



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:02 pm BST

PDB ID : 4J1T
Title : Crystal structure of Thermus thermophilus transhydrogenase heterotrimeric complex of the Alpha1 subunit dimer with the NADP binding domain (domain III) of the Beta subunit in P2(1)
Authors : Yamaguchi, M.; Leung, J.; Schurig Briccio, L.A.; Gennis, R.B.; Stout, C.D.
Deposited on : 2013-02-02
Resolution : 2.37 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

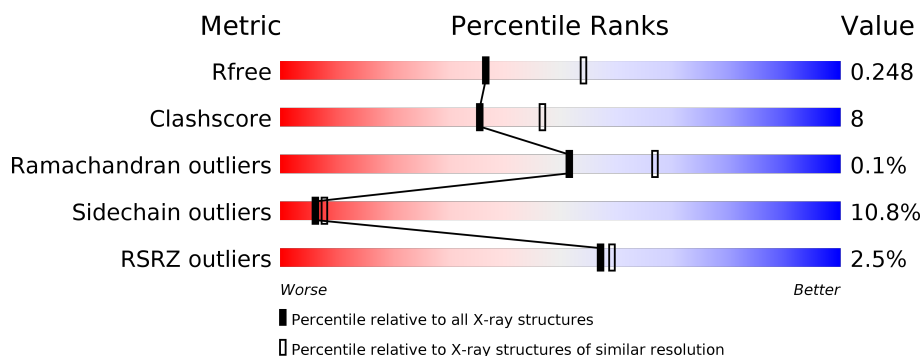
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 on 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	381	<div> <div>2%</div> <div>79%</div> <div>15%</div> <div>.</div> <div>.</div> </div>
1	B	381	<div> <div>2%</div> <div>79%</div> <div>14%</div> <div>.</div> <div>.</div> </div>
1	D	381	<div> <div>2%</div> <div>75%</div> <div>19%</div> <div>.</div> <div>.</div> </div>
1	E	381	<div> <div>4%</div> <div>72%</div> <div>21%</div> <div>.</div> <div>.</div> </div>
2	C	185	<div> <div>3%</div> <div>76%</div> <div>17%</div> <div>.</div> <div>.</div> </div>
2	F	185	<div> <div>%</div> <div>74%</div> <div>18%</div> <div>.</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	401	-	-	X	-
3	GOL	D	401	-	-	X	-
3	GOL	D	402	-	-	X	-
3	GOL	D	403	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14253 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/NADP transhydrogenase alpha subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2770	1757	495	506	12			
1	B	367	Total	C	N	O	S	0	0	0
			2765	1755	496	502	12			
1	D	372	Total	C	N	O	S	0	0	0
			2794	1772	498	512	12			
1	E	373	Total	C	N	O	S	0	0	0
			2798	1774	499	513	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q72GR8
A	-4	HIS	-	EXPRESSION TAG	UNP Q72GR8
A	-3	HIS	-	EXPRESSION TAG	UNP Q72GR8
A	-2	HIS	-	EXPRESSION TAG	UNP Q72GR8
A	-1	HIS	-	EXPRESSION TAG	UNP Q72GR8
A	0	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	-5	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	-4	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	-3	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	-2	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	-1	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	0	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	-5	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	-4	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	-3	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	-2	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	-1	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	0	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

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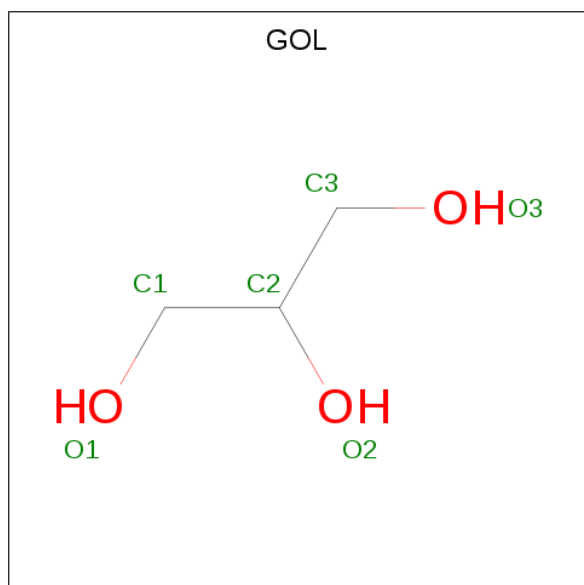
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	HIS	-	EXPRESSION TAG	UNP Q72GR8
E	-1	HIS	-	EXPRESSION TAG	UNP Q72GR8
E	0	HIS	-	EXPRESSION TAG	UNP Q72GR8

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

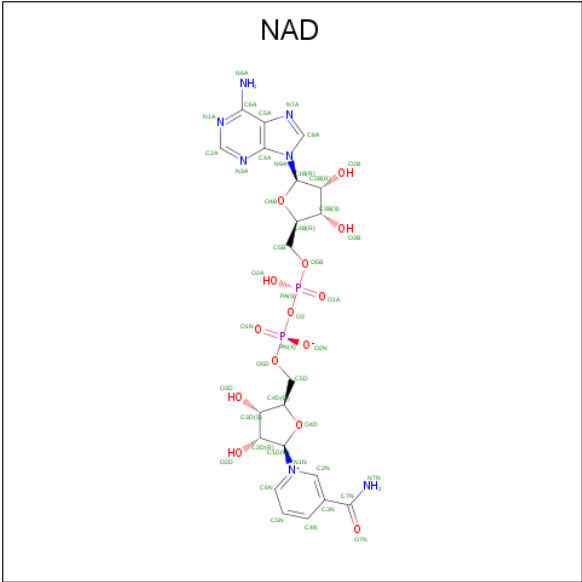
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	177	Total	C	N	O	S	0	0	0
			1343	860	229	248	6			
2	F	177	Total	C	N	O	S	0	0	0
			1343	860	229	248	6			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



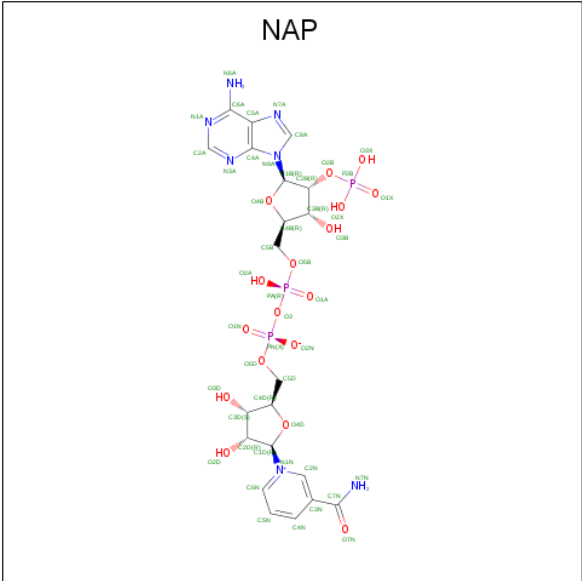
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total	O	0	0
			67	67		
6	B	44	Total	O	0	0
			44	44		
6	C	11	Total	O	0	0
			11	11		
6	D	50	Total	O	0	0
			50	50		
6	E	43	Total	O	0	0
			43	43		
6	F	17	Total	O	0	0
			17	17		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.08Å 68.87Å 132.34Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	132.35 – 2.37 37.14 – 2.37	Depositor EDS
% Data completeness (in resolution range)	95.2 (132.35-2.37) 95.1 (37.14-2.37)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.43 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.205 , 0.253 0.199 , 0.248	Depositor DCC
R_{free} test set	4019 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14253	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAP, 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	0.61	0/2814	0.71	1/3816 (0.0%)
1	B	0.56	0/2812	0.69	0/3814
1	D	0.63	0/2840	0.73	2/3852 (0.1%)
1	E	0.56	0/2844	0.70	1/3857 (0.0%)
2	C	0.51	0/1366	0.64	0/1848
2	F	0.58	0/1366	0.70	1/1848 (0.1%)
All	All	0.58	0/14042	0.70	5/19035 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	188	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	E	123	ILE	N-CA-C	-6.00	94.80	111.00
1	A	188	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	188	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	F	358	LEU	CA-CB-CG	5.13	127.10	115.30

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	2770	0	2888	34	0
1	B	2765	0	2881	39	0
1	D	2794	0	2911	66	0
1	E	2798	0	2914	64	0
2	C	1343	0	1378	20	0
2	F	1343	0	1378	30	0
3	A	6	0	8	7	0
3	D	18	0	24	16	0
4	B	44	0	26	3	0
4	E	44	0	26	5	0
5	C	48	0	25	0	0
5	F	48	0	25	1	0
6	A	67	0	0	1	0
6	B	44	0	0	1	0
6	C	11	0	0	0	0
6	D	50	0	0	3	0
6	E	43	0	0	4	0
6	F	17	0	0	3	0
All	All	14253	0	14484	232	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 8.

