



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:13 AM UTC

PDB ID : 7SIT / pdb_00007sit
Title : Crystal structure of Voltage gated potassium ion channel, Kv 1.2 chimera-3m
Authors : Reddi, R.; Matulef, K.; Riederer, E.A.; Whorton, M.R.; Valiyaveetil, F.I.
Deposited on : 2021-10-14
Resolution : 3.32 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

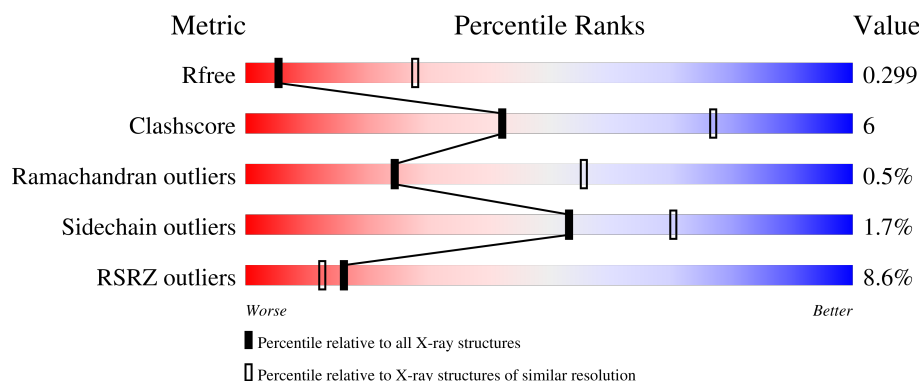
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	333	 3% 77% 20% ..
1	C	333	 2% 87% 11% .
2	B	514	 6% 53% 10% . 37%
2	D	514	 12% 55% 8% 37%

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
5	O	B	503	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10442 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 Voltage-gated potassium channel subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			
1	C	326	Total	C	N	O	S	12	0	0
			2556	1627	443	470	16			

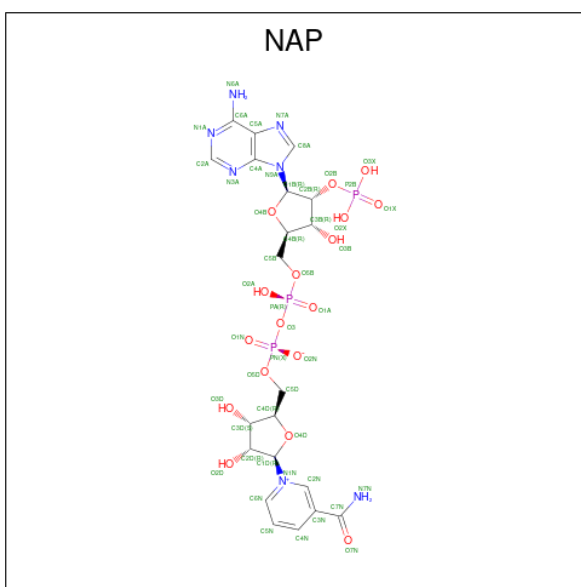
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	initiating methionine	UNP P62483
C	35	MET	-	initiating methionine	UNP P62483

- Molecule 2 is a protein called Voltage gated potassium channel Kv1.2-Kv2.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	325	Total	C	N	O	S	0	0	0
			2629	1737	422	457	13			
2	D	325	Total	C	N	O	S	11	0	0
			2600	1716	413	458	13			

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total K 2 2	0	0
4	D	2	Total K 2 2	0	0

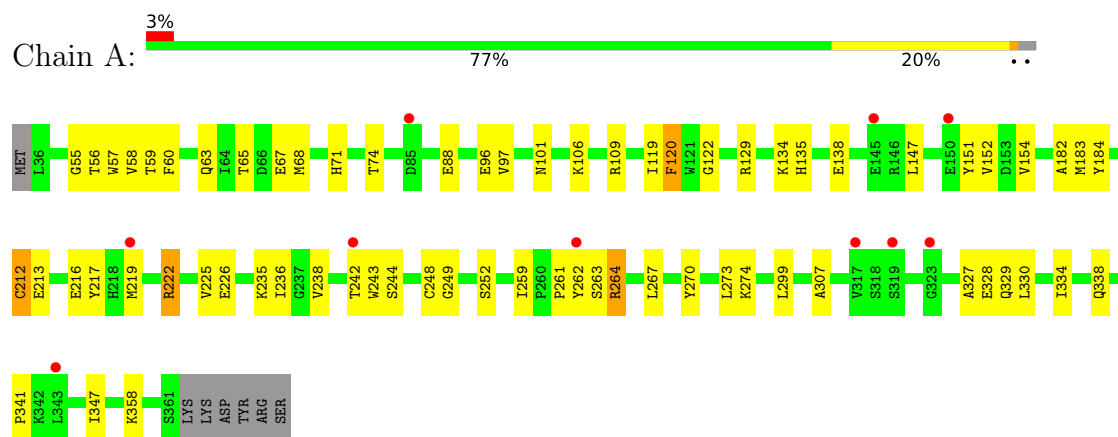
- Molecule 5 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 1 1	0	0

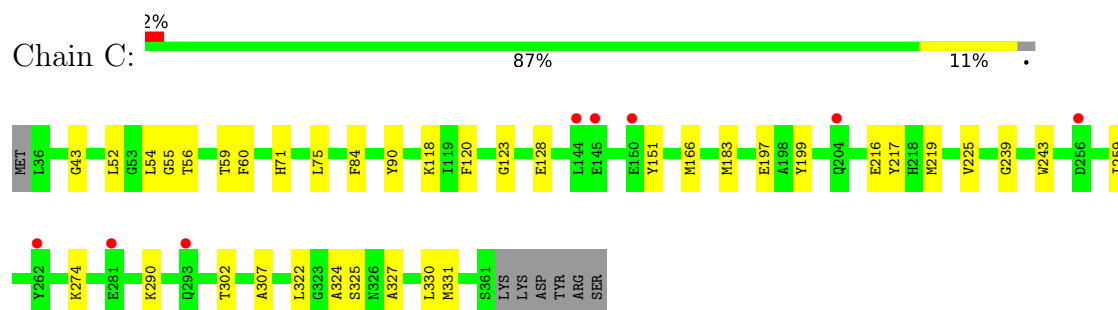
3 Residue-property plots [i](#)

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.

