



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:49 PM UTC

PDB ID : 1PQU / pdb_00001pqu
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 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

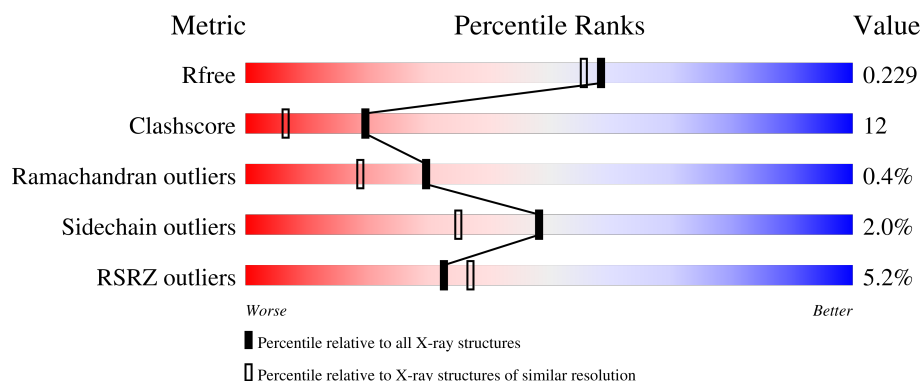
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	5% 74% 25% .
1	B	371	3% 78% 20% .
1	C	371	2% 75% 18% . .
1	D	371	11% 74% 24% .

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	A	1375	-	X	-	-
2	CAC	B	2375	-	X	X	-
2	CAC	C	3374	-	X	X	-
2	CAC	D	4375	-	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.

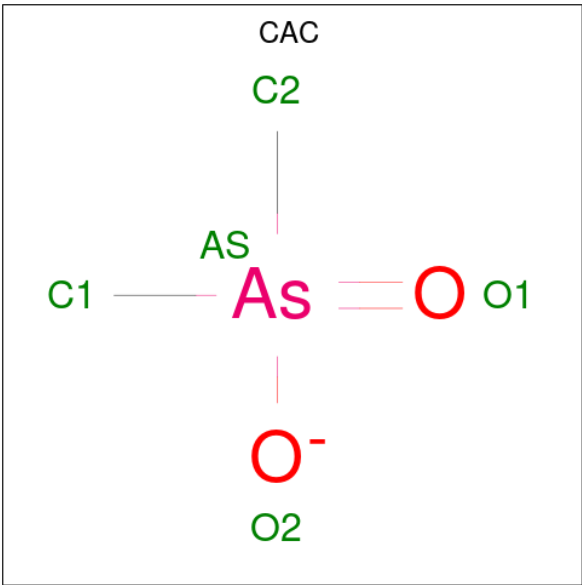
- Molecule 1 is a protein called Aspartate-semialdehyde dehydrogenase.

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:

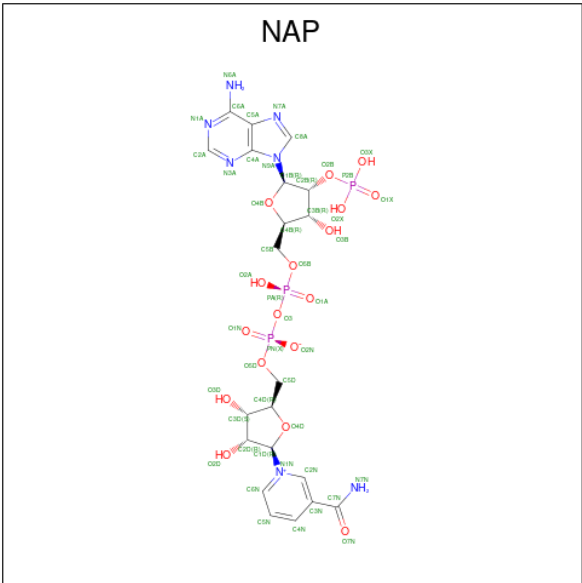
Chain	Residue	Modelled	Actual	Comment	Reference
A	277	ASN	HIS	engineered mutation	UNP P44801
B	277	ASN	HIS	engineered mutation	UNP P44801
C	277	ASN	HIS	engineered mutation	UNP P44801
D	277	ASN	HIS	engineered mutation	UNP P44801

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



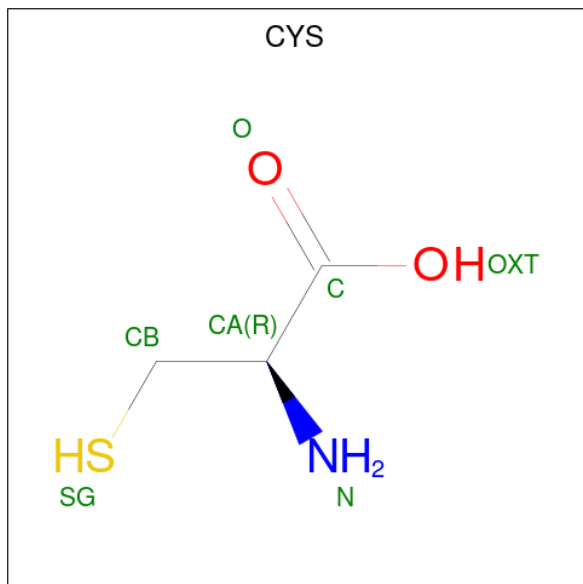
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	As	C	O	0	0
			5	1	2	2		
2	B	1	Total	As	C	O	0	0
			5	1	2	2		
2	C	1	Total	As	C	O	0	0
			5	1	2	2		
2	D	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: 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 (CCD ID: 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		

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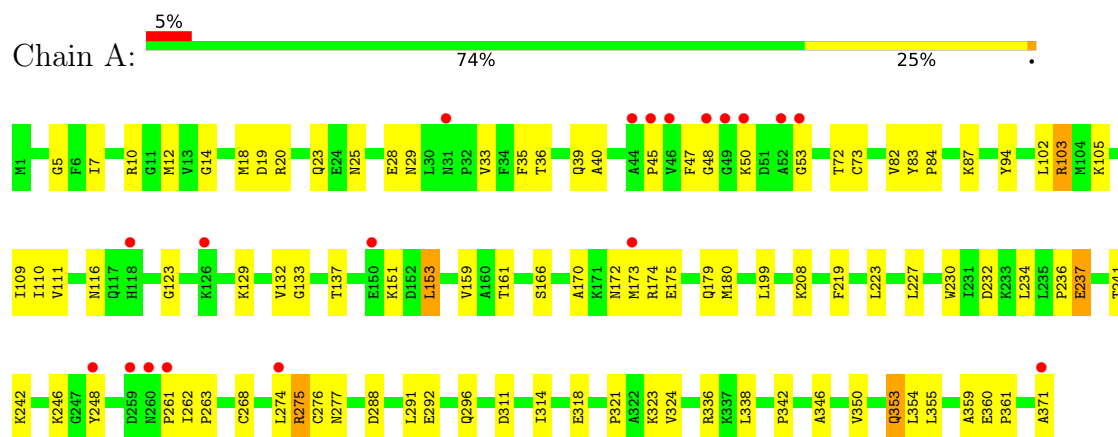
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	145	Total	O	0	0
			145	145		

