



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:16 PM UTC

PDB ID : 1P1H / pdb_00001p1h
Title : Crystal structure of the 1L-myo-inositol/NAD⁺ complex
Authors : Jin, X.; Geiger, J.H.
Deposited on : 2003-04-12
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

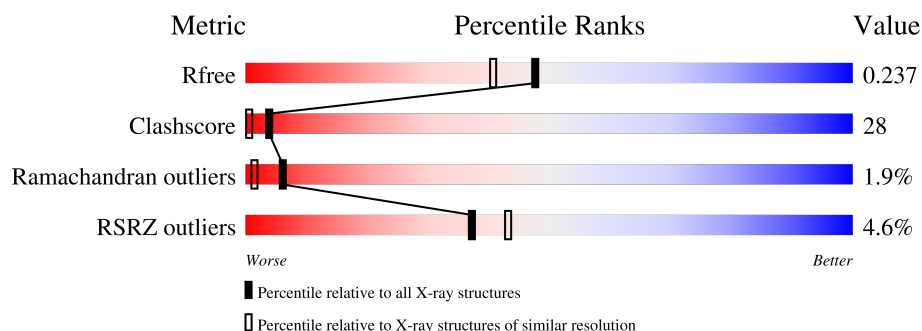
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	5% 54% 38% • 5%
1	B	533	4% 53% 37% • 8%
1	C	533	4% 56% 38% • •
1	D	533	4% 52% 37% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17489 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 Inositol-3-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3988	2538	669	765	16			
1	B	491	Total	C	N	O	S	0	0	0
			3876	2467	652	741	16			
1	C	517	Total	C	N	O	S	0	0	0
			4081	2596	686	783	16			
1	D	487	Total	C	N	O	S	0	0	0
			3839	2439	643	743	14			

There are 40 discrepancies between the modelled and reference sequences:

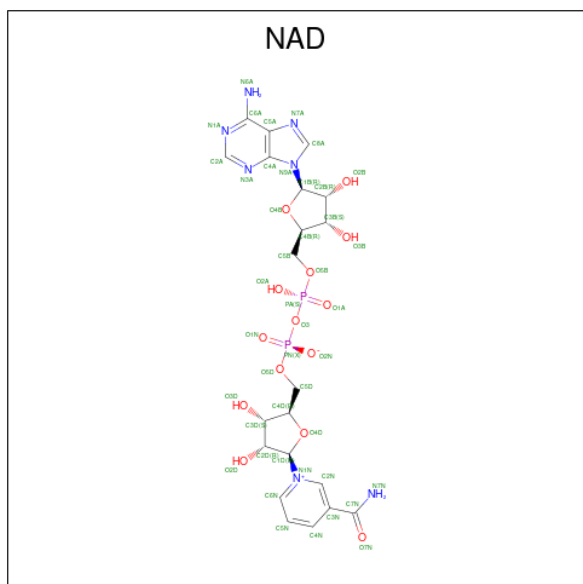
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	SEE REMARK 999	UNP P11986
A	14	VAL	LEU	SEE REMARK 999	UNP P11986
A	?	-	PHE	SEE REMARK 999	UNP P11986
A	60	LEU	GLU	SEE REMARK 999	UNP P11986
A	?	-	ALA	SEE REMARK 999	UNP P11986
A	98	GLU	LYS	SEE REMARK 999	UNP P11986
A	140	ASN	LYS	SEE REMARK 999	UNP P11986
A	141	ASP	HIS	SEE REMARK 999	UNP P11986
A	201	ASN	GLN	SEE REMARK 999	UNP P11986
A	444	PRO	ALA	SEE REMARK 999	UNP P11986
B	?	-	ARG	SEE REMARK 999	UNP P11986
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	?	-	ALA	SEE REMARK 999	UNP P11986
B	98	GLU	LYS	SEE REMARK 999	UNP P11986
B	140	ASN	LYS	SEE REMARK 999	UNP P11986
B	141	ASP	HIS	SEE REMARK 999	UNP P11986
B	201	ASN	GLN	SEE REMARK 999	UNP P11986
B	444	PRO	ALA	SEE REMARK 999	UNP P11986
C	?	-	ARG	SEE REMARK 999	UNP P11986

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Chain	Residue	Modelled	Actual	Comment	Reference
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	?	-	ALA	SEE REMARK 999	UNP P11986
C	98	GLU	LYS	SEE REMARK 999	UNP P11986
C	140	ASN	LYS	SEE REMARK 999	UNP P11986
C	141	ASP	HIS	SEE REMARK 999	UNP P11986
C	201	ASN	GLN	SEE REMARK 999	UNP P11986
C	444	PRO	ALA	SEE REMARK 999	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
D	60	LEU	GLU	SEE REMARK 999	UNP P11986
D	?	-	ALA	SEE REMARK 999	UNP P11986
D	98	GLU	LYS	SEE REMARK 999	UNP P11986
D	140	ASN	LYS	SEE REMARK 999	UNP P11986
D	141	ASP	HIS	SEE REMARK 999	UNP P11986
D	201	ASN	GLN	SEE REMARK 999	UNP P11986
D	444	PRO	ALA	SEE REMARK 999	UNP P11986

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

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

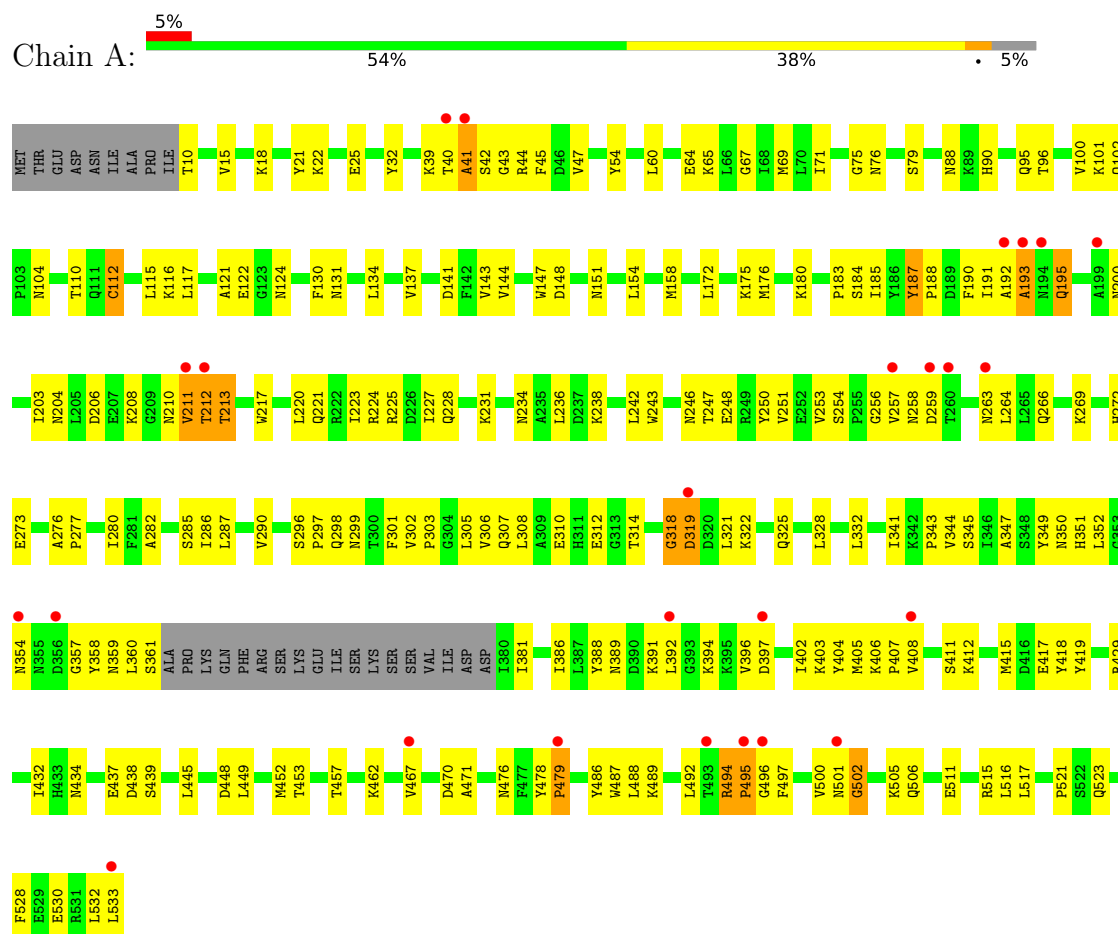
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	425	Total	O	0	0
			425	425		
3	B	354	Total	O	0	0
			354	354		
3	C	383	Total	O	0	0
			383	383		
3	D	367	Total	O	0	0
			367	367		

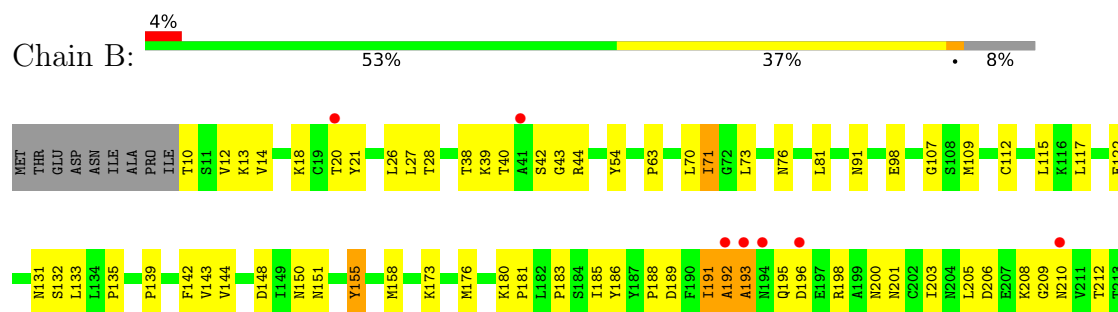
3 Residue-property plots [i](#)

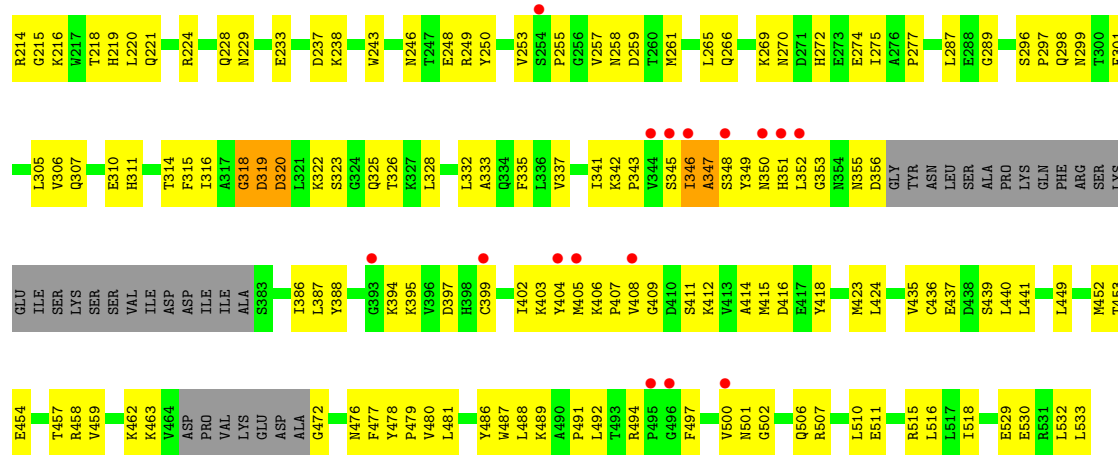
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Inositol-3-phosphate synthase

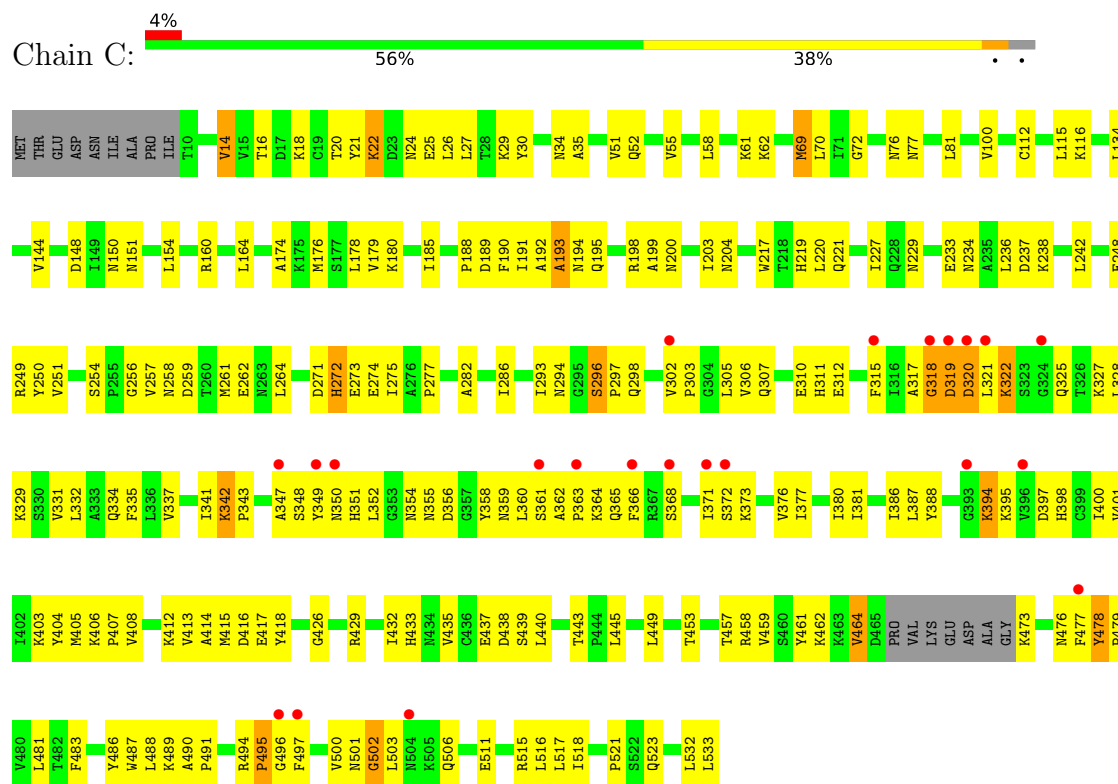


• Molecule 1: Inositol-3-phosphate synthase

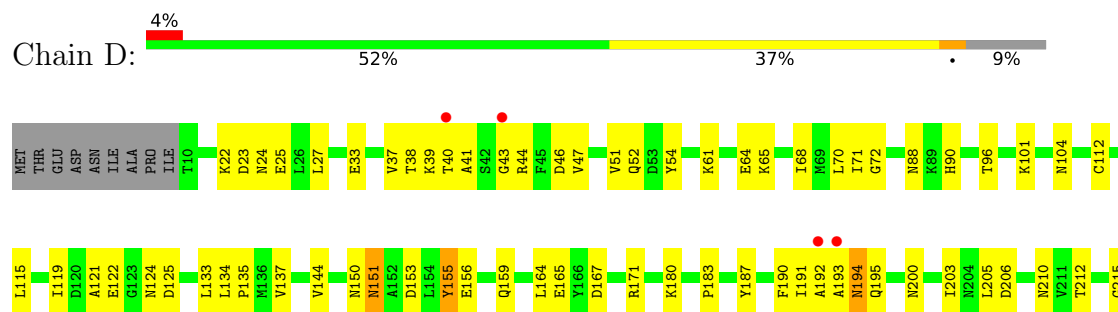


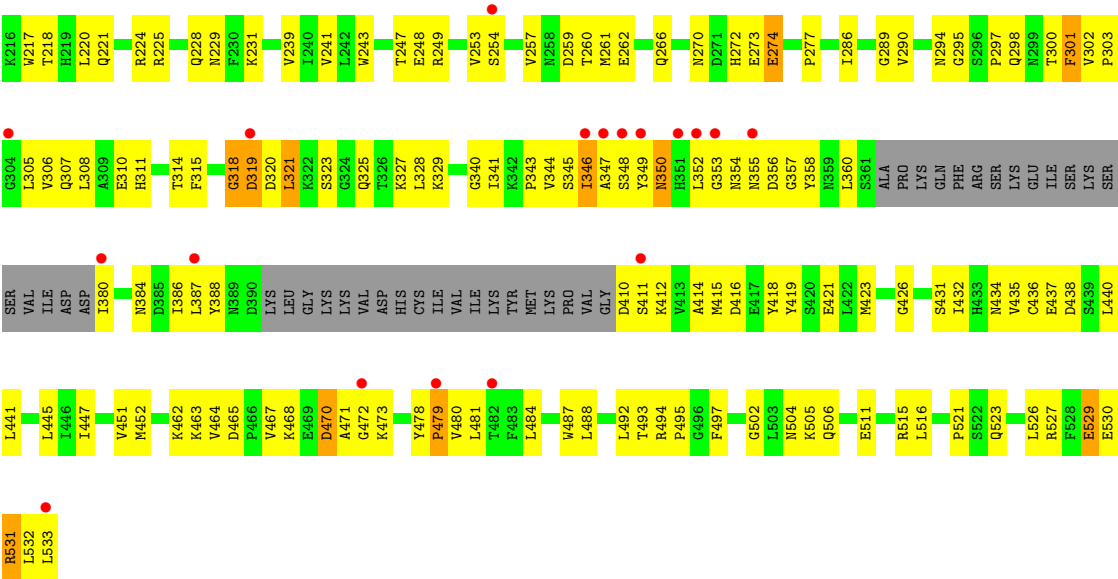


• Molecule 1: Inositol-3-phosphate synthase



• Molecule 1: Inositol-3-phosphate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.79Å 185.58Å 94.08Å 90.00° 114.77° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95 10.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.95) 97.0 (10.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.249 (Not available) , 0.237	Depositor DCC
R_{free} test set	10775 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 104.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17489	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	0/4066	0.93	14/5513 (0.3%)
1	B	0.41	0/3951	0.89	8/5354 (0.1%)
1	C	0.44	1/4160 (0.0%)	0.91	11/5637 (0.2%)
1	D	0.44	0/3913	0.92	12/5308 (0.2%)
All	All	0.43	1/16090 (0.0%)	0.91	45/21812 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	69	MET	SD-CE	-5.49	1.65	1.79

