



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 08:11 PM EDT

PDB ID : 1PQU
Title : Crystal Structure of the H277N Mutant of Aspartate Semialdehyde Dehydrogenase from Haemophilus influenzae Bound with NADP, S-methyl cysteine sulfoxide and cacodylate
Authors : Blanco, J.; Moore, R.A.; Viola, R.E.
Deposited on : 2003-06-19
Resolution : 1.92 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 : 2.23.2
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) : 2.23.2

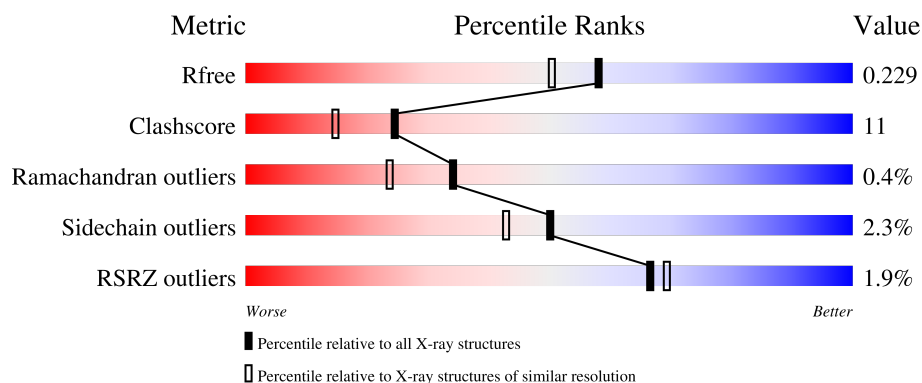
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	371	<div> <div>5%</div> <div>78% 22%</div> </div>
1	B	371	<div> <div>80% 20%</div> </div>
1	C	371	<div> <div>79% 15%</div> </div>
1	D	371	<div> <div>5% 76% 22%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CAC	B	2375	-	-	X	-
2	CAC	C	3374	-	-	X	-
4	CYS	B	2374	-	-	X	-
4	CYS	C	3373	-	-	X	-
4	CYS	D	4374	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12272 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.

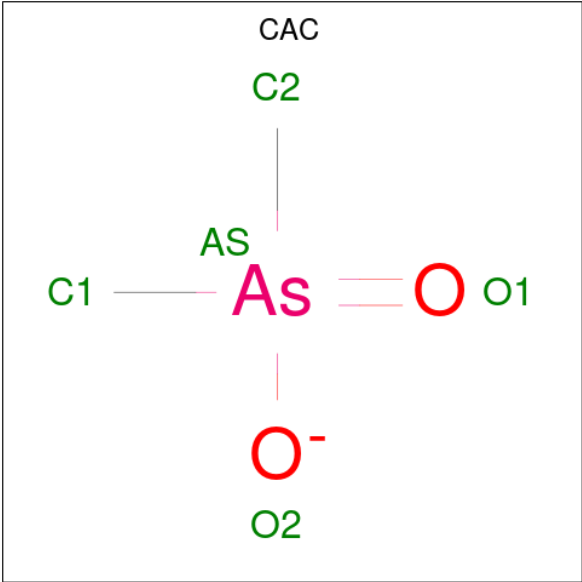
- Molecule 1 is a protein called Aspartate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2845	1814	479	537	15			
1	B	371	Total	C	N	O	S	0	0	0
			2845	1814	479	537	15			
1	C	356	Total	C	N	O	S	0	0	0
			2746	1752	461	518	15			
1	D	371	Total	C	N	O	S	0	0	0
			2845	1814	479	537	15			

There are 4 discrepancies between the modelled and reference sequences:

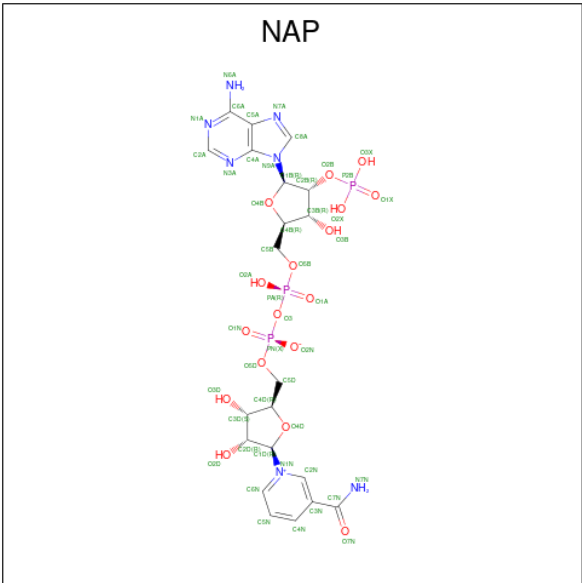
Chain	Residue	Modelled	Actual	Comment	Reference
A	277	ASN	HIS	engineered mutation	UNP P44801
B	277	ASN	HIS	engineered mutation	UNP P44801
C	277	ASN	HIS	engineered mutation	UNP P44801
D	277	ASN	HIS	engineered mutation	UNP P44801

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).



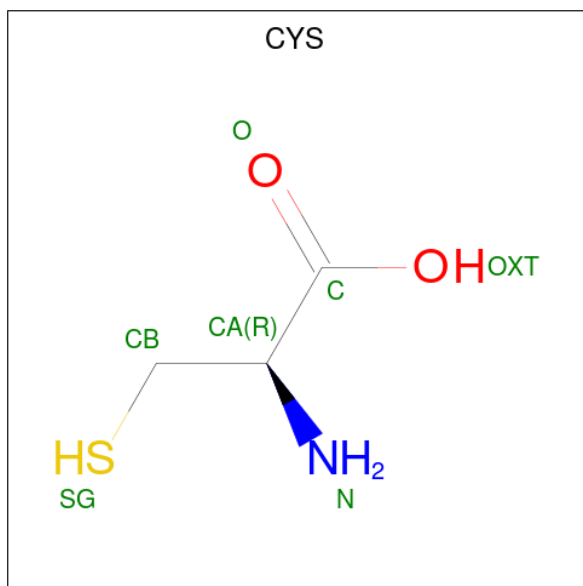
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	As	C	O	0	0
			5	1	2	2		
2	B	1	Total	As	C	O	0	0
			5	1	2	2		
2	C	1	Total	As	C	O	0	0
			5	1	2	2		
2	D	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 4 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	C	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	D	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	216	Total	O	0	0
			216	216		
5	B	205	Total	O	0	0
			205	205		
5	C	233	Total	O	0	0
			233	233		

Continued on next page...

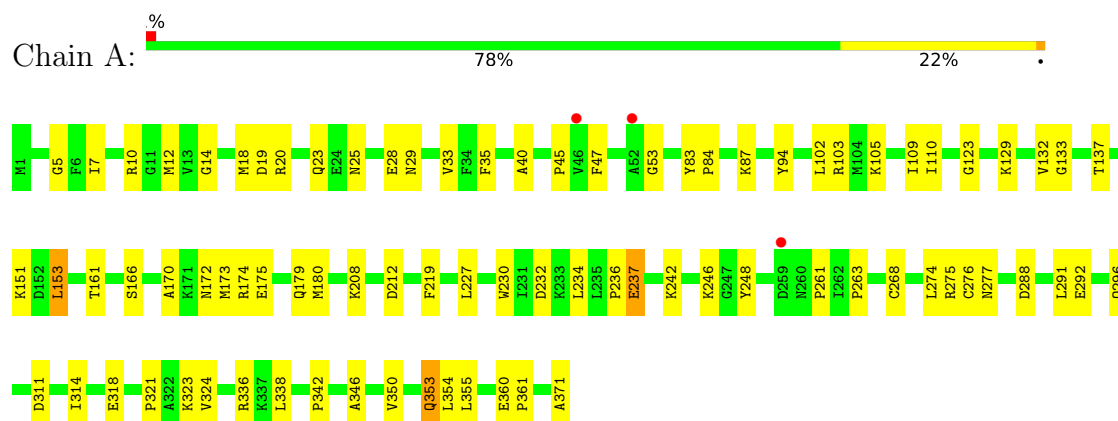
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	145	Total	O	0	0
			145	145		

