



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:18 PM UTC

PDB ID : 4FW8 / pdb_00004fw8
Title : Crystal structure of FABG4 complexed with Coenzyme NADH
Authors : Dutta, D.; Bhattacharyya, S.; Das, A.K.
Deposited on : 2012-06-30
Resolution : 2.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

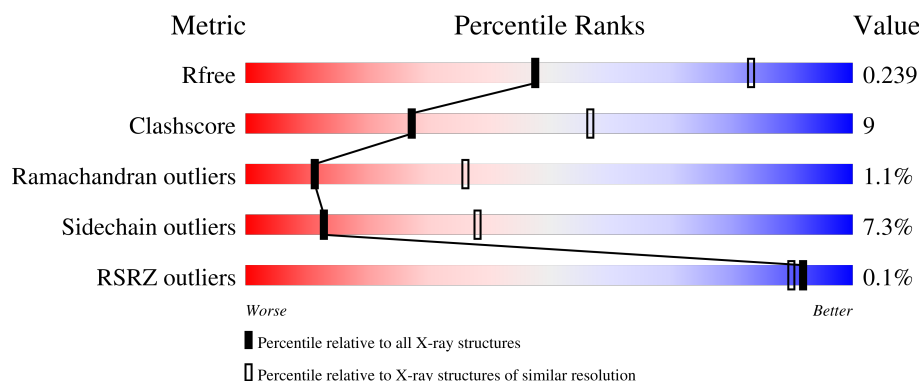
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	454	72% 20% • 6%
1	B	454	74% 16% • 6%
1	C	454	74% 17% • 8%
1	D	454	63% 25% • 10%

2 Entry composition ⓘ

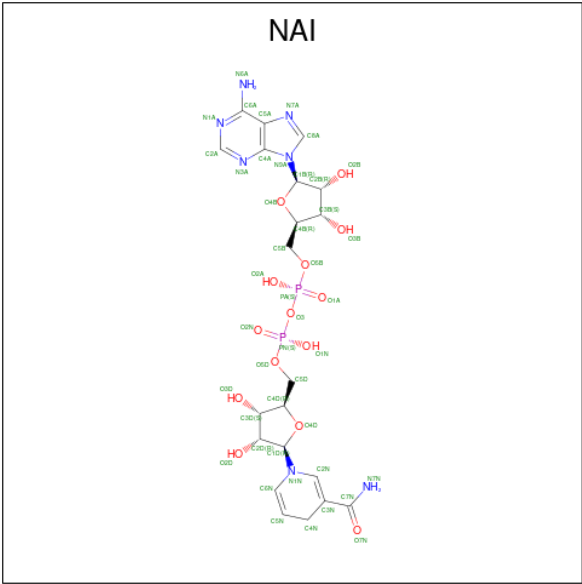
There are 4 unique types of molecules in this entry. The entry contains 12462 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-oxoacyl-(Acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3080	1925	553	595	7			
1	B	425	Total	C	N	O	S	0	0	0
			3059	1916	543	593	7			
1	C	418	Total	C	N	O	S	0	0	0
			2991	1871	530	584	6			
1	D	409	Total	C	N	O	S	0	0	0
			2927	1836	514	571	6			

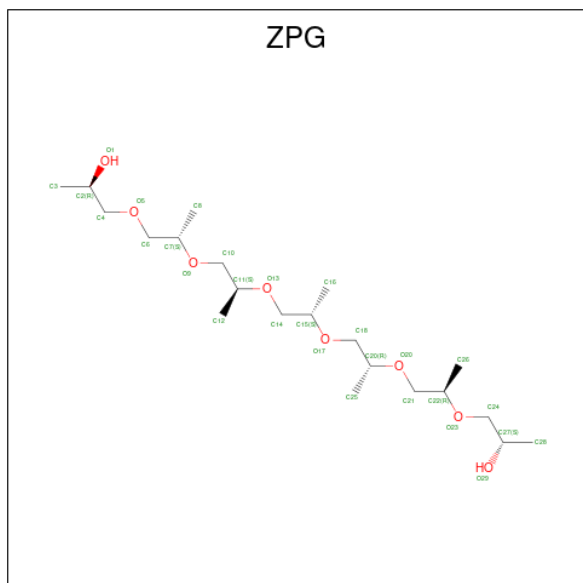
- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



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

- Molecule 3 is (2S,5R,8R,11S,14S,17S,21R)-5,8,11,14,17-PENTAMETHYL-4,7,10,13,16,19-H EXAOXADOCOSANE-2,21-DIOL (CCD ID: ZPG) (formula: C₂₁H₄₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	9	4		

- Molecule 4 is water.

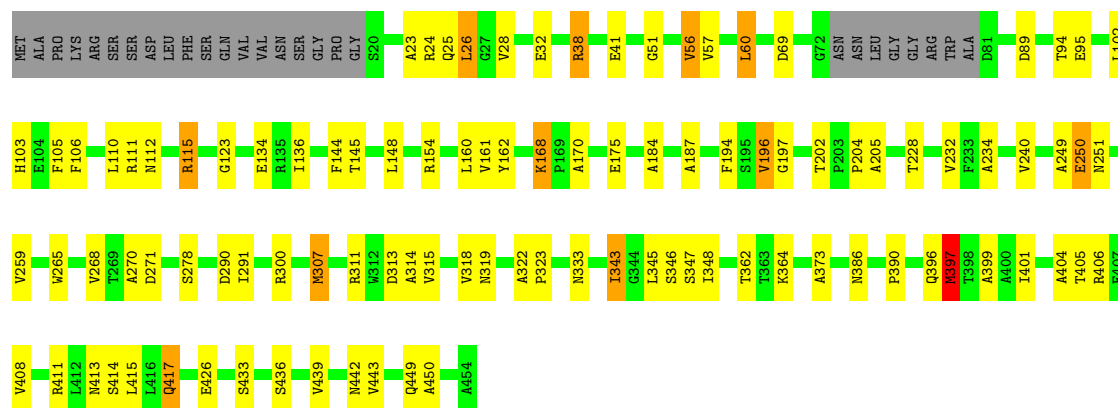
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	68	Total	O	0	0
			68	68		
4	C	38	Total	O	0	0
			38	38		
4	D	31	Total	O	0	0
			31	31		

3 Residue-property plots

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

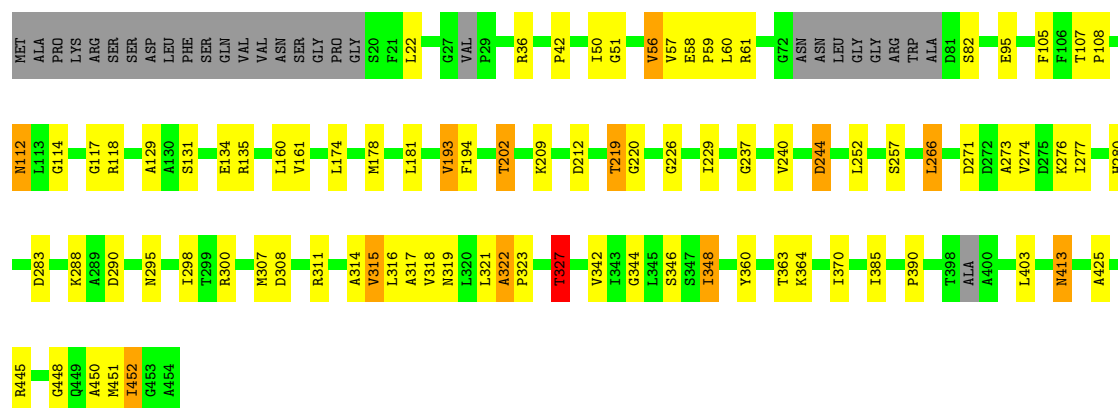
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase

Chain A: 



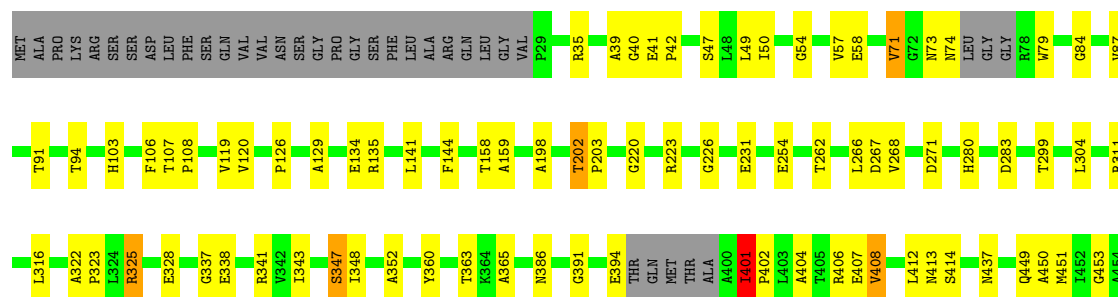
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase

Chain B: 



