



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:43 PM UTC

PDB ID : 3C1M / pdb_00003c1m
Title : Crystal Structure of threonine-sensitive aspartokinase from *Methanococcus jannaschii* with MgAMP-PNP and L-aspartate
Authors : Liu, X.
Deposited on : 2008-01-23
Resolution : 2.30 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

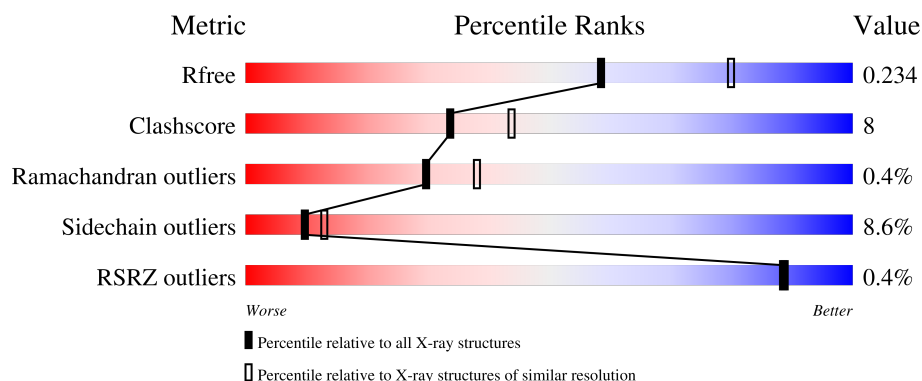
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	473	 80% 15% ..
1	B	473	 78% 17% ..
1	C	473	 79% 18% ..
1	D	473	 80% 15% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15032 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.

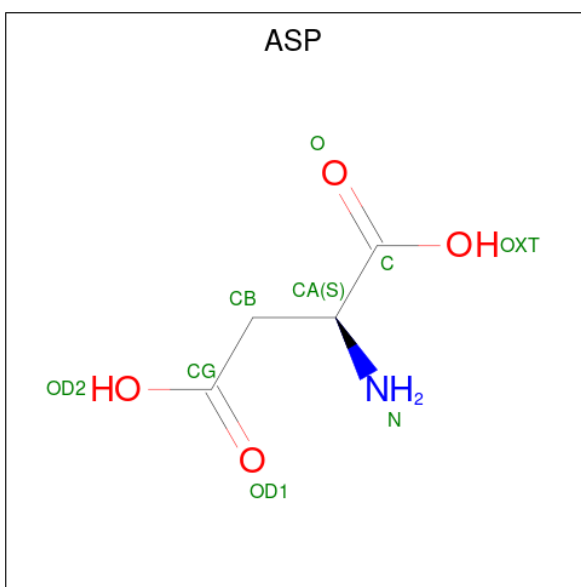
- Molecule 1 is a protein called Probable aspartokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3546	2246	596	693	11			
1	B	465	Total	C	N	O	S	0	1	0
			3554	2251	599	693	11			
1	C	468	Total	C	N	O	S	0	1	0
			3574	2265	602	696	11			
1	D	466	Total	C	N	O	S	0	0	0
			3555	2252	598	694	11			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

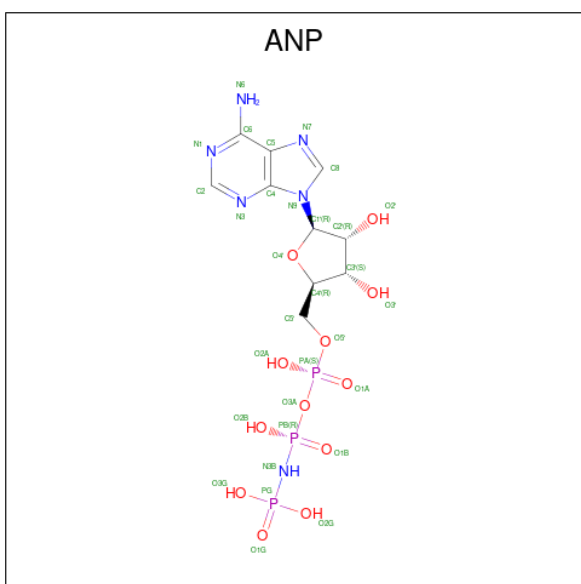
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ASPARTIC ACID (CCD ID: ASP) (formula: C₄H₇NO₄).



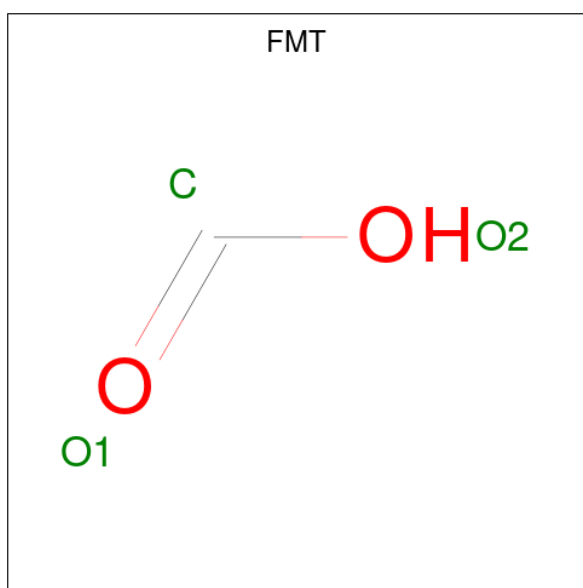
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	4	1	4		
3	B	1	Total	C	N	O	0	0
			9	4	1	4		
3	C	1	Total	C	N	O	0	0
			9	4	1	4		
3	D	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		

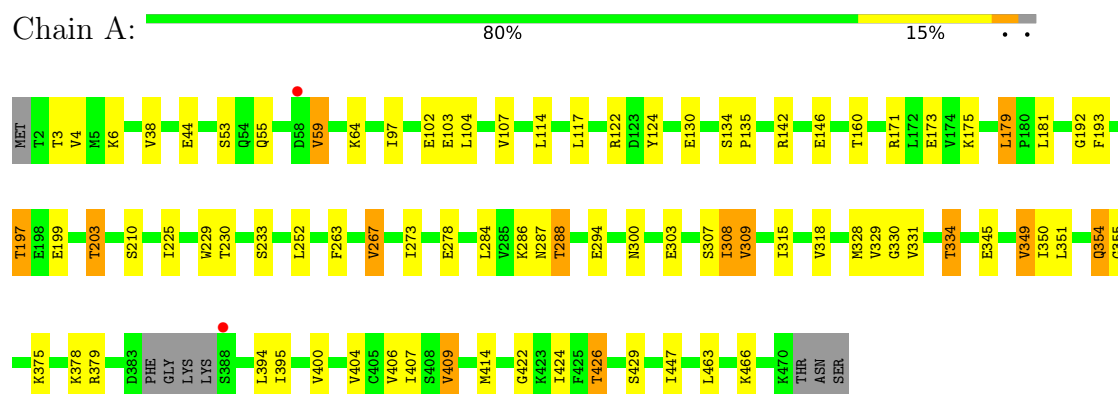
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	168	Total 168	O 168	0	0
6	B	150	Total 150	O 150	0	0
6	C	122	Total 122	O 122	0	0
6	D	181	Total 181	O 181	0	0

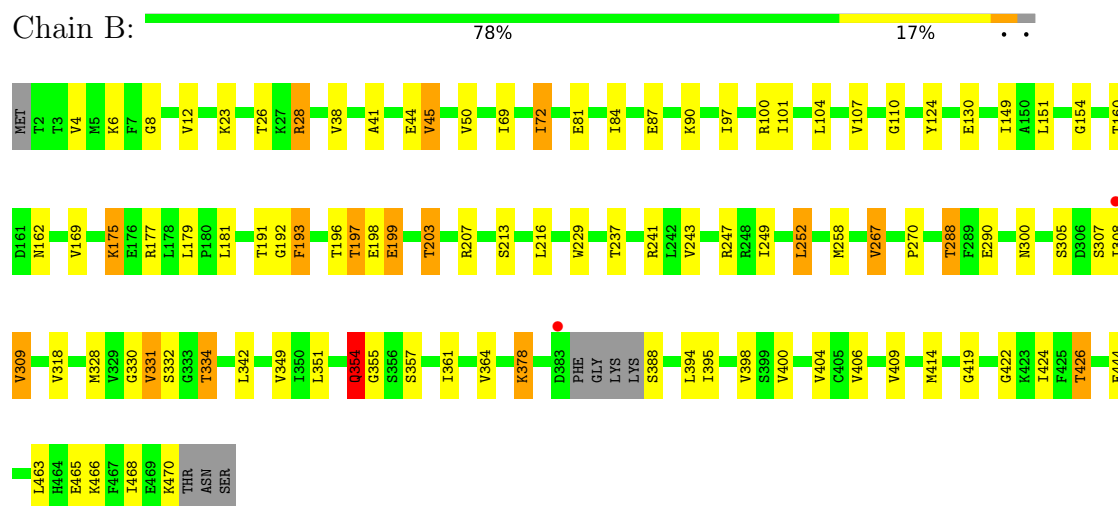
3 Residue-property plots

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.

