



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:09 pm BST

PDB ID : 3NJ4
Title : Fluoro-neplanocin A in Human S-Adenosylhomocysteine Hydrolase
Authors : Jeong, L.S.; Lee, K.M.; Hwang, K.Y.; Choi, S.; Heo, Y.S.
Deposited on : 2010-06-17
Resolution : 2.50 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

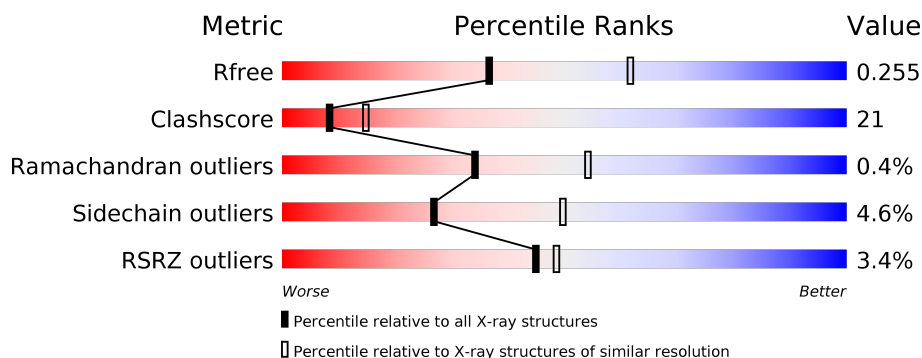
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	435	<div> <div>5%</div> <div> <div></div> <div>62%</div> <div>35%</div> <div>..</div> </div> </div>
1	B	435	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>33%</div> <div>..</div> </div> </div>
1	C	435	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>36%</div> <div>..</div> </div> </div>
1	D	435	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>34%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13846 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 Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3336	2115	572	624	25			
1	B	430	Total	C	N	O	S	0	0	0
			3330	2112	571	622	25			
1	C	431	Total	C	N	O	S	0	0	0
			3336	2115	572	624	25			
1	D	430	Total	C	N	O	S	0	0	0
			3330	2112	571	622	25			

There are 12 discrepancies between the modelled and reference sequences:

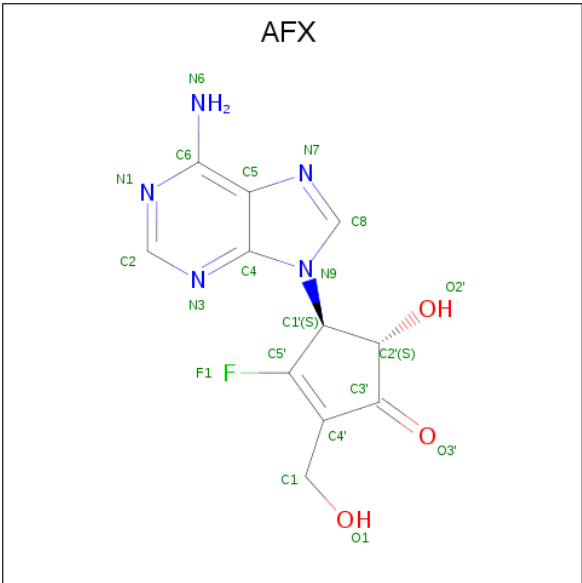
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P23526
A	-1	SER	-	EXPRESSION TAG	UNP P23526
A	0	HIS	-	EXPRESSION TAG	UNP P23526
B	-2	GLY	-	EXPRESSION TAG	UNP P23526
B	-1	SER	-	EXPRESSION TAG	UNP P23526
B	0	HIS	-	EXPRESSION TAG	UNP P23526
C	-2	GLY	-	EXPRESSION TAG	UNP P23526
C	-1	SER	-	EXPRESSION TAG	UNP P23526
C	0	HIS	-	EXPRESSION TAG	UNP P23526
D	-2	GLY	-	EXPRESSION TAG	UNP P23526
D	-1	SER	-	EXPRESSION TAG	UNP P23526
D	0	HIS	-	EXPRESSION TAG	UNP P23526

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is (4S,5S)-4-(6-amino-9H-purin-9-yl)-3-fluoro-5-hydroxy-2-(hydroxymethyl)cyclopent-2-en-1-one (three-letter code: AFX) (formula: C₁₁H₁₀FN₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			20	11	1	5	3		
3	B	1	Total	C	F	N	O	0	0
			20	11	1	5	3		
3	C	1	Total	C	F	N	O	0	0
			20	11	1	5	3		
3	D	1	Total	C	F	N	O	0	0
			20	11	1	5	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	92	Total	O	0	0
			92	92		
4	C	41	Total	O	0	0
			41	41		
4	D	58	Total	O	0	0
			58	58		

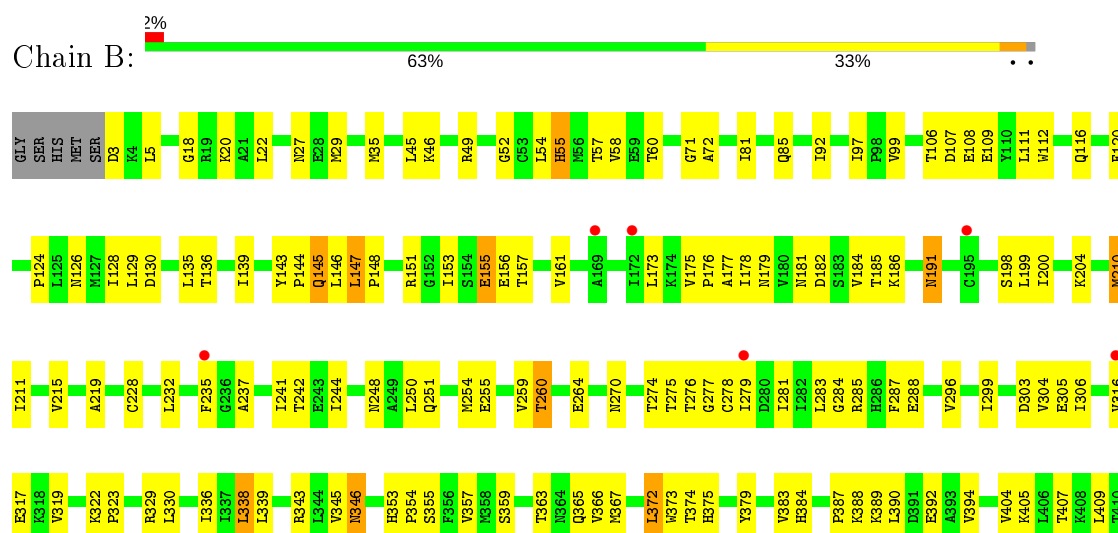
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Adenosylhomocysteinase

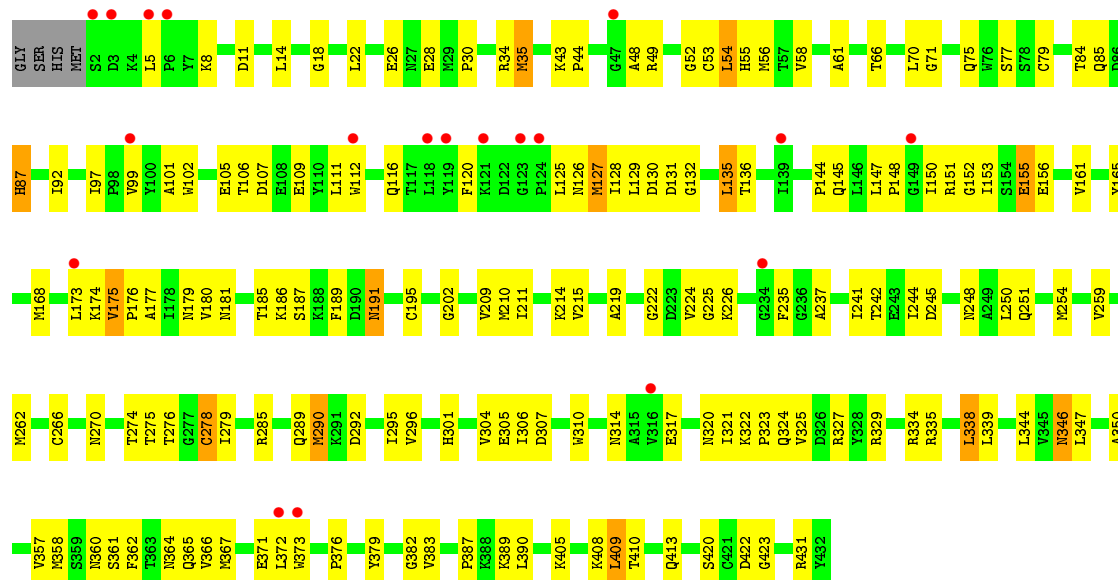


• Molecule 1: Adenosylhomocysteinase

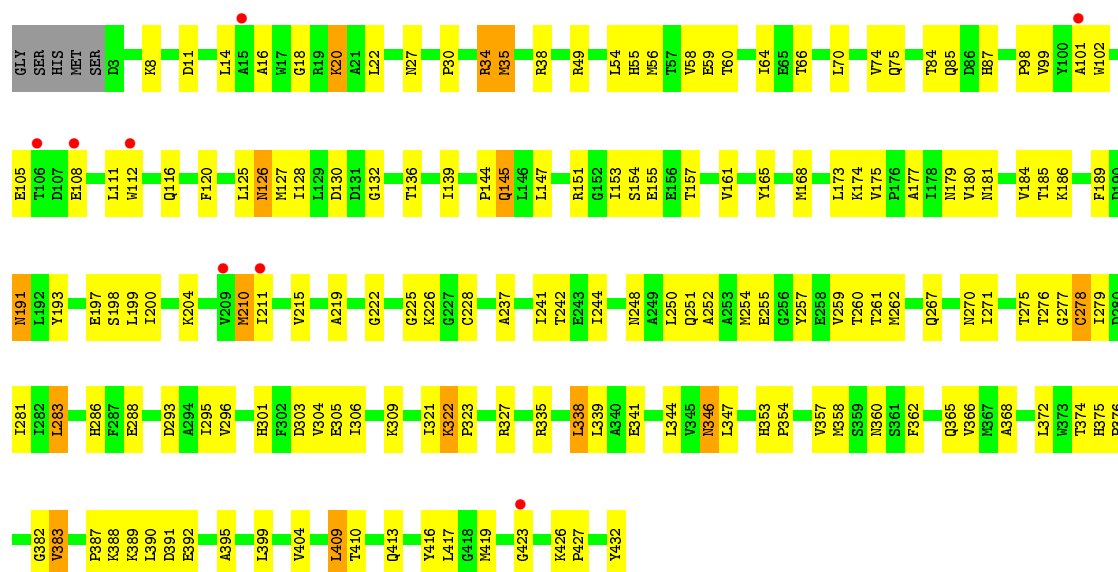




• Molecule 1: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.20 Å 81.94 Å 129.60 Å 90.00° 107.01° 90.00°	Depositor
Resolution (Å)	43.61 – 2.50 43.61 – 2.49	Depositor EDS
% Data completeness (in resolution range)	87.1 (43.61-2.50) 86.3 (43.61-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.48 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.261 0.201 , 0.255	Depositor DCC
R_{free} test set	3954 reflections (6.81%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13846	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: AFX, 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	0.38	0/3400	0.60	0/4601
1	B	0.40	0/3394	0.61	0/4593
1	C	0.36	0/3400	0.57	0/4601
1	D	0.38	0/3394	0.60	0/4593
All	All	0.38	0/13588	0.60	0/18388

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3336	0	3348	164	0
1	B	3330	0	3343	146	0
1	C	3336	0	3348	160	0
1	D	3330	0	3343	137	0
2	A	44	0	25	2	0
2	B	44	0	25	0	0
2	C	44	0	26	0	0
2	D	44	0	25	1	0
3	A	20	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	10	0	0
3	C	20	0	10	0	0
3	D	20	0	10	0	0
4	A	67	0	0	2	0
4	B	92	0	0	4	0
4	C	41	0	0	3	0
4	D	58	0	0	3	0
All	All	13846	0	13523	566	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 21.