All (232) 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:D:146:HIS:ND1	1:D:149:ARG:NH1	1.89	1.19
1:D:188:ARG:HB2	3:D:401:GOL:H12	1.29	1.11
1:D:188:ARG:CB	3:D:401:GOL:H12	1.89	1.03
1:D:188:ARG:CB	3:D:401:GOL:C1	2.42	0.97
1:D:188:ARG:HB2	3:D:401:GOL:C1	1.96	0.95
2:F:422:GLU:HG2	6:F:604:HOH:O	1.67	0.94
1:E:157:MET:CE	2:F:355:LEU:HD23	1.97	0.93
1:A:187:LYS:HE2	1:A:210:GLY:O	1.70	0.91
1:D:124:THR:HG21	2:F:390:PRO:O	1.74	0.87
1:D:188:ARG:HB3	3:D:401:GOL:C1	2.05	0.87
1:B:65:LEU:HD21	1:B:71:LEU:HG	1.58	0.83
2:F:431:MET:HG2	6:F:607:HOH:O	1.77	0.83
2:F:405:VAL:HB	2:F:429:THR:HB	1.59	0.81
1:E:157:MET:HE3	2:F:355:LEU:HD23	1.61	0.81
3:D:401:GOL:H2	2:F:347:GLU:HA	1.65	0.78
1:D:236:ARG:HG2	1:D:236:ARG:HH11	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:500:NAD:H3B	4:E:500:NAD:O2A	1.87	0.75
1:D:188:ARG:CB	3:D:401:GOL:H11	2.16	0.74
1:A:149:ARG:HE	3:A:401:GOL:C1	2.01	0.73
1:D:188:ARG:HD3	1:E:188:ARG:O	1.88	0.72
1:A:149:ARG:HG2	3:A:401:GOL:O1	1.88	0.72
1:B:3:THR:H	1:B:69:HIS:HD2	1.38	0.71
1:E:123:ILE:HG13	1:E:123:ILE:O	1.90	0.69
2:C:358:LEU:HA	2:C:361:ILE:HG22	1.73	0.69
1:B:256:ALA:HA	4:B:500:NAD:H51A	1.72	0.69
1:D:187:LYS:HE2	1:D:210:GLY:O	1.93	0.69
1:E:65:LEU:HD22	1:E:85:LEU:HD23	1.74	0.68
1:D:188:ARG:HB3	3:D:401:GOL:H11	1.76	0.67
1:E:122:ARG:NH1	4:E:500:NAD:H51N	2.09	0.67
1:B:105:ARG:HG3	1:B:372:LEU:HD11	1.77	0.67
1:E:122:ARG:HH11	4:E:500:NAD:H51N	1.60	0.67
1:A:149:ARG:NE	3:A:401:GOL:H12	2.10	0.67
1:A:111:LYS:O	1:A:360:GLU:HA	1.95	0.67
1:B:261:ARG:HG3	1:B:262:ARG:N	2.09	0.66
1:D:111:LYS:NZ	3:D:402:GOL:H31	2.11	0.66
2:F:373:VAL:HG13	2:F:376:ALA:HB3	1.77	0.66
1:E:75:GLN:HB3	1:E:76:PRO:HD2	1.78	0.66
1:B:114:VAL:HG13	1:B:358:MET:HG2	1.78	0.65
1:B:101:LEU:HD11	1:B:372:LEU:HD13	1.79	0.65
1:A:149:ARG:HE	3:A:401:GOL:H12	1.61	0.65
1:D:236:ARG:HG2	1:D:236:ARG:NH1	2.12	0.65
1:D:368:THR:O	1:D:372:LEU:HG	1.97	0.64
1:B:365:HIS:ND1	1:B:368:THR:OG1	2.22	0.64
2:C:373:VAL:HG13	2:C:376:ALA:HB3	1.80	0.63
2:C:281:ASP:OD1	2:C:283:GLU:HG2	1.99	0.63
1:D:111:LYS:HZ2	3:D:402:GOL:H31	1.63	0.61
1:D:284:LEU:HD11	1:D:314:LEU:CD2	2.30	0.61
1:B:107:LEU:HD13	1:B:114:VAL:HG11	1.83	0.61
1:E:218:ILE:O	1:E:238:GLN:NE2	2.32	0.61
1:A:3:THR:HB	1:A:33:ARG:HB2	1.82	0.60
1:D:124:THR:CG2	2:F:390:PRO:O	2.47	0.60
2:F:426:ALA:HB3	2:F:429:THR:CG2	2.30	0.60
1:B:-1:HIS:HB2	1:B:342:ALA:HB1	1.83	0.60
1:B:7:PRO:HG3	1:B:73:THR:HG22	1.82	0.60
1:D:188:ARG:HD2	1:E:189:LEU:HA	1.84	0.59
1:B:233:GLU:HG2	1:B:236:ARG:HH12	1.68	0.59
1:D:3:THR:HB	1:D:33:ARG:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:GLN:HB3	1:D:76:PRO:HD2	1.85	0.59
1:D:334:SER:HB2	1:D:338:ILE:HD12	1.85	0.58
1:D:57:GLU:HB2	6:D:544:HOH:O	2.02	0.58
1:E:230:LEU:HD12	1:E:230:LEU:H	1.68	0.58
1:E:261:ARG:HG2	1:E:262:ARG:N	2.19	0.57
2:F:423:LEU:O	2:F:429:THR:HG21	2.03	0.57
1:E:223:GLU:C	1:E:225:GLY:H	2.06	0.57
1:B:307:ARG:HH11	1:B:307:ARG:HB3	1.69	0.57
1:D:200:LYS:O	1:D:204:GLU:HG3	2.05	0.57
1:E:98:HIS:H	1:E:98:HIS:CD2	2.20	0.56
1:D:146:HIS:CE1	1:D:149:ARG:NH1	2.71	0.56
1:E:285:ALA:O	1:E:289:GLY:O	2.23	0.56
1:A:124:THR:HG21	2:C:390:PRO:O	2.06	0.56
1:D:6:VAL:HG13	1:D:36:VAL:HG22	1.87	0.56
1:E:235:LYS:O	1:E:238:GLN:HB2	2.06	0.56
1:A:6:VAL:HG13	1:A:36:VAL:HG22	1.88	0.55
1:B:2:VAL:HA	1:B:69:HIS:CD2	2.41	0.55
1:D:188:ARG:HD3	3:D:401:GOL:H12	1.88	0.55
3:D:401:GOL:H31	1:E:188:ARG:HA	1.87	0.55
1:B:98:HIS:HB2	6:B:642:HOH:O	2.06	0.55
1:E:230:LEU:HD12	1:E:230:LEU:N	2.21	0.55
1:E:157:MET:HE1	2:F:355:LEU:HD23	1.87	0.55
1:E:65:LEU:HD21	1:E:71:LEU:HG	1.89	0.55
1:E:273:GLU:HA	1:E:304:ARG:HH12	1.71	0.55
1:A:149:ARG:CG	3:A:401:GOL:O1	2.53	0.54
1:E:199:ARG:HH22	4:E:500:NAD:H2D	1.71	0.54
1:E:111:LYS:HA	1:E:361:GLY:CA	2.37	0.54
1:E:124:THR:HG23	1:E:127:GLN:OE1	2.07	0.54
1:B:3:THR:H	1:B:69:HIS:CD2	2.22	0.54
1:D:311:PRO:HB2	1:D:314:LEU:HD13	1.90	0.54
1:B:187:LYS:HE2	1:B:210:GLY:O	2.07	0.54
1:B:91:VAL:HB	1:B:114:VAL:HB	1.89	0.54
3:A:401:GOL:H11	1:B:149:ARG:HH21	1.73	0.53
1:E:122:ARG:NH1	4:E:500:NAD:O2N	2.41	0.53
1:A:307:ARG:NH2	1:B:45:TYR:OH	2.39	0.53
1:A:275:LEU:HD22	1:A:279:THR:HG21	1.90	0.52
1:D:111:LYS:NZ	3:D:402:GOL:C3	2.72	0.52
1:E:166:ARG:HG3	1:E:167:PRO:HD2	1.91	0.52
1:E:96:GLN:HB2	1:E:98:HIS:CE1	2.45	0.52
1:B:138:VAL:HG11	1:B:315:PRO:HA	1.92	0.52
1:A:373:GLY:O	1:D:111:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:ARG:HG2	1:E:262:ARG:H	1.75	0.52
1:A:138:VAL:HG11	1:A:315:PRO:HA	1.91	0.52
1:D:359:LYS:O	1:D:362:GLU:HB2	2.10	0.52
1:D:188:ARG:NH2	2:F:343:VAL:HG12	2.25	0.52
1:A:367:PRO:HA	6:D:509:HOH:O	2.09	0.51
1:D:203:LEU:HG	1:D:213:PRO:HB3	1.91	0.51
1:E:217:PRO:HB2	1:E:237:ILE:HD11	1.92	0.51
1:B:197:ASP:OD2	4:B:500:NAD:H1B	2.10	0.51
1:A:157:MET:HB2	1:A:167:PRO:HD3	1.92	0.51
1:D:307:ARG:HD3	6:D:523:HOH:O	2.11	0.51
1:A:128:SER:HB2	1:A:332:ASN:ND2	2.27	0.50
1:A:125:ARG:NH2	1:A:349:ASP:OD2	2.42	0.50
1:D:188:ARG:CD	1:E:188:ARG:O	2.58	0.50
2:C:280:ILE:HD12	2:C:430:ARG:HD2	1.92	0.50
1:D:111:LYS:HZ3	3:D:402:GOL:C3	2.25	0.49
1:E:154:PHE:HB3	1:E:156:PRO:HD2	1.94	0.49
1:E:114:VAL:CG1	1:E:358:MET:HG2	2.43	0.49
1:D:332:ASN:O	1:D:335:SER:HB3	2.12	0.49
1:D:236:ARG:CG	1:D:236:ARG:HH11	2.24	0.48
1:D:244:ASP:OD1	1:D:274:ARG:NH1	2.42	0.48
1:A:75:GLN:HB3	1:A:76:PRO:HD2	1.95	0.48
1:B:147:ALA:HB1	1:B:251:VAL:HG11	1.96	0.48