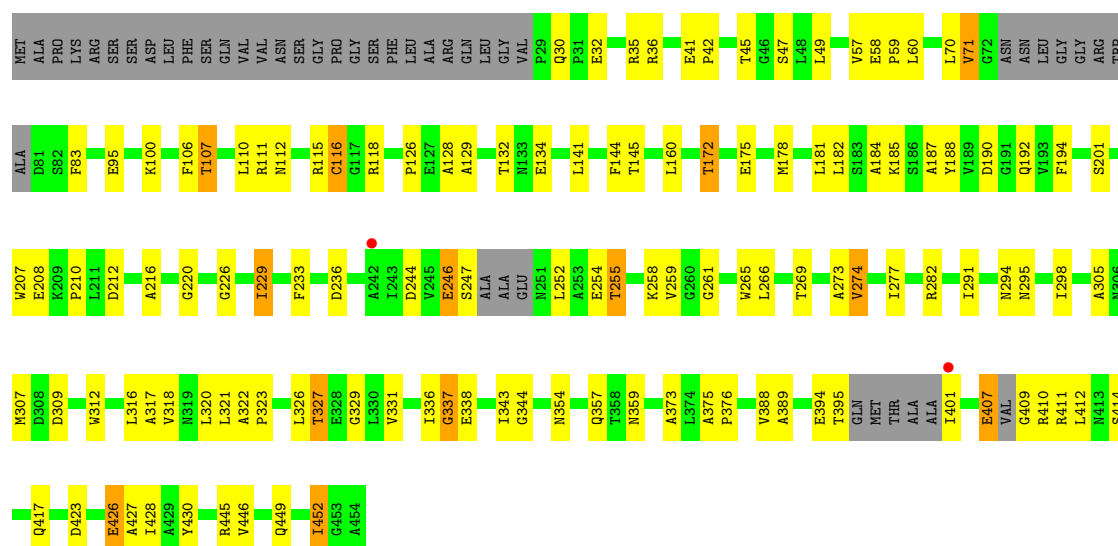
- Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase

Chain C: 



• Molecule 1: 3-oxoacyl-(Acyl-carrier-protein) reductase

Chain D: 63% 25% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.33Å 71.30Å 93.29Å 104.99° 97.08° 93.66°	Depositor
Resolution (Å)	19.86 – 2.79 19.86 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.86-2.79) 96.5 (19.86-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.238 0.166 , 0.239	Depositor DCC
R_{free} test set	1889 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12462	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: NAI, ZPG

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	0.88	1/3125 (0.0%)	1.10	9/4248 (0.2%)
1	B	0.86	2/3102 (0.1%)	1.09	8/4212 (0.2%)
1	C	0.86	1/3036 (0.0%)	1.06	6/4132 (0.1%)
1	D	0.81	1/2968 (0.0%)	1.04	5/4032 (0.1%)
All	All	0.85	5/12231 (0.0%)	1.07	28/16624 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	VAL	CA-CB	6.81	1.62	1.54
1	B	327	THR	CA-CB	5.73	1.62	1.53
1	B	193	VAL	CA-CB	5.65	1.61	1.54
1	C	401	ILE	CA-CB	5.12	1.60	1.54
1	D	327	THR	CA-CB	5.07	1.61	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	LYS	CA-C-N	-8.66	110.81	119.56
1	A	168	LYS	C-N-CA	-8.66	110.81	119.56
1	A	202	THR	CA-C-N	7.93	128.54	120.38
1	A	202	THR	C-N-CA	7.93	128.54	120.38
1	C	406	ARG	N-CA-C	-7.53	103.71	113.12
1	A	175	GLU	N-CA-C	6.85	118.54	111.14
1	C	365	ALA	N-CA-C	-6.17	104.64	111.36
1	D	192	GLN	N-CA-C	5.97	118.23	110.53
1	B	202	THR	CA-C-N	5.93	123.93	119.66
1	B	202	THR	C-N-CA	5.93	123.93	119.66
1	B	42	PRO	CA-C-N	-5.82	113.75	120.04
1	B	42	PRO	C-N-CA	-5.82	113.75	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	SER	N-CA-C	5.76	123.06	110.80
1	A	417	GLN	N-CA-C	5.73	116.97	108.60
1	A	240	VAL	N-CA-C	5.62	116.04	108.17
1	B	161	VAL	CB-CA-C	-5.57	102.39	110.63
1	D	107	THR	CA-C-N	-5.48	113.38	119.19
1	D	107	THR	C-N-CA	-5.48	113.38	119.19
1	C	283	ASP	N-CA-C	5.31	117.07	111.28
1	C	87	VAL	CB-CA-C	-5.29	104.38	110.41
1	B	322	ALA	O-C-N	5.28	123.92	120.27
1	C	198	ALA	N-CA-C	5.25	119.83	113.38
1	A	313	ASP	N-CA-C	5.19	117.61	111.33
1	D	411	ARG	N-CA-C	-5.12	107.08	113.38
1	A	362	THR	N-CA-C	-5.10	105.62	111.07
1	D	175	GLU	N-CA-C	5.06	117.19	111.11
1	B	240	VAL	N-CA-C	5.03	116.05	109.21
1	B	114	GLY	N-CA-C	5.02	120.80	112.66

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	3080	0	3100	65	0
1	B	3059	0	3073	52	0
1	C	2991	0	2963	45	0
1	D	2927	0	2916	69	0
2	A	44	0	27	3	0
2	B	44	0	27	1	0
2	C	44	0	27	1	0
2	D	44	0	27	1	0
3	A	13	0	19	1	0
4	A	79	0	0	2	0
4	B	68	0	0	3	0
4	C	38	0	0	2	0
4	D	31	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12462	0	12179	223	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 9.