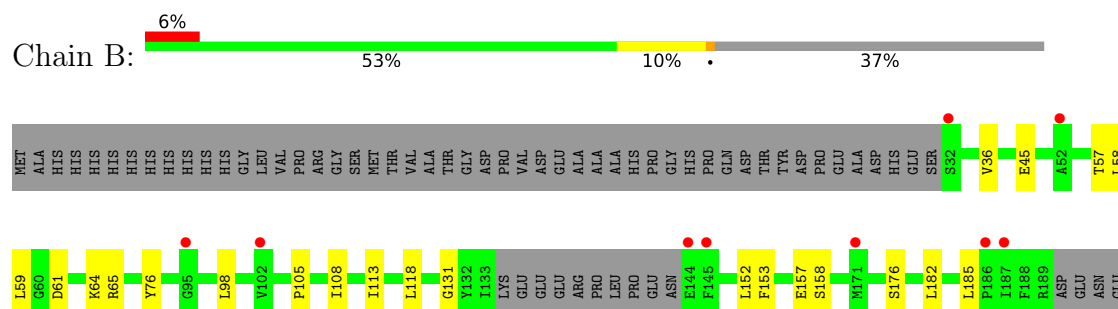
- Molecule 1: Voltage-gated potassium channel subunit beta-2

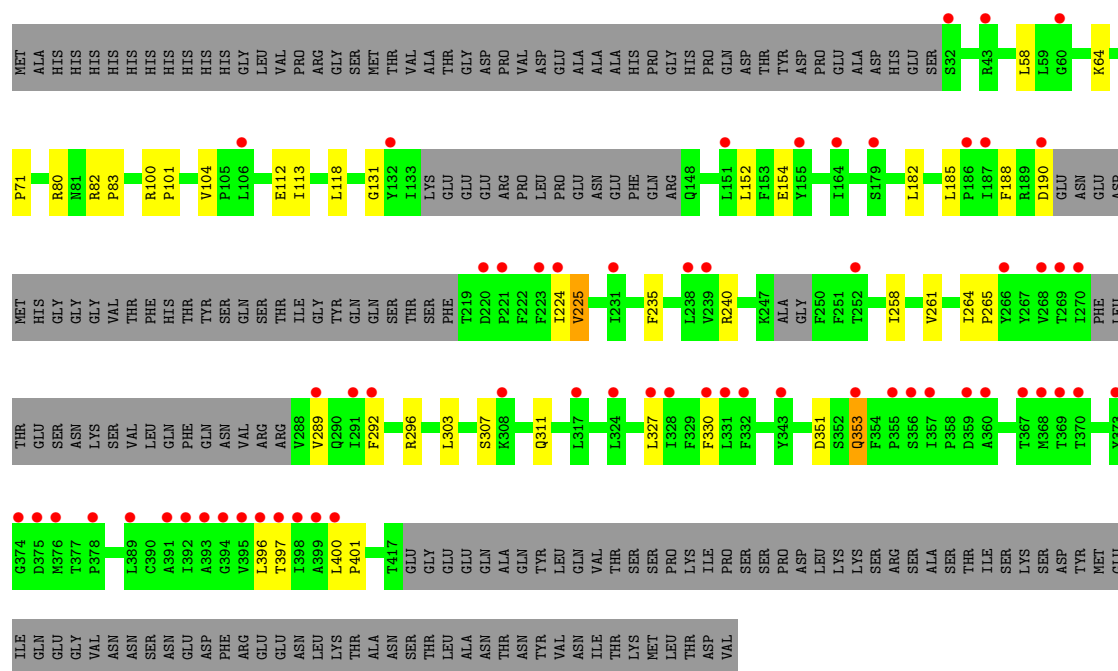


- Molecule 1: Voltage-gated potassium channel subunit beta-2



- Molecule 2: Voltage gated potassium channel Kv1.2-Kv2.1





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.59Å 129.59Å 278.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.16 – 3.32 49.16 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.16-3.32) 99.3 (49.16-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.251 , 0.289 0.267 , 0.299	Depositor DCC
R_{free} test set	1819 reflections (1.71%)	wwPDB-VP
Wilson B-factor (Å ²)	110.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10442	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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, O, K

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	0.23	0/2608	0.33	0/3524
1	C	0.15	0/2608	0.30	0/3524
2	B	0.17	0/2695	0.36	2/3649 (0.1%)
2	D	0.15	0/2662	0.32	1/3608 (0.0%)
All	All	0.18	0/10573	0.33	3/14305 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	264	ILE	CA-C-N	-8.23	113.34	121.65
2	B	264	ILE	C-N-CA	-8.23	113.34	121.65
2	D	265	PRO	N-CA-CB	6.59	110.17	103.25

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	2556	0	2582	60	0
1	C	2556	0	2582	20	0
2	B	2629	0	2620	30	0
2	D	2600	0	2588	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	25	16	0
3	C	48	0	25	2	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
5	B	1	0	0	0	0
All	All	10442	0	10422	132	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 6.

