Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:24 PM EDT

PDB ID	:	7SIT
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:

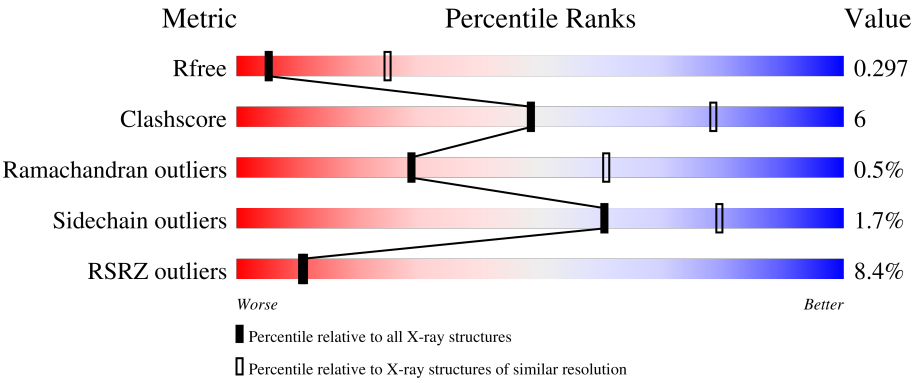
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 <=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	4% 79% 18%
1	C	333	3% 89% 9%
2	B	514	7% 53% 10% 37%
2	D	514	10% 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 (i)

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 2556	C 1627	N 443	O 470	S 16	0	0	0
1	C	326	Total 2556	C 1627	N 443	O 470	S 16	12	0	0

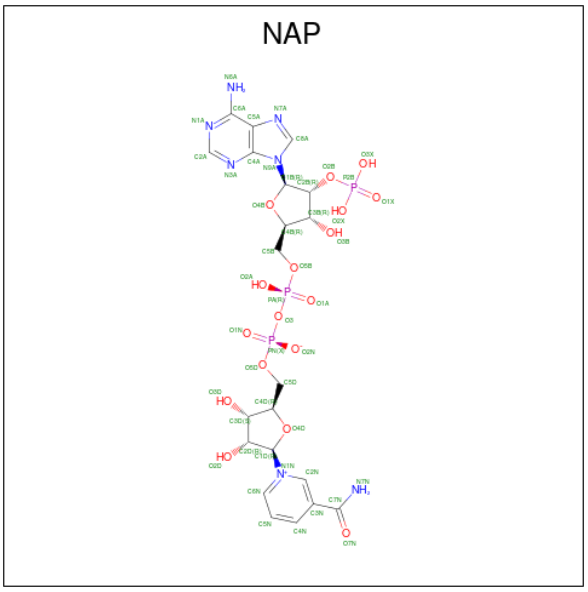
There are 2 discrepancies between the modelled and reference sequences:

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 2629	C 1737	N 422	O 457	S 13	0	0	0
2	D	325	Total 2600	C 1716	N 413	O 458	S 13	11	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 4 is POTASSIUM ION (three-letter code: 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 (three-letter code: O) (formula: O).

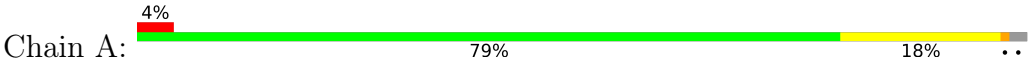
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 1 1	0	0

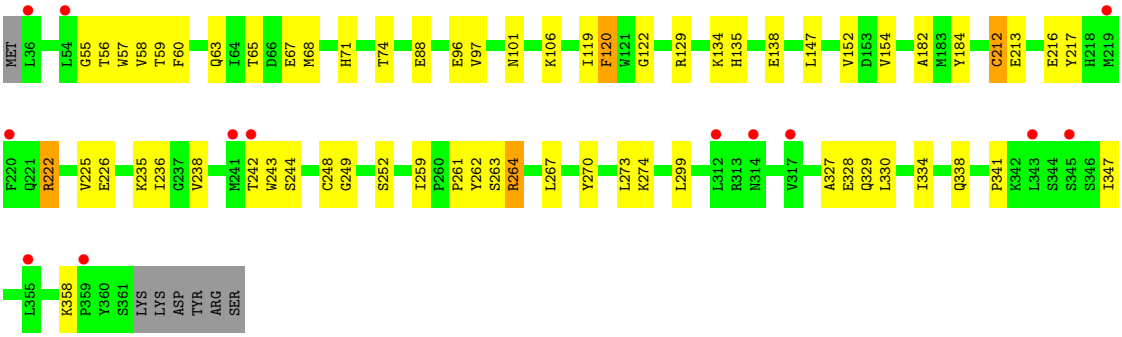
3 Residue-property plots (i)

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

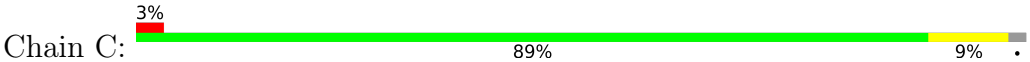
Chain A:

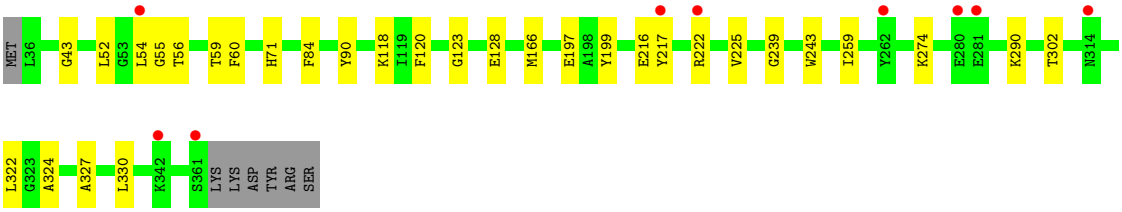




• Molecule 1: Voltage-gated potassium channel subunit beta-2

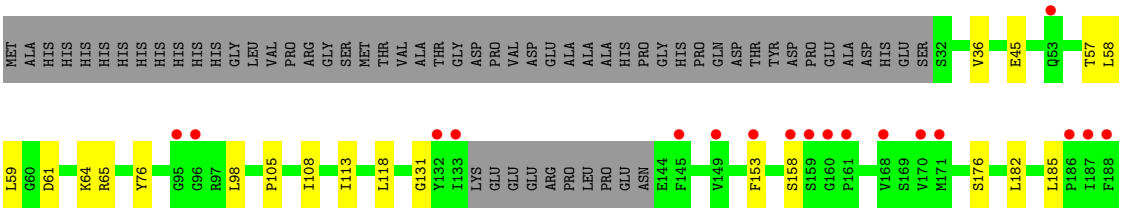
Chain C:

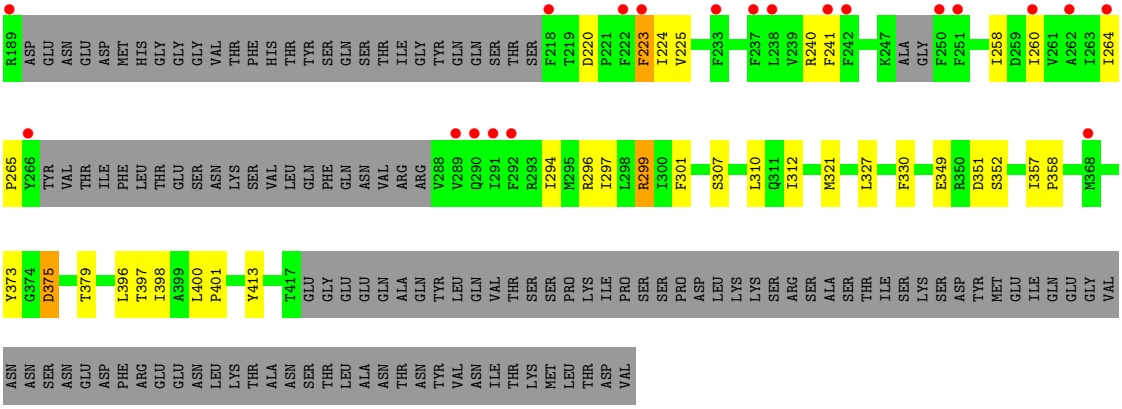




• Molecule 2: Voltage gated potassium channel Kv1.2-Kv2.1

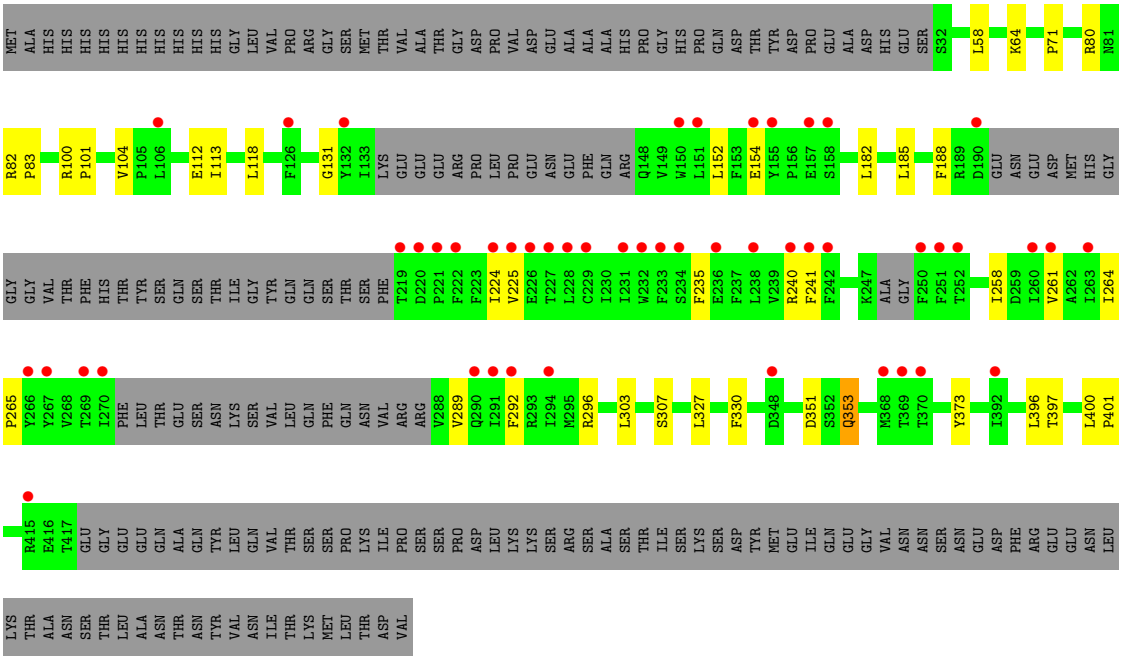
Chain B:





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

Chain D:



4 Data and refinement statistics (i)

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) 99.4 (49.16-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.251 , 0.289 0.263 , 0.297	Depositor DCC
R_{free} test set	1819 reflections (5.09%)	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)	0.32 , 99.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, K, O