All (223) 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:337:GLY:HA2	1:D:338:GLU:HB2	1.38	1.03
1:A:38:ARG:HG2	1:A:38:ARG:HH11	1.33	0.93
1:B:323:PRO:O	1:B:327:THR:HG22	1.78	0.82
1:B:322:ALA:HB3	1:B:323:PRO:HD3	1.60	0.82
1:A:115:ARG:NH2	1:A:154:ARG:HD2	1.99	0.78
1:A:249:ALA:O	1:A:250:GLU:HB2	1.84	0.78
1:D:41:GLU:HG3	1:D:42:PRO:HD2	1.68	0.74
1:C:316:LEU:HD13	1:C:363:THR:HG22	1.71	0.72
1:D:407:GLU:O	1:D:409:GLY:N	2.23	0.72
1:D:57:VAL:HG13	1:D:58:GLU:HG2	1.73	0.71
1:B:413:ASN:HB3	1:B:450:ALA:HA	1.76	0.66
1:A:426:GLU:OE1	1:A:426:GLU:HA	1.96	0.66
1:C:103:HIS:HE1	1:D:307:MET:O	1.79	0.66
1:C:311:ARG:NE	4:C:624:HOH:O	2.28	0.66
1:D:337:GLY:CA	1:D:338:GLU:HB2	2.19	0.65
1:A:404:ALA:O	1:A:408:VAL:HG23	1.97	0.65
1:A:315:VAL:O	1:A:319:ASN:HB2	1.98	0.64
1:D:181:LEU:HD21	1:D:194:PHE:CZ	2.32	0.64
1:C:129:ALA:HB1	1:C:134:GLU:HB3	1.79	0.64
1:A:38:ARG:HH11	1:A:38:ARG:CG	2.09	0.64
1:B:244:ASP:HB2	1:B:252:LEU:HD13	1.80	0.63
1:B:319:ASN:HB2	1:B:363:THR:HG21	1.80	0.63
1:C:49:LEU:HD13	1:C:71:VAL:HG22	1.80	0.63
1:A:278:SER:OG	1:A:333:ASN:ND2	2.32	0.63
1:B:129:ALA:HB1	1:B:134:GLU:HB3	1.81	0.63
1:C:135:ARG:HD3	1:D:373:ALA:CB	2.29	0.63
1:C:107:THR:HB	1:C:108:PRO:HD3	1.81	0.62
1:B:308:ASP:OD1	1:B:311:ARG:HD2	2.01	0.61
1:C:325:ARG:HH12	1:C:328:GLU:HB2	1.64	0.61
1:A:401:ILE:O	1:A:406:ARG:NH1	2.34	0.61
1:C:220:GLY:O	1:C:226:GLY:HA3	2.00	0.60
1:A:414:SER:HB2	1:A:449:GLN:HB3	1.81	0.60
1:C:103:HIS:CE1	1:D:307:MET:O	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:THR:HG21	4:D:615:HOH:O	2.00	0.60
1:B:311:ARG:O	1:B:315:VAL:HG23	2.01	0.60
1:C:41:GLU:HB2	1:C:42:PRO:HD2	1.83	0.60
1:A:249:ALA:O	1:A:250:GLU:CB	2.49	0.59
1:A:103:HIS:HE1	1:B:307:MET:O	1.85	0.59
1:D:244:ASP:HB2	1:D:252:LEU:HD13	1.84	0.59
1:D:318:VAL:O	1:D:323:PRO:HD3	2.03	0.59
1:B:226:GLY:HA2	1:B:229:ILE:HD12	1.84	0.59
1:B:360:TYR:O	1:B:363:THR:OG1	2.21	0.59
1:B:60:LEU:HD11	1:B:178:MET:HG3	1.84	0.58
1:C:135:ARG:HD3	1:D:373:ALA:HB2	1.84	0.58
1:A:322:ALA:HB3	1:A:323:PRO:HD3	1.85	0.58
1:A:38:ARG:HG2	1:A:38:ARG:NH1	2.10	0.58
1:D:307:MET:HE3	1:D:312:TRP:HE3	1.68	0.58
1:C:126:PRO:O	1:C:135:ARG:HG3	2.04	0.57
1:A:268:VAL:HG22	2:A:501:NAI:N1A	2.19	0.57
1:D:273:ALA:O	1:D:277:ILE:HG13	2.03	0.57
1:A:145:THR:HG21	1:A:160:LEU:HB2	1.85	0.57
1:A:343:ILE:HD12	1:A:343:ILE:N	2.20	0.57
1:D:32:GLU:OE2	1:D:115:ARG:HD2	2.04	0.57
1:B:344:GLY:HA3	4:B:666:HOH:O	2.05	0.57
1:D:190:ASP:HB3	1:D:449:GLN:HB2	1.87	0.57
1:C:343:ILE:HA	1:C:386:ASN:O	2.04	0.57
1:B:266:LEU:CD1	1:B:273:ALA:HA	2.35	0.55
1:D:410:ARG:CB	4:D:629:HOH:O	2.54	0.55
1:C:401:ILE:HD13	1:C:401:ILE:H	1.71	0.55
1:C:413:ASN:HB3	1:C:450:ALA:HA	1.88	0.55
1:C:268:VAL:HG22	2:C:501:NAI:N1A	2.22	0.55
1:D:36:ARG:NH2	1:D:423:ASP:OD2	2.36	0.54
1:D:210:PRO:HD2	1:D:236:ASP:HB3	1.89	0.54
1:B:220:GLY:O	1:B:226:GLY:HA3	2.08	0.54
1:D:41:GLU:CG	1:D:42:PRO:HD2	2.36	0.54
1:D:427:ALA:O	1:D:430:TYR:HB3	2.08	0.54
1:C:120:VAL:HG22	1:C:159:ALA:HB3	1.90	0.54
1:D:110:LEU:C	1:D:112:ASN:H	2.15	0.54
1:D:118:ARG:NH2	1:D:187:ALA:HA	2.22	0.54
1:C:322:ALA:HB3	1:C:323:PRO:HD3	1.90	0.54
1:D:172:THR:HB	1:D:201:SER:H	1.73	0.54
1:B:342:VAL:O	1:B:385:ILE:HA	2.07	0.53
1:B:107:THR:HB	1:B:108:PRO:HD3	1.89	0.53
1:A:23:ALA:O	1:A:26:LEU:O	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ASN:HB2	1:D:344:GLY:HA2	1.89	0.53
1:A:433:SER:HB3	1:A:436:SER:OG	2.09	0.53
1:B:413:ASN:HB2	1:B:448:GLY:O	2.09	0.53
1:D:188:TYR:HD2	1:D:446:VAL:HG12	1.74	0.53
1:A:115:ARG:CZ	1:A:154:ARG:HD2	2.39	0.53
1:D:259:VAL:HG23	1:D:261:GLY:H	1.74	0.53
1:A:290:ASP:C	1:A:291:ILE:HG13	2.32	0.52
1:C:262:THR:OG1	1:C:280:HIS:NE2	2.39	0.52
1:B:266:LEU:HD11	1:B:273:ALA:HA	1.91	0.52
1:D:322:ALA:O	1:D:326:LEU:HG	2.09	0.52
1:D:229:ILE:HD11	1:D:428:ILE:HD13	1.90	0.52
1:D:266:LEU:HD21	1:D:273:ALA:HB1	1.92	0.52
1:B:219:THR:O	1:B:295:ASN:HB3	2.10	0.52
1:C:49:LEU:HD13	1:C:71:VAL:CG2	2.41	0.51
1:D:317:ALA:HA	1:D:321:LEU:HB2	1.92	0.51
1:A:38:ARG:CG	1:A:38:ARG:NH1	2.70	0.50
1:A:110:LEU:C	1:A:112:ASN:H	2.20	0.50
1:D:60:LEU:HD21	1:D:178:MET:HE2	1.94	0.50
1:A:413:ASN:HB3	1:A:450:ALA:HA	1.94	0.49
1:B:117:GLY:C	1:B:118:ARG:HG2	2.37	0.49
1:B:322:ALA:HB3	1:B:323:PRO:CD	2.39	0.49
1:D:244:ASP:OD1	2:D:501:NAI:H1B	2.13	0.49
1:C:408:VAL:O	1:C:412:LEU:HB2	2.13	0.49
1:A:249:ALA:HB2	1:A:265:TRP:HE1	1.76	0.49
1:C:50:ILE:HG22	1:C:57:VAL:HG23	1.94	0.49
1:D:207:TRP:O	1:D:210:PRO:HG3	2.12	0.49
1:C:141:LEU:O	1:C:144:PHE:HB3	2.13	0.49
1:B:58:GLU:HB3	1:B:59:PRO:CD	2.42	0.48
1:B:229:ILE:HA	1:B:425:ALA:HB1	1.95	0.48
1:C:394:GLU:HB3	4:C:634:HOH:O	2.13	0.48
1:D:337:GLY:HA2	1:D:338:GLU:CB	2.15	0.48
1:A:56:VAL:O	1:A:60:LEU:HB2	2.12	0.48
1:B:50:ILE:HD12	1:B:61:ARG:HG2	1.95	0.48
1:D:320:LEU:C	1:D:323:PRO:HD2	2.38	0.48
1:A:204:PRO:O	1:A:205:ALA:C	2.56	0.48
1:D:220:GLY:O	1:D:226:GLY:HA3	2.13	0.48
1:A:396:GLN:O	1:A:397:MET:HB3	2.12	0.48
1:C:106:PHE:O	1:C:107:THR:C	2.57	0.48
1:D:255:THR:O	1:D:259:VAL:HG22	2.13	0.48
1:A:234:ALA:HB2	1:A:259:VAL:HB	1.96	0.48
1:B:56:VAL:O	1:B:60:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:HG13	1:C:58:GLU:H	1.79	0.48
1:D:452:ILE:HG22	4:D:623:HOH:O	2.13	0.48
1:B:314:ALA:O	1:B:318:VAL:HG23	2.14	0.48
1:B:445:ARG:NH2	1:B:450:ALA:HB3	2.29	0.47
1:C:35:ARG:NH2	1:C:42:PRO:O	2.42	0.47
1:A:249:ALA:HB2	1:A:265:TRP:NE1	2.30	0.47
1:A:249:ALA:CB	1:A:265:TRP:HE1	2.28	0.47
1:B:82:SER:HA	1:B:112:ASN:ND2	2.29	0.47
1:B:131:SER:HB2	4:B:640:HOH:O	2.15	0.47
1:A:390:PRO:HB2	2:A:501:NAI:C5N	2.45	0.47
1:A:373:ALA:HA	1:B:135:ARG:HD3	1.97	0.47
1:B:390:PRO:HB2	2:B:501:NAI:C5N	2.45	0.47
1:A:228:THR:O	1:A:232:VAL:HG23	2.15	0.46
1:C:337:GLY:O	1:C:338:GLU:C	2.59	0.46
1:B:58:GLU:HB3	1:B:59:PRO:HD3	1.97	0.46
1:D:49:LEU:HB2	1:D:71:VAL:HG23	1.97	0.46
1:B:212:ASP:HA	1:B:237:GLY:HA3	1.96	0.46
1:D:216:ALA:HB2	1:D:291:ILE:HD12	1.98	0.46
1:A:110:LEU:C	1:A:112:ASN:N	2.73	0.46
1:D:375:ALA:N	1:D:376:PRO:HD2	2.31	0.46
1:B:58:GLU:N	1:B:59:PRO:HD2	2.31	0.45
1:D:274:VAL:HG11	1:D:329:GLY:HA3	1.98	0.45
1:B:174:LEU:HG	1:B:178:MET:HG2	1.98	0.45
1:A:404:ALA:O	1:A:405:THR:C	2.59	0.45
1:A:415:LEU:O	1:A:417:GLN:HG2	2.17	0.45
1:C:413:ASN:CB	1:C:450:ALA:HA	2.46	0.45
1:C:54:GLY:HA3	1:C:91:THR:OG1	2.16	0.45
1:A:123:GLY:O	1:A:162:TYR:HA	2.16	0.45
1:D:178:MET:O	1:D:182:LEU:HB2	2.17	0.45
1:A:314:ALA:O	1:A:318:VAL:HG23	2.17	0.45
1:B:298:ILE:HG13	1:B:300:ARG:NH1	2.32	0.45
1:A:26:LEU:HD23	1:B:22:LEU:CD1	2.47	0.44
1:A:161:VAL:HG22	1:A:194:PHE:HB2	1.99	0.44
3:A:502:ZPG:H212	4:B:602:HOH:O	2.17	0.44
1:B:82:SER:HA	1:B:112:ASN:HD22	1.82	0.44
1:D:47:SER:O	1:D:83:PHE:HA	2.18	0.44
1:A:300:ARG:HB3	1:A:311:ARG:HG2	2.00	0.44
1:D:190:ASP:HB3	1:D:449:GLN:CB	2.47	0.44
1:D:35:ARG:NH1	1:D:184:ALA:HB2	2.33	0.44
1:A:443:VAL:HG23	4:A:622:HOH:O	2.17	0.44
1:C:57:VAL:HG13	1:C:58:GLU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:PRO:C	1:C:135:ARG:HG3	2.43	0.44
1:B:348:ILE:HD12	1:B:348:ILE:HA	1.83	0.43
1:D:343:ILE:N	1:D:343:ILE:HD12	2.33	0.43
1:A:346:SER:OG	1:A:347:SER:N	2.48	0.43
1:C:47:SER:N	1:C:84:GLY:H	2.16	0.43
1:C:119:VAL:O	1:C:158:THR:HA	2.18	0.43
1:A:106:PHE:O	1:A:110:LEU:HG	2.18	0.43
1:A:110:LEU:O	1:A:112:ASN:N	2.51	0.43
1:A:270:ALA:O	1:A:271:ASP:C	2.60	0.43
1:D:115:ARG:O	1:D:116:CYS:C	2.61	0.43
1:A:115:ARG:NH2	1:A:154:ARG:CD	2.77	0.43
1:C:348:ILE:HG12	1:C:391:GLY:HA2	2.00	0.43
1:B:452:ILE:HD13	1:B:452:ILE:HG21	1.77	0.43
1:B:160:LEU:O	1:B:193:VAL:HA	2.18	0.43
1:B:209:LYS:HG2	1:B:212:ASP:HB2	2.01	0.43
1:A:32:GLU:OE2	1:A:115:ARG:HG2	2.20	0.42
1:A:364:LYS:NZ	2:A:501:NAI:O3D	2.51	0.42
1:D:126:PRO:C	1:D:128:ALA:H	2.27	0.42
1:A:396:GLN:O	1:A:397:MET:CB	2.67	0.42
1:B:57:VAL:O	1:B:61:ARG:HG3	2.19	0.42
1:D:185:LYS:HB3	1:D:426:GLU:HG2	2.00	0.42
1:B:364:LYS:HD3	1:B:364:LYS:HA	1.80	0.42
1:D:58:GLU:O	1:D:59:PRO:C	2.62	0.42
1:A:170:ALA:HB3	4:A:671:HOH:O	2.19	0.42
1:B:317:ALA:HA	1:B:321:LEU:HB2	2.00	0.42
1:D:307:MET:HE3	1:D:312:TRP:CE3	2.51	0.42
1:C:299:THR:HG22	1:C:360:TYR:CD1	2.54	0.42
1:D:129:ALA:HB1	1:D:134:GLU:HB3	2.00	0.42
1:A:196:VAL:HG22	1:A:439:VAL:HG22	2.01	0.42
1:D:312:TRP:CE3	1:D:359:ASN:HB3	2.55	0.42
1:A:89:ASP:OD1	1:A:89:ASP:C	2.63	0.42
1:A:184:ALA:O	1:A:187:ALA:HB2	2.20	0.41
1:A:386:ASN:OD1	1:A:442:ASN:HB2	2.20	0.41
1:D:354:ASN:O	1:D:357:GLN:HB2	2.20	0.41
1:A:102:LEU:HD13	1:A:144:PHE:CD1	2.55	0.41
1:A:397:MET:O	1:A:397:MET:SD	2.78	0.41
1:D:145:THR:HG21	1:D:160:LEU:HB2	2.02	0.41
1:A:94:THR:O	1:A:134:GLU:HA	2.20	0.41
1:D:389:ALA:O	1:D:445:ARG:HA	2.20	0.41
1:C:41:GLU:CB	1:C:42:PRO:HD2	2.49	0.41
1:D:60:LEU:HD12	1:D:60:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA3	1:A:105:PHE:CE1	2.55	0.41
1:C:401:ILE:HA	1:C:402:PRO:HD2	1.76	0.41
1:C:414:SER:HB2	1:C:449:GLN:HB3	2.02	0.41
1:C:202:THR:HA	1:C:203:PRO:HD2	1.85	0.41
1:A:102:LEU:HD13	1:A:144:PHE:CG	2.55	0.41
1:A:307:MET:HE2	1:A:307:MET:HB2	2.00	0.41
1:D:414:SER:HB2	1:D:449:GLN:HB3	2.01	0.41
1:A:148:LEU:HD12	1:A:148:LEU:HA	1.87	0.41
1:B:244:ASP:O	1:B:266:LEU:N	2.46	0.41
1:C:341:ARG:HH22	1:C:437:ASN:HB3	1.85	0.41
1:C:352:ALA:HB2	1:C:453:GLY:HA2	2.02	0.41
1:D:190:ASP:HB3	1:D:449:GLN:N	2.36	0.41
1:D:210:PRO:HD2	1:D:236:ASP:CB	2.50	0.41
1:D:246:GLU:O	1:D:247:SER:C	2.63	0.41
1:D:295:ASN:O	1:D:295:ASN:CG	2.64	0.41
1:B:181:LEU:HD21	1:B:194:PHE:CZ	2.56	0.41
1:C:304:LEU:HD21	1:D:106:PHE:HB2	2.03	0.41
1:B:51:GLY:HA3	1:B:105:PHE:CE1	2.57	0.40
1:D:141:LEU:O	1:D:144:PHE:HB3	2.20	0.40
1:A:136:ILE:HG12	1:B:370:ILE:HA	2.02	0.40
1:A:397:MET:SD	1:A:397:MET:C	3.04	0.40
1:B:273:ALA:O	1:B:277:ILE:HG13	2.22	0.40
1:D:331:VAL:HG23	1:D:336:ILE:HD12	2.02	0.40
1:B:280:HIS:CD2	1:B:280:HIS:C	2.99	0.40
1:C:266:LEU:HG	1:C:267:ASP:N	2.36	0.40
1:D:110:LEU:C	1:D:112:ASN:N	2.79	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	423/454 (93%)	392 (93%)	26 (6%)	5 (1%)	10	34
1	B	417/454 (92%)	390 (94%)	25 (6%)	2 (0%)	24	55
1	C	412/454 (91%)	384 (93%)	22 (5%)	6 (2%)	8	28
1	D	399/454 (88%)	360 (90%)	34 (8%)	5 (1%)	9	31
All	All	1651/1816 (91%)	1526 (92%)	107 (6%)	18 (1%)	11	36