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	318	GLY	N-CA-C	10.96	126.59	110.60
1	A	318	GLY	N-CA-C	10.90	122.56	111.56
1	B	318	GLY	N-CA-C	9.85	122.99	110.38
1	C	318	GLY	N-CA-C	7.87	120.68	110.45
1	A	213	THR	N-CA-C	-7.07	103.76	112.88
1	D	144	VAL	N-CA-C	7.05	118.75	108.53
1	C	144	VAL	N-CA-C	6.95	118.61	108.53
1	A	494	ARG	CA-C-N	6.63	128.13	119.84
1	A	494	ARG	C-N-CA	6.63	128.13	119.84
1	A	144	VAL	N-CA-C	6.53	118.44	108.71
1	D	151	ASN	N-CA-C	6.51	120.84	113.02
1	C	14	VAL	N-CA-C	6.41	116.86	107.37
1	D	464	VAL	N-CA-C	6.30	117.17	109.30
1	B	143	VAL	N-CA-C	-6.17	98.24	107.37
1	B	112	CYS	N-CA-C	6.13	120.64	112.30
1	B	144	VAL	N-CA-C	5.91	117.10	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	GLY	N-CA-C	-5.81	106.43	115.67
1	A	143	VAL	N-CA-C	-5.76	98.84	107.37
1	D	72	GLY	N-CA-C	-5.76	107.03	115.72
1	A	71	ILE	N-CA-C	-5.75	99.44	108.23
1	C	478	TYR	N-CA-C	-5.58	102.09	109.84
1	C	296	SER	CA-C-N	5.54	125.16	119.56
1	C	296	SER	C-N-CA	5.54	125.16	119.56
1	D	164	LEU	N-CA-C	5.54	119.00	110.42
1	A	112	CYS	N-CA-C	5.53	120.74	112.94
1	C	164	LEU	N-CA-C	5.47	118.89	110.42
1	D	321	LEU	N-CA-C	-5.42	102.02	110.10
1	A	41	ALA	CB-CA-C	-5.42	110.34	116.63
1	B	71	ILE	N-CA-C	-5.39	99.99	108.23
1	B	441	LEU	N-CA-C	-5.38	107.26	113.88
1	D	155	TYR	N-CA-C	-5.37	105.35	111.14
1	C	237	ASP	N-CA-C	-5.36	107.39	114.04
1	D	274	GLU	N-CA-C	5.28	119.44	113.15
1	D	301	PHE	N-CA-C	5.26	117.75	109.39
1	C	342	LYS	N-CA-C	5.25	118.88	108.59
1	A	187	TYR	CA-C-N	5.25	126.40	119.84
1	A	187	TYR	C-N-CA	5.25	126.40	119.84
1	A	121	ALA	N-CA-C	5.23	117.06	111.36
1	D	350	ASN	N-CA-C	5.23	116.79	108.79
1	A	386	ILE	N-CA-C	-5.18	105.49	110.72
1	D	529	GLU	N-CA-C	-5.16	105.78	111.71
1	B	155	TYR	N-CA-C	-5.12	105.39	111.69
1	C	394	LYS	N-CA-C	-5.12	106.78	112.57
1	B	237	ASP	N-CA-C	-5.08	107.02	114.39
1	A	467	VAL	N-CA-C	5.03	115.70	110.82

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	3988	0	3989	225	0
1	B	3876	0	3879	230	0
1	C	4081	0	4088	274	0
1	D	3839	0	3816	240	0
2	A	44	0	26	3	0
2	B	44	0	26	3	0
2	C	44	0	26	5	0
2	D	44	0	26	1	0
3	A	425	0	0	28	0
3	B	354	0	0	20	0
3	C	383	0	0	25	0
3	D	367	0	0	17	0
All	All	17489	0	15876	902	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 28.