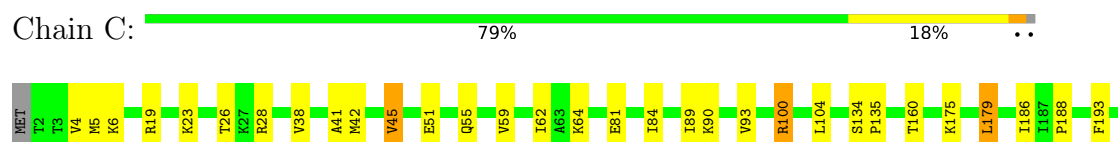
• Molecule 1: Probable aspartokinase

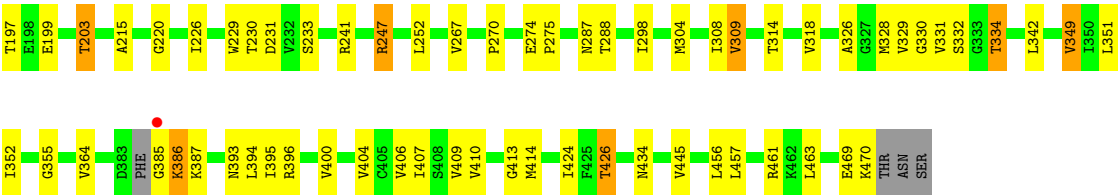


• Molecule 1: Probable aspartokinase

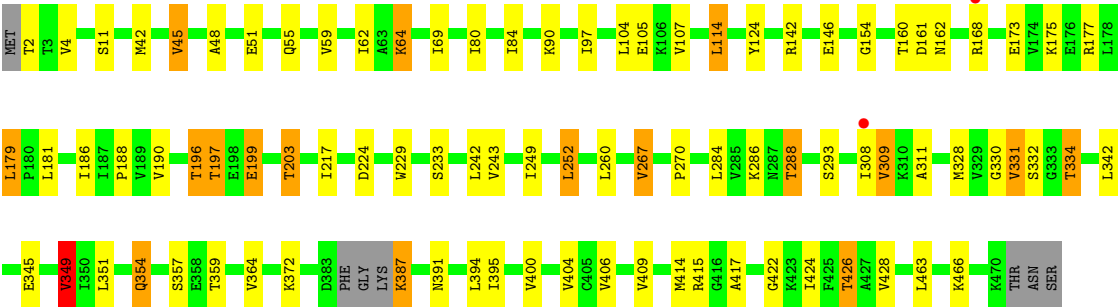
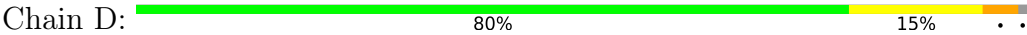


• Molecule 1: Probable aspartokinase





● Molecule 1: Probable aspartokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.41Å 104.48Å 192.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (50.00-2.30) 95.6 (50.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.246 0.186 , 0.234	Depositor DCC
R_{free} test set	4369 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15032	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, FMT, MG

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	0.63	0/3585	0.93	1/4828 (0.0%)
1	B	0.63	1/3596 (0.0%)	0.94	5/4842 (0.1%)
1	C	0.58	0/3616	0.90	0/4866
1	D	0.64	1/3594 (0.0%)	0.95	4/4839 (0.1%)
All	All	0.62	2/14391 (0.0%)	0.93	10/19375 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	GLU	CD-OE2	-6.96	1.12	1.25
1	D	349	VAL	CA-CB	5.09	1.60	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	267	VAL	CB-CA-C	-7.22	101.50	112.05
1	A	267	VAL	CB-CA-C	-5.94	103.38	112.05
1	B	331	VAL	N-CA-C	5.87	116.65	110.72
1	D	331	VAL	N-CA-C	5.47	116.25	110.72
1	B	243	VAL	CA-C-N	5.38	126.57	119.84
1	B	243	VAL	C-N-CA	5.38	126.57	119.84
1	B	267	VAL	CB-CA-C	-5.19	104.47	112.05
1	B	354	GLN	CB-CA-C	5.16	118.68	109.65
1	D	243	VAL	CA-C-N	5.08	126.19	119.84
1	D	243	VAL	C-N-CA	5.08	126.19	119.84

