:C:307:GLN:HG2	1.87	0.56
1:D:516:LEU:HD12	1:D:517:LEU:N	2.19	0.56
1:C:14:VAL:HG22	1:D:47:VAL:HB	1.87	0.56
1:C:423:MSE:CE	1:D:444:PRO:HG3	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:THR:HA	1:B:307:GLN:NE2	2.20	0.56
1:C:96:THR:HG21	1:C:101:LYS:HE3	1.86	0.56
1:D:264:LEU:O	1:D:268:ILE:HG13	2.05	0.56
1:D:465:ASP:CG	1:D:466:PRO:HD2	2.31	0.56
1:B:337:VAL:HG21	1:B:380:ILE:HG21	1.87	0.56
1:C:242:LEU:HD12	1:C:244:THR:OG1	2.05	0.56
1:B:302:VAL:HB	1:B:303:PRO:HD2	1.87	0.56
1:B:445:LEU:HD21	1:B:487:TRP:HB3	1.86	0.56
1:A:329:LYS:HA	1:A:418:TYR:OH	2.06	0.56
1:D:454:GLU:O	1:D:457:THR:HB	2.05	0.56
1:A:229:ASN:O	1:A:233:GLU:HG3	2.05	0.56
1:B:117:LEU:HD21	1:B:133:LEU:HD21	1.86	0.56
1:B:247:THR:HA	1:B:298:GLN:NE2	2.20	0.56
1:B:414:ALA:HB3	1:B:434:ASN:HB3	1.87	0.56
1:C:200:ASN:C	1:C:200:ASN:HD22	2.14	0.56
1:A:242:LEU:HD22	1:A:293:ILE:HB	1.88	0.55
1:D:246:ASN:HD22	2:D:903:NAD:H8A	1.70	0.55
1:D:388:TYR:HB3	1:D:394:LYS:HA	1.89	0.55
1:B:261:MSE:HG3	1:B:307:GLN:HG2	1.88	0.55
1:B:293:ILE:HA	1:B:317:ALA:O	2.06	0.55
1:C:475:GLU:HG3	3:C:992:HOH:O	2.06	0.55
1:A:260:THR:HB	1:A:263:ASN:CG	2.31	0.55
1:B:18:LYS:O	1:B:28:THR:HA	2.06	0.55
1:C:16:THR:HG22	1:C:18:LYS:N	2.17	0.55
1:D:200:ASN:H	1:D:200:ASN:HD22	1.55	0.55
1:A:32:TYR:HE2	1:B:529:GLU:OE2	1.89	0.55
1:B:354:ASN:ND2	1:B:354:ASN:H	2.05	0.55
1:B:468:LYS:HG2	1:B:471:ALA:HB2	1.89	0.55
1:D:247:THR:HA	1:D:298:GLN:NE2	2.21	0.55
1:C:458:ARG:HB2	1:C:458:ARG:HH11	1.72	0.55
1:A:428:ASN:HD21	1:A:430:ILE:HD11	1.72	0.55
1:C:329:LYS:HD3	1:C:416:ASP:OD2	2.07	0.55
1:A:203:ILE:HD13	1:A:222:ARG:CG	2.35	0.55
1:D:406:LYS:N	1:D:407:PRO:HD2	2.22	0.55
1:A:389:ASN:C	1:A:389:ASN:HD22	2.15	0.55
1:B:347:ALA:HB1	1:B:349:TYR:CE1	2.41	0.55
1:B:452:MSE:HE2	1:B:510:LEU:HD22	1.89	0.55
1:D:441:LEU:O	1:D:444:PRO:HD2	2.07	0.55
1:C:33:GLU:HG2	1:C:51:VAL:HG22	1.87	0.54
1:A:468:LYS:HE3	1:A:471:ALA:CB	2.37	0.54
1:D:96:THR:HG23	1:D:98:GLU:N	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:LEU:HD12	1:D:516:LEU:C	2.32	0.54
1:B:260:THR:HA	1:B:307:GLN:HE22	1.72	0.54
1:A:251:VAL:HG12	1:A:299:ASN:ND2	2.22	0.54
1:C:216:LYS:HD2	1:C:271:ASP:HA	1.89	0.54
1:C:500:VAL:HG11	1:D:527:ARG:NE	2.22	0.54
1:C:513:PHE:O	1:C:517:LEU:HG	2.07	0.54
1:B:216:LYS:HD2	1:B:271:ASP:HA	1.90	0.54
1:B:356:ASP:O	1:B:360:LEU:HG	2.07	0.54
1:A:158:MSE:HE2	1:A:176:MSE:HG3	1.88	0.54
1:A:445:LEU:HG	1:A:487:TRP:CD1	2.42	0.54
1:B:158:MSE:SE	1:B:176:MSE:HE2	2.58	0.54
1:B:186:TYR:CE1	1:B:191:ILE:HD11	2.42	0.54
1:C:67:GLY:C	1:C:68:ILE:HD12	2.33	0.54
1:D:337:VAL:HG21	1:D:380:ILE:CG2	2.38	0.54
1:D:468:LYS:NZ	1:D:468:LYS:HB3	2.22	0.54
1:A:153:ASP:OD2	1:A:155:TYR:HB3	2.07	0.54
1:D:527:ARG:HB2	1:D:531:ARG:NH1	2.22	0.54
1:B:96:THR:HG22	1:B:97:LYS:N	2.23	0.54
1:B:329:LYS:HA	1:B:418:TYR:OH	2.06	0.54
1:A:110:THR:HG22	1:A:448:ASP:OD1	2.07	0.54
1:A:530:GLU:HB2	1:B:497:PHE:CD2	2.43	0.54
1:A:73:LEU:HD11	1:A:154:LEU:HD11	1.90	0.54
1:A:242:LEU:CD2	1:A:293:ILE:HB	2.38	0.54
1:A:224:ARG:HH11	1:A:287:LEU:HB3	1.73	0.53
1:B:67:GLY:C	1:B:68:ILE:HD12	2.33	0.53
1:B:115:LEU:HD22	1:B:511:GLU:HG2	1.90	0.53
1:B:251:VAL:HG21	1:B:274:GLU:O	2.08	0.53
1:C:316:ILE:HD12	1:C:316:ILE:C	2.33	0.53
1:A:502:GLY:O	1:A:506:GLN:HG3	2.09	0.53
1:B:22:LYS:O	1:B:22:LYS:HG3	2.08	0.53
1:B:66:LEU:HB2	1:B:137:VAL:HG11	1.91	0.53
1:B:321:LEU:HD21	1:B:446:ILE:HG13	1.91	0.53
1:D:70:LEU:CD2	1:D:242:LEU:HB3	2.39	0.53
1:B:164:LEU:O	1:D:97:LYS:HG3	2.07	0.53
1:C:117:LEU:HD21	1:C:133:LEU:CD2	2.38	0.53
1:D:18:LYS:O	1:D:28:THR:HA	2.08	0.53
1:D:69:MSE:HE1	1:D:227:ILE:HG23	1.90	0.53
1:D:437:GLU:HB3	3:D:945:HOH:O	2.07	0.53
1:D:310:GLU:HA	1:D:479:PRO:HG2	1.90	0.53
1:A:516:LEU:C	1:A:516:LEU:HD12	2.34	0.53
1:B:69:MSE:HE1	1:B:227:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ASN:HA	1:D:200:ASN:HD21	1.72	0.53
1:B:445:LEU:HG	1:B:487:TRP:CD1	2.41	0.53
1:C:458:ARG:HH11	1:C:458:ARG:CB	2.22	0.53
1:C:468:LYS:HG2	1:C:471:ALA:HB2	1.90	0.53
1:D:67:GLY:C	1:D:68:ILE:HD12	2.33	0.53
1:D:203:ILE:HD13	1:D:222:ARG:HG2	1.90	0.53
1:A:432:ILE:HD12	1:B:432:ILE:HD12	1.89	0.53
1:B:350:ASN:HD22	1:B:350:ASN:N	2.06	0.53
1:D:208:LYS:HE3	1:D:208:LYS:N	2.24	0.53
1:D:220:LEU:C	1:D:220:LEU:HD23	2.33	0.53
1:A:305:LEU:HD23	1:A:308:LEU:HD23	1.91	0.53
1:B:70:LEU:CD2	1:B:242:LEU:HB3	2.39	0.53
1:B:354:ASN:ND2	1:B:357:GLY:H	2.07	0.53
1:C:101:LYS:HE2	3:C:923:HOH:O	2.09	0.53
1:D:70:LEU:HD23	1:D:242:LEU:HB3	1.90	0.53
1:A:158:MSE:SE	1:A:176:MSE:HE2	2.59	0.53
1:C:187:TYR:OH	1:C:216:LYS:HG2	2.09	0.53
1:A:220:LEU:HD21	1:A:287:LEU:HD12	1.91	0.52
1:A:248:GLU:OE2	1:A:277:PRO:HG2	2.09	0.52
1:D:69:MSE:HE1	1:D:227:ILE:CG1	2.37	0.52
1:D:282:ALA:O	1:D:286:ILE:HG13	2.09	0.52
1:A:14:VAL:HG22	1:B:47:VAL:HB	1.91	0.52
1:B:224:ARG:HD2	1:B:288:GLU:OE2	2.09	0.52
1:D:151:ASN:H	1:D:200:ASN:ND2	2.07	0.52
1:A:40:THR:HG22	1:A:42:SER:H	1.74	0.52
1:B:346:ILE:O	1:B:398:HIS:HA	2.10	0.52
1:C:57:LYS:HB3	1:C:460:SER:OG	2.09	0.52
1:C:110:THR:HG22	1:C:448:ASP:OD1	2.09	0.52
1:C:192:ALA:HB3	1:C:359:ASN:HD22	1.74	0.52
1:A:203:ILE:HG21	1:A:222:ARG:HG2	1.91	0.52
1:B:147:TRP:HB3	1:B:184:SER:HB2	1.92	0.52
1:B:394:LYS:HE3	3:B:967:HOH:O	2.09	0.52
1:D:117:LEU:HD21	1:D:133:LEU:CD2	2.40	0.52
1:B:516:LEU:HD12	1:B:516:LEU:C	2.34	0.52
1:A:247:THR:HA	1:A:298:GLN:OE1	2.10	0.52
1:A:251:VAL:HG21	1:A:274:GLU:O	2.10	0.52
1:B:441:LEU:C	1:B:444:PRO:HD2	2.35	0.52
1:D:452:MSE:HE2	1:D:510:LEU:HD22	1.91	0.52
1:A:66:LEU:HB2	1:A:137:VAL:HG11	1.92	0.52
1:A:492:LEU:H	1:A:492:LEU:CD2	2.18	0.52
1:B:421:GLU:HG2	3:B:1044:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ASN:HB3	1:C:359:ASN:OD1	2.10	0.52
1:D:258:ASN:HB2	1:D:302:VAL:HG21	1.91	0.52
1:A:67:GLY:C	1:A:68:ILE:HD12	2.34	0.52
1:A:203:ILE:HG23	1:A:222:ARG:NH1	2.25	0.51
1:A:300:THR:HA	3:A:910:HOH:O	2.09	0.51
1:A:407:PRO:HG3	1:D:397:ASP:HB2	1.92	0.51
1:A:515:ARG:NH1	1:A:523:GLN:HG2	2.25	0.51
1:B:22:LYS:HE2	1:B:27:LEU:HD11	1.92	0.51
1:B:150:ASN:HA	1:B:200:ASN:ND2	2.25	0.51
1:B:445:LEU:HD23	1:B:445:LEU:C	2.36	0.51
1:D:111:GLN:HG3	3:D:918:HOH:O	2.09	0.51
1:C:247:THR:HA	1:C:298:GLN:NE2	2.25	0.51
1:D:445:LEU:HG	1:D:487:TRP:CD1	2.42	0.51
1:A:115:LEU:HD21	1:A:507:ARG:HH12	1.74	0.51
1:A:261:MSE:CE	1:A:307:GLN:HG2	2.40	0.51
1:D:12:VAL:HG21	1:D:133:LEU:HD23	1.92	0.51
1:D:465:ASP:OD1	1:D:466:PRO:HD2	2.10	0.51
1:A:261:MSE:HE2	1:A:307:GLN:O	2.11	0.51
1:B:150:ASN:HA	1:B:200:ASN:HD21	1.75	0.51
1:D:76:ASN:HD21	1:D:354:ASN:HB2	1.75	0.51
1:D:216:LYS:HA	1:D:219:HIS:ND1	2.25	0.51
1:A:242:LEU:HD13	1:A:243:TRP:N	2.26	0.51
1:A:300:THR:O	1:A:305:LEU:HD12	2.11	0.51
1:A:346:ILE:O	1:A:398:HIS:HA	2.11	0.51
1:A:500:VAL:HA	3:A:1020:HOH:O	2.10	0.51
1:B:110:THR:HG22	1:B:448:ASP:OD1	2.11	0.51
1:C:242:LEU:CD2	1:C:293:ILE:HB	2.41	0.51
1:D:94:PHE:CD2	1:D:168:LEU:HD13	2.46	0.51
1:A:147:TRP:HB3	1:A:184:SER:HB2	1.91	0.51
1:B:258:ASN:HD22	1:B:302:VAL:HG11	1.75	0.51
1:C:351:HIS:CE1	1:C:413:VAL:HB	2.46	0.51
1:C:354:ASN:OD1	1:C:410:ASP:HA	2.10	0.51
1:A:246:ASN:ND2	1:A:359:ASN:HB2	2.26	0.51
1:A:69:MSE:HE1	1:A:227:ILE:CG1	2.38	0.50
1:B:261:MSE:HG3	1:B:307:GLN:CG	2.41	0.50
1:B:268:ILE:HG12	1:B:275:ILE:HG12	1.93	0.50
1:B:190:PHE:O	1:B:248:GLU:HA	2.12	0.50
1:D:225:ARG:HG3	1:D:225:ARG:HH11	1.77	0.50
1:B:192:ALA:O	1:B:195:GLN:HG2	2.10	0.50
1:B:310:GLU:HA	1:B:479:PRO:HG2	1.93	0.50
1:C:197:GLU:CD	1:C:197:GLU:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ASN:HD22	1:C:389:ASN:C	2.18	0.50
1:D:302:VAL:HB	1:D:303:PRO:HD2	1.94	0.50
1:A:63:PRO:HG2	1:A:238:LYS:HD2	1.92	0.50
1:D:116:LYS:HZ2	1:D:527:ARG:HH22	1.60	0.50
1:B:195:GLN:HA	1:B:195:GLN:NE2	2.26	0.50
1:C:246:ASN:HD22	2:C:902:NAD:H8A	1.76	0.50
1:C:482:THR:OG1	1:D:531:ARG:HG2	2.12	0.50
1:C:527:ARG:HB2	1:C:531:ARG:NH1	2.26	0.50
1:D:388:TYR:HA	1:D:393:GLY:O	2.12	0.50
1:D:447:ILE:O	1:D:451:VAL:HG23	2.12	0.50
1:A:376:VAL:HG22	1:A:501:ASN:HB3	1.93	0.50
1:C:261:MSE:CE	1:C:307:GLN:HG2	2.42	0.50
1:D:66:LEU:HB2	1:D:137:VAL:HG11	1.92	0.50
1:D:223:ILE:HD12	1:D:280:ILE:HG22	1.93	0.50
1:A:66:LEU:HD13	1:A:68:ILE:HD11	1.94	0.50
1:A:441:LEU:C	1:A:444:PRO:HD2	2.37	0.50
1:B:200:ASN:H	1:B:200:ASN:HD22	1.58	0.50
1:B:329:LYS:HD3	1:B:416:ASP:OD2	2.12	0.50
1:D:314:THR:HG22	1:D:315:PHE:N	2.27	0.50
1:A:59:ASP:HB3	1:A:458:ARG:HB3	1.94	0.49
1:B:286:ILE:HA	1:B:314:THR:HG21	1.94	0.49
1:C:260:THR:HB	1:C:262:GLU:OE2	2.11	0.49
1:C:406:LYS:N	1:C:407:PRO:HD2	2.27	0.49
1:A:316:ILE:O	1:A:317:ALA:HB2	2.12	0.49
1:C:444:PRO:HG3	1:D:423:MSE:HE3	1.94	0.49
1:D:513:PHE:O	1:D:516:LEU:HG	2.12	0.49
1:B:272:HIS:ND1	1:B:274:GLU:HB2	2.27	0.49
1:C:166:TYR:O	1:C:170:GLN:HG2	2.13	0.49
1:A:388:TYR:HA	1:A:393:GLY:O	2.12	0.49
1:B:298:GLN:C	1:B:300:THR:H	2.21	0.49
1:C:238:LYS:NZ	1:C:457:THR:HG21	2.27	0.49
1:C:394:LYS:HG2	1:C:394:LYS:O	2.11	0.49
1:A:321:LEU:HG	1:A:445:LEU:HD22	1.95	0.49
1:C:66:LEU:HB2	1:C:137:VAL:HG11	1.94	0.49
1:C:377:ILE:O	1:C:381:ILE:HG13	2.13	0.49
1:C:516:LEU:HD12	1:C:517:LEU:N	2.27	0.49
1:A:386:ILE:HD11	1:B:129:PRO:HB3	1.93	0.49
1:A:531:ARG:HG2	1:B:482:THR:OG1	2.12	0.49