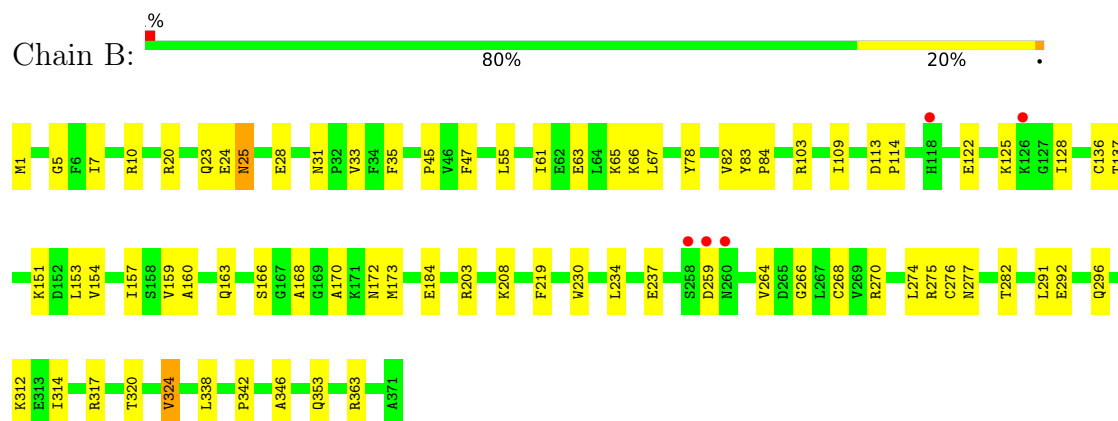
3 Residue-property plots

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.

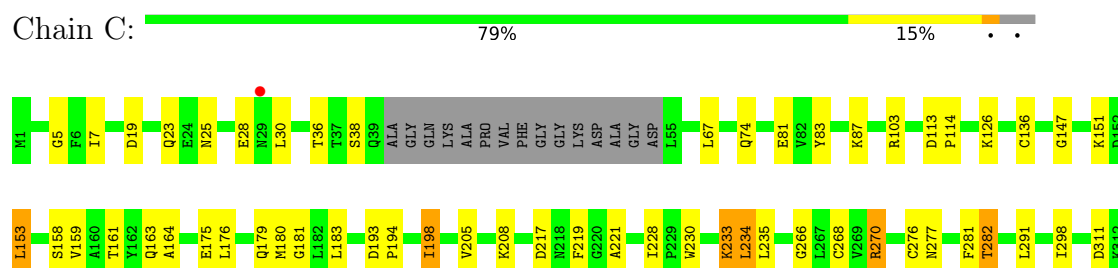
- Molecule 1: Aspartate-semialdehyde dehydrogenase



- Molecule 1: Aspartate-semialdehyde dehydrogenase

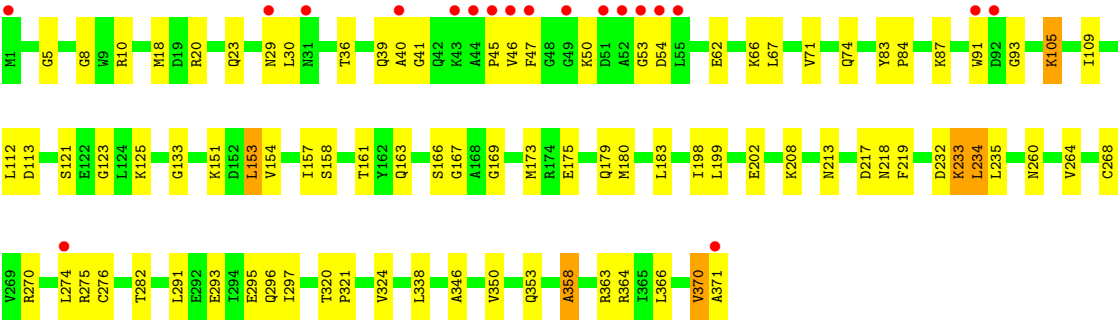
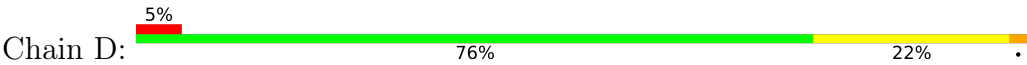


- Molecule 1: Aspartate-semialdehyde dehydrogenase





● Molecule 1: Aspartate-semialdehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.93Å 76.58Å 134.10Å 90.00° 92.59° 90.00°	Depositor
Resolution (Å)	44.65 – 1.92 44.65 – 1.92	Depositor EDS
% Data completeness (in resolution range)	85.7 (44.65-1.92) 85.8 (44.65-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.92Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.182 , 0.234 0.178 , 0.229	Depositor DCC
R_{free} test set	9603 reflections (9.64%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12272	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: CAC, NAP

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	0.33	0/2896	0.63	0/3918
1	B	0.33	0/2896	0.63	1/3918 (0.0%)
1	C	0.34	0/2792	0.64	1/3776 (0.0%)
1	D	0.32	0/2896	0.61	0/3918
All	All	0.33	0/11480	0.63	2/15530 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	THR	N-CA-C	-5.40	96.41	111.00
1	C	282	THR	N-CA-C	-5.03	97.42	111.00

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	2845	0	2901	61	0
1	B	2845	0	2901	62	0
1	C	2746	0	2802	54	0
1	D	2845	0	2901	74	0
2	A	5	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	5	0
2	C	5	0	0	4	0
2	D	5	0	0	3	0
3	A	48	0	25	3	0
3	B	48	0	25	1	0
3	D	48	0	25	3	0
4	A	7	0	3	1	0
4	B	7	0	3	5	0
4	C	7	0	3	5	0
4	D	7	0	3	6	0
5	A	216	0	0	4	0
5	B	205	0	0	3	0
5	C	233	0	0	1	0
5	D	145	0	0	1	0
All	All	12272	0	11592	252	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 11.