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	GLU
1	C	347	SER
1	D	100	LYS
1	D	337	GLY
1	A	111	ARG
1	A	197	GLY
1	A	397	MET
1	C	39	ALA
1	C	79	TRP
1	D	111	ARG
1	B	283	ASP
1	C	404	ALA
1	D	116	CYS
1	A	399	ALA
1	B	346	SER
1	C	73	ASN
1	D	305	ALA
1	C	40	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	306/331 (92%)	286 (94%)	20 (6%)	15	43
1	B	303/331 (92%)	281 (93%)	22 (7%)	13	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	292/331 (88%)	279 (96%)	13 (4%)	24	58
1	D	287/331 (87%)	255 (89%)	32 (11%)	6	20
All	All	1188/1324 (90%)	1101 (93%)	87 (7%)	13	38

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

Mol	Chain	Res	Type
1	A	24	ARG
1	A	25	GLN
1	A	26	LEU
1	A	28	VAL
1	A	38	ARG
1	A	41	GLU
1	A	56	VAL
1	A	57	VAL
1	A	60	LEU
1	A	69	ASP
1	A	95	GLU
1	A	115	ARG
1	A	168	LYS
1	A	251	ASN
1	A	307	MET
1	A	343	ILE
1	A	345	LEU
1	A	348	ILE
1	A	397	MET
1	A	411	ARG
1	B	36	ARG
1	B	56	VAL
1	B	95	GLU
1	B	112	ASN
1	B	202	THR
1	B	219	THR
1	B	244	ASP
1	B	257	SER
1	B	266	LEU
1	B	271	ASP
1	B	274	VAL
1	B	276	LYS
1	B	288	LYS
1	B	290	ASP

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Mol	Chain	Res	Type
1	B	315	VAL
1	B	316	LEU
1	B	327	THR
1	B	348	ILE
1	B	403	LEU
1	B	413	ASN
1	B	451	MET
1	B	452	ILE
1	C	71	VAL
1	C	74	ASN
1	C	94	THR
1	C	202	THR
1	C	223	ARG
1	C	231	GLU
1	C	254	GLU
1	C	271	ASP
1	C	325	ARG
1	C	401	ILE
1	C	407	GLU
1	C	408	VAL
1	C	451	MET
1	D	30	GLN
1	D	45	THR
1	D	70	LEU
1	D	71	VAL
1	D	95	GLU
1	D	107	THR
1	D	172	THR
1	D	208	GLU
1	D	212	ASP
1	D	229	ILE
1	D	233	PHE
1	D	246	GLU
1	D	254	GLU
1	D	255	THR
1	D	258	LYS
1	D	265	TRP
1	D	269	THR
1	D	274	VAL
1	D	282	ARG
1	D	298	ILE
1	D	309	ASP

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Mol	Chain	Res	Type
1	D	316	LEU
1	D	327	THR
1	D	388	VAL
1	D	394	GLU
1	D	395	THR
1	D	401	ILE
1	D	407	GLU
1	D	412	LEU
1	D	417	GLN
1	D	426	GLU
1	D	452	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	103	HIS
1	A	192	GLN
1	A	251	ASN
1	A	285	HIS
1	A	372	GLN
1	B	25	GLN
1	B	192	GLN
1	B	251	ASN
1	B	280	HIS
1	B	294	ASN
1	B	354	ASN
1	B	357	GLN
1	B	413	ASN
1	B	449	GLN
1	C	103	HIS
1	C	192	GLN
1	C	251	ASN
1	C	284	HIS
1	C	285	HIS
1	D	192	GLN
1	D	306	ASN
1	D	417	GLN
1	D	420	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 ⓘ

5 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	ZPG	A	502	-	12,12,28	0.73	0	14,14,34	1.16	2 (14%)
2	NAI	D	501	-	47,48,48	2.19	16 (34%)	64,73,73	2.19	17 (26%)
2	NAI	A	501	-	47,48,48	1.99	14 (29%)	64,73,73	1.90	15 (23%)
2	NAI	C	501	-	47,48,48	2.39	15 (31%)	64,73,73	2.21	16 (25%)
2	NAI	B	501	-	47,48,48	1.94	14 (29%)	64,73,73	2.32	17 (26%)

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	ZPG	A	502	-	-	4/12/12/31	-
2	NAI	D	501	-	-	7/29/72/72	0/5/5/5
2	NAI	A	501	-	-	5/29/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	C	501	-	-	5/29/72/72	0/5/5/5
2	NAI	B	501	-	-	9/29/72/72	0/5/5/5

