



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2025 – 09:55 PM JST

PDB ID : 8YSW
Title : phosphinothricin dehydrogenase
Authors : Xue, Y.P.; Cheng, F.; Zhou, S.P.; Xu, J.M.; Jin, L.Q.; Ma, C.J.; Zheng, Y.G.
Deposited on : 2024-03-23
Resolution : 2.61 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

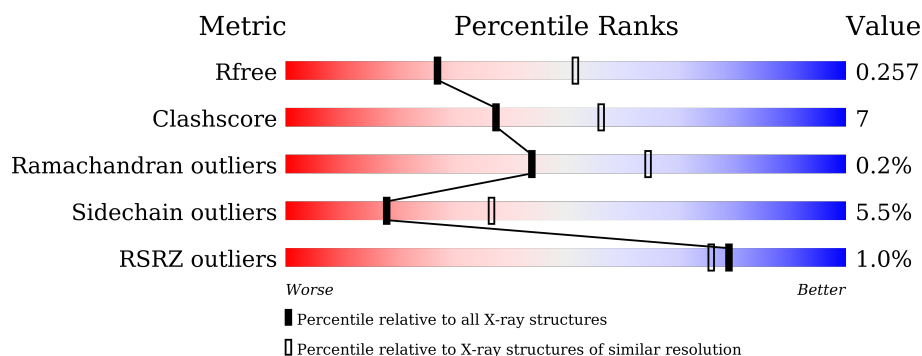
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	164625	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (2.64-2.60)

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	415	
1	B	415	
1	C	415	
1	D	415	
1	E	415	
1	F	415	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18918 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3212	2028	545	619	20			
1	B	410	Total	C	N	O	S	0	0	0
			3173	2005	539	609	20			
1	C	410	Total	C	N	O	S	0	0	0
			3173	2005	539	609	20			
1	D	304	Total	C	N	O	S	0	0	0
			2366	1498	401	449	18			
1	E	413	Total	C	N	O	S	0	0	0
			3195	2017	543	615	20			
1	F	410	Total	C	N	O	S	0	0	0
			3173	2005	539	609	20			

There are 36 discrepancies between the modelled and reference sequences:

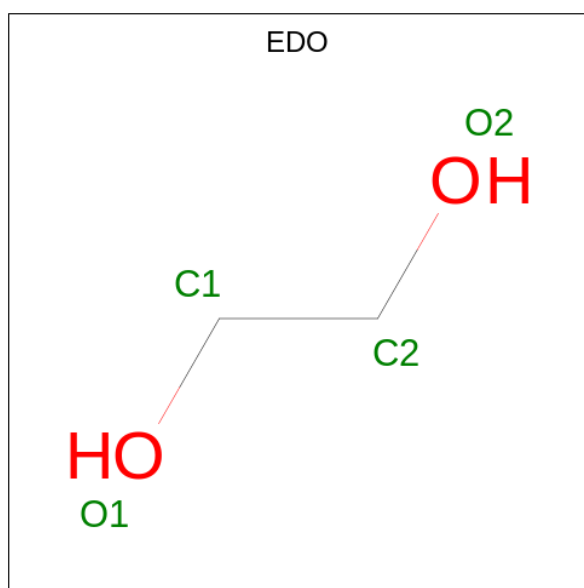
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLY	ALA	conflict	UNP A0A3N9UCW8
A	141	MET	VAL	conflict	UNP A0A3N9UCW8
A	339	ALA	VAL	conflict	UNP A0A3N9UCW8
A	369	TYR	VAL	conflict	UNP A0A3N9UCW8
A	409	LEU	-	expression tag	UNP A0A3N9UCW8
A	410	GLU	-	expression tag	UNP A0A3N9UCW8
B	138	GLY	ALA	conflict	UNP A0A3N9UCW8
B	141	MET	VAL	conflict	UNP A0A3N9UCW8
B	339	ALA	VAL	conflict	UNP A0A3N9UCW8
B	369	TYR	VAL	conflict	UNP A0A3N9UCW8
B	409	LEU	-	expression tag	UNP A0A3N9UCW8
B	410	GLU	-	expression tag	UNP A0A3N9UCW8
C	138	GLY	ALA	conflict	UNP A0A3N9UCW8
C	141	MET	VAL	conflict	UNP A0A3N9UCW8
C	339	ALA	VAL	conflict	UNP A0A3N9UCW8
C	369	TYR	VAL	conflict	UNP A0A3N9UCW8
C	409	LEU	-	expression tag	UNP A0A3N9UCW8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	410	GLU	-	expression tag	UNP A0A3N9UCW8
D	138	GLY	ALA	conflict	UNP A0A3N9UCW8
D	141	MET	VAL	conflict	UNP A0A3N9UCW8
D	339	ALA	VAL	conflict	UNP A0A3N9UCW8
D	369	TYR	VAL	conflict	UNP A0A3N9UCW8
D	409	LEU	-	expression tag	UNP A0A3N9UCW8
D	410	GLU	-	expression tag	UNP A0A3N9UCW8
E	138	GLY	ALA	conflict	UNP A0A3N9UCW8
E	141	MET	VAL	conflict	UNP A0A3N9UCW8
E	339	ALA	VAL	conflict	UNP A0A3N9UCW8
E	369	TYR	VAL	conflict	UNP A0A3N9UCW8
E	409	LEU	-	expression tag	UNP A0A3N9UCW8
E	410	GLU	-	expression tag	UNP A0A3N9UCW8
F	138	GLY	ALA	conflict	UNP A0A3N9UCW8
F	141	MET	VAL	conflict	UNP A0A3N9UCW8
F	339	ALA	VAL	conflict	UNP A0A3N9UCW8
F	369	TYR	VAL	conflict	UNP A0A3N9UCW8
F	409	LEU	-	expression tag	UNP A0A3N9UCW8
F	410	GLU	-	expression tag	UNP A0A3N9UCW8

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0

- # NAD

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



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

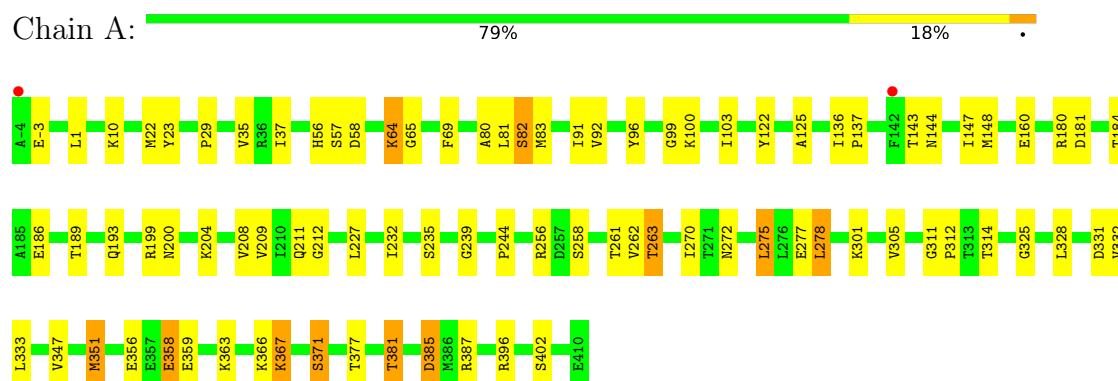
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	71	Total	O	0	0
			71	71		
4	C	56	Total	O	0	0
			56	56		
4	D	58	Total	O	0	0
			58	58		
4	E	60	Total	O	0	0
			60	60		
4	F	63	Total	O	0	0
			63	63		

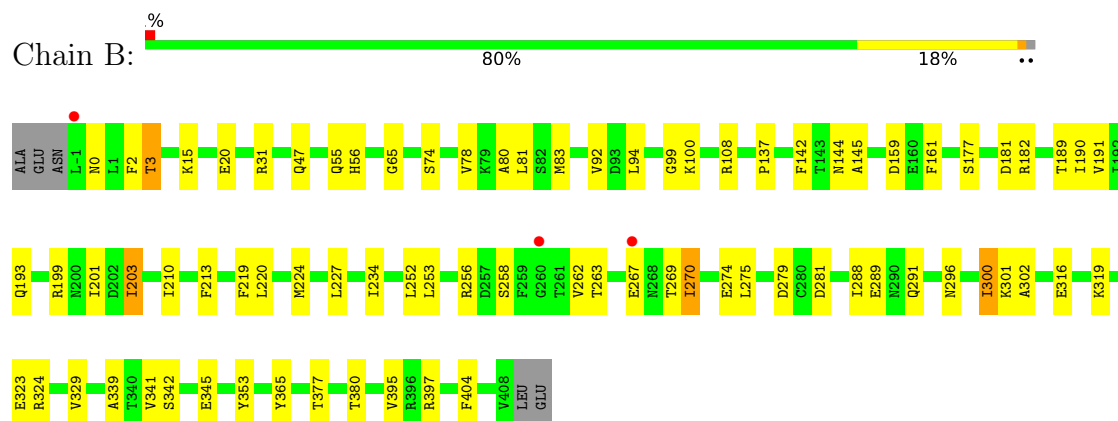
3 Residue-property plots [i](#)

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.