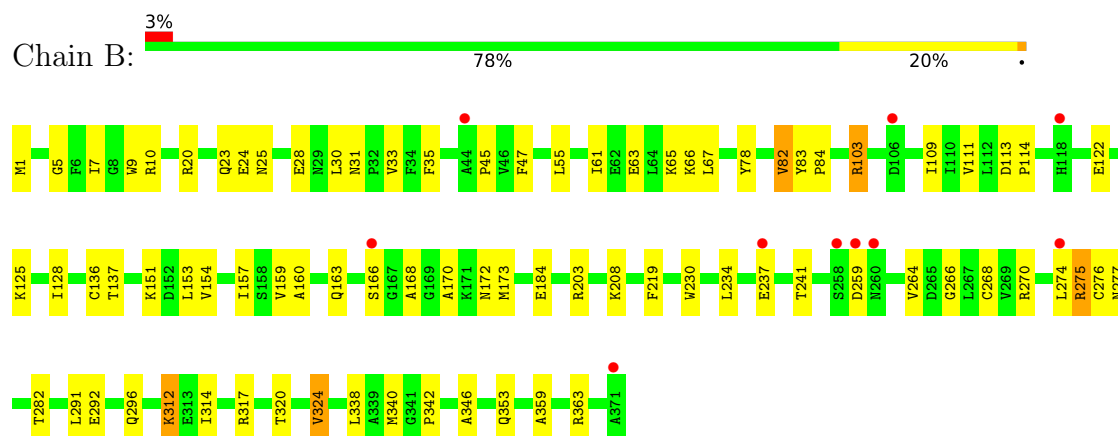
3 Residue-property plots [i](#)

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

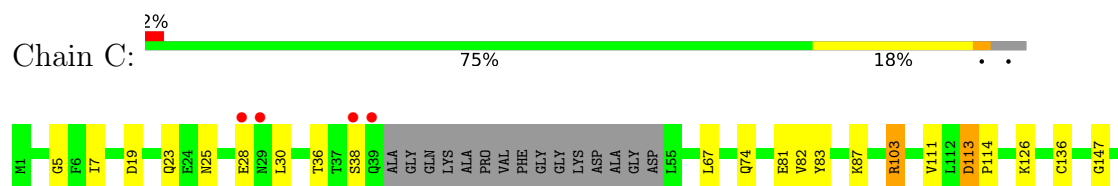
- Molecule 1: Aspartate-semialdehyde dehydrogenase

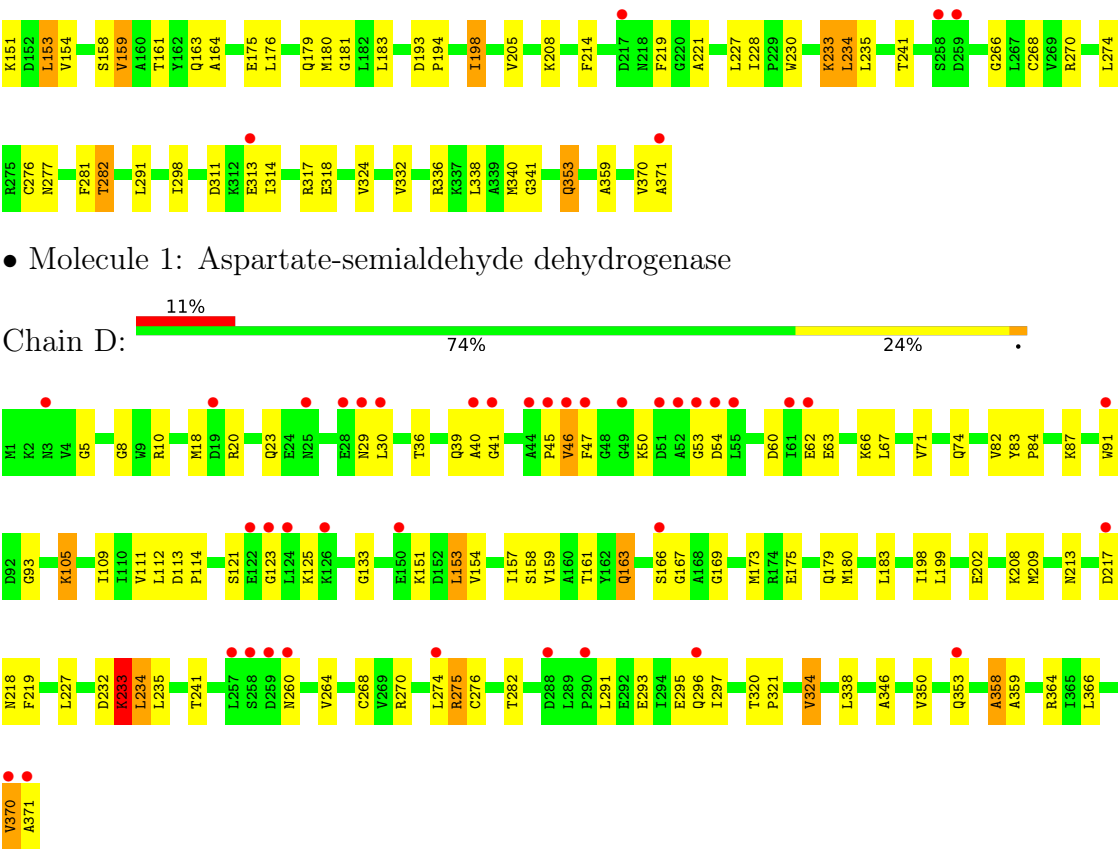


- Molecule 1: Aspartate-semialdehyde dehydrogenase



- Molecule 1: Aspartate-semialdehyde dehydrogenase





● Molecule 1: Aspartate-semialdehyde dehydrogenase

Chain D: 11% 74% 24%

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 0.179 , 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 , 56.1	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, CAC