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	0.30	0/2608	0.42	0/3524
1	C	0.27	0/2608	0.42	0/3524
2	B	0.28	0/2695	0.39	0/3649
2	D	0.26	0/2662	0.39	1/3608 (0.0%)
All	All	0.28	0/10573	0.40	1/14305 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	265	PRO	N-CA-CB	5.72	110.17	103.30

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	57	0
1	C	2556	0	2582	16	0
2	B	2629	0	2620	30	0
2	D	2600	0	2588	22	0
3	A	48	0	25	16	0
3	C	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	124	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 (124) 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: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
1:A:65:THR:HG23	1:A:68:MET:H	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:244:SER:OG	3:A:1001:NAP:O2N	2.25	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
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: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
2:D:182:LEU:HA	2:D:185:LEU:CD1	2.49	0.42
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
1:A:329:GLN:C	3:A:1001:NAP:H61A	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:258:ILE:HA	2:D:261:VAL:HG22	2.03	0.40
2:B:375:ASP:N	2:B:375:ASP:OD1	2.54	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%)	41	71
1	C	324/333 (97%)	312 (96%)	11 (3%)	1 (0%)	41	71
2	B	315/514 (61%)	291 (92%)	22 (7%)	2 (1%)	25	57
2	D	315/514 (61%)	285 (90%)	28 (9%)	2 (1%)	25	57
All	All	1278/1694 (75%)	1202 (94%)	70 (6%)	6 (0%)	29	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
2	B	158	SER
1	C	120	PHE

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Mol	Chain	Res	Type
2	D	264	ILE
2	D	131	GLY
2	B	131	GLY

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	273/280 (98%)	269 (98%)	4 (2%)	65	81
1	C	273/280 (98%)	271 (99%)	2 (1%)	84	91
2	B	284/459 (62%)	276 (97%)	8 (3%)	43	71
2	D	281/459 (61%)	276 (98%)	5 (2%)	59	79
All	All	1111/1478 (75%)	1092 (98%)	19 (2%)	60	79

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

Mol	Chain	Res	Type
1	A	119	ILE
1	A	212	CYS
1	A	222	ARG
1	A	264	ARG
2	B	223	PHE
2	B	241	PHE
2	B	265	PRO
2	B	299	ARG
2	B	321	MET
2	B	373	TYR
2	B	375	ASP
2	B	379	THR
1	C	222	ARG
1	C	302	THR
2	D	152	LEU
2	D	235	PHE
2	D	241	PHE
2	D	353	GLN

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Mol	Chain	Res	Type
2	D	373	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	221	GLN
1	A	228	GLN
1	A	286	GLN
1	A	329	GLN
2	B	53	GLN
1	C	71	HIS
1	C	204	GLN
1	C	286	GLN
1	C	326	ASN
1	C	333	ASN
2	D	53	GLN
2	D	148	GLN
2	D	256	ASN
2	D	353	GLN
2	D	408	ASN

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

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	C	401	-	45,52,52	2.27	10 (22%)	56,80,80	1.58	15 (26%)
3	NAP	A	1001	-	45,52,52	0.94	0	56,80,80	1.24	6 (10%)

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	C	401	-	-	12/31/67/67	0/5/5/5
3	NAP	A	1001	-	-	7/31/67/67	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	NAP	O4D-C1D	6.98	1.50	1.41
3	C	401	NAP	O4B-C1B	6.24	1.49	1.41
3	C	401	NAP	C7N-N7N	6.19	1.44	1.33
3	C	401	NAP	C2D-C1D	-3.63	1.48	1.53
3	C	401	NAP	C2D-C3D	-3.31	1.44	1.53
3	C	401	NAP	C6A-N6A	3.24	1.45	1.34
3	C	401	NAP	P2B-O2B	3.22	1.65	1.59
3	C	401	NAP	C3B-C2B	-2.79	1.46	1.52
3	C	401	NAP	O7N-C7N	-2.55	1.19	1.24
3	C	401	NAP	O4D-C4D	2.47	1.50	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	NAP	PN-O3-PA	-4.23	118.30	132.83
3	C	401	NAP	C3D-C2D-C1D	3.86	106.79	100.98
3	C	401	NAP	N3A-C2A-N1A	-3.41	123.36	128.68
3	C	401	NAP	C4A-C5A-N7A	-3.24	106.02	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	NAP	C2D-C3D-C4D	3.22	108.91	102.64
3	C	401	NAP	PN-O3-PA	-3.13	122.07	132.83
3	C	401	NAP	C3N-C7N-N7N	3.05	121.41	117.75
3	A	1001	NAP	C3D-C2D-C1D	2.91	105.37	100.98
3	A	1001	NAP	N3A-C2A-N1A	-2.88	124.18	128.68
3	A	1001	NAP	C4A-C5A-N7A	-2.80	106.48	109.40
3	C	401	NAP	C3B-C2B-C1B	2.67	107.90	102.89
3	C	401	NAP	C2B-C3B-C4B	2.65	107.75	101.99
3	C	401	NAP	C5D-C4D-C3D	-2.44	106.03	115.18
3	C	401	NAP	O7N-C7N-N7N	-2.36	119.23	122.58
3	A	1001	NAP	O3X-P2B-O2X	2.25	116.22	107.64
3	C	401	NAP	C5B-C4B-C3B	-2.19	106.98	115.18
3	C	401	NAP	O4B-C4B-C3B	2.14	109.35	105.11
3	A	1001	NAP	C5N-C4N-C3N	-2.14	117.81	120.34
3	C	401	NAP	O4D-C1D-C2D	2.11	110.02	106.93
3	C	401	NAP	C1B-N9A-C4A	-2.10	122.95	126.64
3	C	401	NAP	O3D-C3D-C2D	-2.02	105.28	111.82

There are no chirality outliers.

