



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:32 AM UTC

PDB ID : 4O9U / pdb_00004o9u
Title : Mechanism of transhydrogenase coupling proton translocation and hydride transfer
Authors : Leung, J.H.; Yamaguchi, M.; Moeller, A.; Schurig-Briccio, L.A.; Gennis, R.B.; Potter, C.S.; Carragher, B.; Stout, C.D.
Deposited on : 2014-01-02
Resolution : 6.93 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:

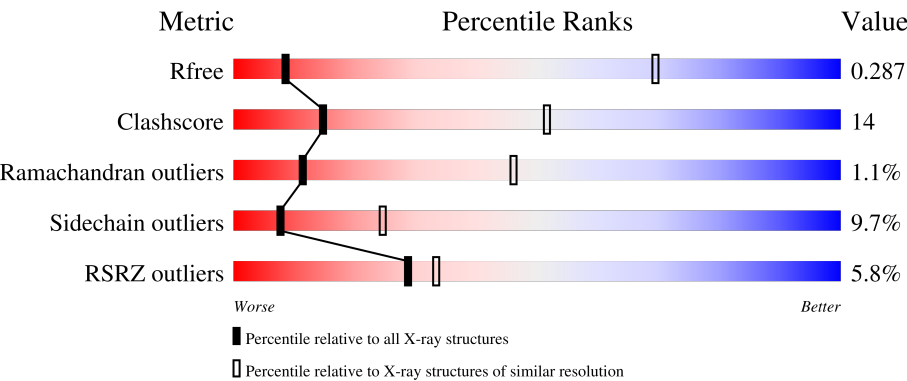
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 6.93 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	1166 (9.70-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1053 (9.70-4.00)
Sidechain outliers	187428	1016 (9.70-4.00)
RSRZ outliers	180081	1159 (9.70-4.00)

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	100	11% 68% 22% • 6%
1	C	100	3% 58% 30% • 10%
2	B	450	6% 66% 28% • •
2	D	450	4% 63% 31% • •

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Mol	Chain	Length	Quality of chain
3	E	384	6% 68% 24%
3	F	384	6% 70% 22%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13618 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 NAD(P) transhydrogenase subunit alpha 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			713	475	114	119	5			
1	C	90	Total	C	N	O	S	0	0	0
			677	453	106	113	5			

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	440	Total	C	N	O	S	0	0	0
			3250	2131	534	563	22			
2	D	437	Total	C	N	O	S	0	0	0
			3235	2122	531	560	22			

- Molecule 3 is a protein called NAD/NADP transhydrogenase alpha subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	372	Total	C	N	O	S	0	0	0
			2794	1772	498	512	12			
3	F	369	Total	C	N	O	S	0	0	0
			2765	1753	494	506	12			

There are 18 discrepancies between the modelled and reference sequences:

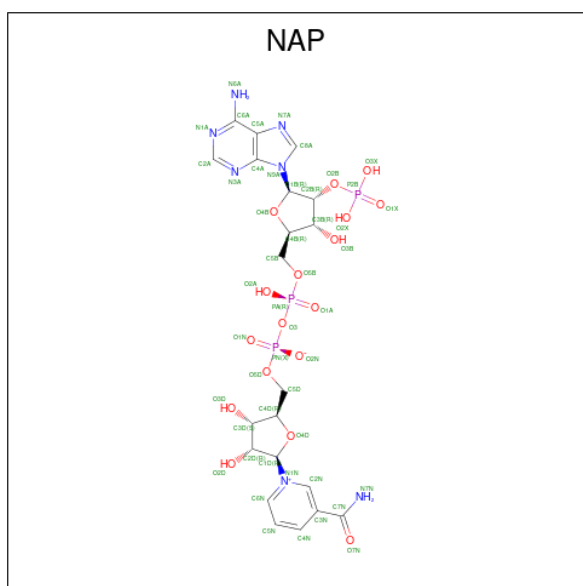
Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	MET	-	expression tag	UNP Q72GR8
E	-7	HIS	-	expression tag	UNP Q72GR8
E	-6	HIS	-	expression tag	UNP Q72GR8
E	-5	HIS	-	expression tag	UNP Q72GR8
E	-4	HIS	-	expression tag	UNP Q72GR8
E	-3	HIS	-	expression tag	UNP Q72GR8
E	-2	HIS	-	expression tag	UNP Q72GR8
E	-1	HIS	-	expression tag	UNP Q72GR8

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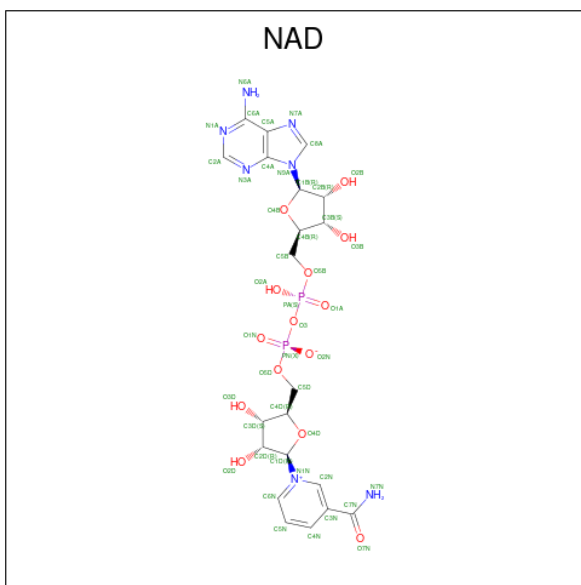
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP Q72GR8
F	-8	MET	-	expression tag	UNP Q72GR8
F	-7	HIS	-	expression tag	UNP Q72GR8
F	-6	HIS	-	expression tag	UNP Q72GR8
F	-5	HIS	-	expression tag	UNP Q72GR8
F	-4	HIS	-	expression tag	UNP Q72GR8
F	-3	HIS	-	expression tag	UNP Q72GR8
F	-2	HIS	-	expression tag	UNP Q72GR8
F	-1	HIS	-	expression tag	UNP Q72GR8
F	0	HIS	-	expression tag	UNP Q72GR8

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

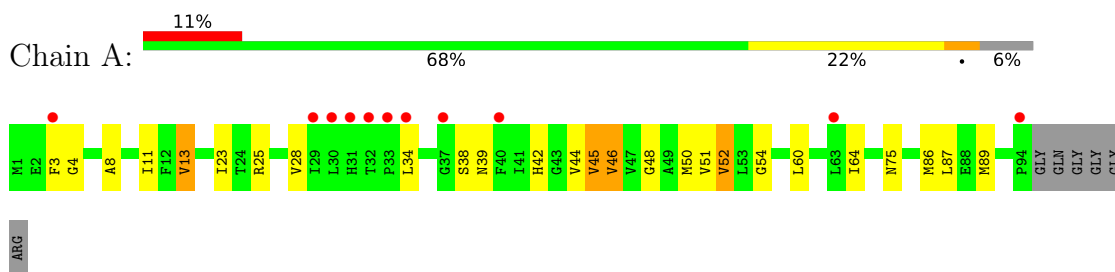


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total 44	C 21	N 7	O 14	P 2	0	0
5	F	1	Total 44	C 21	N 7	O 14	P 2	0	0

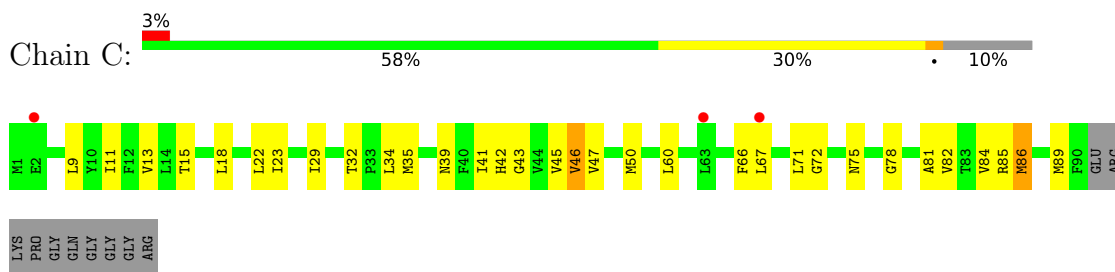
3 Residue-property plots [i](#)

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

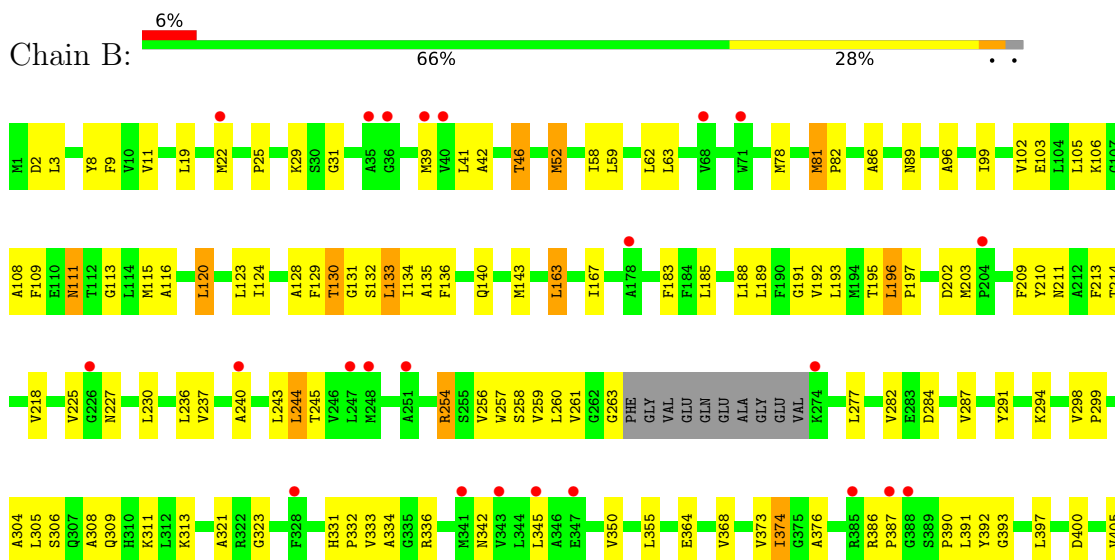
- Molecule 1: NAD(P) transhydrogenase subunit alpha 2