All (902) 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:494:ARG:HB3	1:C:495:PRO:HD2	1.34	1.08
1:C:494:ARG:HH22	1:D:533:LEU:HB3	0.94	1.06
1:A:352:LEU:HD21	1:A:357:GLY:HA3	1.37	1.06
1:D:191:ILE:HG22	1:D:192:ALA:H	1.25	1.01
1:B:191:ILE:HG13	1:B:192:ALA:H	1.20	1.00
1:C:320:ASP:HB3	1:C:489:LYS:HB3	1.39	1.00
1:A:69:MET:HE1	1:A:227:ILE:HA	1.44	0.99
1:C:494:ARG:NH2	1:D:533:LEU:HB3	1.78	0.97
1:B:322:LYS:HA	1:B:489:LYS:HG3	1.46	0.96
1:A:318:GLY:HA2	1:A:488:LEU:HG	1.48	0.96
1:B:437:GLU:HG3	1:B:440:LEU:HD12	1.47	0.94
1:A:115:LEU:HD22	1:A:511:GLU:HG3	1.50	0.93
1:D:437:GLU:HG3	1:D:440:LEU:HD22	1.49	0.93
1:A:502:GLY:HA3	1:A:505:LYS:HE2	1.50	0.93
1:C:69:MET:HE1	1:C:227:ILE:HG12	1.51	0.92
1:C:533:LEU:HB3	1:D:494:ARG:HH22	1.36	0.90
1:B:323:SER:H	1:B:489:LYS:HE3	1.36	0.89
1:C:494:ARG:HH22	1:D:533:LEU:CB	1.83	0.89
1:B:347:ALA:HA	1:B:399:CYS:HB3	1.53	0.89
1:C:302:VAL:HG22	1:C:303:PRO:HD2	1.57	0.87
1:B:151:ASN:H	1:B:200:ASN:HD21	1.21	0.87
1:B:109:MET:HE2	1:B:507:ARG:HE	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:LYS:HE3	1:D:27:LEU:HD11	1.57	0.86
1:C:22:LYS:HZ2	1:C:25:GLU:HB2	1.41	0.85
1:B:289:GLY:HA2	1:B:314:THR:HG21	1.59	0.84
1:B:408:VAL:HG21	3:B:1000:HOH:O	1.76	0.84
1:C:533:LEU:HD13	1:D:494:ARG:HH12	1.41	0.84
1:B:191:ILE:HG13	1:B:192:ALA:N	1.92	0.84
1:C:24:ASN:HD22	1:C:61:LYS:HB2	1.42	0.84
1:A:381:ILE:HD11	1:A:396:VAL:HG23	1.58	0.84
1:C:337:VAL:HG21	1:C:380:ILE:HG23	1.57	0.83
1:D:225:ARG:HH21	1:D:229:ASN:HB2	1.42	0.83
1:B:198:ARG:HD2	3:B:973:HOH:O	1.79	0.82
1:D:40:THR:HG21	1:D:44:ARG:NH1	1.95	0.82
1:C:254:SER:HB2	1:C:257:VAL:HG11	1.62	0.81
1:B:195:GLN:HG3	1:B:198:ARG:HH21	1.43	0.81
1:B:423:MET:HE3	1:B:424:LEU:HD22	1.60	0.81
1:D:115:LEU:HD22	1:D:511:GLU:HG3	1.60	0.80
1:C:515:ARG:NH1	1:C:521:PRO:O	2.15	0.80
1:D:325:GLN:HA	1:D:325:GLN:HE21	1.45	0.80
1:D:352:LEU:HA	1:D:412:LYS:HA	1.64	0.79
1:C:261:MET:HG2	1:C:307:GLN:NE2	1.97	0.79
1:D:191:ILE:HG22	1:D:192:ALA:N	1.98	0.78
1:C:310:GLU:HG2	1:C:479:PRO:HG2	1.65	0.78
1:C:494:ARG:HB3	1:C:495:PRO:CD	2.13	0.78
1:B:342:LYS:HB2	1:B:387:LEU:HD22	1.66	0.78
1:C:347:ALA:HB2	3:C:920:HOH:O	1.82	0.78
1:C:494:ARG:HH12	1:D:533:LEU:HG	1.49	0.78
1:C:69:MET:CE	1:C:227:ILE:HG12	2.13	0.78
1:C:302:VAL:CG2	1:C:303:PRO:HD2	2.14	0.78
1:D:306:VAL:O	1:D:310:GLU:HG3	1.83	0.78
1:A:532:LEU:HB3	1:A:533:LEU:HD12	1.66	0.78
1:C:191:ILE:HG22	1:C:192:ALA:H	1.48	0.77
1:A:389:ASN:HD21	1:A:392:LEU:HD21	1.48	0.77
1:C:191:ILE:HG22	1:C:192:ALA:N	1.99	0.77
1:B:20:THR:HB	1:B:27:LEU:HB2	1.65	0.76
1:D:352:LEU:HD11	1:D:357:GLY:HA3	1.66	0.76
1:B:212:THR:HG22	1:B:214:ARG:H	1.49	0.76
1:C:151:ASN:H	1:C:200:ASN:HD21	1.30	0.76
1:B:478:TYR:HD2	1:B:480:VAL:HG22	1.51	0.76
1:D:156:GLU:HA	1:D:159:GLN:HE21	1.51	0.76
1:D:318:GLY:HA2	1:D:488:LEU:HD13	1.68	0.76
1:C:478:TYR:HB2	1:C:494:ARG:HH21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:H	1:A:299:ASN:HD21	1.35	0.74
1:D:515:ARG:NH1	1:D:521:PRO:O	2.21	0.74
1:A:352:LEU:HD23	1:A:354:ASN:ND2	2.02	0.74
1:C:322:LYS:CD	1:C:327:LYS:HG2	2.18	0.73
1:D:33:GLU:HG2	1:D:51:VAL:HG22	1.69	0.73
1:C:62:LYS:HB3	1:C:458:ARG:CZ	2.19	0.73
1:B:248:GLU:H	1:B:298:GLN:HG2	1.50	0.73
1:C:500:VAL:HG21	1:D:527:ARG:NE	2.04	0.73
1:C:264:LEU:HD21	1:C:305:LEU:HD13	1.69	0.73
1:C:377:ILE:O	1:C:381:ILE:HG13	1.88	0.72
1:B:310:GLU:HG2	1:B:479:PRO:HG3	1.70	0.72
1:A:407:PRO:HG3	1:C:395:LYS:HE2	1.72	0.72
1:B:205:LEU:HA	1:B:210:ASN:O	1.90	0.72
1:A:352:LEU:CD2	1:A:357:GLY:HA3	2.18	0.72
1:B:478:TYR:CD2	1:B:480:VAL:HG22	2.25	0.71
1:C:533:LEU:HD13	1:D:494:ARG:NH1	2.05	0.71
1:B:437:GLU:HG3	1:B:440:LEU:CD1	2.21	0.71
1:D:352:LEU:HB3	1:D:412:LYS:HB2	1.72	0.71
1:C:320:ASP:CB	1:C:489:LYS:HB3	2.19	0.71
1:B:318:GLY:O	1:B:319:ASP:HB2	1.91	0.70
1:A:221:GLN:HG2	3:A:881:HOH:O	1.90	0.70
1:D:261:MET:HE1	1:D:311:HIS:HB2	1.74	0.70
1:B:14:VAL:HG11	1:B:518:ILE:O	1.90	0.70
1:C:69:MET:HE1	1:C:227:ILE:HA	1.74	0.70
1:C:272:HIS:CD2	1:C:274:GLU:H	2.09	0.70
1:D:310:GLU:HG2	1:D:479:PRO:HG3	1.73	0.70
1:A:352:LEU:HD21	1:A:357:GLY:CA	2.19	0.70
1:C:337:VAL:HG21	1:C:380:ILE:CG2	2.21	0.70
1:A:256:GLY:HA2	1:A:263:ASN:HD22	1.56	0.69
1:C:373:LYS:HE3	1:C:489:LYS:HD3	1.72	0.69
1:D:532:LEU:O	1:D:533:LEU:HB2	1.90	0.69
1:D:415:MET:CE	1:D:431:SER:HB2	2.23	0.69
1:C:150:ASN:ND2	1:C:160:ARG:HH12	1.90	0.69
1:C:331:VAL:HA	1:C:334:GLN:NE2	2.06	0.69
1:A:257:VAL:HG13	1:A:258:ASN:H	1.58	0.69
1:C:115:LEU:CD2	1:C:511:GLU:HG2	2.23	0.69
1:A:415:MET:SD	1:C:415:MET:HE2	2.34	0.68
1:A:39:LYS:O	1:A:40:THR:HG23	1.93	0.68
1:A:328:LEU:HD13	3:A:935:HOH:O	1.92	0.68
1:A:486:TYR:HA	1:A:506:GLN:NE2	2.09	0.68
1:B:318:GLY:HA2	1:B:488:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:O	1:A:65:LYS:HD2	1.93	0.67
1:C:22:LYS:HZ2	1:C:22:LYS:HB3	1.59	0.67
1:A:254:SER:O	1:A:257:VAL:HG12	1.94	0.67
1:A:243:TRP:CD1	1:A:296:SER:HG	2.13	0.67
1:C:154:LEU:HD22	1:C:179:VAL:HG11	1.77	0.67
1:C:334:GLN:HG2	1:C:335:PHE:N	2.05	0.67
1:C:350:ASN:HD22	1:C:412:LYS:HE3	1.59	0.67
1:A:318:GLY:O	1:A:319:ASP:HB2	1.93	0.67
1:C:515:ARG:HD2	3:C:911:HOH:O	1.94	0.67
1:C:362:ALA:HB3	1:C:365:GLN:HG2	1.77	0.67
1:A:10:THR:HG22	1:B:43:GLY:HA3	1.76	0.67
1:C:154:LEU:HD22	1:C:179:VAL:CG1	2.25	0.67
1:C:494:ARG:CB	1:C:495:PRO:HD2	2.20	0.67
1:B:404:TYR:OH	1:B:406:LYS:HE3	1.94	0.66
1:C:70:LEU:HD11	1:C:81:LEU:HD23	1.76	0.66
1:A:217:TRP:O	1:A:221:GLN:HG3	1.95	0.66
1:B:261:MET:HE1	1:B:311:HIS:HB2	1.78	0.66
1:C:478:TYR:CD1	1:C:479:PRO:HD2	2.31	0.66
1:C:533:LEU:HB3	1:D:494:ARG:NH2	2.08	0.66
1:B:98:GLU:HB2	3:B:806:HOH:O	1.95	0.66
1:B:352:LEU:HD13	1:B:352:LEU:H	1.61	0.66
1:B:415:MET:HE2	1:D:415:MET:HE2	1.78	0.66
1:C:296:SER:HB2	1:C:298:GLN:OE1	1.96	0.66
1:D:437:GLU:HG3	1:D:440:LEU:CD2	2.24	0.66
1:B:388:TYR:HB3	1:B:394:LYS:HA	1.77	0.66
1:D:38:THR:HG23	1:D:46:ASP:HB2	1.76	0.66
1:A:256:GLY:HA2	1:A:263:ASN:ND2	2.10	0.65
1:D:191:ILE:CG2	1:D:192:ALA:H	2.06	0.65
1:D:341:ILE:O	1:D:343:PRO:HD3	1.95	0.65
1:A:151:ASN:HB2	1:A:180:LYS:HE2	1.77	0.65
1:C:115:LEU:HD21	1:C:511:GLU:HG2	1.78	0.65
1:D:318:GLY:CA	1:D:488:LEU:HD13	2.26	0.65
1:B:405:MET:SD	1:D:347:ALA:HB2	2.36	0.65
1:C:321:LEU:HD23	1:C:321:LEU:O	1.96	0.65
1:A:47:VAL:HG22	1:B:14:VAL:HA	1.79	0.65
1:D:273:GLU:HG2	3:D:822:HOH:O	1.96	0.65
1:D:434:ASN:HD22	1:D:435:VAL:N	1.95	0.65
1:C:178:LEU:HD12	3:C:936:HOH:O	1.95	0.65
1:C:322:LYS:HA	1:C:489:LYS:HE3	1.79	0.64
1:D:318:GLY:O	1:D:319:ASP:HB2	1.96	0.64
1:A:322:LYS:NZ	1:A:506:GLN:HE22	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:SER:HB3	1:D:419:TYR:HB3	1.78	0.64
1:D:473:LYS:HA	3:D:895:HOH:O	1.97	0.64
1:B:200:ASN:C	1:B:200:ASN:HD22	2.05	0.64
1:B:322:LYS:NZ	1:B:506:GLN:HE22	1.96	0.64
1:B:42:SER:C	1:B:44:ARG:H	2.06	0.64
1:C:273:GLU:H	1:C:273:GLU:CD	2.05	0.64
1:B:486:TYR:HA	1:B:506:GLN:NE2	2.13	0.64
1:C:69:MET:HE1	1:C:227:ILE:CG1	2.28	0.64
1:C:361:SER:HB2	3:C:1031:HOH:O	1.97	0.63
1:C:191:ILE:HG21	1:C:195:GLN:HG3	1.80	0.63
1:C:516:LEU:C	1:C:516:LEU:HD23	2.22	0.63
1:A:505:LYS:HG3	3:A:777:HOH:O	1.97	0.63
1:C:322:LYS:HD3	1:C:327:LYS:HG2	1.79	0.63
1:B:195:GLN:HG3	1:B:198:ARG:NH2	2.14	0.63
1:C:14:VAL:HG22	1:D:47:VAL:HB	1.79	0.63
1:B:409:GLY:HA3	3:B:844:HOH:O	1.99	0.63
1:C:322:LYS:HA	1:C:489:LYS:HB2	1.80	0.63
1:C:426:GLY:HA3	1:D:440:LEU:HD23	1.81	0.63
1:B:405:MET:O	1:B:408:VAL:HG22	1.99	0.62
1:B:353:GLY:HA3	1:B:406:LYS:HA	1.80	0.62
1:B:395:LYS:HE2	1:B:397:ASP:OD2	1.99	0.62
1:C:258:ASN:C	1:C:258:ASN:HD22	2.07	0.62
1:C:302:VAL:HG22	1:C:303:PRO:CD	2.29	0.62
1:A:158:MET:HE2	1:A:176:MET:HG3	1.80	0.62
1:C:248:GLU:OE1	1:C:277:PRO:HD2	2.00	0.62
1:D:321:LEU:HB3	3:D:712:HOH:O	2.00	0.62
1:A:321:LEU:HD22	1:A:445:LEU:CD2	2.30	0.62
1:A:478:TYR:CD2	1:A:479:PRO:HD2	2.34	0.62
1:B:395:LYS:HD2	3:B:825:HOH:O	1.99	0.62
1:C:151:ASN:N	1:C:200:ASN:HD21	1.97	0.62
1:C:248:GLU:H	1:C:298:GLN:HG2	1.65	0.62
1:C:445:LEU:HD21	1:C:487:TRP:HB3	1.82	0.62
1:B:12:VAL:HG21	1:B:133:LEU:HD23	1.83	0.61
1:D:329:LYS:HD2	1:D:416:ASP:OD2	2.00	0.61
1:C:58:LEU:HD22	1:C:134:LEU:HD13	1.80	0.61
1:D:357:GLY:O	1:D:360:LEU:HB3	2.00	0.61
1:B:341:ILE:O	1:B:343:PRO:HD3	2.00	0.61
1:C:328:LEU:O	1:C:332:LEU:HG	2.01	0.61
1:B:186:TYR:OH	1:B:196:ASP:HA	2.01	0.61
1:B:191:ILE:CG1	1:B:192:ALA:H	2.02	0.61
1:A:392:LEU:HB3	3:B:854:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:GLN:H	1:B:195:GLN:NE2	1.98	0.61
1:D:192:ALA:HA	3:D:970:HOH:O	2.00	0.61
1:B:478:TYR:CD1	1:B:479:PRO:HD2	2.36	0.60
1:B:109:MET:HE2	1:B:507:ARG:NE	2.13	0.60
1:C:250:TYR:HD1	1:C:368:SER:HG	1.49	0.60
1:D:289:GLY:HA2	1:D:314:THR:CG2	2.31	0.60
1:A:501:ASN:HA	1:A:506:GLN:OE1	2.01	0.60
1:C:387:LEU:HD11	1:D:112:CYS:HB3	1.82	0.60
1:A:332:LEU:HD21	1:B:328:LEU:HD12	1.82	0.60
1:C:432:ILE:HG13	3:C:1034:HOH:O	2.01	0.60
1:B:480:VAL:HG23	1:B:480:VAL:O	2.01	0.60
1:D:225:ARG:NH2	1:D:229:ASN:HB2	2.14	0.60
1:D:289:GLY:HA2	1:D:314:THR:HG21	1.83	0.60
1:C:394:LYS:HB3	1:C:394:LYS:NZ	2.17	0.60
1:C:478:TYR:CB	1:C:494:ARG:HH21	2.14	0.60
1:A:257:VAL:HG13	1:A:258:ASN:N	2.15	0.60
1:A:449:LEU:HD21	1:A:487:TRP:HB2	1.82	0.60
1:B:325:GLN:HE21	1:B:325:GLN:HA	1.67	0.60
1:C:100:VAL:HG12	3:C:797:HOH:O	2.00	0.60
1:D:96:THR:HG22	1:D:165:GLU:HG2	1.84	0.60
1:A:341:ILE:O	1:A:343:PRO:HD3	2.01	0.60
1:B:70:LEU:HD11	1:B:81:LEU:HD23	1.84	0.60
1:D:220:LEU:C	1:D:220:LEU:HD23	2.27	0.60
1:A:75:GLY:O	1:A:79:SER:HB2	2.01	0.60
1:C:22:LYS:NZ	1:C:25:GLU:HB2	2.16	0.60
1:D:511:GLU:O	1:D:515:ARG:HG3	2.02	0.60
1:C:150:ASN:HA	1:C:200:ASN:ND2	2.17	0.59
1:B:437:GLU:CG	1:B:440:LEU:HD12	2.28	0.59
1:C:453:THR:O	1:C:457:THR:HG23	2.02	0.59
1:A:352:LEU:HD13	1:A:352:LEU:N	2.17	0.59
1:D:412:LYS:HE3	1:D:438:ASP:OD1	2.02	0.59
1:A:286:ILE:HG22	1:A:312:GLU:HG3	1.84	0.59
1:B:266:GLN:HE21	1:B:270:ASN:HD21	1.48	0.59
1:C:440:LEU:HD23	1:D:426:GLY:HA3	1.84	0.59
1:D:261:MET:HE1	1:D:311:HIS:CB	2.31	0.59
1:C:325:GLN:NE2	1:C:412:LYS:HD3	2.17	0.59
1:C:329:LYS:HG3	1:C:418:TYR:OH	2.03	0.59
1:D:344:VAL:HG11	1:D:421:GLU:OE2	2.03	0.59
1:B:215:GLY:O	1:B:218:THR:HB	2.02	0.59
1:D:415:MET:HE1	1:D:431:SER:HB2	1.83	0.59
1:A:116:LYS:HB3	1:A:523:GLN:NE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLU:HG2	1:A:479:PRO:HG3	1.84	0.59
1:B:131:ASN:HD22	1:B:131:ASN:C	2.10	0.59
1:C:18:LYS:HE2	3:C:820:HOH:O	2.03	0.59
1:B:185:ILE:HG12	1:B:203:ILE:HD11	1.85	0.59
1:C:325:GLN:HB3	3:C:1035:HOH:O	2.02	0.59
1:A:21:TYR:HD2	1:A:60:LEU:HD11	1.67	0.58
1:A:332:LEU:HG	1:A:432:ILE:HD11	1.84	0.58
1:A:438:ASP:HB3	2:A:650:NAD:O7N	2.03	0.58
1:A:220:LEU:HD23	1:A:280:ILE:HG23	1.85	0.58
1:C:191:ILE:CG2	1:C:195:GLN:HG3	2.33	0.58
1:C:523:GLN:HE21	1:C:523:GLN:HA	1.67	0.58
1:B:193:ALA:N	1:B:196:ASP:HB2	2.17	0.58
1:C:254:SER:HB2	1:C:257:VAL:CG1	2.32	0.58
1:B:318:GLY:CA	1:B:488:LEU:HD13	2.33	0.58
1:C:272:HIS:HB3	1:C:275:ILE:HG12	1.85	0.58
1:C:319:ASP:HB3	1:C:490:ALA:HB3	1.85	0.58
1:A:351:HIS:HD2	1:C:349:TYR:OH	1.87	0.58
1:B:323:SER:H	1:B:489:LYS:CE	2.12	0.58
1:C:154:LEU:HB3	1:C:176:MET:HE2	1.86	0.58
1:C:351:HIS:HA	1:C:403:LYS:O	2.03	0.58
1:A:264:LEU:HD21	1:A:305:LEU:HD13	1.86	0.58
1:B:63:PRO:HG3	1:B:238:LYS:HG3	1.85	0.58
1:C:302:VAL:O	1:C:306:VAL:HG23	2.04	0.58
1:C:494:ARG:HH12	1:D:533:LEU:CG	2.16	0.58
1:D:346:ILE:HG12	1:D:418:TYR:CD2	2.38	0.58
1:A:47:VAL:HG22	1:B:14:VAL:HB	1.85	0.57
1:D:411:SER:HB3	3:D:867:HOH:O	2.04	0.57
1:B:478:TYR:CE2	1:B:494:ARG:HG2	2.38	0.57
1:C:191:ILE:CG2	1:C:192:ALA:H	2.16	0.57
1:B:306:VAL:O	1:B:310:GLU:HG3	2.04	0.57
1:D:286:ILE:HG21	1:D:308:LEU:HD13	1.84	0.57
1:C:25:GLU:HB3	3:C:922:HOH:O	2.03	0.57
1:C:192:ALA:O	1:C:193:ALA:HB2	2.04	0.57
1:D:122:GLU:HB2	1:D:124:ASN:OD1	2.04	0.57
1:D:325:GLN:HA	1:D:325:GLN:NE2	2.16	0.57
1:A:15:VAL:HG11	3:A:788:HOH:O	2.04	0.57
1:C:302:VAL:HG12	1:C:305:LEU:HB2	1.86	0.57
1:C:297:PRO:HB3	1:C:320:ASP:OD1	2.04	0.57
1:D:516:LEU:HD12	1:D:516:LEU:C	2.29	0.57
1:A:497:PHE:CD2	1:B:530:GLU:HG2	2.40	0.56
1:A:407:PRO:CG	1:C:395:LYS:HE2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LYS:HA	3:A:1072:HOH:O	2.05	0.56
1:C:405:MET:O	1:C:408:VAL:HG22	2.06	0.56
1:C:221:GLN:HG2	3:C:799:HOH:O	2.06	0.56
1:C:432:ILE:HD12	1:D:432:ILE:HD12	1.88	0.56
1:C:533:LEU:CD1	1:D:494:ARG:HH12	2.14	0.56
1:D:360:LEU:HD13	1:D:360:LEU:C	2.30	0.56
1:D:380:ILE:N	1:D:380:ILE:HD13	2.21	0.56
1:A:231:LYS:HE3	3:A:790:HOH:O	2.05	0.56
1:C:350:ASN:ND2	1:C:412:LYS:HE3	2.20	0.56
1:B:158:MET:SD	1:B:176:MET:HE2	2.45	0.56
1:D:38:THR:CG2	1:D:46:ASP:HB2	2.36	0.56
1:D:183:PRO:HB2	1:D:203:ILE:HG23	1.88	0.56
1:D:259:ASP:HA	1:D:303:PRO:HG2	1.88	0.56
1:C:191:ILE:CG2	1:C:192:ALA:N	2.69	0.56
1:A:39:LYS:HB2	1:A:45:PHE:CD1	2.41	0.55
1:B:348:SER:HB3	1:B:399:CYS:O	2.06	0.55
1:C:77:ASN:ND2	2:C:670:NAD:N7N	2.54	0.55
1:B:10:THR:HG22	1:B:132:SER:HB2	1.87	0.55
1:D:434:ASN:HD22	1:D:434:ASN:C	2.12	0.55
1:A:124:ASN:HB3	3:B:991:HOH:O	2.05	0.55
1:A:248:GLU:H	1:A:298:GLN:NE2	2.04	0.55
1:D:300:THR:O	1:D:305:LEU:HD12	2.07	0.55
1:D:350:ASN:OD1	1:D:412:LYS:HD3	2.06	0.55
1:B:506:GLN:HG3	3:B:916:HOH:O	2.07	0.55
1:C:417:GLU:OE1	1:C:429:ARG:HD3	2.05	0.55
1:A:256:GLY:CA	1:A:263:ASN:HD22	2.18	0.55
1:D:318:GLY:HA2	1:D:488:LEU:CD1	2.36	0.55
1:B:348:SER:HB2	1:B:416:ASP:OD2	2.07	0.55
1:D:470:ASP:O	1:D:471:ALA:HB3	2.06	0.55
1:A:154:LEU:HB3	1:A:176:MET:HE3	1.89	0.55
1:B:353:GLY:CA	1:B:406:LYS:HA	2.37	0.55
1:D:321:LEU:HG	1:D:445:LEU:HD22	1.88	0.55
1:D:415:MET:HE3	1:D:431:SER:HB2	1.86	0.55
1:A:185:ILE:CD1	1:A:223:ILE:HD11	2.37	0.55
1:A:325:GLN:NE2	3:A:935:HOH:O	2.40	0.55
1:D:478:TYR:CD2	1:D:479:PRO:HD2	2.42	0.55
1:C:403:LYS:NZ	1:C:403:LYS:HB3	2.21	0.55
1:D:191:ILE:HG21	1:D:195:GLN:HG3	1.88	0.55
1:A:351:HIS:HA	1:A:403:LYS:O	2.07	0.54
1:B:155:TYR:CE2	1:B:173:LYS:HE3	2.42	0.54
1:B:200:ASN:C	1:B:200:ASN:ND2	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:THR:CG2	1:D:44:ARG:HB3	2.37	0.54
1:C:318:GLY:O	1:C:319:ASP:HB2	2.07	0.54
1:B:76:ASN:HB3	1:B:439:SER:OG	2.07	0.54
1:A:325:GLN:HE22	1:A:434:ASN:HB2	1.72	0.54
1:B:459:VAL:HB	1:B:477:PHE:HE1	1.73	0.54
1:C:24:ASN:ND2	1:C:61:LYS:HB2	2.19	0.54
1:A:301:PHE:HB2	3:A:942:HOH:O	2.08	0.54
1:C:296:SER:HB3	1:C:297:PRO:HD2	1.89	0.54
1:A:299:ASN:ND2	1:A:299:ASN:H	2.06	0.54
1:A:381:ILE:HD11	1:A:396:VAL:CG2	2.35	0.54
1:C:297:PRO:HB3	1:C:320:ASP:CG	2.33	0.54
1:D:302:VAL:HB	1:D:303:PRO:HD2	1.88	0.54
1:A:116:LYS:HB3	1:A:523:GLN:HE22	1.72	0.54
1:A:158:MET:CE	1:A:176:MET:HG3	2.37	0.54
1:C:238:LYS:HG2	3:C:1015:HOH:O	2.08	0.54
1:C:354:ASN:HB2	3:C:688:HOH:O	2.08	0.54
1:A:47:VAL:CG2	1:B:14:VAL:HB	2.38	0.53
1:A:246:ASN:HD22	1:A:359:ASN:ND2	2.06	0.53
1:C:341:ILE:O	1:C:343:PRO:HD3	2.08	0.53
1:A:210:ASN:O	1:A:211:VAL:O	2.26	0.53
1:B:20:THR:HG22	1:B:21:TYR:N	2.23	0.53
1:B:117:LEU:HD21	1:B:133:LEU:HD21	1.90	0.53
1:B:352:LEU:HD13	1:B:352:LEU:N	2.23	0.53
1:B:454:GLU:OE2	1:B:458:ARG:HD3	2.08	0.53
1:C:21:TYR:CE2	1:C:26:LEU:HD13	2.43	0.53
1:D:151:ASN:H	1:D:200:ASN:HD21	1.55	0.53
1:D:480:VAL:HG11	1:D:492:LEU:HD22	1.90	0.53
1:C:18:LYS:HA	1:C:29:LYS:HE2	1.90	0.53
1:C:234:ASN:HB2	1:C:236:LEU:HD22	1.90	0.53
1:D:502:GLY:O	1:D:506:GLN:HG3	2.08	0.53
1:D:225:ARG:NH2	3:D:819:HOH:O	2.40	0.53
1:B:325:GLN:HG2	1:B:414:ALA:HB1	1.90	0.53
1:C:352:LEU:HD23	1:C:352:LEU:H	1.74	0.53
1:C:381:ILE:HG23	1:C:388:TYR:CG	2.44	0.53
1:D:261:MET:HE2	1:D:308:LEU:HA	1.89	0.53
1:B:224:ARG:O	1:B:228:GLN:HG3	2.09	0.53
1:B:351:HIS:HB3	1:B:403:LYS:HB2	1.91	0.53
1:D:165:GLU:HG3	3:D:734:HOH:O	2.09	0.53
1:C:58:LEU:HD13	1:C:459:VAL:HG22	1.91	0.53
1:B:346:ILE:HG23	1:B:418:TYR:CE2	2.44	0.53
1:C:325:GLN:HE21	1:C:412:LYS:HD3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ALA:C	1:D:195:GLN:H	2.17	0.53
1:D:206:ASP:HB3	1:D:212:THR:HB	1.90	0.53
1:A:500:VAL:HG22	3:A:943:HOH:O	2.07	0.53
1:B:180:LYS:HE3	3:B:982:HOH:O	2.08	0.53
1:C:533:LEU:HD22	1:D:494:ARG:HH12	1.72	0.53
1:D:224:ARG:O	1:D:228:GLN:HG3	2.09	0.53
1:A:183:PRO:HB2	1:A:203:ILE:HG23	1.91	0.52
1:B:491:PRO:HD2	1:B:501:ASN:HD21	1.74	0.52
1:B:255:PRO:HA	1:B:259:ASP:OD1	2.09	0.52
1:C:134:LEU:HD21	1:C:518:ILE:HG22	1.91	0.52
1:B:188:PRO:O	1:B:192:ALA:HB2	2.09	0.52
1:B:350:ASN:ND2	1:B:402:ILE:HG12	2.24	0.52
1:C:112:CYS:HB3	1:D:387:LEU:CD1	2.39	0.52
1:C:192:ALA:HB2	1:C:359:ASN:OD1	2.09	0.52
1:C:328:LEU:CD2	1:C:432:ILE:HG21	2.38	0.52
1:C:532:LEU:HD23	1:D:54:TYR:CE2	2.44	0.52
1:D:183:PRO:HB2	1:D:203:ILE:CG2	2.40	0.52
1:D:467:VAL:O	1:D:467:VAL:HG13	2.08	0.52
1:A:67:GLY:HA3	1:A:236:LEU:HD13	1.91	0.52
1:A:360:LEU:HD23	3:A:1059:HOH:O	2.09	0.52
1:B:208:LYS:HE3	3:B:974:HOH:O	2.10	0.52
1:D:360:LEU:HD22	1:D:360:LEU:O	2.10	0.52
1:A:272:HIS:ND1	1:A:273:GLU:N	2.57	0.52
1:A:328:LEU:HD21	1:B:332:LEU:CD2	2.39	0.52
1:B:326:THR:OG1	1:B:489:LYS:HE2	2.09	0.52
1:C:55:VAL:HG23	1:C:464:VAL:HG11	1.90	0.52
1:C:200:ASN:C	1:C:200:ASN:HD22	2.17	0.52
1:C:294:ASN:HB3	1:C:318:GLY:HA3	1.92	0.52
1:C:400:ILE:HG23	1:C:400:ILE:O	2.10	0.52
1:D:151:ASN:C	1:D:151:ASN:HD22	2.17	0.52
1:B:12:VAL:HG21	1:B:133:LEU:CD2	2.40	0.52
1:A:238:LYS:HG3	3:A:1034:HOH:O	2.09	0.52
1:A:470:ASP:O	1:A:471:ALA:HB3	2.09	0.52
1:B:452:MET:HE2	1:B:510:LEU:HD22	1.92	0.52
1:C:373:LYS:CE	1:C:489:LYS:HD3	2.37	0.52
1:D:484:LEU:HA	1:D:487:TRP:CZ3	2.45	0.52
1:A:307:GLN:HA	1:A:310:GLU:OE1	2.09	0.52
1:D:88:ASN:HD21	1:D:104:ASN:CA	2.23	0.52
1:A:206:ASP:HB3	1:A:212:THR:OG1	2.09	0.51
1:A:515:ARG:NH1	1:A:521:PRO:O	2.43	0.51
1:A:417:GLU:OE2	1:A:429:ARG:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:SER:C	1:C:320:ASP:H	2.18	0.51
1:A:341:ILE:HD13	1:B:107:GLY:HA2	1.92	0.51
1:A:502:GLY:HA3	1:A:505:LYS:CE	2.30	0.51
1:C:306:VAL:O	1:C:310:GLU:HG3	2.10	0.51
1:C:348:SER:HA	1:C:416:ASP:OD1	2.11	0.51
1:C:440:LEU:CD2	1:D:426:GLY:HA3	2.40	0.51
1:D:200:ASN:C	1:D:200:ASN:HD22	2.16	0.51
1:C:329:LYS:HE2	1:C:348:SER:OG	2.10	0.51
1:B:131:ASN:C	1:B:131:ASN:ND2	2.69	0.51
1:A:358:TYR:O	1:A:361:SER:HB3	2.10	0.51
1:B:301:PHE:CD1	1:B:492:LEU:HD22	2.45	0.51
1:B:301:PHE:HD1	1:B:492:LEU:HD22	1.75	0.51
1:B:352:LEU:C	1:B:352:LEU:HD22	2.34	0.51
1:C:478:TYR:HB2	1:C:494:ARG:NH2	2.23	0.51
1:A:405:MET:HG3	3:C:920:HOH:O	2.10	0.51
1:B:325:GLN:HA	1:B:325:GLN:NE2	2.26	0.51
1:C:438:ASP:HB3	2:C:670:NAD:O7N	2.10	0.51
1:D:295:GLY:HA3	1:D:321:LEU:HD13	1.93	0.51
1:D:438:ASP:OD2	1:D:438:ASP:N	2.44	0.51
1:B:489:LYS:C	1:B:491:PRO:HD3	2.36	0.51
1:C:347:ALA:HB1	1:C:349:TYR:CE2	2.45	0.51
1:B:248:GLU:OE1	1:B:277:PRO:HD2	2.11	0.51
1:A:39:LYS:HD2	1:A:45:PHE:CZ	2.46	0.50
1:A:350:ASN:HD21	1:A:402:ILE:HG23	1.76	0.50
1:A:437:GLU:HG3	3:A:658:HOH:O	2.11	0.50
1:A:516:LEU:C	1:A:516:LEU:HD12	2.35	0.50
1:C:445:LEU:HG	1:C:487:TRP:HD1	1.76	0.50
1:A:192:ALA:O	1:A:193:ALA:C	2.53	0.50
1:A:306:VAL:O	1:A:310:GLU:HG3	2.11	0.50
1:B:356:ASP:HB2	2:B:660:NAD:H3D	1.93	0.50
1:C:185:ILE:HG12	1:C:203:ILE:HD11	1.92	0.50
1:A:344:VAL:HG22	1:A:419:TYR:O	2.12	0.50
1:C:282:ALA:HB3	1:C:305:LEU:HD21	1.93	0.50
2:C:670:NAD:O5D	2:C:670:NAD:H2N	2.11	0.50
1:A:296:SER:HA	2:A:650:NAD:O2D	2.11	0.50
1:A:302:VAL:HB	1:A:303:PRO:HD2	1.92	0.50
1:D:340:GLY:O	1:D:387:LEU:HD21	2.10	0.50
1:A:253:VAL:HG13	1:A:253:VAL:O	2.10	0.50
1:B:122:GLU:N	1:B:122:GLU:OE2	2.42	0.50
1:B:150:ASN:HD22	1:B:198:ARG:HG3	1.77	0.50
1:B:310:GLU:HG2	1:B:479:PRO:CG	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LYS:HE3	3:A:988:HOH:O	2.11	0.50
1:A:158:MET:SD	1:A:176:MET:HE2	2.51	0.50
1:B:476:ASN:HB3	3:B:827:HOH:O	2.10	0.50
1:C:150:ASN:HA	1:C:200:ASN:HD21	1.77	0.50
1:C:354:ASN:OD1	1:C:356:ASP:HB3	2.12	0.50
1:C:433:HIS:HB3	1:D:431:SER:OG	2.12	0.50
1:B:348:SER:C	1:B:349:TYR:CD1	2.90	0.50
1:C:500:VAL:HG11	3:D:864:HOH:O	2.11	0.50
1:C:372:SER:CB	1:C:490:ALA:HB2	2.42	0.50
1:A:286:ILE:HG23	1:A:314:THR:HG21	1.94	0.49
1:C:319:ASP:O	1:C:320:ASP:HB2	2.11	0.49
1:D:445:LEU:C	1:D:445:LEU:HD23	2.37	0.49
1:B:221:GLN:HG2	3:B:983:HOH:O	2.12	0.49
1:C:51:VAL:HG22	1:C:52:GLN:N	2.27	0.49
1:C:516:LEU:HD23	1:C:517:LEU:N	2.27	0.49
1:A:47:VAL:HG22	1:B:14:VAL:CB	2.42	0.49
1:D:40:THR:HG22	1:D:44:ARG:HB3	1.93	0.49
1:D:412:LYS:HE3	1:D:438:ASP:CG	2.38	0.49
1:A:191:ILE:HD12	1:A:195:GLN:HG2	1.94	0.49