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	3546	0	3673	55	0
1	B	3554	0	3686	65	0
1	C	3574	0	3715	63	0
1	D	3555	0	3686	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	9	0	3	2	0
3	B	9	0	3	0	0
3	C	9	0	3	2	0
3	D	9	0	3	0	0
4	A	31	0	13	0	0
4	B	31	0	13	1	0
4	C	31	0	13	1	0
4	D	31	0	13	0	0
5	A	12	0	4	0	0
5	C	3	0	1	0	0
5	D	3	0	1	0	0
6	A	168	0	0	5	0
6	B	150	0	0	8	0
6	C	122	0	0	0	0
6	D	181	0	0	2	0
All	All	15032	0	14830	224	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (224) 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:414:MET:HE1	1:A:424:ILE:HD11	1.37	1.05
1:C:414:MET:HE1	1:C:424:ILE:HD11	1.38	1.05
1:C:386:LYS:CB	1:C:387:LYS:HA	1.81	1.03
1:D:308:ILE:O	1:D:309:VAL:HG23	1.57	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:VAL:HG22	1:D:409:VAL:CG1	1.90	1.00
1:C:386:LYS:HB2	1:C:387:LYS:CA	1.90	0.99
1:B:28:ARG:CG	1:B:28:ARG:HH11	1.78	0.96
1:A:330:GLY:O	1:A:334:THR:HG23	1.66	0.95
1:B:193:PHE:N	6:B:595:HOH:O	2.00	0.94
1:C:270:PRO:HB2	1:D:328:MET:HE1	1.49	0.94
1:A:308:ILE:O	1:A:309:VAL:HG23	1.68	0.94
1:B:192:GLY:O	1:B:213:SER:OG	1.87	0.92
1:C:386:LYS:HB2	1:C:387:LYS:HA	0.94	0.92
1:D:414:MET:HE1	1:D:424:ILE:HD11	1.53	0.91
1:B:28:ARG:HH11	1:B:28:ARG:HG2	1.36	0.90
1:B:422:GLY:O	1:B:426:THR:HG23	1.72	0.89
1:A:422:GLY:O	1:A:426:THR:HG23	1.73	0.88
1:C:414:MET:CE	1:C:424:ILE:HD11	2.04	0.88
1:C:386:LYS:HE2	1:C:393:ASN:HB3	1.55	0.88
1:C:330:GLY:O	1:C:334:THR:HG23	1.76	0.85
1:D:414:MET:CE	1:D:424:ILE:HD11	2.10	0.82
1:D:422:GLY:O	1:D:426:THR:HG23	1.80	0.81
1:A:107:VAL:HG21	1:A:124:TYR:HE2	1.45	0.80
1:A:354:GLN:NE2	6:A:569:HOH:O	2.04	0.80
1:A:328:MET:HE2	1:B:258:MET:HE3	1.62	0.79
1:D:309:VAL:HG22	1:D:409:VAL:HG13	1.66	0.78
1:B:229:TRP:HB3	1:B:288:THR:HG22	1.64	0.77
1:D:330:GLY:O	1:D:334:THR:HG22	1.83	0.77
1:B:197:THR:HG22	1:B:199:GLU:H	1.51	0.75
1:A:309:VAL:HG22	1:A:409:VAL:CG1	2.18	0.73
1:A:414:MET:CE	1:A:424:ILE:HD11	2.18	0.72
1:C:426:THR:HG22	6:D:476:HOH:O	1.89	0.71
1:B:414:MET:HE1	1:B:424:ILE:HD11	1.72	0.71
1:D:107:VAL:HG21	1:D:124:TYR:HE2	1.56	0.71
1:A:107:VAL:HG21	1:A:124:TYR:CE2	2.26	0.71
1:D:309:VAL:HG22	1:D:409:VAL:HG11	1.71	0.71
1:D:160:THR:OG1	1:D:203:THR:HG21	1.91	0.70
1:B:192:GLY:C	6:B:595:HOH:O	2.27	0.70
1:B:28:ARG:HG2	1:B:28:ARG:NH1	2.05	0.69
1:A:414:MET:HE1	1:A:424:ILE:CD1	2.20	0.69
1:A:349:VAL:CG1	1:B:332:SER:HB3	2.22	0.69
1:C:270:PRO:HB2	1:D:328:MET:CE	2.22	0.68
1:D:330:GLY:O	1:D:334:THR:CG2	2.41	0.68
1:B:160:THR:OG1	1:B:203:THR:HG21	1.94	0.67
1:C:326:ALA:CB	1:C:386:LYS:HE3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:GLY:HA3	1:D:196:THR:HB	1.77	0.65
1:C:247:ARG:HH12	1:C:469:GLU:HG2	1.61	0.65
1:A:171:ARG:NH1	1:A:173:GLU:OE2	2.29	0.65
1:C:414:MET:CE	1:C:424:ILE:CD1	2.74	0.65
1:C:229:TRP:HB3	1:C:288:THR:HG22	1.78	0.65
1:A:309:VAL:HG22	1:A:409:VAL:HG13	1.78	0.64
1:B:28:ARG:HH11	1:B:28:ARG:HG3	1.61	0.64
1:C:329:VAL:HG23	1:C:334:THR:HG21	1.79	0.64
1:A:308:ILE:O	1:A:309:VAL:CG2	2.45	0.63
1:A:414:MET:CE	1:A:447:ILE:HD12	2.28	0.63
1:B:81:GLU:HA	1:B:90:LYS:HE2	1.81	0.63
1:C:349:VAL:CG1	1:D:332:SER:HB3	2.29	0.63
1:D:308:ILE:O	1:D:309:VAL:CG2	2.43	0.63
1:C:309:VAL:HG13	1:C:409:VAL:HG13	1.81	0.62
1:C:175:LYS:O	1:C:179:LEU:HB2	2.00	0.61
1:A:229:TRP:HB3	1:A:288:THR:HG22	1.82	0.61
1:B:318:VAL:HG21	1:B:406:VAL:HG23	1.83	0.61
1:B:110:GLY:HA3	1:D:114:LEU:HD13	1.82	0.61
1:A:103:GLU:O	1:A:107:VAL:HG23	2.02	0.60
1:A:300:ASN:HB2	6:A:497:HOH:O	2.03	0.59
1:D:175:LYS:O	1:D:179:LEU:HB2	2.02	0.59
1:C:160:THR:OG1	1:C:203:THR:HG21	2.04	0.58
1:C:326:ALA:HB1	1:C:386:LYS:HE3	1.85	0.58
1:A:6:LYS:HE3	1:A:210:SER:HB3	1.85	0.58
1:A:107:VAL:CG2	1:A:124:TYR:HE2	2.15	0.58
1:B:107:VAL:HG21	1:B:124:TYR:CD2	2.39	0.58
1:B:249:ILE:HG21	1:B:252:LEU:HD13	1.86	0.57
1:D:42:MET:O	1:D:45:VAL:HG13	2.04	0.57
1:A:318:VAL:HG21	1:A:406:VAL:HG23	1.87	0.57
1:C:318:VAL:HG21	1:C:406:VAL:HG23	1.86	0.57
1:A:160:THR:OG1	1:A:203:THR:HG21	2.04	0.57
1:D:11:SER:OG	1:D:288:THR:HG21	2.05	0.56
1:D:387:LYS:HB2	1:D:391:ASN:HD21	1.70	0.56
1:B:308:ILE:H	1:B:308:ILE:HD12	1.70	0.56
1:C:332:SER:HB3	1:D:349:VAL:CG1	2.35	0.56
1:A:307:SER:O	1:A:308:ILE:O	2.24	0.55
1:B:107:VAL:HG21	1:B:124:TYR:CE2	2.41	0.55
1:D:107:VAL:HG21	1:D:124:TYR:CE2	2.38	0.55
1:B:154:GLY:HA3	1:B:196:THR:HB	1.88	0.55
1:B:241:ARG:HD2	4:B:473:ANP:O2'	2.07	0.55
1:C:233:SER:HA	1:C:287:ASN:HB2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLU:HG3	6:B:607:HOH:O	2.07	0.54
1:A:414:MET:CE	1:A:424:ILE:CD1	2.82	0.54
1:C:308:ILE:HD12	1:C:308:ILE:H	1.73	0.54
1:A:294:GLU:HG2	6:A:626:HOH:O	2.08	0.54
1:A:414:MET:HE2	1:A:447:ILE:HD12	1.90	0.54
1:A:334:THR:HG22	1:A:394:LEU:HG	1.90	0.53
1:B:388:SER:N	6:B:599:HOH:O	2.41	0.53
1:C:241:ARG:HD2	4:C:473:ANP:O2'	2.08	0.53
1:C:308:ILE:O	1:C:309:VAL:HB	2.08	0.53
1:D:309:VAL:CG2	1:D:409:VAL:HG11	2.37	0.53
1:C:270:PRO:CB	1:D:328:MET:HE1	2.31	0.53
1:D:334:THR:CG2	1:D:359:THR:HG21	2.39	0.53
1:B:41:ALA:HB1	1:B:45:VAL:HG22	1.92	0.52
1:C:193:PHE:CD2	3:C:472:ASP:N	2.78	0.52
1:A:414:MET:HE3	1:A:447:ILE:HD12	1.91	0.52
1:D:334:THR:HG21	1:D:359:THR:HG21	1.91	0.52
1:C:352:ILE:HD12	1:D:354:GLN:HG2	1.92	0.51
1:D:229:TRP:HB3	1:D:288:THR:HG22	1.91	0.51
1:A:142:ARG:NH2	6:A:597:HOH:O	2.42	0.51
1:B:309:VAL:HG13	1:B:409:VAL:HG13	1.92	0.51
1:B:309:VAL:HG22	1:B:409:VAL:CG1	2.40	0.51
1:C:193:PHE:CG	3:C:472:ASP:N	2.79	0.51
1:A:329:VAL:HG23	1:A:334:THR:HG21	1.92	0.51
1:C:309:VAL:HG22	1:C:409:VAL:CG1	2.41	0.51
1:B:169:VAL:HG21	1:B:216:LEU:HD11	1.91	0.51
1:B:330:GLY:O	1:B:334:THR:HG23	2.11	0.51
1:C:386:LYS:CE	1:C:393:ASN:HB3	2.35	0.50
1:C:326:ALA:HB2	1:C:386:LYS:HE3	1.92	0.50
1:B:300:ASN:HB2	6:B:561:HOH:O	2.11	0.50
1:D:354:GLN:NE2	6:D:556:HOH:O	2.19	0.50
1:D:55:GLN:OE1	1:D:64:LYS:HE3	2.12	0.50
1:C:328:MET:HE1	1:D:270:PRO:HB2	1.94	0.50
1:D:80:ILE:HG22	1:D:90:LYS:HG2	1.95	0.49
1:A:284:LEU:HD21	1:A:286:LYS:HD2	1.95	0.49
1:B:28:ARG:CG	1:B:28:ARG:NH1	2.49	0.49
1:C:41:ALA:HB1	1:C:45:VAL:HG22	1.94	0.49
1:B:84:ILE:O	1:B:90:LYS:HE3	2.12	0.48
1:C:84:ILE:O	1:C:90:LYS:HE3	2.14	0.48
1:D:186:ILE:O	1:D:188:PRO:HD3	2.13	0.48
1:D:309:VAL:CG2	1:D:409:VAL:CG1	2.78	0.48
1:C:175:LYS:HG3	1:C:220:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LYS:HA	1:B:38:VAL:O	2.14	0.48
1:B:364:VAL:HG11	1:B:406:VAL:HG21	1.95	0.48
1:D:84:ILE:O	1:D:90:LYS:HD2	2.14	0.48
1:C:6:LYS:HA	1:C:38:VAL:O	2.14	0.48
1:A:328:MET:SD	1:B:270:PRO:HB2	2.54	0.48
1:D:345:GLU:O	1:D:372:LYS:NZ	2.46	0.48
1:A:197:THR:HG22	1:A:199:GLU:H	1.79	0.47
1:C:274:GLU:HB2	1:C:275:PRO:HD3	1.96	0.47
1:C:328:MET:CE	1:D:270:PRO:HB2	2.45	0.47
1:A:142:ARG:HA	1:A:146:GLU:O	2.15	0.47
1:C:55:GLN:CD	1:C:64:LYS:HE2	2.40	0.47
1:A:197:THR:CG2	1:A:199:GLU:OE1	2.63	0.47
1:B:307:SER:O	1:B:308:ILE:C	2.57	0.47
1:C:352:ILE:HD12	1:D:354:GLN:CG	2.44	0.47
1:C:387:LYS:HE3	1:C:396:ARG:HD3	1.97	0.47
1:C:304:MET:SD	1:C:413:GLY:HA3	2.54	0.46
1:C:364:VAL:HG11	1:C:406:VAL:HG21	1.96	0.46
1:D:142:ARG:HA	1:D:146:GLU:O	2.15	0.46
1:B:50:VAL:HG21	1:B:207[B]:ARG:HH21	1.81	0.46
1:A:3:THR:HG23	1:A:225:ILE:HG23	1.97	0.46
1:A:192:GLY:O	1:A:193:PHE:HB3	2.15	0.46
1:B:197:THR:CG2	1:B:199:GLU:OE1	2.64	0.46
1:A:53:SER:HB3	1:A:117:LEU:HD21	1.98	0.46
1:A:122:ARG:NH1	6:A:551:HOH:O	2.49	0.46
1:D:197:THR:CG2	1:D:199:GLU:HG2	2.46	0.46
1:D:260:LEU:HD11	1:D:311:ALA:HB3	1.98	0.46
1:B:72:ILE:HG22	1:B:101:ILE:CD1	2.45	0.46
1:B:328:MET:HE2	1:B:357:SER:HB2	1.97	0.46
1:A:308:ILE:O	1:A:309:VAL:CB	2.63	0.46
1:B:175:LYS:O	1:B:179:LEU:HB2	2.16	0.46
1:B:229:TRP:HB3	1:B:288:THR:CG2	2.41	0.45
1:D:48:ALA:HA	1:D:51:GLU:HG2	1.98	0.45
1:C:19:ARG:HG2	1:C:23:LYS:HE3	1.96	0.45
1:C:215:ALA:HA	1:C:226:ILE:HD13	1.97	0.45
1:C:426:THR:HG23	1:D:422:GLY:HA3	1.98	0.45
1:D:55:GLN:CD	1:D:64:LYS:HE3	2.41	0.45
1:B:309:VAL:HG22	1:B:409:VAL:HG11	1.99	0.45
1:B:8:GLY:O	1:B:12:VAL:HG22	2.17	0.45
1:A:175:LYS:O	1:A:179:LEU:HB2	2.17	0.45
1:C:252:LEU:O	1:C:298:ILE:HA	2.17	0.44
1:B:149:ILE:HD11	1:B:181:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASP:OD2	1:D:168:ARG:HG2	2.18	0.44
1:B:414:MET:HE1	1:B:424:ILE:CD1	2.45	0.44
1:D:173:GLU:O	1:D:177:ARG:HG2	2.18	0.44
1:D:249:ILE:HG21	1:D:252:LEU:HD13	1.98	0.44
1:D:284:LEU:HG	1:D:286:LYS:HG3	2.00	0.44
1:D:84:ILE:HB	1:D:90:LYS:HG3	1.99	0.44
1:D:424:ILE:O	1:D:428:VAL:HG23	2.18	0.44
1:C:100:ARG:HA	1:C:100:ARG:HD3	1.73	0.43
1:A:134:SER:OG	1:A:135:PRO:HD3	2.18	0.43
1:B:354:GLN:HB2	1:B:361:ILE:HG13	1.99	0.43
1:B:364:VAL:HG11	1:B:406:VAL:CG2	2.49	0.43
1:C:457:LEU:HD13	1:C:461:ARG:HH12	1.84	0.43
1:B:308:ILE:O	1:B:309:VAL:HB	2.19	0.43
1:C:186:ILE:O	1:C:188:PRO:HD3	2.18	0.43
1:A:309:VAL:HG22	1:A:409:VAL:HG11	1.99	0.43
1:D:364:VAL:HG11	1:D:406:VAL:HG21	2.00	0.43
1:B:307:SER:O	1:B:307:SER:OG	2.33	0.43
1:B:468:ILE:HD12	1:B:468:ILE:N	2.34	0.43
1:D:69:ILE:HG13	1:D:105:GLU:HG3	1.99	0.42
1:C:81:GLU:HA	1:C:90:LYS:HE2	1.99	0.42
1:B:197:THR:CG2	1:B:199:GLU:H	2.26	0.42
1:C:385:GLY:O	1:C:386:LYS:HG3	2.18	0.42
1:D:2:THR:N	1:D:224:ASP:OD2	2.53	0.42
1:A:349:VAL:HG13	1:B:332:SER:HB3	1.96	0.42
1:B:354:GLN:NE2	6:B:498:HOH:O	2.23	0.42
1:D:233:SER:HB3	1:D:293:SER:OG	2.19	0.42
1:B:23:LYS:HA	1:B:26:THR:HG22	2.01	0.42
1:C:364:VAL:HG11	1:C:406:VAL:CG2	2.50	0.42
1:D:190:VAL:HG11	1:D:217:ILE:HD11	2.02	0.42
1:D:308:ILE:HD13	1:D:417:ALA:HB1	2.00	0.41
1:A:345:GLU:OE1	1:A:379:ARG:NH2	2.53	0.41
1:B:444:GLU:HG2	6:B:527:HOH:O	2.20	0.41
1:A:210:SER:HB2	3:A:471:ASP:OD2	2.20	0.41
1:D:328:MET:HE2	1:D:357:SER:HB2	2.01	0.41
1:B:69:ILE:HG23	1:B:101:ILE:HG23	2.03	0.41
1:B:378:LYS:HE2	1:B:378:LYS:HB3	1.87	0.41
1:C:89:ILE:O	1:C:93:VAL:HG23	2.21	0.41
1:A:429:SER:HB2	1:B:419:GLY:HA2	2.01	0.41
1:A:263:PHE:HA	1:A:315:ILE:HD11	2.02	0.41
1:A:328:MET:HE2	1:B:258:MET:CE	2.43	0.41
1:B:100:ARG:HA	1:B:100:ARG:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:HB3	1:B:191:THR:HB	2.03	0.41
1:A:6:LYS:HA	1:A:38:VAL:O	2.20	0.41
1:C:314:THR:HG22	1:C:407:ILE:HG13	2.03	0.41
1:A:55:GLN:O	1:A:59:VAL:HG22	2.21	0.41
1:A:230:THR:O	1:A:288:THR:HG23	2.21	0.41
1:B:237:THR:HB	1:B:468:ILE:HG12	2.02	0.41
1:C:134:SER:N	1:C:135:PRO:HD2	2.36	0.41
1:A:130:GLU:OE2	3:A:471:ASP:N	2.54	0.41
1:C:230:THR:OG1	1:C:231:ASP:N	2.54	0.41
1:C:5:MET:CE	1:C:28:ARG:HG3	2.52	0.40
1:C:410:VAL:HA	1:C:445:VAL:O	2.21	0.40
1:C:456:LEU:C	1:C:456:LEU:HD23	2.46	0.40
1:B:388:SER:HA	6:B:599:HOH:O	2.21	0.40
1:A:233:SER:HA	1:A:287:ASN:HB2	2.04	0.40
1:C:42:MET:O	1:C:45:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/473 (98%)	447 (97%)	11 (2%)	3 (1%)	18	23
1	B	462/473 (98%)	444 (96%)	16 (4%)	2 (0%)	30	38
1	C	465/473 (98%)	448 (96%)	15 (3%)	2 (0%)	30	38
1	D	462/473 (98%)	451 (98%)	10 (2%)	1 (0%)	43	55
All	All	1850/1892 (98%)	1790 (97%)	52 (3%)	8 (0%)	30	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	ILE
1	A	309	VAL
1	B	309	VAL
1	D	309	VAL
1	C	309	VAL
1	A	355	GLY
1	B	355	GLY
1	C	355	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	390/397 (98%)	356 (91%)	34 (9%)	9	12
1	B	391/397 (98%)	353 (90%)	38 (10%)	8	10
1	C	393/397 (99%)	365 (93%)	28 (7%)	13	19
1	D	391/397 (98%)	357 (91%)	34 (9%)	9	12
All	All	1565/1588 (99%)	1431 (91%)	134 (9%)	10	13