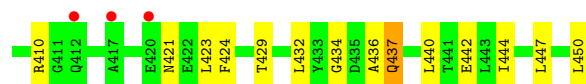


- Molecule 1: NAD(P) transhydrogenase subunit alpha 2

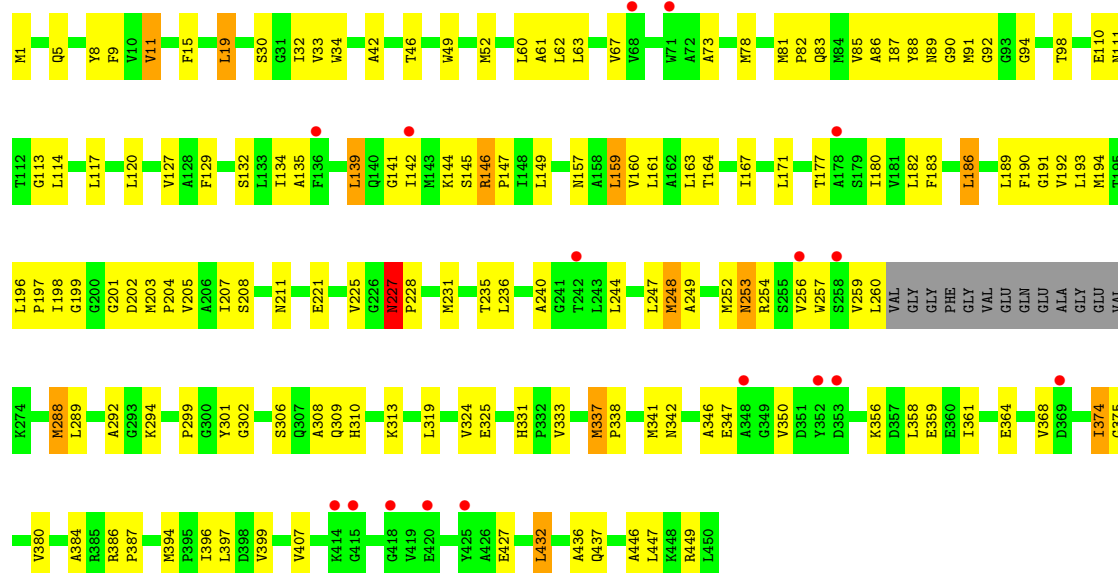


- Molecule 2: NAD(P) transhydrogenase subunit beta

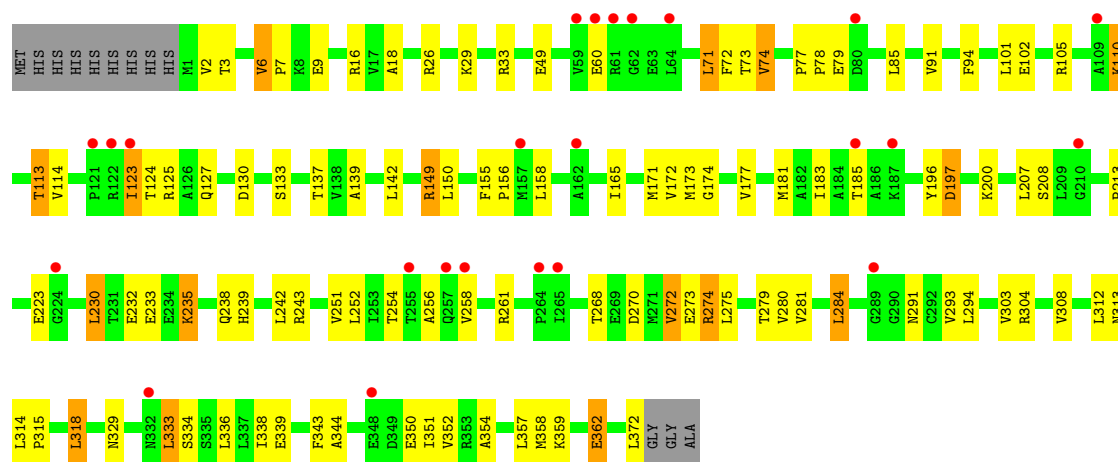




• Molecule 2: NAD(P) transhydrogenase subunit beta

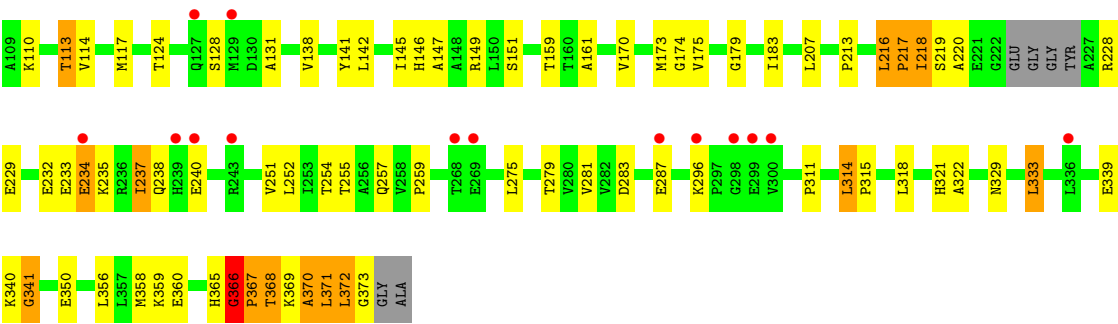


• Molecule 3: NAD/NADP transhydrogenase alpha subunit 1



• Molecule 3: NAD/NADP transhydrogenase alpha subunit 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.33Å 160.59Å 139.62Å 90.00° 128.36° 90.00°	Depositor
Resolution (Å)	38.90 – 6.93 38.90 – 6.93	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.90-6.93) 98.1 (38.90-6.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 6.64Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.213 , 0.284 0.217 , 0.287	Depositor DCC
R_{free} test set	228 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	176.7	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 136.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	13618	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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, NAP

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	0.48	0/730	0.90	0/990
1	C	0.45	0/693	0.86	0/941
2	B	0.45	0/3314	0.89	2/4503 (0.0%)
2	D	0.45	0/3299	0.90	2/4483 (0.0%)
3	E	0.49	0/2840	0.86	0/3852
3	F	0.52	2/2809 (0.1%)	0.86	2/3810 (0.1%)
All	All	0.47	2/13685 (0.0%)	0.88	6/18579 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	366	GLY	C-N	5.36	1.40	1.33
3	F	367	PRO	N-CD	5.27	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	366	GLY	CA-C-N	-5.90	112.80	119.28
3	F	366	GLY	C-N-CA	-5.90	112.80	119.28
2	B	227	ASN	CA-C-N	5.62	125.28	119.05
2	B	227	ASN	C-N-CA	5.62	125.28	119.05
2	D	227	ASN	CA-C-N	5.47	124.99	119.19
2	D	227	ASN	C-N-CA	5.47	124.99	119.19

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	713	0	739	20	0
1	C	677	0	700	31	0
2	B	3250	0	3399	104	0
2	D	3235	0	3384	120	0
3	E	2794	0	2911	78	0
3	F	2765	0	2881	78	0
4	B	48	0	25	1	0
4	D	48	0	25	5	0
5	E	44	0	26	5	0
5	F	44	0	26	2	0
All	All	13618	0	14116	384	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 14.