3:C:996:HOH:O	1:D:463:LYS:HD2	2.13	0.49
1:D:115:LEU:HD22	1:D:511:GLU:CG	2.39	0.49
1:D:231:LYS:HE2	1:D:239:VAL:HG13	1.94	0.49
1:A:349:TYR:O	1:A:350:ASN:HB3	2.13	0.49
1:B:216:LYS:HA	1:B:219:HIS:ND1	2.28	0.49
1:B:253:VAL:HG13	1:B:253:VAL:O	2.12	0.49
1:B:272:HIS:HE1	1:B:274:GLU:HG2	1.77	0.49
1:C:55:VAL:HG23	1:C:464:VAL:CG1	2.42	0.49
1:C:180:LYS:HB3	3:C:881:HOH:O	2.11	0.49
1:A:88:ASN:HD21	1:A:104:ASN:CA	2.25	0.49
1:B:491:PRO:CD	1:B:501:ASN:HD21	2.25	0.49
1:C:34:ASN:CG	1:C:35:ALA:H	2.20	0.49
1:A:204:ASN:O	1:A:211:VAL:O	2.30	0.49
1:A:408:VAL:HG12	1:A:411:SER:O	2.12	0.49
1:B:272:HIS:CE1	1:B:274:GLU:HG2	2.48	0.49
1:C:502:GLY:O	1:C:506:GLN:HG3	2.13	0.49
1:D:44:ARG:NH1	1:D:44:ARG:HB3	2.28	0.49
1:A:151:ASN:CB	1:A:180:LYS:HE2	2.42	0.49
1:B:63:PRO:CG	1:B:238:LYS:HG3	2.43	0.49
1:A:211:VAL:O	1:A:212:THR:HB	2.13	0.48
1:A:391:LYS:HD3	3:A:761:HOH:O	2.12	0.48
1:B:296:SER:O	1:B:320:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:MET:HE3	1:B:424:LEU:CD2	2.37	0.48
1:C:116:LYS:NZ	3:C:1036:HOH:O	2.45	0.48
1:C:310:GLU:CG	1:C:479:PRO:HG2	2.41	0.48
1:D:68:ILE:HG22	1:D:70:LEU:HD13	1.95	0.48
1:A:88:ASN:HD21	1:A:104:ASN:HA	1.77	0.48
1:B:318:GLY:HA2	1:B:488:LEU:CD1	2.42	0.48
1:C:500:VAL:HG21	1:D:527:ARG:CZ	2.43	0.48
1:D:286:ILE:CG2	1:D:308:LEU:HD13	2.43	0.48
1:D:328:LEU:HD23	1:D:432:ILE:HG21	1.94	0.48
1:D:504:ASN:HB2	1:D:505:LYS:NZ	2.28	0.48
1:B:297:PRO:HB3	1:B:320:ASP:OD2	2.13	0.48
1:D:88:ASN:HD21	1:D:104:ASN:HA	1.79	0.48
1:A:45:PHE:HE2	1:B:10:THR:HG21	1.78	0.48
1:A:47:VAL:HG22	1:B:14:VAL:CA	2.43	0.48
1:A:95:GLN:NE2	1:A:100:VAL:HG22	2.28	0.48
1:A:183:PRO:HB2	1:A:203:ILE:CG2	2.43	0.48
1:C:272:HIS:HD2	1:C:274:GLU:HB2	1.77	0.48
1:C:445:LEU:C	1:C:445:LEU:HD23	2.38	0.48
1:D:343:PRO:HD2	1:D:388:TYR:OH	2.13	0.48
1:A:39:LYS:HD2	1:A:45:PHE:CE1	2.48	0.48
1:A:452:MET:HG3	1:A:487:TRP:CH2	2.49	0.48
1:C:328:LEU:HD22	1:C:432:ILE:HG21	1.95	0.48
1:C:334:GLN:HB2	3:C:980:HOH:O	2.14	0.48
1:D:261:MET:H	1:D:307:GLN:NE2	2.11	0.48
1:A:151:ASN:ND2	1:A:200:ASN:HD21	2.12	0.48
1:A:308:LEU:O	1:A:312:GLU:HG2	2.13	0.48
1:A:494:ARG:CG	1:A:495:PRO:HD2	2.43	0.48
1:C:257:VAL:HG13	1:C:258:ASN:N	2.29	0.48
1:C:533:LEU:HD22	1:D:494:ARG:NH1	2.28	0.48
1:B:435:VAL:O	1:B:436:CYS:HB3	2.14	0.48
1:C:343:PRO:HD2	1:C:388:TYR:OH	2.14	0.48
1:C:376:VAL:HG22	1:C:501:ASN:HB3	1.96	0.48
1:D:441:LEU:HD12	3:D:946:HOH:O	2.14	0.48
1:A:225:ARG:HG3	3:A:882:HOH:O	2.13	0.48
1:A:322:LYS:HZ2	1:A:506:GLN:HE22	1.59	0.48
1:B:407:PRO:HB3	1:D:344:VAL:HG23	1.95	0.48
1:B:515:ARG:HD2	3:B:851:HOH:O	2.14	0.48
1:D:24:ASN:OD1	1:D:61:LYS:HB2	2.14	0.48
1:A:131:ASN:N	1:A:131:ASN:HD22	2.10	0.48
1:A:299:ASN:N	1:A:299:ASN:HD22	2.11	0.48
1:C:256:GLY:H	1:C:259:ASP:CG	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:GLU:O	1:D:65:LYS:HE3	2.14	0.48
1:D:180:LYS:HD2	3:D:928:HOH:O	2.13	0.48
1:D:325:GLN:HE21	1:D:325:GLN:CA	2.17	0.48
1:A:112:CYS:HA	1:B:386:ILE:HG21	1.96	0.47
1:A:122:GLU:N	1:A:122:GLU:OE1	2.48	0.47
1:B:257:VAL:HG13	1:B:272:HIS:CD2	2.49	0.47
1:D:200:ASN:C	1:D:200:ASN:ND2	2.71	0.47
1:D:247:THR:CG2	1:D:297:PRO:HG2	2.43	0.47
1:B:20:THR:CG2	1:B:21:TYR:N	2.77	0.47
1:B:229:ASN:O	1:B:233:GLU:HG3	2.15	0.47
1:C:386:ILE:HG21	1:D:112:CYS:HA	1.95	0.47
1:C:394:LYS:HB3	1:C:394:LYS:HZ3	1.78	0.47
1:D:71:ILE:HD13	1:D:243:TRP:HE3	1.79	0.47
1:D:137:VAL:HG13	3:D:696:HOH:O	2.14	0.47
1:D:360:LEU:HD13	1:D:360:LEU:O	2.14	0.47
1:C:412:LYS:HE2	1:C:414:ALA:HB2	1.96	0.47
1:D:220:LEU:O	1:D:224:ARG:HG3	2.14	0.47
1:B:500:VAL:HG13	1:B:500:VAL:O	2.13	0.47
1:D:248:GLU:H	1:D:298:GLN:NE2	2.12	0.47
1:D:254:SER:HB2	1:D:257:VAL:HB	1.97	0.47
1:D:266:GLN:NE2	1:D:270:ASN:HD21	2.12	0.47
1:B:224:ARG:HD2	1:B:287:LEU:HD23	1.96	0.47
1:C:251:VAL:HG21	1:C:274:GLU:O	2.14	0.47
1:C:372:SER:HB3	1:C:490:ALA:HB2	1.96	0.47
1:D:504:ASN:ND2	3:D:827:HOH:O	2.47	0.47
1:D:253:VAL:O	1:D:253:VAL:HG13	2.15	0.47
1:A:39:LYS:HB2	1:A:45:PHE:CE1	2.49	0.47
1:B:332:LEU:O	1:B:335:PHE:HB3	2.15	0.47
1:C:229:ASN:HB3	1:C:233:GLU:OE1	2.14	0.47
1:C:342:LYS:HB2	1:C:387:LEU:HG	1.97	0.47
1:C:481:LEU:HA	3:C:852:HOH:O	2.15	0.47
1:D:325:GLN:HG2	1:D:414:ALA:HB1	1.96	0.47
1:C:445:LEU:HG	1:C:487:TRP:CD1	2.50	0.47
1:D:71:ILE:HG21	1:D:243:TRP:CE3	2.49	0.47
1:A:354:ASN:C	1:A:354:ASN:HD22	2.22	0.47
1:B:261:MET:HE2	1:B:307:GLN:HG2	1.96	0.47
1:B:405:MET:C	1:B:407:PRO:HD2	2.40	0.47
1:C:272:HIS:CD2	1:C:274:GLU:HB2	2.49	0.47
2:D:680:NAD:N7N	2:D:680:NAD:O2N	2.48	0.47
1:D:231:LYS:HE2	1:D:239:VAL:CG1	2.45	0.47
1:A:151:ASN:HB2	1:A:180:LYS:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:SER:HA	1:A:397:ASP:O	2.15	0.46
1:B:193:ALA:H	1:B:196:ASP:HB2	1.79	0.46
1:B:489:LYS:O	1:B:491:PRO:HD3	2.15	0.46
1:C:342:LYS:NZ	3:C:1025:HOH:O	2.47	0.46
1:C:443:THR:HG21	1:D:423:MET:HE1	1.97	0.46
1:A:415:MET:HE1	3:A:878:HOH:O	2.15	0.46
1:A:476:ASN:HB3	3:A:875:HOH:O	2.15	0.46
1:C:257:VAL:HG13	1:C:258:ASN:H	1.79	0.46
1:D:22:LYS:HB2	1:D:25:GLU:HB3	1.97	0.46
1:A:54:TYR:CE2	1:B:532:LEU:HD23	2.50	0.46
1:B:38:THR:HG22	1:B:39:LYS:N	2.30	0.46
1:B:198:ARG:NH2	1:B:355:ASN:HD21	2.12	0.46
1:D:167:ASP:O	1:D:171:ARG:HG3	2.15	0.46
1:B:216:LYS:O	1:B:219:HIS:HB2	2.15	0.46
1:C:217:TRP:O	1:C:220:LEU:HB3	2.14	0.46
1:A:131:ASN:HD22	1:A:131:ASN:H	1.63	0.46
1:B:73:LEU:HD23	1:B:181:PRO:HB3	1.98	0.46
1:A:206:ASP:OD1	1:A:208:LYS:N	2.48	0.46
1:D:37:VAL:HG22	1:D:47:VAL:HG22	1.97	0.46
1:D:206:ASP:N	1:D:210:ASN:O	2.38	0.46
1:D:262:GLU:OE2	1:D:262:GLU:HA	2.16	0.46
1:D:530:GLU:O	1:D:531:ARG:C	2.58	0.46
1:A:45:PHE:HB2	1:B:12:VAL:HG22	1.98	0.46
1:A:453:THR:O	1:A:457:THR:HG23	2.15	0.46
1:D:527:ARG:C	1:D:529:GLU:H	2.23	0.46
1:B:10:THR:N	3:B:917:HOH:O	2.48	0.46
1:C:193:ALA:C	1:C:195:GLN:H	2.23	0.46
1:B:39:LYS:HE2	1:B:43:GLY:HA2	1.98	0.46
1:B:248:GLU:HB2	1:B:298:GLN:HG2	1.97	0.46
1:C:262:GLU:HB2	3:C:830:HOH:O	2.16	0.46
1:A:32:TYR:OH	1:B:529:GLU:OE2	2.33	0.46
1:A:299:ASN:H	1:A:299:ASN:HD22	1.64	0.46
1:A:494:ARG:HG3	1:A:495:PRO:HD2	1.98	0.46
1:A:528:PHE:C	1:A:530:GLU:H	2.24	0.46
1:D:38:THR:HG23	1:D:38:THR:O	2.16	0.46
1:D:40:THR:CG2	1:D:44:ARG:H	2.28	0.46
1:D:121:ALA:HB3	1:D:122:GLU:OE2	2.16	0.46
1:D:153:ASP:OD2	1:D:155:TYR:HB3	2.16	0.46
1:B:21:TYR:CE1	1:B:26:LEU:HD23	2.51	0.45
1:C:473:LYS:O	1:C:473:LYS:HG2	2.16	0.45
1:D:329:LYS:NZ	1:D:348:SER:HB2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:MET:HG3	1:D:487:TRP:CH2	2.50	0.45
1:A:256:GLY:C	1:A:263:ASN:HD22	2.24	0.45
1:B:250:TYR:HD1	3:B:858:HOH:O	1.98	0.45
1:B:453:THR:O	1:B:457:THR:HG23	2.16	0.45
1:C:363:PRO:HA	1:C:366:PHE:HB3	1.98	0.45
1:C:413:VAL:HG22	1:C:435:VAL:HG22	1.97	0.45
1:D:150:ASN:HA	1:D:200:ASN:ND2	2.31	0.45
1:A:131:ASN:H	1:A:131:ASN:ND2	2.14	0.45
1:A:187:TYR:HA	1:A:188:PRO:HD2	1.79	0.45
1:A:389:ASN:OD1	1:A:392:LEU:HD23	2.16	0.45
1:A:404:TYR:OH	1:A:406:LYS:HG2	2.17	0.45
1:B:18:LYS:O	1:B:28:THR:HA	2.16	0.45
1:B:220:LEU:O	1:B:220:LEU:HD23	2.16	0.45
1:B:246:ASN:HB3	3:B:987:HOH:O	2.15	0.45
1:D:41:ALA:C	1:D:43:GLY:H	2.24	0.45
1:A:76:ASN:HB3	1:A:439:SER:OG	2.17	0.45
1:A:147:TRP:HB3	1:A:184:SER:HB2	1.96	0.45
1:B:323:SER:N	1:B:489:LYS:HE3	2.17	0.45
1:C:261:MET:HE1	1:C:311:HIS:ND1	2.31	0.45
1:D:71:ILE:HG21	1:D:243:TRP:CZ3	2.52	0.45
1:B:480:VAL:O	1:B:480:VAL:CG2	2.63	0.45
1:D:354:ASN:C	1:D:356:ASP:H	2.25	0.45
1:A:328:LEU:HD21	1:B:332:LEU:HD23	1.98	0.45
1:A:405:MET:O	1:A:408:VAL:HG23	2.16	0.45
1:B:115:LEU:HG	1:B:511:GLU:HG3	1.97	0.45
1:B:220:LEU:HD23	1:B:220:LEU:C	2.42	0.45
1:C:198:ARG:NH2	1:C:355:ASN:ND2	2.65	0.45
1:C:293:ILE:HA	1:C:317:ALA:O	2.17	0.45
1:A:248:GLU:OE2	1:A:277:PRO:HD2	2.17	0.45
1:B:139:PRO:HA	1:B:142:PHE:CE2	2.52	0.45
1:B:198:ARG:HH22	1:B:355:ASN:ND2	2.15	0.45
1:A:208:LYS:HB2	1:A:210:ASN:OD1	2.17	0.45
1:B:192:ALA:O	1:B:193:ALA:HB3	2.17	0.45
1:B:206:ASP:OD1	1:B:209:GLY:N	2.49	0.45
1:C:271:ASP:O	1:C:272:HIS:C	2.59	0.45
1:C:364:LYS:HB2	1:C:365:GLN:NE2	2.31	0.45
1:B:195:GLN:NE2	1:B:195:GLN:N	2.65	0.45
1:B:452:MET:HG3	1:B:487:TRP:CH2	2.52	0.45
1:C:371:ILE:HG22	1:C:372:SER:N	2.31	0.45
1:C:500:VAL:HG21	1:D:527:ARG:HE	1.79	0.45
1:D:121:ALA:N	3:D:740:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:TRP:O	1:D:221:GLN:HG3	2.17	0.45
1:A:225:ARG:HH11	1:A:228:GLN:NE2	2.14	0.45
1:A:489:LYS:HD3	3:A:986:HOH:O	2.16	0.45
1:B:315:PHE:CD1	1:B:481:LEU:HD11	2.51	0.45
1:B:322:LYS:HA	1:B:489:LYS:CG	2.32	0.45
1:B:516:LEU:HD12	1:B:516:LEU:C	2.41	0.45
1:D:352:LEU:HA	1:D:412:LYS:CA	2.42	0.45
1:D:526:LEU:O	1:D:531:ARG:NE	2.43	0.45
1:A:496:GLY:C	1:A:497:PHE:CD1	2.95	0.44
1:B:218:THR:HG23	3:B:984:HOH:O	2.18	0.44
1:C:55:VAL:CG2	1:C:464:VAL:HG11	2.47	0.44
1:C:352:LEU:HD23	1:C:352:LEU:N	2.32	0.44
1:A:65:LYS:NZ	3:A:996:HOH:O	2.50	0.44
1:B:272:HIS:HB3	1:B:275:ILE:HG12	1.99	0.44
1:C:22:LYS:HB3	1:C:22:LYS:NZ	2.32	0.44
1:C:315:PHE:CD1	1:C:481:LEU:HD11	2.53	0.44
1:C:319:ASP:HB2	1:C:490:ALA:O	2.18	0.44
1:D:190:PHE:O	1:D:249:ARG:HG3	2.17	0.44
1:A:351:HIS:CD2	1:C:349:TYR:OH	2.69	0.44
1:C:148:ASP:HA	2:C:670:NAD:N3A	2.32	0.44
1:C:204:ASN:HB3	1:C:219:HIS:CE1	2.52	0.44
1:A:282:ALA:HB3	1:A:305:LEU:HD21	1.99	0.44
1:A:452:MET:HG3	1:A:487:TRP:HH2	1.83	0.44
1:A:532:LEU:O	1:A:533:LEU:C	2.60	0.44
1:B:148:ASP:HA	2:B:660:NAD:N3A	2.32	0.44
1:C:69:MET:HE1	1:C:227:ILE:CA	2.45	0.44
1:C:335:PHE:HE2	1:D:327:LYS:HB3	1.82	0.44
1:A:69:MET:HE1	1:A:227:ILE:CA	2.30	0.44
1:A:352:LEU:O	1:A:352:LEU:HD22	2.18	0.44
1:B:180:LYS:HB3	3:B:732:HOH:O	2.17	0.44
1:B:198:ARG:NH2	1:B:355:ASN:ND2	2.66	0.44
1:D:505:LYS:HG2	3:D:950:HOH:O	2.15	0.44
1:A:224:ARG:NH1	1:A:287:LEU:HD13	2.33	0.44
1:B:501:ASN:HA	1:B:506:GLN:OE1	2.17	0.44
1:C:335:PHE:CE2	1:D:327:LYS:HB3	2.53	0.44
1:C:497:PHE:CD2	1:D:530:GLU:HG2	2.53	0.44
1:D:247:THR:HG21	1:D:297:PRO:HG2	1.99	0.44
1:D:523:GLN:HE21	1:D:523:GLN:HA	1.83	0.44
1:B:349:TYR:CD1	1:B:349:TYR:N	2.85	0.44
1:C:188:PRO:C	1:C:190:PHE:H	2.25	0.44
1:C:296:SER:O	1:C:319:ASP:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:SER:O	1:C:489:LYS:HG2	2.17	0.44
1:D:134:LEU:HB3	1:D:135:PRO:HD2	1.99	0.44
1:D:308:LEU:O	1:D:308:LEU:HD22	2.18	0.44
1:D:315:PHE:CZ	1:D:481:LEU:HD21	2.52	0.44
1:A:234:ASN:HB2	1:A:236:LEU:HG	2.00	0.44
1:A:492:LEU:C	1:A:492:LEU:HD13	2.43	0.44
1:C:200:ASN:ND2	1:C:200:ASN:C	2.73	0.44
1:C:503:LEU:HA	1:C:506:GLN:OE1	2.18	0.44
1:A:246:ASN:HD22	1:A:359:ASN:HD22	1.66	0.43
1:D:96:THR:HG21	1:D:101:LYS:HD2	1.99	0.43
1:D:347:ALA:HB1	1:D:349:TYR:CE2	2.52	0.43
1:A:352:LEU:HD22	1:A:352:LEU:C	2.42	0.43
1:B:71:ILE:HG21	1:B:243:TRP:CZ3	2.53	0.43
1:B:348:SER:CB	1:B:416:ASP:OD2	2.66	0.43
1:C:516:LEU:C	1:C:516:LEU:CD2	2.90	0.43
1:D:119:ILE:HA	1:D:124:ASN:O	2.18	0.43
1:D:315:PHE:CD1	1:D:481:LEU:HD11	2.53	0.43
1:D:527:ARG:C	1:D:529:GLU:N	2.74	0.43
1:A:117:LEU:HB3	3:A:798:HOH:O	2.18	0.43
1:A:134:LEU:HD11	1:A:517:LEU:HB2	2.00	0.43
1:A:172:LEU:O	1:A:176:MET:HG2	2.18	0.43
1:B:91:ASN:HB3	3:B:752:HOH:O	2.17	0.43
1:B:352:LEU:HD21	1:B:356:ASP:O	2.18	0.43
1:C:112:CYS:HB3	1:D:387:LEU:HD11	1.99	0.43
1:C:259:ASP:OD2	1:C:259:ASP:N	2.51	0.43
1:D:22:LYS:HE3	1:D:27:LEU:CD1	2.40	0.43
1:D:122:GLU:CD	1:D:122:GLU:N	2.76	0.43
1:D:272:HIS:CD2	1:D:274:GLU:H	2.36	0.43
1:D:352:LEU:HB3	1:D:412:LYS:CB	2.46	0.43
1:B:310:GLU:HA	1:B:479:PRO:HG3	2.00	0.43
1:B:462:LYS:HD2	1:B:472:GLY:O	2.17	0.43
1:C:358:TYR:HB2	1:C:404:TYR:CE1	2.54	0.43
1:D:465:ASP:HB3	1:D:468:LYS:HB3	2.00	0.43
1:A:381:ILE:HG23	1:A:388:TYR:CB	2.49	0.43
1:B:117:LEU:HD21	1:B:133:LEU:CD2	2.48	0.43
1:B:183:PRO:HB2	1:B:203:ILE:CG2	2.48	0.43
1:B:355:ASN:HB3	2:B:660:NAD:O1A	2.18	0.43
1:C:533:LEU:C	1:C:533:LEU:HD23	2.43	0.43
1:D:295:GLY:CA	1:D:321:LEU:HD13	2.48	0.43
1:D:447:ILE:O	1:D:451:VAL:HG23	2.18	0.43
1:B:333:ALA:O	1:B:337:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LYS:HB3	1:C:25:GLU:HB2	2.00	0.43
1:C:350:ASN:HB3	1:C:414:ALA:HA	2.00	0.43
1:C:478:TYR:CE2	1:C:494:ARG:HG2	2.53	0.43
1:A:148:ASP:HA	2:A:650:NAD:N3A	2.33	0.43
1:B:352:LEU:N	1:B:352:LEU:CD1	2.82	0.43
1:C:174:ALA:HB2	3:C:933:HOH:O	2.18	0.43
1:C:257:VAL:HG21	1:C:272:HIS:NE2	2.33	0.43
1:C:449:LEU:HD21	1:C:487:TRP:HB2	2.01	0.43
1:D:40:THR:HG21	1:D:44:ARG:HH12	1.75	0.43
1:D:266:GLN:HE21	1:D:270:ASN:ND2	2.16	0.43
1:A:224:ARG:O	1:A:228:GLN:HG3	2.19	0.43
1:A:286:ILE:HG23	1:A:314:THR:CG2	2.48	0.43
1:B:266:GLN:HE21	1:B:270:ASN:ND2	2.14	0.43
1:B:415:MET:HE2	1:D:415:MET:CE	2.48	0.43
1:C:282:ALA:O	1:C:286:ILE:HG13	2.19	0.43
1:D:352:LEU:HD22	1:D:354:ASN:OD1	2.18	0.43
1:A:134:LEU:HD11	1:A:517:LEU:CB	2.49	0.43
1:A:496:GLY:C	1:A:497:PHE:CG	2.97	0.43
1:A:501:ASN:ND2	3:A:795:HOH:O	2.51	0.43
1:C:115:LEU:HD22	1:C:511:GLU:HG2	1.99	0.43
1:C:272:HIS:HD2	1:C:274:GLU:H	1.62	0.43
1:D:286:ILE:HG23	1:D:314:THR:OG1	2.19	0.43
1:D:452:MET:HG3	1:D:487:TRP:HH2	1.84	0.43
1:D:497:PHE:CD1	1:D:497:PHE:N	2.87	0.43
1:A:286:ILE:HG21	1:A:308:LEU:HD22	2.01	0.43
1:B:195:GLN:HG2	1:B:246:ASN:ND2	2.34	0.43
1:B:299:ASN:O	1:B:299:ASN:CG	2.62	0.43
1:C:14:VAL:O	1:C:16:THR:HG22	2.18	0.43
1:C:483:PHE:HA	1:D:531:ARG:NH2	2.34	0.43
1:D:504:ASN:HB2	1:D:505:LYS:HZ3	1.84	0.43
1:B:351:HIS:CD2	1:D:349:TYR:OH	2.72	0.42
1:C:476:ASN:HA	3:C:991:HOH:O	2.18	0.42
1:D:90:HIS:HE1	3:D:790:HOH:O	2.01	0.42
1:B:40:THR:OG1	1:B:44:ARG:HB3	2.19	0.42
1:B:412:LYS:HE3	1:B:412:LYS:HB2	1.78	0.42
1:B:449:LEU:HD21	1:B:487:TRP:HB2	2.01	0.42
1:C:112:CYS:HB3	1:D:387:LEU:HD13	2.01	0.42
1:C:335:PHE:CE1	1:D:328:LEU:CD1	3.03	0.42
1:D:301:PHE:CD1	1:D:492:LEU:HD12	2.54	0.42
1:D:435:VAL:O	1:D:436:CYS:HB3	2.19	0.42
1:A:22:LYS:O	1:A:25:GLU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:CD2	1:A:354:ASN:ND2	2.78	0.42
1:B:261:MET:O	1:B:265:LEU:HG	2.19	0.42
2:C:670:NAD:N7N	2:C:670:NAD:O2N	2.52	0.42
1:A:250:TYR:CE2	1:A:298:GLN:HA	2.54	0.42
1:A:406:LYS:HE2	3:A:699:HOH:O	2.19	0.42
1:A:448:ASP:HB3	1:A:487:TRP:CE2	2.54	0.42
1:C:362:ALA:HB3	1:C:365:GLN:CG	2.46	0.42
1:D:194:ASN:HB2	1:D:358:TYR:CE2	2.55	0.42
1:A:96:THR:HG21	1:A:101:LYS:HD2	2.02	0.42
1:A:220:LEU:CD2	1:A:280:ILE:HG23	2.47	0.42
1:A:418:TYR:O	1:A:429:ARG:HA	2.20	0.42
1:B:189:ASP:O	1:B:249:ARG:HD2	2.19	0.42
1:B:201:ASN:HD22	1:B:201:ASN:HA	1.65	0.42
1:C:18:LYS:HA	1:C:29:LYS:CE	2.50	0.42
1:C:112:CYS:HA	1:D:386:ILE:HG21	2.00	0.42
1:C:461:TYR:OH	1:D:533:LEU:N	2.52	0.42
1:C:495:PRO:HG2	1:C:496:GLY:H	1.82	0.42
1:D:155:TYR:O	1:D:159:GLN:HG3	2.20	0.42
1:D:187:TYR:CD1	1:D:277:PRO:HG3	2.55	0.42
1:A:110:THR:HA	1:A:130:PHE:CD2	2.54	0.42
1:A:137:VAL:HG12	3:A:651:HOH:O	2.19	0.42
1:A:210:ASN:O	1:A:211:VAL:C	2.62	0.42
1:A:407:PRO:HG3	1:C:395:LYS:CE	2.47	0.42
1:B:139:PRO:HA	1:B:142:PHE:CD2	2.54	0.42
1:B:459:VAL:HB	1:B:477:PHE:CE1	2.54	0.42
1:C:76:ASN:HB3	1:C:439:SER:OG	2.19	0.42
1:C:322:LYS:HD2	1:C:327:LYS:HE2	2.00	0.42
1:D:215:GLY:O	1:D:218:THR:OG1	2.36	0.42
1:A:187:TYR:CD1	1:A:213:THR:HG22	2.55	0.42
1:A:259:ASP:HA	1:A:303:PRO:HG2	2.02	0.42
1:B:42:SER:O	1:B:44:ARG:N	2.50	0.42
1:B:310:GLU:CG	1:B:479:PRO:HG3	2.45	0.42
1:D:205:LEU:HA	1:D:210:ASN:O	2.20	0.42
1:D:239:VAL:O	1:D:290:VAL:HG13	2.20	0.42
1:A:405:MET:CE	1:C:397:ASP:HB3	2.50	0.42
1:B:345:SER:C	1:B:346:ILE:HG13	2.45	0.42
1:B:350:ASN:HD21	1:B:402:ILE:HG12	1.85	0.42
1:B:26:LEU:HD22	1:B:27:LEU:N	2.34	0.42
1:B:454:GLU:OE1	1:B:458:ARG:NH2	2.53	0.42
1:C:489:LYS:C	1:C:491:PRO:HD3	2.45	0.42
1:D:325:GLN:HG2	3:D:785:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:SER:HB3	3:A:740:HOH:O	2.19	0.42
1:A:90:HIS:HE1	3:A:784:HOH:O	2.02	0.42
1:A:184:SER:OG	1:A:185:ILE:N	2.52	0.42
1:B:183:PRO:HB2	1:B:203:ILE:HG23	2.02	0.42
1:A:389:ASN:ND2	1:A:392:LEU:HD21	2.25	0.41
1:C:406:LYS:HB3	1:C:407:PRO:HD3	2.01	0.41
1:D:241:VAL:HG23	1:D:290:VAL:HG11	2.02	0.41
1:D:294:ASN:ND2	3:D:726:HOH:O	2.53	0.41
1:A:350:ASN:ND2	1:A:412:LYS:HE3	2.35	0.41
1:C:258:ASN:C	1:C:258:ASN:ND2	2.76	0.41
1:D:434:ASN:C	1:D:434:ASN:ND2	2.76	0.41
1:D:492:LEU:HD23	1:D:493:THR:N	2.35	0.41
1:A:185:ILE:HD11	1:A:223:ILE:CD1	2.51	0.41
1:A:247:THR:CG2	1:A:297:PRO:HG2	2.51	0.41
1:B:350:ASN:O	1:B:402:ILE:HA	2.20	0.41
1:C:22:LYS:HE3	3:C:773:HOH:O	2.20	0.41
1:C:273:GLU:CD	1:C:273:GLU:N	2.77	0.41
1:C:398:HIS:CD2	1:C:398:HIS:N	2.89	0.41
1:C:462:LYS:HD2	1:C:473:LYS:HD3	2.02	0.41
1:C:486:TYR:CD1	1:C:486:TYR:C	2.98	0.41
1:D:266:GLN:HE21	1:D:270:ASN:HD21	1.69	0.41
1:D:384:ASN:O	1:D:388:TYR:HB2	2.21	0.41
1:A:95:GLN:CD	1:A:100:VAL:HG22	2.46	0.41
1:B:27:LEU:N	1:B:27:LEU:HD22	2.35	0.41
1:C:321:LEU:O	1:C:322:LYS:C	2.63	0.41
1:D:39:LYS:HE2	1:D:43:GLY:HA2	2.03	0.41
1:D:352:LEU:HD11	1:D:357:GLY:CA	2.44	0.41
1:A:486:TYR:CD1	1:A:486:TYR:C	2.98	0.41
1:B:253:VAL:O	1:B:253:VAL:HG22	2.21	0.41
1:C:437:GLU:H	1:C:437:GLU:CD	2.25	0.41
1:D:353:GLY:O	1:D:410:ASP:N	2.53	0.41
1:A:190:PHE:CE2	1:A:276:ALA:HB2	2.56	0.41
1:A:285:SER:HB3	1:A:290:VAL:CG2	2.51	0.41
1:A:343:PRO:HD2	1:A:388:TYR:OH	2.21	0.41
1:B:253:VAL:HA	1:B:258:ASN:OD1	2.21	0.41
1:B:408:VAL:HB	1:B:411:SER:O	2.21	0.41
1:C:30:TYR:CD1	1:C:516:LEU:HG	2.56	0.41
1:C:254:SER:N	1:C:258:ASN:HD21	2.18	0.41
1:C:312:GLU:OE1	3:C:873:HOH:O	2.22	0.41
1:C:532:LEU:O	1:C:533:LEU:OXT	2.39	0.41
1:C:327:LYS:O	1:C:331:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ASP:O	1:C:360:LEU:HD23	2.20	0.41
1:C:477:PHE:HD1	3:C:991:HOH:O	2.04	0.41
1:D:125:ASP:CG	1:D:527:ARG:HH12	2.27	0.41
1:D:530:GLU:O	1:D:532:LEU:N	2.53	0.41
1:A:532:LEU:HD23	1:B:54:TYR:CE2	2.56	0.41
1:B:351:HIS:HD2	1:D:349:TYR:OH	2.03	0.41
1:C:242:LEU:C	1:C:242:LEU:HD23	2.46	0.41
1:C:298:GLN:H	1:C:298:GLN:HG3	1.45	0.41
1:C:481:LEU:C	1:C:483:PHE:N	2.77	0.41
1:D:323:SER:O	1:D:327:LYS:HG3	2.21	0.41
1:D:494:ARG:HB3	1:D:495:PRO:HD2	2.03	0.41
1:A:41:ALA:C	1:A:43:GLY:H	2.29	0.41
1:A:44:ARG:HH11	1:B:13:LYS:CB	2.34	0.41
1:A:65:LYS:HE2	1:A:141:ASP:HA	2.03	0.41
1:A:175:LYS:NZ	3:A:806:HOH:O	2.48	0.41
1:A:206:ASP:OD1	1:A:206:ASP:C	2.64	0.41
1:A:285:SER:HB3	1:A:290:VAL:HG23	2.01	0.41
1:A:347:ALA:HB1	1:A:349:TYR:CE2	2.55	0.41
1:B:212:THR:HG22	1:B:214:ARG:N	2.27	0.41
1:B:248:GLU:N	1:B:298:GLN:HG2	2.27	0.41
1:C:134:LEU:HD21	1:C:518:ILE:CG2	2.51	0.41
1:C:150:ASN:HB2	1:C:198:ARG:HG2	2.03	0.41
1:C:249:ARG:HG3	1:C:249:ARG:HH21	1.86	0.41
1:C:349:TYR:CD1	1:C:401:VAL:HB	2.56	0.41
1:C:362:ALA:HA	1:C:363:PRO:HD2	1.90	0.41
1:D:289:GLY:HA2	1:D:314:THR:HG22	2.01	0.41
1:C:112:CYS:SG	1:D:387:LEU:HD11	2.61	0.41
1:D:437:GLU:H	1:D:437:GLU:HG2	1.44	0.41
1:A:394:LYS:CG	1:A:394:LYS:O	2.69	0.40
1:A:533:LEU:HD21	1:B:463:LYS:HE2	2.03	0.40
1:B:198:ARG:HH22	1:B:355:ASN:CG	2.29	0.40
1:B:404:TYR:OH	1:B:406:LYS:HB2	2.21	0.40
1:B:494:ARG:HB2	1:B:497:PHE:CD1	2.56	0.40
1:D:52:GLN:HG3	1:D:54:TYR:CE1	2.56	0.40
1:D:122:GLU:CD	1:D:122:GLU:H	2.29	0.40
1:D:297:PRO:HD3	1:D:320:ASP:OD1	2.21	0.40
1:D:523:GLN:HA	1:D:523:GLN:NE2	2.36	0.40
1:A:266:GLN:HA	1:A:269:LYS:HD2	2.04	0.40
1:A:403:LYS:HE3	1:C:401:VAL:HG22	2.04	0.40
1:B:325:GLN:HE21	1:B:325:GLN:CA	2.29	0.40
1:C:20:THR:HB	1:C:27:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:GLY:HA2	1:C:488:LEU:HD21	2.03	0.40
1:D:133:LEU:HD12	1:D:133:LEU:N	2.37	0.40
1:A:242:LEU:C	1:A:242:LEU:HD23	2.46	0.40
1:A:322:LYS:NZ	3:A:847:HOH:O	2.50	0.40
1:B:316:ILE:HD11	1:B:480:VAL:HG12	2.03	0.40
1:A:191:ILE:HG22	1:A:359:ASN:HD21	1.85	0.40
1:A:445:LEU:HG	1:A:487:TRP:CD1	2.56	0.40
1:B:135:PRO:HG2	1:B:458:ARG:NH1	2.36	0.40
1:B:183:PRO:HD2	3:B:811:HOH:O	2.21	0.40
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.96	0.40
1:D:462:LYS:HE2	1:D:472:GLY:O	2.22	0.40
1:A:102:GLN:NE2	3:A:811:HOH:O	2.46	0.40
1:A:478:TYR:HA	1:B:533:LEU:HD21	2.04	0.40
1:B:70:LEU:HD11	1:B:81:LEU:CD2	2.50	0.40
1:B:265:LEU:O	1:B:269:LYS:HG3	2.20	0.40
1:B:486:TYR:CD1	1:B:486:TYR:C	2.99	0.40
1:C:248:GLU:HB2	1:C:298:GLN:HE21	1.85	0.40
1:D:206:ASP:OD2	1:D:206:ASP:C	2.65	0.40
1:D:260:THR:HB	1:D:307:GLN:HE22	1.86	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	502/533 (94%)	465 (93%)	28 (6%)	9 (2%)	6	1
1	B	485/533 (91%)	445 (92%)	32 (7%)	8 (2%)	7	2
1	C	513/533 (96%)	474 (92%)	27 (5%)	12 (2%)	5	1
1	D	481/533 (90%)	445 (92%)	28 (6%)	8 (2%)	7	2
All	All	1981/2132 (93%)	1829 (92%)	115 (6%)	37 (2%)	6	1