All (566) 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:276:THR:HG22	1:A:278:CYS:H	1.17	1.07
1:B:276:THR:HG22	1:B:278:CYS:H	1.14	1.03
1:D:276:THR:HG22	1:D:278:CYS:H	1.25	1.02
1:C:276:THR:HG22	1:C:278:CYS:H	1.26	0.97
1:D:49:ARG:H	1:D:126:ASN:HD21	1.11	0.96
1:D:191:ASN:H	1:D:191:ASN:HD22	1.14	0.95
1:D:389:LYS:HE2	1:D:423:GLY:HA2	1.49	0.95
1:A:154:SER:HB3	1:A:365:GLN:HE22	1.29	0.94
1:D:144:PRO:HA	1:D:147:LEU:HD13	1.50	0.93
1:A:387:PRO:HD2	1:A:390:LEU:HD12	1.52	0.92
1:C:144:PRO:HA	1:C:147:LEU:HD13	1.49	0.91
1:A:215:VAL:H	1:A:270:ASN:HD22	1.19	0.90
1:C:387:PRO:HD2	1:C:390:LEU:HD12	1.53	0.89
1:D:191:ASN:N	1:D:191:ASN:HD22	1.72	0.86
1:A:154:SER:HB3	1:A:365:GLN:NE2	1.91	0.85
1:A:417:LEU:HD21	1:B:278:CYS:HB3	1.55	0.85
1:A:50:ILE:HB	1:A:74:VAL:HG12	1.56	0.85
1:B:144:PRO:HA	1:B:147:LEU:HD22	1.58	0.84
1:B:317:GLU:HB2	1:B:329:ARG:HB3	1.58	0.84
1:A:49:ARG:H	1:A:126:ASN:HB2	1.39	0.84
1:A:276:THR:HG22	1:A:278:CYS:N	1.92	0.84
1:C:321:ILE:HD11	1:C:327:ARG:HB2	1.61	0.81
1:C:215:VAL:H	1:C:270:ASN:HD22	1.26	0.81
1:A:389:LYS:HE2	1:A:423:GLY:HA2	1.62	0.81
1:B:276:THR:HG22	1:B:278:CYS:N	1.97	0.80
1:A:144:PRO:HA	1:A:147:LEU:HD13	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:VAL:H	1:B:270:ASN:HD22	1.30	0.79
1:C:276:THR:HG22	1:C:278:CYS:N	1.98	0.78
1:A:317:GLU:HB2	1:A:329:ARG:HB3	1.65	0.77
1:D:22:LEU:HD23	1:D:58:VAL:HG13	1.67	0.77
1:C:58:VAL:HG23	1:C:85:GLN:NE2	1.99	0.77
1:C:322:LYS:HB2	1:C:323:PRO:HD2	1.66	0.76
1:B:276:THR:CG2	1:B:278:CYS:H	1.97	0.76
1:A:404:VAL:HG13	1:B:259:VAL:HB	1.68	0.75
1:C:389:LYS:NZ	1:C:423:GLY:HA2	2.00	0.75
1:B:354:PRO:HB2	1:D:210:MET:HB2	1.68	0.75
1:B:49:ARG:H	1:B:126:ASN:HB2	1.52	0.74
1:D:215:VAL:H	1:D:270:ASN:HD22	1.33	0.74
1:D:34:ARG:HH21	1:D:38:ARG:HB2	1.52	0.74
1:C:244:ILE:HG21	1:D:409:LEU:HD13	1.68	0.74
1:B:276:THR:HG21	1:B:281:ILE:HD11	1.70	0.74
1:A:191:ASN:N	1:A:191:ASN:HD22	1.86	0.73
1:C:409:LEU:HD13	1:D:244:ILE:HG21	1.70	0.73
1:B:58:VAL:H	1:B:85:GLN:NE2	1.86	0.73
1:C:276:THR:CG2	1:C:278:CYS:HB3	2.18	0.73
1:C:389:LYS:HZ3	1:C:423:GLY:HA2	1.52	0.73
1:C:191:ASN:HD22	1:C:191:ASN:N	1.84	0.73
1:C:321:ILE:HD12	1:C:321:ILE:H	1.53	0.73
1:C:259:VAL:HB	1:D:404:VAL:HG13	1.72	0.72
1:A:32:LEU:HD23	1:A:62:VAL:HG12	1.70	0.72
1:D:11:ASP:HB3	1:D:14:LEU:HD13	1.69	0.72
1:C:56:MET:HB3	1:C:84:THR:HG23	1.70	0.71
1:A:34:ARG:HH12	1:A:38:ARG:HB2	1.53	0.71
1:B:155:GLU:HG2	4:B:439:HOH:O	1.91	0.71
1:D:387:PRO:HD2	1:D:390:LEU:HD12	1.70	0.71
1:A:259:VAL:HB	1:B:404:VAL:HG13	1.73	0.70
1:C:222:GLY:O	1:C:226:LYS:HG3	1.91	0.70
1:A:54:LEU:HD11	1:A:156:GLU:HG3	1.74	0.70
1:C:307:ASP:OD2	1:C:310:TRP:HB2	1.92	0.70
1:A:354:PRO:HB2	1:C:210:MET:HB2	1.72	0.70
1:D:147:LEU:HD23	1:D:174:LYS:HB2	1.73	0.69
1:A:412:LYS:HD2	1:B:279:ILE:HD11	1.74	0.69
1:A:45:LEU:HB3	1:A:72:ALA:HB2	1.73	0.69
1:A:50:ILE:HG12	1:A:127:MET:HB2	1.75	0.68
1:B:179:ASN:ND2	1:B:182:ASP:HB2	2.07	0.68
1:B:191:ASN:HD22	1:B:191:ASN:H	1.41	0.68
1:C:211:ILE:HG22	1:C:237:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:HB3	1:C:87:HIS:HA	1.77	0.67
1:C:278:CYS:HB2	1:D:417:LEU:HD11	1.76	0.67
1:D:186:LYS:NZ	1:D:191:ASN:HD21	1.93	0.66
1:A:276:THR:HG21	1:A:278:CYS:HB3	1.76	0.66
1:C:49:ARG:N	1:C:126:ASN:HD22	1.93	0.66
1:A:130:ASP:OD2	1:A:136:THR:HG23	1.96	0.66
1:B:279:ILE:HG22	1:B:304:VAL:HB	1.77	0.66
1:D:276:THR:HG22	1:D:278:CYS:N	2.05	0.66
1:C:125:LEU:H	1:C:125:LEU:HD23	1.61	0.66
1:B:426:LYS:HE3	4:B:457:HOH:O	1.95	0.65
1:C:346:ASN:HD22	1:C:346:ASN:N	1.93	0.65
1:B:199:LEU:HD22	1:B:228:CYS:HB3	1.79	0.65
1:C:49:ARG:H	1:C:126:ASN:HD22	1.42	0.65
1:B:211:ILE:HG22	1:B:237:ALA:HB2	1.77	0.65
1:A:346:ASN:HD22	1:A:346:ASN:H	1.45	0.65
1:D:130:ASP:OD2	1:D:136:THR:HG23	1.97	0.65
1:A:410:THR:H	1:A:413:GLN:HE21	1.43	0.64
1:A:34:ARG:NH1	1:A:38:ARG:HB2	2.13	0.64
1:D:151:ARG:HD3	1:D:376:PRO:HG3	1.80	0.64
1:A:210:MET:HE2	1:A:212:ALA:HB3	1.80	0.64
1:C:22:LEU:HD21	1:C:61:ALA:HB3	1.80	0.64
1:A:40:SER:O	1:A:43:LYS:HE3	1.98	0.63
1:C:296:VAL:HG12	1:C:306:ILE:HD13	1.81	0.63
1:B:128:ILE:HB	1:B:153:ILE:HG12	1.79	0.63
1:B:200:ILE:HD11	1:B:232:LEU:HD23	1.79	0.63
1:D:191:ASN:N	1:D:191:ASN:ND2	2.44	0.63
1:B:45:LEU:HB3	1:B:72:ALA:HB2	1.80	0.63
1:A:145:GLN:NE2	1:A:146:LEU:HG	2.13	0.63
1:A:75:GLN:HG2	1:A:98:PRO:HB2	1.81	0.63
1:B:387:PRO:HG2	1:B:390:LEU:HB2	1.81	0.63
1:A:139:ILE:HG22	1:A:147:LEU:HD12	1.81	0.63
1:C:346:ASN:ND2	1:C:347:LEU:H	1.97	0.62
1:D:126:ASN:HD22	1:D:127:MET:N	1.97	0.62
1:C:11:ASP:HB3	1:C:14:LEU:HD13	1.81	0.62
1:D:49:ARG:H	1:D:126:ASN:ND2	1.90	0.62
1:C:274:THR:HB	1:C:305:GLU:OE1	1.99	0.62
1:A:20:LYS:HD2	1:C:321:ILE:HA	1.80	0.62
1:D:279:ILE:HG22	1:D:304:VAL:HB	1.82	0.62
1:D:186:LYS:HZ2	1:D:191:ASN:HD21	1.48	0.61
1:C:387:PRO:HD2	1:C:390:LEU:CD1	2.29	0.61
1:C:151:ARG:HD2	1:C:373:TRP:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ARG:HD3	1:C:335:ARG:N	2.16	0.61
1:D:191:ASN:H	1:D:191:ASN:ND2	1.87	0.61
1:D:155:GLU:O	1:D:180:VAL:HB	2.00	0.60
1:B:210:MET:HB2	1:D:354:PRO:HB2	1.82	0.60
1:A:157:THR:HA	1:A:181:ASN:HD22	1.67	0.60
1:B:128:ILE:HG21	1:B:136:THR:HG22	1.84	0.60
1:D:262:MET:HE3	1:D:262:MET:O	2.01	0.60
1:C:279:ILE:HA	1:C:304:VAL:O	2.01	0.60
1:B:20:LYS:NZ	1:D:321:ILE:HA	2.17	0.60
1:B:92:ILE:HG21	1:B:99:VAL:HG21	1.83	0.60
1:C:54:LEU:HG	1:C:131:ASP:HB2	1.83	0.59
1:C:279:ILE:HG22	1:C:304:VAL:HB	1.84	0.59
1:D:139:ILE:HG22	1:D:147:LEU:HD12	1.85	0.59
1:A:276:THR:O	1:A:305:GLU:OE2	2.19	0.59
1:C:321:ILE:HD12	1:C:321:ILE:N	2.17	0.59
1:C:186:LYS:HG2	1:C:361:SER:HB3	1.85	0.59
1:C:250:LEU:O	1:C:254:MET:HG2	2.01	0.59
1:B:296:VAL:HG12	1:B:306:ILE:HD13	1.85	0.59
1:B:151:ARG:HD2	1:B:373:TRP:CE3	2.38	0.59
1:B:363:THR:HG22	1:B:394:VAL:HG22	1.84	0.59
1:D:128:ILE:HD11	1:D:139:ILE:HD12	1.82	0.59
1:A:147:LEU:HD23	1:A:174:LYS:HB2	1.84	0.59
1:D:181:ASN:HA	1:D:186:LYS:HD2	1.84	0.59
1:A:14:LEU:HB3	1:A:87:HIS:HA	1.85	0.59
1:B:179:ASN:HD21	1:B:182:ASP:HB2	1.67	0.58
1:A:276:THR:CG2	1:A:278:CYS:HB3	2.33	0.58
1:B:186:LYS:HZ2	1:B:191:ASN:HD21	1.50	0.58
1:A:153:ILE:HG22	1:A:154:SER:N	2.18	0.58
1:A:22:LEU:HD23	1:A:58:VAL:HG13	1.84	0.58
1:A:36:ARG:HH21	1:A:66:THR:CA	2.16	0.58
1:A:344:LEU:HD11	1:A:347:LEU:HD12	1.86	0.58
1:B:58:VAL:HG23	1:B:85:GLN:NE2	2.19	0.58
1:D:14:LEU:HB3	1:D:87:HIS:HA	1.86	0.58
1:A:426:LYS:HG2	1:A:430:TYR:CD2	2.39	0.58
1:B:322:LYS:HB2	1:B:323:PRO:HD2	1.86	0.57
1:C:97:ILE:O	1:C:99:VAL:HG23	2.04	0.57
1:B:409:LEU:HD11	1:B:419:MET:HE2	1.87	0.57
1:A:128:ILE:HG21	1:A:136:THR:HG22	1.85	0.57
1:A:276:THR:HB	1:A:305:GLU:OE1	2.03	0.57
1:B:173:LEU:HD11	1:B:175:VAL:O	2.05	0.57
1:B:186:LYS:NZ	1:B:191:ASN:HD21	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:VAL:HG23	1:D:85:GLN:NE2	2.20	0.57
1:B:49:ARG:HD2	1:B:120:PHE:HB2	1.87	0.57
1:A:29:MET:HE3	1:A:62:VAL:HG21	1.86	0.57
1:D:102:TRP:O	1:D:105:GLU:HG3	2.05	0.57
1:A:63:LEU:HD13	1:A:362:PHE:HB3	1.87	0.56
1:C:161:VAL:HG11	1:C:179:ASN:ND2	2.20	0.56
1:C:276:THR:HG22	1:C:278:CYS:HB3	1.87	0.56
1:C:431:ARG:CZ	1:D:184:VAL:HG22	2.35	0.56
1:C:61:ALA:HB1	1:C:92:ILE:HD11	1.86	0.56
1:C:58:VAL:HG23	1:C:85:GLN:HE22	1.69	0.56
1:C:128:ILE:HG23	1:C:135:LEU:HD13	1.87	0.56
1:D:56:MET:HB3	1:D:84:THR:HG23	1.87	0.56
1:C:317:GLU:OE2	1:C:329:ARG:HD2	2.06	0.56
1:A:36:ARG:HH21	1:A:66:THR:N	2.04	0.56
1:D:54:LEU:HD23	1:D:55:HIS:N	2.20	0.56
1:B:128:ILE:HD11	1:B:139:ILE:HD12	1.88	0.56
1:B:157:THR:HA	1:B:181:ASN:HD22	1.71	0.56
1:B:363:THR:O	1:B:367:MET:HG3	2.05	0.56
1:D:388:LYS:HG2	1:D:392:GLU:OE2	2.05	0.56
1:A:354:PRO:CB	1:C:210:MET:HB2	2.35	0.56
1:B:357:VAL:HB	1:D:210:MET:SD	2.46	0.56
1:A:58:VAL:HG23	1:A:85:GLN:NE2	2.21	0.55
1:B:35:MET:CE	1:B:363:THR:HG23	2.36	0.55
1:C:219:ALA:HA	1:C:242:THR:OG1	2.06	0.55
1:D:271:ILE:HD13	1:D:295:ILE:HB	1.87	0.55
1:D:278:CYS:O	1:D:305:GLU:HG2	2.06	0.55
1:D:346:ASN:HD22	1:D:347:LEU:H	1.53	0.55
1:A:76:TRP:HH2	1:A:129:LEU:HD13	1.71	0.55
1:A:55:HIS:ND1	1:A:347:LEU:HD13	2.21	0.55
1:B:284:GLY:O	1:B:288:GLU:HG3	2.06	0.55
1:D:173:LEU:HD11	1:D:175:VAL:O	2.06	0.55
1:A:346:ASN:HD21	2:A:501:NAD:H72N	1.55	0.55
1:D:211:ILE:HG22	1:D:237:ALA:HB2	1.88	0.55
1:A:346:ASN:HD22	1:A:346:ASN:N	2.04	0.55
1:B:191:ASN:N	1:B:191:ASN:HD22	2.02	0.55
1:D:296:VAL:HG12	1:D:306:ILE:HD13	1.88	0.55
1:C:106:THR:OG1	1:C:109:GLU:HG3	2.06	0.55
1:C:66:THR:O	1:C:70:LEU:HD13	2.07	0.54
1:A:155:GLU:O	1:A:180:VAL:HB	2.07	0.54
1:C:276:THR:HG21	1:C:278:CYS:HB3	1.89	0.54
1:D:112:TRP:O	1:D:116:GLN:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:PHE:HD1	1:B:336:ILE:HD13	1.72	0.54
1:D:189:PHE:HA	1:D:193:TYR:CD2	2.42	0.54
1:D:20:LYS:HE3	1:D:20:LYS:HA	1.89	0.54
1:A:197:GLU:HG2	1:C:235:PHE:CD1	2.43	0.54
1:B:49:ARG:H	1:B:126:ASN:HD22	1.55	0.54
1:C:8:LYS:HD2	1:C:102:TRP:CZ3	2.43	0.54
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.72	0.54
1:D:362:PHE:O	1:D:366:VAL:HG23	2.07	0.54
1:B:251:GLN:O	1:B:255:GLU:HG2	2.08	0.54
1:B:316:VAL:HG12	1:B:329:ARG:O	2.08	0.53
1:C:102:TRP:O	1:C:105:GLU:HG3	2.08	0.53
1:B:287:PHE:CD1	1:B:336:ILE:HD13	2.43	0.53
1:D:161:VAL:HG11	1:D:179:ASN:ND2	2.23	0.53
1:A:145:GLN:HE21	1:A:146:LEU:HG	1.73	0.53
1:C:367:MET:O	1:C:371:GLU:HB2	2.09	0.53
1:A:296:VAL:HG12	1:A:306:ILE:HD13	1.91	0.53
1:B:346:ASN:HD22	1:B:346:ASN:N	2.06	0.53
1:C:180:VAL:HG21	1:C:365:GLN:OE1	2.09	0.52
1:D:375:HIS:N	1:D:376:PRO:HD3	2.24	0.52
1:A:410:THR:H	1:A:413:GLN:NE2	2.07	0.52
1:B:143:TYR:HA	1:B:145:GLN:OE1	2.10	0.52
1:B:156:GLU:O	1:B:181:ASN:HB2	2.09	0.52
1:B:363:THR:CG2	1:B:394:VAL:HG22	2.39	0.52
1:A:147:LEU:HB2	1:A:148:PRO:HD3	1.91	0.52
1:C:54:LEU:HD23	1:C:55:HIS:H	1.75	0.52
1:B:145:GLN:CD	1:B:145:GLN:H	2.12	0.52
1:B:283:LEU:N	1:B:283:LEU:HD22	2.25	0.52
1:C:53:CYS:O	1:C:79:CYS:HB3	2.10	0.52
1:A:260:THR:HG22	1:B:405:LYS:HD2	1.92	0.52
1:C:191:ASN:HD22	1:C:191:ASN:H	1.55	0.52
1:C:5:LEU:HD22	1:C:5:LEU:H	1.75	0.52
1:A:11:ASP:O	1:A:14:LEU:HB2	2.10	0.52
1:A:390:LEU:O	1:A:394:VAL:HG23	2.10	0.52
1:C:191:ASN:ND2	1:C:191:ASN:N	2.55	0.52
1:C:248:ASN:HA	1:C:251:GLN:HE21	1.75	0.52
1:C:5:LEU:HD22	1:C:5:LEU:N	2.25	0.52
1:C:153:ILE:HD11	1:C:175:VAL:HG13	1.92	0.51
1:A:164:LEU:HD23	1:A:167:MET:HE3	1.92	0.51
1:A:417:LEU:CD2	1:B:278:CYS:HB3	2.34	0.51
1:A:28:GLU:OE2	1:A:401:LYS:HE3	2.10	0.51
1:B:49:ARG:HD2	1:B:120:PHE:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ALA:HB3	4:D:481:HOH:O	2.10	0.51
1:B:219:ALA:HB3	1:B:274:THR:HA	1.91	0.51
1:C:405:LYS:HE3	1:D:260:THR:HG22	1.93	0.51
1:B:81:ILE:HG12	4:B:441:HOH:O	2.10	0.51
1:C:214:LYS:HE3	4:C:446:HOH:O	2.10	0.51
1:C:195:CYS:SG	1:C:224:VAL:HG13	2.50	0.51
1:A:112:TRP:O	1:A:116:GLN:HG2	2.10	0.51
1:A:396:GLU:HA	1:A:399:LEU:HD13	1.93	0.50
1:A:248:ASN:HA	1:A:251:GLN:HE21	1.76	0.50
1:A:54:LEU:CD1	1:A:156:GLU:HG3	2.40	0.50
1:B:175:VAL:HG23	1:B:176:PRO:HD2	1.93	0.50
1:A:278:CYS:O	1:A:305:GLU:HG2	2.12	0.50
1:C:346:ASN:O	1:C:350:ALA:HB3	2.12	0.50
1:D:219:ALA:HA	1:D:242:THR:OG1	2.11	0.50
1:A:154:SER:CB	1:A:365:GLN:NE2	2.70	0.50
1:A:155:GLU:HB3	1:A:161:VAL:HG23	1.92	0.50
1:A:172:ILE:HG22	1:A:172:ILE:O	2.11	0.50
1:A:191:ASN:H	1:A:191:ASN:HD22	1.56	0.50
1:B:139:ILE:HG22	1:B:147:LEU:HD13	1.93	0.50
1:D:151:ARG:HD3	1:D:376:PRO:CG	2.40	0.50
1:B:184:VAL:C	1:B:186:LYS:H	2.15	0.50
1:A:405:LYS:HB2	1:B:260:THR:HA	1.94	0.50
1:C:128:ILE:HB	1:C:153:ILE:HG23	1.93	0.50
1:A:198:SER:OG	1:A:353:HIS:HD2	1.95	0.49
1:C:338:LEU:HD13	1:C:339:LEU:N	2.26	0.49
1:A:127:MET:SD	1:A:151:ARG:HB3	2.52	0.49
1:B:46:LYS:HA	1:B:71:GLY:O	2.11	0.49
1:C:413:GLN:HG2	1:D:278:CYS:SG	2.52	0.49
1:D:250:LEU:O	1:D:254:MET:HG2	2.13	0.49
1:A:155:GLU:HG3	1:A:161:VAL:N	2.28	0.49
1:A:29:MET:CE	1:A:62:VAL:HG21	2.43	0.49
1:C:155:GLU:O	1:C:180:VAL:HB	2.12	0.49
1:C:410:THR:H	1:C:413:GLN:HE21	1.58	0.49
1:C:175:VAL:HG23	1:C:176:PRO:HD2	1.94	0.49
1:D:126:ASN:HD22	1:D:126:ASN:C	2.14	0.49
1:A:431:ARG:HA	1:B:431:ARG:HD3	1.93	0.49
1:C:128:ILE:HD11	1:C:150:ILE:HD13	1.94	0.49
1:D:30:PRO:O	1:D:34:ARG:HB2	2.13	0.49
1:A:285:ARG:HG3	1:A:286:HIS:N	2.28	0.49
1:A:426:LYS:HG2	1:A:430:TYR:CG	2.48	0.49
1:B:147:LEU:HB2	1:B:148:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LYS:C	1:C:186:LYS:HD3	2.32	0.49
1:A:241:ILE:HD12	1:A:252:ALA:HB1	1.94	0.49
1:B:108:GLU:CD	1:B:108:GLU:H	2.16	0.49
1:C:35:MET:HA	1:C:35:MET:HE2	1.94	0.49
1:D:225:GLY:HA2	1:D:275:THR:HG21	1.93	0.49
1:A:276:THR:HG22	1:A:277:GLY:N	2.27	0.49
1:C:292:ASP:N	1:C:334:ARG:HD2	2.28	0.49
1:C:334:ARG:C	1:C:335:ARG:HD3	2.34	0.48
1:C:357:VAL:O	1:C:360:ASN:HB2	2.13	0.48
1:D:177:ALA:O	1:D:383:VAL:HA	2.12	0.48
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.28	0.48
1:D:153:ILE:HG22	1:D:154:SER:N	2.27	0.48
1:A:411:GLU:OE2	1:A:411:GLU:HA	2.14	0.48
1:C:48:ALA:HB2	1:C:373:TRP:CE2	2.48	0.48
1:B:241:ILE:HG22	1:B:242:THR:N	2.28	0.48
1:B:276:THR:O	1:B:305:GLU:OE2	2.31	0.48