All (384) 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)
3:F:365:HIS:ND1	3:F:368:THR:CG2	1.96	1.26
3:F:371:LEU:O	3:F:373:GLY:N	1.66	1.26
3:F:365:HIS:CB	3:F:368:THR:HG21	1.74	1.16
3:F:114:VAL:HG12	3:F:358:MET:HG2	1.30	1.12
2:B:103:GLU:OE2	2:B:225:VAL:HG11	1.50	1.10
2:D:164:THR:HG22	2:D:186:LEU:HB3	1.34	1.10
3:F:365:HIS:HB3	3:F:368:THR:CG2	1.84	1.06
3:E:274:ARG:HG3	3:E:274:ARG:HH11	1.17	1.05
3:F:365:HIS:ND1	3:F:368:THR:HG23	1.66	1.05
3:F:365:HIS:HB3	3:F:368:THR:HG21	1.00	0.98
3:F:367:PRO:O	3:F:370:ALA:N	1.98	0.96
3:F:371:LEU:O	3:F:373:GLY:O	1.84	0.95
3:F:367:PRO:O	3:F:368:THR:C	2.11	0.94
3:F:365:HIS:CG	3:F:368:THR:CG2	2.51	0.92
3:F:216:LEU:HB3	3:F:217:PRO:HA	1.52	0.92
2:B:202:ASP:HB3	2:B:259:VAL:HG13	1.51	0.91
1:A:51:VAL:HA	2:B:52:MET:HE1	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:3:THR:HG22	3:E:33:ARG:HB2	1.56	0.86
2:B:103:GLU:OE2	2:B:225:VAL:CG1	2.23	0.86
3:E:133:SER:HA	3:E:177:VAL:HG11	1.58	0.86
2:D:252:MET:HA	2:D:333:VAL:HG11	1.60	0.84
3:F:371:LEU:O	3:F:371:LEU:HD12	1.77	0.84
3:F:371:LEU:O	3:F:372:LEU:C	2.18	0.84
3:F:365:HIS:ND1	3:F:368:THR:HG22	1.90	0.83
3:F:371:LEU:HD12	3:F:373:GLY:O	1.78	0.83
2:D:201:GLY:C	4:D:500:NAP:H5N	2.04	0.82
3:F:216:LEU:HB3	3:F:217:PRO:CA	2.08	0.82
3:F:365:HIS:CG	3:F:368:THR:HG21	2.12	0.82
2:D:384:ALA:HB1	2:D:394:MET:HB3	1.61	0.82
3:F:91:VAL:HB	3:F:114:VAL:HG23	1.63	0.81
2:B:25:PRO:HB3	2:B:291:TYR:OH	1.82	0.79
3:E:238:GLN:O	3:E:242:LEU:HB2	1.82	0.77
1:C:47:VAL:HG13	2:D:46:THR:HG21	1.66	0.77
3:F:371:LEU:C	3:F:373:GLY:N	2.42	0.77
2:D:198:ILE:HD12	2:D:259:VAL:HG12	1.66	0.77
2:D:198:ILE:HD11	2:D:260:LEU:HD23	1.66	0.76
1:C:39:ASN:HA	1:C:42:HIS:CE1	2.19	0.76
2:D:30:SER:O	2:D:34:TRP:HD1	1.70	0.75
1:C:35:MET:HE1	2:D:338:PRO:HG2	1.68	0.75
3:E:274:ARG:HG3	3:E:274:ARG:NH1	1.97	0.74
2:D:225:VAL:HG23	2:D:227:ASN:HB2	1.69	0.74
3:F:365:HIS:CB	3:F:368:THR:CG2	2.51	0.74
2:D:248:MET:SD	2:D:338:PRO:HB3	2.28	0.73
3:F:365:HIS:CG	3:F:368:THR:HG23	2.22	0.73
3:F:367:PRO:O	3:F:369:LYS:N	2.22	0.73
2:B:392:TYR:O	3:E:125:ARG:HA	1.91	0.71
2:B:86:ALA:O	2:B:132:SER:HB3	1.90	0.71
2:B:261:VAL:HG12	2:B:263:GLY:H	1.53	0.71
3:F:371:LEU:HD12	3:F:371:LEU:C	2.16	0.70
3:E:272:VAL:HG11	3:E:294:LEU:HD11	1.73	0.69
3:E:274:ARG:HH11	3:E:274:ARG:CG	2.00	0.69
2:D:201:GLY:O	2:D:204:PRO:HD2	1.93	0.69
1:A:86:MET:HE3	2:B:81:MET:HG2	1.76	0.68
2:B:209:PHE:HD1	2:B:245:THR:HG21	1.58	0.68
3:E:110:LYS:HE3	3:E:110:LYS:HA	1.75	0.68
3:F:113:THR:HG23	3:F:359:LYS:HA	1.75	0.68
2:B:103:GLU:OE1	2:B:225:VAL:HG13	1.94	0.68
2:B:103:GLU:CD	2:B:225:VAL:CG1	2.68	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:GLY:O	2:B:195:THR:HG22	1.92	0.67
2:B:261:VAL:HG12	2:B:263:GLY:N	2.09	0.67
2:D:81:MET:N	2:D:82:PRO:HD2	2.09	0.67
3:F:117:MET:HE3	3:F:131:ALA:HB2	1.77	0.66
2:D:63:LEU:O	2:D:67:VAL:HG22	1.93	0.66
3:E:149:ARG:HH11	3:F:146:HIS:HE1	1.43	0.66
3:E:114:VAL:HG13	3:E:357:LEU:HB3	1.77	0.66
2:D:82:PRO:HG2	2:D:83:GLN:OE1	1.95	0.65
2:D:204:PRO:HG2	4:D:500:NAP:H4N	1.77	0.65
2:B:131:GLY:HA2	2:B:195:THR:HG21	1.79	0.65
3:E:149:ARG:NH2	3:F:149:ARG:HH21	1.95	0.65
1:C:86:MET:HE3	2:D:81:MET:HG2	1.80	0.64
3:F:218:ILE:HG22	3:F:219:SER:H	1.62	0.64
3:E:127:GLN:HA	3:E:130:ASP:HB2	1.80	0.64
3:E:256:ALA:HB3	3:E:291:ASN:HD21	1.61	0.64
2:B:103:GLU:CD	2:B:225:VAL:HG11	2.24	0.63
1:C:39:ASN:HD21	2:D:88:TYR:HB2	1.62	0.63
2:B:299:PRO:HA	2:B:374:ILE:HG23	1.79	0.63
2:B:103:GLU:OE1	2:B:225:VAL:CG1	2.47	0.63
3:F:371:LEU:O	3:F:373:GLY:CA	2.47	0.63
2:D:204:PRO:HG3	2:D:337:MET:HA	1.82	0.62
3:F:275:LEU:HD22	3:F:279:THR:HG21	1.81	0.62
2:D:319:LEU:HB3	2:D:324:VAL:HB	1.80	0.62
3:F:371:LEU:O	3:F:373:GLY:C	2.42	0.62
3:E:137:THR:O	3:E:181:MET:HG2	2.00	0.62
3:E:171:MET:HB3	3:E:252:LEU:HD13	1.82	0.62
2:D:160:VAL:O	2:D:164:THR:HG23	1.99	0.61
3:F:365:HIS:O	3:F:368:THR:OG1	2.18	0.61
3:E:174:GLY:HA2	5:E:500:NAD:O2A	2.00	0.61
2:B:391:LEU:HA	3:E:124:THR:OG1	2.00	0.61
2:D:253:ASN:HA	2:D:394:MET:HA	1.83	0.60
2:B:254:ARG:HG2	2:B:258:SER:OG	2.01	0.60
2:D:193:LEU:HD23	2:D:196:LEU:HD22	1.83	0.60
2:D:8:TYR:HA	2:D:11:VAL:HB	1.83	0.59
2:D:177:THR:HA	2:D:180:ILE:HD12	1.84	0.59
3:E:16:ARG:HH21	3:E:313:ASN:HD21	1.50	0.59
2:B:256:VAL:O	2:B:260:LEU:HG	2.02	0.59
3:E:171:MET:HB3	3:E:252:LEU:CD1	2.33	0.59
1:C:35:MET:CE	2:D:338:PRO:HG2	2.32	0.59
3:F:311:PRO:HB2	3:F:314:LEU:HD13	1.85	0.59
1:A:42:HIS:CE1	1:A:75:ASN:HD21	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:LEU:HA	2:D:91:MET:HE3	1.84	0.59
2:D:198:ILE:CD1	2:D:259:VAL:HG12	2.33	0.59
3:E:238:GLN:O	3:E:242:LEU:CB	2.51	0.58
3:E:256:ALA:HB1	5:E:500:NAD:H52A	1.86	0.58
1:A:42:HIS:HD2	2:B:237:VAL:HG11	1.68	0.58
2:B:89:ASN:HD21	2:B:211:ASN:HA	1.68	0.58
2:B:400:ASP:HB3	2:B:423:LEU:HD13	1.83	0.58
2:B:282:VAL:HG11	2:B:442:GLU:OE1	2.03	0.58
1:C:43:GLY:O	1:C:46:VAL:HG23	2.04	0.58
1:A:54:GLY:HA3	2:B:52:MET:HE2	1.86	0.58
3:E:139:ALA:HB1	3:E:284:LEU:HD21	1.85	0.58
1:C:11:ILE:O	1:C:15:THR:HG22	2.05	0.57
2:B:306:SER:CB	2:B:436:ALA:HB3	2.35	0.57
3:E:155:PHE:N	3:E:156:PRO:HD2	2.20	0.57
2:D:358:LEU:HG	2:D:359:GLU:HG3	1.86	0.57
3:E:243:ARG:HH11	3:E:270:ASP:HB2	1.69	0.57
3:F:367:PRO:C	3:F:369:LYS:N	2.63	0.57
2:D:87:ILE:O	2:D:91:MET:HG2	2.04	0.57
2:B:332:PRO:HB3	3:F:161:ALA:HA	1.85	0.56
3:F:371:LEU:C	3:F:373:GLY:H	2.07	0.56
2:D:30:SER:O	2:D:34:TRP:CD1	2.57	0.56
2:B:294:LYS:HG2	2:B:368:VAL:HG22	1.88	0.56
2:D:8:TYR:OH	2:D:46:THR:HG22	2.06	0.56
3:F:114:VAL:CG1	3:F:358:MET:HG2	2.21	0.56
3:E:173:MET:HB2	3:E:254:THR:HG22	1.87	0.56
3:E:350:GLU:O	3:E:354:ALA:HB3	2.05	0.56
3:F:90:ILE:HG12	3:F:113:THR:HB	1.88	0.56
2:D:252:MET:C	2:D:254:ARG:H	2.12	0.56
2:D:331:HIS:ND1	2:D:333:VAL:HG22	2.21	0.56
2:D:289:LEU:HB3	2:D:319:LEU:HD21	1.87	0.55
3:F:141:TYR:O	3:F:145:ILE:HG12	2.05	0.55
2:B:116:ALA:O	2:B:120:LEU:HB2	2.06	0.55
2:D:82:PRO:HB3	2:D:337:MET:HB2	1.87	0.55
3:E:273:GLU:HG2	3:E:304:ARG:HH22	1.70	0.55
1:A:3:PHE:N	1:A:4:GLY:HA2	2.21	0.55
3:F:175:VAL:HA	3:F:179:GLY:HA3	1.87	0.55
3:F:76:PRO:HB3	3:F:95:VAL:HA	1.88	0.55
1:A:52:VAL:HG21	2:B:99:ILE:HG23	1.88	0.55
2:D:86:ALA:O	2:D:132:SER:HB3	2.06	0.55
2:D:146:ARG:HB3	2:D:147:PRO:CD	2.37	0.55
2:D:288:MET:O	2:D:292:ALA:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:ALA:O	2:B:46:THR:HG22	2.07	0.54
3:E:114:VAL:HG12	3:E:358:MET:HB2	1.90	0.54
3:F:1:MET:HA	3:F:341:GLY:O	2.07	0.54
2:B:261:VAL:CG1	2:B:263:GLY:C	2.81	0.54
2:B:313:LYS:HG3	2:B:350:VAL:HG22	1.89	0.54
3:E:233:GLU:O	3:E:233:GLU:HG3	2.08	0.54
3:F:173:MET:HB2	3:F:254:THR:HG22	1.87	0.54
2:B:374:ILE:HD11	2:B:436:ALA:HB1	1.88	0.54
3:F:9:GLU:HG3	3:F:74:VAL:HB	1.89	0.54
2:B:311:LYS:O	2:B:444:ILE:HD11	2.08	0.54
3:E:6:VAL:HG23	3:E:18:ALA:HB3	1.90	0.54
2:D:374:ILE:HD11	2:D:436:ALA:HB1	1.90	0.54
2:B:390:PRO:O	3:E:124:THR:OG1	2.24	0.54
2:B:58:ILE:O	2:B:62:LEU:HG	2.08	0.54
1:C:71:LEU:O	2:D:91:MET:HB3	2.08	0.53
1:C:29:ILE:H	1:C:29:ILE:HD12	1.71	0.53
2:D:81:MET:N	2:D:82:PRO:CD	2.72	0.53
3:E:275:LEU:HD22	3:E:279:THR:HG21	1.88	0.53
2:B:111:ASN:HD22	2:B:113:GLY:H	1.57	0.53
2:B:261:VAL:HG12	2:B:263:GLY:C	2.34	0.53
2:B:440:LEU:O	2:B:444:ILE:HG13	2.08	0.53
2:D:157:ASN:HD21	2:D:193:LEU:HD22	1.73	0.53
2:B:89:ASN:ND2	2:B:211:ASN:HA	2.24	0.53
2:B:25:PRO:CB	2:B:291:TYR:OH	2.54	0.52
3:F:368:THR:OG1	3:F:369:LYS:N	2.39	0.52
1:A:38:SER:HB2	2:B:237:VAL:HG13	1.92	0.52
2:B:421:ASN:HB3	2:B:424:PHE:CE2	2.43	0.52
3:F:311:PRO:HB2	3:F:314:LEU:CD1	2.40	0.52
2:D:306:SER:HB2	4:D:500:NAP:N6A	2.24	0.52
3:E:105:ARG:HH12	3:E:372:LEU:HA	1.75	0.52
1:A:46:VAL:HG21	2:B:39:MET:HE1	1.90	0.52
3:F:175:VAL:HG11	3:F:183:ILE:HD11	1.90	0.52
1:C:89:MET:HB3	2:D:346:ALA:HB1	1.92	0.52
2:B:106:LYS:HD3	2:B:108:ALA:HB2	1.92	0.52
3:E:336:LEU:HD23	3:E:352:VAL:HG23	1.92	0.52
2:D:201:GLY:O	4:D:500:NAP:H5N	2.09	0.51
3:F:283:ASP:O	3:F:311:PRO:HD2	2.10	0.51
1:A:13:VAL:HG21	2:D:9:PHE:HZ	1.75	0.51
2:D:231:MET:O	2:D:235:THR:HG22	2.11	0.51
2:B:96:ALA:HB2	2:B:218:VAL:HG12	1.93	0.51
2:B:294:LYS:NZ	2:B:364:GLU:HG2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ARG:O	1:C:89:MET:HG2	2.11	0.51
2:B:210:TYR:HA	2:B:213:PHE:HB2	1.92	0.51
1:A:42:HIS:CD2	2:B:237:VAL:HG11	2.45	0.51
2:D:253:ASN:N	2:D:253:ASN:OD1	2.42	0.51
2:B:391:LEU:HD23	3:E:124:THR:HG21	1.93	0.51
2:D:198:ILE:HD12	2:D:259:VAL:CG1	2.39	0.51
2:D:204:PRO:HB3	2:D:338:PRO:HG3	1.93	0.50
3:E:230:LEU:HD21	3:E:238:GLN:HG3	1.93	0.50
2:D:78:MET:HB2	2:D:347:GLU:OE1	2.10	0.50
2:D:289:LEU:HD22	2:D:319:LEU:HD11	1.93	0.50
3:E:239:HIS:HE1	3:E:268:THR:HG21	1.77	0.50
2:B:89:ASN:O	2:B:214:THR:HG21	2.11	0.50
2:B:192:VAL:O	2:B:196:LEU:HD13	2.11	0.50