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	44	GLU
1	A	59	VAL
1	A	64	LYS
1	A	97	ILE
1	A	102	GLU
1	A	104	LEU
1	A	114	LEU
1	A	179	LEU
1	A	181	LEU
1	A	197	THR
1	A	203	THR
1	A	252	LEU
1	A	267	VAL

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Mol	Chain	Res	Type
1	A	273	ILE
1	A	278	GLU
1	A	288	THR
1	A	303	GLU
1	A	331	VAL
1	A	334	THR
1	A	349	VAL
1	A	350	ILE
1	A	351	LEU
1	A	354	GLN
1	A	375	LYS
1	A	378	LYS
1	A	395	ILE
1	A	400	VAL
1	A	404	VAL
1	A	407	ILE
1	A	409	VAL
1	A	426	THR
1	A	463	LEU
1	A	466	LYS
1	B	4	VAL
1	B	28	ARG
1	B	45	VAL
1	B	72	ILE
1	B	97	ILE
1	B	104	LEU
1	B	151	LEU
1	B	162	ASN
1	B	175	LYS
1	B	177	ARG
1	B	193	PHE
1	B	197	THR
1	B	198	GLU
1	B	199	GLU
1	B	203	THR
1	B	247	ARG
1	B	252	LEU
1	B	267	VAL
1	B	288	THR
1	B	290	GLU
1	B	305	SER
1	B	331	VAL

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Mol	Chain	Res	Type
1	B	334	THR
1	B	342	LEU
1	B	349	VAL
1	B	351	LEU
1	B	354	GLN
1	B	378	LYS
1	B	394	LEU
1	B	395	ILE
1	B	398	VAL
1	B	400	VAL
1	B	404	VAL
1	B	426	THR
1	B	463	LEU
1	B	465	GLU
1	B	466	LYS
1	B	470	LYS
1	C	4	VAL
1	C	26	THR
1	C	45	VAL
1	C	51	GLU
1	C	59	VAL
1	C	62	ILE
1	C	100	ARG
1	C	104	LEU
1	C	179	LEU
1	C	197	THR
1	C	199	GLU
1	C	203	THR
1	C	247	ARG
1	C	267	VAL
1	C	331	VAL
1	C	334	THR
1	C	342	LEU
1	C	349	VAL
1	C	351	LEU
1	C	386	LYS
1	C	394	LEU
1	C	395	ILE
1	C	400	VAL
1	C	404	VAL
1	C	426	THR
1	C	434	ASN