All (132) 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:264:ARG:HG2	1:A:264:ARG:HH11	1.38	0.88
2:B:220:ASP:HB3	2:B:223:PHE:HB2	1.63	0.79
1:A:55:GLY:HA3	3:A:1001:NAP:O3D	1.83	0.79
1:A:329:GLN:HB3	3:A:1001:NAP:N7A	1.99	0.77
2:B:260:ILE:O	2:B:264:ILE:HG13	1.86	0.76
2:B:58:LEU:HD12	2:B:64:LYS:HB3	1.70	0.73
1:A:264:ARG:HG2	1:A:264:ARG:NH1	1.99	0.72
1:C:217:TYR:HB2	1:C:225:VAL:HG21	1.72	0.71
2:B:260:ILE:O	2:B:264:ILE:CG1	2.40	0.70
1:A:329:GLN:HA	3:A:1001:NAP:N6A	2.07	0.69
1:A:58:VAL:HG22	1:A:270:TYR:OH	1.95	0.67
1:A:329:GLN:HB3	3:A:1001:NAP:C5A	2.23	0.67
1:A:58:VAL:HG11	1:A:264:ARG:HE	1.59	0.67
1:A:329:GLN:CA	3:A:1001:NAP:N6A	2.61	0.63
1:C:90:TYR:OH	1:C:118:LYS:NZ	2.31	0.62
1:C:216:GLU:HB2	1:C:243:TRP:CH2	2.36	0.61
1:A:212:CYS:SG	1:A:213:GLU:N	2.74	0.60
1:A:97:VAL:O	1:A:101:ASN:ND2	2.35	0.58
2:B:334:GLY:HA3	2:B:368:MET:HE1	1.85	0.58
2:B:264:ILE:HG22	2:B:264:ILE:O	2.04	0.58
2:B:349:GLU:HB2	2:B:352:SER:HB3	1.86	0.58
1:A:56:THR:HB	1:A:60:PHE:HB2	1.86	0.58
1:A:244:SER:HA	3:A:1001:NAP:O2A	2.04	0.58
1:A:236:ILE:HG13	1:A:238:VAL:HG23	1.84	0.58
1:A:217:TYR:HB2	1:A:225:VAL:HG21	1.86	0.57
2:D:351:ASP:O	2:D:353:GLN:NE2	2.38	0.57
1:A:261:PRO:O	1:A:262:TYR:HB2	2.02	0.57
1:A:56:THR:HG22	1:A:60:PHE:CD2	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:HG23	1:A:68:MET:H	1.71	0.56
1:A:219:MET:HE3	1:A:307:ALA:HA	1.87	0.56
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.15	0.56
1:A:57:TRP:O	1:A:59:THR:N	2.34	0.55
2:D:400:LEU:HB2	2:D:401:PRO:HD3	1.89	0.55
3:A:1001:NAP:H8A	3:A:1001:NAP:H3B	1.89	0.54
2:D:224:ILE:HG23	2:D:225:VAL:H	1.71	0.54
2:D:289:VAL:HA	2:D:292:PHE:HB3	1.88	0.54
1:A:263:SER:O	1:A:267:LEU:HG	2.07	0.54
2:B:312:ILE:HD13	2:B:413:TYR:HA	1.90	0.54
1:A:329:GLN:NE2	3:A:1001:NAP:C8A	2.71	0.54
2:D:154:GLU:OE1	2:D:240:ARG:NH2	2.40	0.54
1:A:259:ILE:HG13	1:A:274:LYS:HE3	1.90	0.53
1:A:222:ARG:NH1	1:A:226:GLU:OE2	2.42	0.53
2:B:59:LEU:O	2:B:65:ARG:NH1	2.41	0.53
2:B:57:THR:OG1	2:B:58:LEU:N	2.42	0.53
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.91	0.52
1:A:329:GLN:CA	3:A:1001:NAP:H61A	2.22	0.52
1:A:96:GLU:HB3	1:A:147:LEU:HG	1.91	0.52
1:A:264:ARG:HG3	1:A:273:LEU:CD2	2.40	0.52
2:B:330:PHE:HB3	2:B:397:THR:HG23	1.92	0.52
1:C:219:MET:HE3	1:C:307:ALA:HA	1.92	0.52
1:A:249:GLY:O	1:A:252:SER:OG	2.20	0.51
2:B:176:SER:O	2:B:299:ARG:NH1	2.44	0.51
1:C:199:TYR:OH	2:D:71:PRO:O	2.26	0.50
2:D:58:LEU:HD12	2:D:64:LYS:HB3	1.94	0.50
1:C:166:MET:HG2	1:C:197:GLU:HG2	1.94	0.50
2:B:224:ILE:HG23	2:B:225:VAL:HG23	1.93	0.49
1:A:328:GLU:OE1	1:A:328:GLU:N	2.46	0.49
1:A:55:GLY:CA	3:A:1001:NAP:O3D	2.57	0.48
1:C:55:GLY:HA3	3:C:401:NAP:O3D	2.13	0.48
1:C:75:LEU:HG	1:C:331:MET:HE2	1.95	0.48
1:A:74:THR:OG1	1:A:106:LYS:HE3	2.13	0.48
1:A:329:GLN:CB	3:A:1001:NAP:N6A	2.77	0.48
1:A:243:TRP:CE3	3:A:1001:NAP:C5N	2.96	0.48
1:A:120:PHE:O	1:A:129:ARG:HA	2.14	0.48
1:A:299:LEU:HD11	1:A:347:ILE:HG21	1.94	0.48
1:A:222:ARG:HH21	1:A:358:LYS:HA	1.79	0.48
1:C:52:LEU:HD13	1:C:322:LEU:HD11	1.95	0.47
2:D:188:PHE:CD2	2:D:188:PHE:N	2.81	0.47
1:A:65:THR:OG1	1:A:67:GLU:OE1	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ARG:NH1	2:D:104:VAL:O	2.45	0.47
2:B:327:LEU:HD11	2:B:398:ILE:HD13	1.97	0.47
1:A:329:GLN:C	3:A:1001:NAP:H61A	2.23	0.46
2:B:182:LEU:HA	2:B:185:LEU:HD13	1.97	0.46