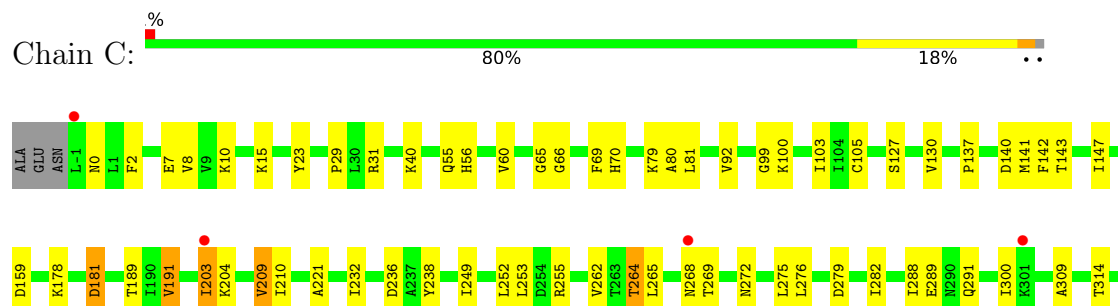
• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase

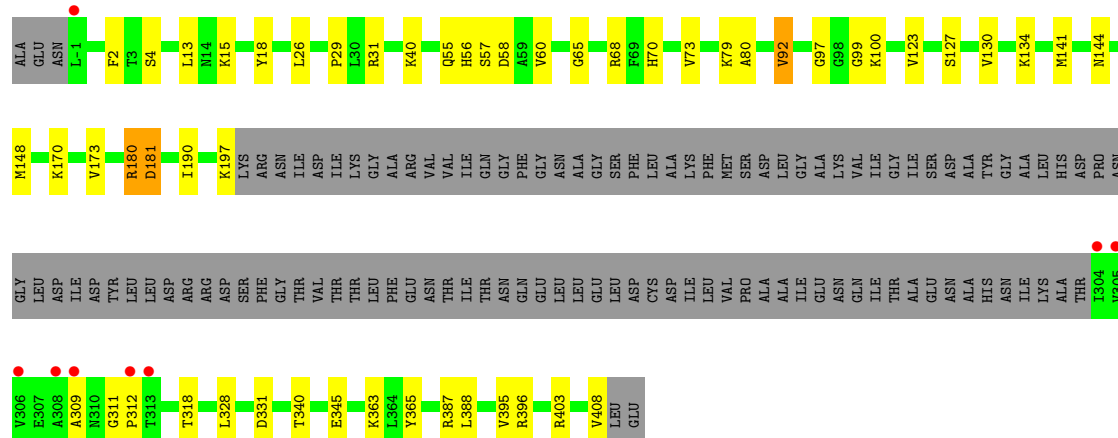


• Molecule 1: Glutamate dehydrogenase

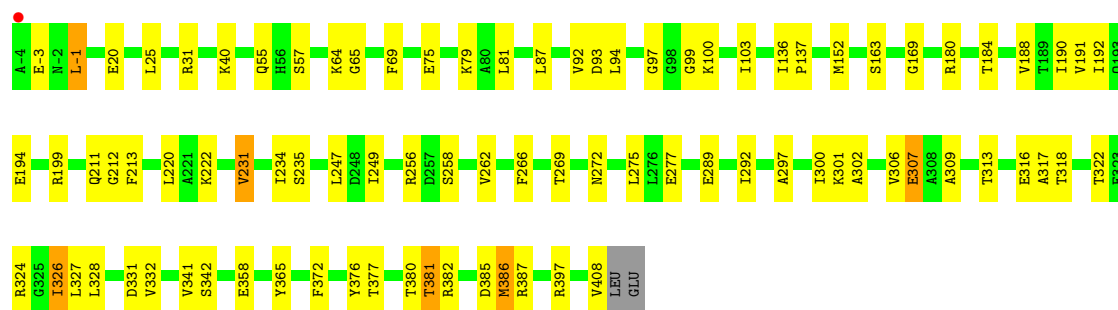
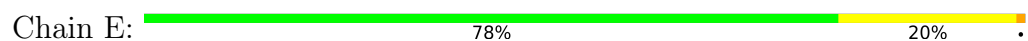




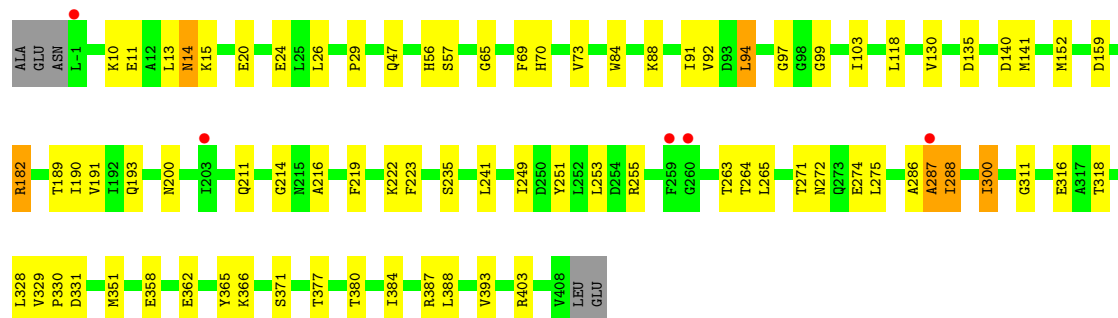
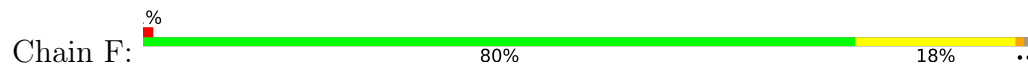
• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.67Å 129.07Å 219.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 2.61 48.36 – 2.61	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.36-2.61) 100.0 (48.36-2.61)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.192 , 0.257 0.193 , 0.257	Depositor DCC
R_{free} test set	3956 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18918	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 2.88% 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: EDO, 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	0.44	0/3269	0.62	0/4422
1	B	0.42	0/3230	0.62	1/4369 (0.0%)
1	C	0.42	0/3230	0.62	1/4369 (0.0%)
1	D	0.42	0/2411	0.59	0/3257
1	E	0.44	0/3252	0.62	0/4399
1	F	0.42	0/3230	0.62	0/4369
All	All	0.43	0/18622	0.62	2/25185 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	LEU	CA-CB-CG	5.78	128.59	115.30
1	B	275	LEU	CA-CB-CG	5.70	128.41	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	267	GLU	Peptide

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	3212	0	3201	47	0
1	B	3173	0	3167	40	0
1	C	3173	0	3167	49	0
1	D	2366	0	2364	33	0
1	E	3195	0	3184	50	0
1	F	3173	0	3166	45	0
2	A	12	0	18	1	0
2	B	8	0	12	0	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
2	F	8	0	12	1	0
3	A	44	0	26	1	0
3	B	44	0	26	0	0
3	C	44	0	26	3	0
3	E	44	0	26	2	0
3	F	44	0	25	3	0
4	A	62	0	0	0	0
4	B	71	0	0	1	0
4	C	56	0	0	4	0
4	D	58	0	0	2	0
4	E	60	0	0	2	0
4	F	63	0	0	1	0
All	All	18918	0	18432	256	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 7.