1:B:35:MET:HG2	1:B:366:VAL:HG11	1.96	0.48
1:C:75:GLN:HG3	1:C:120:PHE:CE2	2.49	0.48
1:D:346:ASN:HD22	1:D:347:LEU:N	2.09	0.48
1:B:173:LEU:HD13	1:B:175:VAL:H	1.79	0.48
1:B:161:VAL:HG11	1:B:179:ASN:ND2	2.29	0.48
1:B:388:LYS:O	1:B:392:GLU:HG3	2.13	0.48
1:D:157:THR:HA	1:D:181:ASN:HD22	1.78	0.48
1:A:164:LEU:HD23	1:A:167:MET:CE	2.43	0.48
1:D:322:LYS:HB2	1:D:323:PRO:HD2	1.96	0.48
1:A:168:MET:SD	1:A:382:GLY:HA2	2.54	0.48
1:A:161:VAL:HG11	1:A:179:ASN:HD21	1.79	0.48
1:B:20:LYS:HZ1	1:D:321:ILE:HA	1.79	0.48
1:C:344:LEU:HD11	1:C:347:LEU:HD12	1.95	0.48
1:B:92:ILE:CG2	1:B:99:VAL:HG21	2.44	0.47
1:A:226:LYS:NZ	1:A:251:GLN:HE22	2.12	0.47
1:A:37:GLU:O	1:A:37:GLU:HG2	2.13	0.47
1:B:49:ARG:HD2	1:B:120:PHE:CG	2.48	0.47
1:D:58:VAL:H	1:D:85:GLN:NE2	2.12	0.47
1:A:151:ARG:O	1:A:176:PRO:HG2	2.13	0.47
1:A:58:VAL:H	1:A:85:GLN:NE2	2.12	0.47
1:C:43:LYS:N	1:C:44:PRO:HD3	2.29	0.47
1:D:251:GLN:O	1:D:255:GLU:HG2	2.14	0.47
1:B:215:VAL:H	1:B:270:ASN:ND2	2.05	0.47
1:C:151:ARG:HD3	1:C:376:PRO:HB3	1.96	0.47
1:C:53:CYS:HA	1:C:77:SER:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:N	1:A:270:ASN:HD22	2.00	0.47
1:B:322:LYS:HB2	1:B:323:PRO:CD	2.45	0.47
1:B:49:ARG:N	1:B:126:ASN:HD22	2.12	0.47
1:B:58:VAL:H	1:B:85:GLN:HE22	1.62	0.47
1:C:321:ILE:HD13	1:C:325:VAL:HG12	1.97	0.47
1:C:58:VAL:HG23	1:C:85:GLN:HE21	1.77	0.47
1:D:346:ASN:ND2	1:D:347:LEU:N	2.62	0.47
1:D:185:THR:HG23	1:D:391:ASP:OD1	2.15	0.47
1:D:54:LEU:HD23	1:D:55:HIS:H	1.80	0.47
1:A:175:VAL:HG23	1:A:176:PRO:HD2	1.97	0.47
1:B:275:THR:HG22	1:B:299:ILE:CG2	2.45	0.47
1:D:139:ILE:HG22	1:D:147:LEU:CD1	2.45	0.47
1:A:278:CYS:SG	1:A:279:ILE:N	2.88	0.47
1:D:49:ARG:N	1:D:126:ASN:HD21	1.95	0.47
1:D:49:ARG:HD2	1:D:120:PHE:HB2	1.96	0.47
1:A:161:VAL:CG1	1:A:179:ASN:ND2	2.78	0.47
1:A:92:ILE:HG22	1:A:97:ILE:HB	1.96	0.47
1:B:161:VAL:HG11	1:B:179:ASN:CG	2.35	0.47
1:C:371:GLU:HG3	1:C:379:TYR:CE1	2.50	0.46
1:C:408:LYS:HD3	4:C:461:HOH:O	2.15	0.46
1:D:145:GLN:HG3	1:D:145:GLN:H	1.30	0.46
1:A:20:LYS:CD	1:C:321:ILE:HA	2.46	0.46
1:B:219:ALA:HA	1:B:242:THR:OG1	2.15	0.46
1:B:389:LYS:CE	1:B:423:GLY:HA2	2.46	0.46
1:D:58:VAL:HG23	1:D:85:GLN:HE21	1.80	0.46
1:A:156:GLU:HG2	1:A:365:GLN:OE1	2.14	0.46
1:A:64:ILE:HG23	1:A:74:VAL:HG21	1.97	0.46
1:C:132:GLY:HA3	1:C:301:HIS:NE2	2.31	0.46
1:C:202:GLY:HA2	1:C:350:ALA:HB2	1.96	0.46
1:D:368:ALA:O	1:D:372:LEU:HD22	2.15	0.46
1:B:153:ILE:O	1:B:177:ALA:HA	2.15	0.46
1:B:186:LYS:C	1:B:186:LYS:HD3	2.36	0.46
1:D:74:VAL:O	1:D:98:PRO:HD2	2.15	0.46
1:A:139:ILE:HG22	1:A:147:LEU:CD1	2.44	0.46
1:A:183:SER:HB2	4:A:461:HOH:O	2.16	0.46
1:A:226:LYS:HZ3	1:A:251:GLN:HE22	1.63	0.46
1:C:180:VAL:HG13	1:C:364:ASN:HB3	1.96	0.46
1:D:8:LYS:HD2	1:D:102:TRP:CZ3	2.51	0.46
1:D:59:GLU:HG2	1:D:358:MET:HG3	1.98	0.46
1:D:199:LEU:HD22	1:D:228:CYS:SG	2.55	0.46
1:A:155:GLU:CD	1:A:160:GLY:HA3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ILE:CD1	1:B:232:LEU:HD23	2.43	0.46
1:D:276:THR:O	1:D:305:GLU:OE2	2.34	0.46
1:B:29:MET:HG2	1:B:355:SER:O	2.16	0.46
1:C:173:LEU:HD11	1:C:175:VAL:O	2.16	0.46
1:D:395:ALA:O	1:D:399:LEU:HD13	2.16	0.46
1:A:32:LEU:HD21	1:A:63:LEU:HA	1.98	0.46
1:A:420:SER:C	1:A:422:ASP:H	2.18	0.46
1:C:5:LEU:CD2	1:C:5:LEU:H	2.29	0.46
1:A:250:LEU:O	1:A:254:MET:HG2	2.15	0.46
1:A:12:ILE:HD11	1:A:94:LYS:HB2	1.98	0.45
1:C:225:GLY:HA2	1:C:275:THR:HG21	1.99	0.45
1:C:147:LEU:HD23	1:C:174:LYS:HB2	1.97	0.45
1:B:319:VAL:HG21	4:B:463:HOH:O	2.15	0.45
1:B:346:ASN:HD22	1:B:346:ASN:H	1.64	0.45
1:C:130:ASP:OD1	1:C:131:ASP:N	2.48	0.45
1:D:125:LEU:HD23	1:D:125:LEU:H	1.80	0.45
1:A:344:LEU:CD1	1:A:347:LEU:HD12	2.46	0.45
1:A:59:GLU:HG3	1:A:355:SER:HA	1.99	0.45
1:C:187:SER:O	1:C:191:ASN:HB2	2.16	0.45
1:D:198:SER:OG	1:D:353:HIS:HD2	2.00	0.45
1:D:60:THR:O	1:D:64:ILE:HG13	2.17	0.45
1:A:102:TRP:CE2	1:A:105:GLU:HG2	2.52	0.45
1:A:151:ARG:HD2	1:A:376:PRO:HB3	1.99	0.45
1:B:112:TRP:O	1:B:116:GLN:HG2	2.17	0.45
1:D:154:SER:OG	1:D:365:GLN:NE2	2.49	0.45
1:A:173:LEU:HD11	1:A:175:VAL:O	2.17	0.45
1:B:430:TYR:CE2	1:B:432:TYR:HA	2.51	0.45
1:C:244:ILE:HD13	1:D:409:LEU:HD13	1.99	0.45
1:D:161:VAL:HG11	1:D:179:ASN:HD21	1.82	0.45
1:A:177:ALA:O	1:A:383:VAL:HA	2.17	0.45
1:A:66:THR:O	1:A:70:LEU:HD13	2.17	0.45
1:C:101:ALA:HA	1:C:105:GLU:OE2	2.17	0.45
1:C:126:ASN:O	1:C:150:ILE:HA	2.17	0.45
1:A:221:TYR:CZ	1:A:226:LYS:HG2	2.52	0.45
1:B:198:SER:OG	1:B:353:HIS:HD2	2.00	0.45
1:D:417:LEU:HD13	1:D:419:MET:HE3	1.99	0.45
1:C:409:LEU:CD2	1:D:244:ILE:HD12	2.47	0.44
1:D:276:THR:HG21	1:D:281:ILE:HD11	1.98	0.44
1:A:11:ASP:OD2	1:A:14:LEU:HD13	2.18	0.44
1:B:210:MET:SD	1:D:357:VAL:HB	2.57	0.44
1:C:186:LYS:HZ2	1:C:191:ASN:HD21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ALA:O	1:C:383:VAL:HA	2.17	0.44
1:D:125:LEU:HD11	1:D:139:ILE:CD1	2.47	0.44
1:D:74:VAL:HG12	1:D:75:GLN:N	2.32	0.44
1:B:198:SER:OG	1:B:353:HIS:CD2	2.70	0.44
1:A:274:THR:HB	1:A:305:GLU:OE1	2.18	0.44
1:C:54:LEU:HD23	1:C:55:HIS:N	2.32	0.44
1:A:102:TRP:O	1:A:105:GLU:HG3	2.18	0.44
1:B:316:VAL:O	1:B:317:GLU:HG3	2.18	0.44
1:B:411:GLU:O	1:B:415:GLN:HG3	2.17	0.44
1:C:262:MET:HE3	1:C:262:MET:O	2.17	0.44
1:C:310:TRP:O	1:C:314:ASN:HB2	2.17	0.44
1:C:126:ASN:HB3	1:C:373:TRP:CZ3	2.53	0.44
1:A:29:MET:HG2	1:A:359:SER:HB2	2.00	0.44
1:D:101:ALA:HA	1:D:105:GLU:OE2	2.18	0.44
1:D:338:LEU:HD13	1:D:339:LEU:N	2.32	0.44
1:D:374:THR:C	1:D:376:PRO:HD3	2.38	0.44
1:A:244:ILE:HG22	1:B:407:THR:O	2.18	0.44
1:B:147:LEU:CB	1:B:148:PRO:HD3	2.48	0.44
1:B:179:ASN:HD21	1:B:182:ASP:CB	2.31	0.44
1:A:420:SER:HB3	1:A:423:GLY:H	1.83	0.43
1:A:346:ASN:ND2	2:A:501:NAD:H72N	2.15	0.43
1:B:35:MET:HE1	1:B:363:THR:HG23	1.98	0.43
1:D:374:THR:HG22	1:D:375:HIS:CD2	2.53	0.43
1:A:153:ILE:HD11	1:A:175:VAL:HG13	1.99	0.43
1:C:52:GLY:HA2	1:C:129:LEU:O	2.17	0.43
1:C:357:VAL:HG13	1:C:358:MET:N	2.32	0.43
1:D:128:ILE:HB	1:D:153:ILE:HG12	1.99	0.43
1:A:24:ILE:HD11	1:C:321:ILE:HG12	2.01	0.43
1:C:54:LEU:HG	1:C:131:ASP:CB	2.47	0.43
1:A:158:THR:N	1:A:181:ASN:ND2	2.66	0.43
1:A:338:LEU:HD13	1:A:339:LEU:N	2.32	0.43
1:B:156:GLU:HG2	1:B:365:GLN:OE1	2.18	0.43
1:B:35:MET:HE2	1:B:363:THR:HG23	2.01	0.43
1:D:261:THR:HB	4:D:471:HOH:O	2.19	0.43
1:D:322:LYS:HB2	1:D:323:PRO:CD	2.49	0.43
1:A:161:VAL:HG11	1:A:179:ASN:ND2	2.34	0.43
1:B:54:LEU:O	1:B:55:HIS:C	2.57	0.43
1:C:245:ASP:HB3	1:C:248:ASN:HB2	2.01	0.43
1:C:389:LYS:HZ2	1:C:423:GLY:HA2	1.79	0.43
1:A:32:LEU:HD23	1:A:62:VAL:CG1	2.43	0.43
1:A:27:ASN:O	1:A:401:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:THR:H	1:D:413:GLN:HE21	1.67	0.43
1:A:36:ARG:HH21	1:A:66:THR:HA	1.84	0.43
1:B:345:VAL:HG13	1:B:346:ASN:N	2.34	0.43
1:C:285:ARG:O	1:C:289:GLN:HG3	2.18	0.43
1:A:54:LEU:HD23	1:A:55:HIS:N	2.34	0.43
1:B:303:ASP:HB3	1:B:343:ARG:HG2	1.99	0.43
1:D:18:GLY:HA3	1:D:87:HIS:O	2.19	0.43
1:B:204:LYS:NZ	1:D:197:GLU:OE1	2.45	0.42
1:A:430:TYR:CE2	1:A:432:TYR:HA	2.53	0.42
1:A:12:ILE:HD13	1:A:93:ALA:HB3	2.01	0.42
1:B:199:LEU:HD22	1:B:228:CYS:CB	2.47	0.42
1:C:186:LYS:NZ	1:C:191:ASN:HD21	2.16	0.42
1:D:222:GLY:HA3	2:D:504:NAD:O1A	2.18	0.42
1:D:226:LYS:HD3	4:D:467:HOH:O	2.18	0.42
1:B:389:LYS:HE2	1:B:423:GLY:HA2	2.01	0.42
1:C:346:ASN:HD22	1:C:346:ASN:H	1.66	0.42
1:D:252:ALA:O	1:D:257:TYR:HB2	2.19	0.42
1:D:168:MET:SD	1:D:382:GLY:HA2	2.59	0.42
1:A:176:PRO:HB3	1:A:380:PRO:O	2.19	0.42
1:A:198:SER:OG	1:A:353:HIS:CD2	2.72	0.42
1:A:55:HIS:NE2	1:A:79:CYS:SG	2.92	0.42
1:B:107:ASP:HB2	1:B:108:GLU:OE1	2.19	0.42
1:A:409:LEU:HD21	1:B:244:ILE:HD13	2.01	0.42
1:C:147:LEU:N	1:C:148:PRO:HD2	2.35	0.42
1:C:168:MET:SD	1:C:382:GLY:HA2	2.59	0.42
1:C:362:PHE:O	1:C:366:VAL:HG23	2.20	0.42
1:D:198:SER:OG	1:D:353:HIS:CD2	2.72	0.42
1:D:35:MET:HG2	1:D:366:VAL:HG11	2.00	0.42
1:A:346:ASN:O	1:A:350:ALA:HB3	2.20	0.42
1:A:364:ASN:OD1	1:A:394:VAL:HG21	2.19	0.42
1:A:411:GLU:HB3	4:A:444:HOH:O	2.19	0.42
1:A:50:ILE:O	1:A:74:VAL:HA	2.19	0.42
1:B:18:GLY:O	1:B:22:LEU:HG	2.19	0.42
1:B:409:LEU:HD11	1:B:419:MET:CE	2.49	0.42
1:C:248:ASN:O	1:C:251:GLN:HB2	2.19	0.42
1:D:293:ASP:OD2	1:D:327:ARG:NH2	2.51	0.42
1:C:276:THR:O	1:C:305:GLU:CD	2.58	0.42
1:C:322:LYS:CB	1:C:323:PRO:HD2	2.45	0.42
1:C:18:GLY:HA3	1:C:87:HIS:O	2.20	0.42
1:A:199:LEU:HD22	1:A:228:CYS:SG	2.60	0.42
1:B:57:THR:H	1:B:60:THR:HB	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:MET:CE	1:C:152:GLY:N	2.82	0.42
1:C:244:ILE:HD12	1:D:409:LEU:HD22	2.01	0.42
1:C:346:ASN:N	1:C:346:ASN:ND2	2.63	0.42
1:D:303:ASP:OD2	1:D:303:ASP:N	2.53	0.42
1:D:66:THR:O	1:D:70:LEU:HD13	2.19	0.42
1:B:191:ASN:ND2	1:B:191:ASN:N	2.67	0.42
1:B:338:LEU:HD13	1:B:339:LEU:N	2.35	0.42
1:C:321:ILE:HD11	1:C:327:ARG:CB	2.43	0.42
1:D:346:ASN:N	1:D:346:ASN:HD22	2.18	0.42
1:B:29:MET:CB	1:B:359:SER:HB2	2.50	0.42
1:C:185:THR:HA	1:C:189:PHE:CD1	2.55	0.42
1:C:266:CYS:O	1:C:290:MET:HA	2.20	0.42
1:C:346:ASN:ND2	1:C:347:LEU:N	2.66	0.42
1:A:153:ILE:HB	1:A:177:ALA:CB	2.50	0.41
1:A:22:LEU:O	1:A:26:GLU:HG3	2.20	0.41
1:B:198:SER:HB2	1:B:346:ASN:HB2	2.01	0.41
1:B:92:ILE:HG21	1:B:99:VAL:CG2	2.49	0.41
1:C:126:ASN:HB3	1:C:373:TRP:HZ3	1.84	0.41
1:C:136:THR:HG23	1:C:153:ILE:HD13	2.02	0.41
1:C:241:ILE:O	1:C:259:VAL:HA	2.21	0.41
1:C:346:ASN:HD22	1:C:347:LEU:H	1.63	0.41
1:C:409:LEU:CD1	1:D:244:ILE:HG21	2.43	0.41
1:D:276:THR:HG22	1:D:277:GLY:N	2.34	0.41
1:A:125:LEU:HD23	1:A:125:LEU:H	1.85	0.41
1:A:32:LEU:HG	1:A:66:THR:OG1	2.20	0.41
1:D:165:TYR:CD1	1:D:383:VAL:HG11	2.56	0.41
1:D:338:LEU:HD12	1:D:341:GLU:HA	2.02	0.41
1:B:130:ASP:OD2	1:B:136:THR:HG23	2.20	0.41
1:B:215:VAL:N	1:B:270:ASN:HD22	2.08	0.41
1:B:354:PRO:CB	1:D:210:MET:HB2	2.45	0.41
1:A:153:ILE:CG2	1:A:154:SER:N	2.84	0.41
1:A:191:ASN:N	1:A:191:ASN:ND2	2.58	0.41
1:C:209:VAL:HG11	1:C:295:ILE:CD1	2.51	0.41
1:C:26:GLU:C	1:C:28:GLU:H	2.24	0.41
1:C:276:THR:O	1:C:305:GLU:OE2	2.38	0.41
1:C:30:PRO:O	1:C:34:ARG:HB2	2.20	0.41
1:D:200:ILE:O	1:D:204:LYS:HG2	2.20	0.41
1:C:153:ILE:O	1:C:177:ALA:HA	2.21	0.41
1:B:81:ILE:HD11	1:B:343:ARG:NE	2.35	0.41
1:B:178:ILE:CD1	1:B:372:LEU:HD13	2.50	0.41
1:A:279:ILE:HD12	1:B:412:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LEU:HD12	1:B:5:LEU:N	2.34	0.41
1:D:357:VAL:O	1:D:360:ASN:HB2	2.20	0.41
1:D:49:ARG:HH11	1:D:49:ARG:HG3	1.85	0.41
1:C:279:ILE:HG23	1:D:416:TYR:CE2	2.55	0.41
1:A:20:LYS:HE2	1:C:320:ASN:O	2.21	0.41
1:D:151:ARG:HG2	1:D:372:LEU:O	2.20	0.41
1:D:358:MET:HA	1:D:358:MET:HE2	2.03	0.41
1:A:76:TRP:CH2	1:A:129:LEU:HD13	2.54	0.41
1:A:63:LEU:HD22	1:A:362:PHE:CD1	2.56	0.41
1:C:420:SER:C	1:C:422:ASP:H	2.23	0.41
1:D:283:LEU:O	1:D:286:HIS:HB2	2.20	0.41
1:C:226:LYS:HE2	1:D:432:TYR:OXT	2.21	0.41
1:A:106:THR:OG1	1:A:109:GLU:HG3	2.21	0.41
1:A:46:LYS:HA	1:A:71:GLY:O	2.21	0.41
1:B:250:LEU:O	1:B:254:MET:HG2	2.21	0.41
1:B:276:THR:CG2	1:B:277:GLY:N	2.84	0.41
1:B:330:LEU:HD11	1:B:336:ILE:HD11	2.03	0.41
1:A:427:PRO:HB2	1:A:429:HIS:CE1	2.56	0.41
1:B:52:GLY:HA2	1:B:129:LEU:O	2.21	0.41
1:B:276:THR:HB	1:B:305:GLU:OE1	2.20	0.41
1:B:387:PRO:CG	1:B:390:LEU:HD22	2.50	0.41
1:D:49:ARG:NH1	1:D:49:ARG:HG3	2.35	0.41
1:B:49:ARG:N	1:B:126:ASN:HB2	2.27	0.40
1:B:200:ILE:HG21	1:B:235:PHE:CE2	2.56	0.40
1:C:156:GLU:O	1:C:181:ASN:HB2	2.20	0.40
1:C:165:TYR:CE1	1:C:383:VAL:HG11	2.57	0.40
1:A:49:ARG:HD2	1:A:120:PHE:HB2	2.03	0.40
1:A:60:THR:O	1:A:64:ILE:HG13	2.22	0.40
1:B:124:PRO:HB3	1:B:146:LEU:HD22	2.03	0.40
1:C:335:ARG:N	1:C:335:ARG:CD	2.84	0.40
1:C:372:LEU:HA	1:C:372:LEU:HD12	1.94	0.40
1:B:374:THR:HG22	1:B:375:HIS:CD2	2.57	0.40
1:B:379:TYR:HD2	1:B:384:HIS:ND1	2.19	0.40
1:A:260:THR:HA	1:B:405:LYS:HB2	2.03	0.40
1:C:28:GLU:HG2	4:C:439:HOH:O	2.20	0.40
1:D:132:GLY:HA3	1:D:301:HIS:NE2	2.37	0.40
1:D:241:ILE:O	1:D:259:VAL:HA	2.22	0.40
1:D:248:ASN:O	1:D:251:GLN:HB2	2.21	0.40
1:B:106:THR:OG1	1:B:109:GLU:HG3	2.22	0.40
1:B:248:ASN:HA	1:B:251:GLN:HE21	1.86	0.40
1:B:92:ILE:CG2	1:B:97:ILE:HB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:TRP:O	1:C:116:GLN:HG2	2.21	0.40
1:D:426:LYS:HA	1:D:427:PRO:HD3	1.93	0.40
1:A:147:LEU:HD23	1:A:174:LYS:CB	2.51	0.40
1:A:431:ARG:CZ	1:B:184:VAL:HG22	2.51	0.40
1:C:323:PRO:O	1:C:324:GLN:HB2	2.22	0.40
1:C:35:MET:HA	1:C:35:MET:CE	2.51	0.40
1:C:43:LYS:HD2	1:C:71:GLY:HA3	2.02	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	429/435 (99%)	396 (92%)	30 (7%)	3 (1%)	22	39
1	B	428/435 (98%)	402 (94%)	24 (6%)	2 (0%)	29	48
1	C	429/435 (99%)	394 (92%)	34 (8%)	1 (0%)	47	68
1	D	428/435 (98%)	398 (93%)	29 (7%)	1 (0%)	47	68
All	All	1714/1740 (98%)	1590 (93%)	117 (7%)	7 (0%)	34	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	B	55	HIS
1	B	185	THR
1	C	290	MET
1	D	344	LEU
1	A	98	PRO
1	A	380	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/358 (99%)	344 (97%)	11 (3%)	40	67
1	B	354/358 (99%)	337 (95%)	17 (5%)	25	48
1	C	355/358 (99%)	340 (96%)	15 (4%)	30	54
1	D	354/358 (99%)	332 (94%)	22 (6%)	18	35
All	All	1418/1432 (99%)	1353 (95%)	65 (5%)	27	50