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	0.40	0/2896	0.96	12/3918 (0.3%)
1	B	0.41	0/2896	0.95	8/3918 (0.2%)
1	C	0.41	0/2792	0.96	15/3776 (0.4%)
1	D	0.39	0/2896	0.93	10/3918 (0.3%)
All	All	0.40	0/11480	0.95	45/15530 (0.3%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	VAL	N-CA-C	8.71	118.71	110.53
1	A	275	ARG	N-CA-C	8.50	121.24	110.61
1	C	82	VAL	N-CA-C	7.57	118.17	110.82
1	D	359	ALA	N-CA-C	7.43	119.38	111.28
1	C	359	ALA	N-CA-C	7.25	119.26	111.36
1	C	241	THR	N-CA-C	-7.24	99.81	110.52
1	B	241	THR	N-CA-C	-7.19	99.88	110.52
1	A	241	THR	N-CA-C	-6.94	100.25	110.52
1	D	241	THR	N-CA-C	-6.91	100.30	110.52
1	A	82	VAL	N-CA-C	6.81	118.42	111.00
1	B	82	VAL	N-CA-C	6.65	117.27	110.82
1	B	275	ARG	N-CA-C	6.48	120.39	111.71
1	C	324	VAL	N-CA-C	6.44	119.14	111.09
1	A	111	VAL	N-CA-C	6.41	117.52	108.36
1	B	111	VAL	N-CA-C	6.21	117.96	108.71
1	B	359	ALA	N-CA-C	6.18	118.10	111.36
1	A	103	ARG	N-CA-C	6.17	118.52	111.11
1	C	113	ASP	CA-C-N	-6.10	113.33	119.56
1	C	113	ASP	C-N-CA	-6.10	113.33	119.56
1	C	111	VAL	N-CA-C	6.10	117.79	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ILE	N-CA-C	-6.05	100.91	108.05
1	C	282	THR	N-CA-C	-5.96	97.42	108.02
1	C	159	VAL	N-CA-C	5.81	116.85	108.48
1	A	223	LEU	N-CA-C	-5.78	105.32	112.72
1	D	233	LYS	N-CA-C	5.74	118.30	110.55
1	D	159	VAL	N-CA-C	5.72	116.71	108.48
1	A	159	VAL	N-CA-C	5.57	117.42	108.85
1	D	46	VAL	N-CA-C	5.53	114.69	106.85
1	C	274	LEU	N-CA-C	5.48	118.08	111.40
1	D	324	VAL	N-CA-C	5.42	117.86	111.09
1	B	312	LYS	N-CA-C	5.41	116.87	110.97
1	B	282	THR	N-CA-C	-5.40	96.41	107.70
1	D	111	VAL	N-CA-C	5.38	116.73	108.71
1	A	359	ALA	N-CA-C	5.38	117.22	111.36
1	B	103	ARG	N-CA-C	5.25	117.68	111.33
1	C	103	ARG	N-CA-C	5.23	117.66	111.33
1	A	73	CYS	N-CA-C	-5.22	105.20	112.30
1	C	214	PHE	N-CA-C	-5.19	103.24	109.72
1	C	154	VAL	N-CA-C	5.16	116.12	108.23
1	C	341	GLY	CA-C-N	5.14	125.22	119.87
1	C	341	GLY	C-N-CA	5.14	125.22	119.87
1	A	72	THR	N-CA-C	5.07	117.16	108.90
1	D	275	ARG	N-CA-C	5.05	118.48	111.71
1	D	163	GLN	N-CA-C	5.03	118.41	109.96
1	A	116	ASN	N-CA-C	5.02	117.30	110.88

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	2845	0	2901	64	0
1	B	2845	0	2901	65	0
1	C	2746	0	2802	57	0
1	D	2845	0	2901	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	2	0
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	266	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 12.

All (266) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:GLY:N	1:D:353:GLN:HE22	1.83	0.76
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:B:270:ARG:HH22	4:B:2374:CYS:C	2.05	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:D:166:SER:C	1:D:353:GLN:HE22	2.05	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:B:166:SER:HB2	1:B:173:MET:HE2	1.80	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:270:ARG:HH22	4:D:4374:CYS:C	2.08	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:5:GLY:HA3	1:B:67:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:276:CYS:SG	1:B:324:VAL:HG22	2.43	0.58
1:A:237:GLU:H	1:A:237:GLU:CD	2.11	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:A:25:ASN:HD22	1:A:28:GLU:CD	2.14	0.56
1:D:166:SER:HA	1:D:173:MET:CG	2.35	0.56
1:D:232:ASP:C	1:D:233:LYS:HE3	2.31	0.55
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:270:ARG:HH22	4:C:3373:CYS:C	2.17	0.52
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: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:B:312:LYS:HE3	1:C:233:LYS:HZ3	1.76	0.51
1:D:36:THR:HG21	1:D:39:GLN:C	2.36	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:B:113:ASP:CG	1:B:114:PRO:HD3	2.36	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: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:B:166:SER:CB	1:B:173:MET:HE2	2.42	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: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:C:113:ASP:CG	1:C:114:PRO:HD3	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:ALA:HB1	1:C:198:ILE:HG13	1.96	0.48
1:D:208:LYS:HZ1	1:D:213:ASN:HD21	1.61	0.48
1:A:83:TYR:O	1:A:87:LYS:HG2	2.13	0.48
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: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:C:30:LEU:C	1:C:30:LEU:HD12	2.39	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:30:LEU:C	1:D:30:LEU:HD12	2.40	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: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:C:25:ASN:HB3	1:C:28:GLU:CD	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LYS:CB	1:B:153:LEU:HD13	2.46	0.45
1:C:338:LEU:HD13	1:C:340:MET:HE1	1.97	0.45
1:D:161:THR:OG1	1:D:268:CYS:HA	2.17	0.45
1:A:227:LEU:C	1:A:227:LEU:HD12	2.42	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
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:C:370:VAL:O	1:C:371:ALA:C	2.61	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:277:ASN:OD1	1:C:353:GLN:CD	2.60	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:B:338:LEU:HD13	1:B:340:MET:HE1	2.00	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:A:48:GLY:C	1:A:50:LYS:H	2.27	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:A:36:THR:HG21	1:A:39:GLN:C	2.45	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:D:113:ASP:CG	1:D:114:PRO:HD3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:LEU:C	1:D:227:LEU:HD12	2.45	0.42
1:A:230:TRP:CZ2	1:A:234:LEU:HB2	2.52	0.42
1:B:30:LEU:HD12	1:B:30:LEU:C	2.44	0.42
1:C:227:LEU:C	1:C:227:LEU:HD12	2.45	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: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
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:A:12:MET:HE3	3:A:1372:NAP:H72N	1.85	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:B:9:TRP:CD1	1:B:9:TRP:H	2.38	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:A:355:LEU:HD23	1:A:355:LEU:HA	1.93	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:D:60:ASP:CG	1:D:63:GLU:HG2	2.47	0.40
1:D:209:MET:HE3	1:D:209:MET:HB2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24	14
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%)	11	3
All	All	1459/1484 (98%)	1395 (96%)	58 (4%)	6 (0%)	30	19