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ALA
1	A	211	VAL
1	A	319	ASP
1	A	495	PRO
1	B	192	ALA
1	B	319	ASP
1	C	193	ALA
1	D	319	ASP
1	B	191	ILE
1	C	199	ALA
1	C	319	ASP
1	D	531	ARG
1	A	195	GLN
1	B	193	ALA
1	B	347	ALA
1	C	22	LYS
1	C	189	ASP
1	C	194	ASN
1	C	272	HIS
1	C	322	LYS
1	D	23	ASP
1	D	470	ASP
1	B	320	ASP
1	A	212	THR
1	C	320	ASP
1	C	502	GLY
1	D	355	ASN
1	A	42	SER
1	A	479	PRO
1	A	502	GLY
1	D	194	ASN
1	B	502	GLY
1	B	346	ILE
1	C	495	PRO
1	D	346	ILE
1	D	479	PRO
1	C	464	VAL

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	680	-	46,48,48	2.31	11 (23%)	64,73,73	1.07	4 (6%)
2	NAD	C	670	-	46,48,48	2.17	11 (23%)	64,73,73	1.08	4 (6%)
2	NAD	B	660	-	46,48,48	2.47	14 (30%)	64,73,73	1.07	5 (7%)
2	NAD	A	650	-	46,48,48	2.32	10 (21%)	64,73,73	1.07	4 (6%)