1:D:49:GLU:OE1	1:D:49:GLU:N	2.42	0.48
1:A:369:LYS:HD2	1:D:87:PRO:HG2	1.96	0.48
1:E:74:VAL:O	1:E:94:PHE:HB2	2.14	0.48
1:A:101:LEU:HD11	1:A:372:LEU:HD13	1.96	0.48
1:B:175:VAL:HG23	1:B:197:ASP:HB2	1.96	0.48
1:E:187:LYS:HE3	1:E:210:GLY:O	2.14	0.48
2:F:351:ASP:HB3	2:F:354:LYS:HD3	1.96	0.48
2:F:387:PRO:HA	2:F:392:TYR:CG	2.48	0.48
1:A:274:ARG:HD3	6:A:517:HOH:O	2.13	0.47
1:E:223:GLU:O	1:E:226:TYR:HB2	2.14	0.47
1:E:228:ARG:HH11	1:E:228:ARG:CB	2.27	0.47
1:E:114:VAL:HG12	1:E:358:MET:HG2	1.96	0.47
1:E:8:LYS:HG3	1:E:40:ALA:HA	1.96	0.47
2:F:337:MET:O	2:F:340:HIS:HB2	2.14	0.47
2:C:316:ALA:O	2:C:320:GLU:HG3	2.14	0.47
1:E:35:ARG:NH1	1:E:63:GLU:O	2.48	0.47
2:C:357:ASP:O	2:C:360:GLU:HG3	2.14	0.47
1:E:233:GLU:O	1:E:237:ILE:HG23	2.15	0.47
1:D:154:PHE:HB3	1:D:156:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ILE:HG23	1:D:193:VAL:HG11	1.97	0.46
2:F:328:PHE:HB2	2:F:355:LEU:HD12	1.97	0.46
1:A:311:PRO:HB2	1:A:314:LEU:HD13	1.96	0.46
1:B:218:ILE:O	1:B:238:GLN:NE2	2.48	0.46
1:D:111:LYS:HZ3	3:D:402:GOL:H32	1.81	0.46
1:A:175:VAL:HG12	1:A:175:VAL:O	2.15	0.46
1:B:199:ARG:NH2	4:B:500:NAD:O3B	2.37	0.46
2:F:282:VAL:HG12	2:F:432:LEU:HD21	1.98	0.46
1:E:302:GLU:OE2	1:E:305:GLY:HA2	2.16	0.46
2:F:430:ARG:HA	6:F:607:HOH:O	2.16	0.45
1:D:307:ARG:HH22	1:E:15:ARG:NH2	2.14	0.45
1:D:349:ASP:O	1:D:353:ARG:HG2	2.17	0.45
1:D:111:LYS:O	1:D:360:GLU:HA	2.16	0.45
2:F:410:ARG:NH2	5:F:500:NAP:O1X	2.35	0.45
1:E:124:THR:CG2	1:E:127:GLN:OE1	2.65	0.45
1:E:222:GLY:HA3	1:E:226:TYR:O	2.17	0.45
2:F:381:ASN:O	2:F:396:ILE:HD13	2.17	0.45
2:C:328:PHE:HB2	2:C:355:LEU:HD12	1.99	0.45
1:B:2:VAL:HA	1:B:69:HIS:HD2	1.80	0.45
1:E:103:LEU:HG	6:E:627:HOH:O	2.17	0.45
1:A:4:VAL:HG13	1:A:34:VAL:HG22	1.99	0.45
1:D:174:GLY:O	1:D:255:THR:OG1	2.34	0.45
1:A:369:LYS:HB3	1:D:87:PRO:HG2	1.98	0.45
3:A:401:GOL:H11	1:B:149:ARG:NH2	2.31	0.44
1:E:138:VAL:HG11	1:E:315:PRO:HA	1.99	0.44
2:C:280:ILE:HD12	2:C:430:ARG:CD	2.47	0.44
1:E:37:GLU:OE1	1:E:61:ARG:NH1	2.48	0.44
1:A:357:LEU:HD23	1:A:358:MET:HB2	1.99	0.44
3:D:401:GOL:H2	2:F:347:GLU:CA	2.41	0.44
1:A:124:THR:CG2	2:C:390:PRO:O	2.65	0.44
1:D:6:VAL:CG1	1:D:36:VAL:HG22	2.47	0.44
2:C:278:LYS:NZ	2:C:426:ALA:O	2.51	0.44
1:D:128:SER:HB2	1:D:332:ASN:ND2	2.32	0.44
2:C:362:ASN:CB	2:C:363:PRO:HD3	2.48	0.43
2:C:380:VAL:O	2:C:382:PRO:HD3	2.18	0.43
1:E:124:THR:HG1	1:E:127:GLN:CG	2.30	0.43
1:A:101:LEU:CD1	1:A:372:LEU:HD13	2.48	0.43
1:E:99:LYS:O	1:E:99:LYS:HG2	2.18	0.43
1:B:203:LEU:HG	1:B:213:PRO:HB3	1.99	0.43
1:B:52:GLN:HG2	1:B:58:VAL:HG23	2.01	0.43
1:D:77:PRO:HA	1:D:78:PRO:HD3	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:PRO:HB2	1:E:314:LEU:HD13	1.99	0.43
1:D:146:HIS:CE1	1:D:149:ARG:HH12	2.25	0.43
1:A:366:GLY:HA3	1:D:86:GLU:HG2	2.01	0.43
2:C:394:MET:CE	2:C:396:ILE:HD12	2.49	0.43
2:C:432:LEU:HD13	2:C:439:VAL:CG1	2.48	0.43
1:B:321:HIS:O	1:B:325:MET:HG3	2.19	0.43
2:C:311:LYS:HD3	2:C:311:LYS:HA	1.77	0.43
2:F:311:LYS:HG3	2:F:437:GLN:HG3	2.02	0.42
1:D:170:VAL:HG22	1:D:251:VAL:HB	2.00	0.42
1:D:131:ALA:O	1:D:135:GLN:HG2	2.19	0.42
1:B:284:LEU:HA	1:B:284:LEU:HD12	1.92	0.42
1:B:24:VAL:HG11	1:B:56:ALA:HB2	2.01	0.42
1:D:11:ALA:HA	1:D:12:PRO:HD3	1.93	0.42
1:D:324:GLU:O	1:D:328:LYS:HG3	2.19	0.42
1:D:320:VAL:HG23	1:E:152:PRO:HB2	2.01	0.42
2:F:380:VAL:CG1	2:F:399:VAL:HG11	2.49	0.42
1:E:52:GLN:HG3	1:E:58:VAL:HG23	2.00	0.42
2:F:423:LEU:O	2:F:429:THR:CG2	2.67	0.42
1:B:77:PRO:HA	1:B:78:PRO:HD3	1.93	0.42
2:C:362:ASN:HB2	2:C:363:PRO:HD3	2.02	0.42
2:F:278:LYS:NZ	2:F:426:ALA:O	2.38	0.42
2:C:358:LEU:N	2:C:358:LEU:HD23	2.35	0.41
1:E:187:LYS:HE2	6:E:640:HOH:O	2.19	0.41
1:E:223:GLU:C	1:E:225:GLY:N	2.73	0.41
1:B:194:PHE:CD1	1:B:194:PHE:N	2.87	0.41
1:A:153:ARG:HB3	1:B:321:HIS:CE1	2.55	0.41
2:C:319:LEU:HB3	2:C:324:VAL:HB	2.02	0.41
1:E:237:ILE:HG13	1:E:238:GLN:N	2.36	0.41
2:F:331:HIS:NE2	2:F:395:PRO:O	2.44	0.41
1:B:229:GLU:HB3	1:B:230:LEU:H	1.61	0.41
1:E:60:GLU:HG3	6:E:615:HOH:O	2.21	0.41
2:F:381:ASN:HA	2:F:382:PRO:HD3	1.87	0.41
1:A:170:VAL:HG22	1:A:251:VAL:HB	2.03	0.41
1:D:300:VAL:HG22	1:D:309:TYR:CD1	2.55	0.41
1:D:314:LEU:HA	1:D:314:LEU:HD12	1.87	0.41
1:E:326:TYR:CE2	1:E:330:LEU:HD11	2.54	0.41
1:E:24:VAL:HG11	1:E:56:ALA:HB2	2.03	0.41
1:D:307:ARG:NH2	1:E:45:TYR:OH	2.54	0.41
1:B:52:GLN:CG	1:B:58:VAL:HG23	2.50	0.41
1:E:258:VAL:HA	1:E:259:PRO:HD3	1.92	0.41
1:A:240:GLU:HG2	1:A:243:ARG:NH2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:VAL:HA	1:D:7:PRO:HD3	1.96	0.40
1:E:131:ALA:O	1:E:135:GLN:HG2	2.22	0.40
1:E:203:LEU:HG	1:E:213:PRO:HB3	2.03	0.40
1:E:328:LYS:CD	6:E:620:HOH:O	2.69	0.40
2:F:311:LYS:HD3	2:F:311:LYS:HA	1.94	0.40
2:C:283:GLU:O	2:C:287:VAL:HG23	2.22	0.40
1:D:149:ARG:HH11	1:D:149:ARG:HD3	1.70	0.40
1:D:171:MET:HB2	1:D:249:MET:HG3	2.04	0.40
1:D:153:ARG:HB3	1:E:321:HIS:CE1	2.56	0.40
2:F:380:VAL:HG12	2:F:399:VAL:CG1	2.52	0.40
1:A:152:PRO:HB2	1:B:320:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/381 (96%)	355 (97%)	10 (3%)	0	100	100
1	B	363/381 (95%)	355 (98%)	8 (2%)	0	100	100
1	D	370/381 (97%)	358 (97%)	12 (3%)	0	100	100
1	E	371/381 (97%)	355 (96%)	14 (4%)	2 (0%)	29	39
2	C	175/185 (95%)	168 (96%)	7 (4%)	0	100	100
2	F	175/185 (95%)	172 (98%)	3 (2%)	0	100	100
All	All	1819/1894 (96%)	1763 (97%)	54 (3%)	2 (0%)	51	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	225	GLY
1	E	224	GLY