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Mol	Chain	Res	Type
1	C	463	LEU
1	C	470	LYS
1	D	4	VAL
1	D	45	VAL
1	D	59	VAL
1	D	62	ILE
1	D	64	LYS
1	D	97	ILE
1	D	104	LEU
1	D	114	LEU
1	D	162	ASN
1	D	179	LEU
1	D	181	LEU
1	D	196	THR
1	D	197	THR
1	D	199	GLU
1	D	203	THR
1	D	242	LEU
1	D	252	LEU
1	D	267	VAL
1	D	288	THR
1	D	331	VAL
1	D	334	THR
1	D	342	LEU
1	D	349	VAL
1	D	351	LEU
1	D	354	GLN
1	D	387	LYS
1	D	394	LEU
1	D	395	ILE
1	D	400	VAL
1	D	404	VAL
1	D	415	ARG
1	D	426	THR
1	D	463	LEU
1	D	466	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	B	54	GLN

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Mol	Chain	Res	Type
1	B	163	ASN
1	B	348	ASN
1	B	392	ASN
1	C	54	GLN
1	C	162	ASN
1	C	434	ASN
1	D	54	GLN
1	D	162	ASN
1	D	434	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

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	ASP	A	471	-	7,8,8	1.18	1 (14%)	6,10,10	1.38	1 (16%)
5	FMT	D	474	-	2,2,2	0.73	0	1,1,1	0.27	0
4	ANP	A	472	2	33,33,33	2.02	9 (27%)	45,52,52	2.02	13 (28%)
4	ANP	D	473	2	33,33,33	1.96	10 (30%)	45,52,52	2.09	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	A	473	-	2,2,2	0.65	0	1,1,1	0.18	0
5	FMT	A	475	-	2,2,2	0.70	0	1,1,1	0.24	0
5	FMT	A	474	-	2,2,2	0.73	0	1,1,1	0.30	0
5	FMT	C	474	-	2,2,2	0.70	0	1,1,1	0.14	0
3	ASP	D	472	-	7,8,8	1.13	1 (14%)	6,10,10	1.46	1 (16%)
4	ANP	B	473	2	33,33,33	1.92	10 (30%)	45,52,52	2.01	12 (26%)
3	ASP	B	472	-	7,8,8	1.20	0	6,10,10	0.96	1 (16%)
4	ANP	C	473	2	33,33,33	2.02	9 (27%)	45,52,52	2.18	14 (31%)
3	ASP	C	472	-	7,8,8	1.22	1 (14%)	6,10,10	1.57	1 (16%)
5	FMT	A	476	-	2,2,2	0.73	0	1,1,1	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASP	A	471	-	-	0/8/8/8	-
4	ANP	A	472	2	-	8/18/38/38	0/3/3/3
4	ANP	D	473	2	-	5/18/38/38	0/3/3/3
3	ASP	D	472	-	-	2/8/8/8	-
4	ANP	B	473	2	-	8/18/38/38	0/3/3/3
3	ASP	B	472	-	-	0/8/8/8	-
4	ANP	C	473	2	-	8/18/38/38	0/3/3/3
3	ASP	C	472	-	-	3/8/8/8	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	473	ANP	C5-C4	5.06	1.48	1.39
4	A	472	ANP	C5-C4	4.86	1.47	1.39
4	C	473	ANP	PB-N3B	4.84	1.76	1.63
4	C	473	ANP	C5-C4	4.84	1.47	1.39
4	C	473	ANP	PG-N3B	4.82	1.76	1.63
4	D	473	ANP	PG-N3B	4.54	1.75	1.63
4	D	473	ANP	C5-C4	4.31	1.46	1.39
4	A	472	ANP	PB-N3B	4.29	1.74	1.63
4	B	473	ANP	PG-N3B	4.27	1.74	1.63
4	A	472	ANP	PG-N3B	4.27	1.74	1.63
4	A	472	ANP	PB-O1B	3.91	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	472	ANP	PG-O1G	3.81	1.51	1.46
4	D	473	ANP	PB-N3B	3.80	1.73	1.63
4	D	473	ANP	PG-O1G	3.70	1.51	1.46
4	B	473	ANP	PB-N3B	3.68	1.73	1.63
4	C	473	ANP	PG-O1G	3.66	1.51	1.46
4	D	473	ANP	PB-O1B	3.24	1.51	1.46
4	B	473	ANP	PG-O1G	3.21	1.51	1.46
4	C	473	ANP	PB-O1B	3.14	1.50	1.46
4	B	473	ANP	PB-O3A	3.08	1.62	1.59
4	D	473	ANP	PB-O3A	2.97	1.62	1.59
4	C	473	ANP	C5-C6	2.90	1.49	1.41
4	D	473	ANP	PG-O3G	-2.69	1.49	1.56
4	A	472	ANP	C5-N7	-2.56	1.34	1.39
4	A	472	ANP	PB-O2B	-2.54	1.50	1.56
4	B	473	ANP	C5-C6	2.48	1.47	1.41
4	B	473	ANP	PB-O2B	-2.37	1.50	1.56
4	B	473	ANP	C8-N7	2.37	1.36	1.31
3	C	472	ASP	OXT-C	-2.34	1.23	1.30
4	A	472	ANP	C5-C6	2.33	1.47	1.41
4	B	473	ANP	C5-N7	-2.32	1.34	1.39
4	D	473	ANP	C5-C6	2.30	1.47	1.41
4	A	472	ANP	PG-O3G	-2.26	1.50	1.56
3	A	471	ASP	OXT-C	-2.20	1.23	1.30
4	D	473	ANP	C8-N7	2.18	1.35	1.31
3	D	472	ASP	OXT-C	-2.17	1.23	1.30
4	C	473	ANP	C5-N7	-2.16	1.35	1.39
4	B	473	ANP	PG-O3G	-2.15	1.51	1.56
4	C	473	ANP	PB-O2B	-2.14	1.51	1.56
4	C	473	ANP	C8-N7	2.13	1.35	1.31
4	D	473	ANP	C5-N7	-2.05	1.35	1.39

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	473	ANP	O1G-PG-N3B	-6.42	102.31	111.77
4	C	473	ANP	C5-C4-N3	-6.02	118.43	126.72
4	D	473	ANP	C5-C4-N3	-5.88	118.62	126.72
4	B	473	ANP	O1G-PG-N3B	-5.57	103.57	111.77
4	B	473	ANP	C5-C4-N3	-5.46	119.20	126.72
4	A	472	ANP	C5-C4-N3	-5.45	119.22	126.72
4	C	473	ANP	N3-C4-N9	4.87	135.45	127.17
4	A	472	ANP	N3-C4-N9	4.86	135.44	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	473	ANP	N3-C4-N9	4.84	135.40	127.17
4	A	472	ANP	O2B-PB-O1B	4.75	120.06	109.87
4	B	473	ANP	N3-C4-N9	4.54	134.88	127.17
4	D	473	ANP	N3-C2-N1	-4.45	121.84	128.58
4	D	473	ANP	C2-N3-C4	4.12	121.89	111.83
4	C	473	ANP	C2-N3-C4	3.92	121.39	111.83
4	A	472	ANP	O1G-PG-N3B	-3.87	106.07	111.77
4	D	473	ANP	O2B-PB-O1B	3.84	118.11	109.87
4	A	472	ANP	N3-C2-N1	-3.83	122.78	128.58
4	C	473	ANP	N3-C2-N1	-3.71	122.97	128.58
4	B	473	ANP	C2-N3-C4	3.54	120.48	111.83
4	D	473	ANP	O1B-PB-N3B	-3.51	106.61	111.77
4	A	472	ANP	C2-N3-C4	3.50	120.38	111.83
4	D	473	ANP	O2G-PG-O3G	3.46	116.88	107.59
4	B	473	ANP	N3-C2-N1	-3.46	123.35	128.58
4	C	473	ANP	C4-C5-N7	-3.33	106.77	110.58
4	C	473	ANP	O3A-PB-N3B	3.21	115.50	106.59
4	D	473	ANP	C4-C5-N7	-3.17	106.95	110.58
4	B	473	ANP	C4-C5-N7	-3.15	106.98	110.58
4	A	472	ANP	O2G-PG-O3G	2.95	115.51	107.59
3	A	471	ASP	OXT-C-O	-2.91	117.48	124.08
4	B	473	ANP	O2B-PB-O1B	2.90	116.09	109.87
3	C	472	ASP	OXT-C-O	-2.88	117.54	124.08
4	A	472	ANP	C4-C5-N7	-2.84	107.33	110.58
4	B	473	ANP	O2G-PG-O3G	2.84	115.21	107.59
4	D	473	ANP	C4-N9-C8	2.83	108.71	105.74
4	C	473	ANP	O2B-PB-O1B	2.82	115.91	109.87
3	D	472	ASP	OXT-C-O	-2.77	117.79	124.08
4	A	472	ANP	C2-N1-C6	2.73	123.22	118.73
4	B	473	ANP	C4-N9-C8	2.65	108.52	105.74
4	A	472	ANP	C4-N9-C8	2.64	108.51	105.74
4	D	473	ANP	O1G-PG-N3B	-2.61	107.93	111.77
4	C	473	ANP	C5-N7-C8	2.59	107.51	103.45
4	B	473	ANP	C2-N1-C6	2.50	122.83	118.73
4	D	473	ANP	C5-N7-C8	2.44	107.28	103.45
4	B	473	ANP	C5-N7-C8	2.41	107.24	103.45
4	D	473	ANP	C2-N1-C6	2.36	122.61	118.73
4	C	473	ANP	C4-N9-C8	2.35	108.20	105.74
4	C	473	ANP	O2A-PA-O1A	2.31	123.19	112.44
4	A	472	ANP	O1B-PB-N3B	-2.26	108.44	111.77
4	A	472	ANP	C5-N7-C8	2.25	106.99	103.45
4	C	473	ANP	C2-N1-C6	2.17	122.30	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	473	ANP	O2G-PG-O3G	2.16	113.40	107.59
4	B	473	ANP	C6-C5-N7	2.14	136.21	132.09
4	C	473	ANP	C6-C5-N7	2.14	136.21	132.09
4	A	472	ANP	C3'-C2'-C1'	2.10	105.44	101.46
4	D	473	ANP	C6-C5-N7	2.10	136.15	132.09
3	B	472	ASP	OXT-C-O	-2.04	119.46	124.08
4	D	473	ANP	N9-C8-N7	-2.01	111.08	113.94