1:B:350:ASN:O	1:B:402:ILE:HA	2.13	0.49
1:A:96:THR:HG21	1:A:101:LYS:HD2	1.95	0.49
1:B:261:MSE:HE2	1:B:307:GLN:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ALA:HB3	1:C:359:ASN:ND2	2.28	0.49
1:C:447:ILE:O	1:C:451:VAL:HG23	2.13	0.49
3:C:989:HOH:O	1:D:423:MSE:HG2	2.12	0.49
1:B:504:ASN:O	1:B:508:THR:HG23	2.12	0.49
1:D:205:LEU:HA	1:D:210:ASN:O	2.12	0.49
1:A:61:LYS:HB3	1:A:61:LYS:HZ3	1.78	0.49
1:B:478:TYR:CE2	1:B:494:ARG:HB3	2.48	0.49
1:D:354:ASN:H	1:D:354:ASN:ND2	2.11	0.49
1:A:315:PHE:HD2	1:A:481:LEU:HD11	1.78	0.49
1:A:533:LEU:HD13	1:A:533:LEU:C	2.38	0.49
1:B:470:ASP:HA	3:B:978:HOH:O	2.11	0.49
1:C:55:VAL:HG23	1:C:464:VAL:CG2	2.43	0.49
1:C:298:GLN:C	1:C:300:THR:H	2.21	0.49
1:C:316:ILE:HD12	1:C:316:ILE:O	2.12	0.49
1:D:264:LEU:HD21	1:D:305:LEU:HG	1.95	0.49
1:A:216:LYS:HD2	1:A:271:ASP:HA	1.94	0.48
1:B:15:VAL:HG23	1:B:15:VAL:O	2.13	0.48
1:B:39:LYS:H	1:B:39:LYS:CD	2.20	0.48
1:D:357:GLY:HA3	1:D:404:TYR:CD1	2.48	0.48
1:C:350:ASN:O	1:C:402:ILE:HA	2.13	0.48
1:A:478:TYR:CD1	1:A:479:PRO:HD2	2.48	0.48
1:B:260:THR:OG1	1:B:263:ASN:ND2	2.47	0.48
1:C:206:ASP:HB3	1:C:212:THR:HG21	1.96	0.48
1:D:244:THR:HG22	2:D:903:NAD:H51N	1.96	0.48
1:A:305:LEU:O	1:A:308:LEU:HB3	2.13	0.48
1:B:195:GLN:NE2	1:B:198:ARG:HD3	2.28	0.48
1:B:244:THR:HG22	2:B:901:NAD:H51N	1.95	0.48
1:B:354:ASN:H	1:B:354:ASN:HD22	1.61	0.48
1:D:437:GLU:HG3	1:D:440:LEU:CD1	2.25	0.48
1:B:354:ASN:HD22	1:B:354:ASN:N	2.11	0.48
1:D:360:LEU:HD13	1:D:402:ILE:HG21	1.96	0.48
1:A:468:LYS:HE3	1:A:471:ALA:HB1	1.94	0.48
1:C:238:LYS:CE	1:C:457:THR:HG21	2.43	0.48
1:D:376:VAL:HG22	1:D:501:ASN:HB3	1.96	0.48
1:C:203:ILE:HG21	1:C:222:ARG:HG2	1.96	0.48
1:C:375:SER:HB2	1:C:378:ASP:OD2	2.14	0.48
1:C:423:MSE:HE3	1:D:444:PRO:CG	2.20	0.48
1:D:58:LEU:HD22	1:D:134:LEU:HD13	1.94	0.48
1:D:446:ILE:O	1:D:450:LEU:HG	2.14	0.48
1:A:423:MSE:HE3	1:B:444:PRO:HG3	1.94	0.48
1:B:96:THR:CG2	1:B:97:LYS:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:TYR:HA	1:C:393:GLY:O	2.14	0.48
1:D:129:PRO:HG2	1:D:132:SER:CB	2.40	0.48
1:A:291:PRO:HB3	1:A:315:PHE:HB2	1.95	0.47
1:A:334:GLN:NE2	1:A:380:ILE:HG12	2.28	0.47
1:A:337:VAL:HG21	1:A:380:ILE:HG21	1.96	0.47
1:B:125:ASP:CG	1:B:527:ARG:HH22	2.22	0.47
1:C:302:VAL:O	1:C:306:VAL:HG23	2.13	0.47
1:A:323:SER:O	1:A:327:LYS:HG3	2.14	0.47
1:A:332:LEU:HD11	1:A:432:ILE:HD11	1.96	0.47
1:C:375:SER:HB3	3:C:929:HOH:O	2.14	0.47
1:D:69:MSE:HA	1:D:145:SER:O	2.14	0.47
1:D:147:TRP:HB3	1:D:184:SER:HB2	1.95	0.47
1:D:322:LYS:HG2	1:D:327:LYS:HG3	1.95	0.47
1:C:203:ILE:HD13	1:C:222:ARG:CG	2.44	0.47
1:A:286:ILE:HA	1:A:314:THR:HG21	1.95	0.47
1:A:325:GLN:OE1	1:A:328:LEU:HD12	2.14	0.47
1:A:527:ARG:HD3	3:A:979:HOH:O	2.13	0.47
1:C:18:LYS:HE3	3:C:1020:HOH:O	2.15	0.47
1:C:81:LEU:C	1:C:81:LEU:HD23	2.40	0.47
1:D:16:THR:HG23	3:D:1018:HOH:O	2.14	0.47
1:A:263:ASN:N	1:A:263:ASN:HD22	2.12	0.47
1:A:356:ASP:O	1:A:360:LEU:HG	2.15	0.47
1:B:65:LYS:HD3	1:B:141:ASP:HB3	1.95	0.47
1:A:158:MSE:CE	1:A:176:MSE:HG3	2.44	0.47
1:A:243:TRP:CE2	1:A:245:ALA:HB3	2.49	0.47
1:A:445:LEU:C	1:A:445:LEU:HD23	2.40	0.47
1:B:447:ILE:O	1:B:451:VAL:HG23	2.14	0.47
1:D:243:TRP:CE2	1:D:245:ALA:HB3	2.50	0.47
1:D:350:ASN:HB3	1:D:412:LYS:HE2	1.97	0.47
1:D:478:TYR:CD1	1:D:479:PRO:HD2	2.50	0.47
1:C:454:GLU:O	1:C:457:THR:HB	2.14	0.47
1:D:218:THR:HA	1:D:221:GLN:NE2	2.26	0.47
1:A:350:ASN:O	1:A:402:ILE:HA	2.15	0.47
1:D:23:ASP:O	1:D:25:GLU:HG3	2.15	0.47
1:A:431:SER:HB2	1:B:433:HIS:HB3	1.97	0.47
1:B:513:PHE:O	1:B:517:LEU:HG	2.15	0.47
1:C:12:VAL:HG21	1:C:133:LEU:HD23	1.97	0.47
1:C:524:ASN:C	1:C:526:LEU:H	2.23	0.47
1:B:63:PRO:CG	1:B:238:LYS:HG3	2.45	0.46
1:C:158:MSE:SE	1:C:176:MSE:HE2	2.64	0.46
1:D:153:ASP:OD2	1:D:155:TYR:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MSE:HE1	1:A:227:ILE:HG23	1.97	0.46
1:A:283:ALA:O	1:A:287:LEU:HG	2.15	0.46
1:B:297:PRO:HD3	1:B:320:ASP:OD2	2.14	0.46
1:C:205:LEU:HA	1:C:210:ASN:O	2.15	0.46
1:C:352:LEU:HD22	1:C:354:ASN:HD22	1.79	0.46
1:A:185:ILE:CD1	1:A:223:ILE:HD11	2.45	0.46
1:A:318:GLY:H	1:A:492:LEU:HD21	1.79	0.46
1:B:116:LYS:HD3	1:B:523:GLN:NE2	2.28	0.46
1:B:242:LEU:HD12	1:B:244:THR:OG1	2.14	0.46
1:A:122:GLU:H	1:A:122:GLU:CD	2.23	0.46
1:A:473:LYS:HG2	1:A:474:PHE:H	1.80	0.46
1:B:184:SER:O	1:B:202:CYS:HA	2.14	0.46
1:C:47:VAL:HG11	1:D:520:LEU:HD21	1.98	0.46
1:C:527:ARG:H	1:C:531:ARG:HH11	1.64	0.46
1:D:257:VAL:HG11	1:D:274:GLU:OE1	2.16	0.46
1:D:260:THR:HA	1:D:307:GLN:NE2	2.31	0.46
1:D:482:THR:C	1:D:484:LEU:H	2.23	0.46
1:A:272:HIS:HB3	1:A:275:ILE:HD13	1.96	0.46
1:B:81:LEU:C	1:B:81:LEU:HD23	2.41	0.46
1:C:432:ILE:HD12	1:D:432:ILE:HD12	1.95	0.46
1:C:513:PHE:O	1:C:516:LEU:HG	2.14	0.46
1:D:73:LEU:CD2	1:D:154:LEU:HD11	2.40	0.46
1:A:406:LYS:N	1:A:407:PRO:CD	2.77	0.46
1:B:243:TRP:CZ2	1:B:245:ALA:HB3	2.51	0.46
1:C:359:ASN:HB2	3:C:952:HOH:O	2.15	0.46
1:A:447:ILE:O	1:A:451:VAL:HG23	2.16	0.46
1:B:82:VAL:HG21	1:B:154:LEU:CD1	2.45	0.46
1:C:37:VAL:HG22	1:C:47:VAL:HG22	1.98	0.46
1:D:515:ARG:HB3	1:D:520:LEU:HB2	1.98	0.46
1:B:69:MSE:CE	1:B:227:ILE:HG12	2.37	0.46
1:A:148:ASP:HA	2:A:900:NAD:N3A	2.31	0.45
1:A:273:GLU:OE1	1:A:273:GLU:O	2.34	0.45
1:D:454:GLU:C	1:D:454:GLU:CD	2.83	0.45
1:A:18:LYS:O	1:A:28:THR:HA	2.16	0.45
1:A:452:MSE:HE2	1:A:510:LEU:HD22	1.98	0.45
1:B:16:THR:CG2	1:B:18:LYS:HG3	2.46	0.45
1:B:248:GLU:H	1:B:298:GLN:NE2	2.14	0.45
1:D:158:MSE:SE	1:D:176:MSE:HE2	2.66	0.45
1:D:377:ILE:O	1:D:381:ILE:HG13	2.15	0.45
1:C:497:PHE:CD2	1:D:530:GLU:HB2	2.51	0.45
1:D:96:THR:C	1:D:98:GLU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:ASN:N	1:D:354:ASN:HD22	2.13	0.45
1:A:243:TRP:CZ2	1:A:245:ALA:HB3	2.51	0.45
1:B:223:ILE:O	1:B:227:ILE:HG13	2.17	0.45
1:C:525:GLU:O	1:C:527:ARG:HG3	2.17	0.45
1:D:349:TYR:C	1:D:350:ASN:HD22	2.24	0.45
1:A:116:LYS:HB3	1:A:523:GLN:HE22	1.81	0.45
1:A:520:LEU:HA	1:A:521:PRO:HD3	1.85	0.45
1:B:225:ARG:HD3	3:B:971:HOH:O	2.17	0.45
1:C:248:GLU:H	1:C:298:GLN:NE2	2.15	0.45
1:D:243:TRP:CZ2	1:D:245:ALA:HB3	2.52	0.45
1:D:452:MSE:HG3	1:D:487:TRP:CH2	2.51	0.45
1:A:220:LEU:C	1:A:220:LEU:HD23	2.42	0.45
1:A:343:PRO:HD2	1:A:388:TYR:OH	2.17	0.45
1:C:105:TYR:HA	1:D:423:MSE:HE2	1.99	0.45
1:D:465:ASP:C	1:D:467:VAL:H	2.24	0.45
1:B:97:LYS:HB3	1:B:98:GLU:OE2	2.16	0.45
1:C:147:TRP:CD2	1:C:281:PHE:HE2	2.35	0.45
1:C:264:LEU:O	1:C:268:ILE:HG13	2.17	0.45
1:A:217:TRP:O	1:A:221:GLN:HG3	2.17	0.45
1:A:224:ARG:HD3	1:A:287:LEU:HB2	1.99	0.45
1:A:465:ASP:HB3	1:A:468:LYS:O	2.16	0.45
1:B:293:ILE:HD11	1:B:453:THR:OG1	2.17	0.45
1:C:500:VAL:HG11	1:D:527:ARG:HE	1.81	0.45
1:D:351:HIS:HB2	1:D:403:LYS:O	2.16	0.45
1:B:326:THR:HG21	1:B:489:LYS:HG2	1.99	0.45
1:B:377:ILE:O	1:B:381:ILE:HG13	2.16	0.45
1:C:33:GLU:HA	1:C:50:THR:O	2.16	0.45
1:C:376:VAL:HG22	1:C:501:ASN:CB	2.40	0.45
1:C:389:ASN:ND2	1:C:392:LEU:N	2.62	0.45
1:D:276:ALA:HB1	1:D:277:PRO:HD2	1.99	0.45
1:D:376:VAL:HG13	1:D:501:ASN:HB2	1.99	0.45
1:A:36:VAL:HA	1:B:119:ILE:O	2.17	0.45
1:B:67:GLY:O	1:B:239:VAL:HA	2.17	0.45
1:B:220:LEU:O	1:B:220:LEU:HD23	2.17	0.45
1:B:446:ILE:O	1:B:450:LEU:HG	2.17	0.45
1:D:154:LEU:HD23	1:D:179:VAL:HG12	1.99	0.45
1:A:276:ALA:HB1	1:A:277:PRO:HD2	1.99	0.44
1:A:518:ILE:HD11	1:A:520:LEU:HD12	1.99	0.44
1:C:482:THR:C	1:C:484:LEU:H	2.24	0.44
1:D:115:LEU:HD12	1:D:133:LEU:HD11	1.98	0.44
1:D:246:ASN:HB3	1:D:359:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ILE:HG21	1:C:243:TRP:CE3	2.53	0.44
1:C:203:ILE:HD13	1:C:222:ARG:HG2	1.98	0.44
1:C:243:TRP:CE2	1:C:245:ALA:HB3	2.52	0.44
1:C:294:ASN:ND2	1:C:319:ASP:HA	2.31	0.44
1:C:355:ASN:HB3	2:C:902:NAD:O1A	2.16	0.44
1:A:190:PHE:CE2	1:A:276:ALA:HB2	2.52	0.44
1:A:316:ILE:O	1:A:480:VAL:HA	2.17	0.44
1:B:200:ASN:HD22	1:B:200:ASN:N	2.13	0.44
1:B:208:LYS:H	1:B:208:LYS:CD	2.31	0.44
1:B:441:LEU:O	1:B:444:PRO:HD2	2.17	0.44
1:C:69:MSE:HE1	1:C:227:ILE:CG1	2.34	0.44
1:A:47:VAL:HB	1:B:14:VAL:HG22	1.98	0.44
1:A:350:ASN:HB2	1:A:402:ILE:HG12	1.98	0.44
1:A:461:TYR:CE2	1:B:532:LEU:HG	2.52	0.44
1:A:513:PHE:O	1:A:516:LEU:HG	2.16	0.44
1:B:44:ARG:HB3	1:B:44:ARG:NH1	2.33	0.44
1:C:109:MSE:HE3	1:C:109:MSE:HB2	1.87	0.44
1:C:524:ASN:O	1:C:524:ASN:CG	2.61	0.44
1:D:272:HIS:HB3	1:D:275:ILE:HD13	1.99	0.44
1:D:272:HIS:HE1	1:D:274:GLU:HG3	1.82	0.44
1:D:351:HIS:CE1	1:D:413:VAL:HB	2.53	0.44
1:A:405:MSE:C	1:A:407:PRO:HD2	2.42	0.44
1:C:200:ASN:C	1:C:200:ASN:ND2	2.75	0.44
1:A:302:VAL:HB	1:A:303:PRO:HD2	1.99	0.44
1:B:148:ASP:C	1:B:150:ASN:H	2.25	0.44
1:B:437:GLU:H	1:B:437:GLU:HG2	1.36	0.44
1:C:37:VAL:HG12	1:C:38:THR:N	2.32	0.44
1:C:349:TYR:C	1:C:350:ASN:ND2	2.73	0.44
1:D:242:LEU:HD13	1:D:243:TRP:N	2.33	0.44
1:A:120:ASP:OD2	1:A:124:ASN:N	2.51	0.44
1:B:191:ILE:HD12	1:B:195:GLN:HG3	2.00	0.44
1:B:200:ASN:HD22	1:B:200:ASN:C	2.26	0.44
1:B:325:GLN:HG2	1:B:414:ALA:HB1	1.99	0.44
1:C:52:GLN:HG3	1:C:54:TYR:CE1	2.53	0.44
1:C:251:VAL:HG13	1:C:251:VAL:O	2.18	0.44
1:C:521:PRO:HG2	1:D:33:GLU:HB3	1.99	0.44
1:D:323:SER:O	1:D:327:LYS:HG3	2.18	0.44
1:D:437:GLU:H	1:D:437:GLU:HG2	1.45	0.44
1:A:69:MSE:CE	1:A:227:ILE:HG12	2.41	0.44