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 [i](#)

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%)	48	35
1	B	305/305 (100%)	301 (99%)	4 (1%)	61	53
1	C	296/305 (97%)	289 (98%)	7 (2%)	43	28
1	D	305/305 (100%)	298 (98%)	7 (2%)	44	30
All	All	1211/1220 (99%)	1187 (98%)	24 (2%)	48	35

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	153	LEU
1	A	199	LEU
1	A	237	GLU
1	A	291	LEU
1	A	353	GLN
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	233	LYS
1	C	234	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN

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Mol	Chain	Res	Type
1	A	25	ASN
1	A	29	ASN
1	A	31	ASN
1	A	39	GLN
1	A	218	ASN
1	A	277	ASN
1	A	279	GLN
1	A	296	GLN
1	A	353	GLN
1	B	23	GLN
1	B	25	ASN
1	B	42	GLN
1	B	74	GLN
1	B	80	ASN
1	B	118	HIS
1	B	163	GLN
1	B	218	ASN
1	B	279	GLN
1	B	296	GLN
1	C	117	GLN
1	C	163	GLN
1	C	260	ASN
1	C	279	GLN
1	C	296	GLN
1	C	353	GLN
1	C	368	GLN
1	D	23	GLN
1	D	39	GLN
1	D	74	GLN
1	D	117	GLN
1	D	163	GLN
1	D	279	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 oligosaccharides 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$
4	CYS	D	4374	1	5,6,6	0.99	0	3,7,7	0.61	0
4	CYS	B	2374	1	5,6,6	0.93	0	3,7,7	1.37	1 (33%)
4	CYS	C	3373	1	5,6,6	0.94	0	3,7,7	0.40	0
2	CAC	A	1375	-	2,4,4	3.80	2 (100%)	4,6,6	3.74	4 (100%)
4	CYS	A	1374	1	5,6,6	0.96	0	3,7,7	0.75	0
2	CAC	C	3374	-	2,4,4	3.36	2 (100%)	4,6,6	3.97	4 (100%)
2	CAC	B	2375	-	2,4,4	3.75	2 (100%)	4,6,6	3.85	4 (100%)
2	CAC	D	4375	-	2,4,4	3.87	2 (100%)	4,6,6	4.41	4 (100%)
3	NAP	B	2372	-	50,52,52	1.86	9 (18%)	71,80,80	1.52	9 (12%)
3	NAP	D	4372	-	50,52,52	1.87	9 (18%)	71,80,80	1.51	10 (14%)
3	NAP	A	1372	-	50,52,52	1.83	9 (18%)	71,80,80	1.50	9 (12%)