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	472	ANP	PB-N3B-PG-O1G
4	A	472	ANP	PG-N3B-PB-O1B
4	B	473	ANP	PB-N3B-PG-O1G
4	B	473	ANP	C5'-O5'-PA-O3A
4	C	473	ANP	PB-N3B-PG-O1G
4	C	473	ANP	PG-N3B-PB-O1B
4	D	473	ANP	PB-N3B-PG-O1G
4	D	473	ANP	PG-N3B-PB-O1B
4	B	473	ANP	PB-O3A-PA-O1A
4	B	473	ANP	C4'-C5'-O5'-PA
4	A	472	ANP	PB-O3A-PA-O1A
3	C	472	ASP	O-C-CA-CB
3	C	472	ASP	OXT-C-CA-CB
4	B	473	ANP	C5'-O5'-PA-O1A
4	A	472	ANP	C4'-C5'-O5'-PA
4	D	473	ANP	C4'-C5'-O5'-PA
3	D	472	ASP	OXT-C-CA-CB
3	D	472	ASP	O-C-CA-CB
4	D	473	ANP	PB-O3A-PA-O1A
4	C	473	ANP	PA-O3A-PB-O2B
4	C	473	ANP	C4'-C5'-O5'-PA
4	A	472	ANP	C2'-C1'-N9-C8
3	C	472	ASP	OXT-C-CA-N
4	C	473	ANP	C2'-C1'-N9-C8
4	A	472	ANP	C2'-C1'-N9-C4
4	B	473	ANP	O4'-C1'-N9-C8
4	C	473	ANP	O4'-C1'-N9-C8
4	D	473	ANP	O4'-C1'-N9-C8
4	A	472	ANP	PB-O3A-PA-O2A
4	B	473	ANP	PB-O3A-PA-O2A

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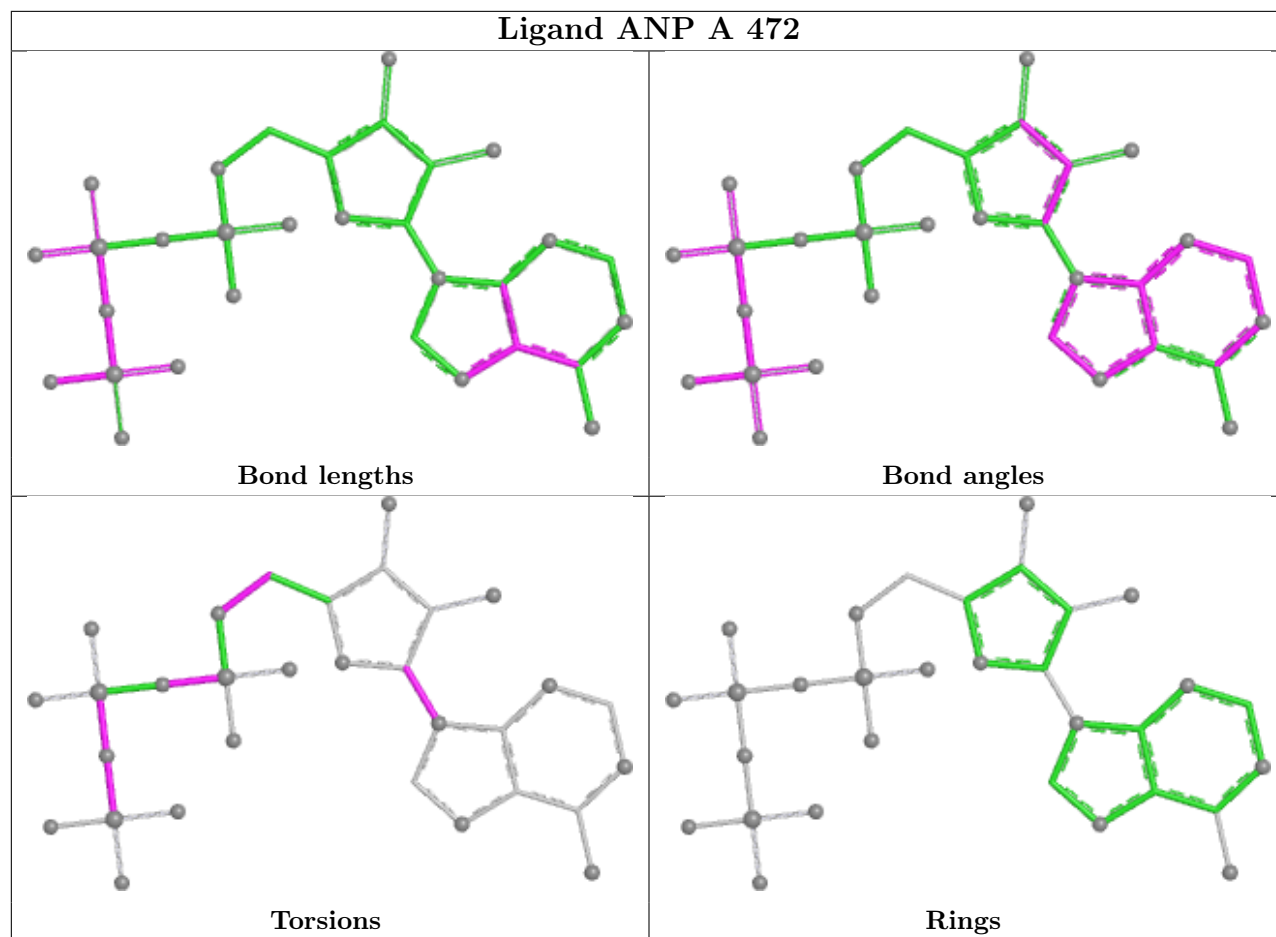
Mol	Chain	Res	Type	Atoms
4	A	472	ANP	O4'-C1'-N9-C8
4	B	473	ANP	C2'-C1'-N9-C8
4	C	473	ANP	PA-O3A-PB-O1B
4	C	473	ANP	C2'-C1'-N9-C4

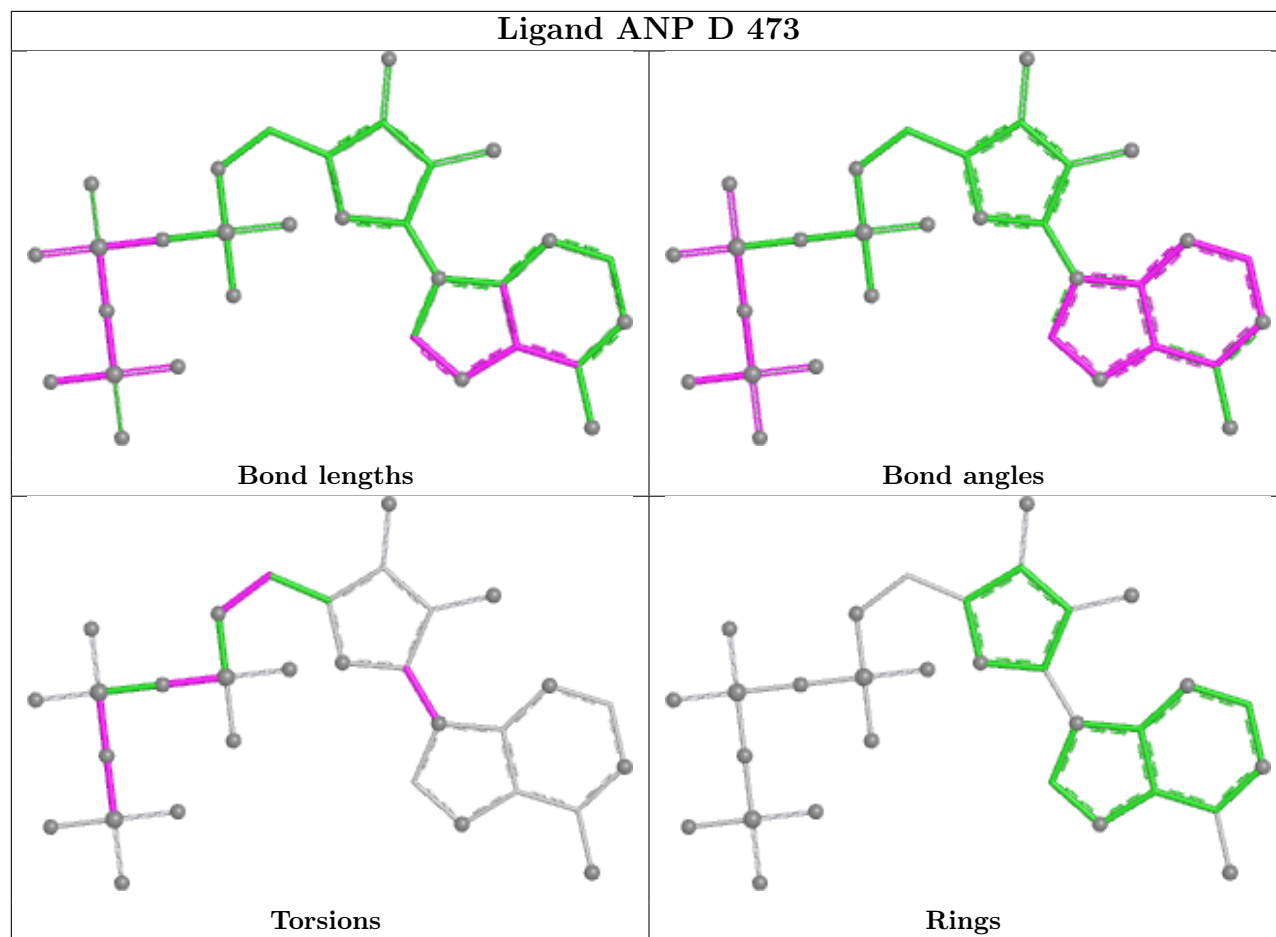
There are no ring outliers.