All (256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG21	1:A:125:ALA:HB1	1.53	0.88
1:B:191:VAL:HG11	1:B:329:VAL:HG11	1.60	0.83
1:D:18:TYR:OH	1:D:396:ARG:NH2	2.15	0.79
1:C:300:ILE:HD11	1:C:321:LEU:HD21	1.65	0.79
1:C:268:ASN:OD1	1:D:396:ARG:NH1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ASP:OD2	1:C:255:ARG:NH2	2.17	0.77
1:F:318:THR:HG23	1:F:328:LEU:HD23	1.67	0.77
1:E:307:GLU:OE2	1:E:387:ARG:NH2	2.19	0.75
1:B:300:ILE:O	1:B:324:ARG:NH2	2.20	0.73
1:A:91:ILE:HD12	1:A:332:VAL:HG12	1.74	0.70
1:F:287:ALA:HB2	3:F:503:NAD:H52N	1.73	0.69
1:B:144:ASN:HB2	1:C:264:THR:HG21	1.73	0.69
1:F:15:LYS:HD2	1:F:388:LEU:HD21	1.74	0.68
1:F:15:LYS:HE3	1:F:384:ILE:HG21	1.78	0.65
1:B:300:ILE:HD12	1:B:302:ALA:H	1.61	0.65
1:F:29:PRO:HA	1:F:56:HIS:HA	1.80	0.63
1:C:321:LEU:HD22	1:C:326:ILE:HD12	1.81	0.62
1:A:199:ARG:NH2	1:A:325:GLY:O	2.33	0.60
1:F:189:THR:HG21	1:F:223:PHE:CE1	2.37	0.60
1:F:47:GLN:HE22	2:F:502:EDO:H22	1.67	0.59
1:E:272:ASN:OD1	3:E:501:NAD:H2A	2.02	0.58
1:C:15:LYS:HD2	1:C:388:LEU:HD21	1.85	0.58
1:C:65:GLY:HA3	1:C:99:GLY:O	2.04	0.57
1:D:65:GLY:HA3	1:D:99:GLY:O	2.05	0.57
1:E:262:VAL:HG12	1:E:266:PHE:HE2	1.68	0.57
1:F:92:VAL:HA	1:F:371:SER:OG	2.04	0.57
1:A:356:GLU:OE2	1:F:366:LYS:HE2	2.05	0.57
1:A:64:LYS:HG3	1:A:96:TYR:CE2	2.39	0.56
1:E:292:ILE:HB	1:E:313:THR:HG22	1.87	0.56
1:A:359:GLU:OE2	1:A:363:LYS:NZ	2.37	0.56
1:E:292:ILE:HG22	1:E:317:ALA:HB1	1.86	0.56
1:E:376:TYR:HA	1:E:386:MET:HE1	1.88	0.56
1:F:91:ILE:HA	1:F:393:VAL:HG12	1.87	0.56
1:C:288:ILE:HG12	1:C:289:GLU:H	1.71	0.56
1:B:270:ILE:HG13	1:B:274:GLU:HB3	1.88	0.56
1:E:377:THR:O	1:E:381:THR:HB	2.05	0.56
1:E:256:ARG:HA	1:E:262:VAL:HG22	1.87	0.55
1:D:180:ARG:NH1	1:D:345:GLU:OE1	2.39	0.55
1:F:311:GLY:N	1:F:331:ASP:OD2	2.38	0.55
1:B:2:PHE:HA	1:B:80:ALA:HB2	1.87	0.55
1:B:92:VAL:HG13	1:B:94:LEU:HG	1.88	0.54
1:C:29:PRO:HG2	1:C:79:LYS:HG2	1.89	0.54
1:F:190:ILE:HD13	1:F:365:TYR:HA	1.89	0.54
1:C:375:VAL:HG12	1:C:386:MET:HE3	1.90	0.54
1:E:277:GLU:O	1:E:301:LYS:HD3	2.07	0.54
1:E:397:ARG:NH2	4:E:601:HOH:O	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:VAL:HG13	1:F:329:VAL:HG11	1.90	0.54
1:B:319:LYS:NZ	1:B:323:GLU:OE1	2.40	0.54
1:F:70:HIS:HB3	1:F:73:VAL:HG23	1.90	0.54
1:A:35:VAL:CG2	1:A:125:ALA:HB1	2.32	0.53
1:A:367:LYS:O	1:A:371:SER:HB3	2.08	0.53
1:B:220:LEU:O	1:B:224:MET:HG2	2.09	0.53
1:B:191:VAL:CG1	1:B:329:VAL:HG11	2.36	0.53
1:A:144:ASN:O	1:A:148:MET:HG2	2.09	0.52
1:D:57:SER:O	1:D:97:GLY:HA3	2.10	0.52
1:B:177:SER:HB2	1:B:345:GLU:HB2	1.92	0.52
1:C:143:THR:HA	1:C:147:ILE:HD12	1.92	0.52
1:B:190:ILE:HG12	1:B:365:TYR:CD2	2.44	0.52
1:B:291:GLN:O	1:B:296:ASN:ND2	2.43	0.52
1:C:8:VAL:HG13	1:C:391:TYR:CD2	2.45	0.52
1:C:236:ASP:HB3	1:C:238:TYR:H	1.75	0.52
1:E:322:THR:HG21	1:E:385:ASP:HB2	1.92	0.52
1:E:382:ARG:NH2	4:E:604:HOH:O	2.42	0.51
1:E:302:ALA:O	1:E:326:ILE:HD13	2.11	0.51
1:C:309:ALA:HA	3:C:502:NAD:H1D	1.92	0.51
1:A:377:THR:O	1:A:381:THR:HB	2.11	0.51
1:B:263:THR:HG23	1:B:269:THR:HG21	1.91	0.51
1:C:140:ASP:OD1	1:C:141:MET:N	2.44	0.51
1:F:57:SER:O	1:F:97:GLY:HA3	2.11	0.51
1:F:84:TRP:O	1:F:88:LYS:HG2	2.11	0.51
1:A:351:MET:HE2	1:F:351:MET:SD	2.50	0.51
1:A:160:GLU:OE1	2:A:501:EDO:H22	2.11	0.50
1:A:64:LYS:HZ3	1:A:136:ILE:HG22	1.76	0.50
1:D:309:ALA:HA	1:D:331:ASP:HB2	1.92	0.50
1:C:81:LEU:HB2	1:C:100:LYS:HG2	1.93	0.50
1:C:191:VAL:CG1	1:C:329:VAL:HG11	2.41	0.50
1:B:74:SER:O	1:B:78:VAL:HG23	2.12	0.50
1:E:93:ASP:OD1	1:E:397:ARG:NH1	2.44	0.50
1:E:57:SER:O	1:E:97:GLY:HA3	2.12	0.50
1:F:377:THR:HA	1:F:380:THR:HG22	1.93	0.50
1:A:347:VAL:O	1:A:351:MET:HG2	2.13	0.49
1:D:92:VAL:HG11	1:D:340:THR:OG1	2.12	0.49
1:E:64:LYS:HE3	1:E:342:SER:HB3	1.95	0.49
1:C:69:PHE:CE1	1:C:103:ILE:HD12	2.47	0.49
1:F:92:VAL:HG13	1:F:94:LEU:HD13	1.95	0.49
1:E:376:TYR:O	1:E:380:THR:HG22	2.13	0.48
1:A:64:LYS:HD3	1:A:136:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASP:OD1	1:A:332:VAL:N	2.45	0.48
1:B:201:ILE:HD13	1:B:281:ASP:HB3	1.95	0.48
1:E:65:GLY:O	1:E:137:PRO:HA	2.13	0.48
1:F:211:GLN:O	1:F:286:ALA:HB2	2.13	0.48
1:C:2:PHE:HA	1:C:80:ALA:HB2	1.96	0.48
1:B:65:GLY:O	1:B:137:PRO:HA	2.13	0.48
1:B:253:LEU:HA	1:B:256:ARG:HD3	1.95	0.48
1:C:0:ASN:ND2	4:C:612:HOH:O	2.47	0.48
1:E:92:VAL:HG23	1:E:94:LEU:HG	1.95	0.48
1:D:190:ILE:HD13	1:D:365:TYR:HA	1.96	0.47
1:E:212:GLY:H	1:E:235:SER:HB3	1.78	0.47
1:F:140:ASP:CG	1:F:141:MET:H	2.17	0.47
1:A:56:HIS:CD2	1:A:83:MET:HG2	2.50	0.47
1:A:212:GLY:H	1:A:235:SER:HB3	1.78	0.47
1:F:330:PRO:HG3	1:F:387:ARG:HA	1.96	0.47
1:A:235:SER:OG	1:A:272:ASN:OD1	2.28	0.47
1:F:182:ARG:NH1	1:F:219:PHE:HE2	2.11	0.47
1:E:231:VAL:HG21	1:E:249:ILE:HD11	1.97	0.47
1:B:190:ILE:HD13	1:B:365:TYR:HA	1.96	0.47
1:B:0:ASN:HB3	1:B:3:THR:CG2	2.44	0.47
1:E:65:GLY:HA3	1:E:99:GLY:O	2.14	0.47
1:F:130:VAL:HG12	1:F:135:ASP:HB3	1.97	0.47
1:C:70:HIS:HD2	1:C:142:PHE:HE2	1.63	0.47
1:E:358:GLU:CD	1:E:358:GLU:H	2.17	0.47
1:B:213:PHE:O	1:B:256:ARG:NH1	2.47	0.47
3:C:502:NAD:N7N	4:C:607:HOH:O	2.35	0.47
1:A:10:LYS:HB2	1:A:23:TYR:CE1	2.49	0.46
1:A:29:PRO:HA	1:A:56:HIS:HA	1.97	0.46
1:B:193:GLN:HG2	1:B:203:ILE:HD13	1.98	0.46
1:C:65:GLY:O	1:C:137:PRO:HA	2.15	0.46
1:B:279:ASP:HA	1:B:301:LYS:HB2	1.96	0.46
1:C:358:GLU:CD	1:C:358:GLU:H	2.19	0.46
1:F:214:GLY:HA3	3:F:503:NAD:O5B	2.15	0.46
1:D:181:ASP:N	1:D:181:ASP:OD1	2.48	0.46
1:C:178:LYS:HE3	4:C:652:HOH:O	2.14	0.46
1:E:-3:GLU:OE1	1:E:-1:LEU:HD11	2.16	0.46
1:A:385:ASP:OD1	1:A:387:ARG:N	2.49	0.46
1:B:81:LEU:HD13	1:B:100:LYS:HE2	1.97	0.46
1:E:31:ARG:HD2	1:E:55:GLN:OE1	2.16	0.46
1:C:203:ILE:HD12	1:C:204:LYS:H	1.81	0.46
1:E:211:GLN:HA	1:E:235:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLN:HA	1:A:235:SER:HB3	1.97	0.46
1:B:65:GLY:HA3	1:B:99:GLY:O	2.16	0.46
1:B:256:ARG:NE	4:B:603:HOH:O	2.29	0.46
1:D:100:LYS:NZ	4:D:606:HOH:O	2.47	0.46
1:A:91:ILE:CD1	1:A:332:VAL:HG12	2.45	0.46