All (19) torsion outliers are listed below:

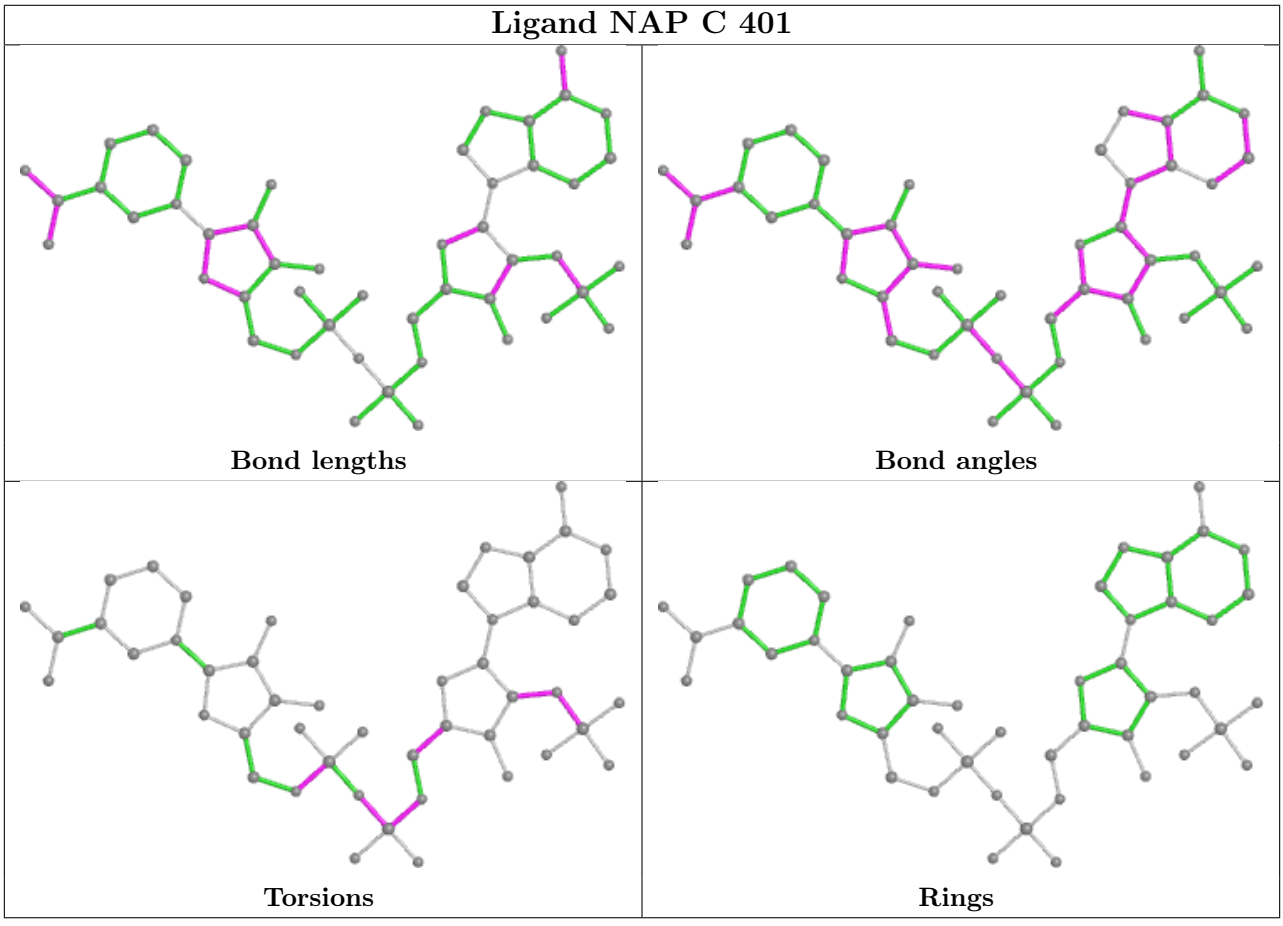
Mol	Chain	Res	Type	Atoms
3	A	1001	NAP	O4D-C4D-C5D-O5D
3	C	401	NAP	C5B-O5B-PA-O1A
3	C	401	NAP	C5B-O5B-PA-O2A
3	C	401	NAP	C3B-C4B-C5B-O5B
3	C	401	NAP	C2B-O2B-P2B-O2X
3	C	401	NAP	C5D-O5D-PN-O3
3	C	401	NAP	C5D-O5D-PN-O1N
3	A	1001	NAP	C2N-C3N-C7N-O7N
3	A	1001	NAP	C2N-C3N-C7N-N7N
3	A	1001	NAP	C4N-C3N-C7N-O7N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

There are no ring outliers.