1:A:73:LEU:HD13	1:A:73:LEU:O	2.17	0.44
1:A:242:LEU:HD13	1:A:242:LEU:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LYS:HE2	1:B:335:PHE:CE1	2.52	0.44
1:A:344:VAL:HG11	1:A:421:GLU:HG3	2.00	0.44
1:B:109:MSE:HG3	1:B:110:THR:N	2.33	0.44
1:C:337:VAL:HG21	1:C:380:ILE:CG2	2.48	0.44
1:A:327:LYS:HE2	1:B:335:PHE:HE1	1.82	0.44
1:B:68:ILE:HG12	1:B:450:LEU:HD13	1.99	0.44
1:B:221:GLN:HG2	3:B:984:HOH:O	2.17	0.44
1:B:259:ASP:HA	1:B:303:PRO:HG2	2.00	0.44
1:C:533:LEU:HD13	1:C:533:LEU:C	2.43	0.44
1:A:224:ARG:HG2	1:A:284:ALA:HB1	2.00	0.43
1:A:461:TYR:O	1:A:474:PHE:HA	2.17	0.43
1:A:529:GLU:OE1	1:A:529:GLU:N	2.49	0.43
1:B:57:LYS:HB2	1:B:474:PHE:CE2	2.53	0.43
1:B:351:HIS:HD2	1:B:405:MSE:HB2	1.82	0.43
1:C:115:LEU:O	1:C:127:TYR:HA	2.17	0.43
1:C:257:VAL:HG23	1:C:258:ASN:H	1.83	0.43
1:C:70:LEU:CD2	1:C:242:LEU:HB3	2.48	0.43
1:C:362:ALA:HB1	1:C:363:PRO:HD2	2.00	0.43
1:D:58:LEU:CD2	1:D:134:LEU:HD13	2.47	0.43
1:D:494:ARG:HG3	1:D:497:PHE:CD1	2.53	0.43
1:C:18:LYS:O	1:C:28:THR:HA	2.18	0.43
1:C:257:VAL:HG23	1:C:258:ASN:N	2.33	0.43
1:A:407:PRO:HD3	1:D:397:ASP:OD2	2.19	0.43
1:C:225:ARG:HH11	1:C:229:ASN:HB2	1.82	0.43
1:A:478:TYR:O	1:A:479:PRO:C	2.61	0.43
1:C:40:THR:HG22	1:C:41:ALA:N	2.33	0.43
1:C:149:ILE:HD11	3:C:978:HOH:O	2.19	0.43
1:C:242:LEU:HD13	1:C:243:TRP:N	2.33	0.43
1:D:40:THR:CG2	1:D:41:ALA:N	2.82	0.43
1:D:203:ILE:HD11	3:D:965:HOH:O	2.18	0.43
1:B:265:LEU:O	1:B:269:LYS:HG3	2.19	0.43
1:C:159:GLN:HG2	3:C:956:HOH:O	2.18	0.43
1:C:459:VAL:HG11	1:C:513:PHE:HZ	1.83	0.43
1:D:16:THR:HB	3:D:975:HOH:O	2.19	0.43
1:A:68:ILE:HG12	1:A:450:LEU:HD13	2.00	0.43
1:A:90:HIS:CD2	1:A:175:LYS:HE2	2.53	0.43
1:B:80:THR:HG22	1:B:443:THR:HG21	2.01	0.43
1:C:482:THR:C	1:C:484:LEU:N	2.77	0.43
1:C:527:ARG:H	1:C:531:ARG:NH1	2.16	0.43
1:D:350:ASN:HD22	1:D:350:ASN:N	2.15	0.43
1:D:354:ASN:H	1:D:354:ASN:HD22	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:ASN:HD22	1:D:354:ASN:C	2.26	0.43
1:D:406:LYS:C	1:D:408:VAL:H	2.26	0.43
1:A:204:ASN:ND2	1:A:211:VAL:HG13	2.33	0.43
1:B:352:LEU:CD1	1:B:357:GLY:HA3	2.48	0.43
1:B:406:LYS:C	1:B:408:VAL:H	2.27	0.43
1:B:513:PHE:O	1:B:516:LEU:HG	2.19	0.43
1:C:318:GLY:HA2	1:C:488:LEU:CD2	2.46	0.43
1:D:189:ASP:O	1:D:249:ARG:NH1	2.52	0.43
1:D:200:ASN:HD22	1:D:200:ASN:C	2.25	0.43
1:B:482:THR:C	1:B:484:LEU:H	2.26	0.43
1:A:232:GLU:C	1:A:232:GLU:CD	2.87	0.43
1:B:115:LEU:CD2	1:B:511:GLU:HG2	2.49	0.43
1:B:350:ASN:N	1:B:350:ASN:ND2	2.66	0.43
1:C:507:ARG:NH1	1:C:511:GLU:OE1	2.52	0.43
1:D:200:ASN:ND2	1:D:200:ASN:H	2.16	0.43
1:D:314:THR:HG22	1:D:315:PHE:H	1.84	0.43
1:A:437:GLU:H	1:A:437:GLU:HG2	1.59	0.42
1:B:153:ASP:OD2	1:B:153:ASP:C	2.61	0.42
1:B:277:PRO:O	1:B:281:PHE:HD1	2.01	0.42
1:B:449:LEU:HD21	1:B:487:TRP:HB2	2.00	0.42
1:D:381:ILE:HG23	1:D:388:TYR:CG	2.54	0.42
1:D:523:GLN:HG3	3:D:923:HOH:O	2.19	0.42
1:A:346:ILE:HD12	1:A:377:ILE:HD13	2.01	0.42
1:A:414:ALA:C	1:A:415:MSE:HG3	2.44	0.42
1:B:251:VAL:HG22	1:B:274:GLU:HG3	2.01	0.42
1:C:276:ALA:HB1	1:C:277:PRO:HD2	2.01	0.42
1:A:47:VAL:O	1:B:15:VAL:HG22	2.19	0.42
1:C:153:ASP:OD2	1:C:153:ASP:C	2.61	0.42
1:D:183:PRO:HG2	3:D:965:HOH:O	2.18	0.42
1:D:203:ILE:HD13	1:D:222:ARG:CG	2.49	0.42
1:A:59:ASP:O	1:A:458:ARG:HD2	2.20	0.42
1:A:398:HIS:HB2	3:A:970:HOH:O	2.19	0.42
1:A:533:LEU:HD23	1:B:463:LYS:HZ2	1.84	0.42
1:B:19:CYS:HA	1:B:27:LEU:O	2.19	0.42
1:B:190:PHE:CE2	1:B:276:ALA:HB2	2.53	0.42
1:B:347:ALA:O	1:B:416:ASP:HA	2.19	0.42
1:B:389:ASN:HD22	1:B:391:LYS:H	1.67	0.42
1:D:342:LYS:HG3	1:D:388:TYR:CZ	2.54	0.42
1:B:206:ASP:OD2	1:B:210:ASN:HB2	2.20	0.42
1:B:405:MSE:HB3	1:B:408:VAL:CG2	2.50	0.42
1:B:412:LYS:HB2	1:B:438:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:HA	1:C:219:HIS:ND1	2.34	0.42
1:D:408:VAL:HG12	1:D:411:SER:HB3	2.00	0.42
1:A:187:TYR:OH	1:A:216:LYS:HG2	2.19	0.42
1:A:318:GLY:HA2	1:A:488:LEU:HD22	2.00	0.42
1:C:337:VAL:HG21	1:C:380:ILE:HG21	2.01	0.42
1:C:532:LEU:HG	1:D:461:TYR:CE2	2.54	0.42
1:D:231:LYS:HG2	1:D:239:VAL:HG21	2.01	0.42
1:A:531:ARG:HG3	1:A:531:ARG:HH11	1.85	0.42
1:B:16:THR:HG22	1:B:18:LYS:HG3	2.02	0.42
1:B:406:LYS:N	1:B:407:PRO:CD	2.83	0.42
1:C:16:THR:HG22	1:C:17:ASP:N	2.35	0.42
1:B:354:ASN:ND2	1:B:354:ASN:N	2.65	0.42
1:C:286:ILE:HA	1:C:314:THR:HG21	2.02	0.42
1:D:329:LYS:HD2	1:D:418:TYR:OH	2.19	0.42
1:D:360:LEU:HD13	1:D:402:ILE:CG2	2.50	0.42
1:D:443:THR:N	1:D:444:PRO:CD	2.83	0.42
1:A:310:GLU:HA	1:A:479:PRO:HG2	2.02	0.42
1:C:134:LEU:HB3	1:C:135:PRO:HD2	2.02	0.42
1:C:192:ALA:HB2	3:C:968:HOH:O	2.20	0.42
1:C:440:LEU:O	1:C:444:PRO:HG2	2.19	0.42
1:C:21:TYR:CZ	1:C:26:LEU:HD13	2.55	0.42
1:D:59:ASP:HB3	1:D:458:ARG:HB3	2.01	0.42
1:D:358:TYR:O	1:D:362:ALA:HB2	2.20	0.42
1:A:256:GLY:HA2	1:A:263:ASN:OD1	2.20	0.41
1:A:494:ARG:HD2	1:B:530:GLU:O	2.19	0.41
1:C:242:LEU:HD13	1:C:242:LEU:C	2.44	0.41
1:C:497:PHE:CE2	1:D:530:GLU:HB2	2.55	0.41
1:A:251:VAL:HG12	1:A:299:ASN:HD21	1.82	0.41
1:A:428:ASN:OD1	1:B:436:CYS:HB3	2.19	0.41
1:B:405:MSE:HB3	1:B:408:VAL:HG23	2.01	0.41
1:C:69:MSE:HE1	1:C:227:ILE:HG23	2.02	0.41
1:C:70:LEU:HD11	1:C:81:LEU:HD13	2.02	0.41
1:C:116:LYS:HD3	1:C:523:GLN:HE22	1.85	0.41
1:D:68:ILE:HD12	1:D:68:ILE:N	2.34	0.41
1:A:352:LEU:HD22	1:A:354:ASN:HD22	1.84	0.41
1:C:158:MSE:HE2	1:C:176:MSE:HG3	2.01	0.41
1:C:428:ASN:HD21	1:C:430:ILE:HD11	1.86	0.41
1:C:478:TYR:O	1:C:479:PRO:C	2.63	0.41
1:D:350:ASN:HB3	1:D:412:LYS:CE	2.51	0.41
1:C:43:GLY:O	1:D:10:THR:HA	2.19	0.41
1:C:291:PRO:HA	1:C:315:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:LYS:HE3	1:C:472:GLY:O	2.20	0.41
1:C:532:LEU:HG	1:D:461:TYR:CD2	2.55	0.41
1:A:423:MSE:CE	1:B:444:PRO:HG3	2.50	0.41
1:C:524:ASN:O	1:C:526:LEU:N	2.54	0.41
1:D:120:ASP:OD2	1:D:124:ASN:N	2.50	0.41
1:D:350:ASN:N	1:D:350:ASN:ND2	2.68	0.41
1:A:337:VAL:HG21	1:A:380:ILE:HG22	2.01	0.41
1:B:37:VAL:HG12	1:B:38:THR:N	2.36	0.41
1:C:492:LEU:H	1:C:492:LEU:CD2	2.29	0.41
1:D:190:PHE:CE2	1:D:276:ALA:HB2	2.55	0.41
1:A:332:LEU:HD13	1:A:418:TYR:CE1	2.55	0.41
1:A:500:VAL:HG21	1:B:527:ARG:NE	2.35	0.41
1:C:212:THR:HA	3:C:997:HOH:O	2.21	0.41
1:C:318:GLY:HA2	1:C:488:LEU:HD13	2.03	0.41
1:D:194:ASN:HB3	1:D:358:TYR:HD2	1.86	0.41
1:A:350:ASN:N	1:A:350:ASN:ND2	2.68	0.41
1:B:58:LEU:HD22	1:B:134:LEU:HD13	2.02	0.41
1:C:520:LEU:HA	1:C:521:PRO:HD3	1.89	0.41
1:D:175:LYS:HG3	3:D:1020:HOH:O	2.20	0.41
1:A:25:GLU:CD	1:A:57:LYS:HD3	2.46	0.41
1:A:244:THR:O	2:A:900:NAD:H51N	2.21	0.41
1:A:294:ASN:O	1:A:319:ASP:N	2.52	0.41
1:A:483:PHE:HD2	1:A:483:PHE:HA	1.76	0.41
1:B:454:GLU:CD	1:B:454:GLU:C	2.89	0.41
1:C:231:LYS:O	1:C:234:ASN:O	2.39	0.41
1:C:234:ASN:HB2	1:C:236:LEU:HG	2.03	0.41
1:C:243:TRP:CZ2	1:C:245:ALA:HB3	2.56	0.41
1:C:408:VAL:O	1:C:408:VAL:HG12	2.21	0.41
1:C:443:THR:N	1:C:444:PRO:CD	2.83	0.41
1:D:96:THR:C	1:D:98:GLU:N	2.76	0.41
1:D:293:ILE:HD11	1:D:453:THR:OG1	2.21	0.41
1:A:318:GLY:HA2	1:A:488:LEU:CD2	2.51	0.41
1:A:344:VAL:CG1	1:A:421:GLU:HG3	2.51	0.41
1:B:68:ILE:HD12	1:B:68:ILE:N	2.36	0.41
1:C:478:TYR:O	1:C:480:VAL:N	2.54	0.41
1:D:115:LEU:CD2	1:D:507:ARG:HH12	2.33	0.41
1:D:249:ARG:O	1:D:249:ARG:HG3	2.21	0.41
1:D:275:ILE:HD12	1:D:275:ILE:N	2.36	0.41
1:D:329:LYS:HA	1:D:418:TYR:OH	2.21	0.41
1:D:354:ASN:ND2	1:D:354:ASN:N	2.69	0.41
1:A:220:LEU:HD23	1:A:224:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:OD1	1:A:489:LYS:HD3	2.20	0.40
1:B:491:PRO:HG2	1:B:499:PRO:HB2	2.03	0.40
1:C:187:TYR:CD1	1:C:277:PRO:HD3	2.56	0.40
1:C:408:VAL:O	1:C:411:SER:HB2	2.22	0.40
1:D:69:MSE:CE	1:D:227:ILE:HG12	2.41	0.40
1:D:478:TYR:CZ	1:D:494:ARG:HB3	2.55	0.40
1:D:482:THR:C	1:D:484:LEU:N	2.79	0.40
1:B:71:ILE:HG21	1:B:243:TRP:CE3	2.57	0.40
1:B:243:TRP:CE2	1:B:245:ALA:HB3	2.57	0.40
1:D:109:MSE:HA	1:D:113:SER:HB2	2.03	0.40
1:D:122:GLU:HB2	3:D:972:HOH:O	2.20	0.40
1:D:286:ILE:HA	1:D:314:THR:HG21	2.03	0.40
1:A:69:MSE:HE1	1:A:227:ILE:HA	2.03	0.40
1:A:318:GLY:N	1:A:492:LEU:HD21	2.36	0.40
1:A:401:VAL:HG11	1:D:401:VAL:HG21	2.03	0.40
1:B:40:THR:C	1:B:42:SER:N	2.80	0.40
1:B:69:MSE:CE	1:B:227:ILE:HG23	2.51	0.40
1:B:318:GLY:O	1:B:319:ASP:CB	2.66	0.40
1:B:389:ASN:O	1:B:393:GLY:N	2.54	0.40
1:C:250:TYR:HA	1:C:299:ASN:OD1	2.21	0.40
1:D:97:LYS:O	1:D:97:LYS:HG2	2.22	0.40
1:D:206:ASP:HB3	1:D:212:THR:HG21	2.03	0.40
1:D:408:VAL:HG12	1:D:411:SER:O	2.22	0.40
1:B:25:GLU:OE2	1:B:57:LYS:HD3	2.20	0.40
1:B:458:ARG:NH1	1:B:458:ARG:HB2	2.37	0.40
1:C:184:SER:O	1:C:202:CYS:HA	2.21	0.40
1:C:334:GLN:HB2	3:C:961:HOH:O	2.22	0.40
1:C:437:GLU:CG	1:C:440:LEU:HD12	2.37	0.40
1:C:524:ASN:C	1:C:526:LEU:N	2.79	0.40
1:D:33:GLU:HA	1:D:50:THR:O	2.21	0.40
1:D:248:GLU:HG3	1:D:298:GLN:CD	2.47	0.40
1:D:493:THR:HG21	1:D:499:PRO:HB3	2.03	0.40
1:A:265:LEU:O	1:A:268:ILE:HB	2.21	0.40
1:B:319:ASP:HB3	1:B:490:ALA:HB3	2.04	0.40
1:C:381:ILE:HG23	1:C:388:TYR:CG	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	510/533 (96%)	471 (92%)	36 (7%)	3 (1%)	21	34
1	B	510/533 (96%)	462 (91%)	41 (8%)	7 (1%)	9	14
1	C	510/533 (96%)	468 (92%)	37 (7%)	5 (1%)	12	20
1	D	510/533 (96%)	456 (89%)	50 (10%)	4 (1%)	16	27
All	All	2040/2132 (96%)	1857 (91%)	164 (8%)	19 (1%)	14	24