1:D:197:LYS:H	1:D:197:LYS:HD2	1.81	0.46
1:F:20:GLU:O	1:F:24:GLU:HG2	2.16	0.46
1:A:65:GLY:O	1:A:137:PRO:HA	2.16	0.45
1:D:311:GLY:H	1:D:312:PRO:HD3	1.81	0.45
1:F:10:LYS:O	1:F:14:ASN:HB2	2.16	0.45
1:F:189:THR:O	1:F:193:GLN:HG3	2.16	0.45
1:D:408:VAL:O	4:D:601:HOH:O	2.20	0.45
1:E:64:LYS:HD2	1:E:136:ILE:HB	1.98	0.45
1:E:318:THR:O	1:E:322:THR:HG23	2.17	0.45
1:D:15:LYS:HD3	1:D:388:LEU:HD21	1.98	0.45
1:D:170:LYS:O	1:D:180:ARG:NH2	2.50	0.45
1:E:327:LEU:HD11	1:E:386:MET:HE3	1.99	0.45
1:F:241:LEU:HG	1:F:263:THR:HG22	1.97	0.45
1:D:123:VAL:O	1:D:127:SER:HB3	2.16	0.45
1:A:180:ARG:HG3	1:A:181:ASP:N	2.32	0.45
1:D:173:VAL:HG12	1:E:397:ARG:HG3	1.98	0.45
1:E:-1:LEU:HD12	1:E:-1:LEU:H	1.81	0.45
1:F:235:SER:HB3	1:F:275:LEU:HG	1.97	0.45
1:F:251:TYR:CZ	1:F:255:ARG:HD2	2.52	0.45
1:B:56:HIS:CD2	1:B:83:MET:HG2	2.51	0.45
1:C:276:LEU:O	1:C:300:ILE:HG22	2.16	0.45
1:A:81:LEU:HD13	1:A:100:LYS:HE2	1.99	0.44
1:A:235:SER:HB2	1:A:275:LEU:HD22	1.98	0.44
1:B:31:ARG:HD2	1:B:55:GLN:OE1	2.18	0.44
1:D:70:HIS:HB3	1:D:73:VAL:HG23	2.00	0.44
1:E:297:ALA:O	1:E:324:ARG:NH1	2.48	0.44
1:A:69:PHE:CE1	1:A:103:ILE:HD12	2.52	0.44
1:B:210:ILE:O	1:B:234:ILE:HA	2.16	0.44
1:C:31:ARG:HD2	1:C:55:GLN:OE1	2.18	0.44
1:E:25:LEU:HD22	1:E:408:VAL:HG13	1.99	0.44
1:F:222:LYS:CG	1:F:253:LEU:HD11	2.48	0.44
1:B:161:PHE:HB3	1:D:134:LYS:HG2	1.98	0.44
1:C:209:VAL:HG12	1:C:232:ILE:HG12	1.99	0.44
1:E:309:ALA:HA	3:E:501:NAD:H1D	2.00	0.44
1:F:286:ALA:O	1:F:288:ILE:N	2.44	0.44
1:A:277:GLU:O	1:A:301:LYS:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ALA:HB1	1:C:249:ILE:HD12	2.00	0.44
1:E:191:VAL:HG23	1:E:372:PHE:CD1	2.53	0.44
1:E:289:GLU:OE1	1:E:289:GLU:N	2.44	0.44
1:B:252:LEU:HD22	1:B:262:VAL:HG11	2.00	0.44
1:D:29:PRO:HB3	1:D:56:HIS:HA	2.00	0.44
1:F:403:ARG:NH2	4:F:609:HOH:O	2.50	0.44
1:E:69:PHE:CE1	1:E:103:ILE:HD12	2.53	0.43
1:C:81:LEU:HB3	1:C:100:LYS:HE3	2.00	0.43
1:C:272:ASN:OD1	3:C:502:NAD:H2A	2.18	0.43
1:D:318:THR:HG23	1:D:328:LEU:HD22	1.99	0.43
1:F:271:THR:OG1	1:F:274:GLU:HG3	2.18	0.43
1:C:249:ILE:O	1:C:253:LEU:HB2	2.19	0.43
1:A:22:MET:HE1	1:A:402:SER:CB	2.49	0.43
1:D:31:ARG:HH22	1:D:58:ASP:CG	2.22	0.43
1:E:75:GLU:O	1:E:79:LYS:HG3	2.18	0.43
1:A:305:VAL:HG22	1:A:328:LEU:HD23	1.99	0.43
1:B:182:ARG:HD2	1:B:219:PHE:CE2	2.54	0.43
1:C:288:ILE:HG12	1:C:289:GLU:N	2.33	0.43
1:E:81:LEU:HB2	1:E:100:LYS:HG2	2.01	0.43
1:E:87:LEU:HB2	1:E:332:VAL:HG21	2.00	0.43
1:A:65:GLY:HA3	1:A:99:GLY:O	2.18	0.43
1:D:144:ASN:O	1:D:148:MET:HG2	2.19	0.43
1:F:222:LYS:HG2	1:F:253:LEU:HD11	2.00	0.43
1:C:70:HIS:CD2	1:C:142:PHE:HE2	2.37	0.43
1:A:184:THR:HG21	3:A:504:NAD:C5N	2.49	0.42
1:B:199:ARG:HD3	1:B:199:ARG:HA	1.85	0.42
1:E:199:ARG:HA	1:E:199:ARG:HD3	1.71	0.42
1:E:213:PHE:O	1:E:256:ARG:NH1	2.50	0.42
1:E:169:GLY:HA2	1:E:180:ARG:HD3	2.00	0.42
1:F:103:ILE:HG21	1:F:118:LEU:HD11	2.01	0.42
1:A:358:GLU:CD	1:A:358:GLU:H	2.22	0.42
1:C:29:PRO:HA	1:C:56:HIS:HA	2.01	0.42
1:C:181:ASP:OD1	1:C:181:ASP:N	2.51	0.42
1:E:231:VAL:CG2	1:E:249:ILE:HD11	2.49	0.42
1:C:407:TRP:N	1:C:407:TRP:CD1	2.87	0.42
1:C:191:VAL:HG13	1:C:329:VAL:HG11	2.02	0.42
1:C:314:THR:HG23	1:C:317:ALA:H	1.83	0.42
1:F:300:ILE:O	1:F:300:ILE:HG13	2.19	0.42
1:D:13:LEU:HD11	1:D:26:LEU:HD12	2.02	0.41
1:D:31:ARG:HD2	1:D:55:GLN:OE1	2.19	0.41
1:A:311:GLY:N	1:A:312:PRO:HD3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ALA:O	1:B:342:SER:HB2	2.20	0.41
1:C:321:LEU:HD23	1:C:321:LEU:HA	1.65	0.41
1:D:13:LEU:HD23	1:D:13:LEU:HA	1.83	0.41
1:E:184:THR:O	1:E:188:VAL:HG23	2.20	0.41
1:A:37:ILE:HD13	1:A:122:TYR:HA	2.01	0.41
1:A:239:GLY:CA	1:A:263:THR:HG21	2.50	0.41
1:C:279:ASP:N	1:C:279:ASP:OD1	2.54	0.41
1:D:68:ARG:HB2	1:D:141:MET:HB2	2.02	0.41
1:E:307:GLU:HG3	1:E:331:ASP:N	2.35	0.41
1:A:80:ALA:HA	1:A:83:MET:HE2	2.01	0.41
1:C:191:VAL:HG11	1:C:329:VAL:HG11	2.01	0.41
1:E:300:ILE:H	1:E:324:ARG:HH12	1.69	0.41
1:F:182:ARG:HH11	1:F:219:PHE:HE2	1.68	0.41
1:A:143:THR:HA	1:A:147:ILE:HD12	2.02	0.41
1:F:13:LEU:HD11	1:F:26:LEU:HD12	2.02	0.41
1:D:328:LEU:HD21	1:D:387:ARG:NH2	2.35	0.41
1:A:-3:GLU:OE2	1:A:314:THR:OG1	2.25	0.41
1:D:2:PHE:HA	1:D:80:ALA:HB2	2.03	0.41
1:D:170:LYS:HB2	1:D:170:LYS:HE2	1.90	0.41
1:E:192:ILE:HG12	1:E:306:VAL:HG21	2.02	0.41
1:A:22:MET:HE1	1:A:402:SER:HB2	2.03	0.41
1:A:209:VAL:HG21	1:A:278:LEU:CD1	2.51	0.41
1:A:232:ILE:HD12	1:A:244:PRO:HA	2.03	0.41
1:C:127:SER:HA	1:C:130:VAL:HG22	2.02	0.41
1:D:127:SER:HA	1:D:130:VAL:HG22	2.03	0.41
1:F:216:ALA:HB2	3:F:503:NAD:C2N	2.51	0.41
1:B:182:ARG:HD2	1:B:219:PHE:CZ	2.56	0.41
1:E:190:ILE:HD12	1:E:365:TYR:CE2	2.56	0.41
1:E:249:ILE:HD13	1:E:249:ILE:HA	1.87	0.41
1:F:65:GLY:HA3	1:F:99:GLY:O	2.21	0.41
1:D:29:PRO:HG2	1:D:79:LYS:HG2	2.03	0.40
1:F:69:PHE:CE1	1:F:103:ILE:HD12	2.56	0.40
1:B:377:THR:HA	1:B:380:THR:HG22	2.03	0.40
1:C:92:VAL:HG23	1:C:371:SER:OG	2.21	0.40
1:F:92:VAL:HA	1:F:371:SER:HG	1.85	0.40
1:F:358:GLU:O	1:F:362:GLU:HG3	2.22	0.40
1:A:64:LYS:HD3	1:A:136:ILE:O	2.22	0.40
1:B:108:ARG:NH1	1:B:142:PHE:HZ	2.19	0.40
1:B:353:TYR:OH	1:D:363:LYS:HE3	2.22	0.40
1:C:10:LYS:HB2	1:C:23:TYR:CE1	2.57	0.40
1:C:66:GLY:O	1:C:100:LYS:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:PHE:HB3	1:C:105:CYS:SG	2.61	0.40
1:A:56:HIS:HB2	1:A:82:SER:OG	2.22	0.40
1:A:189:THR:O	1:A:193:GLN:HG3	2.21	0.40
1:B:145:ALA:HB3	1:C:264:THR:HG23	2.04	0.40
1:C:40:LYS:NZ	4:C:601:HOH:O	2.16	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	413/415 (100%)	403 (98%)	9 (2%)	1 (0%)	44	65
1	B	408/415 (98%)	394 (97%)	13 (3%)	1 (0%)	44	65
1	C	408/415 (98%)	393 (96%)	14 (3%)	1 (0%)	44	65
1	D	300/415 (72%)	290 (97%)	10 (3%)	0	100	100
1	E	411/415 (99%)	402 (98%)	9 (2%)	0	100	100
1	F	408/415 (98%)	395 (97%)	12 (3%)	1 (0%)	44	65
All	All	2348/2490 (94%)	2277 (97%)	67 (3%)	4 (0%)	44	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	ILE
1	F	287	ALA
1	C	262	VAL
1	A	262	VAL