2:D:240:ALA:O	2:D:244:LEU:HB2	2.11	0.49
3:F:233:GLU:HB2	3:F:237:ILE:HD11	1.95	0.49
2:D:249:ALA:O	2:D:252:MET:HB2	2.11	0.49
3:F:232:GLU:O	3:F:233:GLU:HB2	2.13	0.49
1:A:8:ALA:HA	1:A:11:ILE:HB	1.95	0.49
3:E:334:SER:HB2	3:E:338:ILE:HD12	1.95	0.49
3:F:220:ALA:H	3:F:229:GLU:HB2	1.77	0.49
2:B:304:ALA:HB1	3:E:208:SER:HB2	1.95	0.49
1:A:39:ASN:HD21	2:B:89:ASN:HA	1.77	0.49
2:B:129:PHE:O	2:B:133:LEU:HG	2.13	0.49
3:F:339:GLU:C	3:F:341:GLY:H	2.21	0.49
2:D:134:ILE:HG13	2:D:192:VAL:HG13	1.95	0.48
3:F:138:VAL:HG11	3:F:322:ALA:HB2	1.94	0.48
3:E:74:VAL:O	3:E:94:PHE:HB2	2.14	0.48
2:B:135:ALA:HA	2:B:203:MET:HE2	1.96	0.48
2:B:373:VAL:HG13	2:B:376:ALA:HB3	1.95	0.48
2:B:59:LEU:HA	2:B:62:LEU:HD12	1.95	0.48
2:D:446:ALA:HA	2:D:449:ARG:HE	1.78	0.48
3:E:26:ARG:HA	3:E:29:LYS:HB2	1.95	0.48
3:E:339:GLU:HB2	3:E:344:ALA:HB3	1.94	0.48
2:D:159:LEU:O	2:D:163:LEU:HG	2.13	0.48
2:D:164:THR:HG22	2:D:186:LEU:CB	2.25	0.48
2:D:190:PHE:CE2	2:D:194:MET:HE3	2.49	0.48
2:D:49:TRP:HB3	2:D:52:MET:HG3	1.95	0.48
2:B:392:TYR:O	3:E:125:ARG:HG2	2.14	0.48
2:D:135:ALA:O	2:D:139:LEU:HD12	2.14	0.48
2:D:141:GLY:HA2	2:D:144:LYS:HB2	1.96	0.48
3:F:252:LEU:HB2	3:F:281:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:MET:SD	2:D:338:PRO:CB	3.02	0.47
2:D:308:ALA:HA	2:D:437:GLN:HB3	1.96	0.47
2:D:319:LEU:HD22	2:D:324:VAL:HG21	1.96	0.47
3:E:173:MET:HA	3:E:196:TYR:HB3	1.97	0.47
1:A:46:VAL:O	1:A:50:MET:HG3	2.14	0.47
2:D:201:GLY:C	2:D:203:MET:H	2.23	0.47
2:D:356:LYS:HG3	2:D:361:ILE:HD12	1.97	0.47
2:D:380:VAL:HB	2:D:399:VAL:HG11	1.95	0.47
1:A:51:VAL:HA	2:B:52:MET:CE	2.34	0.47
2:B:193:LEU:HA	2:B:196:LEU:HD22	1.97	0.47
2:B:209:PHE:CD1	2:B:245:THR:HG21	2.45	0.47
2:D:194:MET:O	2:D:197:PRO:HD2	2.15	0.47
3:E:293:VAL:HG23	3:E:294:LEU:HG	1.96	0.47
2:B:185:LEU:HD23	2:B:188:LEU:HD12	1.97	0.46
2:B:257:TRP:CE3	2:B:260:LEU:HD12	2.50	0.46
1:C:23:ILE:HD11	2:D:19:LEU:HD22	1.98	0.46
2:B:11:VAL:HG21	2:B:42:ALA:HB2	1.97	0.46
2:D:309:GLN:HE21	2:D:310:HIS:CD2	2.33	0.46
3:E:26:ARG:HA	3:E:29:LYS:HD2	1.98	0.46
3:E:274:ARG:NH1	3:E:274:ARG:CG	2.67	0.46
1:C:66:PHE:CD1	2:D:61:ALA:HB2	2.51	0.46
2:D:94:GLY:O	2:D:98:THR:HG23	2.16	0.46
2:B:9:PHE:CZ	1:C:13:VAL:HG21	2.51	0.46
2:B:214:THR:O	2:B:218:VAL:HG13	2.16	0.46
3:E:71:LEU:C	3:E:72:PHE:HD1	2.23	0.46
3:F:76:PRO:HG3	3:F:100:ASN:ND2	2.31	0.46
3:F:105:ARG:HA	3:F:108:GLN:HG2	1.98	0.46
2:B:331:HIS:HB3	2:B:334:ALA:HB2	1.98	0.46
3:E:314:LEU:N	3:E:315:PRO:CD	2.79	0.46
2:B:321:ALA:C	2:B:323:GLY:H	2.23	0.46
3:E:149:ARG:HG3	3:E:150:LEU:HG	1.98	0.46
3:F:90:ILE:HA	3:F:113:THR:O	2.16	0.46
1:C:78:GLY:O	1:C:82:VAL:HG22	2.15	0.45
2:D:147:PRO:HD3	2:D:199:GLY:HA2	1.98	0.45
2:D:294:LYS:HB3	2:D:368:VAL:HA	1.97	0.45
3:E:230:LEU:HD23	3:E:235:LYS:HG3	1.97	0.45
2:B:336:ARG:NH2	4:B:500:NAP:O2A	2.45	0.45
2:D:90:GLY:O	2:D:129:PHE:HD1	1.98	0.45
2:D:127:VAL:HG13	2:D:191:GLY:HA2	1.99	0.45
3:E:124:THR:HA	3:E:127:GLN:CD	2.41	0.45
3:E:251:VAL:HG22	3:E:280:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:105:ARG:HG3	3:F:372:LEU:HD12	1.97	0.45
2:B:78:MET:HE2	2:B:78:MET:HA	1.97	0.45
2:D:85:VAL:O	2:D:89:ASN:HB2	2.17	0.45
2:D:302:GLY:HA3	2:D:375:GLY:HA3	1.98	0.45
1:C:71:LEU:HB3	2:D:91:MET:O	2.17	0.45
3:E:2:VAL:HG22	3:E:3:THR:N	2.32	0.45
2:B:331:HIS:CE1	2:B:333:VAL:HG22	2.52	0.45
1:C:75:ASN:HD22	2:D:88:TYR:HB3	1.82	0.45
2:D:221:GLU:O	2:D:225:VAL:HG22	2.17	0.45
3:E:77:PRO:HA	3:E:78:PRO:HD3	1.76	0.45
2:B:342:ASN:CG	3:F:159:THR:H	2.23	0.45
3:F:207:LEU:HD23	3:F:213:PRO:HD3	1.98	0.45
3:F:257:GLN:H	5:F:500:NAD:H52A	1.82	0.45
2:D:208:SER:HA	2:D:211:ASN:HB3	1.98	0.45
2:D:364:GLU:O	2:D:368:VAL:HG23	2.17	0.45
3:F:238:GLN:HE22	5:F:500:NAD:H62A	1.65	0.45
2:B:81:MET:N	2:B:82:PRO:CD	2.80	0.45
1:C:50:MET:HE3	2:D:62:LEU:HD11	1.99	0.45
3:E:207:LEU:HD12	3:E:213:PRO:HD3	1.99	0.45
2:B:22:MET:HG3	2:B:31:GLY:HA3	1.99	0.44
1:C:82:VAL:HG13	2:D:73:ALA:HB1	1.98	0.44
3:E:281:VAL:HB	3:E:308:VAL:HG22	1.99	0.44
2:D:42:ALA:O	2:D:46:THR:HG23	2.17	0.44
3:F:371:LEU:CD1	3:F:373:GLY:O	2.57	0.44
3:E:230:LEU:HB2	3:E:235:LYS:HZ1	1.82	0.44
3:E:303:VAL:HG22	3:E:304:ARG:HE	1.81	0.44
1:C:18:LEU:O	1:C:22:LEU:HG	2.17	0.44
1:C:29:ILE:HA	2:D:342:ASN:ND2	2.33	0.44
1:A:23:ILE:HB	2:B:243:LEU:HD13	1.99	0.44
1:A:52:VAL:HG13	2:B:102:VAL:HG11	2.00	0.44
3:F:365:HIS:O	3:F:366:GLY:O	2.36	0.44
2:D:227:ASN:HA	2:D:228:PRO:HD3	1.81	0.44
3:E:230:LEU:HB2	3:E:235:LYS:NZ	2.32	0.44
2:D:144:LYS:HG2	2:D:145:SER:N	2.33	0.44
2:B:130:THR:O	2:B:134:ILE:HG12	2.18	0.43
2:B:284:ASP:O	2:B:287:VAL:HB	2.18	0.43
2:D:11:VAL:HG13	2:D:15:PHE:CE2	2.53	0.43
2:B:196:LEU:N	2:B:197:PRO:CD	2.82	0.43
2:D:113:GLY:O	2:D:117:LEU:HG	2.18	0.43
3:F:314:LEU:N	3:F:315:PRO:CD	2.81	0.43
2:B:109:PHE:CE1	2:B:115:MET:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:74:VAL:O	3:F:94:PHE:HB2	2.19	0.43
2:D:199:GLY:C	2:D:201:GLY:N	2.76	0.43
2:D:358:LEU:HG	2:D:359:GLU:N	2.33	0.43
2:B:410:ARG:HA	2:B:434:GLY:H	1.84	0.42
2:B:128:ALA:HB1	2:B:214:THR:HG23	2.00	0.42
2:D:301:TYR:HB3	4:D:500:NAP:H52A	2.01	0.42
3:E:113:THR:HG23	3:E:359:LYS:HA	2.00	0.42
2:B:128:ALA:HB2	2:B:213:PHE:HB3	2.00	0.42
2:D:252:MET:C	2:D:254:ARG:N	2.77	0.42
3:E:155:PHE:N	3:E:156:PRO:CD	2.81	0.42
2:D:299:PRO:HA	2:D:374:ILE:HG23	2.00	0.42
3:E:139:ALA:CB	3:E:284:LEU:HD21	2.50	0.42
3:E:329:ASN:O	3:E:333:LEU:HB2	2.19	0.42
2:B:29:LYS:H	2:B:29:LYS:HG2	1.68	0.42
2:B:196:LEU:H	2:B:197:PRO:HD3	1.84	0.42
2:D:337:MET:HB2	2:D:338:PRO:CD	2.49	0.42
2:B:240:ALA:O	2:B:244:LEU:HB2	2.19	0.42
3:E:125:ARG:HB3	3:E:351:ILE:HD11	2.01	0.42
3:E:235:LYS:HE3	5:E:500:NAD:H2A	2.02	0.42
2:D:94:GLY:N	2:D:129:PHE:HB2	2.35	0.42
2:D:299:PRO:HB2	2:D:341:MET:SD	2.59	0.42
1:A:13:VAL:HG21	2:D:9:PHE:CZ	2.53	0.42
1:C:86:MET:CE	2:D:81:MET:HG2	2.49	0.42
2:D:111:ASN:HB3	2:D:114:LEU:HG	2.01	0.42
2:D:199:GLY:C	2:D:201:GLY:H	2.26	0.42
1:C:42:HIS:HE1	2:D:211:ASN:OD1	2.02	0.42
2:D:30:SER:O	2:D:33:VAL:HB	2.20	0.42
3:F:147:ALA:O	3:F:151:SER:HB2	2.19	0.42
1:C:41:ILE:C	1:C:43:GLY:H	2.27	0.41
1:C:43:GLY:C	1:C:45:VAL:H	2.27	0.41
1:C:46:VAL:HG22	1:C:72:GLY:C	2.45	0.41
2:D:167:ILE:HG22	2:D:183:PHE:HB2	2.01	0.41
2:D:331:HIS:HD2	2:D:397:LEU:HB2	1.84	0.41
3:E:91:VAL:HB	3:E:114:VAL:HA	2.01	0.41
2:B:202:ASP:CG	2:B:254:ARG:HH12	2.28	0.41
2:B:345:LEU:HD22	2:B:350:VAL:HG21	2.02	0.41
3:E:9:GLU:HG3	3:E:74:VAL:HB	2.01	0.41
2:B:386:ARG:HA	2:B:387:PRO:HD3	1.89	0.41
2:D:201:GLY:O	2:D:203:MET:N	2.53	0.41
3:E:165:ILE:HG12	3:F:321:HIS:CD2	2.55	0.41
3:F:6:VAL:HG13	3:F:18:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PHE:N	1:A:4:GLY:CA	2.83	0.41
2:B:392:TYR:CG	2:B:393:GLY:N	2.88	0.41
3:E:7:PRO:HG3	3:E:73:THR:HG22	2.02	0.41
3:E:172:VAL:HG21	3:E:183:ILE:HG13	2.02	0.41
3:F:329:ASN:O	3:F:333:LEU:HB2	2.21	0.41
1:A:48:GLY:HA3	2:B:230:LEU:HD11	2.03	0.41
1:C:42:HIS:HD2	1:C:75:ASN:OD1	2.04	0.41
2:D:163:LEU:O	2:D:167:ILE:HG13	2.21	0.41
3:E:142:LEU:HD11	3:E:318:LEU:HB2	2.03	0.41
3:F:79:GLU:OE1	3:F:103:LEU:HD23	2.20	0.41
3:F:87:PRO:C	3:F:89:ALA:H	2.27	0.41
2:D:205:VAL:O	2:D:205:VAL:HG12	2.19	0.41
2:D:386:ARG:HA	2:D:387:PRO:HD3	1.90	0.41
2:D:407:VAL:O	2:D:432:LEU:N	2.50	0.41
3:E:197:ASP:OD1	5:E:500:NAD:O1A	2.38	0.41
3:E:358:MET:HA	3:E:362:GLU:O	2.21	0.41
3:F:174:GLY:O	3:F:255:THR:OG1	2.31	0.41
2:B:8:TYR:OH	2:B:46:THR:HB	2.20	0.41
2:B:109:PHE:HE1	2:B:115:MET:HG3	1.86	0.41
2:B:308:ALA:HA	2:B:437:GLN:HB3	2.02	0.41
3:E:174:GLY:CA	5:E:500:NAD:O2A	2.67	0.41
2:B:124:ILE:HG23	2:B:213:PHE:CD2	2.55	0.40
1:C:45:VAL:HG11	2:D:92:GLY:HA2	2.02	0.40
3:F:82:ILE:HG23	3:F:107:LEU:HD23	2.03	0.40
2:B:298:VAL:HB	2:B:373:VAL:HG22	2.03	0.40
2:B:405:VAL:HB	2:B:429:THR:HA	2.03	0.40
2:D:313:LYS:HG3	2:D:350:VAL:HG22	2.03	0.40
3:E:149:ARG:CZ	3:F:149:ARG:HH21	2.33	0.40
2:B:25:PRO:HG2	2:B:450:LEU:HD22	2.03	0.40
2:B:123:LEU:HD12	2:B:183:PHE:HE1	1.85	0.40
2:B:133:LEU:HA	2:B:136:PHE:HB3	2.03	0.40
2:B:163:LEU:O	2:B:167:ILE:HG22	2.22	0.40
3:F:170:VAL:HG22	3:F:251:VAL:HB	2.03	0.40
2:D:86:ALA:HB2	2:D:207:ILE:HG12	2.02	0.40
3:E:251:VAL:HA	3:E:280:VAL:O	2.21	0.40
1:C:81:ALA:HB3	2:D:73:ALA:HB3	2.03	0.40
2:D:207:ILE:O	2:D:211:ASN:N	2.54	0.40
2:D:294:LYS:HE2	2:D:364:GLU:HG2	2.04	0.40
3:F:110:LYS:HD3	3:F:110:LYS:O	2.21	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	92/100 (92%)	82 (89%)	9 (10%)	1 (1%)	11	46
1	C	88/100 (88%)	77 (88%)	11 (12%)	0	100	100
2	B	436/450 (97%)	413 (95%)	22 (5%)	1 (0%)	43	78
2	D	433/450 (96%)	403 (93%)	29 (7%)	1 (0%)	43	78
3	E	370/384 (96%)	333 (90%)	34 (9%)	3 (1%)	16	54
3	F	365/384 (95%)	321 (88%)	31 (8%)	13 (4%)	2	20
All	All	1784/1868 (96%)	1629 (91%)	136 (8%)	19 (1%)	11	46