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	162	HIS
1	A	191	ASN
1	A	260	THR
1	A	285	ARG
1	A	338	LEU
1	A	346	ASN
1	A	372	LEU
1	A	383	VAL
1	A	384	HIS
1	A	391	ASP
1	B	3	ASP
1	B	27	ASN
1	B	111	LEU
1	B	135	LEU
1	B	145	GLN
1	B	147	LEU
1	B	155	GLU
1	B	191	ASN
1	B	210	MET
1	B	260	THR
1	B	264	GLU
1	B	285	ARG
1	B	338	LEU

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Mol	Chain	Res	Type
1	B	346	ASN
1	B	372	LEU
1	B	383	VAL
1	B	411	GLU
1	C	35	MET
1	C	54	LEU
1	C	87	HIS
1	C	107	ASP
1	C	111	LEU
1	C	127	MET
1	C	135	LEU
1	C	145	GLN
1	C	155	GLU
1	C	175	VAL
1	C	191	ASN
1	C	278	CYS
1	C	338	LEU
1	C	346	ASN
1	C	409	LEU
1	D	20	LYS
1	D	27	ASN
1	D	34	ARG
1	D	35	MET
1	D	99	VAL
1	D	108	GLU
1	D	111	LEU
1	D	126	ASN
1	D	145	GLN
1	D	191	ASN
1	D	210	MET
1	D	267	GLN
1	D	278	CYS
1	D	283	LEU
1	D	288	GLU
1	D	309	LYS
1	D	322	LYS
1	D	335	ARG
1	D	338	LEU
1	D	346	ASN
1	D	383	VAL
1	D	409	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	75	GLN
1	A	85	GLN
1	A	181	ASN
1	A	191	ASN
1	A	230	GLN
1	A	248	ASN
1	A	251	GLN
1	A	267	GLN
1	A	270	ASN
1	A	314	ASN
1	A	346	ASN
1	A	353	HIS
1	A	365	GLN
1	A	413	GLN
1	B	27	ASN
1	B	75	GLN
1	B	85	GLN
1	B	126	ASN
1	B	137	ASN
1	B	163	ASN
1	B	181	ASN
1	B	191	ASN
1	B	248	ASN
1	B	251	GLN
1	B	270	ASN
1	B	346	ASN
1	B	353	HIS
1	B	365	GLN
1	B	413	GLN
1	C	27	ASN
1	C	85	GLN
1	C	126	ASN
1	C	145	GLN
1	C	181	ASN
1	C	191	ASN
1	C	248	ASN
1	C	251	GLN
1	C	267	GLN
1	C	270	ASN
1	C	346	ASN
1	C	353	HIS

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Mol	Chain	Res	Type
1	C	369	GLN
1	C	413	GLN
1	C	415	GLN
1	D	27	ASN
1	D	75	GLN
1	D	85	GLN
1	D	116	GLN
1	D	126	ASN
1	D	145	GLN
1	D	181	ASN
1	D	191	ASN
1	D	248	ASN
1	D	251	GLN
1	D	267	GLN
1	D	270	ASN
1	D	346	ASN
1	D	365	GLN
1	D	384	HIS
1	D	403	ASN
1	D	413	GLN