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	341/341 (100%)	314 (92%)	27 (8%)	10	20
1	B	337/341 (99%)	320 (95%)	17 (5%)	20	41
1	C	337/341 (99%)	317 (94%)	20 (6%)	16	33
1	D	251/341 (74%)	243 (97%)	8 (3%)	34	59
1	E	339/341 (99%)	318 (94%)	21 (6%)	15	31
1	F	337/341 (99%)	323 (96%)	14 (4%)	25	48
All	All	1942/2046 (95%)	1835 (94%)	107 (6%)	18	37

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	57	SER
1	A	58	ASP
1	A	64	LYS
1	A	82	SER
1	A	92	VAL
1	A	186	GLU
1	A	200	ASN
1	A	204	LYS
1	A	208	VAL
1	A	227	LEU
1	A	256	ARG
1	A	258	SER
1	A	261	THR
1	A	263	THR
1	A	270	ILE
1	A	275	LEU
1	A	278	LEU
1	A	333	LEU
1	A	351	MET
1	A	358	GLU
1	A	366	LYS

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Mol	Chain	Res	Type
1	A	367	LYS
1	A	371	SER
1	A	381	THR
1	A	385	ASP
1	A	396	ARG
1	B	3	THR
1	B	15	LYS
1	B	20	GLU
1	B	47	GLN
1	B	159	ASP
1	B	189	THR
1	B	203	ILE
1	B	227	LEU
1	B	258	SER
1	B	270	ILE
1	B	289	GLU
1	B	300	ILE
1	B	316	GLU
1	B	341	VAL
1	B	395	VAL
1	B	397	ARG
1	B	404	PHE
1	C	7	GLU
1	C	60	VAL
1	C	159	ASP
1	C	181	ASP
1	C	189	THR
1	C	191	VAL
1	C	203	ILE
1	C	209	VAL
1	C	210	ILE
1	C	252	LEU
1	C	264	THR
1	C	265	LEU
1	C	269	THR
1	C	282	ILE
1	C	291	GLN
1	C	341	VAL
1	C	358	GLU
1	C	386	MET
1	C	395	VAL
1	C	403	ARG

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Mol	Chain	Res	Type
1	D	4	SER
1	D	40	LYS
1	D	60	VAL
1	D	92	VAL
1	D	180	ARG
1	D	181	ASP
1	D	395	VAL
1	D	403	ARG
1	E	-1	LEU
1	E	20	GLU
1	E	40	LYS
1	E	152	MET
1	E	163	SER
1	E	194	GLU
1	E	220	LEU
1	E	222	LYS
1	E	231	VAL
1	E	234	ILE
1	E	247	LEU
1	E	258	SER
1	E	269	THR
1	E	275	LEU
1	E	307	GLU
1	E	316	GLU
1	E	326	ILE
1	E	328	LEU
1	E	341	VAL
1	E	381	THR
1	E	386	MET
1	F	11	GLU
1	F	14	ASN
1	F	94	LEU
1	F	152	MET
1	F	159	ASP
1	F	182	ARG
1	F	200	ASN
1	F	249	ILE
1	F	264	THR
1	F	265	LEU
1	F	272	ASN
1	F	288	ILE
1	F	300	ILE

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Mol	Chain	Res	Type
1	F	316	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	47	GLN

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 ⓘ

14 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	EDO	A	501	-	3,3,3	0.63	0	2,2,2	0.04	0
2	EDO	B	501	-	3,3,3	0.55	0	2,2,2	0.43	0
2	EDO	A	502	-	3,3,3	0.58	0	2,2,2	0.26	0
3	NAD	B	503	-	42,48,48	0.65	1 (2%)	50,73,73	0.91	3 (6%)
2	EDO	F	501	-	3,3,3	0.53	0	2,2,2	0.40	0
2	EDO	F	502	-	3,3,3	0.48	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	F	503	-	42,48,48	0.61	0	50,73,73	0.82	1 (2%)
3	NAD	C	502	-	42,48,48	0.69	1 (2%)	50,73,73	0.87	1 (2%)
2	EDO	A	503	-	3,3,3	0.60	0	2,2,2	0.06	0
2	EDO	D	501	-	3,3,3	0.49	0	2,2,2	0.37	0
3	NAD	E	501	-	42,48,48	0.65	0	50,73,73	0.90	2 (4%)
2	EDO	C	501	-	3,3,3	0.36	0	2,2,2	0.38	0
2	EDO	B	502	-	3,3,3	0.53	0	2,2,2	0.09	0
3	NAD	A	504	-	42,48,48	0.67	0	50,73,73	0.89	4 (8%)

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	EDO	A	501	-	-	1/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
3	NAD	B	503	-	-	7/26/62/62	0/5/5/5
2	EDO	F	501	-	-	1/1/1/1	-
2	EDO	F	502	-	-	1/1/1/1	-
3	NAD	F	503	-	-	5/26/62/62	0/5/5/5
3	NAD	C	502	-	-	7/26/62/62	0/5/5/5
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	D	501	-	-	0/1/1/1	-
3	NAD	E	501	-	-	8/26/62/62	0/5/5/5
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
3	NAD	A	504	-	-	4/26/62/62	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	NAD	C2N-N1N	2.36	1.37	1.35
3	B	503	NAD	C2N-N1N	2.00	1.37	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	NAD	C5A-C6A-N6A	2.62	124.34	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	NAD	PN-O3-PA	2.62	141.82	132.83
3	B	503	NAD	C5A-C6A-N6A	2.42	124.03	120.35
3	F	503	NAD	C5A-C6A-N6A	2.34	123.91	120.35
3	A	504	NAD	O3B-C3B-C2B	-2.29	104.42	111.82
3	A	504	NAD	C5A-C6A-N6A	2.27	123.80	120.35
3	A	504	NAD	C3B-C2B-C1B	-2.26	97.57	100.98
3	E	501	NAD	O4B-C1B-C2B	-2.22	103.67	106.93
3	C	502	NAD	C5A-C6A-N6A	2.19	123.68	120.35
3	A	504	NAD	C6N-N1N-C2N	-2.13	120.03	121.97
3	B	503	NAD	C3B-C2B-C1B	-2.01	97.95	100.98

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	NAD	O4D-C1D-N1N-C2N
3	B	503	NAD	O4D-C1D-N1N-C6N
3	B	503	NAD	C2D-C1D-N1N-C2N
3	B	503	NAD	C2D-C1D-N1N-C6N
3	C	502	NAD	C2D-C1D-N1N-C2N
3	C	502	NAD	C2D-C1D-N1N-C6N
3	E	501	NAD	C5B-O5B-PA-O1A
3	E	501	NAD	PN-O3-PA-O5B
3	E	501	NAD	C5D-O5D-PN-O2N
3	F	503	NAD	O4D-C1D-N1N-C2N
3	F	503	NAD	O4D-C1D-N1N-C6N
3	F	503	NAD	C2D-C1D-N1N-C2N
3	F	503	NAD	C2D-C1D-N1N-C6N
3	B	503	NAD	O4B-C4B-C5B-O5B
2	A	501	EDO	O1-C1-C2-O2
2	F	501	EDO	O1-C1-C2-O2
2	F	502	EDO	O1-C1-C2-O2
3	E	501	NAD	C5B-O5B-PA-O3
3	E	501	NAD	C5D-O5D-PN-O3
3	A	504	NAD	PN-O3-PA-O1A
3	E	501	NAD	C5B-O5B-PA-O2A
3	E	501	NAD	C5D-O5D-PN-O1N
2	B	501	EDO	O1-C1-C2-O2
3	C	502	NAD	C2N-C3N-C7N-O7N
3	C	502	NAD	C2N-C3N-C7N-N7N
3	A	504	NAD	PN-O3-PA-O2A
3	A	504	NAD	O4B-C4B-C5B-O5B

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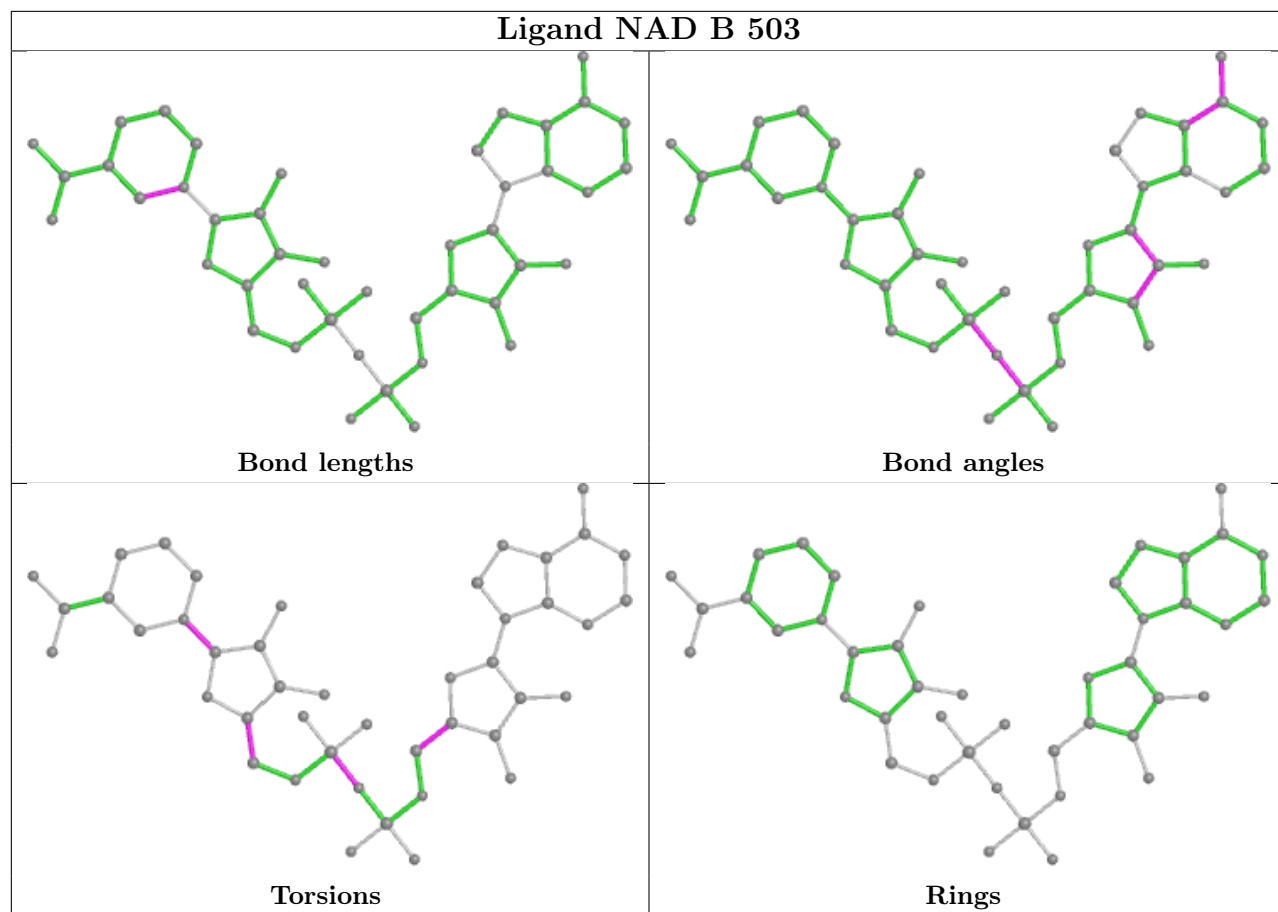
Mol	Chain	Res	Type	Atoms
3	B	503	NAD	O4D-C4D-C5D-O5D
3	C	502	NAD	C4N-C3N-C7N-N7N
3	C	502	NAD	C4N-C3N-C7N-O7N
3	A	504	NAD	C2D-C1D-N1N-C6N
3	F	503	NAD	O4B-C4B-C5B-O5B
3	B	503	NAD	PA-O3-PN-O2N
3	C	502	NAD	O4B-C4B-C5B-O5B
3	E	501	NAD	O4B-C4B-C5B-O5B