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	D	4374	1	-	2/6/6/6	-
4	CYS	B	2374	1	-	2/6/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CYS	C	3373	1	-	1/6/6/6	-
4	CYS	A	1374	1	-	1/6/6/6	-
3	NAP	D	4372	-	-	6/35/67/67	0/5/5/5
3	NAP	A	1372	-	-	7/35/67/67	0/5/5/5
3	NAP	B	2372	-	-	6/35/67/67	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2372	NAP	C2N-N1N	7.34	1.43	1.35
3	D	4372	NAP	C2N-N1N	7.34	1.43	1.35
3	A	1372	NAP	C2N-N1N	6.99	1.42	1.35
3	B	2372	NAP	O4D-C1D	4.77	1.47	1.40
3	A	1372	NAP	O4D-C1D	4.38	1.46	1.40
3	D	4372	NAP	O4D-C1D	4.35	1.46	1.40
2	D	4375	CAC	AS-C1	4.34	2.00	1.90
2	B	2375	CAC	AS-C1	4.33	2.00	1.90
2	A	1375	CAC	AS-C1	4.29	2.00	1.90
2	C	3374	CAC	AS-C1	4.04	1.99	1.90
3	D	4372	NAP	P2B-O1X	3.55	1.61	1.50
3	A	1372	NAP	PN-O3	3.54	1.63	1.59
3	B	2372	NAP	P2B-O1X	3.51	1.61	1.50
3	B	2372	NAP	C5A-N7A	-3.39	1.32	1.39
3	A	1372	NAP	C5A-N7A	-3.36	1.33	1.39
3	D	4372	NAP	PN-O3	3.34	1.63	1.59
2	D	4375	CAC	AS-C2	3.33	1.98	1.90
2	A	1375	CAC	AS-C2	3.23	1.98	1.90
3	D	4372	NAP	C5A-N7A	-3.23	1.33	1.39
3	A	1372	NAP	P2B-O1X	3.18	1.60	1.50
3	D	4372	NAP	PA-O3	3.17	1.62	1.59
2	B	2375	CAC	AS-C2	3.07	1.97	1.90
3	B	2372	NAP	C6N-N1N	3.01	1.42	1.35
3	A	1372	NAP	PA-O3	2.99	1.62	1.59
3	A	1372	NAP	C6N-N1N	2.95	1.42	1.35
3	B	2372	NAP	PA-O3	2.92	1.62	1.59
3	D	4372	NAP	C6N-N1N	2.91	1.42	1.35
3	D	4372	NAP	C3N-C7N	2.60	1.54	1.50
3	A	1372	NAP	O4B-C1B	2.60	1.48	1.42
3	B	2372	NAP	C3N-C7N	2.57	1.54	1.50
3	B	2372	NAP	PN-O3	2.55	1.62	1.59
2	C	3374	CAC	AS-C2	2.50	1.96	1.90
3	B	2372	NAP	O4B-C1B	2.39	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1372	NAP	C3N-C7N	2.31	1.54	1.50
3	D	4372	NAP	O4B-C1B	2.18	1.47	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4375	CAC	O1-AS-C1	-7.45	102.23	111.50
2	C	3374	CAC	O1-AS-C1	-6.31	103.65	111.50
2	B	2375	CAC	O1-AS-C1	-6.31	103.66	111.50
2	A	1375	CAC	O1-AS-C1	-6.13	103.88	111.50
3	A	1372	NAP	N3A-C2A-N1A	-5.34	120.50	128.58
3	D	4372	NAP	N3A-C2A-N1A	-5.31	120.55	128.58
3	B	2372	NAP	N3A-C2A-N1A	-5.30	120.57	128.58
3	B	2372	NAP	C5A-C4A-N3A	-5.11	119.68	126.72
3	D	4372	NAP	C5A-C4A-N3A	-4.95	119.90	126.72
3	A	1372	NAP	C5A-C4A-N3A	-4.92	119.95	126.72
3	B	2372	NAP	C2A-N3A-C4A	3.75	121.00	111.83
3	D	4372	NAP	C2A-N3A-C4A	3.71	120.89	111.83
3	A	1372	NAP	C2A-N3A-C4A	3.68	120.81	111.83
3	B	2372	NAP	N3A-C4A-N9A	3.48	133.09	127.17
2	C	3374	CAC	O1-AS-C2	-3.36	107.32	111.50
3	A	1372	NAP	N3A-C4A-N9A	3.34	132.85	127.17
3	D	4372	NAP	N3A-C4A-N9A	3.33	132.83	127.17
3	A	1372	NAP	N9A-C8A-N7A	-3.31	109.24	113.94
3	D	4372	NAP	N9A-C8A-N7A	-3.29	109.27	113.94
2	D	4375	CAC	O2-AS-C1	3.20	113.60	105.84
3	B	2372	NAP	N9A-C8A-N7A	-3.17	109.44	113.94
3	B	2372	NAP	O3X-P2B-O2X	3.00	119.05	107.80
3	D	4372	NAP	O3X-P2B-O2X	2.97	118.94	107.80
3	A	1372	NAP	O3X-P2B-O2X	2.93	118.80	107.80
3	A	1372	NAP	C5A-N7A-C8A	2.82	107.88	103.45
3	B	2372	NAP	C5A-N7A-C8A	2.79	107.83	103.45
3	D	4372	NAP	C5A-N7A-C8A	2.78	107.82	103.45
2	B	2375	CAC	O1-AS-C2	-2.72	108.11	111.50
2	A	1375	CAC	O1-AS-C2	-2.68	108.16	111.50
2	B	2375	CAC	O2-AS-C1	2.66	112.29	105.84
2	C	3374	CAC	O2-AS-C1	2.57	112.07	105.84
2	D	4375	CAC	O2-AS-C2	2.54	112.00	105.84
2	A	1375	CAC	O2-AS-C1	2.47	111.83	105.84
3	B	2372	NAP	C4A-C5A-N7A	-2.39	107.85	110.58
3	D	4372	NAP	C4A-C5A-N7A	-2.39	107.86	110.58
2	D	4375	CAC	O1-AS-C2	-2.38	108.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2372	NAP	C6N-N1N-C2N	-2.35	119.88	121.88
3	A	1372	NAP	C4A-C5A-N7A	-2.35	107.90	110.58
2	C	3374	CAC	O2-AS-C2	2.32	111.47	105.84
3	D	4372	NAP	C6N-N1N-C2N	-2.31	119.91	121.88
2	A	1375	CAC	O2-AS-C2	2.28	111.36	105.84
2	B	2375	CAC	O2-AS-C2	2.22	111.23	105.84
4	B	2374	CYS	CB-CA-C	-2.17	107.73	109.89
3	A	1372	NAP	C6N-N1N-C2N	-2.09	120.10	121.88
3	D	4372	NAP	O2B-P2B-O1X	-2.05	102.02	109.33

There are no chirality outliers.

All (25) torsion outliers are listed below:

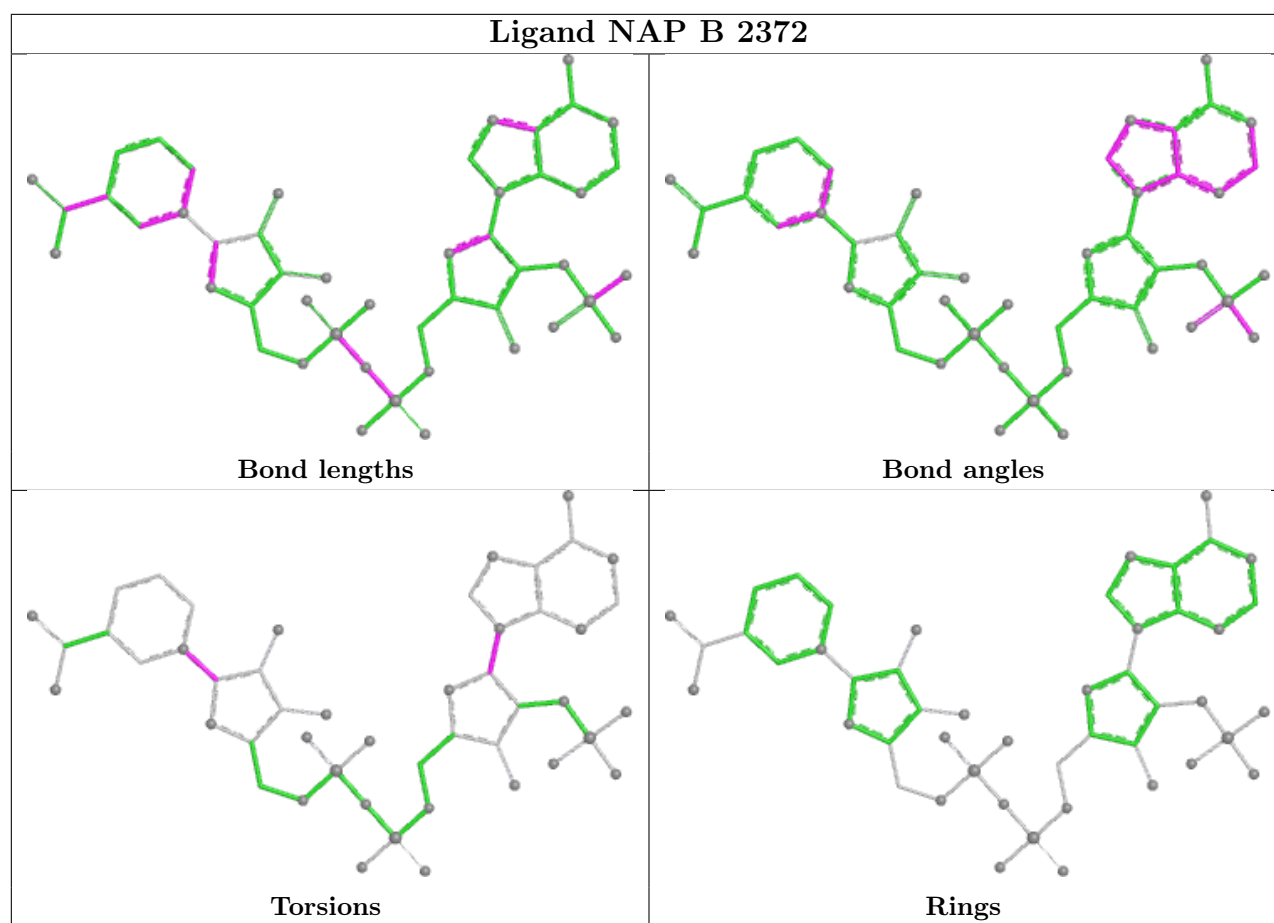
Mol	Chain	Res	Type	Atoms
3	A	1372	NAP	O4D-C1D-N1N-C2N
3	A	1372	NAP	O4D-C1D-N1N-C6N
3	A	1372	NAP	C2D-C1D-N1N-C6N
3	B	2372	NAP	O4D-C1D-N1N-C2N
3	B	2372	NAP	O4D-C1D-N1N-C6N
3	B	2372	NAP	C2D-C1D-N1N-C2N
3	B	2372	NAP	C2D-C1D-N1N-C6N
3	D	4372	NAP	O4D-C1D-N1N-C2N
3	D	4372	NAP	O4D-C1D-N1N-C6N
3	D	4372	NAP	C2D-C1D-N1N-C2N
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
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	B	2372	NAP	O4B-C1B-N9A-C8A
3	A	1372	NAP	C2B-C1B-N9A-C8A
3	A	1372	NAP	C2B-C1B-N9A-C4A
3	B	2372	NAP	C2B-C1B-N9A-C8A
3	D	4372	NAP	PN-O3-PA-O2A
3	A	1372	NAP	O4B-C1B-N9A-C8A
3	D	4372	NAP	O4B-C1B-N9A-C8A