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	285/293 (97%)	251 (88%)	34 (12%)	5	6
1	B	286/293 (98%)	260 (91%)	26 (9%)	9	12
1	D	287/293 (98%)	253 (88%)	34 (12%)	5	6
1	E	287/293 (98%)	253 (88%)	34 (12%)	5	6
2	C	139/146 (95%)	128 (92%)	11 (8%)	12	17
2	F	139/146 (95%)	124 (89%)	15 (11%)	6	8
All	All	1423/1464 (97%)	1269 (89%)	154 (11%)	6	8

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	VAL
1	A	6	VAL
1	A	26	ARG
1	A	60	GLU
1	A	65	LEU
1	A	66	LYS
1	A	99	LYS
1	A	102	GLU
1	A	114	VAL
1	A	122	ARG
1	A	124	THR
1	A	149	ARG
1	A	158	LEU
1	A	203	LEU
1	A	212	LYS
1	A	215	GLU
1	A	219	SER
1	A	228	ARG
1	A	230	LEU
1	A	232	GLU
1	A	261	ARG

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Mol	Chain	Res	Type
1	A	262	ARG
1	A	284	LEU
1	A	303	VAL
1	A	314	LEU
1	A	333	LEU
1	A	336	LEU
1	A	348	GLU
1	A	357	LEU
1	A	360	GLU
1	A	364	LEU
1	A	369	LYS
1	A	372	LEU
1	B	38	ARG
1	B	71	LEU
1	B	108	GLN
1	B	111	LYS
1	B	114	VAL
1	B	124	THR
1	B	142	LEU
1	B	149	ARG
1	B	160	THR
1	B	203	LEU
1	B	216	LEU
1	B	218	ILE
1	B	230	LEU
1	B	233	GLU
1	B	261	ARG
1	B	262	ARG
1	B	284	LEU
1	B	307	ARG
1	B	314	LEU
1	B	316	SER
1	B	318	LEU
1	B	333	LEU
1	B	336	LEU
1	B	339	GLU
1	B	350	GLU
1	B	372	LEU
2	C	277	LEU
2	C	280	ILE
2	C	282	VAL
2	C	283	GLU

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Mol	Chain	Res	Type
2	C	325	GLU
2	C	354	LYS
2	C	427	GLU
2	C	430	ARG
2	C	432	LEU
2	C	437	GLN
2	C	443	LEU
1	D	1	MET
1	D	3	THR
1	D	4	VAL
1	D	6	VAL
1	D	15	ARG
1	D	60	GLU
1	D	71	LEU
1	D	96	GLN
1	D	99	LYS
1	D	108	GLN
1	D	111	LYS
1	D	122	ARG
1	D	124	THR
1	D	149	ARG
1	D	188	ARG
1	D	200	LYS
1	D	203	LEU
1	D	207	LEU
1	D	215	GLU
1	D	219	SER
1	D	228	ARG
1	D	232	GLU
1	D	236	ARG
1	D	262	ARG
1	D	269	GLU
1	D	303	VAL
1	D	314	LEU
1	D	333	LEU
1	D	336	LEU
1	D	348	GLU
1	D	362	GLU
1	D	364	LEU
1	D	371	LEU
1	D	372	LEU
1	E	10	ARG

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Mol	Chain	Res	Type
1	E	49	GLU
1	E	66	LYS
1	E	71	LEU
1	E	86	GLU
1	E	96	GLN
1	E	98	HIS
1	E	110	LYS
1	E	114	VAL
1	E	122	ARG
1	E	124	THR
1	E	125	ARG
1	E	127	GLN
1	E	133	SER
1	E	142	LEU
1	E	203	LEU
1	E	208	SER
1	E	212	LYS
1	E	215	GLU
1	E	218	ILE
1	E	228	ARG
1	E	229	GLU
1	E	230	LEU
1	E	231	THR
1	E	237	ILE
1	E	262	ARG
1	E	303	VAL
1	E	304	ARG
1	E	314	LEU
1	E	316	SER
1	E	333	LEU
1	E	336	LEU
1	E	339	GLU
1	E	371	LEU
2	F	277	LEU
2	F	280	ILE
2	F	282	VAL
2	F	283	GLU
2	F	320	GLU
2	F	325	GLU
2	F	355	LEU
2	F	358	LEU
2	F	360	GLU