1:A:122:GLY:HA3	1:A:135:HIS:HE1	1.80	0.46
1:A:56:THR:HG22	1:A:60:PHE:CG	2.50	0.46
2:B:396:LEU:O	2:B:400:LEU:HG	2.15	0.46
1:C:43:GLY:HA2	1:C:239:GLY:HA3	1.98	0.46
1:C:56:THR:HB	1:C:60:PHE:HB2	1.98	0.45
2:B:105:PRO:HG2	2:B:108:ILE:HD12	1.98	0.45
1:C:59:THR:HG21	1:C:324:ALA:O	2.17	0.45
2:D:327:LEU:HB2	2:D:401:PRO:HG2	1.99	0.45
1:A:338:GLN:O	1:A:341:PRO:HD2	2.17	0.45
2:B:294:ILE:O	2:B:297:ILE:HG22	2.17	0.45
1:A:57:TRP:C	1:A:59:THR:H	2.24	0.45
2:B:36:VAL:HG22	2:B:45:GLU:HG2	1.98	0.45
1:A:71:HIS:CD2	1:A:327:ALA:HB2	2.52	0.44
2:B:307:SER:HB3	2:B:310:LEU:HB2	1.98	0.44
2:D:303:LEU:O	2:D:307:SER:N	2.49	0.44
1:A:216:GLU:HB2	1:A:243:TRP:CZ2	2.53	0.44
1:A:235:LYS:NZ	2:B:76:TYR:OH	2.28	0.44
2:B:357:ILE:HB	2:B:358:PRO:HD3	2.00	0.44
1:C:71:HIS:CD2	1:C:327:ALA:HB2	2.52	0.44
1:A:329:GLN:HB3	3:A:1001:NAP:N6A	2.33	0.44
1:A:88:GLU:HA	1:A:96:GLU:OE2	2.18	0.43
1:A:152:VAL:O	1:A:182:ALA:HA	2.18	0.43
2:D:101:PRO:HB2	2:D:104:VAL:HG23	2.00	0.43
2:B:296:ARG:O	2:B:299:ARG:HD2	2.18	0.43
1:C:259:ILE:HG13	1:C:274:LYS:HE3	2.00	0.43
1:A:59:THR:HA	1:A:63:GLN:HB3	2.01	0.43
1:A:244:SER:OG	3:A:1001:NAP:O2N	2.25	0.43
1:A:56:THR:CG2	1:A:60:PHE:CD2	3.02	0.43
1:A:329:GLN:HB3	3:A:1001:NAP:C6A	2.49	0.43
1:C:290:LYS:HD2	1:C:290:LYS:HA	1.87	0.43
2:B:153:PHE:HB3	2:B:240:ARG:NH1	2.34	0.42
2:D:113:ILE:HG23	2:D:118:LEU:HD12	2.00	0.42
1:A:122:GLY:HA3	1:A:135:HIS:CE1	2.54	0.42
2:B:98:LEU:HD21	2:B:113:ILE:HD13	2.00	0.42
1:C:54:LEU:O	1:C:84:PHE:HA	2.19	0.42
1:C:151:TYR:CE1	1:C:183:MET:HE2	2.54	0.42
2:D:182:LEU:HA	2:D:185:LEU:CD1	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:PHE:H	2:D:188:PHE:HD2	1.66	0.42
2:D:296:ARG:HA	2:D:296:ARG:HD2	1.84	0.42
1:A:248:CYS:HB3	1:A:264:ARG:NH1	2.34	0.42
1:C:54:LEU:HD13	1:C:330:LEU:HD13	2.00	0.42
2:B:351:ASP:OD1	2:B:351:ASP:N	2.51	0.42
1:A:154:VAL:HG22	1:A:184:TYR:HB2	2.01	0.42
2:D:83:PRO:HB2	2:D:104:VAL:HG22	2.02	0.42
2:D:396:LEU:O	2:D:400:LEU:HG	2.19	0.42
1:A:151:TYR:CE1	1:A:183:MET:HE2	2.56	0.41
2:D:82:ARG:HB2	2:D:83:PRO:HD3	2.02	0.41
1:A:217:TYR:HB3	1:A:242:THR:HB	2.02	0.41
2:B:61:ASP:HB3	2:B:64:LYS:HB2	2.03	0.41
1:A:134:LYS:HE3	1:A:138:GLU:OE2	2.20	0.41
2:B:258:ILE:HG12	2:B:301:PHE:HB3	2.02	0.41
2:D:330:PHE:HB3	2:D:397:THR:HG23	2.02	0.41
1:C:123:GLY:HA3	1:C:128:GLU:OE1	2.21	0.41
2:D:80:ARG:NH1	2:D:112:GLU:OE2	2.54	0.41
1:A:330:LEU:O	1:A:334:ILE:HG13	2.21	0.41
2:B:113:ILE:HG23	2:B:118:LEU:HD12	2.03	0.41
1:C:325:SER:OG	3:C:401:NAP:O2X	2.31	0.41
2:D:258:ILE:HA	2:D:261:VAL:HG22	2.03	0.40
2:D:188:PHE:C	2:D:190:ASP:H	2.30	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	324/333 (97%)	314 (97%)	9 (3%)	1 (0%)	36 66
1	C	324/333 (97%)	312 (96%)	11 (3%)	1 (0%)	36 66
2	B	315/514 (61%)	291 (92%)	22 (7%)	2 (1%)	21 52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	315/514 (61%)	285 (90%)	28 (9%)	2 (1%)	21	52
All	All	1278/1694 (75%)	1202 (94%)	70 (6%)	6 (0%)	24	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
2	B	158	SER
1	C	120	PHE
2	D	264	ILE
2	D	131	GLY
2	B	131	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	273/280 (98%)	268 (98%)	5 (2%)	51	69
1	C	273/280 (98%)	272 (100%)	1 (0%)	84	83
2	B	284/459 (62%)	276 (97%)	8 (3%)	38	63
2	D	281/459 (61%)	276 (98%)	5 (2%)	51	69
All	All	1111/1478 (75%)	1092 (98%)	19 (2%)	53	70