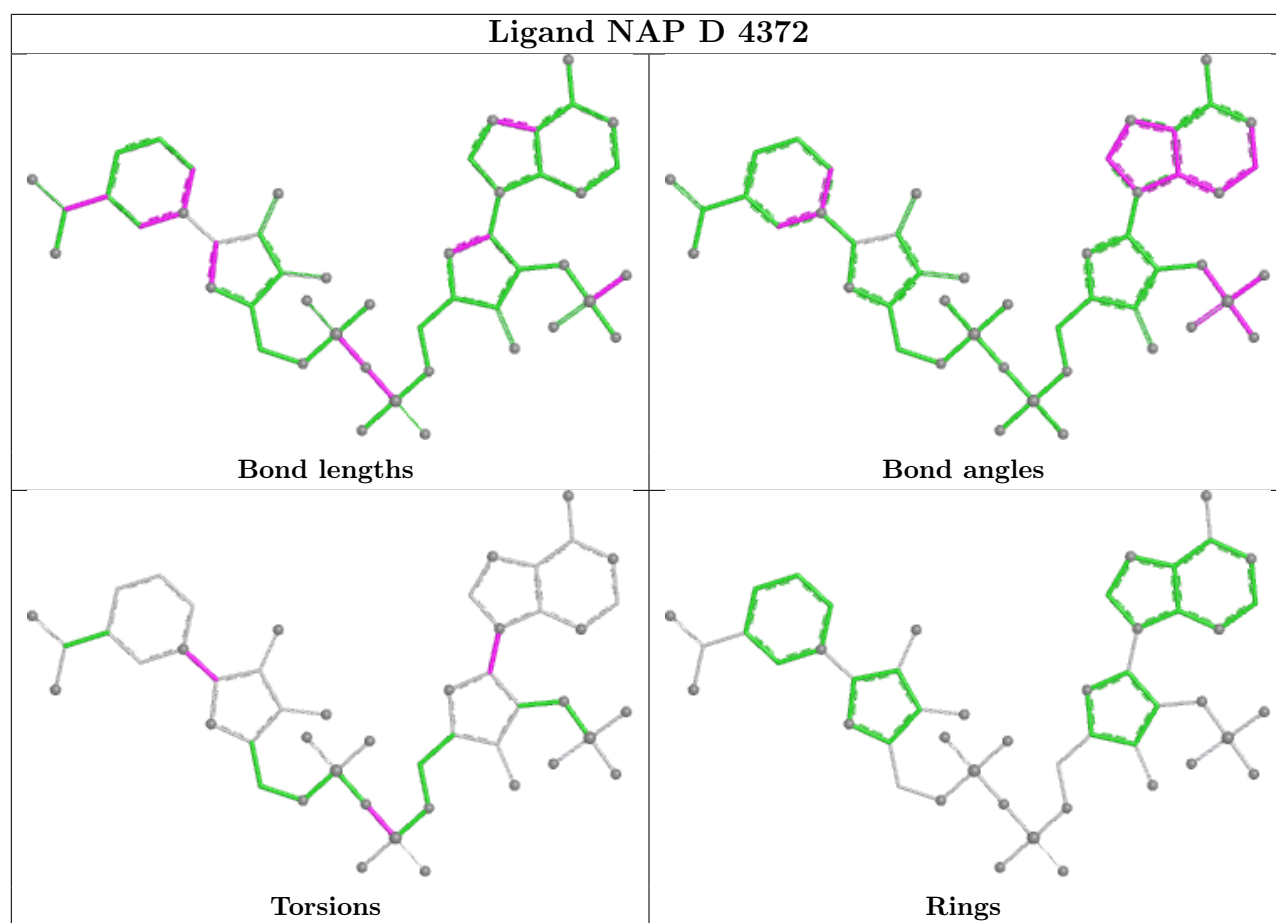
There are no ring outliers.