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAI	PA-O3	7.90	1.68	1.59
2	C	501	NAI	PN-O3	7.14	1.67	1.59
2	D	501	NAI	PA-O3	7.03	1.67	1.59
2	A	501	NAI	PA-O3	6.90	1.66	1.59
2	B	501	NAI	PA-O3	5.00	1.64	1.59
2	A	501	NAI	PA-O1A	4.47	1.66	1.50
2	D	501	NAI	C4N-C3N	-4.42	1.41	1.50
2	C	501	NAI	C4N-C3N	-4.41	1.41	1.50
2	D	501	NAI	PA-O1A	4.26	1.65	1.50
2	B	501	NAI	C4N-C3N	-4.09	1.42	1.50
2	D	501	NAI	C2A-N3A	4.00	1.41	1.33
2	D	501	NAI	C2A-N1A	3.96	1.41	1.33
2	B	501	NAI	PA-O1A	3.94	1.64	1.50
2	A	501	NAI	C2A-N1A	3.89	1.40	1.33
2	B	501	NAI	C2A-N3A	3.80	1.40	1.33
2	B	501	NAI	C2A-N1A	3.73	1.40	1.33
2	C	501	NAI	PA-O1A	3.70	1.63	1.50
2	D	501	NAI	C4N-C5N	-3.54	1.39	1.49
2	C	501	NAI	C7N-C3N	-3.48	1.41	1.48
2	D	501	NAI	C7N-C3N	-3.42	1.41	1.48
2	B	501	NAI	PN-O3	3.38	1.63	1.59
2	C	501	NAI	C2A-N3A	3.37	1.39	1.33
2	C	501	NAI	C2A-N1A	3.34	1.39	1.33
2	B	501	NAI	C4N-C5N	-3.31	1.40	1.49
2	D	501	NAI	PN-O3	3.29	1.63	1.59
2	A	501	NAI	C4N-C3N	-3.27	1.43	1.50
2	B	501	NAI	C7N-C3N	-3.24	1.41	1.48
2	A	501	NAI	C7N-C3N	-3.23	1.41	1.48
2	D	501	NAI	C5A-N7A	-3.15	1.33	1.39
2	A	501	NAI	C5A-N7A	-3.10	1.33	1.39
2	C	501	NAI	C5A-C4A	-3.01	1.33	1.39
2	A	501	NAI	C2A-N3A	2.89	1.39	1.33
2	C	501	NAI	C5A-N7A	-2.80	1.34	1.39
2	A	501	NAI	C5A-C6A	-2.75	1.33	1.41
2	A	501	NAI	C4N-C5N	-2.74	1.41	1.49
2	A	501	NAI	C2N-C3N	2.70	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAI	C6N-C5N	2.67	1.41	1.33
2	B	501	NAI	C5A-C4A	-2.63	1.34	1.39
2	D	501	NAI	C8A-N9A	-2.63	1.33	1.37
2	C	501	NAI	C6N-C5N	2.55	1.40	1.33
2	A	501	NAI	C5A-C4A	-2.54	1.34	1.39
2	C	501	NAI	C4N-C5N	-2.53	1.42	1.49
2	C	501	NAI	C2N-C3N	2.53	1.42	1.35
2	D	501	NAI	C6N-C5N	2.50	1.40	1.33
2	D	501	NAI	C2N-C3N	2.50	1.42	1.35
2	B	501	NAI	C6N-C5N	2.43	1.40	1.33
2	B	501	NAI	C2N-C3N	2.36	1.41	1.35
2	D	501	NAI	C5A-C4A	-2.32	1.35	1.39
2	C	501	NAI	C5A-C6A	-2.30	1.34	1.41
2	B	501	NAI	C5A-N7A	-2.29	1.34	1.39
2	B	501	NAI	PN-O1N	2.21	1.65	1.55
2	A	501	NAI	C8A-N9A	-2.19	1.33	1.37
2	C	501	NAI	C8A-N9A	-2.18	1.33	1.37
2	D	501	NAI	C4A-N9A	-2.16	1.33	1.37
2	B	501	NAI	C8A-N9A	-2.16	1.33	1.37
2	C	501	NAI	O4D-C1D	2.15	1.47	1.42
2	D	501	NAI	O4D-C1D	2.15	1.47	1.42
2	A	501	NAI	C4A-N9A	-2.13	1.33	1.37
2	D	501	NAI	C5A-C6A	-2.09	1.35	1.41

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAI	C6N-N1N-C2N	-9.70	108.94	119.32
2	C	501	NAI	C6N-N1N-C2N	-7.77	111.01	119.32
2	B	501	NAI	N3A-C2A-N1A	-7.58	117.11	128.58
2	B	501	NAI	C6N-N1N-C2N	-7.29	111.52	119.32
2	C	501	NAI	N3A-C2A-N1A	-7.25	117.60	128.58
2	A	501	NAI	N3A-C2A-N1A	-7.19	117.70	128.58
2	D	501	NAI	N3A-C2A-N1A	-5.80	119.80	128.58
2	C	501	NAI	N9A-C8A-N7A	-4.96	106.90	113.94
2	B	501	NAI	N9A-C8A-N7A	-4.77	107.17	113.94
2	B	501	NAI	O4B-C1B-N9A	4.69	117.09	108.09
2	A	501	NAI	C1D-N1N-C6N	-4.62	111.01	120.77
2	D	501	NAI	O4D-C1D-N1N	4.54	116.73	108.08
2	B	501	NAI	C5A-C4A-N3A	-4.42	120.63	126.72
2	D	501	NAI	C1D-N1N-C6N	-4.20	111.89	120.77
2	D	501	NAI	C5A-C4A-N3A	-4.15	121.00	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAI	C5A-C4A-N3A	-4.02	121.17	126.72
2	C	501	NAI	C3N-C2N-N1N	-3.95	117.40	123.20
2	A	501	NAI	N9A-C8A-N7A	-3.85	108.47	113.94
2	D	501	NAI	N9A-C8A-N7A	-3.82	108.52	113.94
2	B	501	NAI	C2A-N3A-C4A	3.72	120.93	111.83
2	A	501	NAI	C5A-C4A-N3A	-3.70	121.62	126.72
2	C	501	NAI	O4B-C4B-C5B	-3.67	97.58	109.33
2	B	501	NAI	C1D-N1N-C6N	-3.65	113.05	120.77
2	C	501	NAI	C5A-N7A-C8A	3.46	108.89	103.45
2	A	501	NAI	C6N-N1N-C2N	-3.44	115.64	119.32
2	B	501	NAI	C5A-N7A-C8A	3.43	108.85	103.45
2	C	501	NAI	C2A-N3A-C4A	3.40	120.14	111.83
2	B	501	NAI	C5B-C4B-C3B	-3.39	103.03	115.21
2	A	501	NAI	O4D-C1D-N1N	3.32	114.42	108.08
2	C	501	NAI	C4A-N9A-C8A	3.27	109.17	105.74
2	A	501	NAI	C2A-N3A-C4A	3.17	119.57	111.83
2	C	501	NAI	O4B-C1B-N9A	3.16	114.15	108.09
2	B	501	NAI	C4A-N9A-C8A	3.07	108.97	105.74
2	B	501	NAI	C4B-O4B-C1B	-3.07	102.68	109.47
2	D	501	NAI	C6A-C5A-C4A	3.01	121.29	117.18
2	D	501	NAI	C5A-N7A-C8A	2.99	108.15	103.45
2	B	501	NAI	C3N-C2N-N1N	-2.93	118.90	123.20
2	C	501	NAI	O1N-PN-O3	2.88	115.05	107.27
2	B	501	NAI	O4D-C1D-N1N	2.84	113.50	108.08
2	B	501	NAI	C4A-C5A-N7A	-2.81	107.37	110.58
2	D	501	NAI	C4A-C5A-N7A	-2.81	107.37	110.58
2	C	501	NAI	C5A-C6A-N6A	-2.81	116.34	123.29
2	D	501	NAI	C2A-N3A-C4A	2.74	118.52	111.83
2	B	501	NAI	N3A-C4A-N9A	2.68	131.72	127.17
2	A	501	NAI	C4A-N9A-C1B	-2.65	120.43	126.63
2	C	501	NAI	N3A-C4A-N9A	2.65	131.68	127.17
3	A	502	ZPG	O20-C20-C18	2.64	115.65	108.64
2	A	501	NAI	O1N-PN-O3	2.63	114.39	107.27
2	D	501	NAI	O2A-PA-O3	2.60	114.29	107.27
2	A	501	NAI	O3-PA-O1A	-2.58	102.93	110.70
2	B	501	NAI	C5A-C6A-N6A	-2.56	116.95	123.29
2	A	501	NAI	C5A-C6A-N6A	-2.50	117.10	123.29
2	D	501	NAI	O4B-C1B-N9A	-2.50	103.29	108.09
2	C	501	NAI	O4D-C1D-N1N	2.46	112.78	108.08
2	D	501	NAI	C5A-C6A-N6A	-2.41	117.32	123.29
2	B	501	NAI	O4B-C1B-C2B	-2.38	101.53	106.62
2	C	501	NAI	C4A-C5A-N7A	-2.36	107.88	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAI	C5A-N7A-C8A	2.32	107.09	103.45
2	D	501	NAI	C3N-C2N-N1N	-2.27	119.87	123.20
2	D	501	NAI	N3A-C4A-N9A	2.18	130.88	127.17
2	C	501	NAI	C1D-N1N-C6N	-2.16	116.21	120.77
2	D	501	NAI	C5A-C4A-N9A	2.12	108.12	105.81
2	A	501	NAI	C4A-N9A-C8A	2.09	107.94	105.74
2	D	501	NAI	C2B-C3B-C4B	2.09	106.65	102.61
2	A	501	NAI	O2A-PA-O3	2.08	112.91	107.27
3	A	502	ZPG	C21-O20-C20	2.06	118.09	115.05
2	A	501	NAI	C1B-N9A-C8A	2.04	131.63	127.09

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAI	C5B-O5B-PA-O1A
2	B	501	NAI	C5B-O5B-PA-O1A
2	B	501	NAI	C5D-O5D-PN-O1N
2	B	501	NAI	O4D-C4D-C5D-O5D
2	D	501	NAI	O4B-C4B-C5B-O5B
2	C	501	NAI	O4D-C4D-C5D-O5D
2	D	501	NAI	O4D-C4D-C5D-O5D
2	D	501	NAI	C3B-C4B-C5B-O5B
2	B	501	NAI	C3D-C4D-C5D-O5D
2	A	501	NAI	C2D-C1D-N1N-C6N
2	C	501	NAI	C3D-C4D-C5D-O5D
2	D	501	NAI	C3D-C4D-C5D-O5D
3	A	502	ZPG	C27-C24-O23-C22
2	D	501	NAI	C4B-C5B-O5B-PA
2	C	501	NAI	C2D-C1D-N1N-C6N
2	A	501	NAI	O4D-C1D-N1N-C6N
3	A	502	ZPG	C26-C22-O23-C24
3	A	502	ZPG	C25-C20-O20-C21
2	A	501	NAI	C5B-O5B-PA-O2A
2	A	501	NAI	C5B-O5B-PA-O3
2	B	501	NAI	C5D-O5D-PN-O3
2	C	501	NAI	O4D-C1D-N1N-C6N
2	B	501	NAI	C2D-C1D-N1N-C6N
2	D	501	NAI	O4D-C1D-N1N-C6N
2	B	501	NAI	O4D-C1D-N1N-C6N
2	D	501	NAI	C2D-C1D-N1N-C6N
2	B	501	NAI	PA-O3-PN-O2N