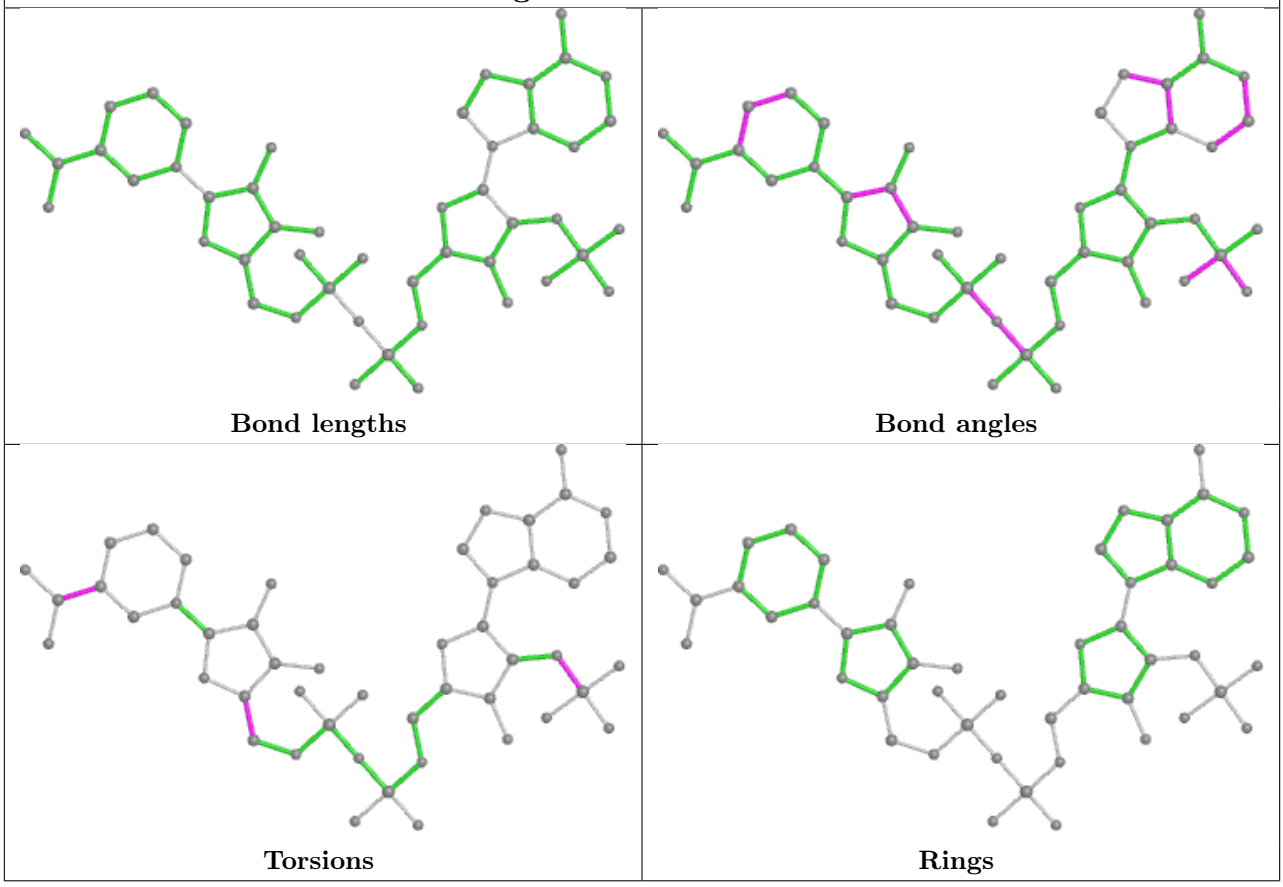
2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	NAP	1	0
3	A	1001	NAP	16	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand NAP A 1001



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, 95^{th} 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%)	0.35	13 (3%) 38 37	67, 92, 133, 164	0
1	C	325/333 (97%)	0.36	9 (2%) 53 51	65, 90, 121, 147	0
2	B	325/514 (63%)	0.58	38 (11%) 4 3	81, 141, 208, 223	0
2	D	324/514 (63%)	0.79	49 (15%) 2 1	75, 176, 250, 280	0
All	All	1300/1694 (76%)	0.52	109 (8%) 11 11	65, 108, 228, 280	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	187	ILE	7.1
2	D	291	ILE	7.0
2	D	231	ILE	6.1
2	B	251	PHE	6.1
2	D	236	GLU	5.6
2	D	368	MET	5.6
2	D	270	ILE	5.4
2	D	229	CYS	5.2
2	B	145	PHE	5.1
2	D	242	PHE	5.1
2	B	186	PRO	5.1
2	D	132	TYR	4.7
2	D	221	PRO	4.7
2	D	224	ILE	4.7
2	D	252	THR	4.7
2	D	233	PHE	4.6
2	D	190	ASP	4.6
2	D	220	ASP	4.5
2	B	238	LEU	4.5
2	B	291	ILE	4.4
2	B	264	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	219	MET	4.3
2	B	171	MET	4.2
2	D	155	TYR	4.2
2	D	158	SER	4.2
2	B	188	PHE	4.2
2	D	241	PHE	4.0
2	B	250	PHE	4.0
2	D	151	LEU	3.8
2	D	225	VAL	3.8
2	B	132	TYR	3.8
2	D	219	THR	3.8
1	A	343	LEU	3.8
2	D	150	TRP	3.7
2	B	189	ARG	3.7
2	B	161	PRO	3.6
2	B	266	TYR	3.6
2	D	232	TRP	3.6
2	B	159	SER	3.6
2	D	238	LEU	3.5
2	D	290	GLN	3.5
2	B	233	PHE	3.5
2	D	369	THR	3.4
2	D	266	TYR	3.4
2	D	269	THR	3.4
2	D	228	LEU	3.3
2	D	250	PHE	3.3
2	B	292	PHE	3.1
2	B	262	ALA	3.1
2	D	251	PHE	3.0
2	D	227	THR	3.0
1	A	220	PHE	3.0
1	C	281	GLU	3.0
2	D	370	THR	3.0
2	B	168	VAL	3.0
2	D	348	ASP	3.0
1	A	36	LEU	2.9
2	D	157	GLU	2.9
1	C	54	LEU	2.9
1	C	280	GLU	2.8
1	C	222	ARG	2.8
2	B	260	ILE	2.8
2	D	222	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	263	ILE	2.7
1	C	262	TYR	2.7
2	B	237	PHE	2.6
2	B	368	MET	2.6
2	B	96	GLY	2.5
2	D	260	ILE	2.5
2	D	392	ILE	2.5
1	A	359	PRO	2.5
2	B	160	GLY	2.5
2	D	126	PHE	2.5
1	A	355	LEU	2.5
2	B	53	GLN	2.5
2	B	241	PHE	2.4
1	A	242	THR	2.4
1	A	317	VAL	2.3
1	C	217	TYR	2.3
2	D	294	ILE	2.3
1	A	54	LEU	2.2
2	D	106	LEU	2.2
1	C	342	LYS	2.2
2	B	242	PHE	2.2
2	B	153	PHE	2.2
2	B	95	GLY	2.2
2	D	261	VAL	2.2
2	B	223	PHE	2.2
1	A	312	LEU	2.2
2	B	133	ILE	2.2
2	B	289	VAL	2.2
2	D	154	GLU	2.2
2	D	292	PHE	2.1
2	D	240	ARG	2.1
2	D	415	ARG	2.1
2	B	218	PHE	2.1
2	B	222	PHE	2.1
1	C	314	ASN	2.1
1	A	345	SER	2.1
1	A	241	MET	2.1
1	A	314	ASN	2.1
2	D	226	GLU	2.1
2	B	149	VAL	2.1
2	B	158	SER	2.1
2	D	267	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	290	GLN	2.0
2	B	170	VAL	2.0
1	C	361	SER	2.0
2	D	234	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