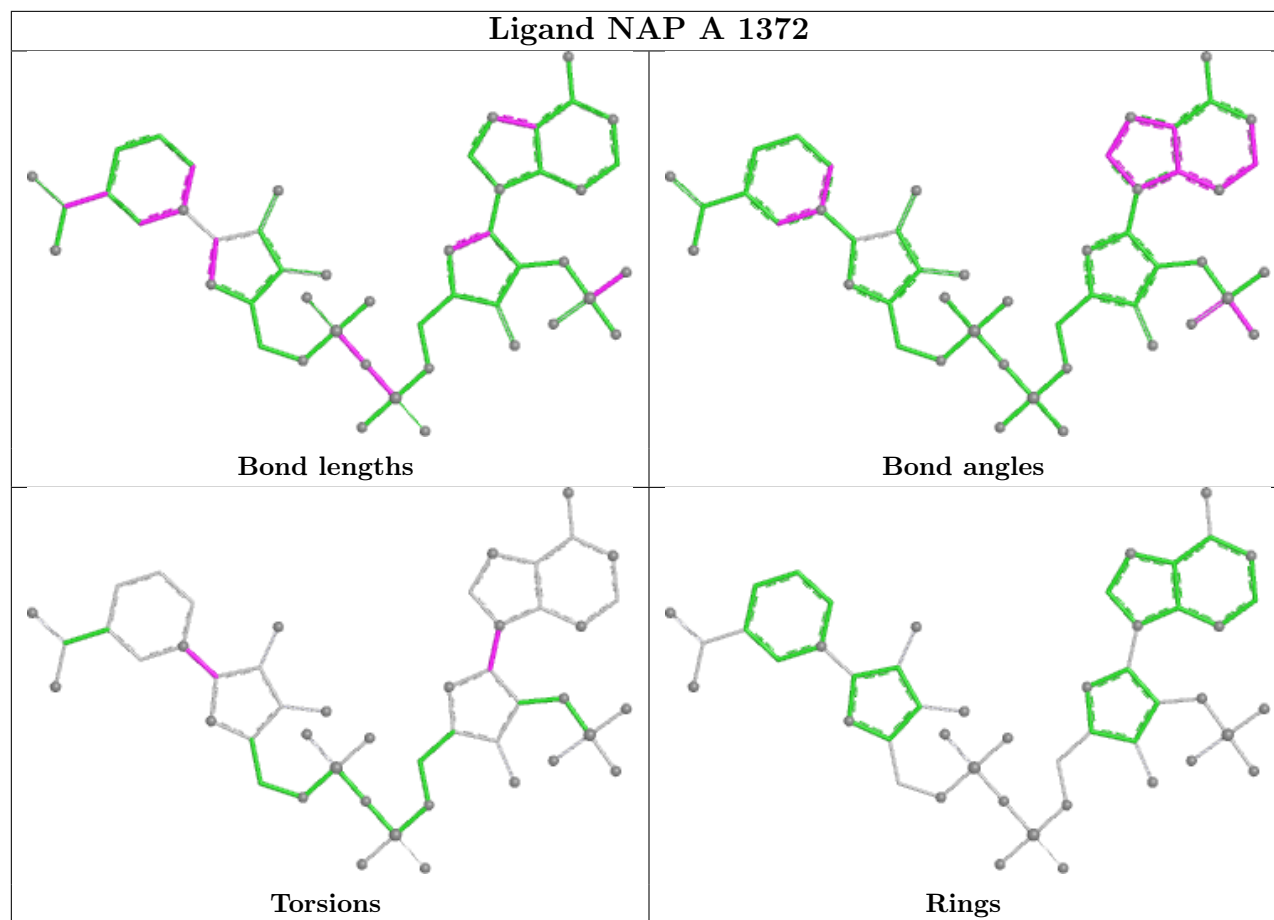
11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4374	CYS	6	0
4	B	2374	CYS	5	0
4	C	3373	CYS	5	0
2	A	1375	CAC	2	0
4	A	1374	CYS	1	0
2	C	3374	CAC	4	0
2	B	2375	CAC	5	0
2	D	4375	CAC	3	0
3	B	2372	NAP	1	0
3	D	4372	NAP	3	0
3	A	1372	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%)	0.10	19 (5%) 33 37	6, 15, 30, 45	0
1	B	371/371 (100%)	0.13	10 (2%) 56 62	6, 16, 30, 43	0
1	C	356/371 (95%)	0.08	9 (2%) 58 64	5, 13, 28, 41	0
1	D	371/371 (100%)	0.60	39 (10%) 11 15	8, 19, 41, 58	0
All	All	1469/1484 (98%)	0.23	77 (5%) 33 37	5, 16, 33, 58	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	371	ALA	7.8
1	D	55	LEU	4.8
1	D	46	VAL	4.7
1	A	46	VAL	4.5
1	B	258	SER	4.2
1	D	52	ALA	4.1
1	D	44	ALA	4.0
1	A	259	ASP	3.9
1	D	53	GLY	3.5
1	D	166	SER	3.4
1	C	39	GLN	3.4
1	B	260	ASN	3.3
1	C	258	SER	3.3
1	D	288	ASP	3.3
1	A	49	GLY	3.3
1	A	52	ALA	3.3
1	D	40	ALA	3.3
1	D	29	ASN	3.2
1	B	274	LEU	3.2
1	B	371	ALA	3.1
1	A	261	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	41	GLY	3.1
1	D	370	VAL	3.1
1	D	45	PRO	3.0
1	B	259	ASP	2.9
1	B	106	ASP	2.9
1	B	44	ALA	2.9
1	D	49	GLY	2.9
1	C	259	ASP	2.9
1	B	118	HIS	2.8
1	C	29	ASN	2.8
1	D	257	LEU	2.7
1	D	353	GLN	2.7
1	B	166	SER	2.7
1	D	259	ASP	2.6
1	D	274	LEU	2.6
1	D	296	GLN	2.6
1	A	371	ALA	2.5
1	D	290	PRO	2.5
1	A	274	LEU	2.5
1	D	258	SER	2.5
1	D	51	ASP	2.5
1	D	123	GLY	2.4
1	C	313	GLU	2.4
1	C	28	GLU	2.4
1	D	28	GLU	2.4
1	D	122	GLU	2.4
1	A	31	ASN	2.4
1	D	61	ILE	2.3
1	A	173	MET	2.3
1	D	217	ASP	2.3
1	A	50	LYS	2.3
1	A	126	LYS	2.3
1	D	47	PHE	2.3
1	D	54	ASP	2.3
1	A	260	ASN	2.3
1	D	260	ASN	2.3
1	D	124	LEU	2.3
1	C	38	SER	2.2
1	D	126	LYS	2.2
1	A	48	GLY	2.2
1	D	19	ASP	2.2
1	D	25	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	44	ALA	2.2
1	C	371	ALA	2.2
1	A	118	HIS	2.2
1	C	217	ASP	2.2
1	D	30	LEU	2.2
1	A	45	PRO	2.2
1	D	3	ASN	2.1
1	D	91	TRP	2.1
1	B	237	GLU	2.1
1	D	62	GLU	2.1
1	A	150	GLU	2.1
1	D	150	GLU	2.0
1	A	53	GLY	2.0
1	A	248	TYR	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CAC	A	1375	5/5	0.72	0.32	73,74,75,77	0
4	CYS	D	4374	7/7	0.82	0.15	34,34,36,37	0
4	CYS	A	1374	7/7	0.84	0.17	30,31,32,32	0
4	CYS	B	2374	7/7	0.85	0.13	26,28,29,31	0
2	CAC	C	3374	5/5	0.86	0.29	73,73,74,74	0
4	CYS	C	3373	7/7	0.87	0.13	31,32,33,36	0
2	CAC	B	2375	5/5	0.87	0.22	70,70,70,72	0
2	CAC	D	4375	5/5	0.88	0.22	62,62,63,64	0
3	NAP	D	4372	48/48	0.93	0.11	25,30,39,41	0