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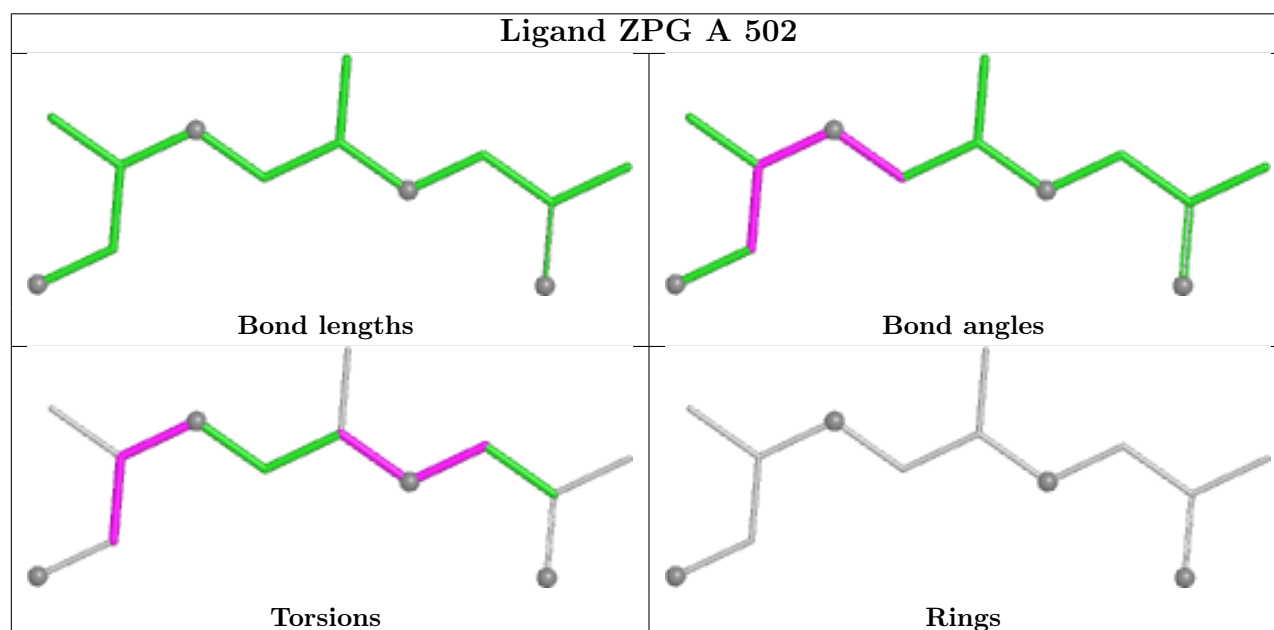
Mol	Chain	Res	Type	Atoms
2	C	501	NAI	O4B-C4B-C5B-O5B
3	A	502	ZPG	O17-C18-C20-C25
2	B	501	NAI	PA-O3-PN-O1N

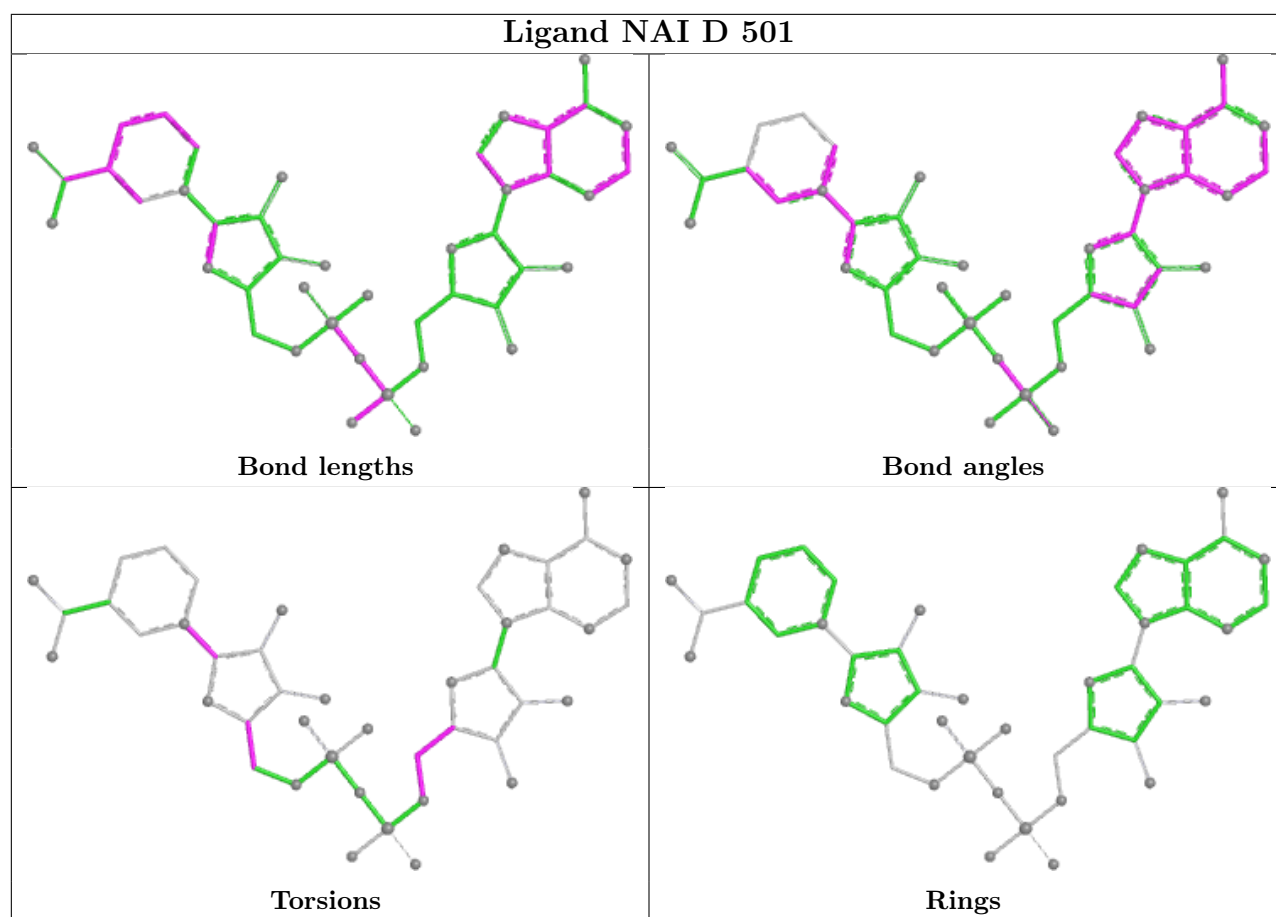
There are no ring outliers.

5 monomers are involved in 7 short contacts:

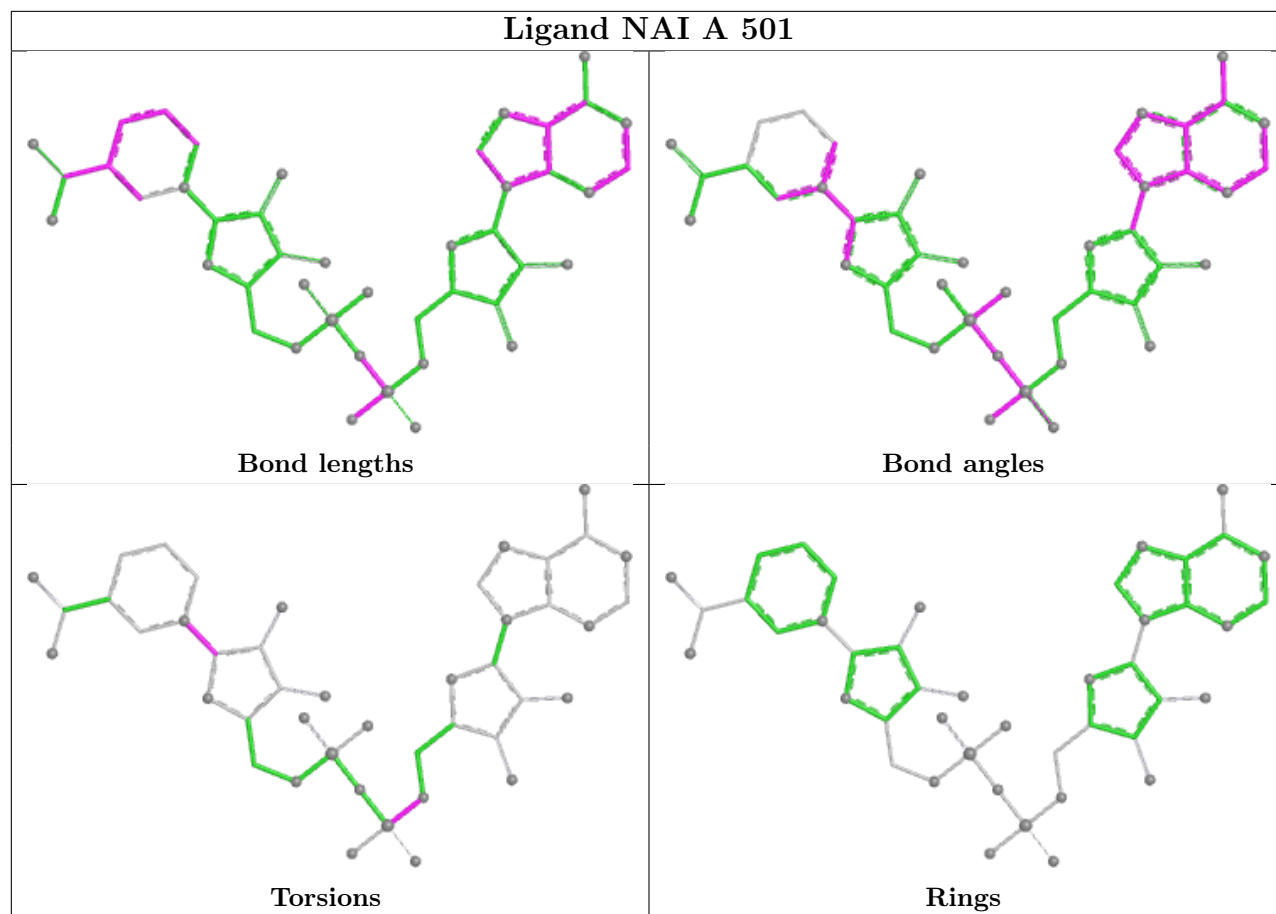
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ZPG	1	0
2	D	501	NAI	1	0
2	A	501	NAI	3	0
2	C	501	NAI	1	0
2	B	501	NAI	1	0