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	D	680	-	-	3/30/62/62	0/5/5/5
2	NAD	C	670	-	-	3/30/62/62	0/5/5/5
2	NAD	B	660	-	-	1/30/62/62	0/5/5/5
2	NAD	A	650	-	-	2/30/62/62	0/5/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	660	NAD	C2N-N1N	8.85	1.44	1.35
2	A	650	NAD	C2N-N1N	7.78	1.43	1.35
2	B	660	NAD	C4N-C3N	6.97	1.50	1.39
2	C	670	NAD	C2N-N1N	6.91	1.42	1.35
2	A	650	NAD	C4N-C3N	6.86	1.49	1.39
2	D	680	NAD	C2N-N1N	6.84	1.42	1.35
2	D	680	NAD	C4N-C3N	6.80	1.49	1.39
2	C	670	NAD	C4N-C3N	6.14	1.48	1.39
2	D	680	NAD	PA-O3	-5.12	1.54	1.59
2	D	680	NAD	C6N-N1N	5.00	1.46	1.35
2	A	650	NAD	C6N-N1N	4.91	1.46	1.35
2	C	670	NAD	C6N-N1N	4.84	1.46	1.35
2	C	670	NAD	PA-O3	-4.55	1.54	1.59
2	B	660	NAD	C5N-C4N	4.49	1.46	1.38
2	B	660	NAD	C6N-N1N	4.45	1.45	1.35
2	A	650	NAD	PA-O3	-4.26	1.54	1.59
2	B	660	NAD	C2A-N1A	4.10	1.41	1.33
2	A	650	NAD	C5N-C4N	3.96	1.45	1.38
2	D	680	NAD	C5N-C4N	3.91	1.45	1.38
2	B	660	NAD	C3N-C7N	3.85	1.56	1.50
2	C	670	NAD	C5N-C4N	3.84	1.45	1.38
2	A	650	NAD	C2A-N1A	3.83	1.40	1.33
2	D	680	NAD	C2A-N1A	3.77	1.40	1.33
2	C	670	NAD	C3N-C7N	3.32	1.55	1.50
2	C	670	NAD	C2A-N1A	3.04	1.39	1.33
2	B	660	NAD	C5A-C6A	2.97	1.49	1.41
2	D	680	NAD	C3N-C7N	2.96	1.55	1.50
2	D	680	NAD	C8A-N7A	2.91	1.37	1.31
2	C	670	NAD	C8A-N7A	2.84	1.37	1.31
2	D	680	NAD	C5A-C4A	2.82	1.44	1.39
2	B	660	NAD	PN-O3	2.81	1.62	1.59
2	A	650	NAD	C3N-C7N	2.67	1.54	1.50
2	B	660	NAD	PA-O3	-2.66	1.56	1.59
2	B	660	NAD	C5A-C4A	2.64	1.43	1.39
2	D	680	NAD	C5A-C6A	2.63	1.48	1.41
2	B	660	NAD	C4A-N3A	2.60	1.39	1.34
2	A	650	NAD	C5A-C6A	2.60	1.48	1.41
2	D	680	NAD	C4A-N3A	2.54	1.39	1.34
2	A	650	NAD	C4A-N3A	2.53	1.39	1.34
2	B	660	NAD	C2N-C3N	2.36	1.42	1.39
2	C	670	NAD	C5A-C4A	2.34	1.43	1.39
2	A	650	NAD	C8A-N7A	2.28	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	670	NAD	C4A-N3A	2.26	1.38	1.34
2	B	660	NAD	C6A-N1A	2.16	1.41	1.35
2	B	660	NAD	C8A-N7A	2.15	1.35	1.31
2	C	670	NAD	C5A-C6A	2.05	1.46	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	660	NAD	C3N-C7N-N7N	3.73	122.34	117.74
2	A	650	NAD	C3N-C7N-N7N	3.45	121.99	117.74
2	C	670	NAD	O7N-C7N-N7N	-3.44	117.64	122.62
2	A	650	NAD	O2A-PA-O3	3.32	116.25	107.27
2	D	680	NAD	O2A-PA-O3	3.26	116.07	107.27
2	D	680	NAD	O7N-C7N-N7N	-3.11	118.12	122.62
2	D	680	NAD	C3N-C7N-N7N	3.08	121.53	117.74
2	C	670	NAD	C6N-N1N-C2N	-2.96	119.36	121.88
2	C	670	NAD	O2A-PA-O3	2.82	114.90	107.27
2	B	660	NAD	O7N-C7N-N7N	-2.82	118.54	122.62
2	A	650	NAD	O7N-C7N-N7N	-2.63	118.82	122.62
2	C	670	NAD	C3N-C7N-N7N	2.63	120.97	117.74
2	A	650	NAD	C6N-N1N-C2N	-2.62	119.65	121.88
2	B	660	NAD	C4D-O4D-C1D	-2.62	107.53	109.92
2	B	660	NAD	O3-PN-O1N	-2.36	103.60	110.70
2	B	660	NAD	C6N-N1N-C2N	-2.17	120.03	121.88
2	D	680	NAD	O4D-C4D-C3D	2.12	109.35	105.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