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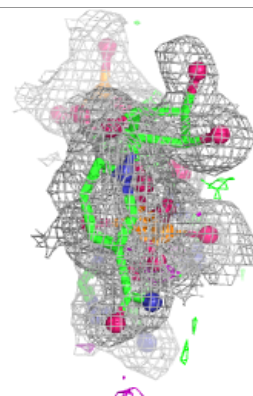
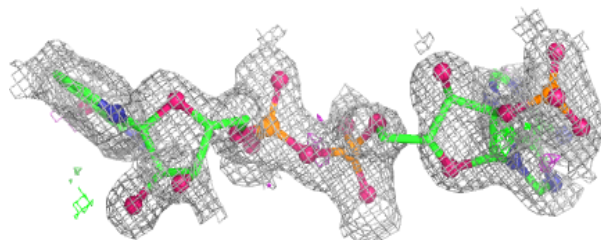
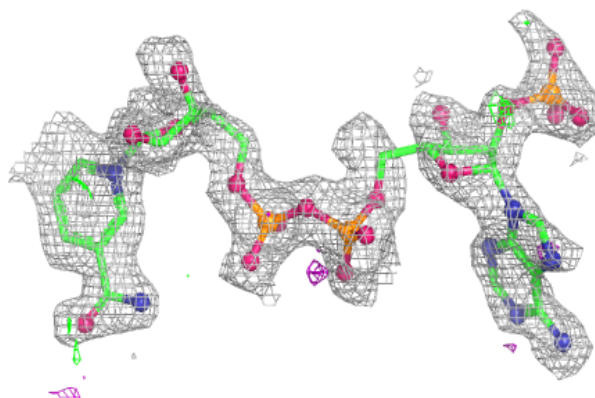
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	B	2372	48/48	0.96	0.08	17,22,25,25	0
3	NAP	A	1372	48/48	0.97	0.07	9,15,27,32	0

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.

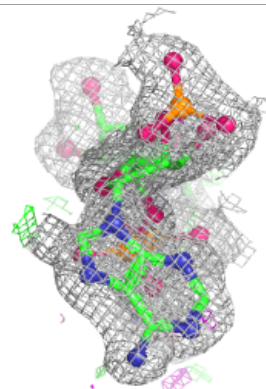
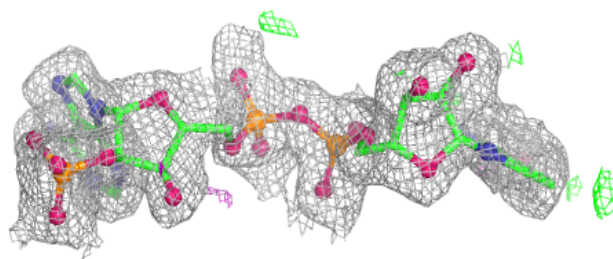
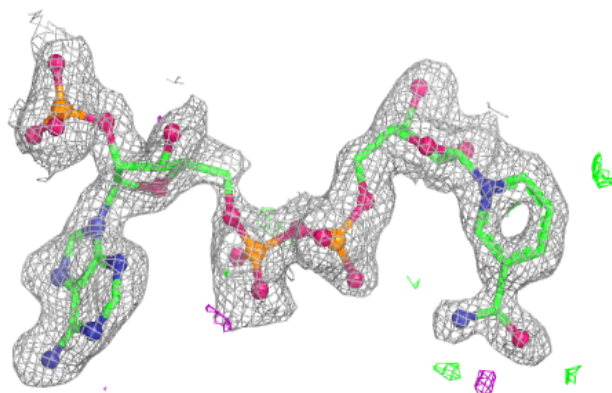
Electron density around NAP D 4372:

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

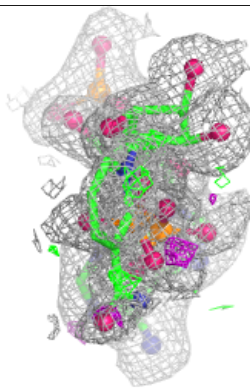
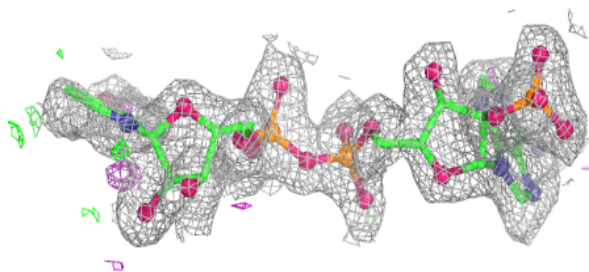
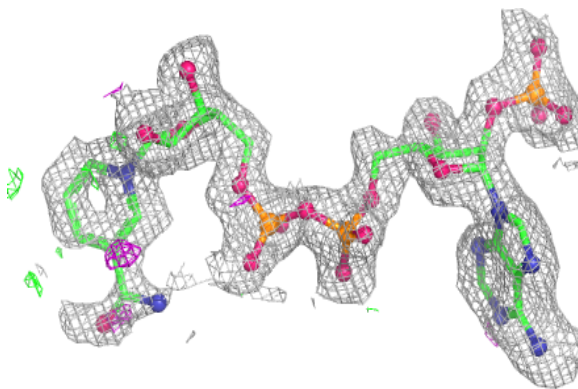


Electron density around NAP B 2372:

$2mF_o-DF_c$ (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.