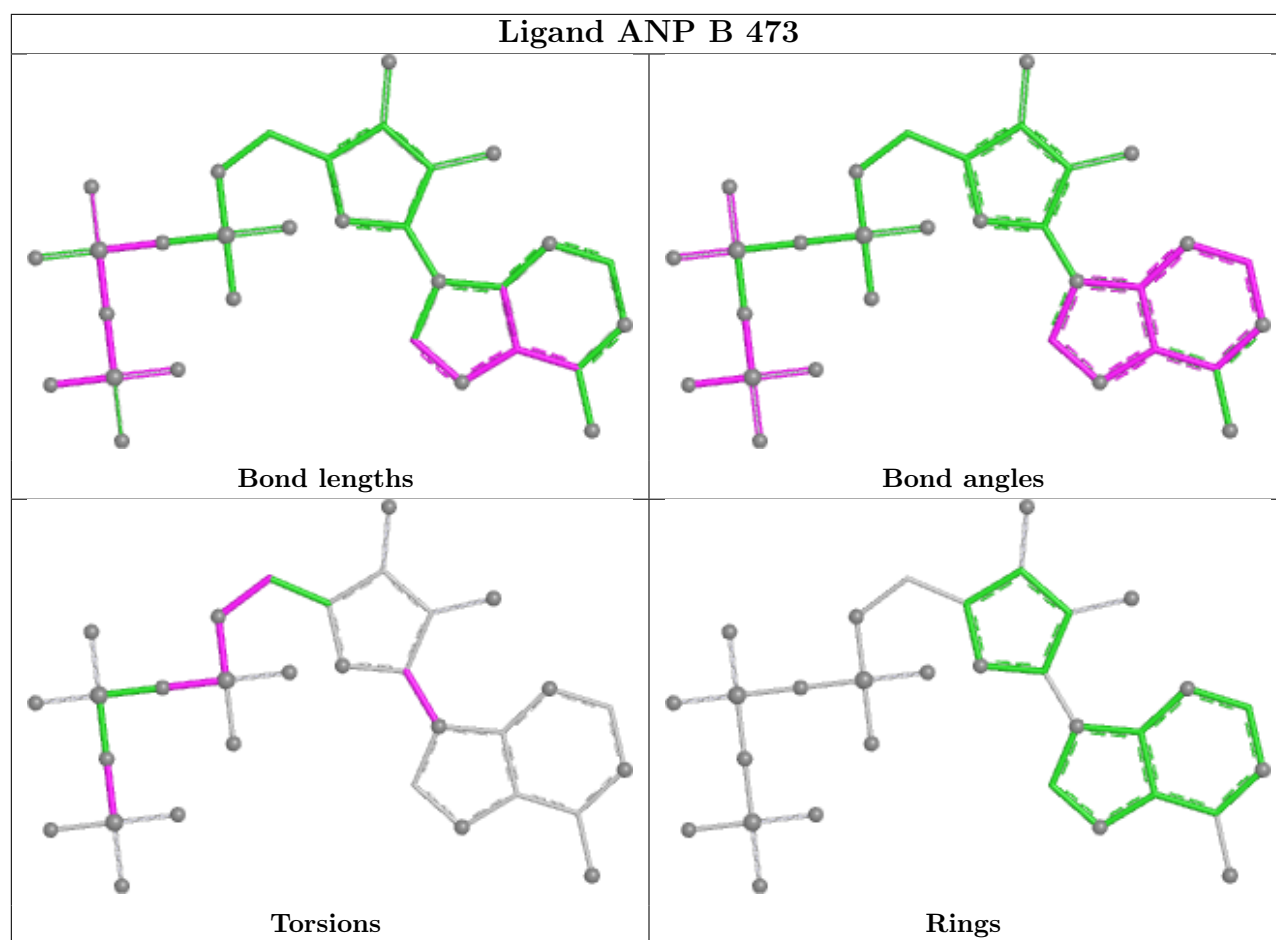
4 monomers are involved in 6 short contacts:

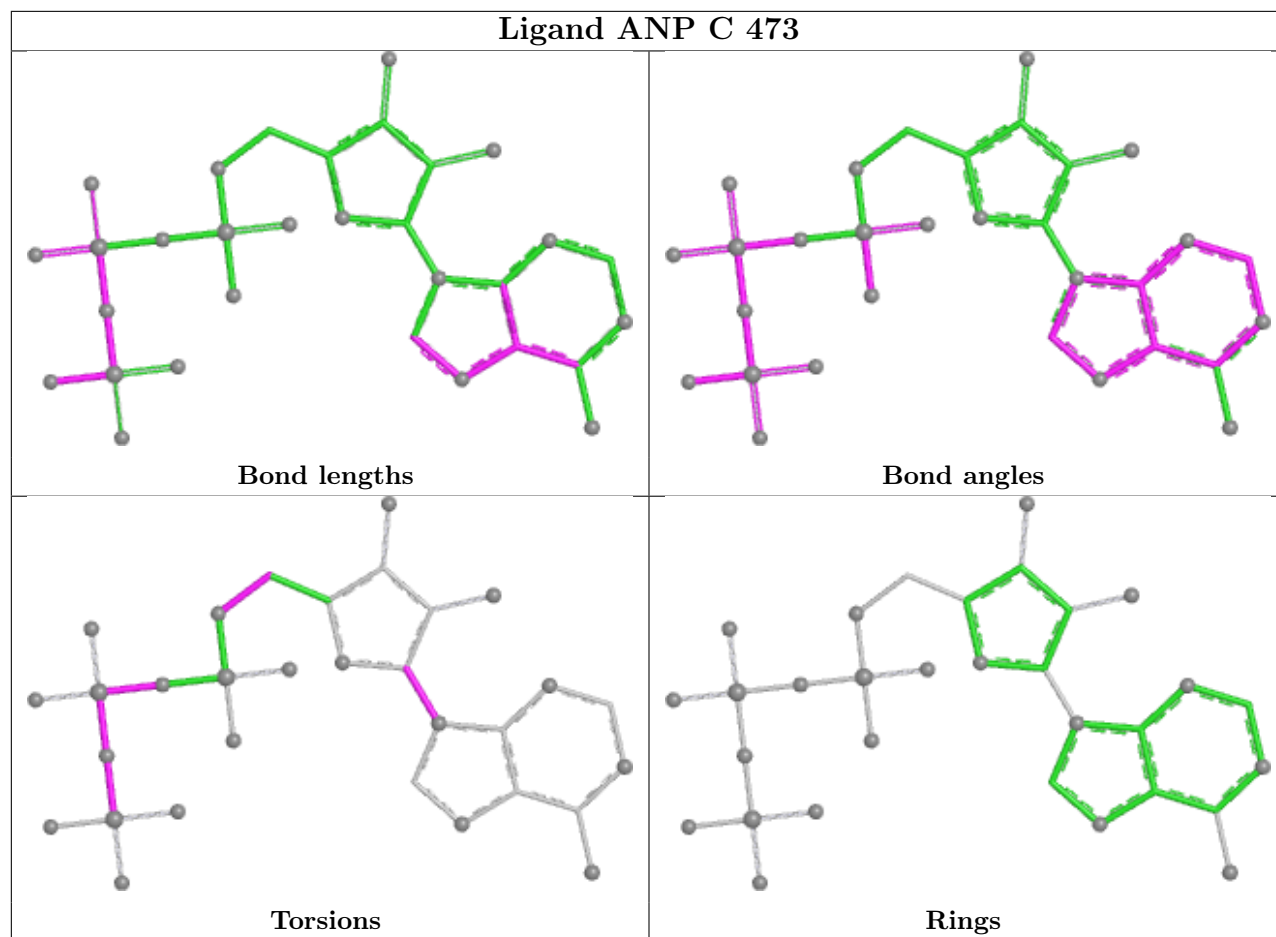
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	471	ASP	2	0
4	B	473	ANP	1	0
4	C	473	ANP	1	0
3	C	472	ASP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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(Å ²)	Q<0.9
1	A	465/473 (98%)	-0.37	2 (0%) 88 89	18, 25, 35, 48	0
1	B	465/473 (98%)	-0.18	2 (0%) 88 89	11, 26, 36, 44	1 (0%)
1	C	468/473 (98%)	-0.22	1 (0%) 91 91	18, 27, 36, 55	1 (0%)
1	D	466/473 (98%)	-0.44	2 (0%) 88 89	18, 25, 34, 51	0
All	All	1864/1892 (98%)	-0.30	7 (0%) 88 89	11, 26, 35, 55	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	308	ILE	2.8
1	A	58	ASP	2.6
1	B	308	ILE	2.3
1	C	385	GLY	2.1
1	D	168	ARG	2.1
1	B	383	ASP	2.1
1	A	388	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