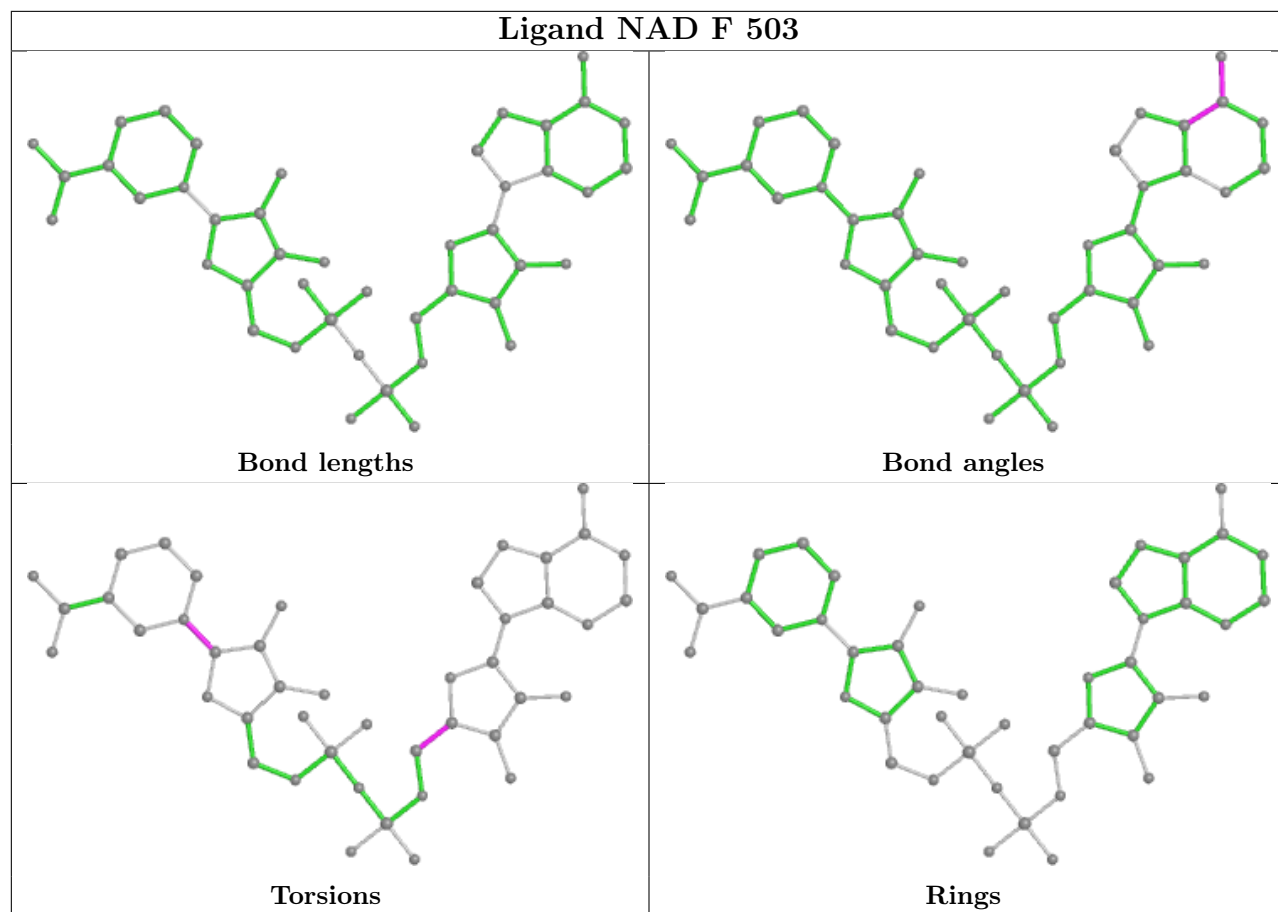
There are no ring outliers.

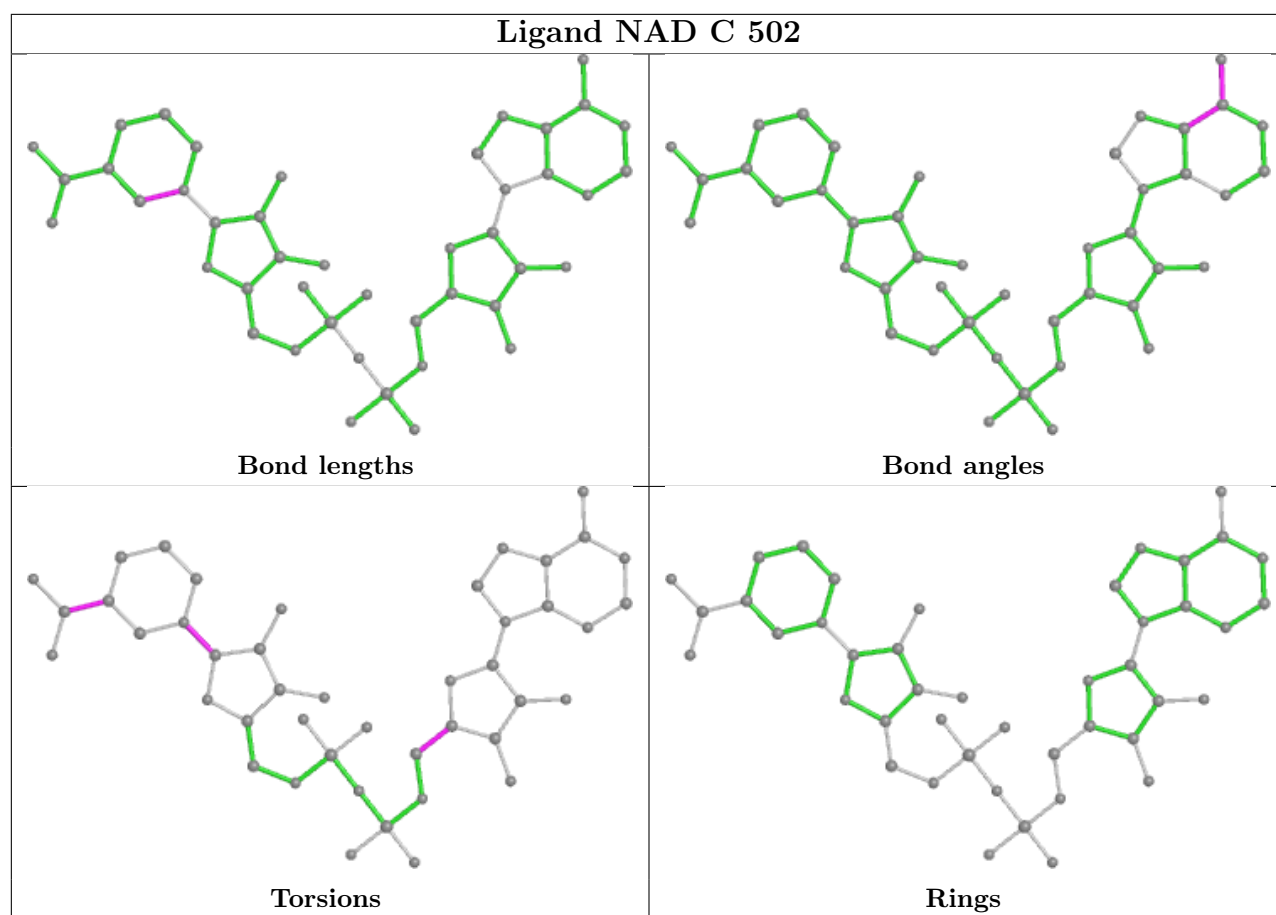
6 monomers are involved in 11 short contacts:

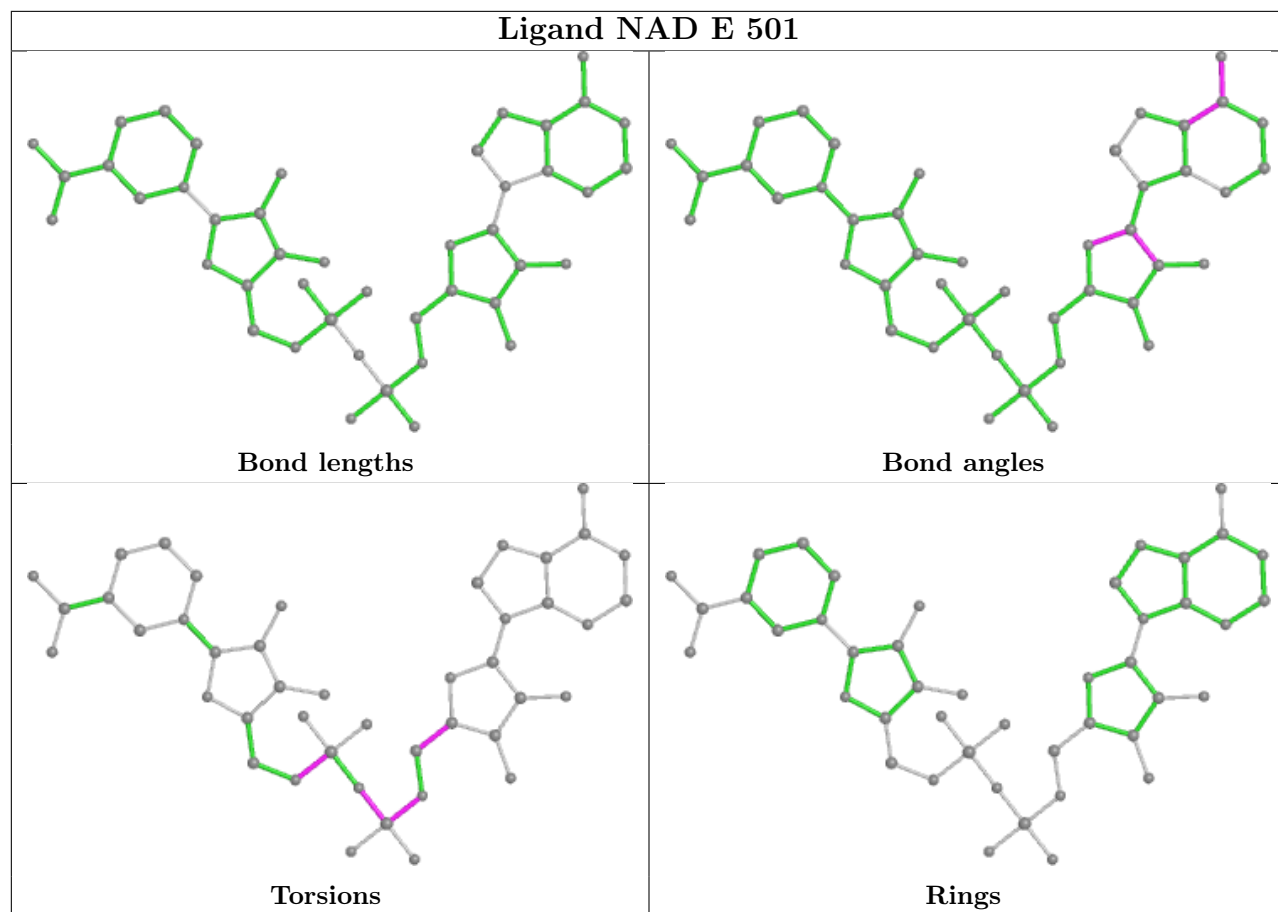
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	EDO	1	0
2	F	502	EDO	1	0
3	F	503	NAD	3	0
3	C	502	NAD	3	0
3	E	501	NAD	2	0
3	A	504	NAD	1	0

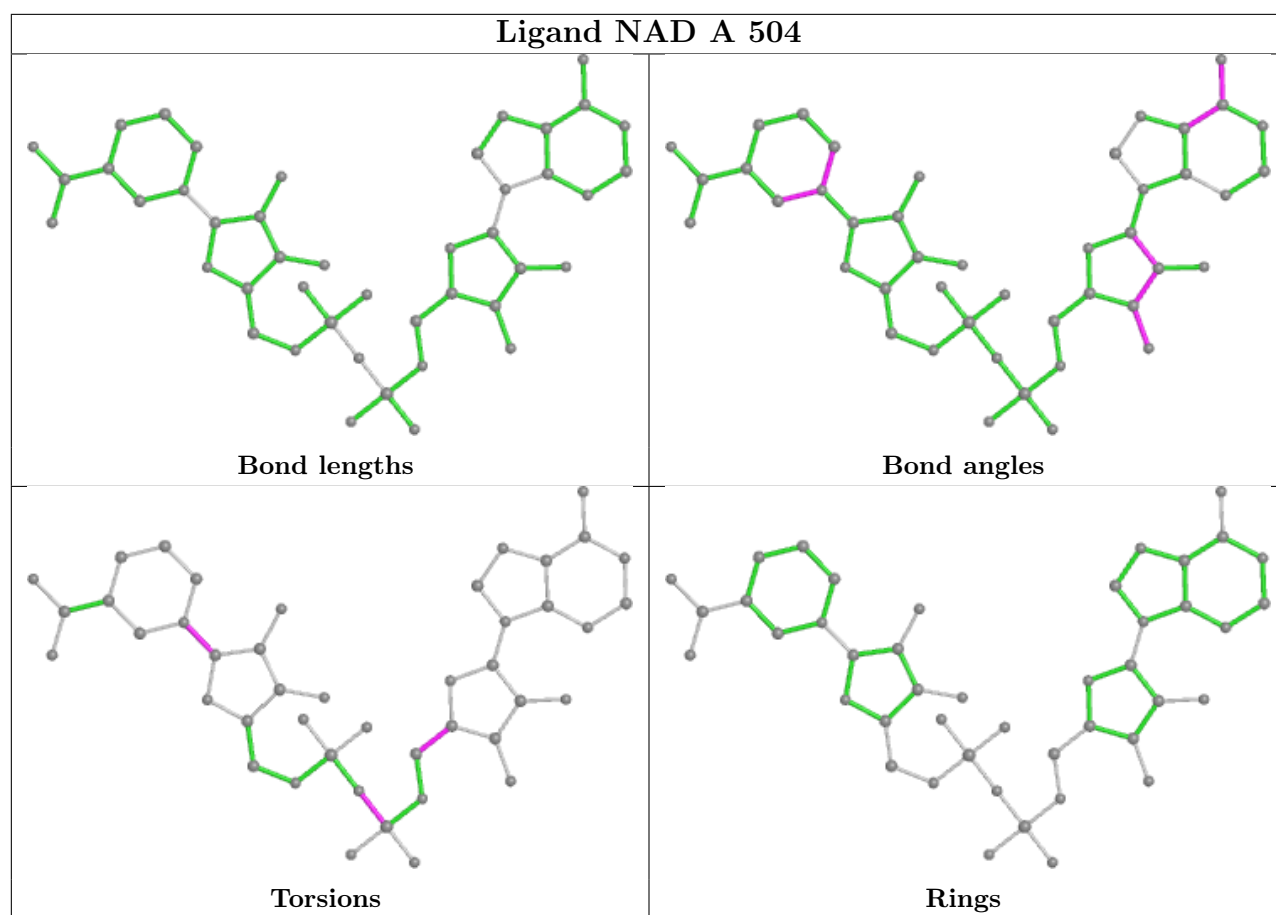
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	415/415 (100%)	-0.40	2 (0%) 87 85	33, 44, 64, 91	0
1	B	410/415 (98%)	-0.25	3 (0%) 84 81	33, 47, 71, 130	0
1	C	410/415 (98%)	-0.34	4 (0%) 79 76	34, 48, 71, 103	0
1	D	304/415 (73%)	-0.18	8 (2%) 57 52	33, 46, 93, 132	0
1	E	413/415 (99%)	-0.35	1 (0%) 92 90	32, 44, 71, 104	0
1	F	410/415 (98%)	-0.35	5 (1%) 76 73	33, 45, 69, 111	0
All	All	2362/2490 (94%)	-0.32	23 (0%) 79 76	32, 46, 73, 132	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	308	ALA	5.2
1	F	287	ALA	5.1
1	E	-4	ALA	4.3
1	D	309	ALA	3.8
1	B	-1	LEU	3.7
1	D	306	VAL	3.7
1	C	-1	LEU	3.5
1	F	259	PHE	3.5
1	F	260	GLY	3.2
1	D	-1	LEU	2.9
1	F	-1	LEU	2.8
1	C	268	ASN	2.8
1	C	301	LYS	2.6
1	B	267	GLU	2.6
1	A	142	PHE	2.6
1	F	203	ILE	2.6
1	D	312	PRO	2.5
1	A	-4	ALA	2.4
1	D	305	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	203	ILE	2.1
1	D	304	ILE	2.1
1	D	313	THR	2.1
1	B	260	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