All (252) 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)
2:B:2375:CAC:C2	4:B:2374:CYS:HB2	1.94	0.98
1:D:29:ASN:HB3	1:D:371:ALA:HB3	1.48	0.95
2:A:1375:CAC:C2	4:A:1374:CYS:HB2	2.00	0.91
1:C:313:GLU:HG2	1:C:317:ARG:HH12	1.34	0.91
1:D:276:CYS:SG	1:D:324:VAL:HG23	2.13	0.88
1:D:324:VAL:HG21	1:D:350:VAL:HG12	1.52	0.88
1:B:20:ARG:HH11	1:B:23:GLN:HE21	1.24	0.84
1:A:276:CYS:SG	1:A:324:VAL:HG23	2.18	0.83
1:B:122:GLU:HA	1:B:125:LYS:HE3	1.60	0.81
1:D:198:ILE:HG23	1:D:199:LEU:HD12	1.62	0.80
1:D:20:ARG:HH11	1:D:23:GLN:NE2	1.80	0.80
2:D:4375:CAC:C1	4:D:4374:CYS:HB2	2.12	0.79
1:B:20:ARG:HH11	1:B:23:GLN:NE2	1.80	0.79
1:D:293:GLU:O	1:D:296:GLN:HG3	1.82	0.79
1:B:109:ILE:HD13	1:B:128:ILE:HG21	1.63	0.78
2:C:3374:CAC:C2	4:C:3373:CYS:HB2	2.12	0.78
1:B:314:ILE:HG23	1:B:317:ARG:NH2	1.99	0.78
1:A:324:VAL:HG21	1:A:350:VAL:HG12	1.65	0.77
1:D:167:GLY:N	1:D:353:GLN:HE22	1.83	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HB2	1:A:353:GLN:NE2	2.01	0.76
1:D:83:TYR:HB3	1:D:84:PRO:HD3	1.66	0.75
1:C:291:LEU:HD11	1:C:336:ARG:HA	1.69	0.75
1:D:154:VAL:HG11	1:D:157:ILE:HD11	1.68	0.74
1:B:154:VAL:HG11	1:B:157:ILE:HD11	1.69	0.74
1:C:317:ARG:HG3	1:C:318:GLU:HG2	1.70	0.73
1:D:157:ILE:HD13	1:D:264:VAL:HG22	1.73	0.71
1:C:151:LYS:HB2	1:C:153:LEU:HD22	1.73	0.70
1:B:83:TYR:HB3	1:B:84:PRO:HD3	1.74	0.70
1:A:166:SER:HB3	1:A:173:MET:SD	2.32	0.70
1:D:234:LEU:HD22	1:D:235:LEU:N	2.07	0.69
1:D:324:VAL:HG21	1:D:350:VAL:CG1	2.21	0.69
1:D:296:GLN:HE21	1:D:297:ILE:HG13	1.57	0.68
1:D:291:LEU:O	1:D:295:GLU:HG3	1.95	0.67
1:B:166:SER:HB3	1:B:353:GLN:OE1	1.95	0.67
1:C:163:GLN:HG2	1:C:277:ASN:ND2	2.09	0.67
1:C:233:LYS:HE3	1:C:233:LYS:HA	1.76	0.67
1:A:336:ARG:HH12	1:A:338:LEU:HD23	1.60	0.66
1:C:7:ILE:HG22	1:C:74:GLN:HB2	1.77	0.65
1:B:172:ASN:HB3	1:B:219:PHE:CZ	2.31	0.65
1:B:292:GLU:O	1:B:296:GLN:HG3	1.96	0.65
1:B:275:ARG:O	1:B:353:GLN:HG2	1.98	0.64
1:D:233:LYS:HE3	1:D:233:LYS:N	2.12	0.64
1:A:151:LYS:HB2	1:A:153:LEU:HD22	1.79	0.63
1:B:25:ASN:ND2	1:B:28:GLU:HG2	2.13	0.63
1:B:24:GLU:HG3	1:B:363:ARG:NE	2.13	0.63
1:B:270:ARG:NH2	4:B:2374:CYS:OXT	2.32	0.63
1:A:137:THR:HG22	1:A:277:ASN:HD22	1.62	0.62
1:A:338:LEU:HD21	1:A:346:ALA:HB2	1.82	0.61
1:B:312:LYS:HE3	1:C:233:LYS:NZ	2.14	0.61
1:D:121:SER:O	1:D:125:LYS:HE2	2.01	0.60
1:C:164:ALA:HB3	1:C:353:GLN:NE2	2.17	0.60
1:B:20:ARG:NH1	1:B:23:GLN:HE21	1.96	0.60
1:C:25:ASN:HB3	1:C:28:GLU:OE1	2.01	0.60
1:D:166:SER:OG	1:D:353:GLN:NE2	2.35	0.60
1:B:270:ARG:HH22	4:B:2374:CYS:C	2.05	0.59
1:B:5:GLY:HA3	1:B:67:LEU:HD13	1.84	0.59
2:B:2375:CAC:C2	4:B:2374:CYS:CB	2.78	0.59
1:C:36:THR:HG22	1:C:38:SER:H	1.68	0.59
1:A:20:ARG:HH11	1:A:23:GLN:NE2	2.00	0.58
1:D:20:ARG:HH11	1:D:23:GLN:HE21	1.51	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:SER:C	1:D:353:GLN:HE22	2.05	0.58
1:B:276:CYS:SG	1:B:324:VAL:HG22	2.43	0.58
1:A:353:GLN:HE22	1:A:354:LEU:HG	1.69	0.57
1:D:167:GLY:HA3	4:D:4374:CYS:OXT	2.04	0.57
1:D:8:GLY:HA2	3:D:4372:NAP:O3B	2.04	0.57
1:D:219:PHE:CE2	1:D:270:ARG:HD3	2.39	0.57
1:C:19:ASP:O	1:C:23:GLN:HG3	2.04	0.57
1:B:166:SER:HB2	1:B:274:LEU:O	2.05	0.56
1:D:166:SER:HA	1:D:173:MET:HG2	1.87	0.56
1:D:270:ARG:HH22	4:D:4374:CYS:C	2.08	0.56
1:D:166:SER:HA	1:D:173:MET:CG	2.35	0.56
1:A:29:ASN:ND2	1:A:371:ALA:HB2	2.22	0.55
1:D:20:ARG:NH1	1:D:23:GLN:HE21	2.04	0.55
1:A:242:LYS:O	1:A:246:LYS:HG3	2.06	0.55
1:D:20:ARG:NH1	1:D:23:GLN:NE2	2.53	0.55
1:A:172:ASN:HB3	1:A:219:PHE:CZ	2.42	0.55
1:A:230:TRP:HZ2	1:A:234:LEU:HB2	1.70	0.55
1:D:370:VAL:HG23	1:D:371:ALA:N	2.22	0.55
1:D:105:LYS:HE3	1:D:105:LYS:HA	1.90	0.55
1:A:336:ARG:NH1	1:A:338:LEU:HD23	2.22	0.54
1:B:122:GLU:HA	1:B:125:LYS:CE	2.32	0.54
1:C:313:GLU:HG2	1:C:317:ARG:NH1	2.13	0.54
1:D:219:PHE:HE2	1:D:270:ARG:HD3	1.73	0.54
1:A:248:TYR:OH	1:A:261:PRO:HB2	2.07	0.54
1:B:7:ILE:HD13	1:B:35:PHE:HB2	1.90	0.54
1:B:208:LYS:O	1:B:208:LYS:HD3	2.08	0.54
1:A:12:MET:CE	3:A:1372:NAP:H72N	2.22	0.53
1:A:45:PRO:HB2	1:A:47:PHE:CE1	2.43	0.53
1:A:20:ARG:HH11	1:A:23:GLN:HE21	1.56	0.53
1:A:237:GLU:H	1:A:237:GLU:CD	2.11	0.53
1:A:353:GLN:NE2	1:A:354:LEU:HG	2.24	0.53
1:D:270:ARG:NH2	4:D:4374:CYS:OXT	2.41	0.53
1:D:41:GLY:O	1:D:54:ASP:HB3	2.09	0.53
1:D:179:GLN:O	1:D:183:LEU:HG	2.09	0.53
1:A:276:CYS:HB2	1:A:321:PRO:HB3	1.91	0.52
1:B:338:LEU:HD21	1:B:346:ALA:HB2	1.90	0.52
1:D:208:LYS:NZ	1:D:213:ASN:HD21	2.07	0.52
1:A:311:ASP:OD2	1:A:314:ILE:HG12	2.09	0.52
1:D:36:THR:HG21	1:D:40:ALA:N	2.25	0.52
1:D:5:GLY:HA3	1:D:67:LEU:HD13	1.91	0.52
1:C:164:ALA:HB3	1:C:353:GLN:HE22	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:SER:CB	1:D:274:LEU:O	2.58	0.52
1:B:137:THR:HG22	1:B:277:ASN:HD22	1.75	0.52
1:C:234:LEU:HD22	1:C:235:LEU:N	2.25	0.52
1:C:353:GLN:OE1	4:C:3373:CYS:SG	2.67	0.51
1:D:296:GLN:NE2	1:D:297:ILE:HG13	2.25	0.51
1:A:25:ASN:HD22	1:A:28:GLU:CD	2.14	0.51
1:B:24:GLU:HG3	1:B:363:ARG:HE	1.74	0.51
1:A:276:CYS:SG	1:A:324:VAL:CG2	2.94	0.51
1:D:166:SER:HB3	1:D:274:LEU:O	2.11	0.51
1:C:270:ARG:NH2	4:C:3373:CYS:OXT	2.44	0.51
1:B:78:TYR:CE1	1:B:82:VAL:HG21	2.45	0.51
1:D:121:SER:O	1:D:125:LYS:HG2	2.11	0.51
1:B:24:GLU:HG3	1:B:363:ARG:CZ	2.40	0.51
1:C:353:GLN:HG2	4:C:3373:CYS:SG	2.51	0.50
1:D:151:LYS:O	1:D:153:LEU:HD13	2.11	0.50
1:D:232:ASP:C	1:D:233:LYS:HE3	2.31	0.50
1:A:29:ASN:HD21	1:A:371:ALA:HB2	1.76	0.50
1:B:103:ARG:NH2	2:B:2375:CAC:O2	2.44	0.50
1:B:20:ARG:HD2	1:B:23:GLN:HE22	1.76	0.50
1:D:166:SER:HB3	1:D:275:ARG:HA	1.93	0.50
1:C:136:CYS:H	2:C:3374:CAC:C2	2.24	0.50
1:D:276:CYS:HB2	1:D:321:PRO:HB3	1.94	0.50
1:A:288:ASP:OD1	1:A:342:PRO:HB2	2.11	0.50
1:A:7:ILE:HD13	1:A:35:PHE:HB2	1.94	0.49
1:B:173:MET:SD	1:B:274:LEU:HD12	2.51	0.49
1:D:338:LEU:HD21	1:D:346:ALA:HB2	1.92	0.49
1:B:63:GLU:HA	1:B:66:LYS:HE2	1.93	0.49
1:D:208:LYS:HZ2	1:D:213:ASN:HD21	1.60	0.49