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
2	NAD	C	503	-	42,48,48	3.48	19 (45%)	50,73,73	2.88	24 (48%)
3	AFX	A	601	-	17,22,22	3.34	7 (41%)	9,33,33	1.30	1 (11%)
2	NAD	B	502	-	42,48,48	3.29	20 (47%)	50,73,73	2.93	23 (46%)
3	AFX	B	602	-	17,22,22	3.23	5 (29%)	9,33,33	1.24	1 (11%)
2	NAD	A	501	-	42,48,48	3.35	19 (45%)	50,73,73	2.92	23 (46%)
3	AFX	C	603	-	17,22,22	3.26	3 (17%)	9,33,33	1.34	1 (11%)
2	NAD	D	504	-	42,48,48	3.41	21 (50%)	50,73,73	2.86	24 (48%)
3	AFX	D	604	-	17,22,22	3.35	4 (23%)	9,33,33	1.31	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	503	-	-	12/26/62/62	0/5/5/5
3	AFX	A	601	-	-	1/2/26/26	0/3/3/3
2	NAD	B	502	-	-	12/26/62/62	0/5/5/5
3	AFX	B	602	-	-	2/2/26/26	0/3/3/3
2	NAD	A	501	-	-	12/26/62/62	0/5/5/5
3	AFX	C	603	-	-	2/2/26/26	0/3/3/3
2	NAD	D	504	-	-	12/26/62/62	0/5/5/5
3	AFX	D	604	-	-	2/2/26/26	0/3/3/3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	604	AFX	C4-N3	12.45	1.52	1.35
3	C	603	AFX	C4-N3	12.24	1.52	1.35
3	A	601	AFX	C4-N3	12.20	1.52	1.35
3	B	602	AFX	C4-N3	11.79	1.51	1.35
2	A	501	NAD	C4A-N3A	9.31	1.48	1.35
2	D	504	NAD	C4A-N3A	9.24	1.48	1.35
2	C	503	NAD	C4A-N3A	9.19	1.48	1.35
2	C	503	NAD	C2A-N3A	9.18	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	NAD	C2A-N3A	8.95	1.46	1.32
2	B	502	NAD	C4A-N3A	8.82	1.47	1.35
2	A	501	NAD	C2A-N3A	8.54	1.45	1.32
2	C	503	NAD	C2N-N1N	8.12	1.44	1.35
2	D	504	NAD	C2N-N1N	8.04	1.44	1.35
2	B	502	NAD	C2A-N3A	7.87	1.44	1.32
2	C	503	NAD	C3N-C7N	7.79	1.62	1.50
2	D	504	NAD	C3N-C7N	7.65	1.62	1.50
2	B	502	NAD	C3N-C7N	7.64	1.62	1.50
2	A	501	NAD	C2N-N1N	7.58	1.44	1.35
2	B	502	NAD	C2N-N1N	7.51	1.44	1.35
2	A	501	NAD	C3N-C7N	6.72	1.60	1.50
2	B	502	NAD	C7N-N7N	5.43	1.43	1.33
2	A	501	NAD	C7N-N7N	5.42	1.43	1.33
2	C	503	NAD	C7N-N7N	5.32	1.43	1.33
2	B	502	NAD	C4N-C3N	5.12	1.48	1.39
2	C	503	NAD	C5N-C4N	5.06	1.49	1.38
2	D	504	NAD	C7N-N7N	5.03	1.42	1.33
2	D	504	NAD	C5N-C4N	4.94	1.49	1.38
2	C	503	NAD	C4N-C3N	4.88	1.47	1.39
2	A	501	NAD	C4N-C3N	4.82	1.47	1.39
2	D	504	NAD	C4N-C3N	4.78	1.47	1.39
2	B	502	NAD	C5N-C4N	4.58	1.48	1.38
2	A	501	NAD	C5N-C4N	4.47	1.48	1.38
2	D	504	NAD	C6N-N1N	3.96	1.45	1.35
2	A	501	NAD	C6N-N1N	3.96	1.45	1.35
2	B	502	NAD	O4D-C4D	3.79	1.53	1.45
2	C	503	NAD	C6N-N1N	3.72	1.44	1.35
2	B	502	NAD	C6N-N1N	3.68	1.44	1.35
2	C	503	NAD	O4D-C4D	3.59	1.53	1.45
2	A	501	NAD	C6A-C5A	3.51	1.56	1.43
2	C	503	NAD	C6A-C5A	3.47	1.56	1.43
2	C	503	NAD	O4B-C1B	-3.46	1.36	1.41
3	B	602	AFX	C1'-N9	-3.45	1.44	1.49
2	D	504	NAD	C6A-C5A	3.40	1.55	1.43
2	A	501	NAD	O4D-C4D	3.14	1.52	1.45
3	C	603	AFX	F1-C5'	3.11	1.40	1.36
3	D	604	AFX	C1'-N9	-3.08	1.44	1.49
2	A	501	NAD	O4B-C1B	-3.04	1.36	1.41
2	D	504	NAD	O4D-C4D	2.98	1.51	1.45
2	D	504	NAD	O4B-C1B	-2.92	1.37	1.41
2	A	501	NAD	C3D-C4D	2.91	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	NAD	C6A-C5A	2.86	1.53	1.43
2	B	502	NAD	O2B-C2B	-2.84	1.36	1.43
3	A	601	AFX	F1-C5'	2.81	1.39	1.36
2	D	504	NAD	C3D-C4D	2.77	1.60	1.53
2	A	501	NAD	O2B-C2B	-2.76	1.36	1.43
2	A	501	NAD	O4D-C1D	2.72	1.44	1.41
2	B	502	NAD	O4B-C1B	-2.72	1.37	1.41
2	A	501	NAD	O4B-C4B	2.71	1.51	1.45
3	A	601	AFX	C1'-N9	-2.71	1.45	1.49
2	D	504	NAD	O2B-C2B	-2.66	1.36	1.43
2	C	503	NAD	C3D-C4D	2.63	1.59	1.53
2	B	502	NAD	C3D-C4D	2.62	1.59	1.53
2	D	504	NAD	O4B-C4B	2.60	1.50	1.45
2	C	503	NAD	O4B-C4B	2.59	1.50	1.45
2	D	504	NAD	C3B-C4B	2.59	1.59	1.53
2	C	503	NAD	C3B-C4B	2.55	1.59	1.53
2	A	501	NAD	C3B-C4B	2.51	1.59	1.53
2	A	501	NAD	C2D-C1D	-2.40	1.50	1.53
2	D	504	NAD	O3B-C3B	2.40	1.48	1.43
2	B	502	NAD	C5B-C4B	-2.38	1.44	1.51
2	C	503	NAD	O2B-C2B	-2.37	1.37	1.43
2	D	504	NAD	C2N-C3N	2.35	1.42	1.39
2	B	502	NAD	O4B-C4B	2.35	1.50	1.45
3	A	601	AFX	C6-C5	2.33	1.52	1.43
3	A	601	AFX	C3'-C4'	2.33	1.52	1.46
2	B	502	NAD	O3D-C3D	-2.31	1.37	1.43
2	C	503	NAD	PN-O5D	2.30	1.68	1.59
2	D	504	NAD	O4D-C1D	2.29	1.44	1.41
3	D	604	AFX	F1-C5'	2.28	1.39	1.36
3	A	601	AFX	C5-C4	2.27	1.46	1.40
2	B	502	NAD	C3B-C4B	2.26	1.58	1.53
2	A	501	NAD	C5B-C4B	-2.24	1.44	1.51
2	D	504	NAD	C5B-C4B	-2.23	1.44	1.51
3	B	602	AFX	C6-C5	2.22	1.51	1.43
2	C	503	NAD	C8A-N7A	-2.19	1.30	1.34
3	B	602	AFX	C5-C4	2.18	1.46	1.40
2	B	502	NAD	O2D-C2D	-2.15	1.37	1.43
3	B	602	AFX	C3'-C4'	2.15	1.51	1.46
3	C	603	AFX	C5-C4	2.13	1.46	1.40
3	A	601	AFX	C8-N7	2.12	1.38	1.34
2	B	502	NAD	C6A-N1A	2.08	1.46	1.37
3	D	604	AFX	C5-C4	2.08	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	504	NAD	PN-O1N	-2.06	1.43	1.50
2	C	503	NAD	C6A-N1A	2.05	1.46	1.37
2	A	501	NAD	PN-O5D	2.03	1.67	1.59
2	C	503	NAD	O4D-C1D	2.02	1.43	1.41
2	D	504	NAD	C6A-N1A	2.02	1.46	1.37
2	B	502	NAD	C2N-C3N	2.00	1.42	1.39

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAD	C3N-C2N-N1N	-7.86	112.75	120.43
2	B	502	NAD	C3N-C2N-N1N	-7.77	112.83	120.43
2	C	503	NAD	C3N-C2N-N1N	-7.16	113.43	120.43
2	A	501	NAD	C2N-C3N-C4N	7.09	126.30	118.26
2	B	502	NAD	C2N-C3N-C4N	7.07	126.28	118.26
2	D	504	NAD	C3N-C2N-N1N	-6.91	113.67	120.43
2	D	504	NAD	C2N-C3N-C4N	6.88	126.06	118.26
2	C	503	NAD	C2N-C3N-C4N	6.88	126.05	118.26
2	C	503	NAD	O5D-PN-O1N	-5.50	87.59	109.07
2	B	502	NAD	O5D-PN-O1N	-5.49	87.60	109.07
2	A	501	NAD	O5D-PN-O1N	-5.45	87.76	109.07
2	B	502	NAD	N3A-C2A-N1A	-5.44	120.18	128.68
2	D	504	NAD	O5D-PN-O1N	-5.43	87.85	109.07
2	D	504	NAD	N3A-C2A-N1A	-5.29	120.42	128.68
2	A	501	NAD	C6N-N1N-C2N	5.27	126.78	121.97
2	B	502	NAD	C6N-N1N-C2N	5.26	126.78	121.97
2	A	501	NAD	N3A-C2A-N1A	-5.08	120.74	128.68
2	C	503	NAD	N3A-C2A-N1A	-5.05	120.78	128.68
2	C	503	NAD	C6N-N1N-C2N	4.96	126.50	121.97
2	C	503	NAD	O5D-C5D-C4D	4.71	125.20	108.99
2	D	504	NAD	O5D-C5D-C4D	4.64	124.98	108.99
2	D	504	NAD	O2N-PN-O5D	-4.64	86.20	107.75
2	C	503	NAD	O2N-PN-O5D	-4.63	86.25	107.75
2	B	502	NAD	O2N-PN-O5D	-4.62	86.27	107.75
2	A	501	NAD	O2N-PN-O5D	-4.58	86.49	107.75
2	D	504	NAD	C2A-N1A-C6A	4.50	126.46	118.75
2	B	502	NAD	C2A-N1A-C6A	4.50	126.44	118.75
2	D	504	NAD	C5N-C4N-C3N	-4.44	115.09	120.34
2	A	501	NAD	C2A-N1A-C6A	4.44	126.34	118.75
2	D	504	NAD	C6N-N1N-C2N	4.36	125.95	121.97
2	C	503	NAD	C2A-N1A-C6A	4.31	126.13	118.75
2	C	503	NAD	C5N-C4N-C3N	-4.31	115.25	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	NAD	C5N-C4N-C3N	-4.30	115.26	120.34
2	B	502	NAD	O5D-C5D-C4D	4.14	123.23	108.99
2	A	501	NAD	O2A-PA-O1A	4.08	132.44	112.24
2	C	503	NAD	O2A-PA-O1A	4.05	132.27	112.24
2	B	502	NAD	O2A-PA-O1A	4.03	132.17	112.24
2	A	501	NAD	O5D-C5D-C4D	3.98	122.69	108.99
2	A	501	NAD	C5N-C4N-C3N	-3.95	115.66	120.34
2	D	504	NAD	O2A-PA-O1A	3.92	131.63	112.24
2	D	504	NAD	O5B-C5B-C4B	3.90	122.43	108.99
2	A	501	NAD	O5B-C5B-C4B	3.76	121.94	108.99
2	C	503	NAD	O5B-C5B-C4B	3.73	121.82	108.99
2	B	502	NAD	O5B-C5B-C4B	3.68	121.66	108.99
3	C	603	AFX	C4-C5-N7	3.63	113.19	109.40
2	B	502	NAD	PN-O3-PA	3.54	144.97	132.83
3	D	604	AFX	C4-C5-N7	3.52	113.07	109.40
2	B	502	NAD	O4B-C1B-C2B	3.30	111.75	106.93
2	C	503	NAD	PN-O3-PA	3.26	144.01	132.83
2	A	501	NAD	O4B-C1B-C2B	3.24	111.67	106.93
2	D	504	NAD	PN-O3-PA	3.23	143.91	132.83
2	A	501	NAD	C5A-C6A-N6A	3.23	125.26	120.35
2	C	503	NAD	C5A-C6A-N6A	3.23	125.25	120.35
3	B	602	AFX	C4-C5-N7	3.17	112.70	109.40
2	D	504	NAD	O4B-C1B-C2B	3.15	111.53	106.93
2	D	504	NAD	C5A-C6A-N6A	3.14	125.13	120.35
2	A	501	NAD	PN-O3-PA	3.13	143.57	132.83
3	A	601	AFX	C4-C5-N7	3.05	112.58	109.40
2	D	504	NAD	O4D-C4D-C5D	3.02	119.31	109.37
2	A	501	NAD	O7N-C7N-C3N	-2.96	116.08	119.63
2	B	502	NAD	C2B-C3B-C4B	2.92	108.32	102.64
2	C	503	NAD	O4B-C1B-C2B	2.92	111.20	106.93
2	C	503	NAD	O2N-PN-O1N	2.88	126.48	112.24
2	B	502	NAD	O2N-PN-O1N	2.87	126.43	112.24
2	C	503	NAD	C5A-C6A-N1A	-2.87	113.86	120.35
2	D	504	NAD	O2N-PN-O1N	2.86	126.36	112.24
2	B	502	NAD	C5A-C6A-N1A	-2.85	113.89	120.35
2	B	502	NAD	C5A-C6A-N6A	2.83	124.65	120.35
2	C	503	NAD	C2N-C3N-C7N	-2.81	111.31	119.46
2	A	501	NAD	C5A-C6A-N1A	-2.80	114.00	120.35
2	B	502	NAD	C2N-C3N-C7N	-2.77	111.42	119.46
2	A	501	NAD	O2N-PN-O1N	2.77	125.92	112.24
2	C	503	NAD	O4D-C4D-C5D	2.73	118.35	109.37
2	D	504	NAD	C2N-C3N-C7N	-2.72	111.56	119.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	504	NAD	C5A-C6A-N1A	-2.69	114.24	120.35
2	A	501	NAD	C2B-C3B-C4B	2.63	107.75	102.64
2	C	503	NAD	C2B-C3B-C4B	2.55	107.59	102.64
2	A	501	NAD	O4D-C4D-C5D	2.54	117.72	109.37
2	A	501	NAD	C2N-C3N-C7N	-2.52	112.14	119.46
2	D	504	NAD	C2B-C3B-C4B	2.51	107.53	102.64
2	B	502	NAD	O4D-C4D-C5D	2.38	117.20	109.37
2	C	503	NAD	C5N-C6N-N1N	-2.30	117.10	120.40
2	A	501	NAD	O3D-C3D-C4D	-2.30	104.41	111.05
2	A	501	NAD	O4D-C4D-C3D	-2.27	100.62	105.11
2	D	504	NAD	O2D-C2D-C1D	2.27	119.23	110.85
2	B	502	NAD	O7N-C7N-C3N	-2.26	116.92	119.63
2	B	502	NAD	O3D-C3D-C4D	-2.25	104.53	111.05
2	A	501	NAD	C5N-C6N-N1N	-2.25	117.17	120.40
2	C	503	NAD	O4D-C4D-C3D	-2.23	100.70	105.11
2	D	504	NAD	C5N-C6N-N1N	-2.19	117.26	120.40
2	C	503	NAD	O7N-C7N-C3N	-2.15	117.06	119.63
2	D	504	NAD	O7N-C7N-C3N	-2.14	117.06	119.63
2	C	503	NAD	O3D-C3D-C4D	-2.13	104.90	111.05
2	D	504	NAD	O4D-C4D-C3D	-2.12	100.92	105.11
2	C	503	NAD	O2D-C2D-C1D	2.12	118.67	110.85
2	B	502	NAD	C5N-C6N-N1N	-2.08	117.42	120.40
2	D	504	NAD	O3D-C3D-C4D	-2.04	105.15	111.05
2	B	502	NAD	O2D-C2D-C1D	2.00	118.25	110.85