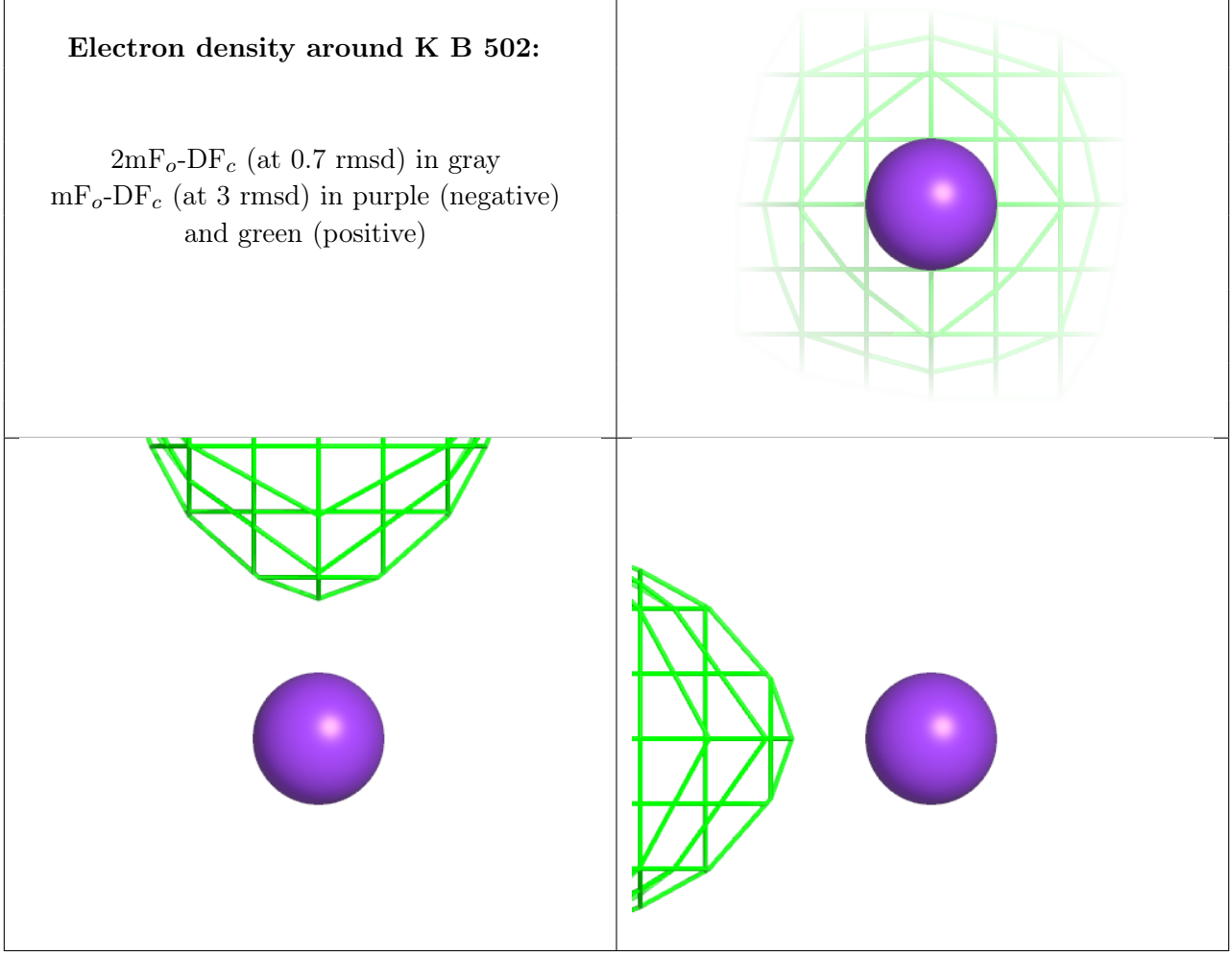
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.07	1.47	154,154,154,154	1
4	K	B	502	1/1	0.39	0.20	122,122,122,122	1
4	K	D	501	1/1	0.85	0.07	159,159,159,159	1
4	K	D	502	1/1	0.86	0.24	158,158,158,158	1
3	NAP	C	401	48/48	0.93	0.24	79,96,118,121	0
3	NAP	A	1001	48/48	0.94	0.21	20,20,20,20	0
4	K	B	501	1/1	0.98	0.34	118,118,118,118	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.