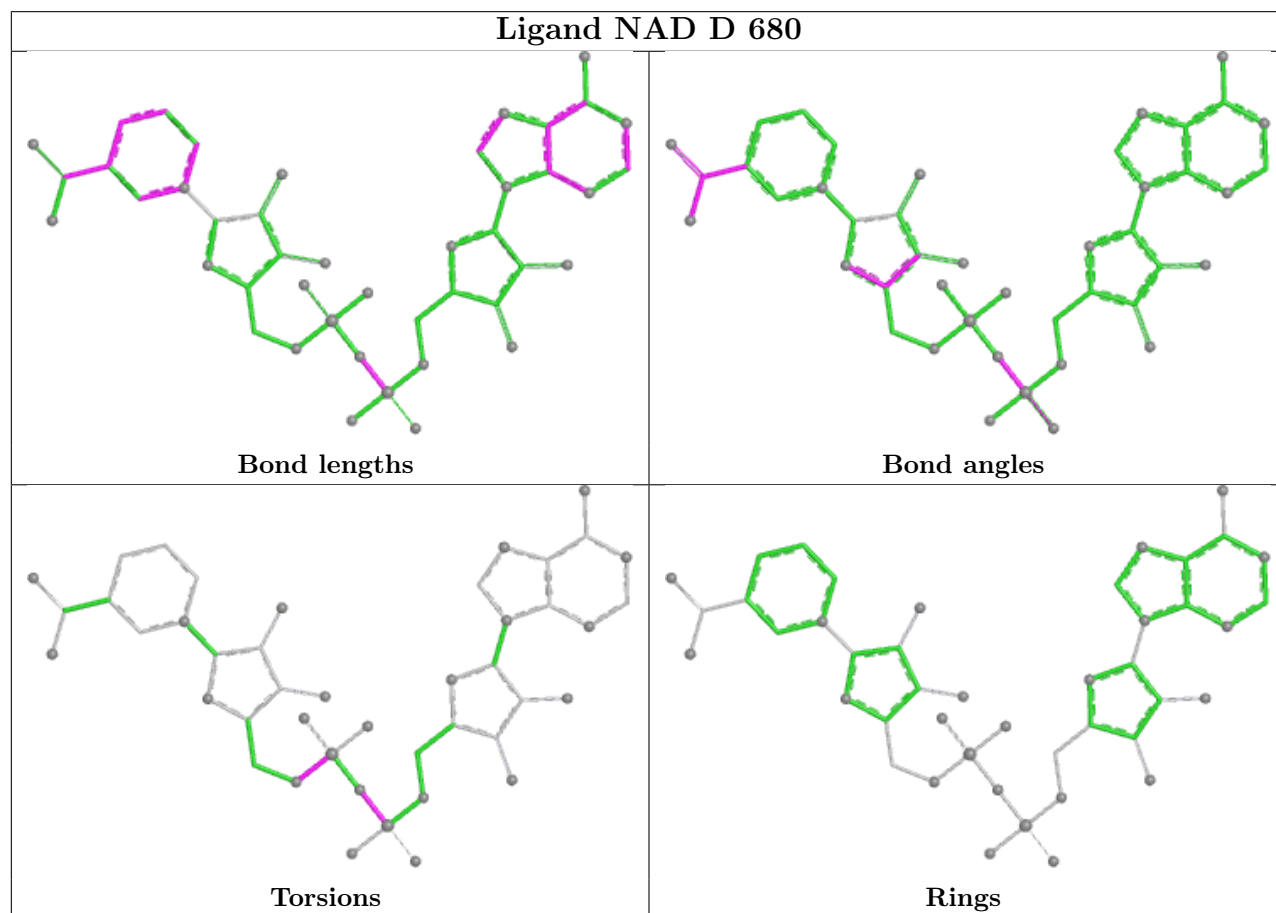
Mol	Chain	Res	Type	Atoms
2	D	680	NAD	C5D-O5D-PN-O1N
2	D	680	NAD	PN-O3-PA-O1A
2	C	670	NAD	PN-O3-PA-O1A
2	C	670	NAD	PN-O3-PA-O2A
2	D	680	NAD	PN-O3-PA-O2A
2	B	660	NAD	PA-O3-PN-O2N
2	A	650	NAD	O4B-C4B-C5B-O5B
2	C	670	NAD	O4B-C4B-C5B-O5B
2	A	650	NAD	PN-O3-PA-O2A

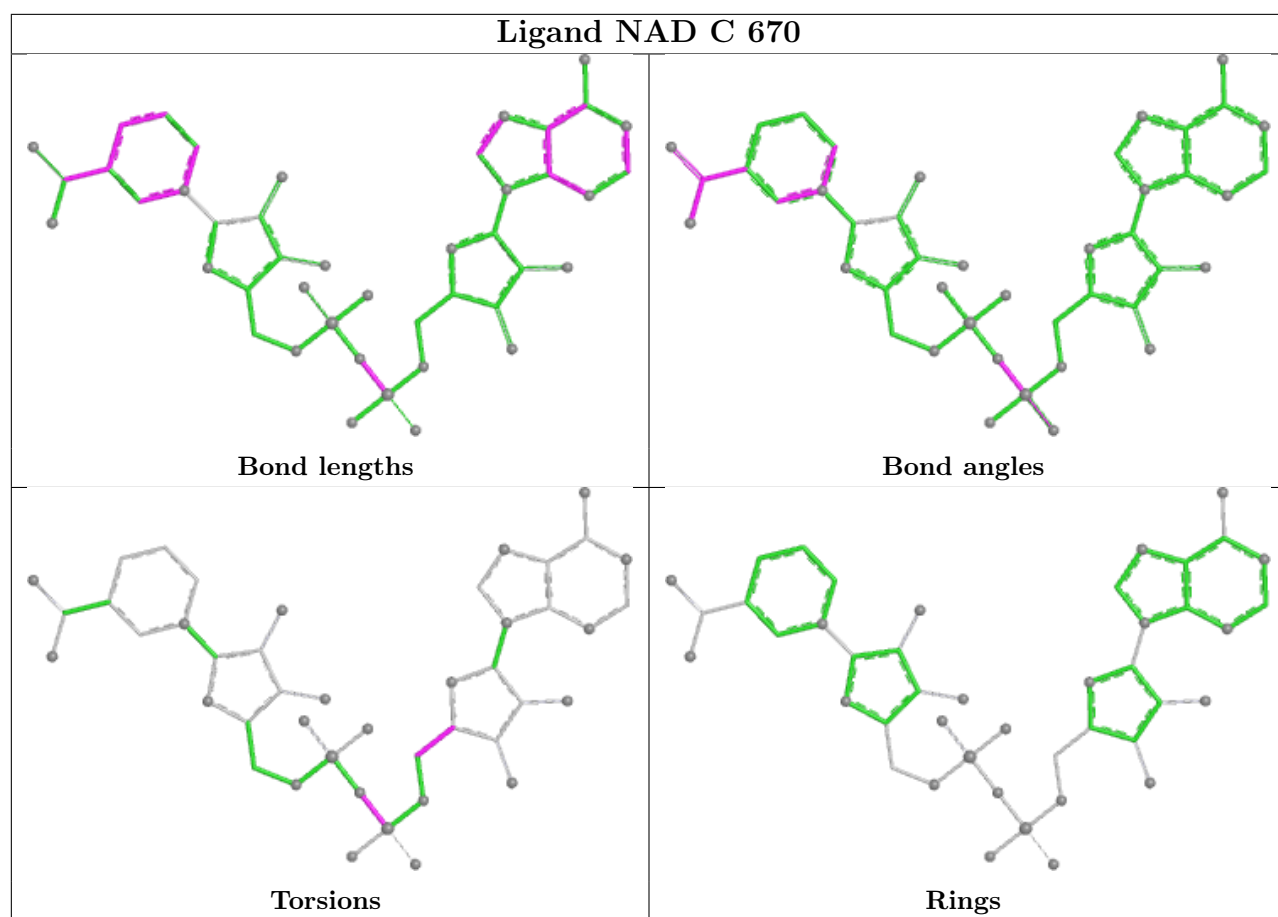
There are no ring outliers.

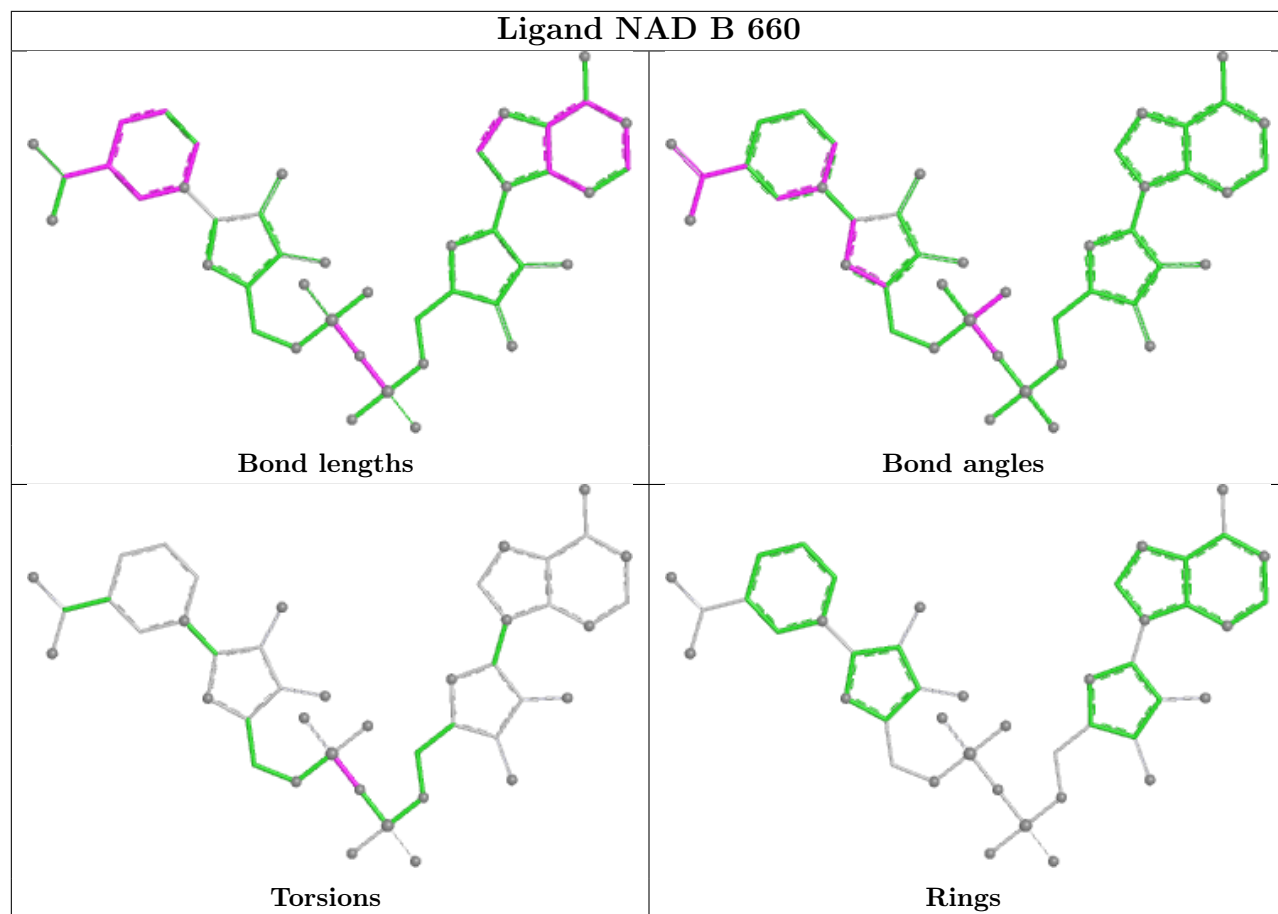
4 monomers are involved in 12 short contacts:

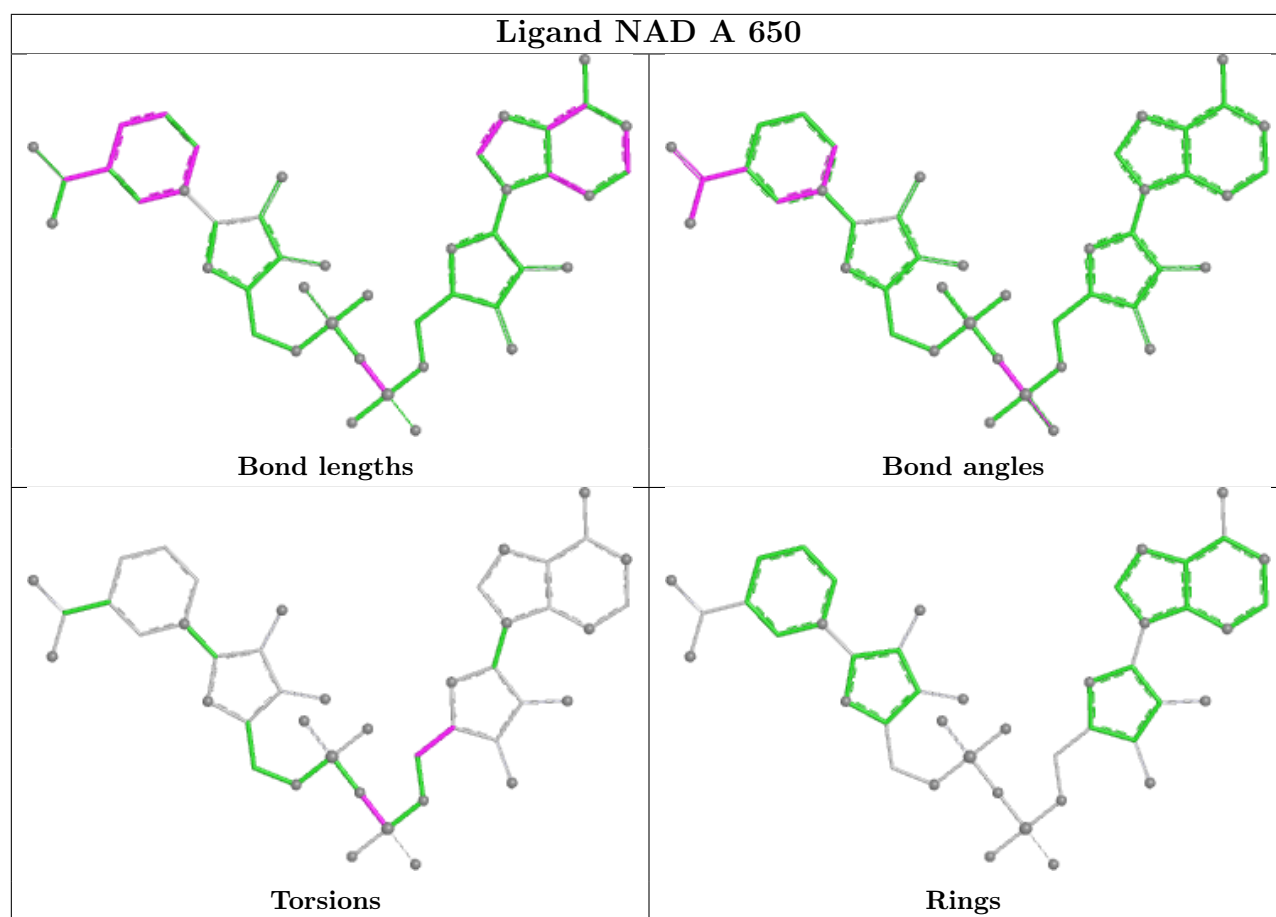
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	680	NAD	1	0
2	C	670	NAD	5	0
2	B	660	NAD	3	0
2	A	650	NAD	3	0