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	503	NAD	C5B-O5B-PA-O2A
2	C	503	NAD	C4B-C5B-O5B-PA
2	C	503	NAD	O4D-C4D-C5D-O5D
2	C	503	NAD	C3D-C4D-C5D-O5D
2	C	503	NAD	O4D-C1D-N1N-C2N
2	C	503	NAD	O4D-C1D-N1N-C6N
2	C	503	NAD	C2D-C1D-N1N-C2N
2	C	503	NAD	C2D-C1D-N1N-C6N
2	B	502	NAD	C5B-O5B-PA-O2A
2	B	502	NAD	C4B-C5B-O5B-PA
2	B	502	NAD	O4D-C4D-C5D-O5D
2	B	502	NAD	C3D-C4D-C5D-O5D
2	B	502	NAD	O4D-C1D-N1N-C2N

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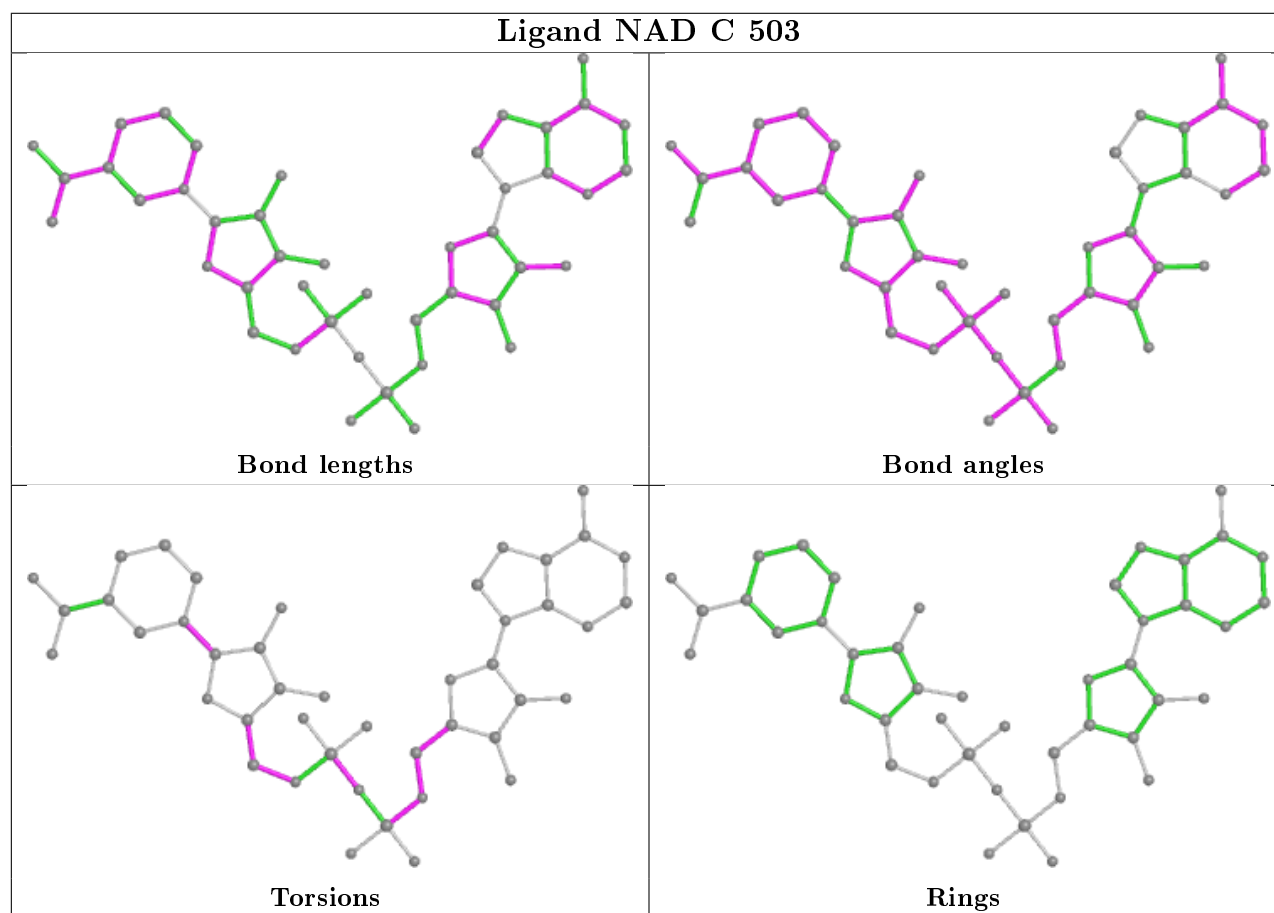
Mol	Chain	Res	Type	Atoms
2	B	502	NAD	O4D-C1D-N1N-C6N
2	B	502	NAD	C2D-C1D-N1N-C2N
2	B	502	NAD	C2D-C1D-N1N-C6N
2	A	501	NAD	C5B-O5B-PA-O2A
2	A	501	NAD	C4B-C5B-O5B-PA
2	A	501	NAD	O4D-C4D-C5D-O5D
2	A	501	NAD	C3D-C4D-C5D-O5D
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
3	C	603	AFX	O1-C1-C4'-C3'
3	C	603	AFX	O1-C1-C4'-C5'
2	D	504	NAD	C5B-O5B-PA-O2A
2	D	504	NAD	C4B-C5B-O5B-PA
2	D	504	NAD	O4D-C4D-C5D-O5D
2	D	504	NAD	C3D-C4D-C5D-O5D
2	D	504	NAD	O4D-C1D-N1N-C2N
2	D	504	NAD	O4D-C1D-N1N-C6N
2	D	504	NAD	C2D-C1D-N1N-C2N
2	D	504	NAD	C2D-C1D-N1N-C6N
3	D	604	AFX	O1-C1-C4'-C3'
2	C	503	NAD	PA-O3-PN-O1N
2	B	502	NAD	PA-O3-PN-O1N
2	A	501	NAD	PA-O3-PN-O1N
2	D	504	NAD	PA-O3-PN-O1N
2	C	503	NAD	C5B-O5B-PA-O1A
2	B	502	NAD	C5B-O5B-PA-O1A
2	A	501	NAD	C5B-O5B-PA-O1A
2	D	504	NAD	C5B-O5B-PA-O1A
3	B	602	AFX	O1-C1-C4'-C5'
3	D	604	AFX	O1-C1-C4'-C5'
3	A	601	AFX	O1-C1-C4'-C3'
3	B	602	AFX	O1-C1-C4'-C3'
2	D	504	NAD	C4D-C5D-O5D-PN
2	C	503	NAD	C4D-C5D-O5D-PN
2	B	502	NAD	C4D-C5D-O5D-PN
2	A	501	NAD	O4B-C4B-C5B-O5B
2	D	504	NAD	O4B-C4B-C5B-O5B
2	C	503	NAD	O4B-C4B-C5B-O5B
2	B	502	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	C4D-C5D-O5D-PN

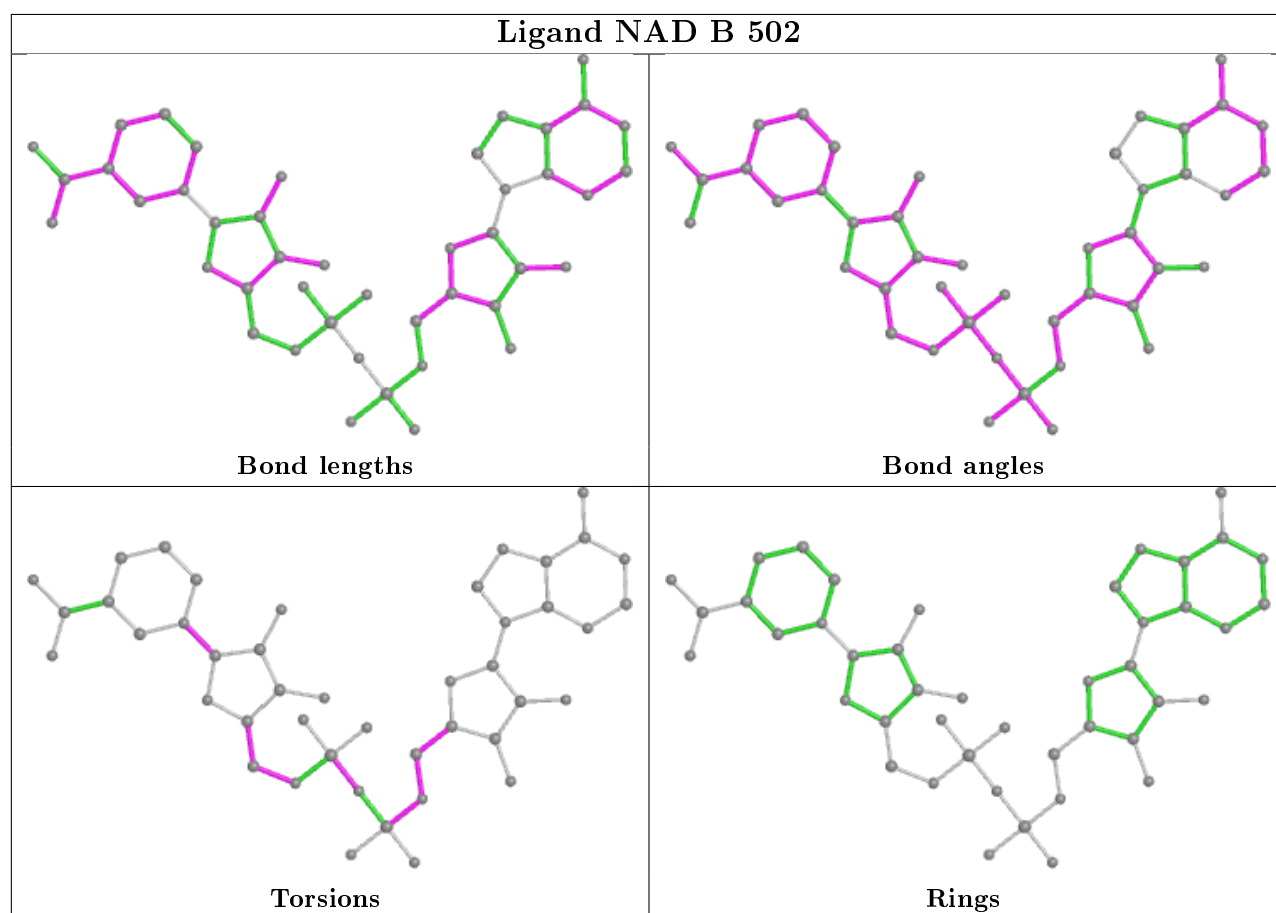
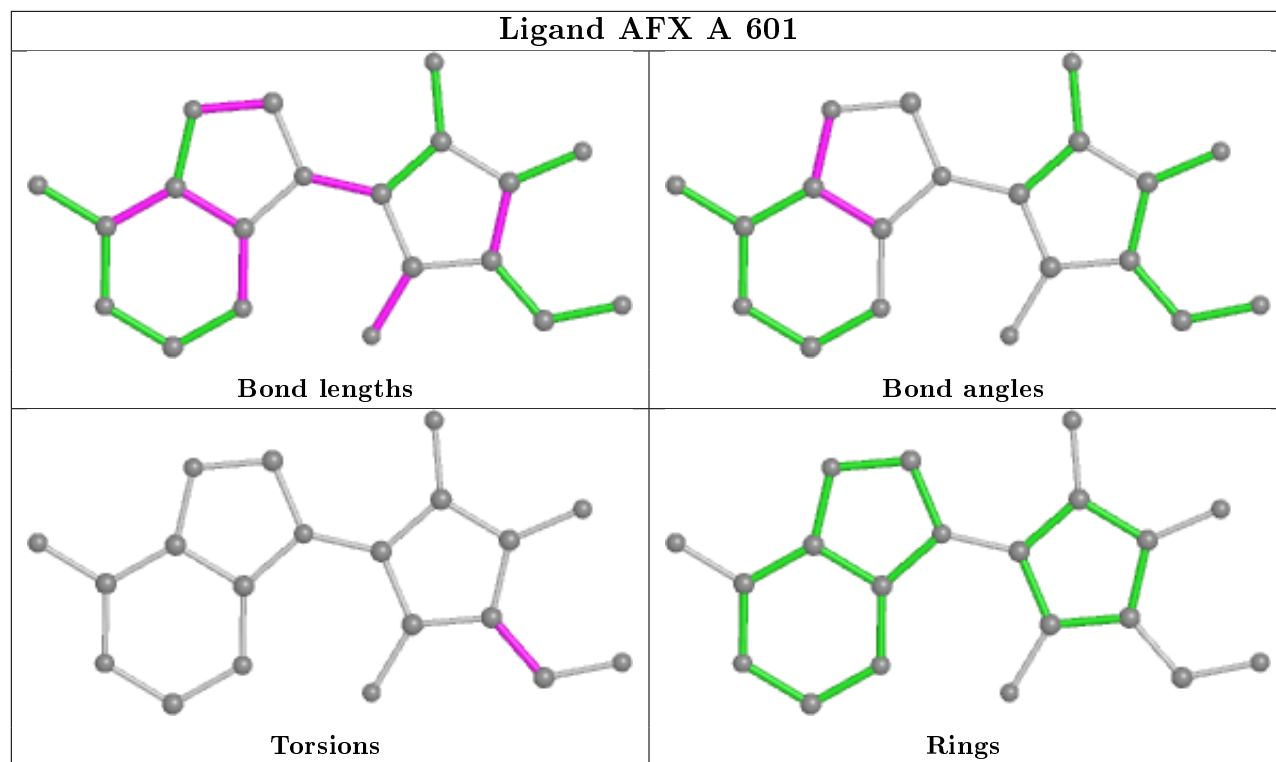
There are no ring outliers.

2 monomers are involved in 3 short contacts:

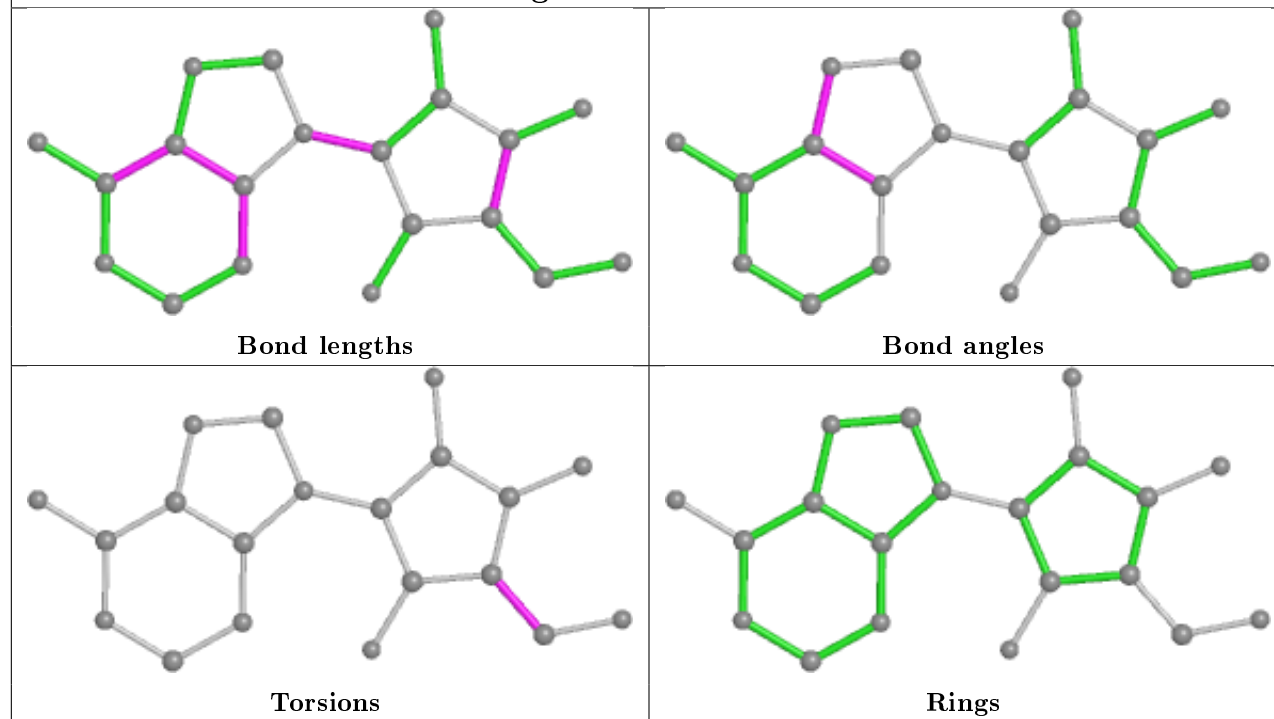
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAD	2	0
2	D	504	NAD	1	0

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.