1:B:237:GLU:HG3	5:B:2534:HOH:O	2.11	0.49
1:A:275:ARG:HB2	1:A:353:GLN:HE22	1.73	0.49
1:B:20:ARG:HD2	1:B:23:GLN:NE2	2.28	0.49
1:C:221:ALA:HB3	1:C:228:ILE:HD12	1.93	0.49
2:D:4375:CAC:C1	4:D:4374:CYS:CB	2.86	0.49
1:B:157:ILE:HD13	1:B:264:VAL:HG22	1.94	0.49
1:D:109:ILE:CD1	1:D:123:GLY:HA3	2.42	0.49
1:B:103:ARG:HH22	2:B:2375:CAC:AS	2.56	0.49
1:C:233:LYS:HE3	1:C:233:LYS:CA	2.42	0.48
1:B:173:MET:HE3	1:C:198:ILE:HD12	1.95	0.48
1:B:312:LYS:HE3	1:C:233:LYS:HZ3	1.78	0.48
1:B:170:ALA:HB1	1:C:198:ILE:HG13	1.96	0.48
1:A:83:TYR:O	1:A:87:LYS:HG2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLU:HG3	1:C:181:GLY:HA3	1.96	0.48
1:B:270:ARG:HD2	5:B:2448:HOH:O	2.13	0.47
1:A:170:ALA:O	1:A:174:ARG:HG3	2.14	0.47
1:C:208:LYS:O	1:C:208:LYS:HD3	2.14	0.47
2:D:4375:CAC:C1	4:D:4374:CYS:N	2.78	0.47
1:D:62:GLU:O	1:D:66:LYS:HG3	2.15	0.47
1:B:314:ILE:HG23	1:B:317:ARG:HH21	1.76	0.47
1:C:270:ARG:HH22	4:C:3373:CYS:C	2.17	0.47
1:C:103:ARG:HH22	2:C:3374:CAC:AS	2.58	0.47
1:C:230:TRP:HZ2	1:C:234:LEU:HB2	1.79	0.47
1:C:311:ASP:OD2	1:C:314:ILE:HG12	2.15	0.47
1:D:46:VAL:HG13	1:D:50:LYS:O	2.15	0.47
1:A:103:ARG:NH2	2:A:1375:CAC:O2	2.47	0.47
1:B:320:THR:O	1:B:324:VAL:HG13	2.14	0.47
1:A:208:LYS:HE2	5:A:1518:HOH:O	2.15	0.47
1:C:234:LEU:HD22	1:C:235:LEU:H	1.80	0.47
1:A:318:GLU:HA	1:A:323:LYS:HG2	1.96	0.47
1:C:161:THR:OG1	1:C:268:CYS:HA	2.16	0.46
1:C:219:PHE:HE2	1:C:270:ARG:HD3	1.80	0.46
1:D:36:THR:HG21	1:D:39:GLN:C	2.36	0.46
1:A:12:MET:HE3	3:A:1372:NAP:H72N	1.80	0.46
1:A:360:GLU:HB3	1:A:361:PRO:HD3	1.98	0.46
1:B:159:VAL:O	1:B:266:GLY:HA3	2.16	0.46
1:B:61:ILE:O	1:B:65:LYS:HG3	2.16	0.46
1:D:320:THR:O	1:D:324:VAL:HG22	2.15	0.46
1:B:113:ASP:CG	1:B:114:PRO:HD3	2.36	0.46
1:B:136:CYS:SG	1:B:277:ASN:ND2	2.88	0.46
1:C:5:GLY:HA3	1:C:67:LEU:HD13	1.97	0.46
1:C:158:SER:HB3	1:C:282:THR:HB	1.97	0.46
1:D:157:ILE:N	1:D:157:ILE:HD12	2.31	0.46
1:A:83:TYR:N	1:A:84:PRO:HD2	2.31	0.45
1:A:133:GLY:HA3	5:A:1392:HOH:O	2.15	0.45
5:A:1537:HOH:O	1:C:126:LYS:HD2	2.15	0.45
1:B:10:ARG:O	3:B:2372:NAP:H2A	2.16	0.45
1:D:234:LEU:HD22	1:D:235:LEU:H	1.81	0.45
1:D:133:GLY:HA3	5:D:4432:HOH:O	2.17	0.45
1:B:151:LYS:CB	1:B:153:LEU:HD13	2.46	0.45
1:D:161:THR:OG1	1:D:268:CYS:HA	2.17	0.45
1:A:175:GLU:O	1:A:179:GLN:HG3	2.17	0.44
1:D:18:MET:HB3	1:D:47:PHE:CE2	2.52	0.44
1:D:151:LYS:HB2	1:D:153:LEU:HD22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:O	3:A:1372:NAP:H2A	2.16	0.44
1:B:1:MET:HG3	1:B:31:ASN:OD1	2.18	0.44
1:A:166:SER:CB	1:A:173:MET:SD	3.04	0.44
1:A:166:SER:OG	1:A:275:ARG:HA	2.17	0.44
1:A:248:TYR:CE2	1:A:263:PRO:HA	2.52	0.44
1:D:83:TYR:O	1:D:87:LYS:HG2	2.18	0.44
1:A:109:ILE:HD11	1:A:123:GLY:HA3	2.00	0.44
1:D:29:ASN:CB	1:D:371:ALA:HB3	2.33	0.44
1:D:91:TRP:CZ2	1:D:93:GLY:HA3	2.53	0.44
1:A:110:ILE:HA	1:A:132:VAL:O	2.17	0.44
1:C:113:ASP:CG	1:C:114:PRO:HD3	2.38	0.44
1:C:103:ARG:NH2	2:C:3374:CAC:O2	2.48	0.44
1:D:208:LYS:HD3	1:D:208:LYS:O	2.18	0.44
1:C:298:ILE:HG21	1:C:332:VAL:HG11	1.99	0.43
2:B:2375:CAC:C2	4:B:2374:CYS:N	2.81	0.43
1:C:151:LYS:CB	1:C:153:LEU:HD22	2.45	0.43
1:D:8:GLY:HA2	1:D:74:GLN:NE2	2.34	0.43
1:A:275:ARG:O	1:A:353:GLN:NE2	2.52	0.43
1:B:24:GLU:HG3	1:B:363:ARG:NH2	2.34	0.43
1:C:83:TYR:O	1:C:87:LYS:HG2	2.18	0.43
1:B:166:SER:CB	1:B:274:LEU:O	2.67	0.42
1:D:30:LEU:HD12	1:D:30:LEU:O	2.19	0.42
1:C:147:GLY:O	1:C:151:LYS:HG2	2.19	0.42
1:B:203:ARG:HG3	5:B:2518:HOH:O	2.17	0.42
1:D:175:GLU:OE1	1:D:218:ASN:HB2	2.19	0.42
1:A:180:MET:HB3	1:D:180:MET:HB3	2.00	0.42
1:C:30:LEU:C	1:C:30:LEU:HD12	2.39	0.42
1:D:163:GLN:NE2	1:D:268:CYS:HB3	2.34	0.42
1:A:166:SER:OG	1:A:274:LEU:O	2.38	0.42
1:A:166:SER:HA	1:A:173:MET:CG	2.49	0.42
1:A:230:TRP:CZ2	1:A:234:LEU:HB2	2.52	0.42
1:A:102:LEU:HA	1:A:105:LYS:HD3	2.02	0.42
1:D:10:ARG:O	3:D:4372:NAP:H2A	2.19	0.42
1:D:30:LEU:HD12	1:D:30:LEU:C	2.40	0.42
1:B:168:ALA:HB2	1:B:270:ARG:NH1	2.35	0.41
1:C:176:LEU:O	1:C:180:MET:HG3	2.20	0.41
1:C:314:ILE:HA	1:C:317:ARG:HH11	1.84	0.41
1:D:169:GLY:O	1:D:173:MET:HG3	2.20	0.41
1:A:5:GLY:HA2	1:A:33:VAL:O	2.19	0.41
1:A:94:TYR:CE2	1:A:129:LYS:HD3	2.55	0.41
1:A:161:THR:OG1	1:A:268:CYS:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:VAL:O	1:B:324:VAL:HG23	2.19	0.41
1:D:113:ASP:OD2	1:D:364:ARG:HD3	2.20	0.41
1:C:175:GLU:O	1:C:179:GLN:HG3	2.20	0.41
1:C:193:ASP:HA	1:C:194:PRO:HD2	1.93	0.41
1:C:198:ILE:HD13	1:C:198:ILE:O	2.19	0.41
1:B:163:GLN:NE2	1:B:268:CYS:HB3	2.35	0.41
1:A:336:ARG:NH1	5:A:1388:HOH:O	2.53	0.41
1:C:159:VAL:HG22	1:C:281:PHE:CD2	2.55	0.41
1:A:234:LEU:O	1:A:236:PRO:HD3	2.21	0.41
1:B:5:GLY:HA2	1:B:33:VAL:O	2.20	0.41
1:B:230:TRP:CZ2	1:B:234:LEU:HB2	2.56	0.41
1:D:45:PRO:CG	1:D:47:PHE:HE1	2.34	0.41
1:D:358:ALA:HB2	3:D:4372:NAP:C5N	2.51	0.41
1:B:159:VAL:HG12	1:B:160:ALA:N	2.36	0.41
1:B:166:SER:HB2	1:B:173:MET:HE2	2.03	0.40
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.93	0.40
1:C:25:ASN:HB3	1:C:28:GLU:CD	2.42	0.40
1:C:183:LEU:HD22	1:C:205:VAL:HG13	2.03	0.40
1:C:270:ARG:HD2	5:C:3376:HOH:O	2.20	0.40
1:D:158:SER:HB3	1:D:282:THR:HB	2.03	0.40
1:A:14:GLY:O	1:A:18:MET:HG2	2.21	0.40
1:B:45:PRO:HB2	1:B:47:PHE:CE1	2.56	0.40
1:A:40:ALA:CB	1:B:342:PRO:HD3	2.52	0.40
1:A:227:LEU:HD12	1:A:227:LEU:O	2.20	0.40
1:A:292:GLU:O	1:A:296:GLN:HG3	2.21	0.40
1:C:159:VAL:HG22	1:C:281:PHE:HD2	1.87	0.40
1:C:159:VAL:O	1:C:266:GLY:HA3	2.21	0.40
1:D:71:VAL:HG21	1:D:366:LEU:HD22	2.04	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	369/371 (100%)	355 (96%)	12 (3%)	2 (0%)	29	18
1	B	369/371 (100%)	351 (95%)	18 (5%)	0	100	100
1	C	352/371 (95%)	339 (96%)	13 (4%)	0	100	100
1	D	369/371 (100%)	350 (95%)	15 (4%)	4 (1%)	14	5
All	All	1459/1484 (98%)	1395 (96%)	58 (4%)	6 (0%)	34	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLY
1	D	53	GLY
1	A	232	ASP
1	D	370	VAL
1	D	112	LEU
1	D	358	ALA