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	119	ILE
1	A	212	CYS
1	A	222	ARG
1	A	264	ARG
2	B	152	LEU
2	B	157	GLU
2	B	223	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	260	ILE
2	B	264	ILE
2	B	265	PRO
2	B	310	LEU
2	B	379	THR
1	C	302	THR
2	D	152	LEU
2	D	225	VAL
2	D	235	PHE
2	D	311	GLN
2	D	353	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	221	GLN
1	A	286	GLN
1	A	329	GLN
1	A	333	ASN
2	B	53	GLN
2	B	103	ASN
2	B	253	ASN
1	C	63	GLN
1	C	71	HIS
1	C	204	GLN
1	C	286	GLN
1	C	293	GLN
1	C	326	ASN
1	C	333	ASN
2	D	47	GLN
2	D	148	GLN
2	D	253	ASN
2	D	353	GLN

5.3.3 RNA ⓘ

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 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	NAP	A	1001	-	50,52,52	1.23	5 (10%)	71,80,80	1.63	11 (15%)
3	NAP	C	401	-	50,52,52	2.52	15 (30%)	71,80,80	2.29	20 (28%)

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	NAP	A	1001	-	-	7/35/67/67	0/5/5/5
3	NAP	C	401	-	-	13/35/67/67	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	NAP	O4D-C1D	7.56	1.50	1.40
3	C	401	NAP	C7N-N7N	6.42	1.44	1.33
3	C	401	NAP	C8A-N9A	-5.38	1.28	1.37
3	C	401	NAP	PA-O3	4.86	1.64	1.59
3	C	401	NAP	PN-O3	4.84	1.64	1.59
3	C	401	NAP	C6A-N6A	4.56	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	NAP	C4A-N9A	-3.99	1.29	1.37
3	A	1001	NAP	C5A-C4A	3.77	1.45	1.39
3	C	401	NAP	O4B-C1B	3.37	1.49	1.42
3	C	401	NAP	C2D-C3D	-3.36	1.44	1.53
3	C	401	NAP	P2B-O2B	3.35	1.65	1.59
3	A	1001	NAP	C5A-N7A	-3.11	1.33	1.39
3	C	401	NAP	C3B-C2B	-2.86	1.46	1.53
3	C	401	NAP	O7N-C7N	-2.62	1.19	1.24
3	C	401	NAP	C5A-C4A	2.50	1.43	1.39
3	C	401	NAP	O4D-C4D	2.49	1.50	1.45
3	A	1001	NAP	C8A-N9A	-2.41	1.33	1.37
3	A	1001	NAP	C4A-N9A	-2.39	1.32	1.37
3	C	401	NAP	C4N-C3N	-2.22	1.36	1.39
3	A	1001	NAP	C5A-C6A	2.11	1.46	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	NAP	C4A-N9A-C8A	8.59	114.75	105.74
3	C	401	NAP	C4D-O4D-C1D	-7.19	103.34	109.92
3	C	401	NAP	N3A-C4A-N9A	6.45	138.13	127.17
3	A	1001	NAP	C5A-C4A-N3A	-6.21	118.17	126.72
3	C	401	NAP	C5A-C4A-N3A	-6.06	118.37	126.72
3	A	1001	NAP	N3A-C4A-N9A	4.86	135.43	127.17
3	C	401	NAP	C4A-C5A-N7A	-3.99	106.02	110.58
3	A	1001	NAP	C2B-C1B-N9A	-3.92	107.30	113.75
3	C	401	NAP	N9A-C8A-N7A	-3.78	108.58	113.94
3	A	1001	NAP	C2A-N3A-C4A	3.64	120.72	111.83
3	A	1001	NAP	C4A-C5A-N7A	-3.58	106.48	110.58
3	C	401	NAP	N3A-C2A-N1A	-3.45	123.36	128.58
3	C	401	NAP	C2A-N3A-C4A	3.39	120.11	111.83
3	C	401	NAP	C2D-C3D-C4D	3.26	108.91	102.61
3	C	401	NAP	C3N-C7N-N7N	2.98	121.41	117.74
3	A	1001	NAP	N3A-C2A-N1A	-2.91	124.18	128.58
3	A	1001	NAP	C4A-N9A-C8A	2.75	108.62	105.74
3	A	1001	NAP	C5A-N7A-C8A	2.70	107.69	103.45
3	C	401	NAP	C2B-C3B-C4B	2.68	107.75	101.99
3	C	401	NAP	C3B-C2B-C1B	2.66	107.90	102.81
3	A	1001	NAP	C5N-C4N-C3N	-2.59	117.81	120.36
3	C	401	NAP	C5D-C4D-C3D	-2.55	106.03	115.21
3	C	401	NAP	C5A-N7A-C8A	2.35	107.15	103.45
3	C	401	NAP	O7N-C7N-N7N	-2.34	119.23	122.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	NAP	C5B-C4B-C3B	-2.29	106.98	115.21
3	A	1001	NAP	O3X-P2B-O2X	2.25	116.22	107.80
3	A	1001	NAP	N9A-C8A-N7A	-2.21	110.80	113.94
3	C	401	NAP	C1B-N9A-C8A	-2.17	122.28	127.09
3	C	401	NAP	C5A-C4A-N9A	-2.13	103.49	105.81
3	C	401	NAP	O4B-C4B-C3B	2.11	109.35	105.15
3	C	401	NAP	O3D-C3D-C2D	-2.04	105.28	111.82

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	NAP	O4D-C4D-C5D-O5D
3	C	401	NAP	C5B-O5B-PA-O1A
3	C	401	NAP	C5B-O5B-PA-O2A
3	C	401	NAP	C5B-O5B-PA-O3
3	C	401	NAP	C5D-O5D-PN-O3
3	C	401	NAP	C5D-O5D-PN-O1N
3	A	1001	NAP	C2N-C3N-C7N-O7N
3	A	1001	NAP	C2N-C3N-C7N-N7N
3	C	401	NAP	C3B-C4B-C5B-O5B
3	A	1001	NAP	C4N-C3N-C7N-N7N
3	A	1001	NAP	C4N-C3N-C7N-O7N
3	C	401	NAP	O4B-C4B-C5B-O5B
3	A	1001	NAP	C3D-C4D-C5D-O5D
3	C	401	NAP	PN-O3-PA-O5B
3	A	1001	NAP	C2B-O2B-P2B-O1X
3	C	401	NAP	C5D-O5D-PN-O2N
3	C	401	NAP	C2B-O2B-P2B-O2X
3	C	401	NAP	O4D-C1D-N1N-C6N
3	C	401	NAP	C3B-C2B-O2B-P2B
3	C	401	NAP	C2B-O2B-P2B-O1X

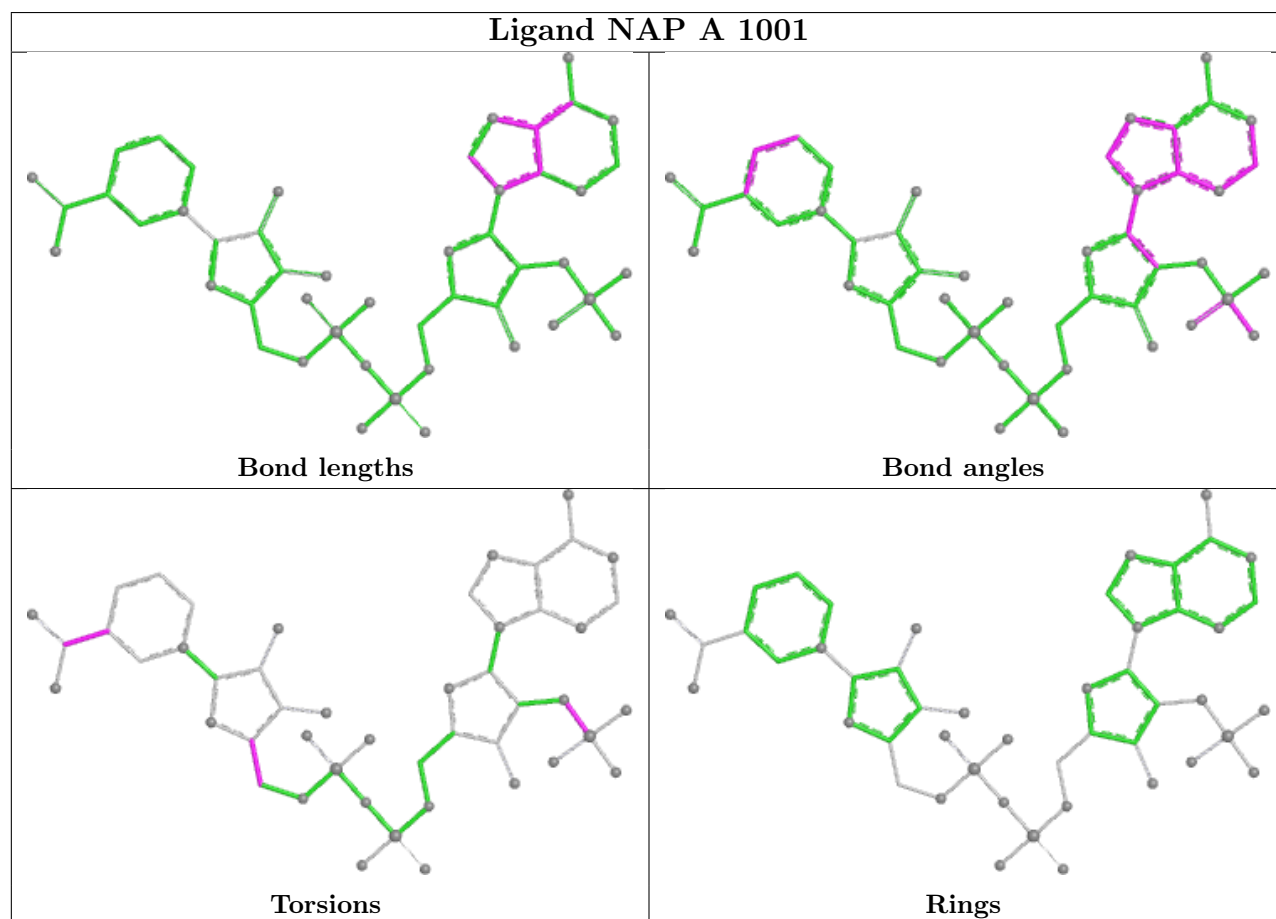
There are no ring outliers.