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 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	506/533 (94%)	0.21	25 (4%)	35 41	24, 45, 85, 90	0
1	B	491/533 (92%)	0.22	23 (4%)	36 42	23, 45, 88, 90	0
1	C	517/533 (96%)	0.28	22 (4%)	40 46	22, 45, 86, 90	0
1	D	487/533 (91%)	0.16	22 (4%)	38 44	21, 41, 88, 90	0
All	All	2001/2132 (93%)	0.22	92 (4%)	37 43	21, 44, 87, 90	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	ALA	5.4
1	D	193	ALA	4.9
1	B	348	SER	4.4
1	D	353	GLY	4.2
1	C	372	SER	4.1
1	A	263	ASN	4.0
1	B	193	ALA	4.0
1	D	351	HIS	3.9
1	C	319	ASP	3.8
1	C	321	LEU	3.8
1	D	43	GLY	3.6
1	B	496	GLY	3.5
1	C	350	ASN	3.4
1	A	319	ASP	3.4
1	C	349	TYR	3.2
1	A	496	GLY	3.2
1	C	324	GLY	3.2
1	A	194	ASN	3.2
1	D	40	THR	3.1
1	B	346	ILE	3.0
1	D	192	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	408	VAL	3.0
1	A	467	VAL	3.0
1	D	349	TYR	2.9
1	B	351	HIS	2.8
1	D	347	ALA	2.8
1	C	318	GLY	2.8
1	C	496	GLY	2.8
1	C	320	ASP	2.7
1	C	302	VAL	2.7
1	A	501	ASN	2.7
1	A	211	VAL	2.7
1	D	411	SER	2.6
1	A	193	ALA	2.6
1	B	194	ASN	2.6
1	B	404	TYR	2.6
1	A	192	ALA	2.6
1	A	199	ALA	2.6
1	D	346	ILE	2.5
1	C	315	PHE	2.5
1	D	352	LEU	2.5
1	C	368	SER	2.5
1	D	387	LEU	2.5
1	D	472	GLY	2.5
1	C	347	ALA	2.4
1	B	210	ASN	2.4
1	A	533	LEU	2.4
1	B	345	SER	2.4
1	C	477	PHE	2.4
1	B	495	PRO	2.4
1	B	500	VAL	2.4
1	B	405	MET	2.4
1	C	361	SER	2.4
1	A	41	ALA	2.3
1	B	393	GLY	2.3
1	C	366	PHE	2.3
1	B	352	LEU	2.3
1	C	371	ILE	2.3
1	B	254	SER	2.3
1	B	20	THR	2.3
1	D	482	THR	2.3
1	A	354	ASN	2.2
1	A	397	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	504	ASN	2.2
1	A	212	THR	2.2
1	B	399	CYS	2.2
1	D	533	LEU	2.2
1	D	304	GLY	2.2
1	B	41	ALA	2.2
1	C	497	PHE	2.2
1	D	380	ILE	2.2
1	B	350	ASN	2.1
1	C	363	PRO	2.1
1	A	356	ASP	2.1
1	D	319	ASP	2.1
1	A	260	THR	2.1
1	A	257	VAL	2.1
1	B	344	VAL	2.1
1	A	392	LEU	2.1
1	A	495	PRO	2.1
1	A	259	ASP	2.1
1	D	355	ASN	2.1
1	A	40	THR	2.0
1	B	196	ASP	2.0
1	D	254	SER	2.0
1	D	348	SER	2.0
1	A	493	THR	2.0
1	C	393	GLY	2.0
1	A	479	PRO	2.0
1	D	479	PRO	2.0
1	B	408	VAL	2.0
1	C	396	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

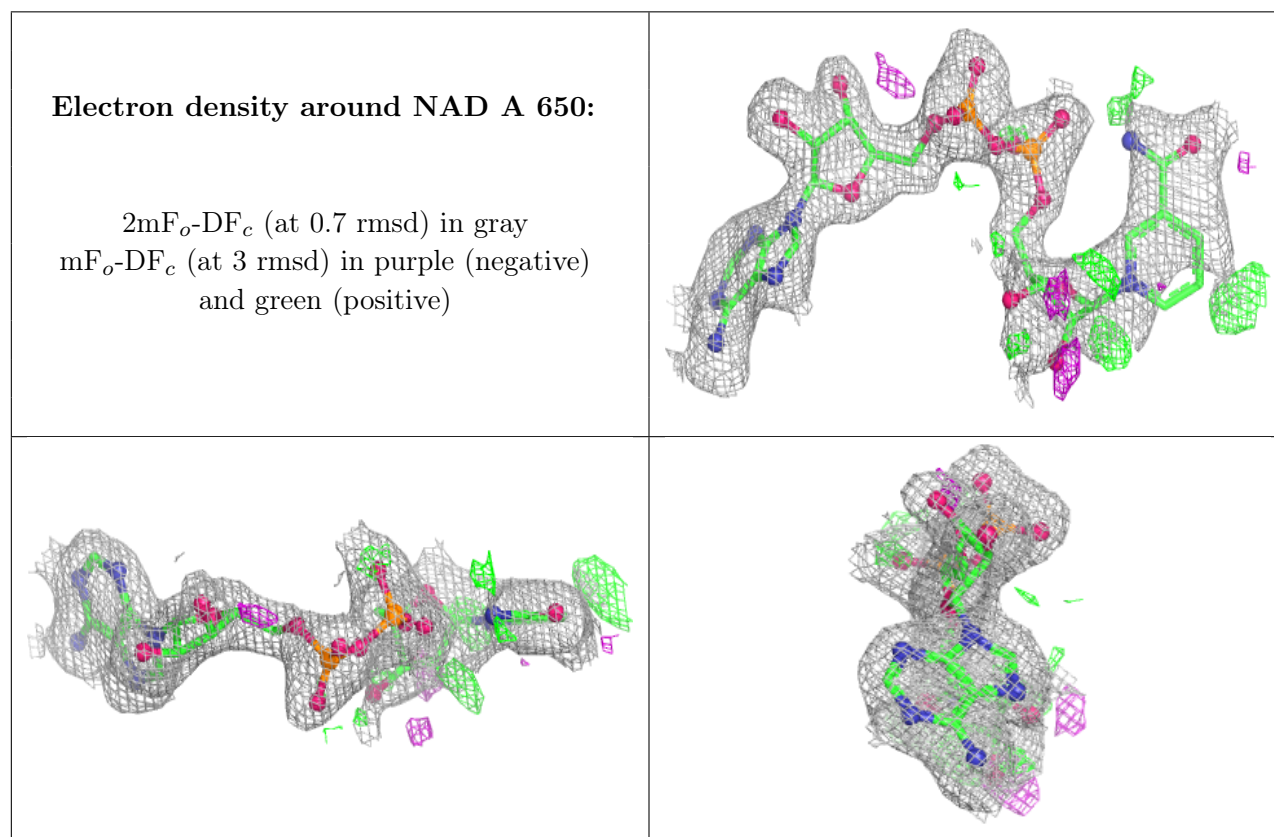
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

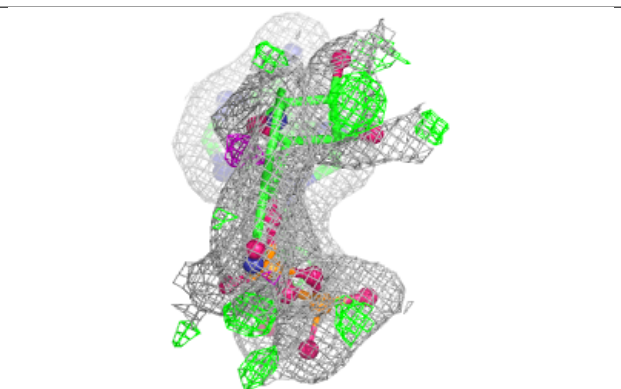
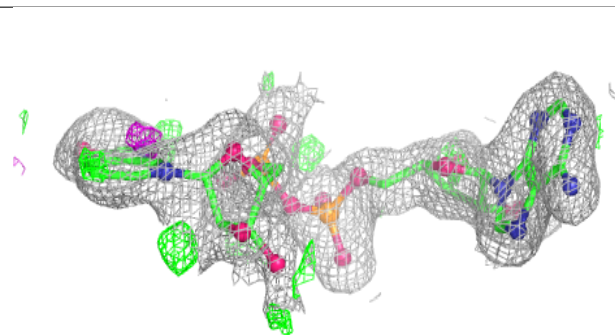
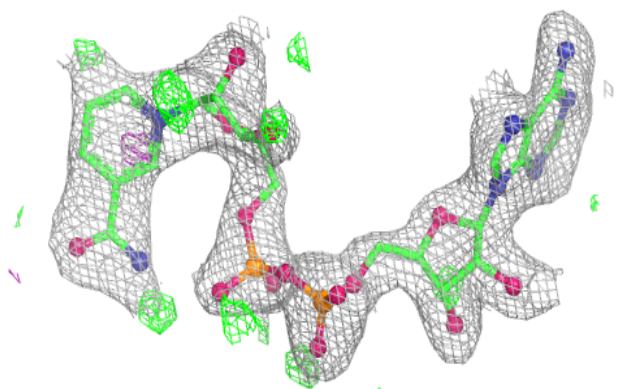
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	A	650	44/44	0.95	0.08	32,40,65,68	0
2	NAD	B	660	44/44	0.96	0.07	29,40,56,57	0
2	NAD	C	670	44/44	0.96	0.07	29,34,65,70	0
2	NAD	D	680	44/44	0.96	0.07	26,35,70,75	0

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

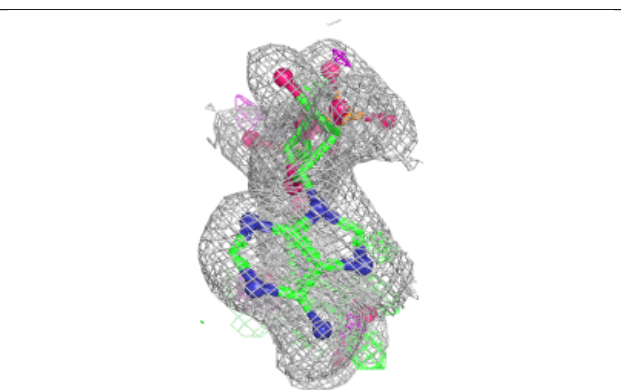
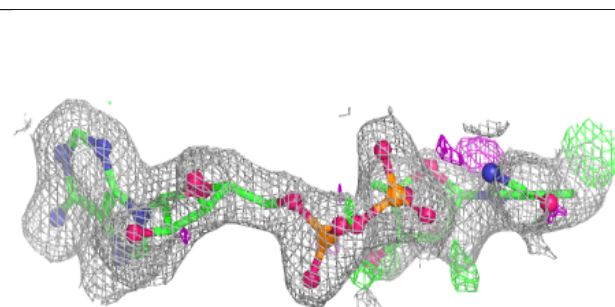
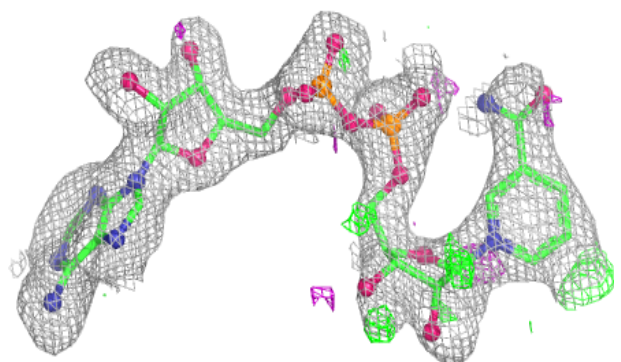


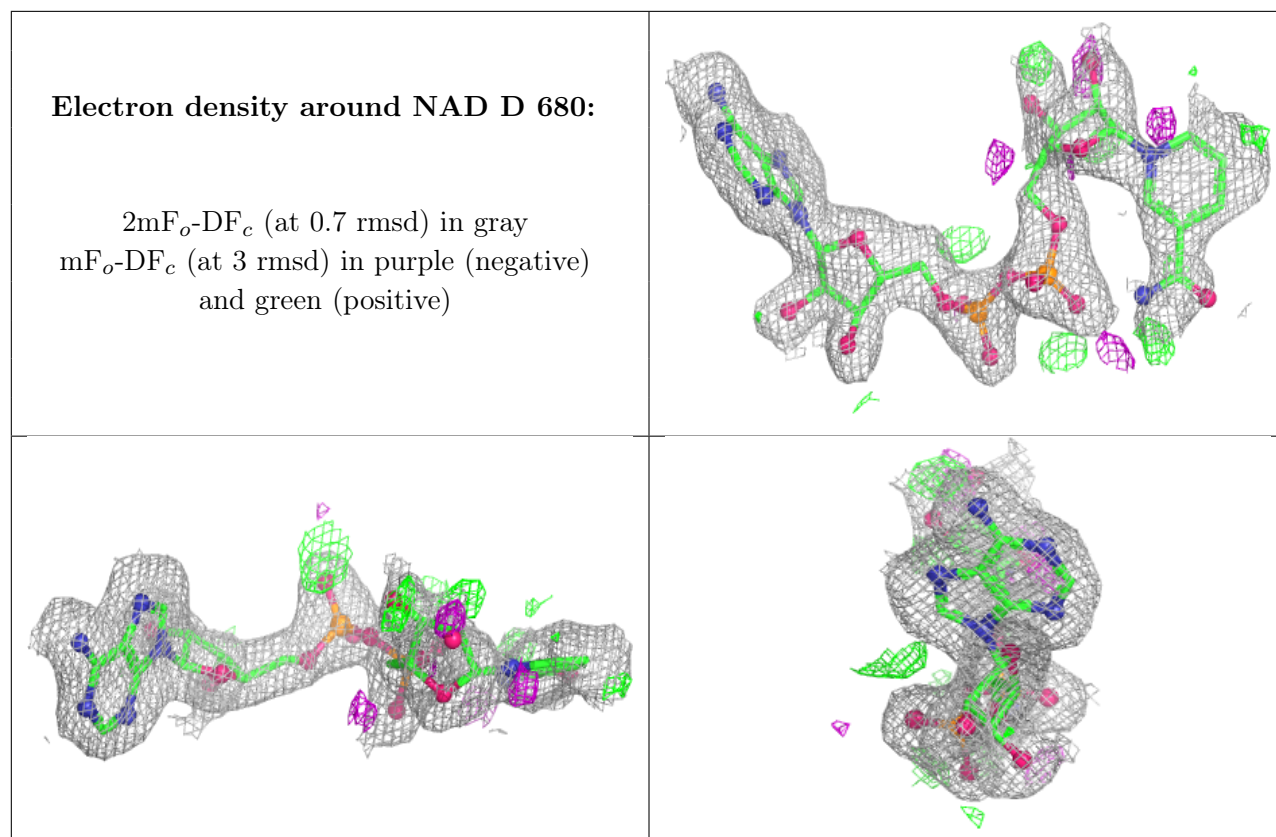
Electron density around NAD B 660:

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

**Electron density around NAD C 670:**

$2mF_o-DF_c$ (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.