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	305/305 (100%)	299 (98%)	6 (2%)	55	49
1	B	305/305 (100%)	300 (98%)	5 (2%)	62	58
1	C	296/305 (97%)	287 (97%)	9 (3%)	41	31
1	D	305/305 (100%)	297 (97%)	8 (3%)	46	37
All	All	1211/1220 (99%)	1183 (98%)	28 (2%)	50	43

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	153	LEU
1	A	212	ASP
1	A	237	GLU
1	A	291	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	353	GLN
1	B	25	ASN
1	B	55	LEU
1	B	259	ASP
1	B	291	LEU
1	B	324	VAL
1	C	81	GLU
1	C	153	LEU
1	C	198	ILE
1	C	217	ASP
1	C	233	LYS
1	C	234	LEU
1	C	270	ARG
1	C	276	CYS
1	C	353	GLN
1	D	105	LYS
1	D	153	LEU
1	D	202	GLU
1	D	217	ASP
1	D	233	LYS
1	D	234	LEU
1	D	260	ASN
1	D	363	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	25	ASN
1	A	29	ASN
1	A	31	ASN
1	A	163	GLN
1	A	277	ASN
1	A	296	GLN
1	B	23	GLN
1	B	25	ASN
1	B	118	HIS
1	B	163	GLN
1	B	218	ASN
1	B	296	GLN
1	C	31	ASN
1	C	163	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	296	GLN
1	C	353	GLN
1	D	23	GLN
1	D	31	ASN
1	D	42	GLN
1	D	74	GLN
1	D	117	GLN
1	D	163	GLN
1	D	296	GLN
1	D	353	GLN
1	D	368	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	CAC	A	1375	-	0,4,4	-	-	0,6,6	-	-
4	CYS	A	1374	1	3,6,6	0.79	0	1,7,7	0.98	0
2	CAC	D	4375	-	0,4,4	-	-	0,6,6	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	A	1372	-	45,52,52	1.72	6 (13%)	56,80,80	1.23	5 (8%)
2	CAC	C	3374	-	0,4,4	-	-	0,6,6	-	-
3	NAP	B	2372	-	45,52,52	1.77	6 (13%)	56,80,80	1.24	5 (8%)
4	CYS	B	2374	1	3,6,6	0.75	0	1,7,7	0.89	0
4	CYS	C	3373	1	3,6,6	0.59	0	1,7,7	0.41	0
2	CAC	B	2375	-	0,4,4	-	-	0,6,6	-	-
4	CYS	D	4374	1	3,6,6	0.75	0	1,7,7	0.69	0
3	NAP	D	4372	-	45,52,52	1.73	6 (13%)	56,80,80	1.24	5 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CYS	A	1374	1	-	1/2/6/6	-
3	NAP	B	2372	-	-	4/31/67/67	0/5/5/5
4	CYS	B	2374	1	-	2/2/6/6	-
3	NAP	A	1372	-	-	4/31/67/67	0/5/5/5
4	CYS	C	3373	1	-	1/2/6/6	-
4	CYS	D	4374	1	-	2/2/6/6	-
3	NAP	D	4372	-	-	5/31/67/67	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2372	NAP	C2N-N1N	6.64	1.43	1.35
3	D	4372	NAP	C2N-N1N	6.63	1.43	1.35
3	A	1372	NAP	C2N-N1N	6.32	1.42	1.35
3	A	1372	NAP	O4B-C1B	4.96	1.48	1.41
3	B	2372	NAP	O4B-C1B	4.62	1.47	1.41
3	B	2372	NAP	O4D-C1D	4.35	1.47	1.41
3	D	4372	NAP	O4B-C1B	4.27	1.47	1.41
3	A	1372	NAP	O4D-C1D	3.98	1.46	1.41
3	D	4372	NAP	O4D-C1D	3.96	1.46	1.41
3	D	4372	NAP	P2B-O1X	3.40	1.61	1.50
3	B	2372	NAP	P2B-O1X	3.36	1.61	1.50
3	A	1372	NAP	P2B-O1X	3.04	1.60	1.50
3	B	2372	NAP	C6N-N1N	2.78	1.42	1.35
3	A	1372	NAP	C6N-N1N	2.72	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4372	NAP	C6N-N1N	2.69	1.42	1.35
3	D	4372	NAP	C3N-C7N	2.59	1.54	1.50
3	B	2372	NAP	C3N-C7N	2.56	1.54	1.50
3	A	1372	NAP	C3N-C7N	2.30	1.54	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1372	NAP	N3A-C2A-N1A	-5.23	120.50	128.68
3	D	4372	NAP	N3A-C2A-N1A	-5.20	120.55	128.68
3	B	2372	NAP	N3A-C2A-N1A	-5.19	120.57	128.68
3	B	2372	NAP	PN-O3-PA	-3.18	121.92	132.83
3	D	4372	NAP	PN-O3-PA	-3.16	121.99	132.83
3	B	2372	NAP	O3X-P2B-O2X	2.99	119.05	107.64
3	A	1372	NAP	PN-O3-PA	-2.97	122.64	132.83
3	D	4372	NAP	O3X-P2B-O2X	2.96	118.94	107.64
3	A	1372	NAP	O3X-P2B-O2X	2.92	118.80	107.64
3	B	2372	NAP	C6N-N1N-C2N	-2.30	119.88	121.97
3	D	4372	NAP	C6N-N1N-C2N	-2.26	119.91	121.97
3	A	1372	NAP	C3N-C7N-N7N	-2.05	115.28	117.75
3	B	2372	NAP	C3N-C7N-N7N	-2.05	115.28	117.75
3	A	1372	NAP	C6N-N1N-C2N	-2.05	120.10	121.97
3	D	4372	NAP	C3N-C7N-N7N	-2.02	115.33	117.75