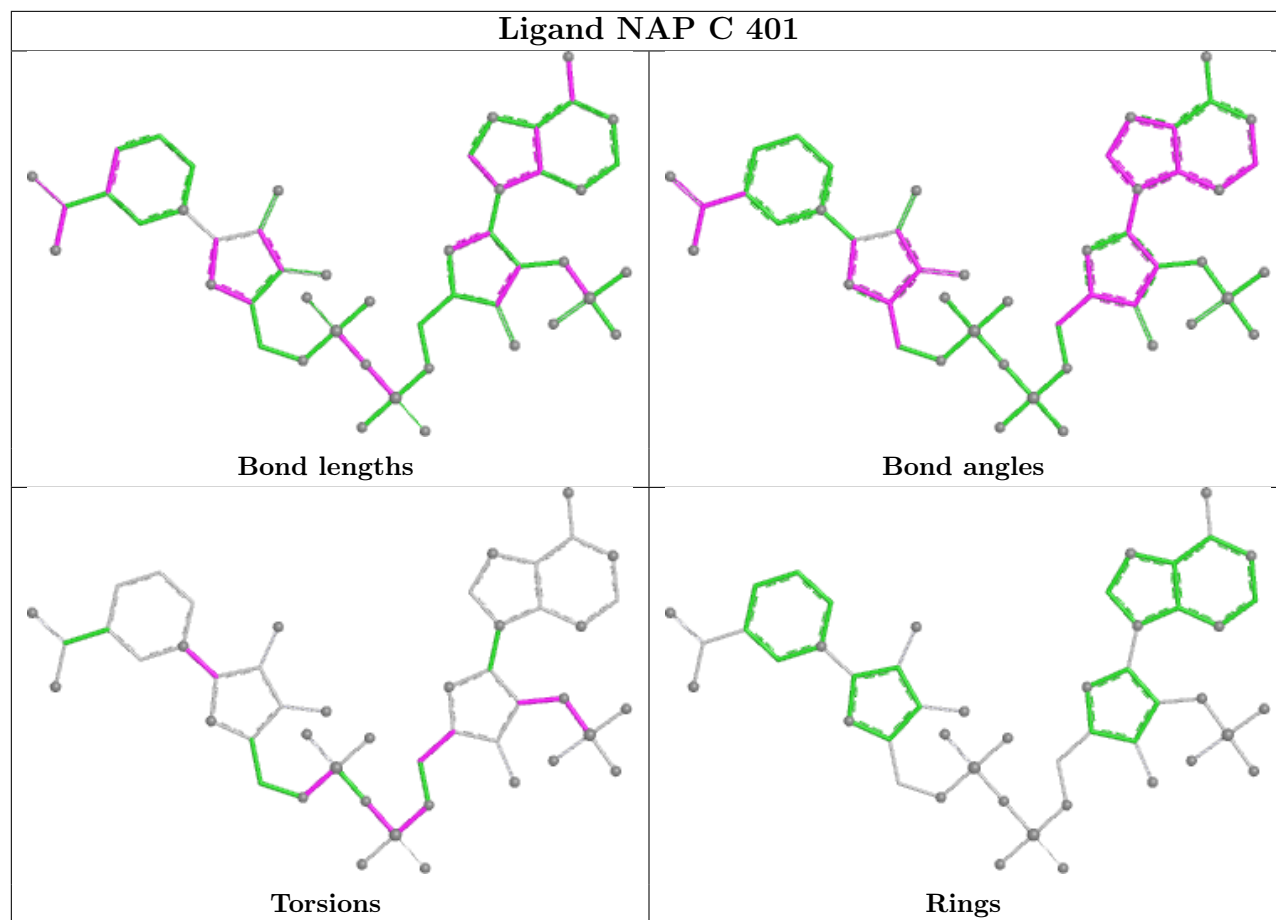
2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	NAP	16	0
3	C	401	NAP	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