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Mol	Chain	Res	Type
2	F	361	ILE
2	F	396	ILE
2	F	399	VAL
2	F	429	THR
2	F	430	ARG
2	F	432	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	HIS
1	E	98	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
3	GOL	A	401	-	5,5,5	0.59	0	5,5,5	1.32	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAP	C	500	-	45,52,52	1.59	6 (13%)	56,80,80	2.00	12 (21%)
5	NAP	F	500	-	45,52,52	1.45	9 (20%)	56,80,80	2.15	12 (21%)
3	GOL	D	401	-	5,5,5	0.52	0	5,5,5	0.92	0
3	GOL	D	402	-	5,5,5	0.48	0	5,5,5	0.85	0
4	NAD	E	500	-	42,48,48	1.35	5 (11%)	50,73,73	2.12	12 (24%)
4	NAD	B	500	-	42,48,48	1.31	5 (11%)	50,73,73	1.46	10 (20%)
3	GOL	D	403	-	5,5,5	0.38	0	5,5,5	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	401	-	-	2/4/4/4	-
5	NAP	C	500	-	-	6/31/67/67	0/5/5/5
5	NAP	F	500	-	-	9/31/67/67	0/5/5/5
3	GOL	D	401	-	-	0/4/4/4	-
3	GOL	D	402	-	-	4/4/4/4	-
4	NAD	E	500	-	-	10/26/62/62	0/5/5/5
4	NAD	B	500	-	-	14/26/62/62	0/5/5/5
3	GOL	D	403	-	-	0/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	500	NAP	P2B-O1X	4.94	1.66	1.50
4	E	500	NAD	PA-O1A	4.56	1.67	1.50
5	C	500	NAP	PA-O1A	4.54	1.67	1.50
5	C	500	NAP	PN-O1N	4.06	1.65	1.50
4	B	500	NAD	PN-O1N	4.05	1.65	1.50
4	E	500	NAD	PN-O1N	4.05	1.65	1.50
4	B	500	NAD	PA-O1A	3.96	1.65	1.50
5	F	500	NAP	PN-O1N	3.95	1.64	1.50
5	F	500	NAP	P2B-O1X	3.72	1.62	1.50
5	F	500	NAP	PA-O1A	3.51	1.63	1.50
5	C	500	NAP	P2B-O2B	3.31	1.65	1.59
4	B	500	NAD	O4D-C1D	2.68	1.44	1.41
5	F	500	NAP	P2B-O2X	2.54	1.64	1.54
5	C	500	NAP	P2B-O2X	2.52	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	500	NAD	PA-O2A	2.51	1.67	1.55
5	C	500	NAP	P2B-O3X	2.48	1.64	1.54
4	E	500	NAD	O4D-C1D	2.43	1.44	1.41
4	B	500	NAD	PN-O2N	2.28	1.66	1.55
4	E	500	NAD	PN-O2N	2.25	1.65	1.55
5	F	500	NAP	O4D-C1D	2.24	1.44	1.41
4	B	500	NAD	PA-O2A	2.17	1.65	1.55
5	F	500	NAP	P2B-O2B	2.17	1.63	1.59
5	F	500	NAP	C2A-N3A	2.11	1.35	1.32
5	F	500	NAP	C4N-C3N	2.10	1.42	1.39
5	F	500	NAP	P2B-O3X	2.02	1.62	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	500	NAD	O5B-PA-O1A	-9.10	73.53	109.07
5	C	500	NAP	C3N-C7N-N7N	7.19	126.38	117.75
5	F	500	NAP	C3N-C7N-N7N	6.91	126.05	117.75
5	C	500	NAP	N3A-C2A-N1A	-6.76	118.11	128.68
5	F	500	NAP	N3A-C2A-N1A	-6.22	118.96	128.68
5	F	500	NAP	C6N-N1N-C2N	-5.11	117.32	121.97
5	F	500	NAP	O3B-C3B-C4B	-5.02	96.53	111.05
4	E	500	NAD	PN-O3-PA	-4.95	115.85	132.83
5	F	500	NAP	O4D-C1D-C2D	-4.80	99.90	106.93
4	E	500	NAD	N3A-C2A-N1A	-4.41	121.78	128.68
4	B	500	NAD	N3A-C2A-N1A	-4.12	122.24	128.68
5	F	500	NAP	O7N-C7N-C3N	-3.79	115.10	119.63
5	C	500	NAP	O7N-C7N-C3N	-3.67	115.23	119.63
5	C	500	NAP	O3B-C3B-C4B	-3.66	100.46	111.05
4	E	500	NAD	O2A-PA-O5B	-3.58	91.12	107.75
5	C	500	NAP	O3D-C3D-C4D	-3.53	100.85	111.05
4	B	500	NAD	O4D-C4D-C3D	-3.50	98.19	105.11
5	C	500	NAP	O7N-C7N-N7N	-2.99	118.33	122.58
4	E	500	NAD	O4B-C4B-C5B	-2.98	99.56	109.37
5	C	500	NAP	O4B-C4B-C3B	-2.96	99.25	105.11
4	E	500	NAD	C5D-C4D-C3D	-2.95	104.13	115.18
4	E	500	NAD	PA-O5B-C5B	-2.94	104.43	121.68
4	B	500	NAD	PN-O3-PA	-2.86	123.01	132.83
4	E	500	NAD	C6N-N1N-C2N	-2.79	119.43	121.97
5	F	500	NAP	O3D-C3D-C4D	-2.79	102.98	111.05
4	B	500	NAD	O4D-C4D-C5D	2.77	118.48	109.37
4	B	500	NAD	O4B-C4B-C5B	-2.69	100.51	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	500	NAP	O7N-C7N-N7N	-2.67	118.78	122.58
4	E	500	NAD	O2A-PA-O1A	2.51	124.67	112.24
4	E	500	NAD	C3D-C2D-C1D	2.47	104.69	100.98
5	C	500	NAP	O4B-C1B-C2B	-2.46	102.32	106.59
4	E	500	NAD	C4A-C5A-N7A	-2.43	106.87	109.40
4	B	500	NAD	C4A-C5A-N7A	-2.42	106.88	109.40
5	F	500	NAP	C5N-C6N-N1N	2.40	123.84	120.40
3	A	401	GOL	O2-C2-C1	-2.40	98.56	109.12
4	B	500	NAD	C2D-C3D-C4D	-2.31	98.16	102.64
5	C	500	NAP	O4D-C1D-C2D	-2.25	103.64	106.93
4	E	500	NAD	C5N-C4N-C3N	-2.25	117.68	120.34
4	B	500	NAD	C5N-C4N-C3N	-2.25	117.68	120.34
5	C	500	NAP	C1B-N9A-C4A	-2.24	122.71	126.64
5	F	500	NAP	O2D-C2D-C3D	-2.20	104.70	111.82
4	B	500	NAD	C6N-N1N-C2N	-2.19	119.98	121.97
5	C	500	NAP	C2A-N1A-C6A	2.19	122.50	118.75
4	B	500	NAD	C2B-C3B-C4B	2.13	106.78	102.64
5	F	500	NAP	C4A-C5A-N7A	-2.13	107.18	109.40
5	C	500	NAP	C2B-C3B-C4B	2.12	106.61	101.99
5	F	500	NAP	C5N-C4N-C3N	-2.02	117.95	120.34

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	500	NAP	O4D-C1D-N1N-C2N
5	F	500	NAP	O4D-C1D-N1N-C2N
5	F	500	NAP	O4D-C1D-N1N-C6N
5	F	500	NAP	C2D-C1D-N1N-C2N
5	F	500	NAP	C2D-C1D-N1N-C6N
3	D	402	GOL	O1-C1-C2-C3
4	E	500	NAD	C5B-O5B-PA-O1A
4	E	500	NAD	C5B-O5B-PA-O2A
4	E	500	NAD	O4D-C1D-N1N-C6N
4	E	500	NAD	C2N-C3N-C7N-O7N
4	E	500	NAD	C2N-C3N-C7N-N7N
4	B	500	NAD	C5D-O5D-PN-O3
4	B	500	NAD	C5D-O5D-PN-O1N
4	E	500	NAD	C4N-C3N-C7N-O7N
4	E	500	NAD	C4N-C3N-C7N-N7N
5	F	500	NAP	O4B-C4B-C5B-O5B
5	F	500	NAP	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	B	500	NAD	O4B-C4B-C5B-O5B
4	B	500	NAD	C3B-C4B-C5B-O5B
3	A	401	GOL	C1-C2-C3-O3
3	D	402	GOL	C1-C2-C3-O3
3	D	402	GOL	O2-C2-C3-O3
4	B	500	NAD	C3D-C4D-C5D-O5D
4	B	500	NAD	C2N-C3N-C7N-O7N
4	B	500	NAD	C2N-C3N-C7N-N7N
3	D	402	GOL	O1-C1-C2-O2
4	E	500	NAD	PN-O3-PA-O1A
4	B	500	NAD	C4N-C3N-C7N-O7N
4	B	500	NAD	C4N-C3N-C7N-N7N
4	B	500	NAD	C4D-C5D-O5D-PN
5	C	500	NAP	PA-O3-PN-O5D
4	E	500	NAD	C4B-C5B-O5B-PA
5	C	500	NAP	C5B-O5B-PA-O3
4	E	500	NAD	O4D-C4D-C5D-O5D
5	F	500	NAP	PN-O3-PA-O1A
4	B	500	NAD	C5D-O5D-PN-O2N
4	B	500	NAD	O4D-C4D-C5D-O5D
3	A	401	GOL	O2-C2-C3-O3
4	B	500	NAD	PA-O3-PN-O1N
4	B	500	NAD	PA-O3-PN-O2N
5	C	500	NAP	C2D-C1D-N1N-C6N
5	C	500	NAP	O4D-C4D-C5D-O5D
5	F	500	NAP	PN-O3-PA-O2A
5	C	500	NAP	O4B-C4B-C5B-O5B
5	F	500	NAP	O4D-C4D-C5D-O5D