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	235	ALA
1	B	319	ASP
1	D	320	ASP
1	D	469	GLU
1	C	319	ASP
1	B	322	LYS
1	C	525	GLU
1	B	261	MSE
1	B	320	ASP
1	D	59	ASP
1	A	319	ASP
1	A	320	ASP
1	B	148	ASP
1	C	320	ASP
1	C	479	PRO
1	D	49	PRO
1	A	479	PRO
1	B	149	ILE
1	C	49	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	452/461 (98%)	435 (96%)	17 (4%)	29	49
1	B	452/461 (98%)	430 (95%)	22 (5%)	22	38
1	C	452/461 (98%)	429 (95%)	23 (5%)	21	36
1	D	452/461 (98%)	427 (94%)	25 (6%)	19	33
All	All	1808/1844 (98%)	1721 (95%)	87 (5%)	23	39

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	44	ARG
1	A	61	LYS
1	A	66	LEU
1	A	91	ASN
1	A	109	MSE
1	A	244	THR
1	A	273	GLU
1	A	332	LEU
1	A	338	ASP
1	A	352	LEU
1	A	389	ASN
1	A	437	GLU
1	A	454	GLU
1	A	475	GLU
1	A	479	PRO
1	A	483	PHE
1	B	34	ASN
1	B	39	LYS
1	B	64	GLU
1	B	66	LEU
1	B	73	LEU
1	B	109	MSE
1	B	200	ASN