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	326/333 (97%)	0.20	10 (3%) 51 35	67, 92, 133, 164	0
1	C	325/333 (97%)	0.21	8 (2%) 58 39	65, 90, 121, 147	0
2	B	325/514 (63%)	0.58	32 (9%) 13 11	81, 141, 208, 223	0
2	D	324/514 (63%)	1.16	62 (19%) 3 3	75, 176, 250, 280	0
All	All	1300/1694 (76%)	0.53	112 (8%) 16 12	65, 108, 228, 280	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	369	THR	10.0
2	D	368	MET	8.8
2	D	392	ILE	7.9
2	D	394	GLY	7.6
2	D	370	THR	7.5
2	B	368	MET	6.6
1	A	145	GLU	6.2
2	D	391	ALA	6.1
2	B	186	PRO	5.7
2	B	395	VAL	5.4
2	D	291	ILE	5.3
2	D	395	VAL	5.3
2	D	238	LEU	5.1
1	A	323	GLY	5.1
2	B	369	THR	5.1
2	D	393	ALA	5.0
2	B	392	ILE	4.9
2	D	328	ILE	4.7
2	D	396	LEU	4.7
2	B	187	ILE	4.7
2	D	398	ILE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	269	THR	4.5
2	B	370	THR	4.3
2	B	394	GLY	4.3
2	D	324	LEU	4.2
2	D	376	MET	4.0
2	B	374	GLY	3.9
2	D	220	ASP	3.9
2	B	389	LEU	3.8
2	D	389	LEU	3.7
2	D	224	ILE	3.7
2	B	52	ALA	3.6
2	B	102	VAL	3.5
2	D	400	LEU	3.5
2	D	270	ILE	3.5
2	B	398	ILE	3.4
2	D	397	THR	3.3
2	D	332	PHE	3.3
2	D	186	PRO	3.3
2	D	106	LEU	3.3
2	D	317	LEU	3.2
2	D	187	ILE	3.2
2	D	231	ILE	3.2
2	B	377	THR	3.2
2	D	330	PHE	3.1
2	D	356	SER	3.0
2	B	95	GLY	3.0
2	B	328	ILE	2.9
2	D	327	LEU	2.9
2	B	324	LEU	2.9
2	B	238	LEU	2.9
2	D	357	ILE	2.9
2	B	393	ALA	2.8
2	D	268	VAL	2.8
2	D	155	TYR	2.8
1	C	204	GLN	2.8
2	B	331	LEU	2.8
1	C	145	GLU	2.7
1	A	319	SER	2.7
2	D	373	TYR	2.7
1	A	317	VAL	2.7
2	B	294	ILE	2.7
2	D	375	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	372	GLY	2.6
2	B	32	SER	2.6
1	A	150	GLU	2.6
1	C	262	TYR	2.6
2	D	399	ALA	2.6
2	D	343	TYR	2.5
2	D	32	SER	2.5
2	D	43	ARG	2.5
1	A	343	LEU	2.5
2	D	359	ASP	2.5
2	D	308	LYS	2.5
2	D	179	SER	2.5
2	D	360	ALA	2.5
2	D	190	ASP	2.5
1	A	219	MET	2.5
2	D	367	THR	2.5
1	C	256	ASP	2.4
2	D	164	ILE	2.4
1	C	150	GLU	2.4
2	B	373	TYR	2.4
2	D	60	GLY	2.4
1	C	281	GLU	2.4
2	D	378	PRO	2.4
2	B	144	GLU	2.3
2	D	289	VAL	2.3
1	C	293	GLN	2.3
2	D	374	GLY	2.3
2	B	171	MET	2.3
1	A	242	THR	2.3
2	B	292	PHE	2.2
2	D	223	PHE	2.2
1	A	262	TYR	2.2
2	D	151	LEU	2.2
2	B	266	TYR	2.2
2	D	353	GLN	2.2
2	B	327	LEU	2.2
2	D	355	PRO	2.2
2	B	145	PHE	2.2
2	D	292	PHE	2.2
2	B	263	ILE	2.1
2	D	331	LEU	2.1
1	A	85	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	239	VAL	2.1
1	C	144	LEU	2.1
2	D	132	TYR	2.1
2	D	221	PRO	2.1
2	B	376	MET	2.0
2	D	252	THR	2.0
2	D	266	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](#)

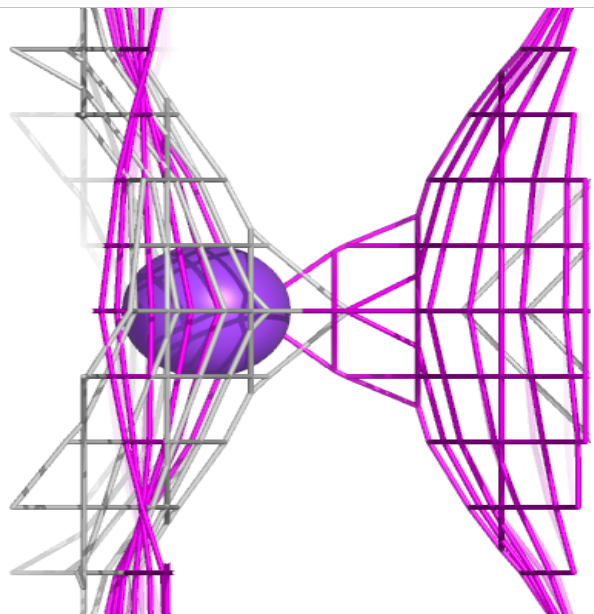
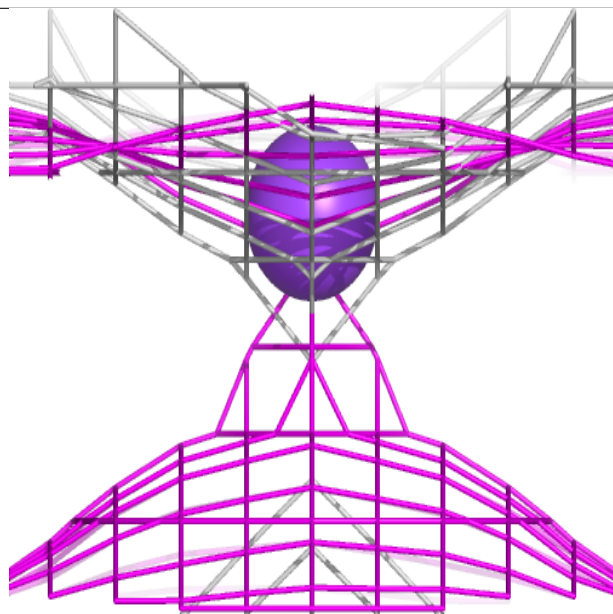
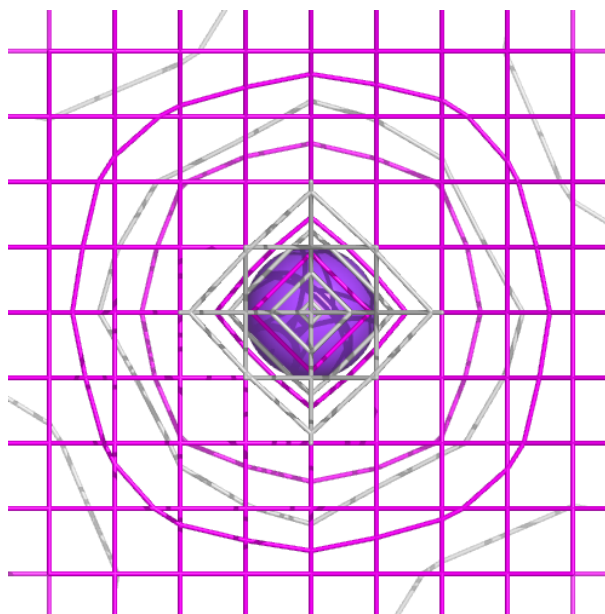
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	O	B	503	1/1	-0.30	0.80	154,154,154,154	1
4	K	D	502	1/1	0.47	0.34	158,158,158,158	1
4	K	B	501	1/1	0.68	0.23	118,118,118,118	1
3	NAP	A	1001	48/48	0.84	0.14	20,20,20,20	0
3	NAP	C	401	48/48	0.88	0.10	79,96,118,121	0
4	K	B	502	1/1	0.94	0.05	122,122,122,122	1
4	K	D	501	1/1	0.99	0.07	159,159,159,159	1

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.