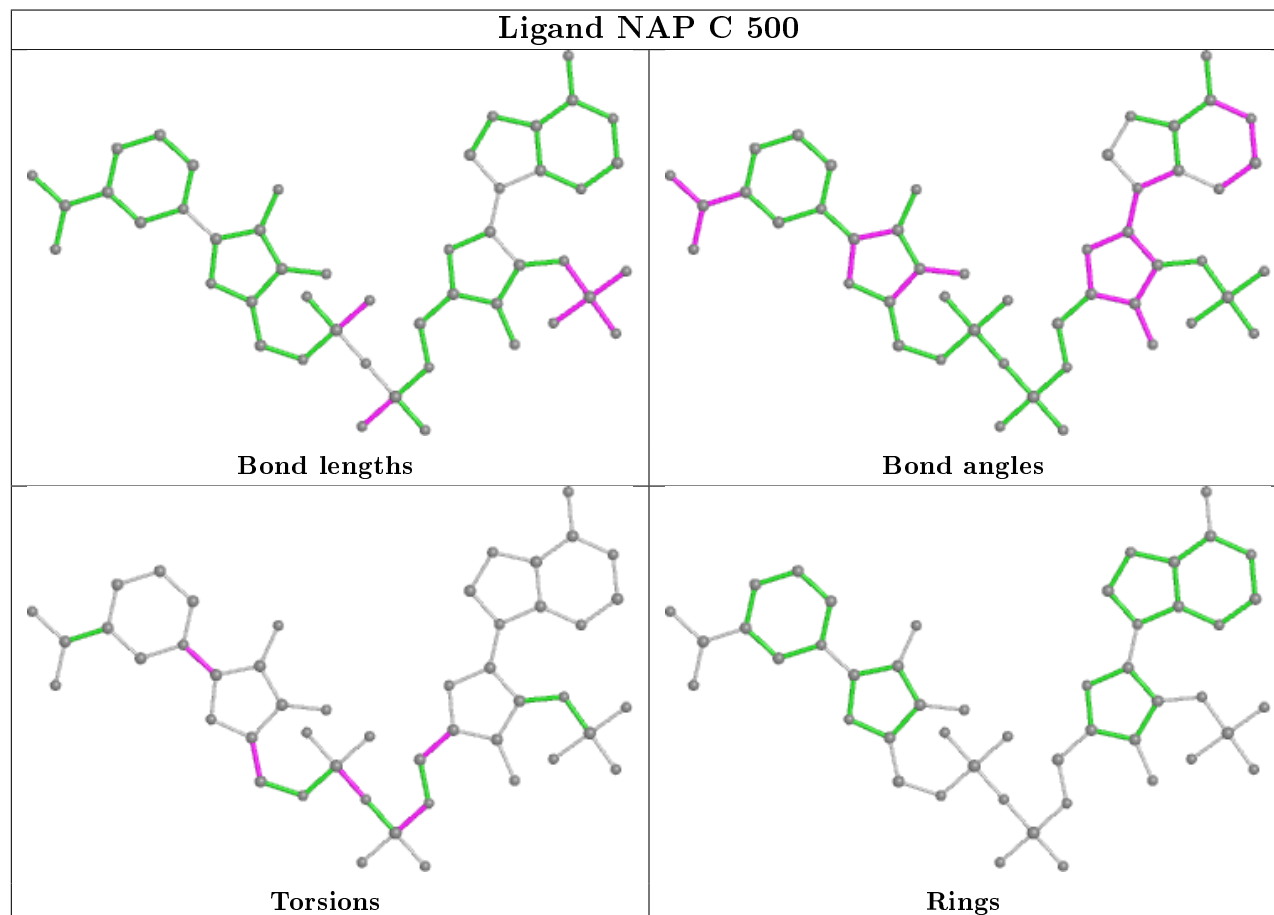
There are no ring outliers.

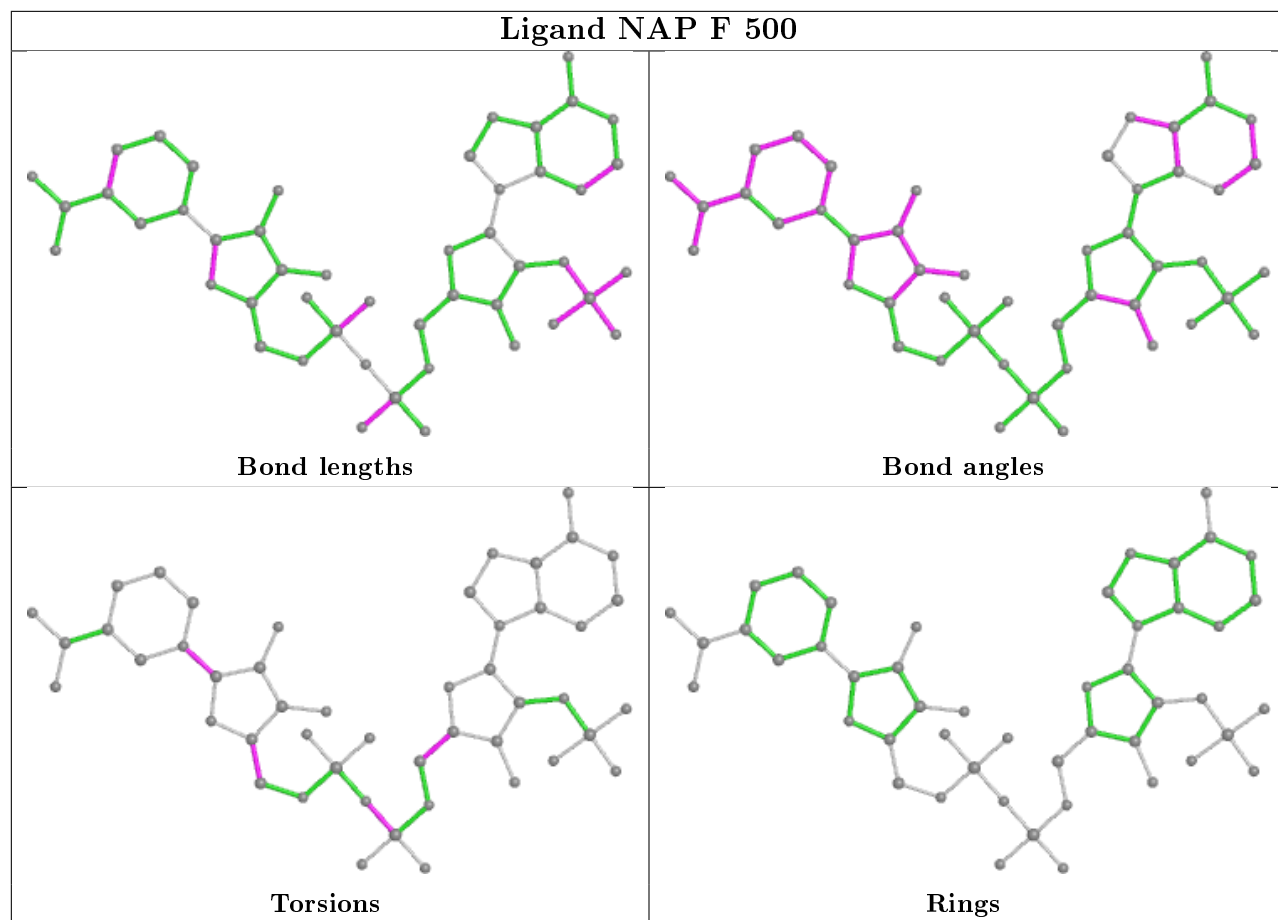
6 monomers are involved in 32 short contacts:

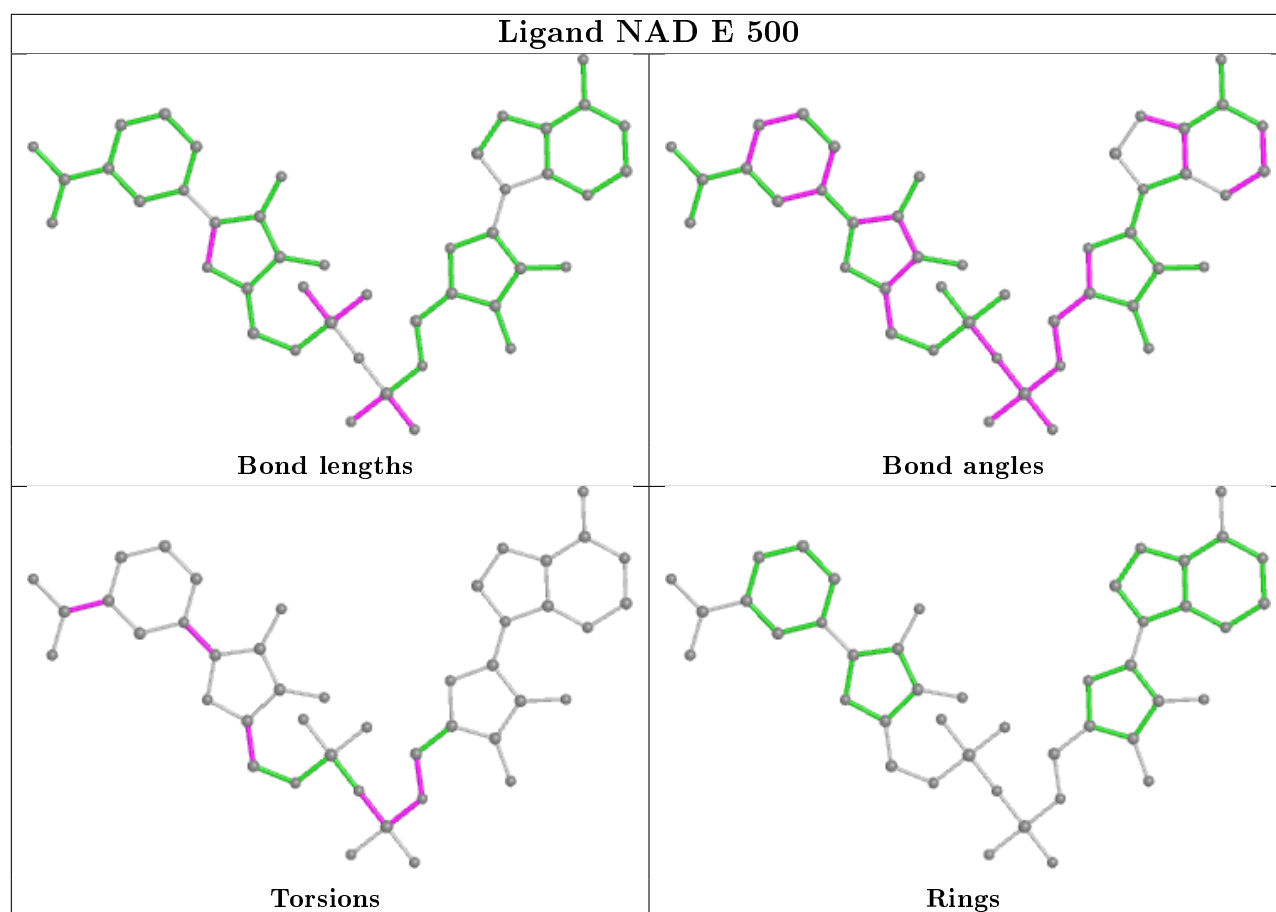
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GOL	7	0
5	F	500	NAP	1	0
3	D	401	GOL	11	0
3	D	402	GOL	5	0
4	E	500	NAD	5	0
4	B	500	NAD	3	0