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	370	ALA
3	F	372	LEU
3	E	123	ILE
3	E	343	PHE
3	F	216	LEU
3	F	366	GLY
2	B	309	GLN
2	D	202	ASP
3	F	217	PRO
3	F	235	LYS
3	F	368	THR
1	A	45	VAL
3	F	356	LEU
3	F	234	GLU
3	F	340	LYS
3	E	74	VAL
3	F	341	GLY
3	F	96	GLN
3	F	259	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	73/75 (97%)	61 (84%)	12 (16%)	2	10
1	C	69/75 (92%)	61 (88%)	8 (12%)	5	18
2	B	327/335 (98%)	298 (91%)	29 (9%)	9	28
2	D	326/335 (97%)	293 (90%)	33 (10%)	7	23
3	E	287/296 (97%)	258 (90%)	29 (10%)	7	23
3	F	284/296 (96%)	262 (92%)	22 (8%)	12	32
All	All	1366/1412 (97%)	1233 (90%)	133 (10%)	8	24

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	25	ARG
1	A	28	VAL
1	A	34	LEU
1	A	44	VAL
1	A	45	VAL
1	A	46	VAL
1	A	52	VAL
1	A	60	LEU
1	A	64	ILE
1	A	87	LEU
1	A	89	MET
2	B	2	ASP
2	B	3	LEU
2	B	19	LEU
2	B	41	LEU
2	B	46	THR
2	B	52	MET
2	B	63	LEU
2	B	81	MET
2	B	105	LEU
2	B	111	ASN

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Mol	Chain	Res	Type
2	B	120	LEU
2	B	130	THR
2	B	133	LEU
2	B	140	GLN
2	B	143	MET
2	B	163	LEU
2	B	189	LEU
2	B	196	LEU
2	B	236	LEU
2	B	244	LEU
2	B	254	ARG
2	B	277	LEU
2	B	305	LEU
2	B	355	LEU
2	B	374	ILE
2	B	397	LEU
2	B	432	LEU
2	B	437	GLN
2	B	447	LEU
1	C	9	LEU
1	C	32	THR
1	C	34	LEU
1	C	46	VAL
1	C	60	LEU
1	C	67	LEU
1	C	84	VAL
1	C	86	MET
2	D	1	MET
2	D	5	GLN
2	D	11	VAL
2	D	19	LEU
2	D	32	ILE
2	D	60	LEU
2	D	110	GLU
2	D	120	LEU
2	D	139	LEU
2	D	142	ILE
2	D	146	ARG
2	D	149	LEU
2	D	159	LEU
2	D	161	LEU
2	D	171	LEU

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Mol	Chain	Res	Type
2	D	182	LEU
2	D	186	LEU
2	D	189	LEU
2	D	227	ASN
2	D	236	LEU
2	D	247	LEU
2	D	248	MET
2	D	253	ASN
2	D	256	VAL
2	D	257	TRP
2	D	288	MET
2	D	325	GLU
2	D	337	MET
2	D	374	ILE
2	D	396	ILE
2	D	427	GLU
2	D	432	LEU
2	D	447	LEU
3	E	6	VAL
3	E	49	GLU
3	E	60	GLU
3	E	71	LEU
3	E	79	GLU
3	E	85	LEU
3	E	101	LEU
3	E	102	GLU
3	E	110	LYS
3	E	113	THR
3	E	123	ILE
3	E	149	ARG
3	E	158	LEU
3	E	185	THR
3	E	197	ASP
3	E	200	LYS
3	E	223	GLU
3	E	230	LEU
3	E	232	GLU
3	E	235	LYS
3	E	258	VAL
3	E	261	ARG
3	E	272	VAL
3	E	274	ARG

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Mol	Chain	Res	Type
3	E	284	LEU
3	E	312	LEU
3	E	318	LEU
3	E	333	LEU
3	E	362	GLU
3	F	49	GLU
3	F	71	LEU
3	F	83	GLN
3	F	86	GLU
3	F	105	ARG
3	F	113	THR
3	F	124	THR
3	F	128	SER
3	F	142	LEU
3	F	218	ILE
3	F	228	ARG
3	F	234	GLU
3	F	237	ILE
3	F	240	GLU
3	F	287	GLU
3	F	296	LYS
3	F	314	LEU
3	F	318	LEU
3	F	333	LEU
3	F	350	GLU
3	F	360	GLU
3	F	371	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	75	ASN
2	B	54	ASN
2	B	89	ASN
2	B	111	ASN
2	B	140	GLN
2	B	310	HIS
2	B	437	GLN
1	C	39	ASN
1	C	42	HIS
1	C	55	HIS