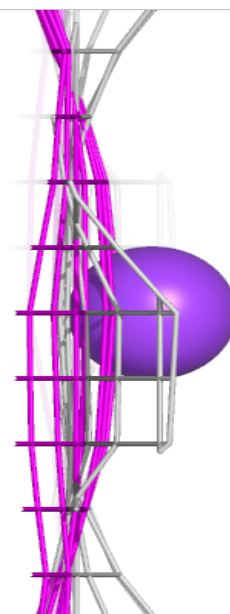
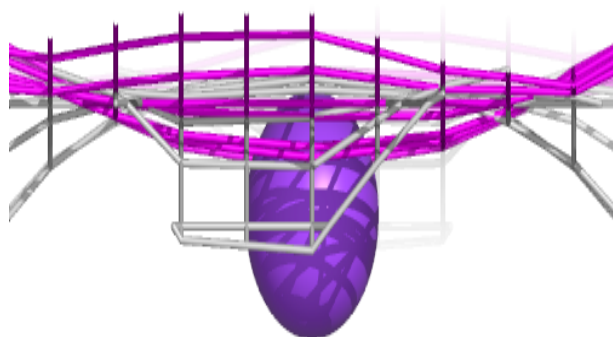
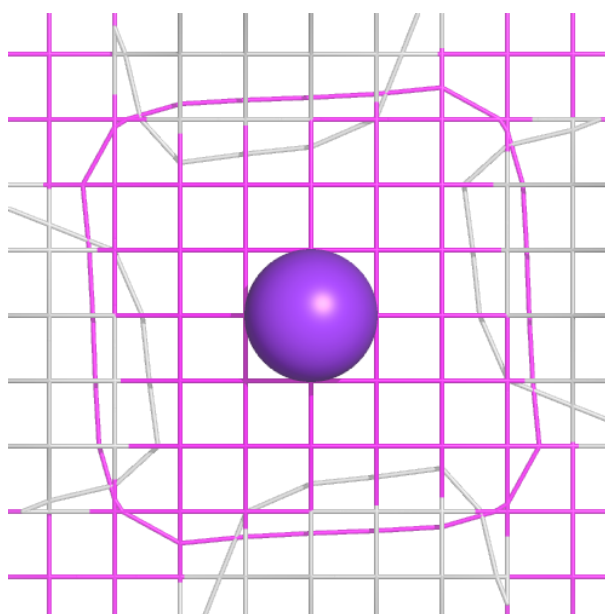
Electron density around K D 502:

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



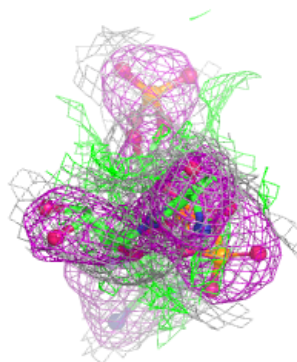
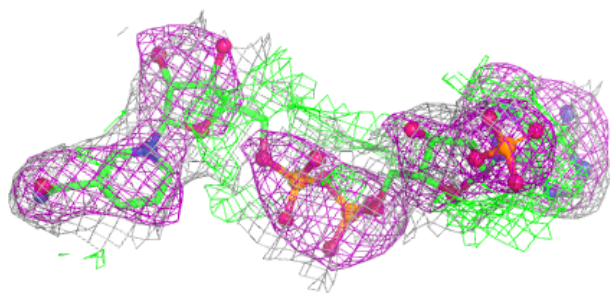
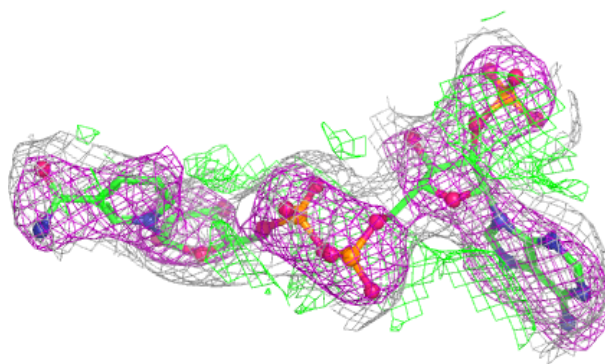
Electron density around K B 501:

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

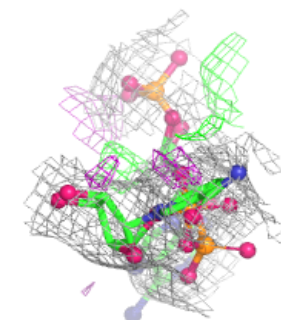
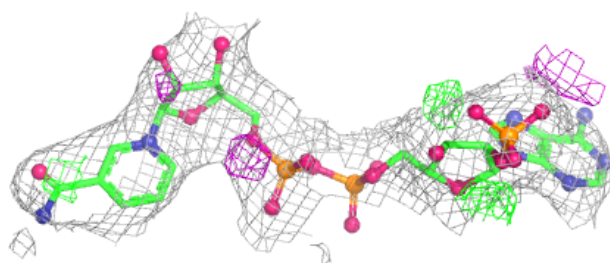
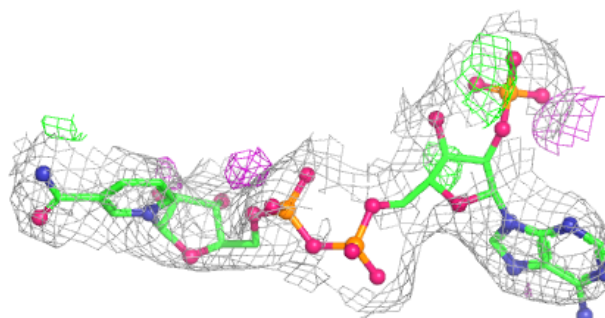


Electron density around NAP A 1001:

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

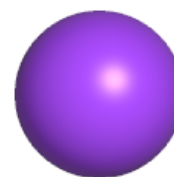
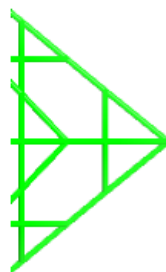
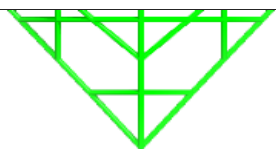
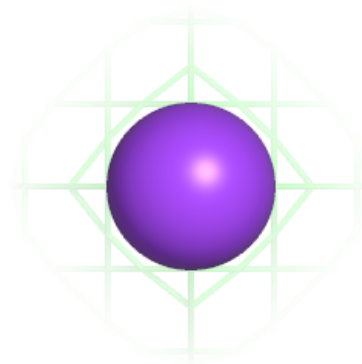
**Electron density around NAP C 401:**

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

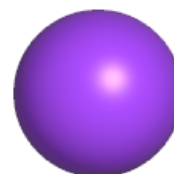
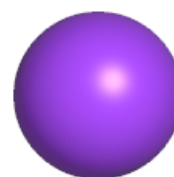


Electron density around K B 502:

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

**Electron density around K D 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.