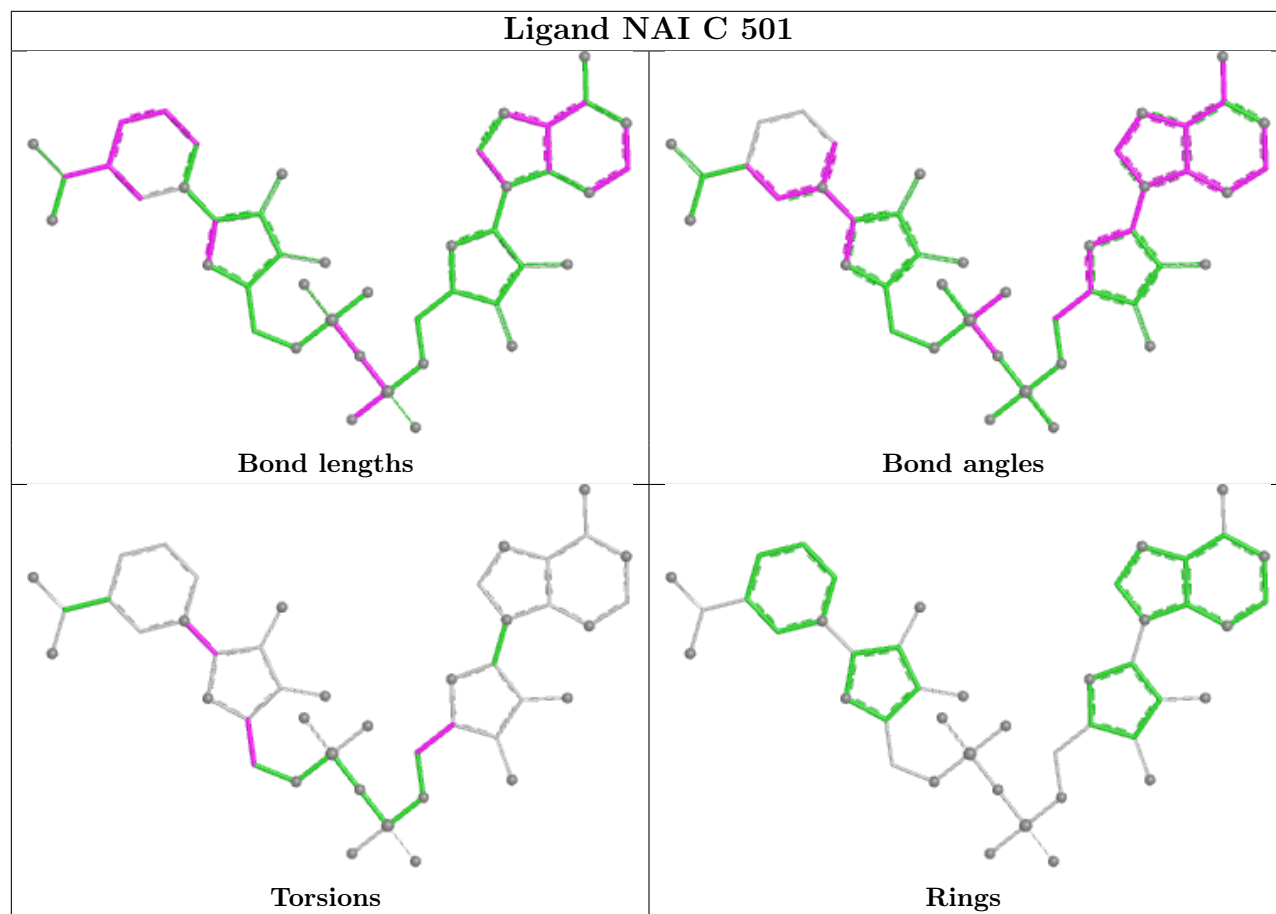
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

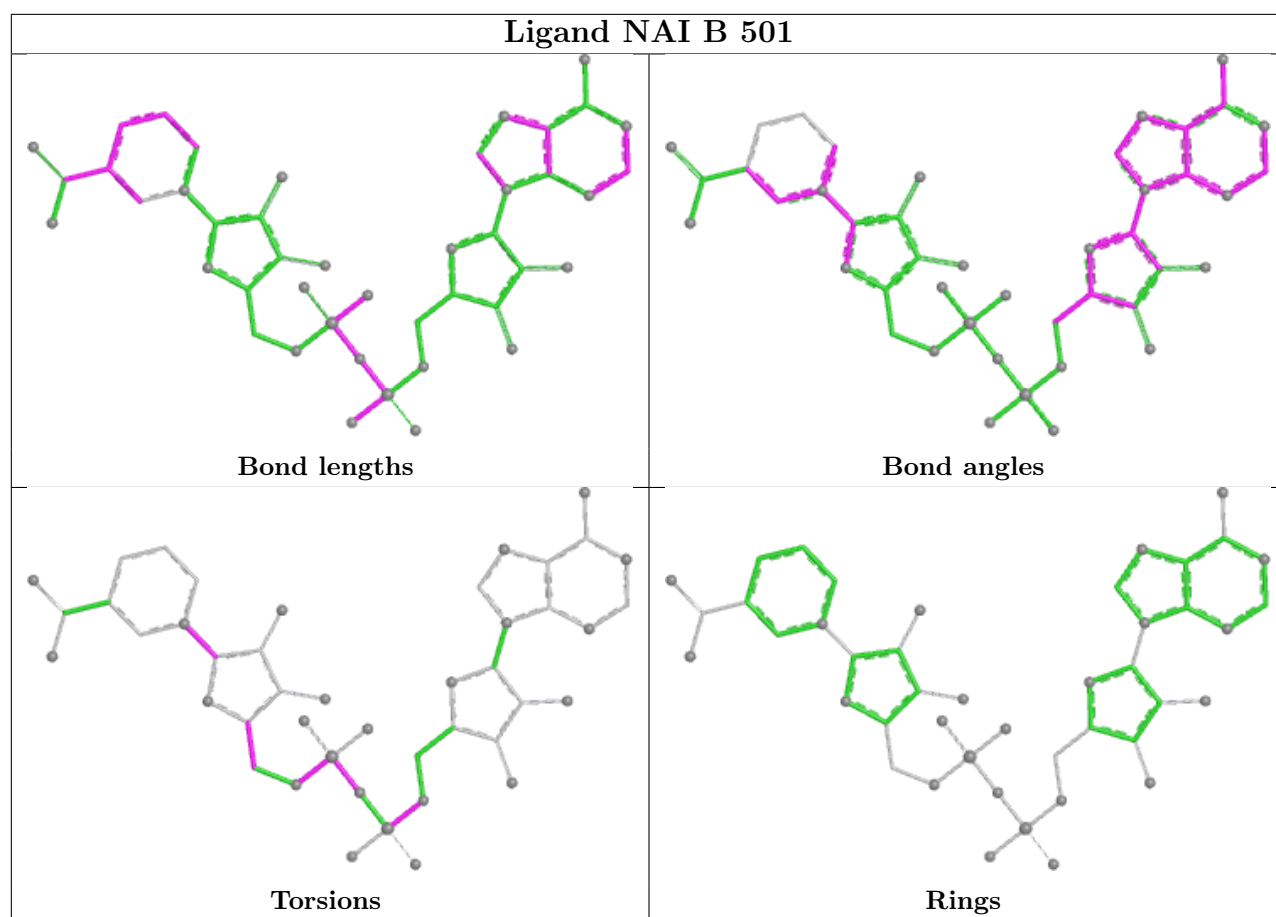




Ligand NAI A 501







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9
1	A	427/454 (94%)	-0.87	0	100100	13, 31, 51, 62	0
1	B	425/454 (93%)	-0.75	0	100100	11, 35, 66, 79	0
1	C	418/454 (92%)	-0.71	0	100100	21, 39, 61, 76	0
1	D	409/454 (90%)	-0.43	2 (0%)	8782	26, 52, 82, 93	0
All	All	1679/1816 (92%)	-0.69	2 (0%)	9290	11, 39, 71, 93	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	401	ILE	2.5
1	D	242	ALA	2.4