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Mol	Chain	Res	Type
1	B	233	GLU
1	B	242	LEU
1	B	262	GLU
1	B	320	ASP
1	B	352	LEU
1	B	354	ASN
1	B	405	MSE
1	B	437	GLU
1	B	454	GLU
1	B	465	ASP
1	B	475	GLU
1	B	479	PRO
1	B	483	PHE
1	B	492	LEU
1	B	533	LEU
1	C	34	ASN
1	C	50	THR
1	C	66	LEU
1	C	73	LEU
1	C	109	MSE
1	C	200	ASN
1	C	232	GLU
1	C	242	LEU
1	C	249	ARG
1	C	252	GLU
1	C	262	GLU
1	C	273	GLU
1	C	319	ASP
1	C	325	GLN
1	C	328	LEU
1	C	352	LEU
1	C	389	ASN
1	C	405	MSE
1	C	437	GLU
1	C	454	GLU
1	C	457	THR
1	C	475	GLU
1	C	479	PRO
1	D	11	SER
1	D	66	LEU
1	D	73	LEU
1	D	97	LYS

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Mol	Chain	Res	Type
1	D	109	MSE
1	D	111	GLN
1	D	200	ASN
1	D	208	LYS
1	D	232	GLU
1	D	237	ASP
1	D	242	LEU
1	D	249	ARG
1	D	262	GLU
1	D	266	GLN
1	D	273	GLU
1	D	328	LEU
1	D	329	LYS
1	D	352	LEU
1	D	354	ASN
1	D	437	GLU
1	D	445	LEU
1	D	454	GLU
1	D	475	GLU
1	D	483	PHE
1	D	523	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	34	ASN
1	A	111	GLN
1	A	159	GLN
1	A	170	GLN
1	A	194	ASN
1	A	195	GLN
1	A	246	ASN
1	A	263	ASN
1	A	266	GLN
1	A	334	GLN
1	A	350	ASN
1	A	351	HIS
1	A	389	ASN
1	A	427	HIS
1	B	24	ASN
1	B	34	ASN

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Mol	Chain	Res	Type
1	B	95	GLN
1	B	195	GLN
1	B	200	ASN
1	B	246	ASN
1	B	263	ASN
1	B	298	GLN
1	B	307	GLN
1	B	334	GLN
1	B	350	ASN
1	B	351	HIS
1	B	354	ASN
1	B	355	ASN
1	B	389	ASN
1	B	427	HIS
1	B	476	ASN
1	B	501	ASN
1	B	523	GLN
1	C	34	ASN
1	C	77	ASN
1	C	111	GLN
1	C	159	GLN
1	C	194	ASN
1	C	195	GLN
1	C	200	ASN
1	C	246	ASN
1	C	298	GLN
1	C	325	GLN
1	C	350	ASN
1	C	351	HIS
1	C	354	ASN
1	C	359	ASN
1	C	389	ASN
1	C	427	HIS
1	C	501	ASN
1	C	523	GLN
1	C	524	ASN
1	D	24	ASN
1	D	34	ASN
1	D	77	ASN
1	D	90	HIS
1	D	111	GLN
1	D	124	ASN