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Mol	Chain	Res	Type
1	C	75	ASN
2	D	5	GLN
2	D	24	HIS
2	D	140	GLN
2	D	153	GLN
2	D	157	ASN
2	D	310	HIS
2	D	437	GLN
3	E	98	HIS
3	E	239	HIS
3	E	291	ASN
3	E	329	ASN
3	F	83	GLN
3	F	108	GLN
3	F	127	GLN
3	F	146	HIS
3	F	238	GLN
3	F	245	HIS
3	F	313	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	$\# Z > 2$
4	NAP	D	500	-	50,52,52	1.21	5 (10%)	71,80,80	1.57	10 (14%)
5	NAD	E	500	-	46,48,48	1.38	7 (15%)	64,73,73	1.64	8 (12%)
4	NAP	B	500	-	50,52,52	1.23	5 (10%)	71,80,80	1.56	11 (15%)
5	NAD	F	500	-	46,48,48	1.29	6 (13%)	64,73,73	1.65	11 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	D	500	-	-	13/35/67/67	0/5/5/5
5	NAD	E	500	-	-	13/30/62/62	0/5/5/5
4	NAP	B	500	-	-	4/35/67/67	0/5/5/5
5	NAD	F	500	-	-	13/30/62/62	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	500	NAD	C5A-C4A	5.29	1.48	1.39
5	F	500	NAD	C5A-C4A	4.99	1.48	1.39
4	D	500	NAP	C5A-C4A	4.90	1.47	1.39
4	B	500	NAP	C5A-C4A	4.87	1.47	1.39
5	E	500	NAD	C5A-C6A	3.04	1.49	1.41
5	F	500	NAD	C5A-C6A	2.97	1.49	1.41
5	E	500	NAD	PA-O3	2.90	1.62	1.59
4	B	500	NAP	C5A-C6A	2.90	1.49	1.41
5	E	500	NAD	PN-O3	2.87	1.62	1.59
4	D	500	NAP	C5A-C6A	2.82	1.48	1.41
5	F	500	NAD	O4D-C1D	2.58	1.44	1.40
5	E	500	NAD	C8A-N7A	2.57	1.36	1.31
4	B	500	NAP	O4D-C1D	2.51	1.44	1.40
5	F	500	NAD	C8A-N7A	2.41	1.36	1.31
4	D	500	NAP	C8A-N7A	2.39	1.36	1.31
4	B	500	NAP	C8A-N7A	2.34	1.36	1.31
4	B	500	NAP	C5A-N7A	-2.28	1.34	1.39
4	D	500	NAP	C5A-N7A	-2.26	1.35	1.39
5	F	500	NAD	C5A-N7A	-2.24	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	500	NAD	C5A-N7A	-2.22	1.35	1.39
4	D	500	NAP	O4D-C1D	2.20	1.43	1.40
5	E	500	NAD	O4D-C1D	2.13	1.43	1.40
5	F	500	NAD	PA-O3	2.03	1.61	1.59

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	500	NAD	C5A-C4A-N3A	-6.50	117.77	126.72
5	F	500	NAD	C5A-C4A-N3A	-6.13	118.28	126.72
4	B	500	NAP	C5A-C4A-N3A	-6.08	118.35	126.72
4	D	500	NAP	C5A-C4A-N3A	-5.85	118.66	126.72
4	B	500	NAP	N3A-C4A-N9A	4.74	135.23	127.17
5	F	500	NAD	N3A-C4A-N9A	4.73	135.21	127.17
5	E	500	NAD	N3A-C4A-N9A	4.72	135.20	127.17
4	D	500	NAP	N3A-C4A-N9A	4.69	135.15	127.17
5	E	500	NAD	C2A-N3A-C4A	3.98	121.54	111.83
5	F	500	NAD	C2A-N3A-C4A	3.95	121.47	111.83
4	B	500	NAP	C2A-N3A-C4A	3.85	121.22	111.83
4	D	500	NAP	C2A-N3A-C4A	3.79	121.08	111.83
5	E	500	NAD	C4A-C5A-N7A	-3.77	106.27	110.58
4	B	500	NAP	C4A-C5A-N7A	-3.49	106.59	110.58
4	D	500	NAP	N3A-C2A-N1A	-3.48	123.31	128.58
5	F	500	NAD	C4A-C5A-N7A	-3.48	106.60	110.58
5	F	500	NAD	N3A-C2A-N1A	-3.47	123.33	128.58
4	D	500	NAP	C4A-C5A-N7A	-3.35	106.75	110.58
5	E	500	NAD	N3A-C2A-N1A	-3.29	123.61	128.58
4	B	500	NAP	N3A-C2A-N1A	-3.28	123.62	128.58
4	B	500	NAP	C2B-C1B-N9A	-2.82	109.10	113.75
4	B	500	NAP	O4B-C1B-N9A	2.66	113.20	108.09
5	E	500	NAD	C3B-C2B-C1B	2.64	106.46	101.46
5	F	500	NAD	C6N-N1N-C2N	-2.62	119.65	121.88
5	E	500	NAD	C5A-N7A-C8A	2.55	107.46	103.45
4	B	500	NAP	C5A-N7A-C8A	2.55	107.45	103.45
4	D	500	NAP	C5A-N7A-C8A	2.53	107.43	103.45
4	D	500	NAP	C4A-N9A-C8A	2.51	108.38	105.74
5	F	500	NAD	C5A-N7A-C8A	2.51	107.39	103.45
4	D	500	NAP	O4B-C1B-N9A	2.42	112.73	108.09
5	F	500	NAD	O5D-C5D-C4D	2.42	117.22	108.99
4	B	500	NAP	C4A-N9A-C8A	2.29	108.15	105.74
4	D	500	NAP	C2B-C1B-N9A	-2.26	110.03	113.75
5	F	500	NAD	C6A-C5A-N7A	2.13	136.20	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	500	NAD	C6A-C5A-N7A	2.13	136.19	132.09
4	B	500	NAP	C6N-N1N-C2N	-2.13	120.07	121.88
5	F	500	NAD	C4A-N9A-C8A	2.10	107.94	105.74
4	B	500	NAP	C6A-C5A-N7A	2.09	136.12	132.09
4	D	500	NAP	C6A-C5A-N7A	2.08	136.10	132.09
5	F	500	NAD	C3B-C2B-C1B	2.02	105.28	101.46

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	500	NAP	PA-O3-PN-O5D
4	D	500	NAP	O4D-C1D-N1N-C2N
4	D	500	NAP	C2N-C3N-C7N-N7N
5	E	500	NAD	C5D-O5D-PN-O3
5	E	500	NAD	O4D-C1D-N1N-C2N
5	E	500	NAD	O4D-C1D-N1N-C6N
5	E	500	NAD	C2D-C1D-N1N-C2N
5	E	500	NAD	C2D-C1D-N1N-C6N
5	F	500	NAD	C5D-O5D-PN-O3
5	F	500	NAD	C5D-O5D-PN-O2N
5	F	500	NAD	C2N-C3N-C7N-O7N
4	D	500	NAP	C4N-C3N-C7N-N7N
4	D	500	NAP	C2N-C3N-C7N-O7N
5	F	500	NAD	C2N-C3N-C7N-N7N
4	D	500	NAP	C4N-C3N-C7N-O7N
4	D	500	NAP	O4B-C4B-C5B-O5B
4	D	500	NAP	C3B-C4B-C5B-O5B
5	E	500	NAD	O4B-C4B-C5B-O5B
4	D	500	NAP	O4D-C4D-C5D-O5D
5	E	500	NAD	C3B-C4B-C5B-O5B
5	F	500	NAD	O4B-C4B-C5B-O5B
5	F	500	NAD	C3B-C4B-C5B-O5B
5	F	500	NAD	C4N-C3N-C7N-O7N
5	F	500	NAD	C4N-C3N-C7N-N7N
4	B	500	NAP	O4B-C4B-C5B-O5B
4	B	500	NAP	C3B-C4B-C5B-O5B
4	D	500	NAP	C3D-C4D-C5D-O5D
5	F	500	NAD	C2B-C1B-N9A-C8A
5	E	500	NAD	C5D-O5D-PN-O1N
5	E	500	NAD	C5D-O5D-PN-O2N
5	F	500	NAD	C5D-O5D-PN-O1N

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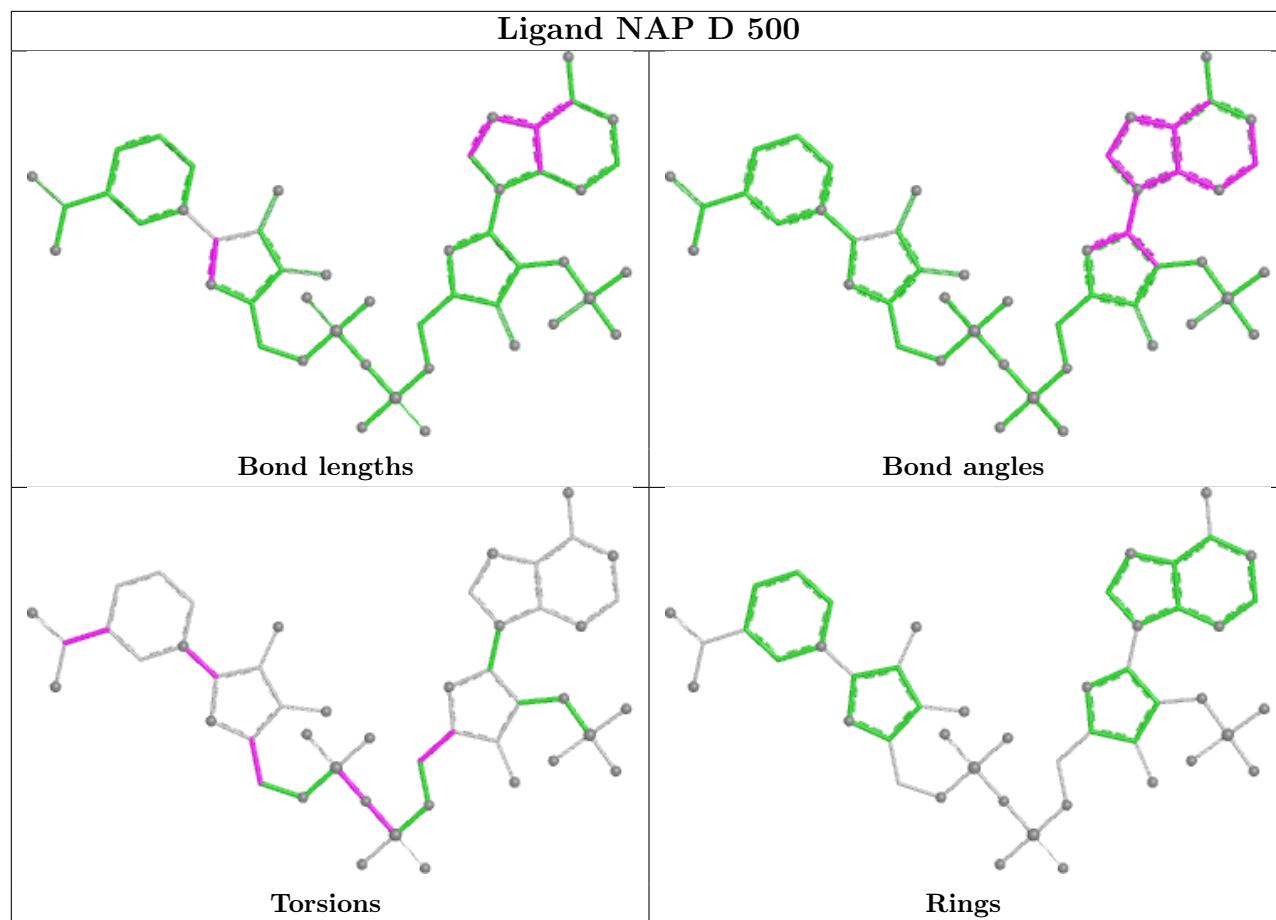
Mol	Chain	Res	Type	Atoms
5	E	500	NAD	C4B-C5B-O5B-PA
5	F	500	NAD	O4D-C4D-C5D-O5D
5	F	500	NAD	O4B-C1B-N9A-C8A
4	D	500	NAP	O4D-C1D-N1N-C6N
5	E	500	NAD	O4D-C4D-C5D-O5D
4	D	500	NAP	PN-O3-PA-O1A
4	B	500	NAP	PN-O3-PA-O1A
5	E	500	NAD	C3D-C4D-C5D-O5D
5	E	500	NAD	C4D-C5D-O5D-PN
5	F	500	NAD	C2B-C1B-N9A-C4A
4	B	500	NAP	PN-O3-PA-O2A
4	D	500	NAP	PN-O3-PA-O2A