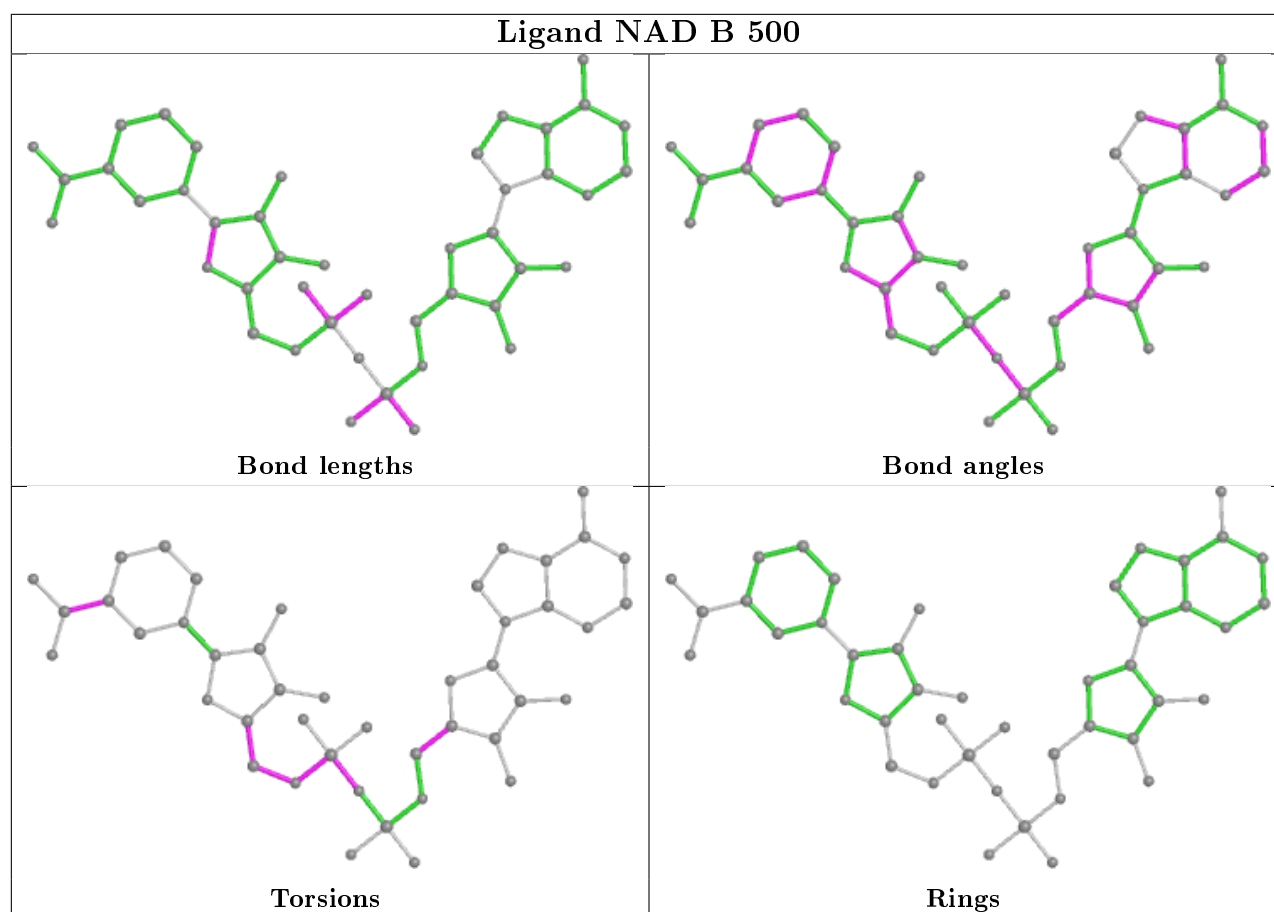
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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	369/381 (96%)	0.20	8 (2%) 62 63	21, 35, 50, 70	0
1	B	367/381 (96%)	0.16	8 (2%) 62 63	21, 40, 59, 70	0
1	D	372/381 (97%)	0.12	6 (1%) 72 73	18, 35, 55, 69	0
1	E	373/381 (97%)	0.32	16 (4%) 35 38	20, 43, 72, 88	0
2	C	177/185 (95%)	0.12	5 (2%) 53 55	25, 44, 60, 70	0
2	F	177/185 (95%)	0.10	2 (1%) 80 81	21, 38, 53, 63	0
All	All	1835/1894 (96%)	0.18	45 (2%) 57 59	18, 38, 59, 88	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	220	ALA	7.5
1	A	219	SER	6.8
1	E	218	ILE	5.4
2	F	274	LYS	5.2
1	A	220	ALA	5.1
1	E	217	PRO	4.2
1	A	218	ILE	3.8
2	C	275	GLY	3.8
1	A	228	ARG	3.5
1	D	371	LEU	3.5
1	E	215	GLU	3.4
1	E	219	SER	3.4
1	B	218	ILE	3.2
1	E	124	THR	3.2
1	A	-1	HIS	3.1
1	E	230	LEU	3.1
1	B	-2	HIS	2.8
2	C	274	LYS	2.7
2	C	387	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	362	GLU	2.7
1	B	371	LEU	2.6
1	B	219	SER	2.6
1	B	229	GLU	2.5
1	E	123	ILE	2.5
1	B	230	LEU	2.5
1	E	189	LEU	2.5
1	B	236	ARG	2.4
1	D	108	GLN	2.4
1	A	33	ARG	2.3
1	A	98	HIS	2.3
2	C	425	TYR	2.3
1	A	215	GLU	2.3
2	F	392	TYR	2.3
1	B	237	ILE	2.2
1	D	230	LEU	2.2
1	E	371	LEU	2.2
1	D	236	ARG	2.1
1	E	49	GLU	2.1
1	E	231	THR	2.1
1	E	200	LYS	2.1
1	E	348	GLU	2.1
1	D	148	ALA	2.1
1	D	370	ALA	2.1
1	E	198	VAL	2.1
2	C	391	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

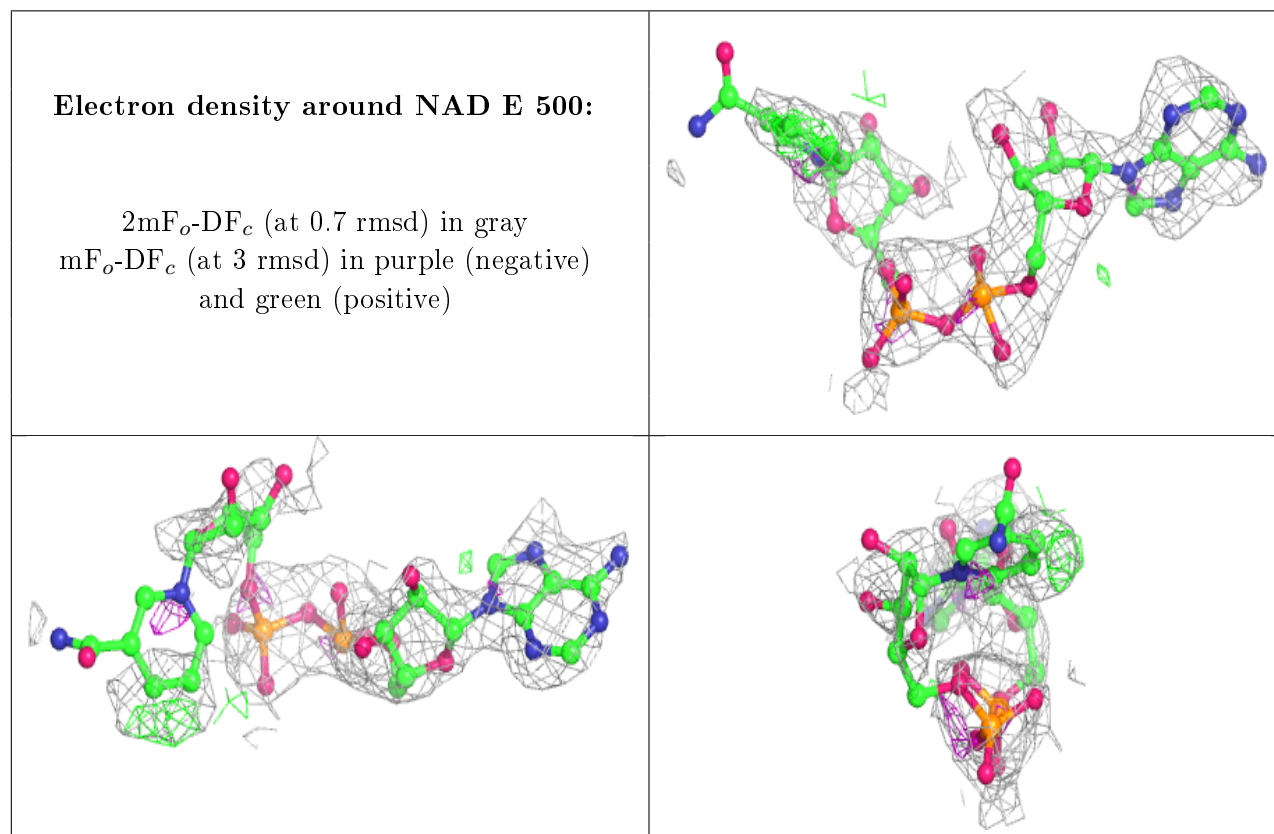
There are no carbohydrates in this entry.