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Mol	Chain	Res	Type
1	D	151	ASN
1	D	200	ASN
1	D	221	GLN
1	D	228	GLN
1	D	234	ASN
1	D	246	ASN
1	D	263	ASN
1	D	270	ASN
1	D	298	GLN
1	D	307	GLN
1	D	334	GLN
1	D	350	ASN
1	D	351	HIS
1	D	354	ASN
1	D	359	ASN
1	D	427	HIS
1	D	433	HIS
1	D	524	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	A	900	-	46,48,48	2.79	9 (19%)	64,73,73	1.55	9 (14%)
2	NAD	C	902	-	46,48,48	2.78	9 (19%)	64,73,73	1.61	9 (14%)
2	NAD	B	901	-	46,48,48	2.80	10 (21%)	64,73,73	1.56	8 (12%)
2	NAD	D	903	-	46,48,48	2.79	12 (26%)	64,73,73	1.57	8 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	900	-	-	7/30/62/62	0/5/5/5
2	NAD	C	902	-	-	3/30/62/62	0/5/5/5
2	NAD	B	901	-	-	2/30/62/62	0/5/5/5
2	NAD	D	903	-	-	3/30/62/62	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	NAD	C2N-N1N	9.38	1.45	1.35
2	C	902	NAD	C2N-N1N	9.26	1.45	1.35
2	B	901	NAD	C2N-N1N	9.15	1.45	1.35
2	D	903	NAD	C2N-N1N	8.98	1.44	1.35
2	D	903	NAD	C5N-C4N	8.79	1.53	1.38
2	A	900	NAD	C5N-C4N	8.77	1.53	1.38
2	B	901	NAD	C5N-C4N	8.77	1.53	1.38
2	C	902	NAD	C5N-C4N	8.72	1.53	1.38
2	B	901	NAD	C4N-C3N	8.01	1.51	1.39
2	D	903	NAD	C4N-C3N	7.95	1.51	1.39
2	A	900	NAD	C4N-C3N	7.94	1.51	1.39
2	C	902	NAD	C4N-C3N	7.90	1.51	1.39
2	C	902	NAD	C2N-C3N	5.82	1.48	1.39
2	A	900	NAD	C2N-C3N	5.81	1.48	1.39
2	B	901	NAD	C2N-C3N	5.70	1.48	1.39
2	D	903	NAD	C2N-C3N	5.61	1.47	1.39
2	C	902	NAD	C6N-N1N	4.69	1.46	1.35
2	B	901	NAD	C6N-N1N	4.69	1.46	1.35
2	D	903	NAD	C6N-N1N	4.63	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	NAD	C6N-N1N	4.62	1.45	1.35
2	D	903	NAD	C2A-N1A	3.68	1.40	1.33
2	B	901	NAD	C2A-N1A	3.66	1.40	1.33
2	C	902	NAD	C2A-N1A	3.64	1.40	1.33
2	A	900	NAD	C2A-N1A	3.59	1.40	1.33
2	D	903	NAD	PN-O3	3.32	1.63	1.59
2	B	901	NAD	PN-O3	3.19	1.62	1.59
2	C	902	NAD	PN-O3	3.03	1.62	1.59
2	A	900	NAD	PN-O3	2.96	1.62	1.59
2	A	900	NAD	O4D-C1D	2.69	1.44	1.40
2	B	901	NAD	O4D-C1D	2.64	1.44	1.40
2	D	903	NAD	O4D-C1D	2.56	1.44	1.40
2	B	901	NAD	C7N-N7N	2.51	1.37	1.33
2	D	903	NAD	C7N-N7N	2.45	1.37	1.33
2	C	902	NAD	O4D-C1D	2.42	1.44	1.40
2	C	902	NAD	C7N-N7N	2.41	1.37	1.33
2	A	900	NAD	C7N-N7N	2.25	1.37	1.33
2	B	901	NAD	O4B-C1B	-2.20	1.36	1.42
2	D	903	NAD	PA-O3	2.11	1.61	1.59
2	D	903	NAD	O4B-C1B	-2.08	1.37	1.42
2	D	903	NAD	PN-O5D	2.05	1.67	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	NAD	C3N-C7N-N7N	5.78	124.86	117.74
2	C	902	NAD	C3N-C7N-N7N	5.65	124.70	117.74
2	D	903	NAD	C3N-C7N-N7N	5.61	124.65	117.74
2	B	901	NAD	C3N-C7N-N7N	5.58	124.61	117.74
2	C	902	NAD	O7N-C7N-C3N	-5.28	113.14	119.60
2	D	903	NAD	O7N-C7N-C3N	-5.24	113.19	119.60
2	A	900	NAD	O7N-C7N-C3N	-5.21	113.23	119.60
2	B	901	NAD	O7N-C7N-C3N	-5.19	113.25	119.60
2	C	902	NAD	C6N-N1N-C2N	-4.05	118.44	121.88
2	A	900	NAD	C6N-N1N-C2N	-3.89	118.56	121.88
2	B	901	NAD	C6N-N1N-C2N	-3.87	118.58	121.88
2	D	903	NAD	C6N-N1N-C2N	-3.72	118.71	121.88
2	B	901	NAD	C5N-C4N-C3N	-3.31	117.11	120.36
2	D	903	NAD	C5N-C4N-C3N	-3.28	117.14	120.36
2	D	903	NAD	O2N-PN-O3	3.27	116.11	107.27
2	C	902	NAD	C5N-C4N-C3N	-3.26	117.16	120.36
2	B	901	NAD	O2N-PN-O3	3.24	116.03	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	NAD	O2N-PN-O3	3.22	115.98	107.27
2	A	900	NAD	C5N-C4N-C3N	-3.22	117.20	120.36
2	D	903	NAD	O4B-C1B-C2B	-3.11	99.97	106.62
2	A	900	NAD	O2N-PN-O3	3.07	115.57	107.27
2	B	901	NAD	O4B-C1B-C2B	-2.99	100.21	106.62
2	C	902	NAD	C5N-C6N-N1N	2.87	124.30	120.38
2	A	900	NAD	C5N-C6N-N1N	2.79	124.18	120.38
2	C	902	NAD	O4B-C1B-C2B	-2.76	100.70	106.62
2	B	901	NAD	C5N-C6N-N1N	2.75	124.13	120.38
2	D	903	NAD	C5N-C6N-N1N	2.72	124.10	120.38
2	B	901	NAD	O3-PN-O1N	2.48	118.16	110.70
2	C	902	NAD	O3-PN-O1N	2.47	118.14	110.70
2	D	903	NAD	O3-PN-O1N	2.44	118.04	110.70
2	A	900	NAD	O4B-C1B-C2B	-2.37	101.53	106.62
2	A	900	NAD	O3-PN-O1N	2.35	117.76	110.70
2	C	902	NAD	C2D-C3D-C4D	2.22	106.91	102.61
2	A	900	NAD	O5D-PN-O1N	-2.18	100.29	108.94

There are no chirality outliers.

All (15) torsion outliers are listed below:

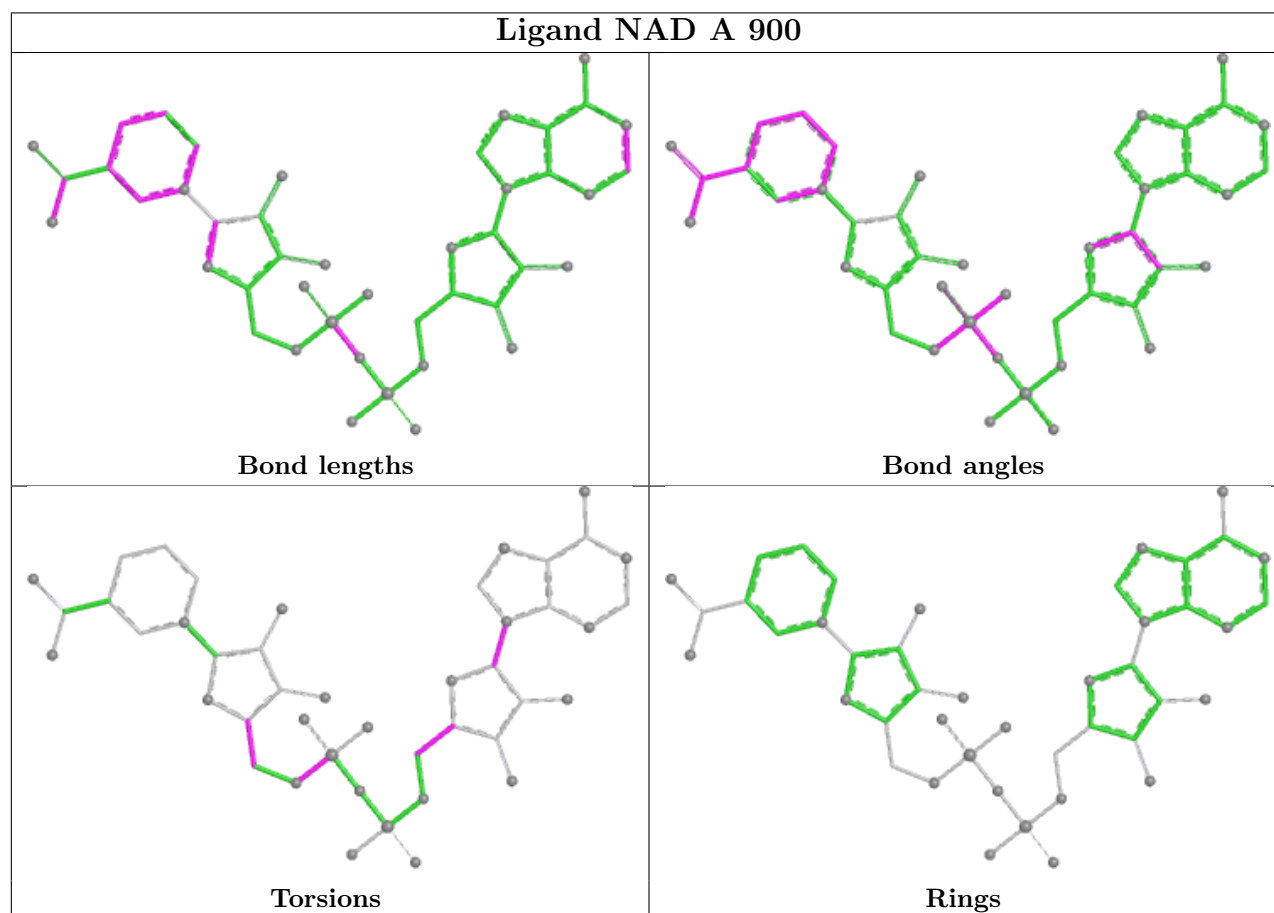
Mol	Chain	Res	Type	Atoms
2	A	900	NAD	C5D-O5D-PN-O1N
2	A	900	NAD	O4D-C4D-C5D-O5D
2	A	900	NAD	C3D-C4D-C5D-O5D
2	A	900	NAD	C2B-C1B-N9A-C8A
2	C	902	NAD	O4D-C4D-C5D-O5D
2	A	900	NAD	C2B-C1B-N9A-C4A
2	D	903	NAD	C2B-C1B-N9A-C8A
2	A	900	NAD	O4B-C1B-N9A-C8A
2	A	900	NAD	O4B-C4B-C5B-O5B
2	C	902	NAD	O4B-C4B-C5B-O5B
2	B	901	NAD	O4B-C4B-C5B-O5B
2	D	903	NAD	O4B-C4B-C5B-O5B
2	C	902	NAD	C2B-C1B-N9A-C8A
2	B	901	NAD	PA-O3-PN-O2N
2	D	903	NAD	PA-O3-PN-O2N