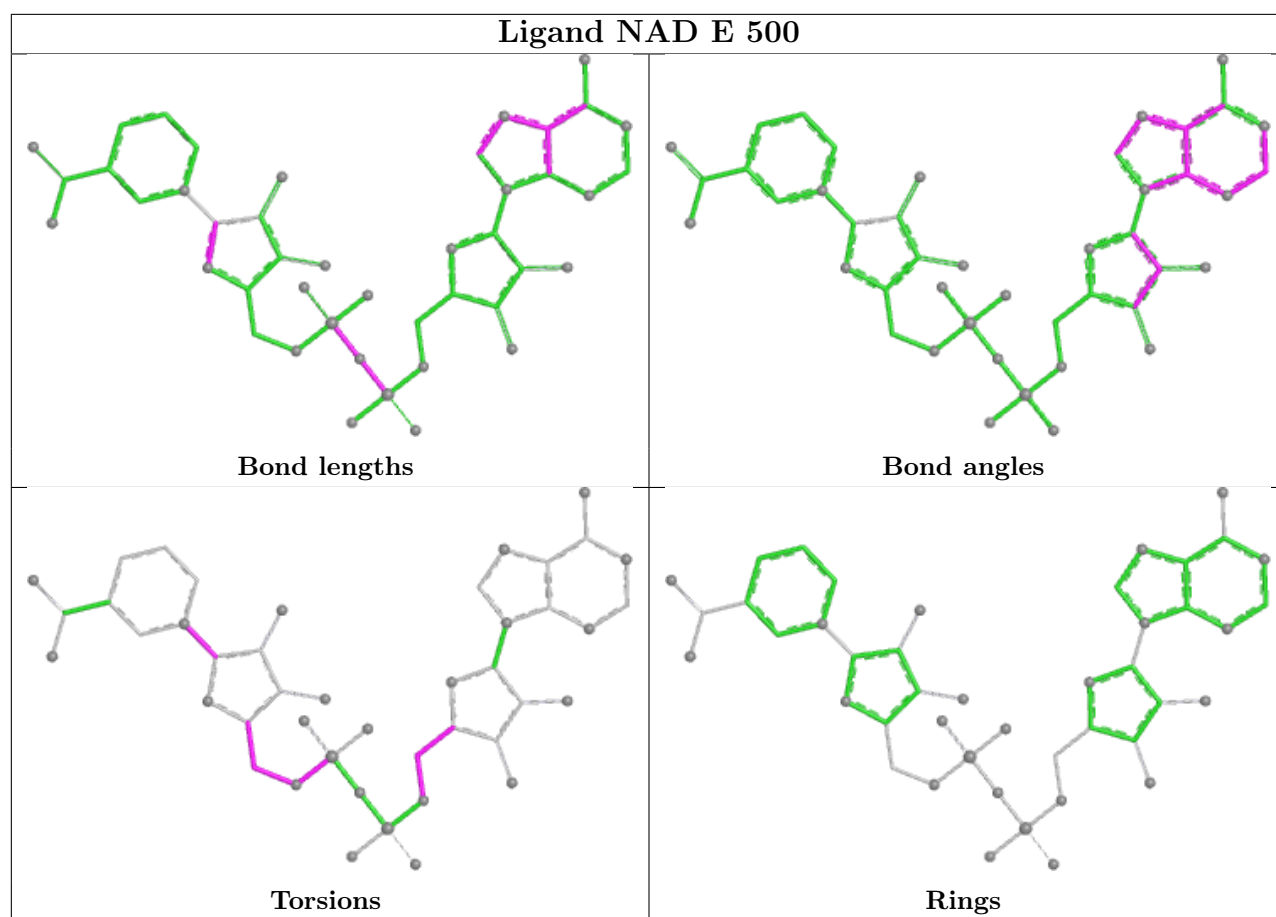
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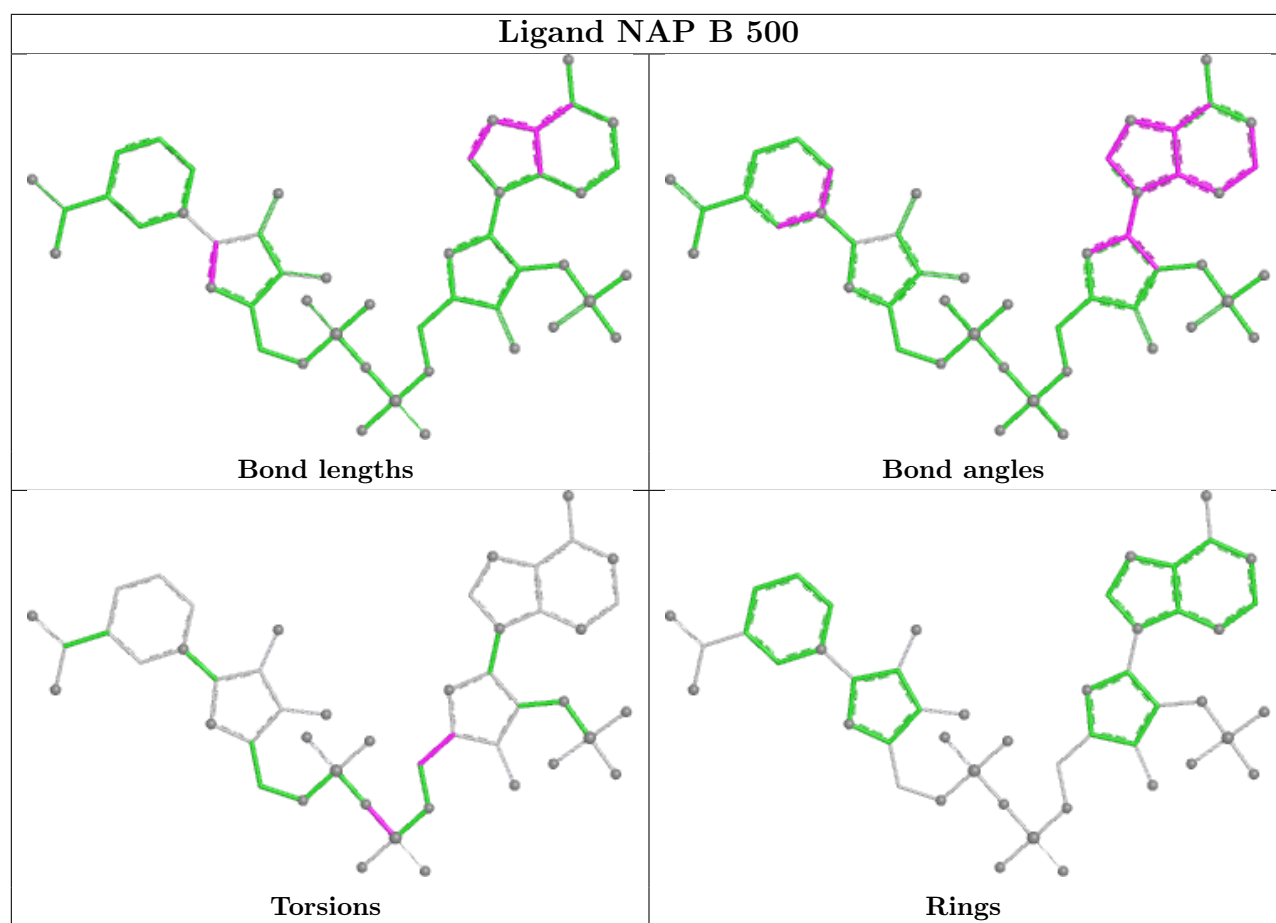
4 monomers are involved in 13 short contacts:

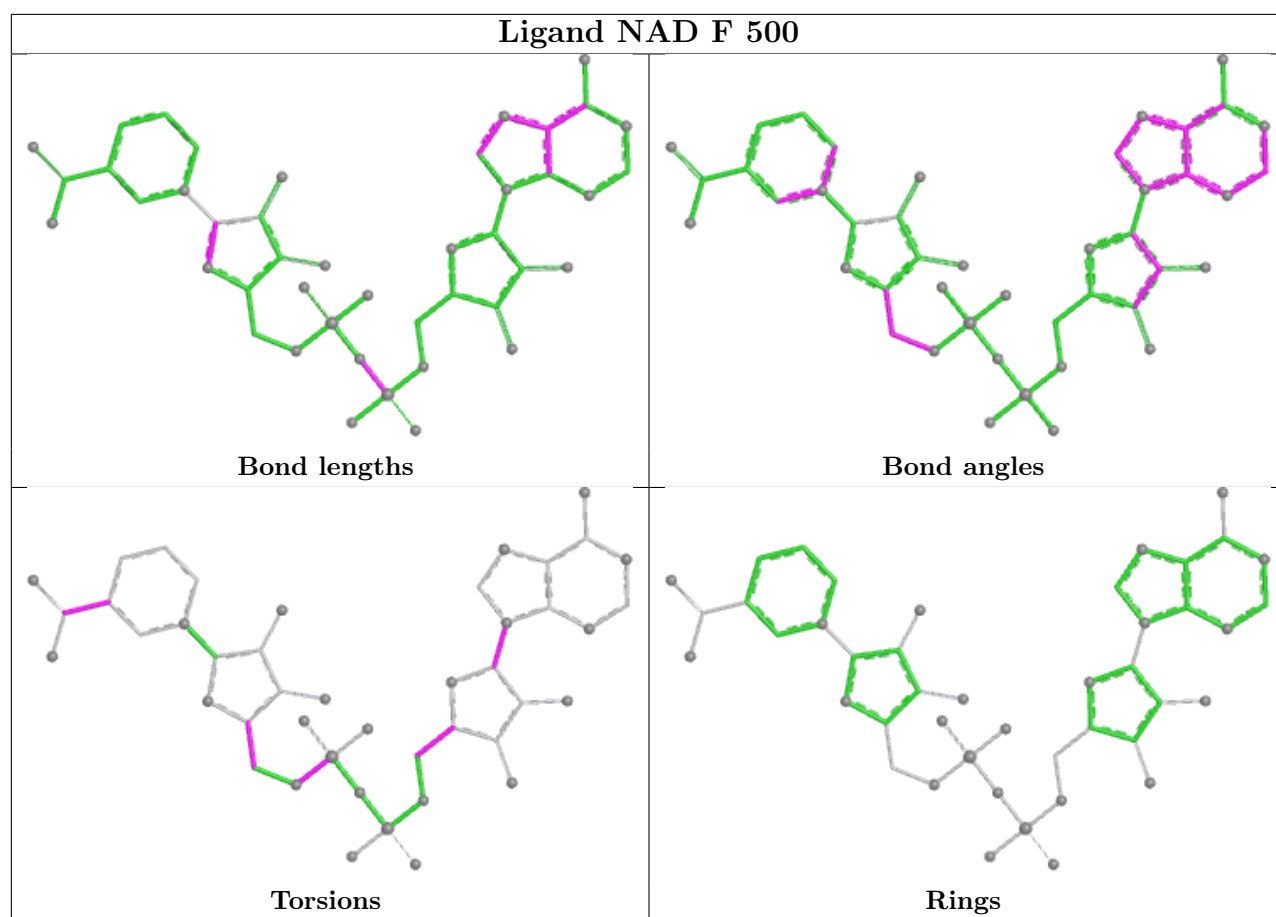
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	500	NAP	5	0
5	E	500	NAD	5	0
4	B	500	NAP	1	0
5	F	500	NAD	2	0