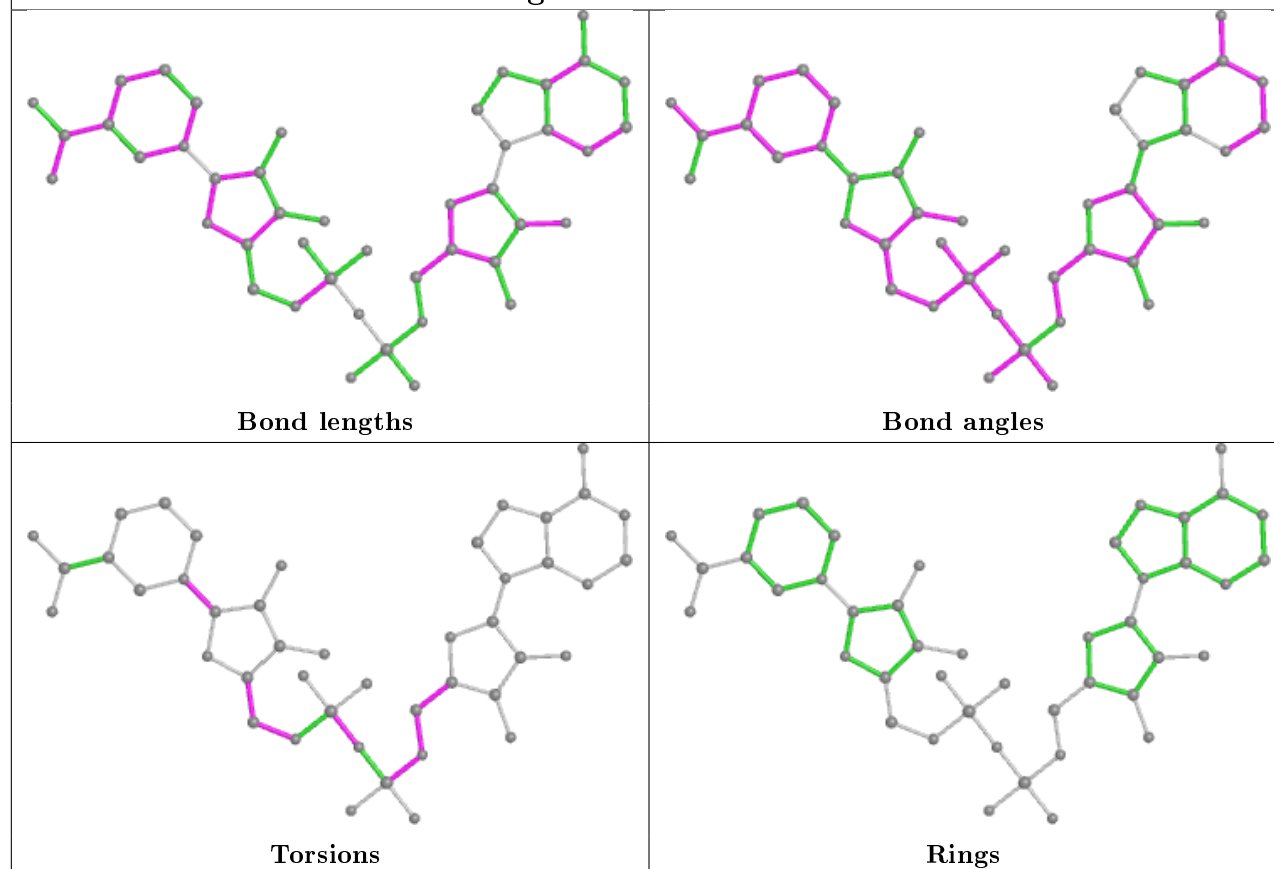




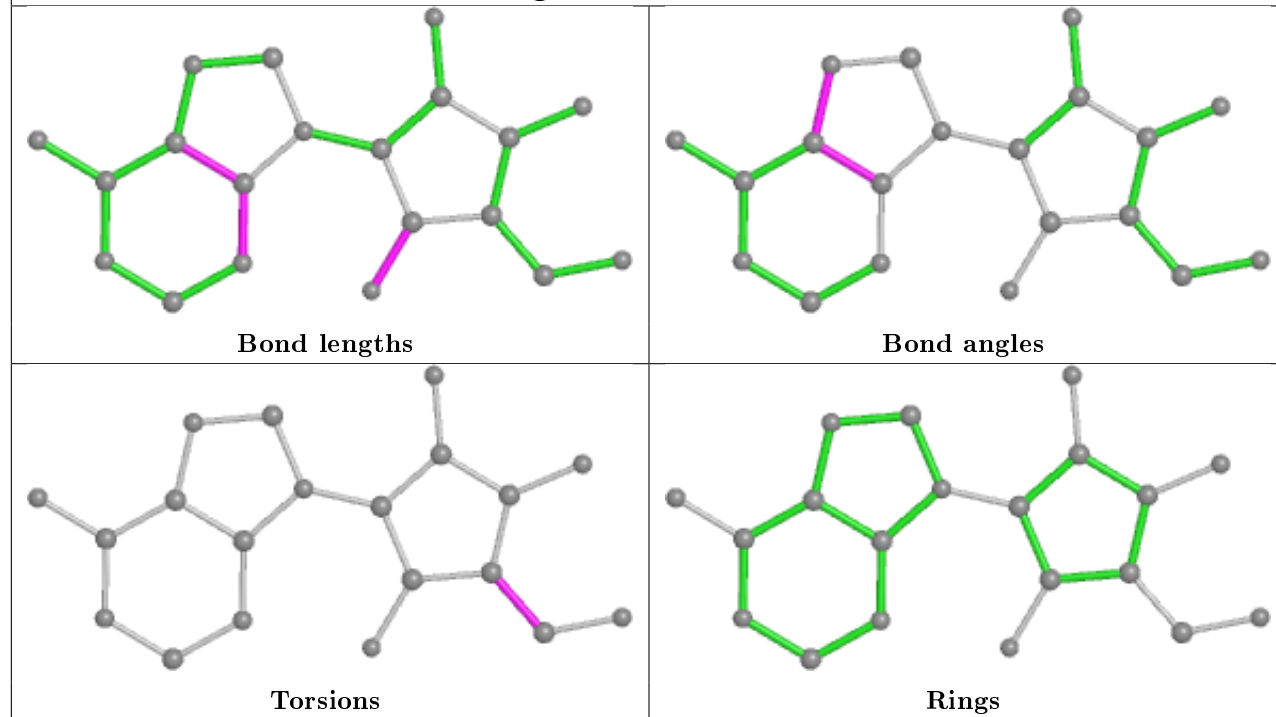
Ligand AFX B 602



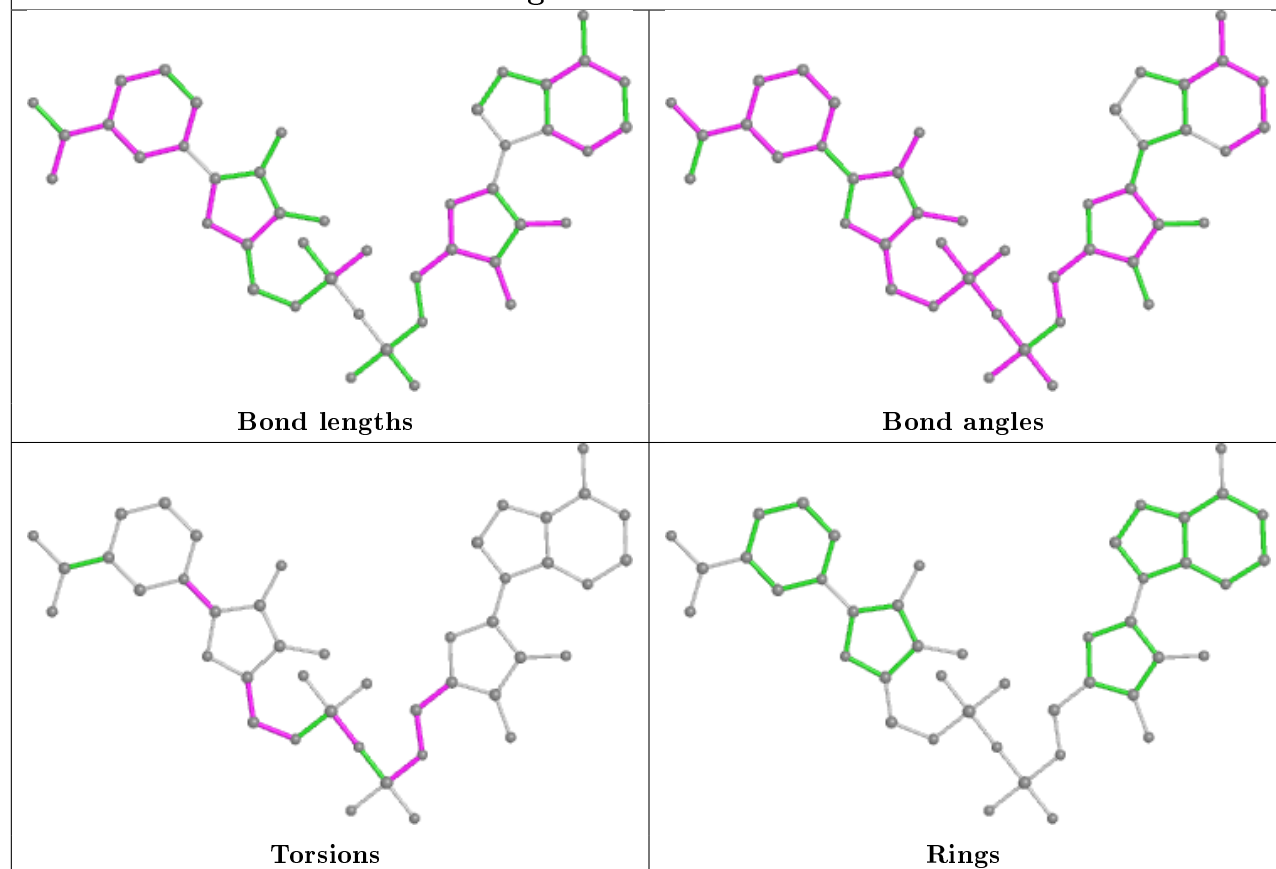
Ligand NAD A 501

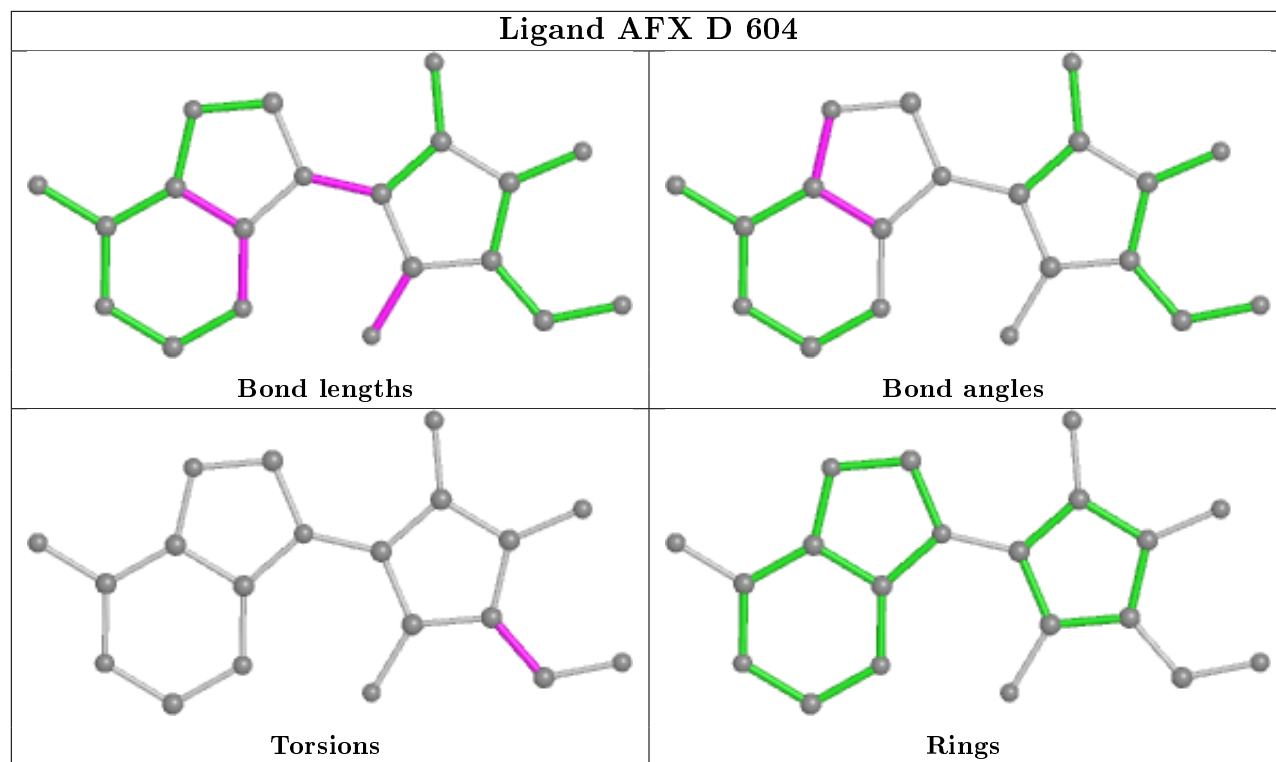


Ligand AFX C 603



Ligand NAD D 504





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	431/435 (99%)	0.38	23 (5%) 26 28	17, 36, 54, 84	0
1	B	430/435 (98%)	0.25	8 (1%) 66 69	16, 32, 47, 66	0
1	C	431/435 (99%)	0.36	19 (4%) 34 37	19, 40, 60, 84	0
1	D	430/435 (98%)	0.18	8 (1%) 66 69	15, 34, 50, 64	0
All	All	1722/1740 (98%)	0.29	58 (3%) 45 48	15, 35, 55, 84	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	SER	5.0
1	A	2	SER	4.3
1	C	3	ASP	4.0
1	C	372	LEU	3.8
1	A	149	GLY	3.8
1	B	172	ILE	3.5
1	C	121	LYS	3.3
1	C	124	PRO	3.3
1	A	421	CYS	3.3
1	A	150	ILE	3.2
1	C	316	VAL	3.2
1	C	118	LEU	3.2
1	B	279	ILE	3.1
1	C	119	TYR	3.0
1	A	45	LEU	2.9
1	C	123	GLY	2.8
1	B	316	VAL	2.8
1	B	421	CYS	2.8
1	C	5	LEU	2.8
1	D	106	THR	2.7
1	A	120	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	373	TRP	2.6
1	A	409	LEU	2.6
1	C	112	TRP	2.6
1	C	149	GLY	2.5
1	C	99	VAL	2.5
1	A	377	ASP	2.5
1	A	176	PRO	2.5
1	D	15	ALA	2.5
1	D	423	GLY	2.5
1	D	211	ILE	2.4
1	A	152	GLY	2.4
1	A	119	TYR	2.4
1	C	173	LEU	2.4
1	A	9	VAL	2.3
1	B	235	PHE	2.3
1	C	234	GLY	2.3
1	A	151	ARG	2.3
1	A	126	ASN	2.3
1	C	6	PRO	2.3
1	B	195	CYS	2.3
1	A	376	PRO	2.2
1	C	47	GLY	2.2
1	A	145	GLN	2.2
1	D	112	TRP	2.2
1	A	420	SER	2.2
1	D	209	VAL	2.2
1	C	139	ILE	2.2
1	A	423	GLY	2.2
1	D	108	GLU	2.2
1	B	169	ALA	2.1
1	B	420	SER	2.1
1	A	374	THR	2.1
1	A	200	ILE	2.1
1	A	195	CYS	2.1
1	A	47	GLY	2.1
1	A	17	TRP	2.1
1	D	101	ALA	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