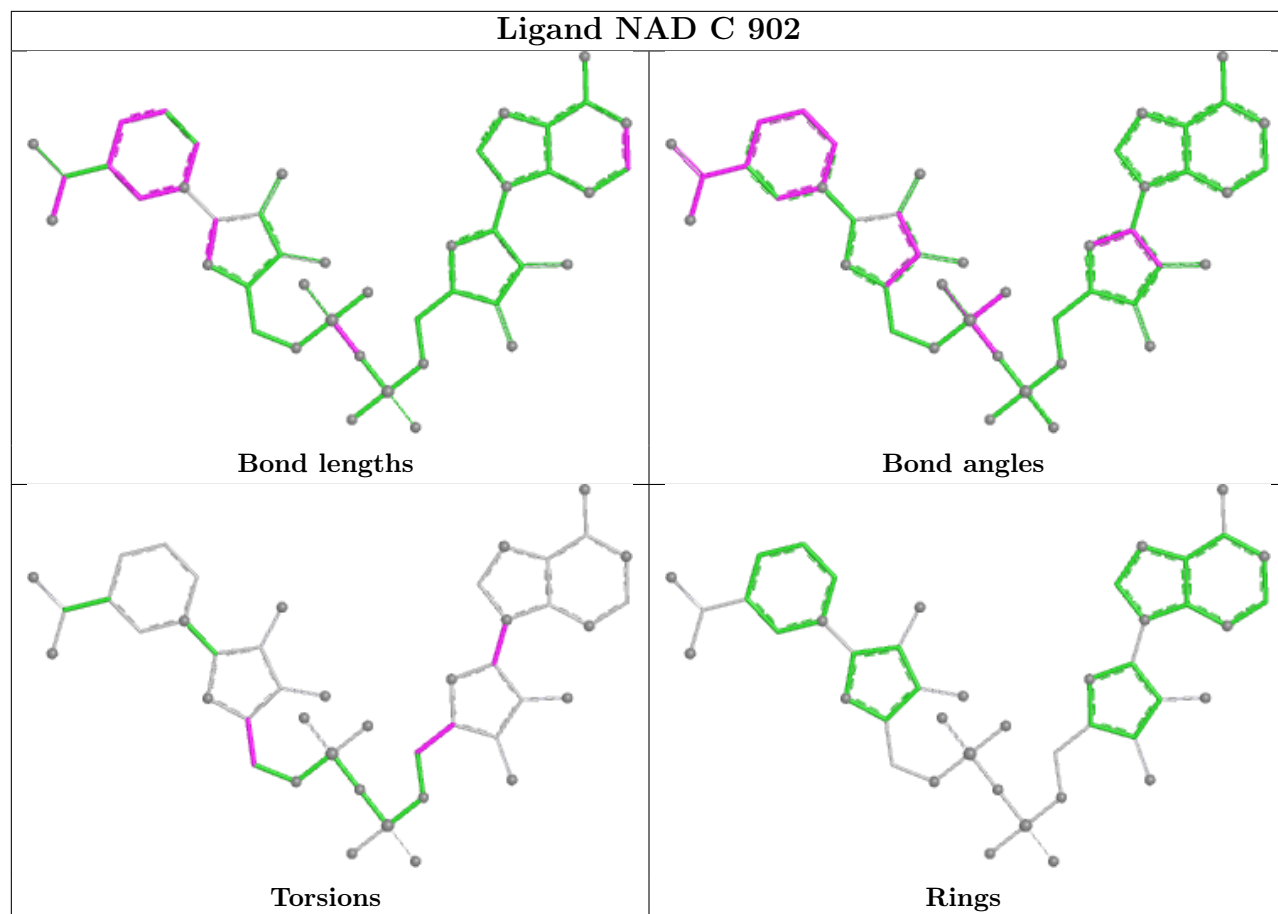
There are no ring outliers.

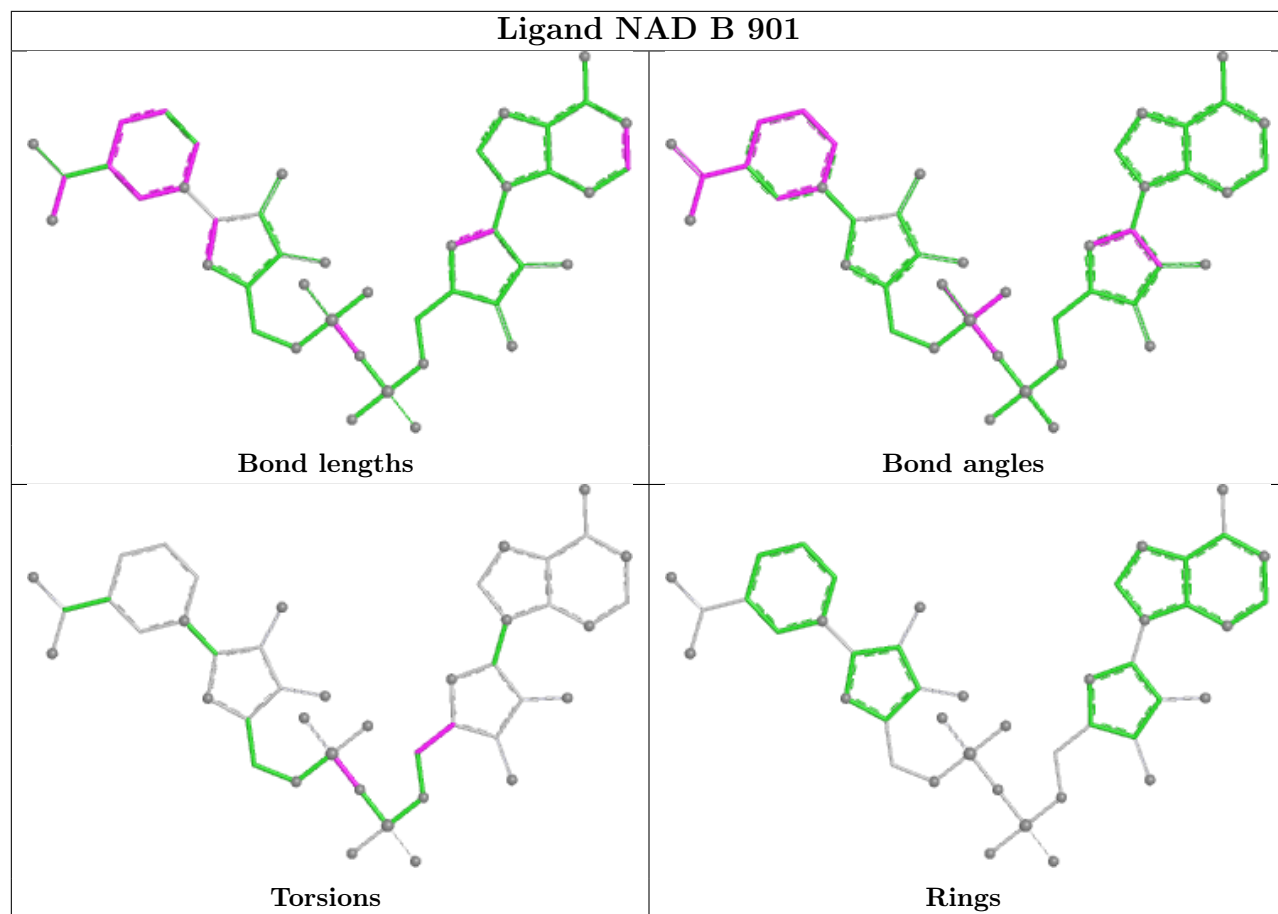
4 monomers are involved in 7 short contacts:

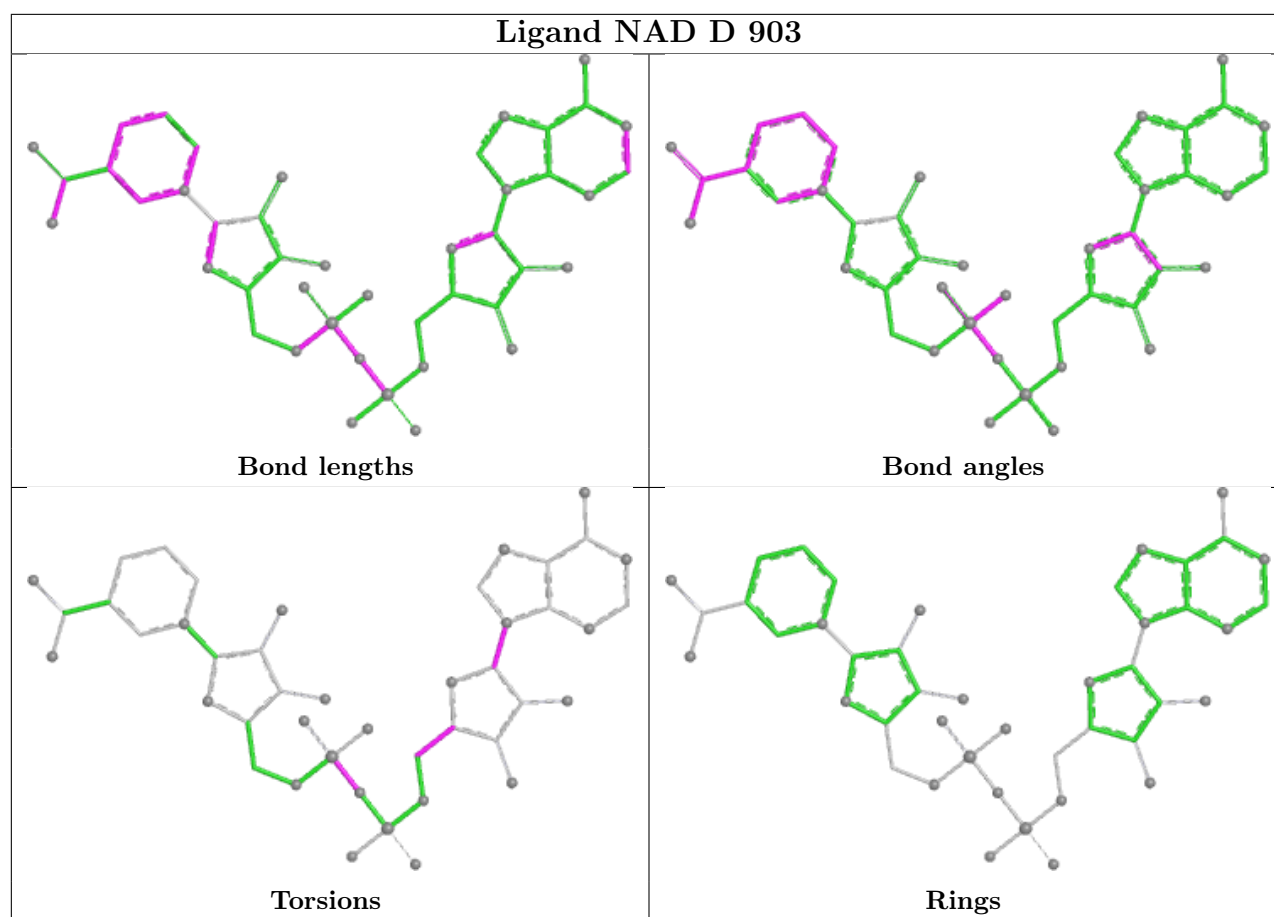
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	NAD	2	0
2	C	902	NAD	2	0
2	B	901	NAD	1	0
2	D	903	NAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	504/533 (94%)	0.26	39 (7%)	19	14	13, 37, 79, 119	0
1	B	504/533 (94%)	0.17	27 (5%)	31	25	13, 38, 75, 117	0
1	C	504/533 (94%)	0.12	22 (4%)	39	31	12, 36, 70, 109	0
1	D	504/533 (94%)	0.22	28 (5%)	30	24	13, 38, 84, 117	0
All	All	2016/2132 (94%)	0.19	116 (5%)	29	22	12, 37, 77, 119	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	356	ASP	5.7
1	C	358	TYR	5.3
1	C	359	ASN	4.9
1	D	467	VAL	4.9
1	D	351	HIS	4.6
1	A	408	VAL	4.6
1	C	360	LEU	4.6
1	A	196	ASP	4.4
1	A	195	GLN	4.3
1	D	376	VAL	4.3
1	B	471	ALA	4.2
1	A	360	LEU	4.2
1	B	318	GLY	4.1
1	B	364	LYS	4.1
1	A	354	ASN	4.0
1	A	358	TYR	4.0
1	A	356	ASP	4.0
1	A	364	LYS	4.0
1	A	359	ASN	3.9
1	B	467	VAL	3.8
1	D	466	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	359	ASN	3.7
1	A	357	GLY	3.7
1	B	358	TYR	3.6
1	A	355	ASN	3.6
1	A	362	ALA	3.6
1	A	363	PRO	3.5
1	D	352	LEU	3.5
1	A	361	SER	3.5
1	A	259	ASP	3.4
1	D	358	TYR	3.3
1	C	408	VAL	3.3
1	B	362	ALA	3.3
1	A	318	GLY	3.2
1	A	352	LEU	3.2
1	D	355	ASN	3.2
1	D	360	LEU	3.2
1	D	468	LYS	3.1
1	A	533	LEU	3.1
1	B	363	PRO	3.1
1	A	251	VAL	3.1
1	B	470	ASP	3.0
1	A	189	ASP	3.0
1	A	193	ALA	3.0
1	A	197	GLU	2.9
1	D	407	PRO	2.9
1	D	363	PRO	2.9
1	D	359	ASN	2.9
1	C	362	ALA	2.9
1	A	407	PRO	2.8
1	B	464	VAL	2.8
1	D	350	ASN	2.8
1	C	258	ASN	2.7
1	D	318	GLY	2.7
1	B	360	LEU	2.7
1	B	375	SER	2.7
1	D	408	VAL	2.7
1	A	260	THR	2.7
1	C	207	GLU	2.6
1	A	406	LYS	2.6
1	A	192	ALA	2.6
1	B	356	ASP	2.6
1	A	353	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	471	ALA	2.6
1	B	194	ASN	2.5
1	B	407	PRO	2.5
1	A	532	LEU	2.5
1	D	349	TYR	2.5
1	B	193	ALA	2.5
1	B	408	VAL	2.5
1	A	347	ALA	2.5
1	A	191	ILE	2.4
1	C	318	GLY	2.4
1	B	468	LYS	2.4
1	D	533	LEU	2.4
1	B	469	GLU	2.4
1	B	357	GLY	2.4
1	A	194	ASN	2.4
1	C	254	SER	2.4
1	C	273	GLU	2.4
1	D	464	VAL	2.4
1	B	321	LEU	2.3
1	A	255	PRO	2.3
1	D	465	ASP	2.3
1	C	533	LEU	2.3
1	D	406	LYS	2.3
1	B	466	PRO	2.3
1	C	356	ASP	2.3
1	B	472	GLY	2.3
1	A	349	TYR	2.2
1	A	404	TYR	2.2
1	A	258	ASN	2.2
1	C	363	PRO	2.2
1	C	357	GLY	2.2
1	C	364	LYS	2.2
1	D	496	GLY	2.2
1	C	192	ALA	2.2
1	B	355	ASN	2.2
1	C	524	ASN	2.2
1	A	319	ASP	2.2
1	A	351	HIS	2.2
1	A	403	LYS	2.1
1	B	39	LYS	2.1
1	D	273	GLU	2.1
1	D	42	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	122	GLU	2.1
1	D	122	GLU	2.1
1	B	16	THR	2.1
1	C	39	LYS	2.0
1	D	195	GLN	2.0
1	C	124	ASN	2.0
1	C	354	ASN	2.0
1	C	355	ASN	2.0
1	A	253	VAL	2.0
1	C	253	VAL	2.0
1	D	375	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

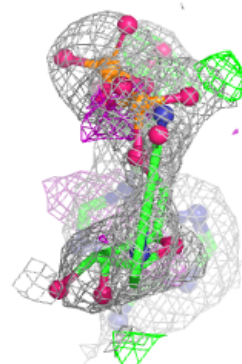
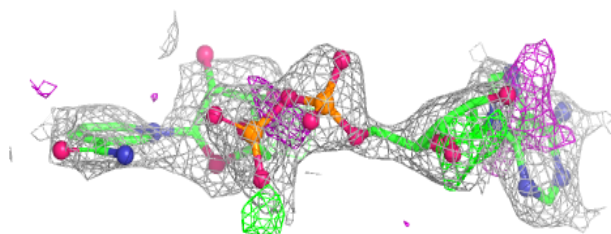
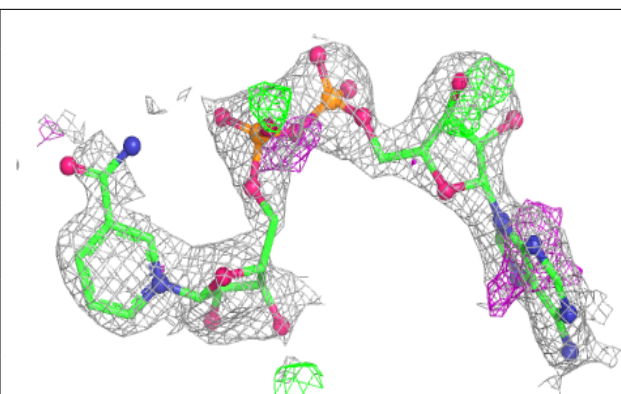
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	D	903	44/44	0.80	0.20	50,72,82,83	0
2	NAD	B	901	44/44	0.83	0.17	46,67,79,80	0
2	NAD	A	900	44/44	0.84	0.17	61,78,86,88	0
2	NAD	C	902	44/44	0.89	0.14	47,60,62,64	0

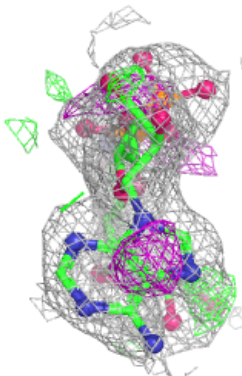
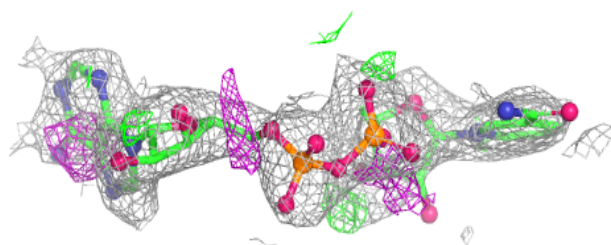
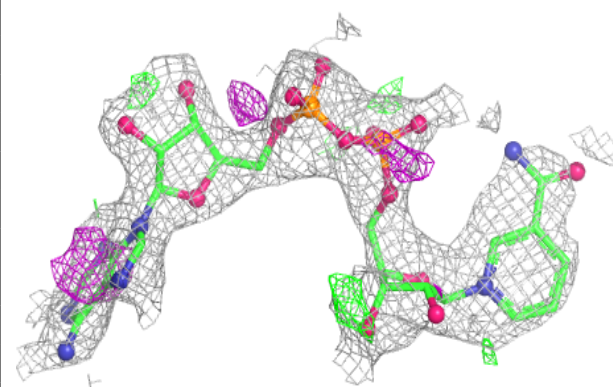
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 903:

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

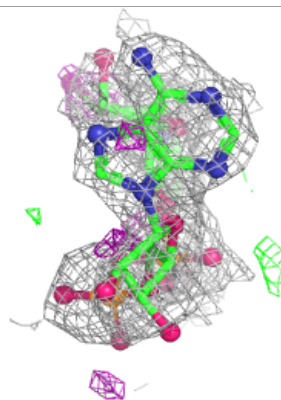
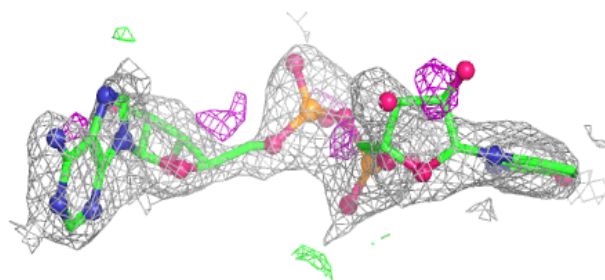
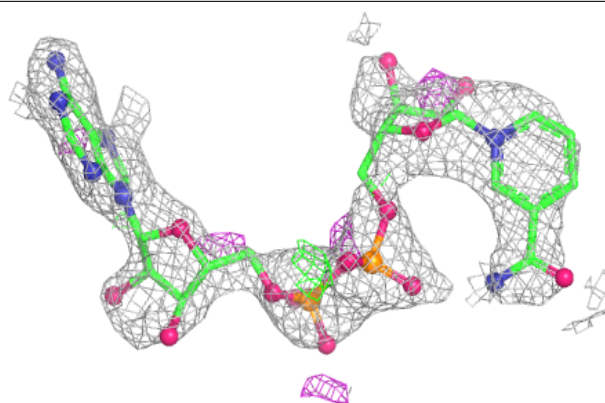
**Electron density around NAD B 901:**

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

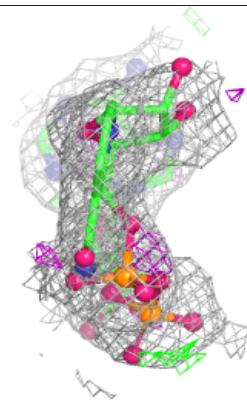
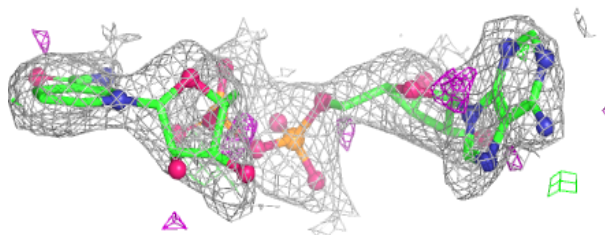
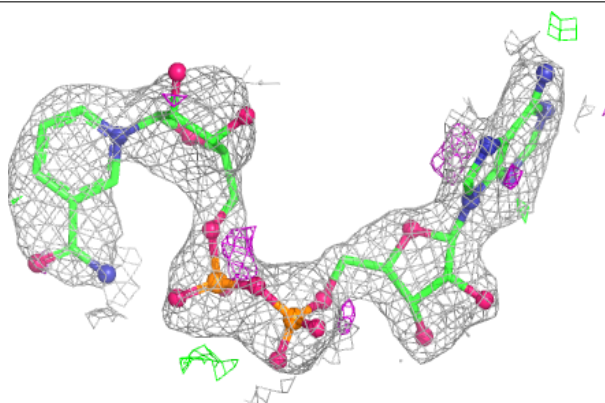


Electron density around NAD A 900:

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

**Electron density around NAD C 902:**

$2mF_o-DF_c$ (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.