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1372	NAP	O4D-C1D-N1N-C2N
3	A	1372	NAP	O4D-C1D-N1N-C6N
3	A	1372	NAP	C2D-C1D-N1N-C6N
3	B	2372	NAP	O4D-C1D-N1N-C2N
3	B	2372	NAP	O4D-C1D-N1N-C6N
3	B	2372	NAP	C2D-C1D-N1N-C2N
3	B	2372	NAP	C2D-C1D-N1N-C6N
3	D	4372	NAP	O4D-C1D-N1N-C2N
3	D	4372	NAP	O4D-C1D-N1N-C6N
3	D	4372	NAP	C2D-C1D-N1N-C2N
3	D	4372	NAP	C2D-C1D-N1N-C6N
4	B	2374	CYS	N-CA-CB-SG
4	D	4374	CYS	N-CA-CB-SG
4	D	4374	CYS	C-CA-CB-SG

Continued on next page...

Continued from previous page...

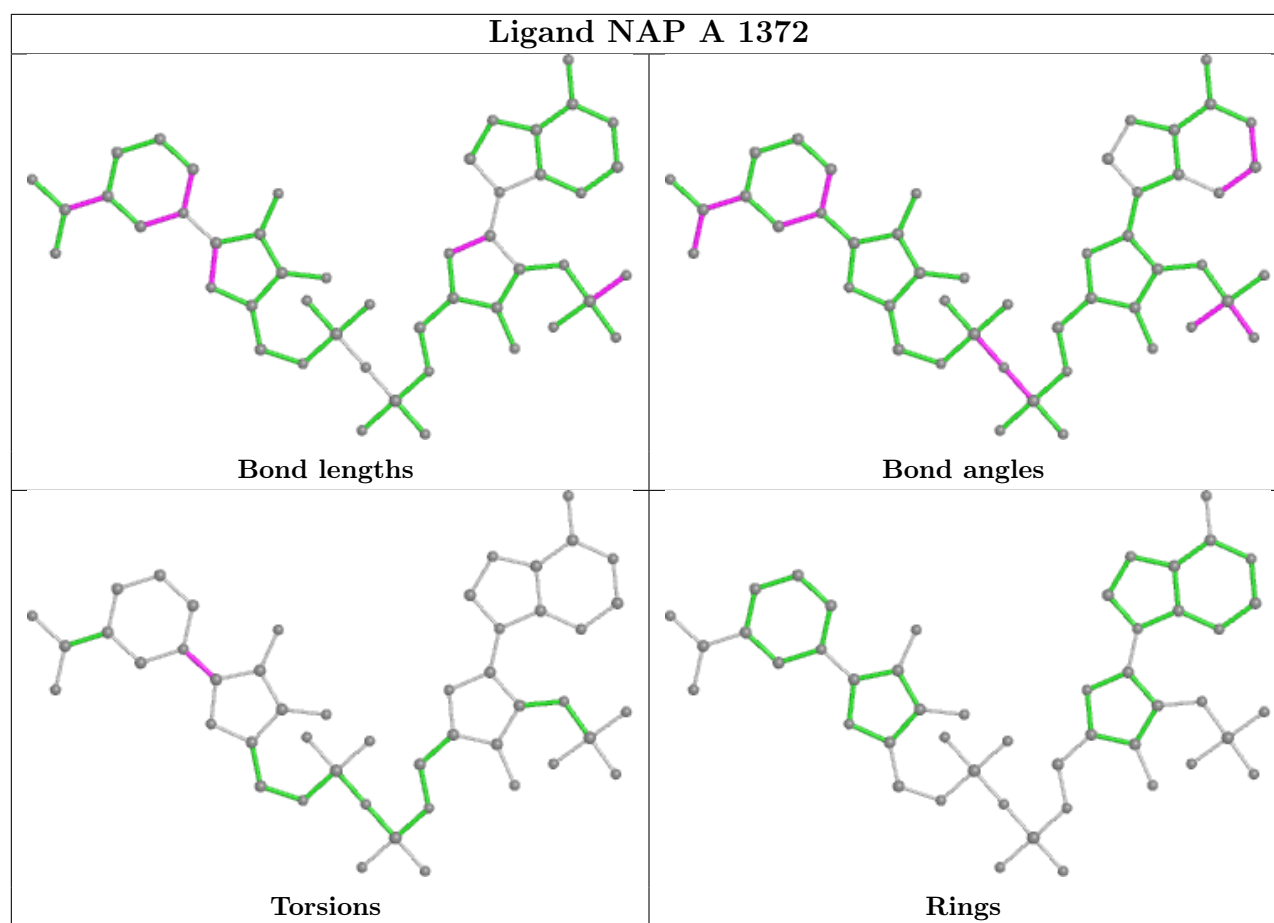
Mol	Chain	Res	Type	Atoms
4	B	2374	CYS	C-CA-CB-SG
4	A	1374	CYS	N-CA-CB-SG
4	C	3373	CYS	N-CA-CB-SG
3	A	1372	NAP	C2D-C1D-N1N-C2N
3	D	4372	NAP	PN-O3-PA-O2A