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	94/100 (94%)	0.30	11 (11%) 9 17	107, 187, 276, 328	0
1	C	90/100 (90%)	-0.39	3 (3%) 49 45	84, 136, 201, 285	0
2	B	440/450 (97%)	-0.09	26 (5%) 28 33	65, 148, 218, 287	0
2	D	437/450 (97%)	-0.25	17 (3%) 43 42	73, 152, 251, 298	0
3	E	372/384 (96%)	0.04	24 (6%) 25 30	50, 145, 221, 249	0
3	F	369/384 (96%)	-0.07	23 (6%) 26 31	84, 173, 238, 275	0
All	All	1802/1868 (96%)	-0.09	104 (5%) 29 33	50, 154, 236, 328	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	40	ALA	10.1
3	F	8	LYS	7.2
3	E	257	GLN	6.8
2	B	39	MET	6.4
2	B	387	PRO	6.2
2	B	412	GLN	5.9
3	E	62	GLY	5.9
3	F	39	GLY	5.9
2	B	178	ALA	5.7
3	E	224	GLY	5.3
3	E	61	ARG	5.1
2	D	418	GLY	5.0
1	A	32	THR	4.9
2	B	68	VAL	4.7
1	A	34	LEU	4.3
1	A	3	PHE	4.3
3	F	239	HIS	4.1
2	D	414	LYS	4.1
3	E	123	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	71	TRP	3.8
2	B	240	ALA	3.8
2	B	251	ALA	3.8
1	A	29	ILE	3.6
3	E	264	PRO	3.6
2	B	385	ARG	3.6
3	F	129	MET	3.6
3	F	269	GLU	3.6
2	B	36	GLY	3.6
2	B	328	PHE	3.5
3	E	258	VAL	3.5
3	E	289	GLY	3.5
1	A	31	HIS	3.4
2	D	352	TYR	3.4
1	C	2	GLU	3.4
2	B	345	LEU	3.4
3	E	157	MET	3.3
3	F	42	GLU	3.3
3	F	10	ARG	3.2
2	D	415	GLY	3.2
2	D	256	VAL	3.1
3	F	15	ARG	3.1
2	B	35	ALA	3.0
2	D	136	PHE	3.0
2	D	71	TRP	3.0
2	B	343	VAL	3.0
1	A	30	LEU	2.9
3	E	255	THR	2.8
2	B	248	MET	2.8
1	A	94	PRO	2.8
3	E	187	LYS	2.8
3	F	99	LYS	2.7
3	F	298	GLY	2.7
2	D	348	ALA	2.7
1	A	63	LEU	2.7
2	B	204	PRO	2.7
3	E	122	ARG	2.7
3	F	300	VAL	2.7
2	D	353	ASP	2.6
3	F	299	GLU	2.6
2	D	68	VAL	2.6
2	D	369	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	121	PRO	2.6
3	F	287	GLU	2.6
2	B	274	LYS	2.5
2	B	22	MET	2.5
3	E	265	ILE	2.5
3	E	162	ALA	2.5
2	B	226	GLY	2.5
2	B	247	LEU	2.4
3	E	348	GLU	2.4
3	E	60	GLU	2.4
2	B	341	MET	2.4
3	F	240	GLU	2.4
3	F	336	LEU	2.4
2	B	388	GLY	2.3
2	B	417	ALA	2.3
3	E	109	ALA	2.3
2	D	425	TYR	2.3
1	C	67	LEU	2.3
3	F	243	ARG	2.3
3	E	210	GLY	2.3
3	F	296	LYS	2.3
2	B	347	GLU	2.3
2	B	40	VAL	2.3
2	D	142	ILE	2.2
2	D	242	THR	2.2
3	E	64	LEU	2.2
3	F	234	GLU	2.2
1	C	63	LEU	2.2
2	B	420	GLU	2.2
1	A	33	PRO	2.1
3	E	80	ASP	2.1
2	D	178	ALA	2.1
3	E	59	VAL	2.1
3	F	88	GLY	2.1
3	E	332	ASN	2.1
3	F	268	THR	2.1
1	A	37	GLY	2.0
2	D	258	SER	2.0
3	F	43	GLY	2.0
3	E	185	THR	2.0
1	A	40	PHE	2.0
3	F	127	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	420	GLU	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](#)

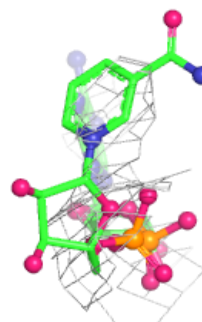
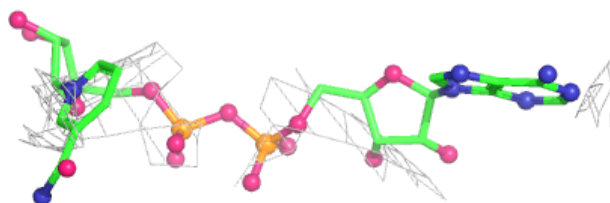
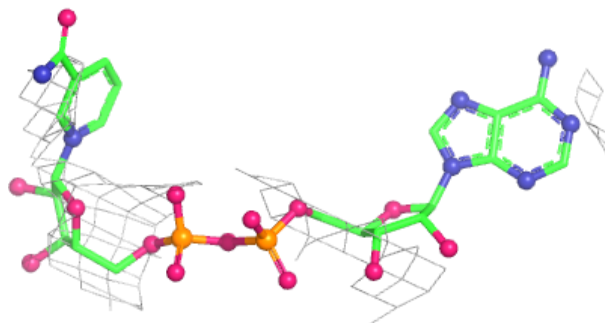
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAD	E	500	44/44	0.85	0.14	137,203,307,312	0
4	NAP	D	500	48/48	0.87	0.07	190,212,228,229	0
5	NAD	F	500	44/44	0.92	0.10	165,193,250,257	0
4	NAP	B	500	48/48	0.98	0.04	89,94,103,107	0

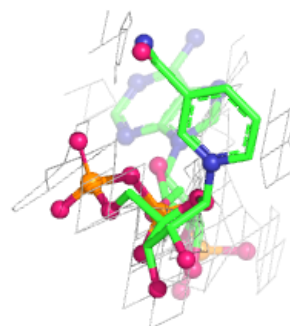
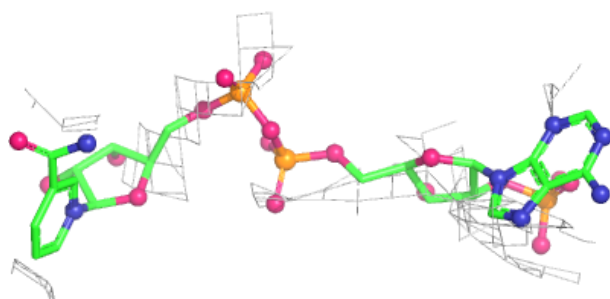
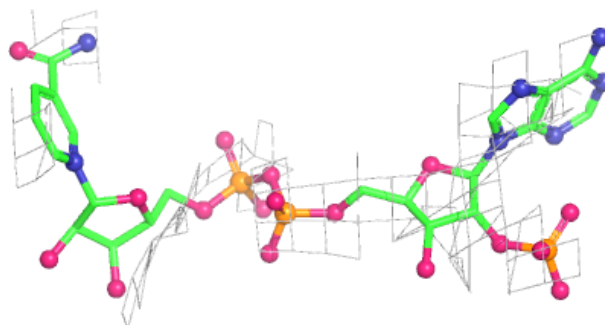
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD E 500:

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

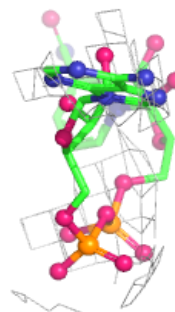
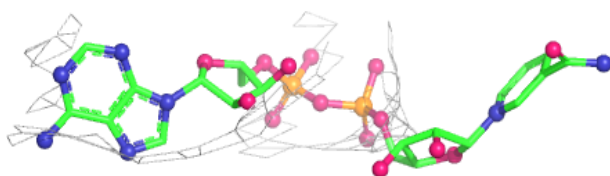
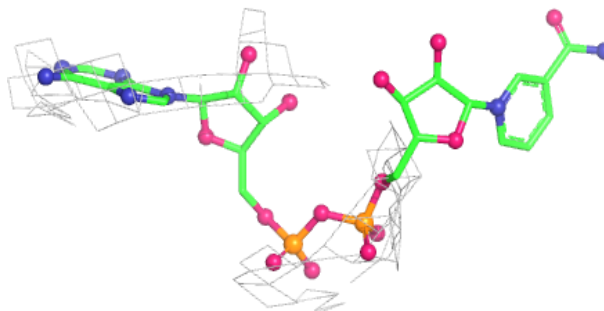
**Electron density around NAP D 500:**

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

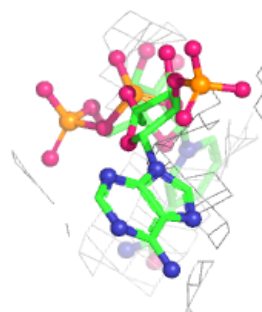
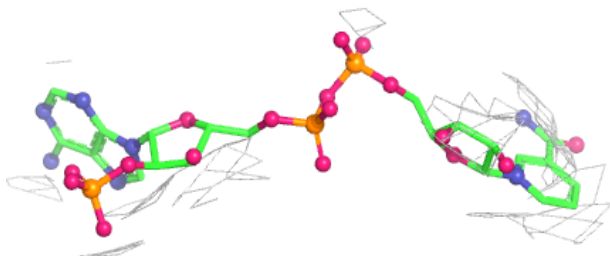
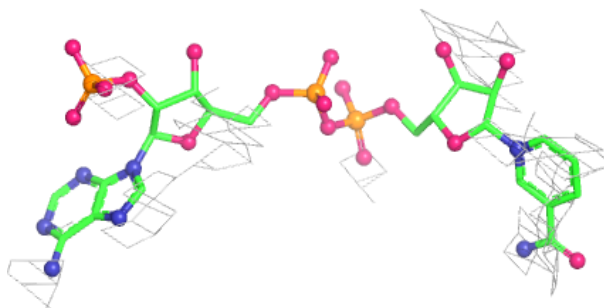


Electron density around NAD F 500:

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

**Electron density around NAP B 500:**

$2mF_o-DF_c$ (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.