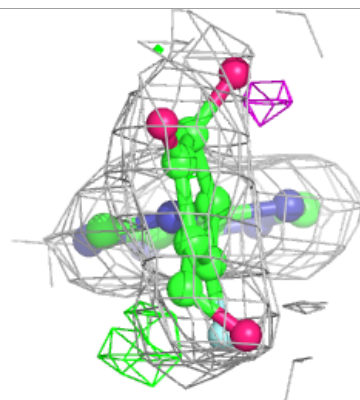
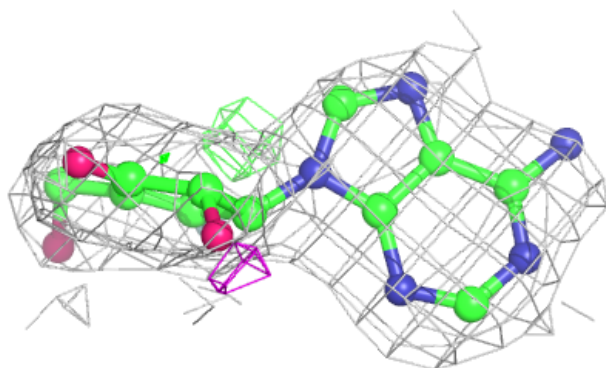
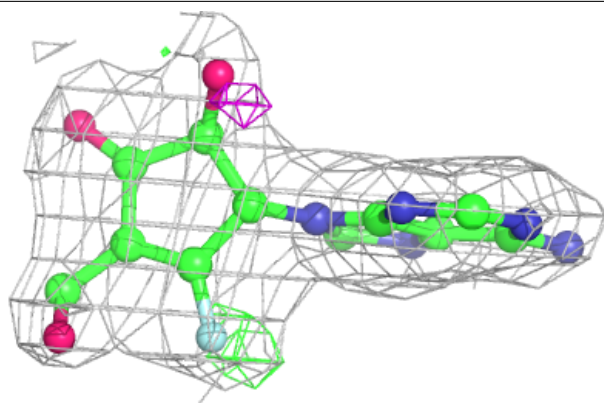
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AFX	C	603	20/20	0.92	0.22	31,34,37,38	0
2	NAD	B	502	44/44	0.94	0.18	22,30,32,36	0
3	AFX	B	602	20/20	0.94	0.24	26,32,35,35	0
3	AFX	A	601	20/20	0.94	0.20	27,33,37,39	0
2	NAD	A	501	44/44	0.95	0.17	27,30,35,37	0
2	NAD	C	503	44/44	0.95	0.17	29,33,36,37	0
3	AFX	D	604	20/20	0.95	0.19	28,30,33,33	0
2	NAD	D	504	44/44	0.96	0.16	21,28,32,34	0

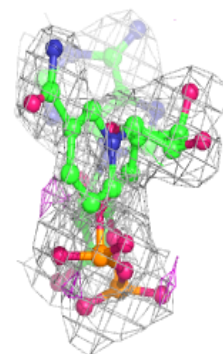
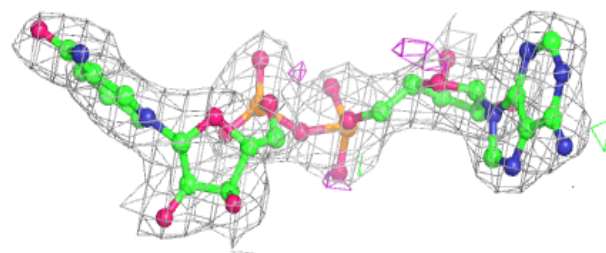
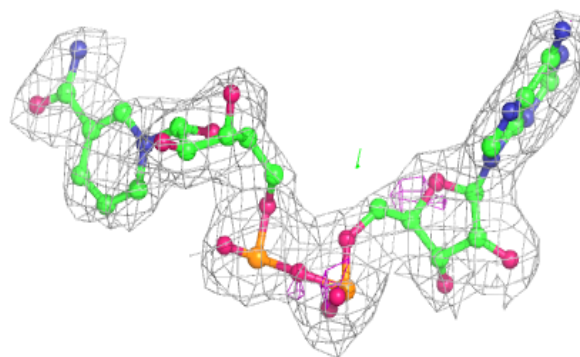
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AFX C 603:

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

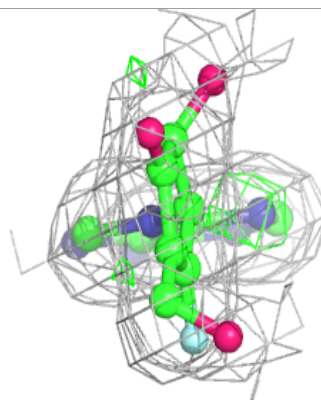
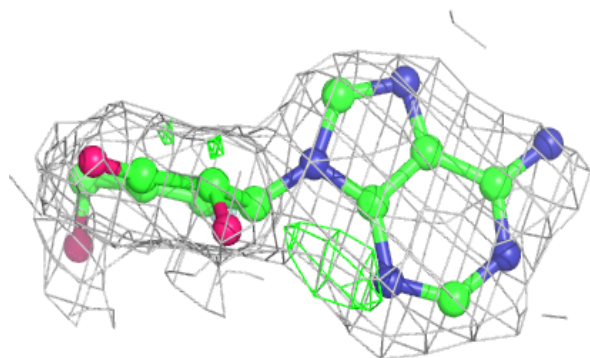
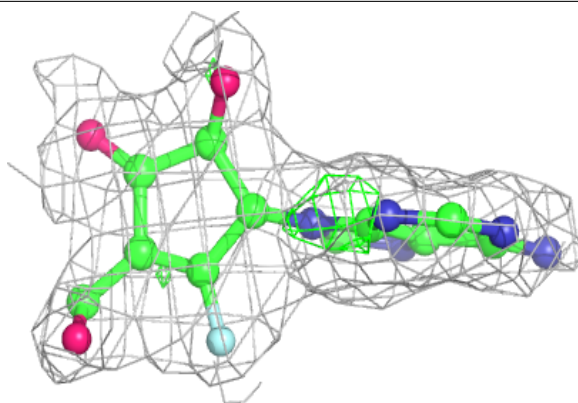
**Electron density around NAD B 502:**

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

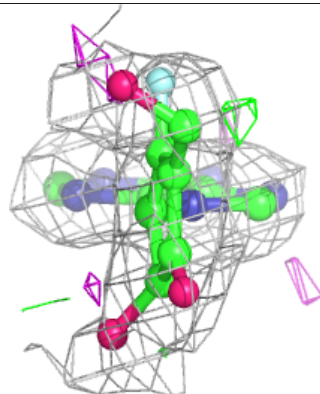
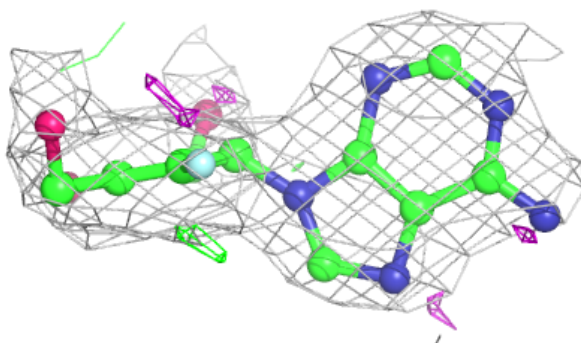
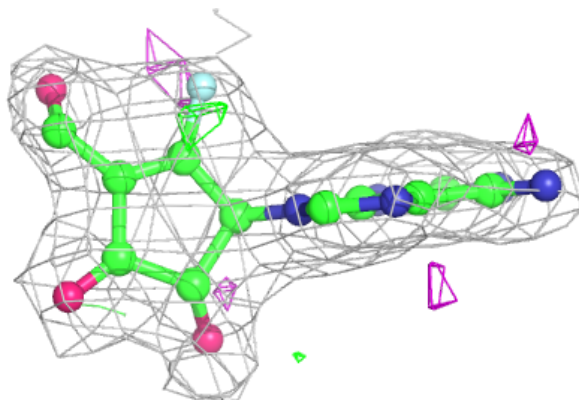


Electron density around AFX B 602:

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

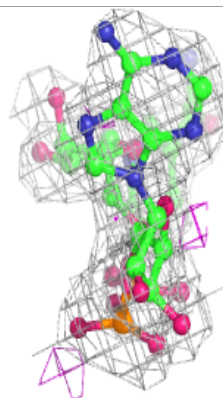
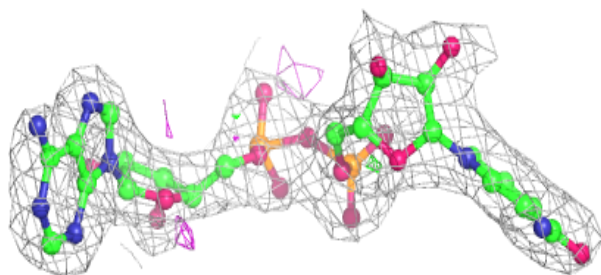
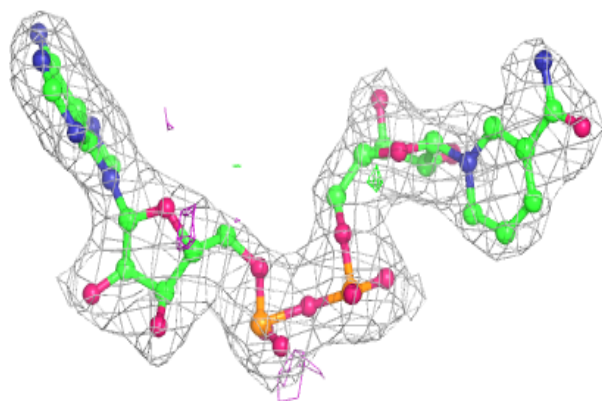
**Electron density around AFX A 601:**

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

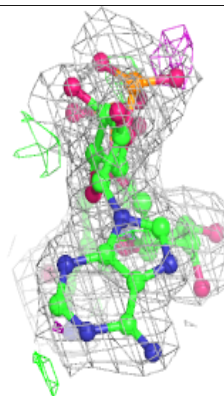
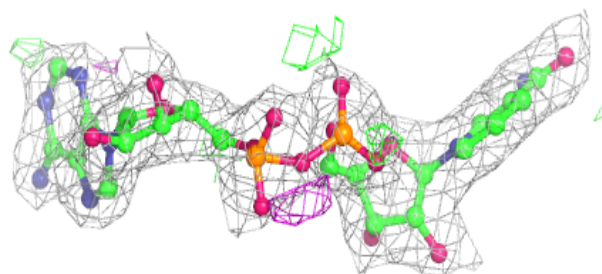
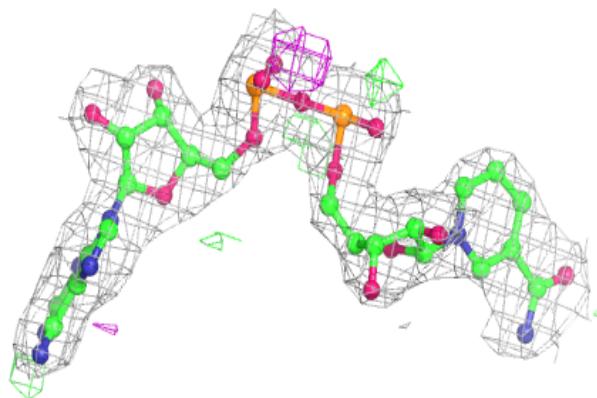


Electron density around NAD A 501:

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

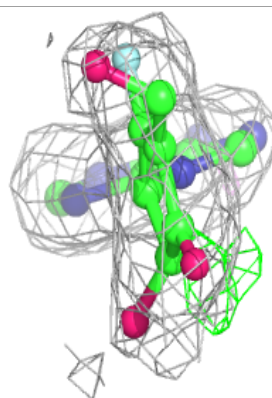
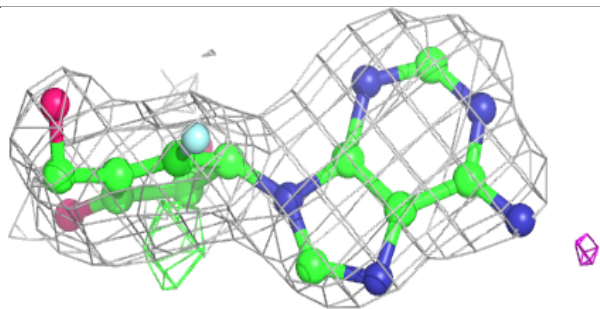
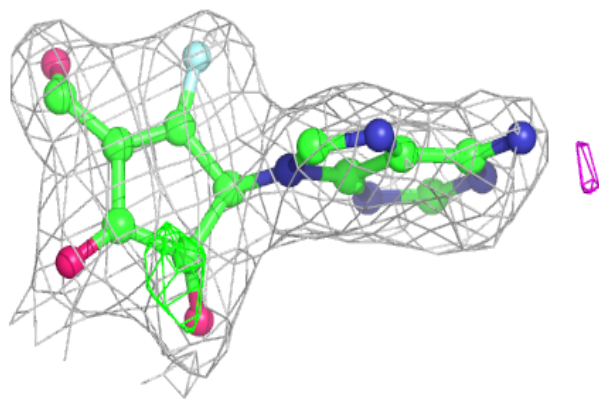
**Electron density around NAD C 503:**

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

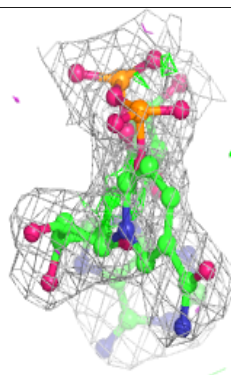
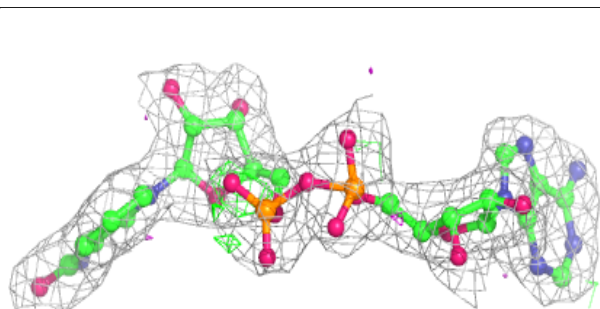
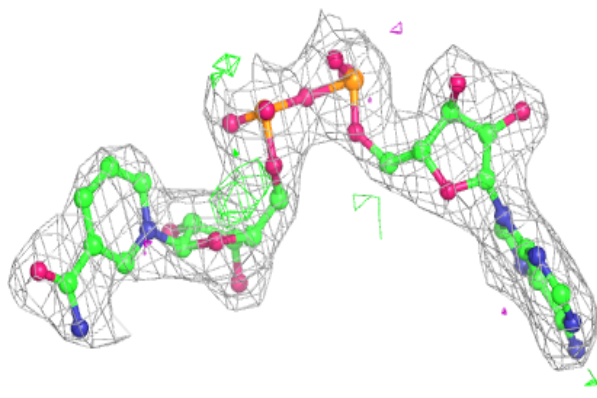


Electron density around AFX D 604:

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

**Electron density around NAD D 504:**

$2mF_o-DF_c$ (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.