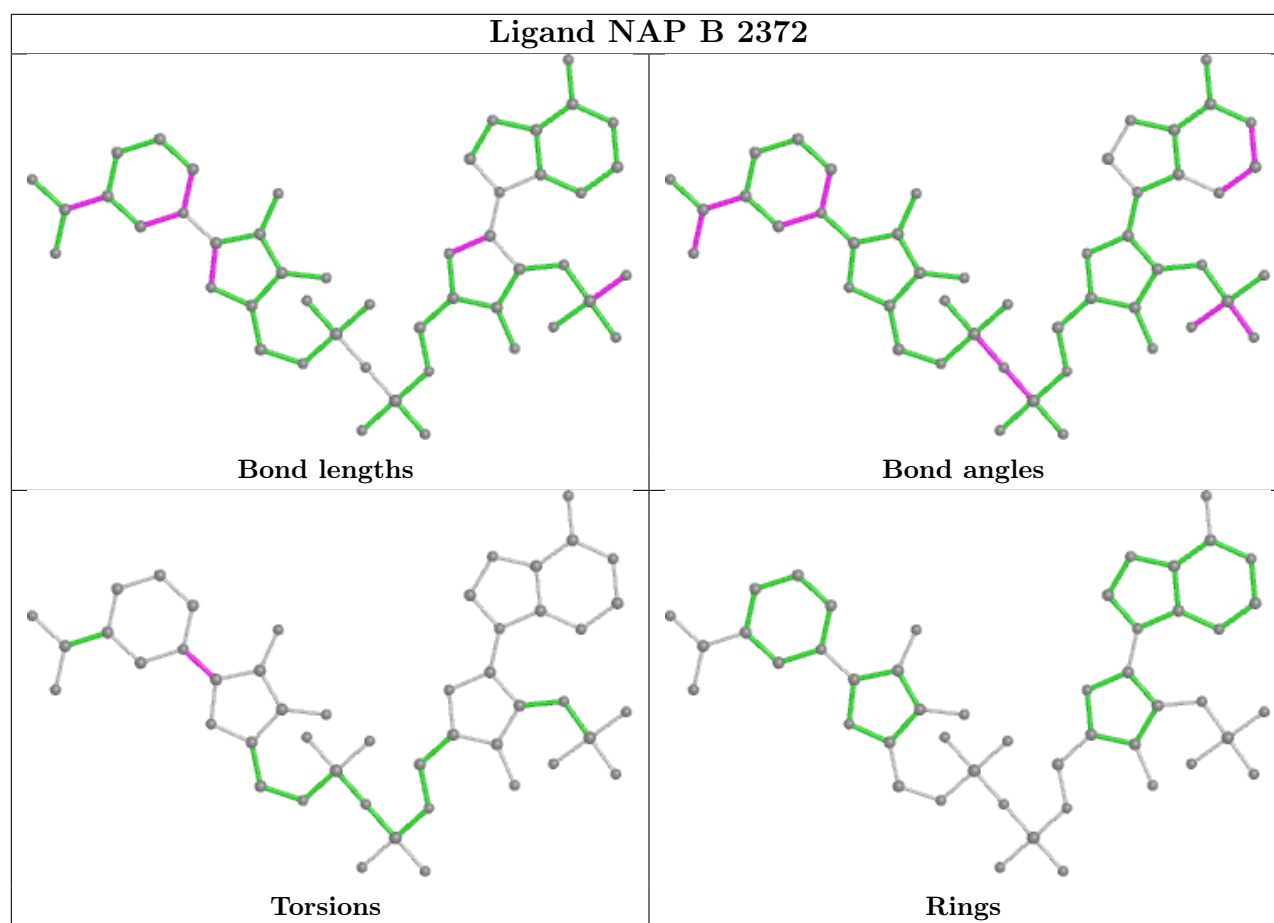
There are no ring outliers.

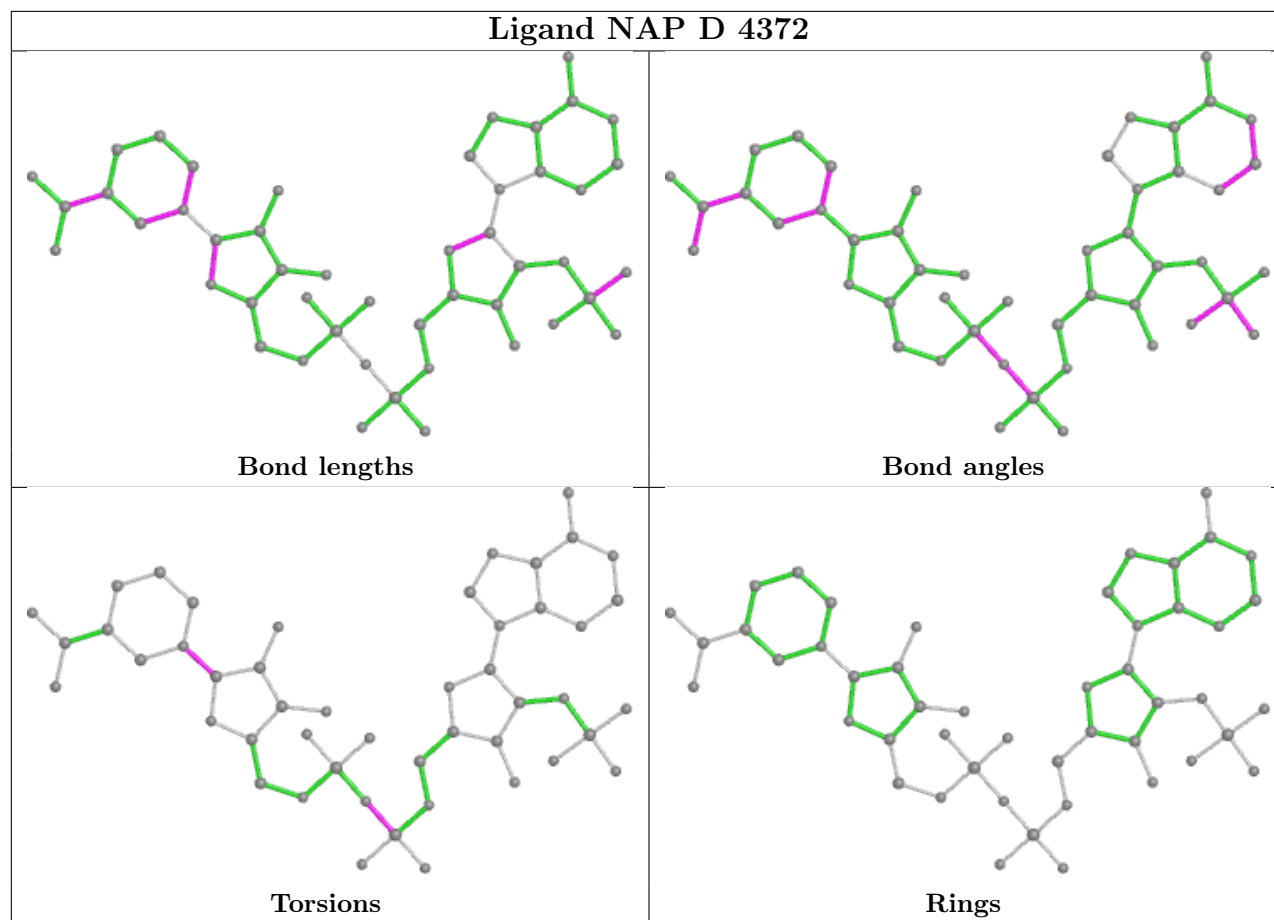
11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1375	CAC	2	0
4	A	1374	CYS	1	0
2	D	4375	CAC	3	0
3	A	1372	NAP	3	0
2	C	3374	CAC	4	0
3	B	2372	NAP	1	0
4	B	2374	CYS	5	0
4	C	3373	CYS	5	0
2	B	2375	CAC	5	0
4	D	4374	CYS	6	0
3	D	4372	NAP	3	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	371/371 (100%)	-0.19	3 (0%) 86 87	6, 15, 30, 45	0
1	B	371/371 (100%)	-0.08	5 (1%) 77 79	6, 16, 30, 43	0
1	C	356/371 (95%)	-0.05	1 (0%) 94 94	5, 13, 28, 41	0
1	D	371/371 (100%)	0.33	19 (5%) 28 31	8, 19, 41, 58	0
All	All	1469/1484 (98%)	0.00	28 (1%) 66 69	5, 16, 33, 58	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	371	ALA	7.1
1	D	52	ALA	6.9
1	B	259	ASP	4.2
1	D	45	PRO	3.6
1	D	51	ASP	3.6
1	D	46	VAL	3.6
1	D	55	LEU	3.4
1	D	47	PHE	3.4
1	A	259	ASP	3.3
1	D	40	ALA	3.2
1	D	49	GLY	3.1
1	A	52	ALA	2.9
1	D	44	ALA	2.9
1	B	258	SER	2.8
1	D	53	GLY	2.8
1	A	46	VAL	2.8
1	D	54	ASP	2.7
1	B	260	ASN	2.6
1	D	29	ASN	2.6
1	D	92	ASP	2.6
1	D	43	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	2.2
1	D	91	TRP	2.2
1	B	126	LYS	2.1
1	C	29	ASN	2.1
1	D	31	ASN	2.1
1	D	274	LEU	2.1
1	B	118	HIS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