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.

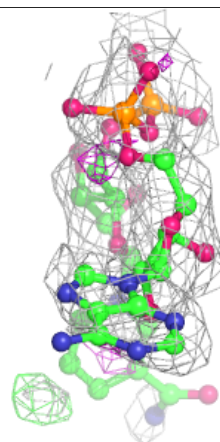
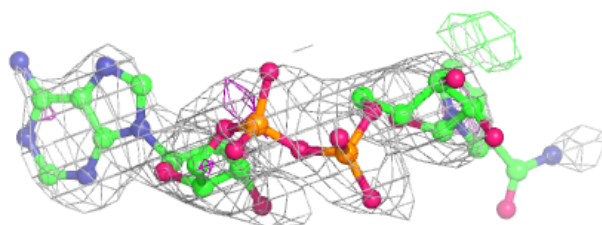
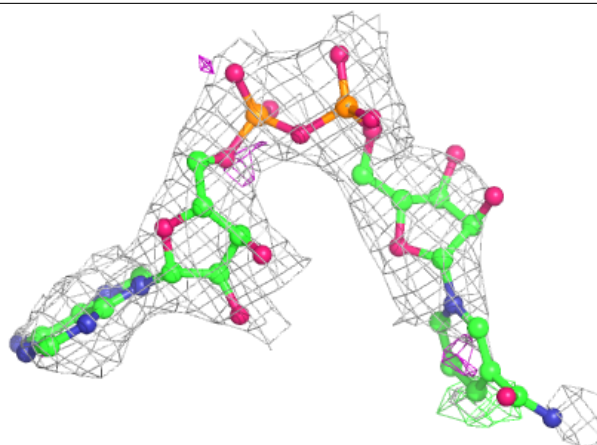
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAD	E	500	44/44	0.73	0.30	72,83,102,103	0
3	GOL	D	403	6/6	0.76	0.41	36,38,38,38	0
3	GOL	D	402	6/6	0.77	0.33	33,34,39,41	0
3	GOL	D	401	6/6	0.79	0.23	33,35,35,36	0
4	NAD	B	500	44/44	0.82	0.27	58,71,91,92	0
3	GOL	A	401	6/6	0.88	0.28	30,32,33,37	0
5	NAP	F	500	48/48	0.96	0.13	19,27,32,35	0
5	NAP	C	500	48/48	0.96	0.11	25,32,36,39	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.

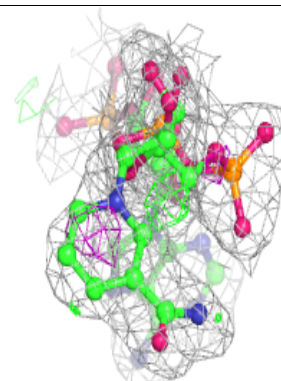
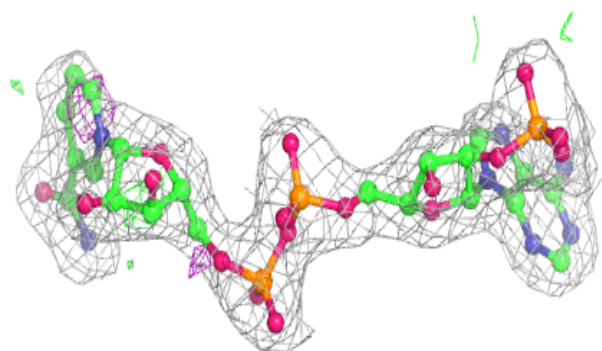
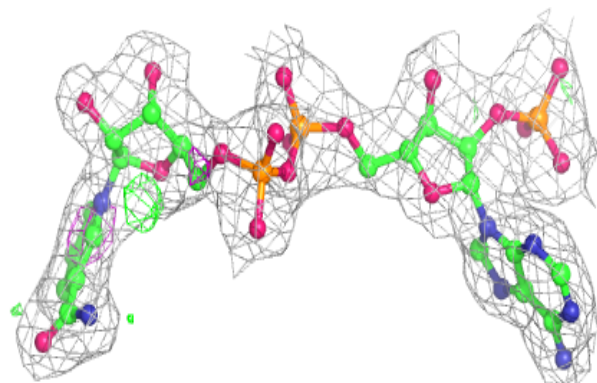


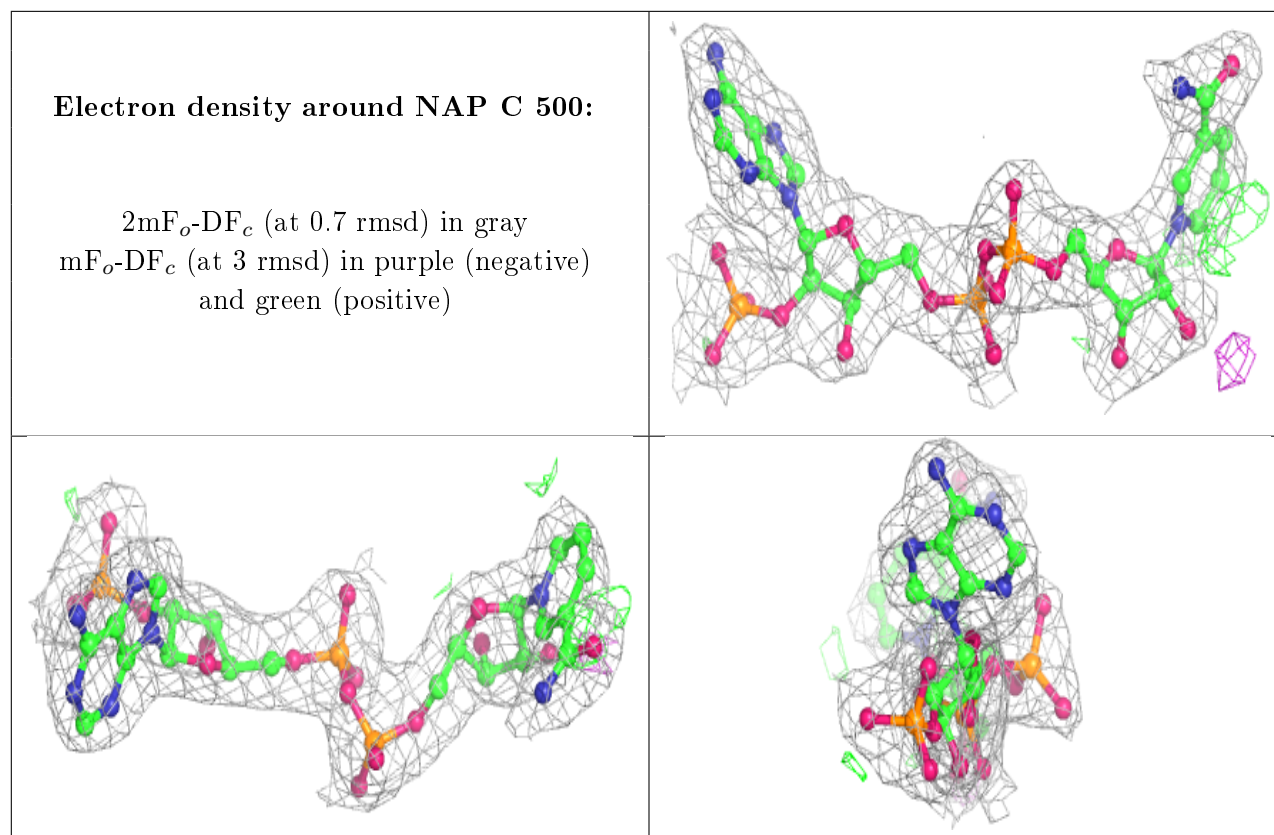
Electron density around NAD B 500:

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

**Electron density around NAP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.