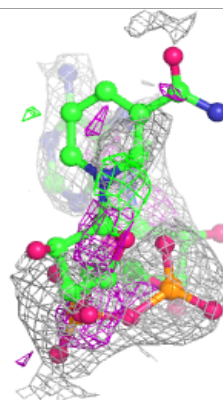
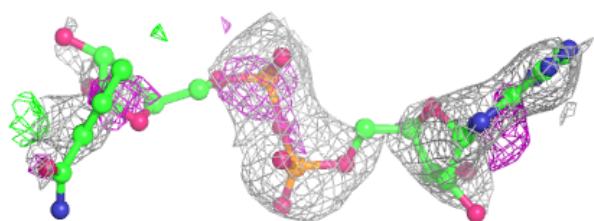
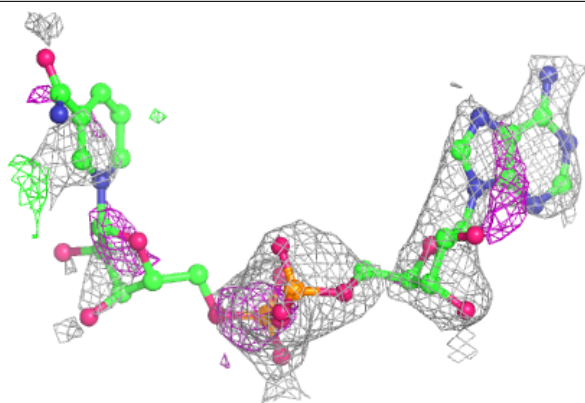
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAD	B	503	44/44	0.65	0.16	68,80,95,96	0
3	NAD	F	503	44/44	0.69	0.14	65,74,85,89	0
3	NAD	E	501	44/44	0.72	0.16	54,66,76,78	0
2	EDO	A	501	4/4	0.82	0.16	39,44,45,49	0
2	EDO	F	501	4/4	0.85	0.12	38,39,42,48	0
2	EDO	F	502	4/4	0.86	0.13	49,50,53,59	0
2	EDO	A	502	4/4	0.88	0.12	36,42,42,47	0
3	NAD	C	502	44/44	0.89	0.10	47,54,60,63	0
2	EDO	B	501	4/4	0.90	0.13	40,43,44,46	0
3	NAD	A	504	44/44	0.90	0.10	47,53,59,64	0
2	EDO	A	503	4/4	0.90	0.12	50,53,55,56	0
2	EDO	D	501	4/4	0.92	0.09	37,38,42,47	0
2	EDO	C	501	4/4	0.92	0.10	35,37,40,46	0
2	EDO	B	502	4/4	0.95	0.08	36,39,40,44	0

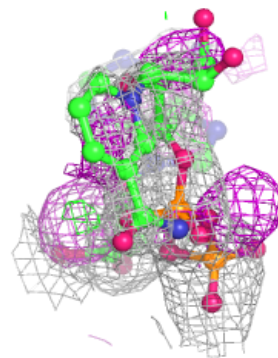
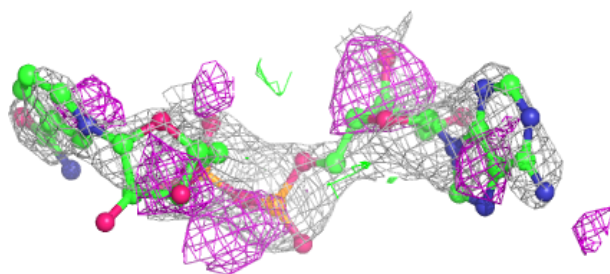
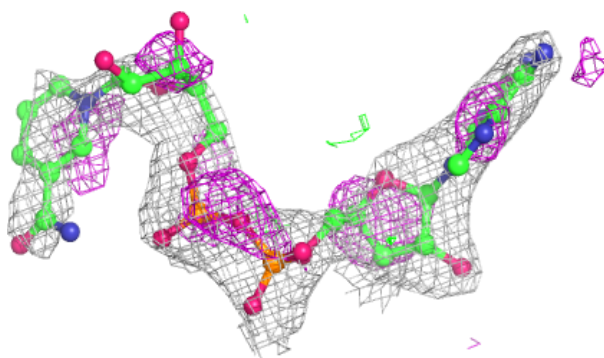
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 503:

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

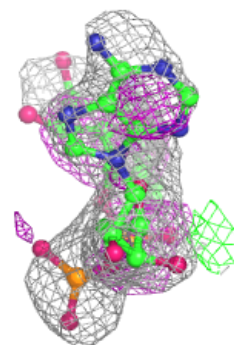
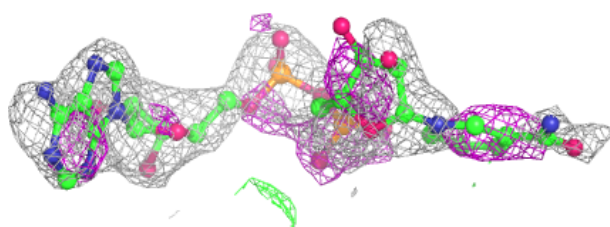
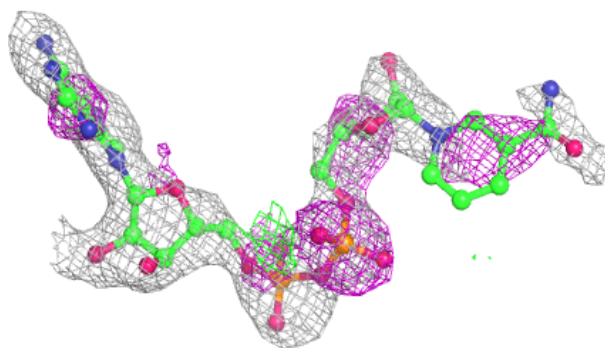
**Electron density around NAD F 503:**

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

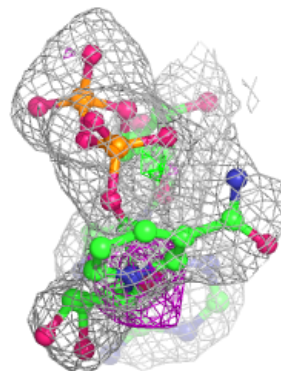
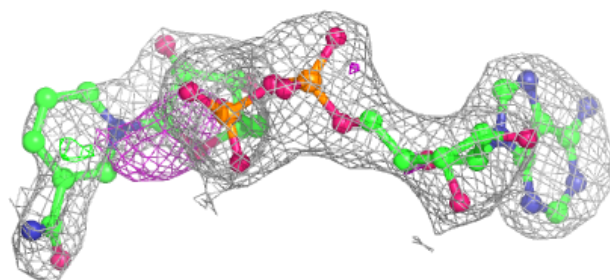
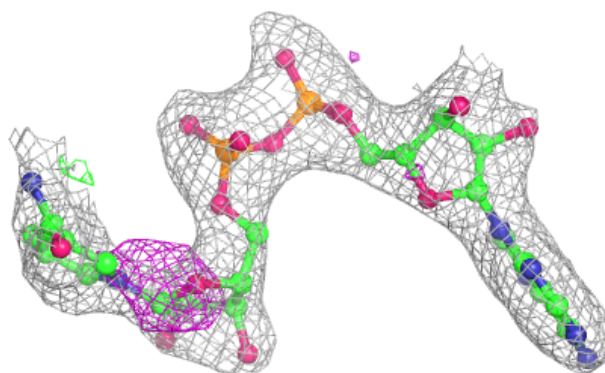


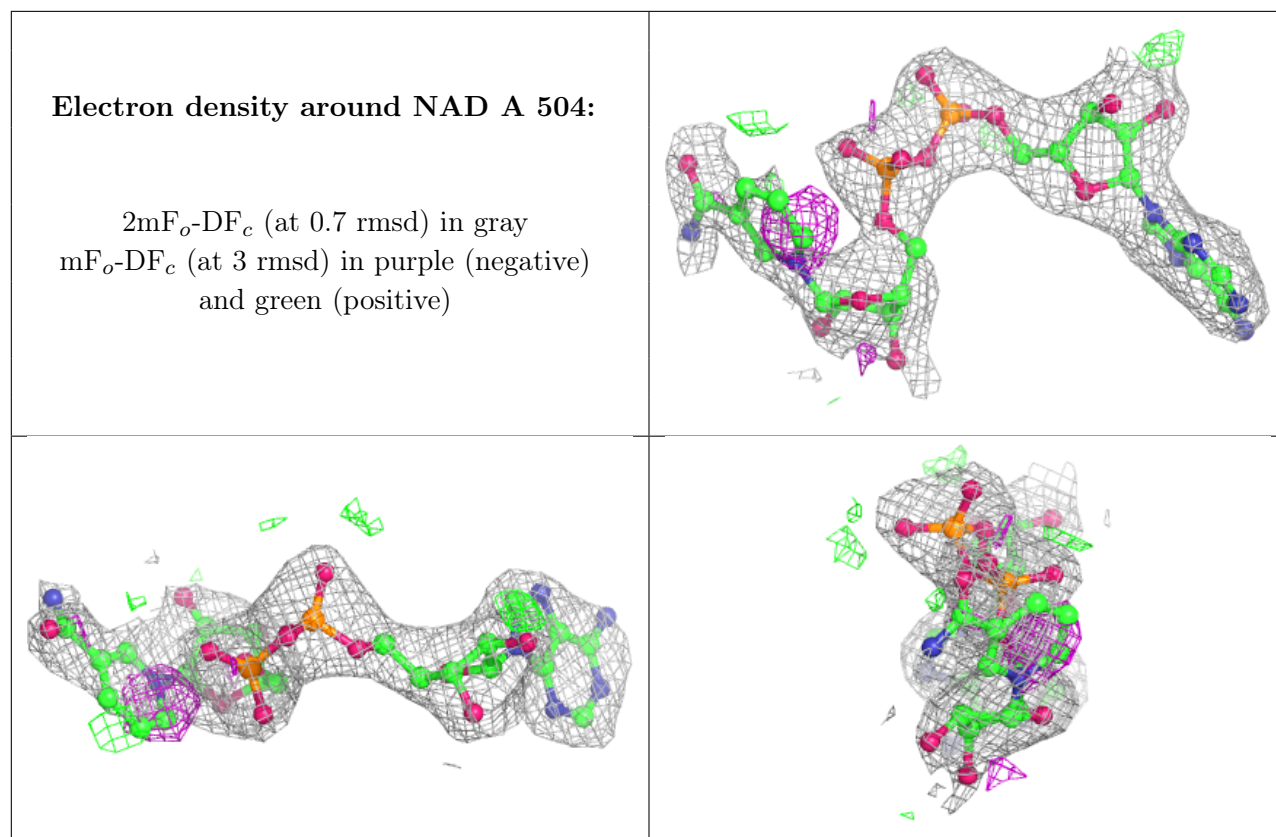
Electron density around NAD E 501:

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

**Electron density around NAD C 502:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.