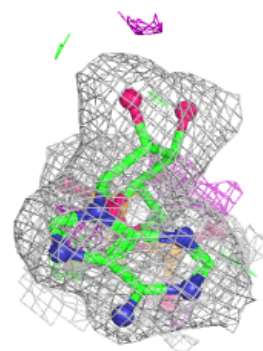
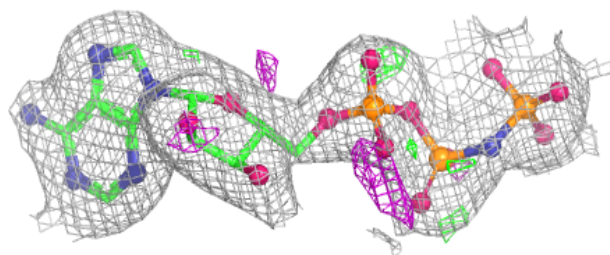
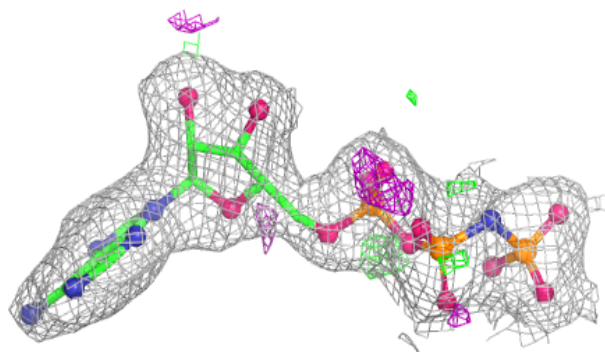
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FMT	A	473	3/3	0.62	0.23	61,61,61,61	0
5	FMT	A	476	3/3	0.78	0.22	74,74,74,74	0
5	FMT	A	475	3/3	0.83	0.22	80,80,80,80	0
5	FMT	A	474	3/3	0.85	0.18	64,64,64,64	0
5	FMT	D	474	3/3	0.85	0.18	64,64,64,65	0
5	FMT	C	474	3/3	0.87	0.17	73,73,73,73	0
3	ASP	C	472	9/9	0.93	0.08	38,39,39,41	0
3	ASP	D	472	9/9	0.93	0.09	29,30,30,33	0
2	MG	C	471	1/1	0.95	0.09	44,44,44,44	0
3	ASP	A	471	9/9	0.96	0.06	34,35,35,37	0
4	ANP	B	473	31/31	0.96	0.07	31,35,43,46	0
4	ANP	C	473	31/31	0.96	0.07	41,47,49,50	0
3	ASP	B	472	9/9	0.97	0.05	34,35,36,36	0
4	ANP	A	472	31/31	0.98	0.05	24,28,31,32	0
2	MG	A	1	1/1	0.98	0.03	32,32,32,32	0
2	MG	D	471	1/1	0.98	0.03	22,22,22,22	0
4	ANP	D	473	31/31	0.98	0.05	27,28,30,30	0
2	MG	B	471	1/1	0.98	0.05	29,29,29,29	0

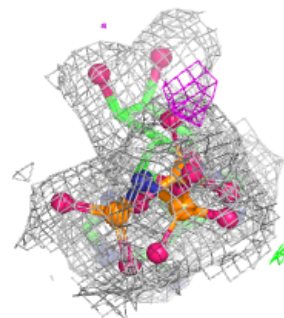
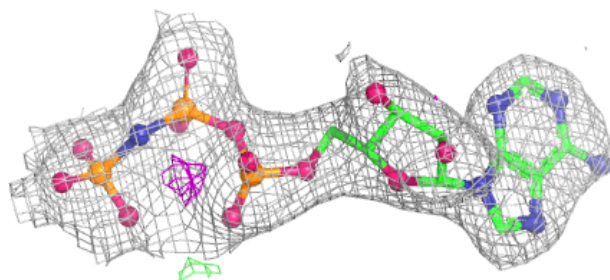
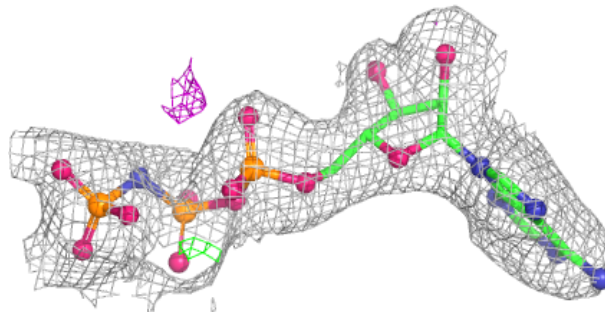
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP B 473:

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

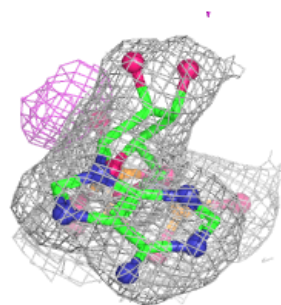
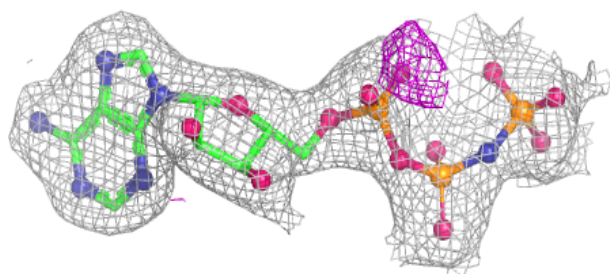
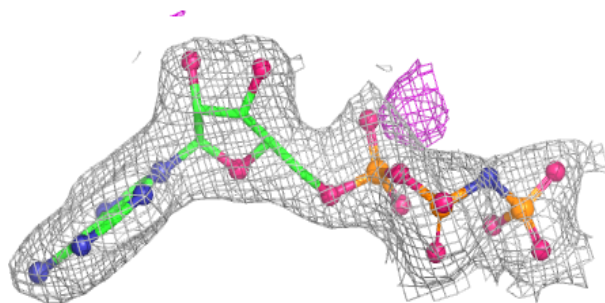
**Electron density around ANP C 473:**

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

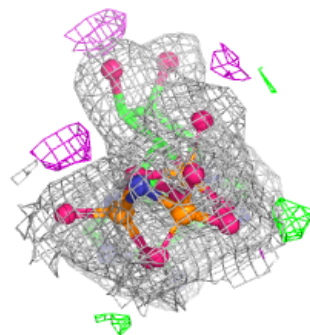
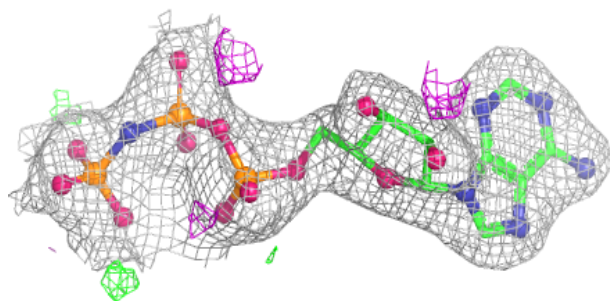
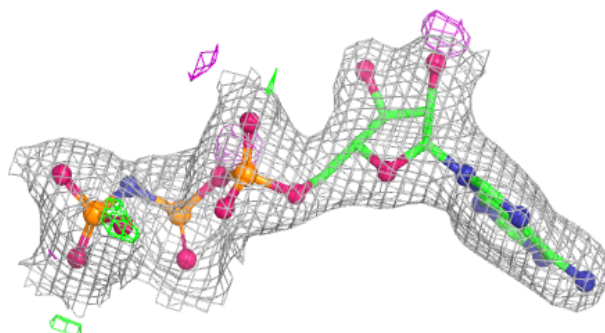


Electron density around ANP A 472:

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

**Electron density around ANP D 473:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.