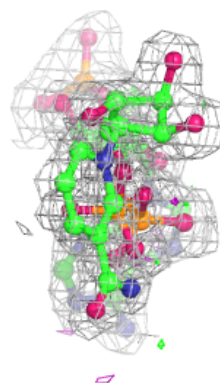
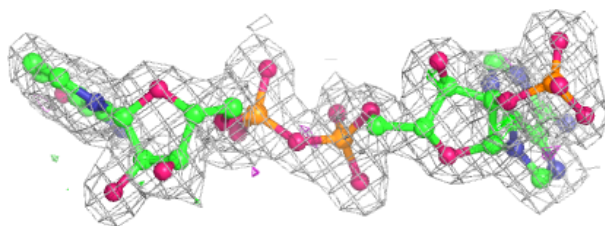
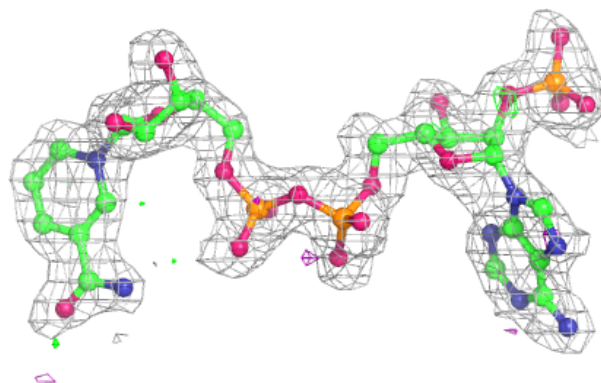
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CYS	D	4374	7/7	0.79	0.21	34,34,36,37	0
4	CYS	A	1374	7/7	0.82	0.17	30,31,32,32	0
4	CYS	C	3373	7/7	0.85	0.16	31,32,33,36	0
4	CYS	B	2374	7/7	0.90	0.14	26,28,29,31	0
2	CAC	A	1375	5/5	0.91	0.19	73,74,75,77	0
2	CAC	C	3374	5/5	0.92	0.21	73,73,74,74	0
3	NAP	D	4372	48/48	0.93	0.12	25,30,39,41	0
2	CAC	D	4375	5/5	0.94	0.18	62,62,63,64	0
2	CAC	B	2375	5/5	0.95	0.19	70,70,70,72	0
3	NAP	B	2372	48/48	0.97	0.10	17,22,25,25	0
3	NAP	A	1372	48/48	0.97	0.09	9,15,27,32	0

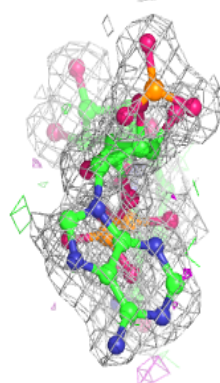
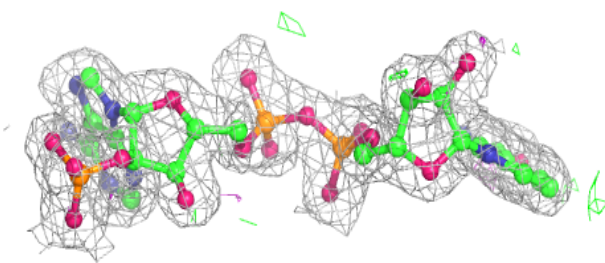
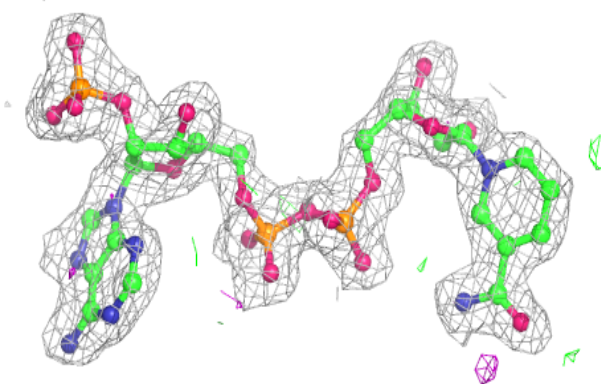
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP D 4372:

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

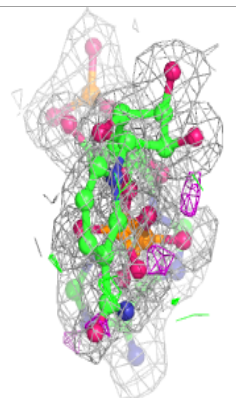
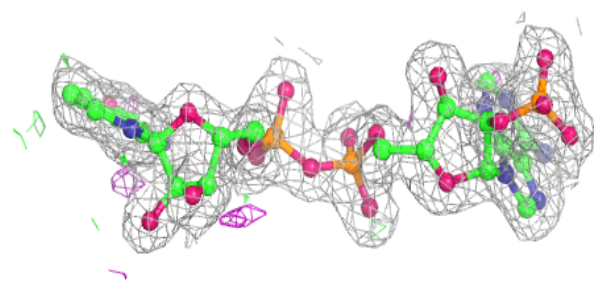
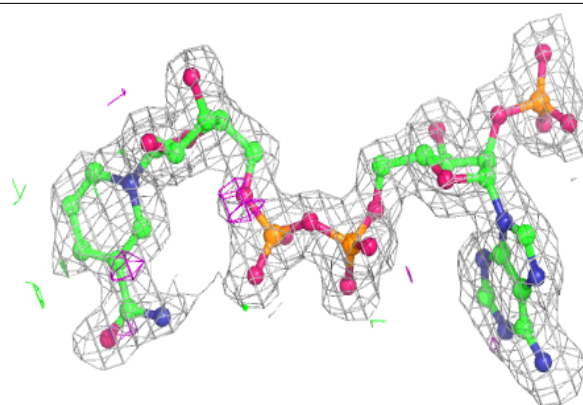
**Electron density around NAP B 2372:**

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



Electron density around NAP A 1372:

$2mF_o-DF_c$ (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.