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

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

6.3 Carbohydrates [i](#)

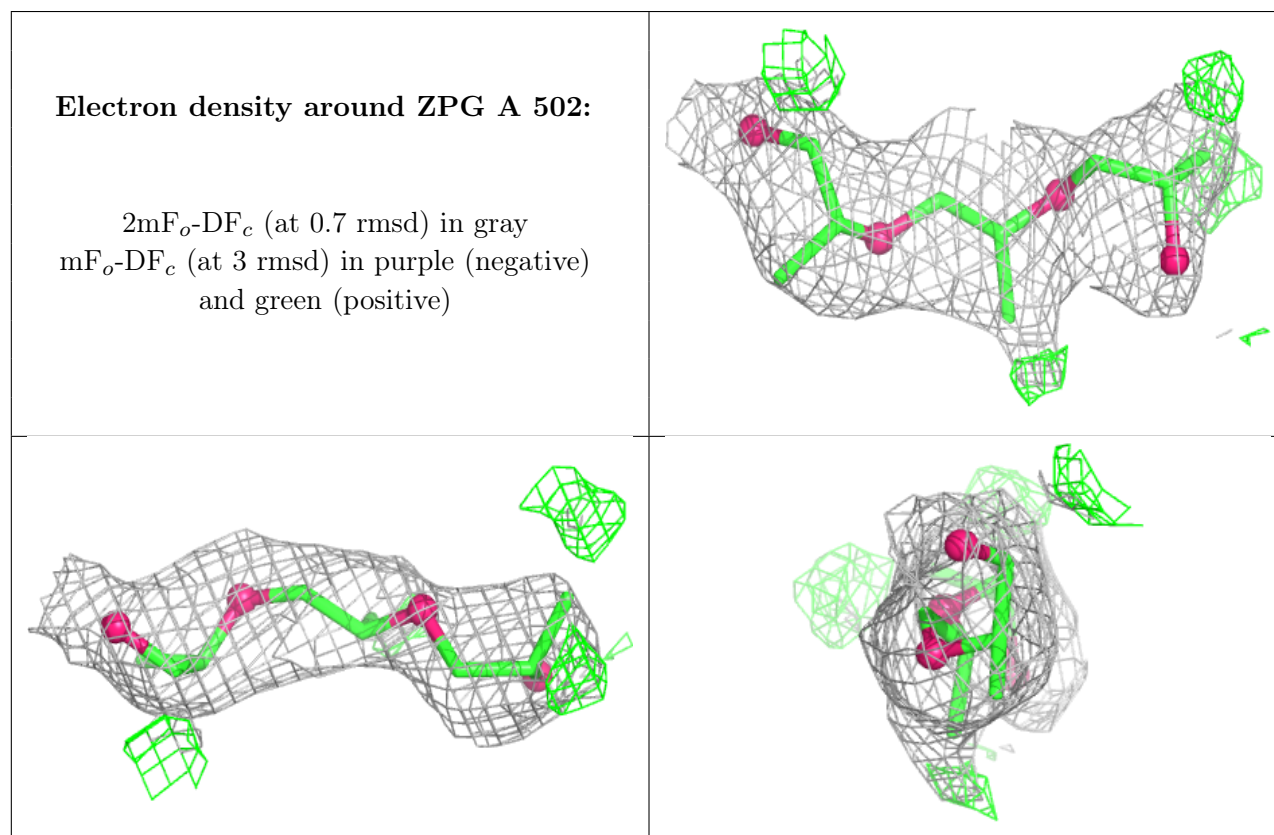
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

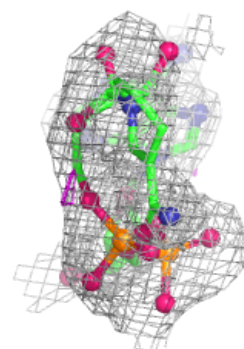
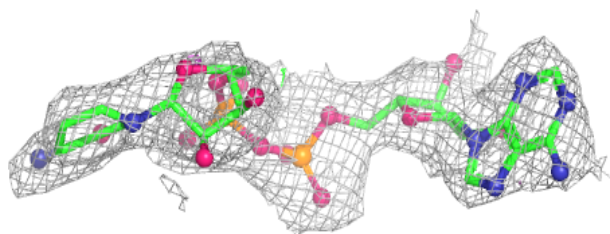
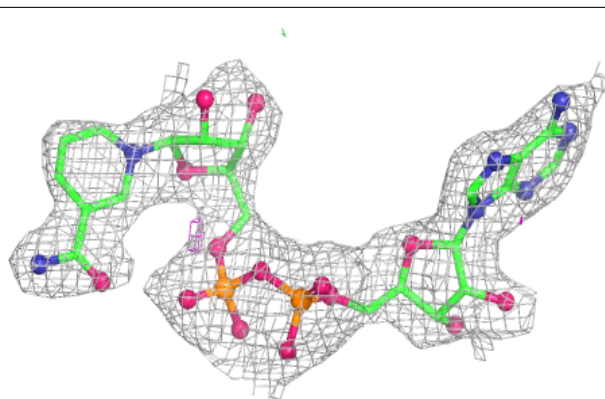
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZPG	A	502	13/29	0.84	0.11	65,67,69,70	0
2	NAI	B	501	44/44	0.90	0.09	63,67,72,73	0
2	NAI	D	501	44/44	0.92	0.08	54,64,74,77	0
2	NAI	C	501	44/44	0.95	0.07	34,45,56,58	0
2	NAI	A	501	44/44	0.96	0.06	29,37,43,46	0

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.

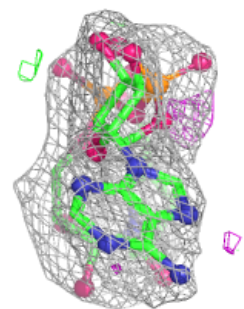
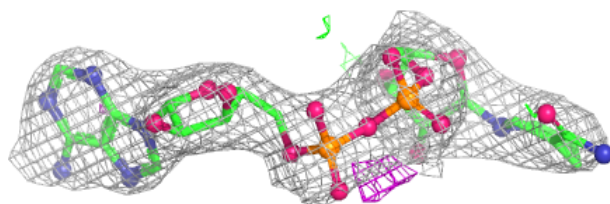
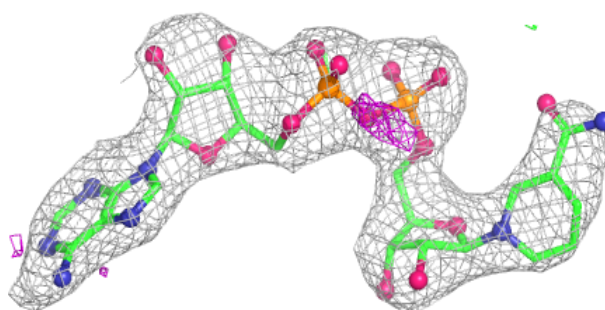


Electron density around NAI B 501:

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

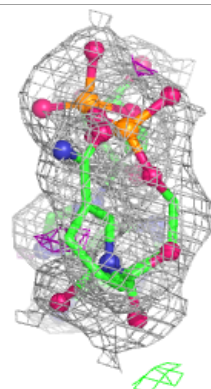
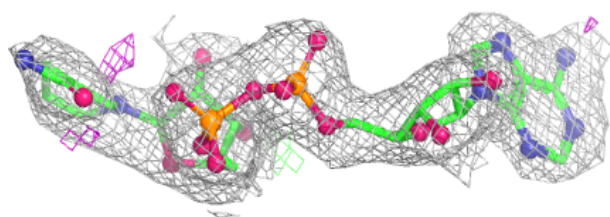
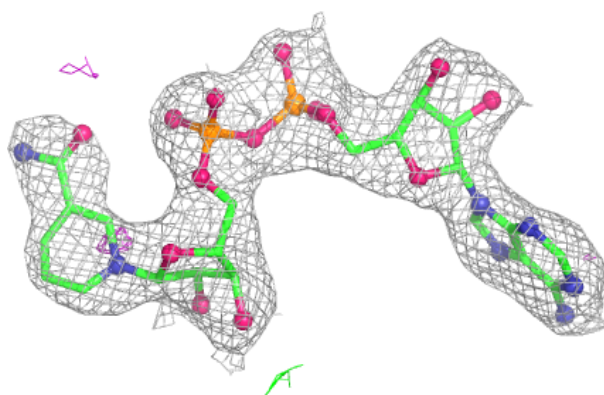
**Electron density around NAI D 501:**

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

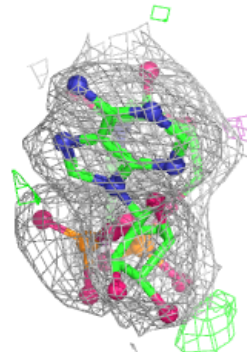
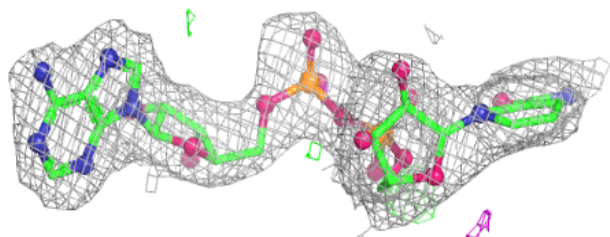
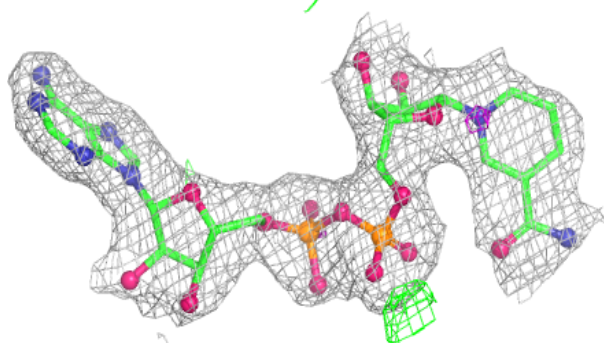


Electron density around NAI C 501:

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

**Electron density around NAI A 501:**

$2mF_o-DF_c$ (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.