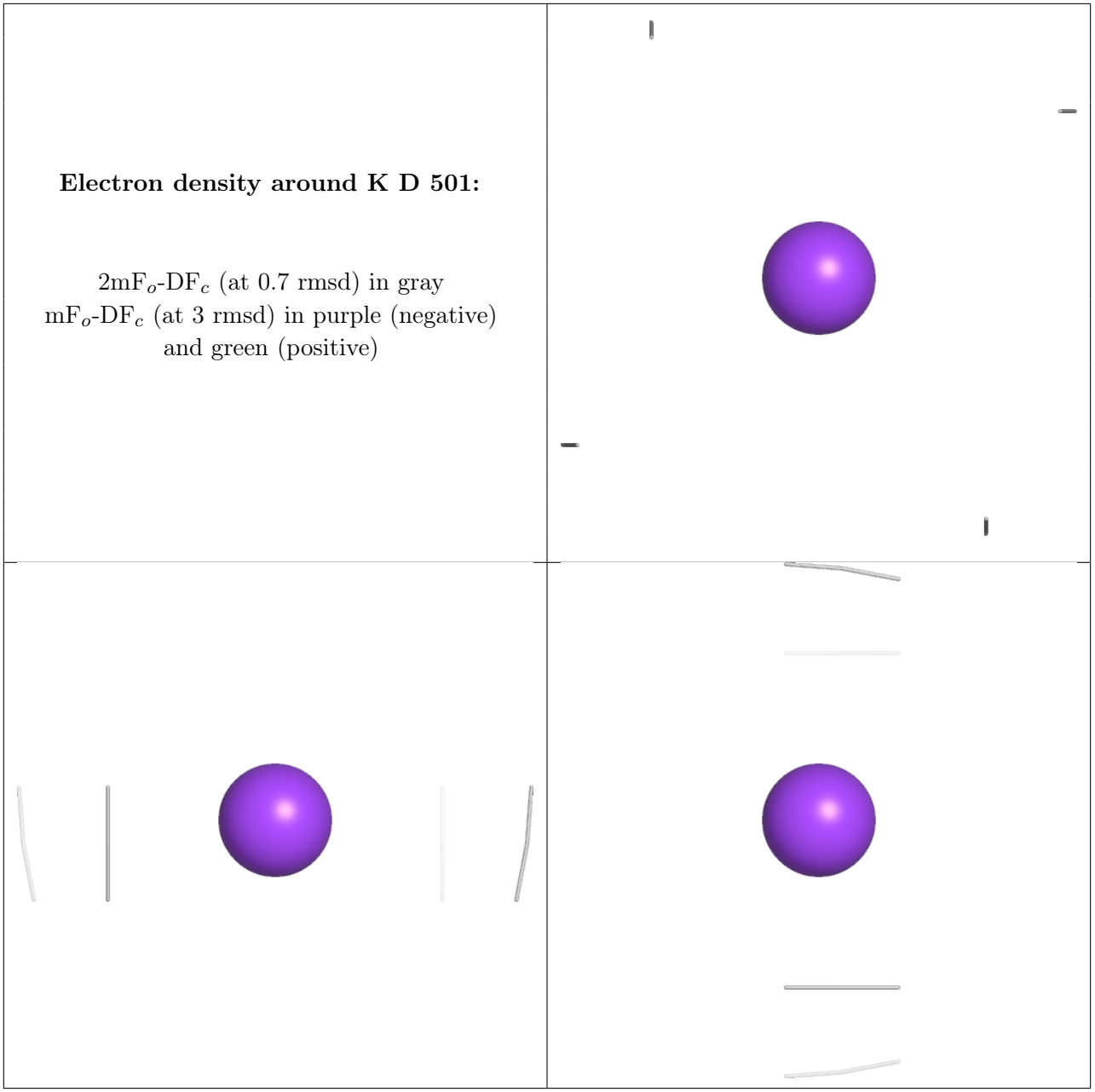
Electron density around K B 502:

$2mF_o$-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)



Electron density around K D 502:

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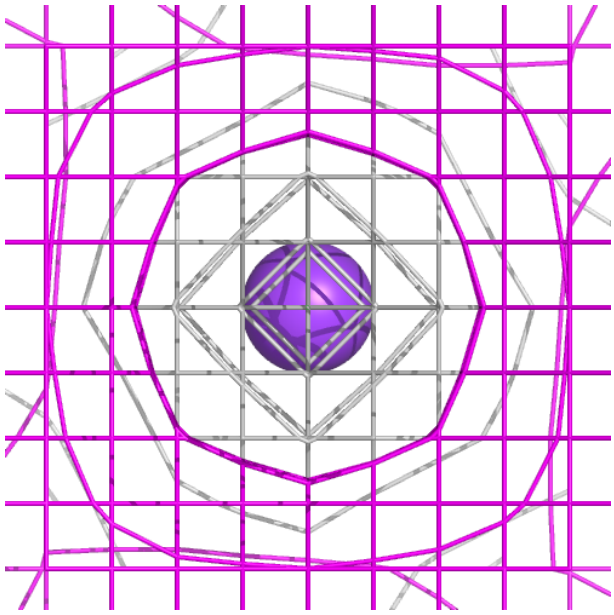
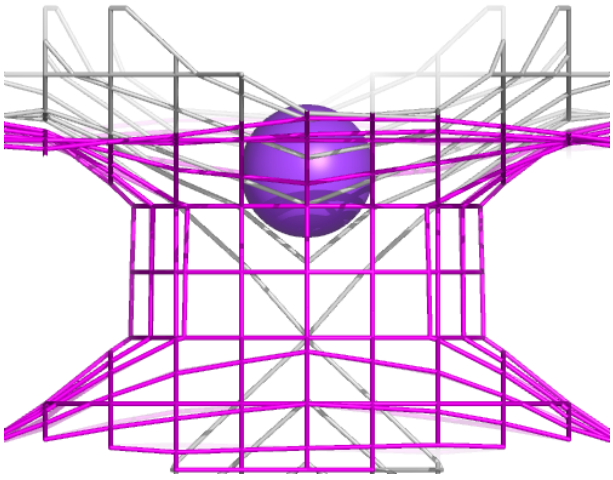
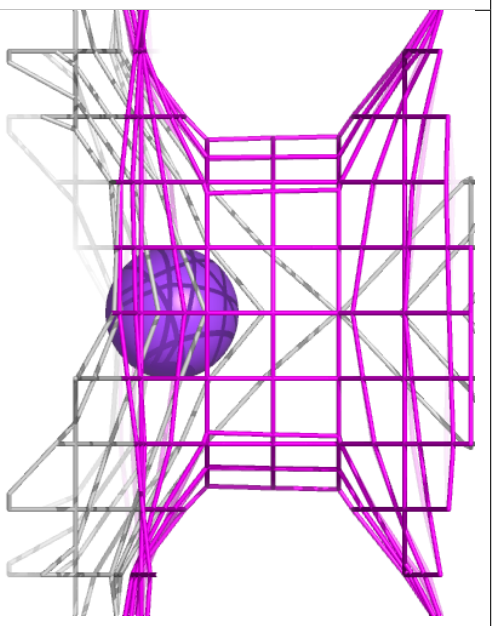
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

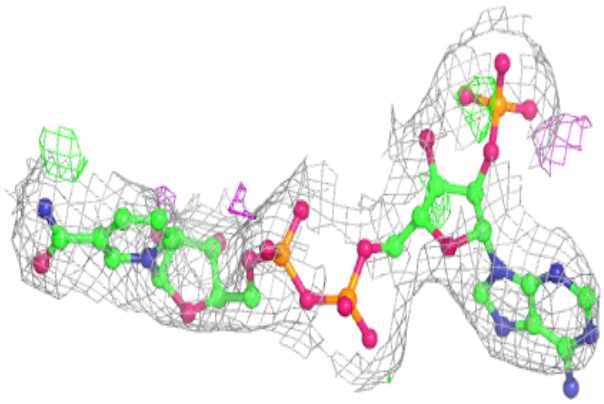


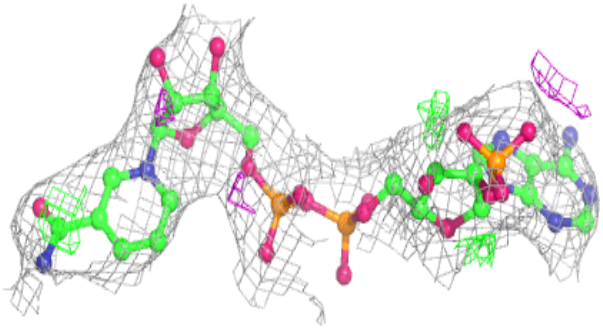


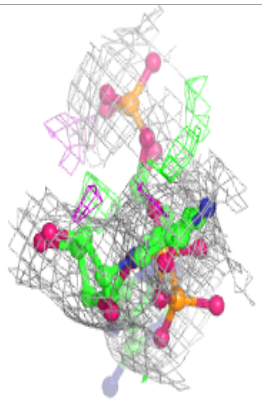


Electron density around NAP C 401:

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

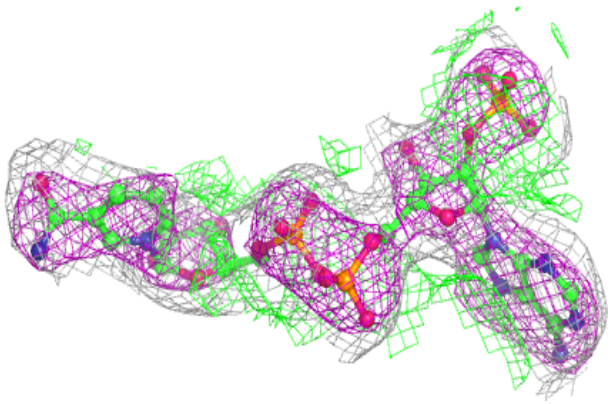


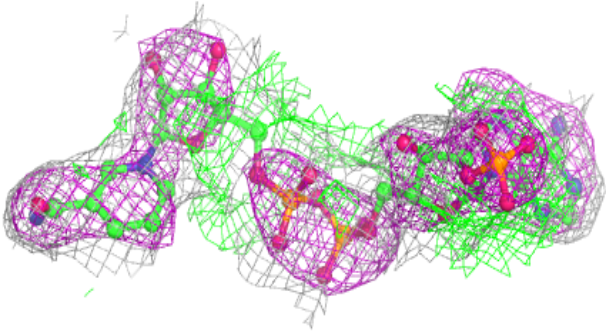


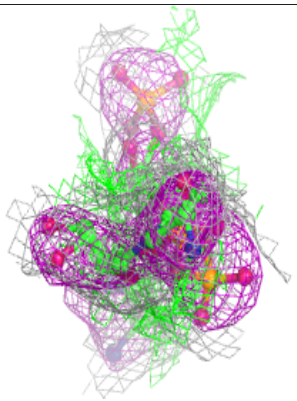


Electron density around NAP A 1001:

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

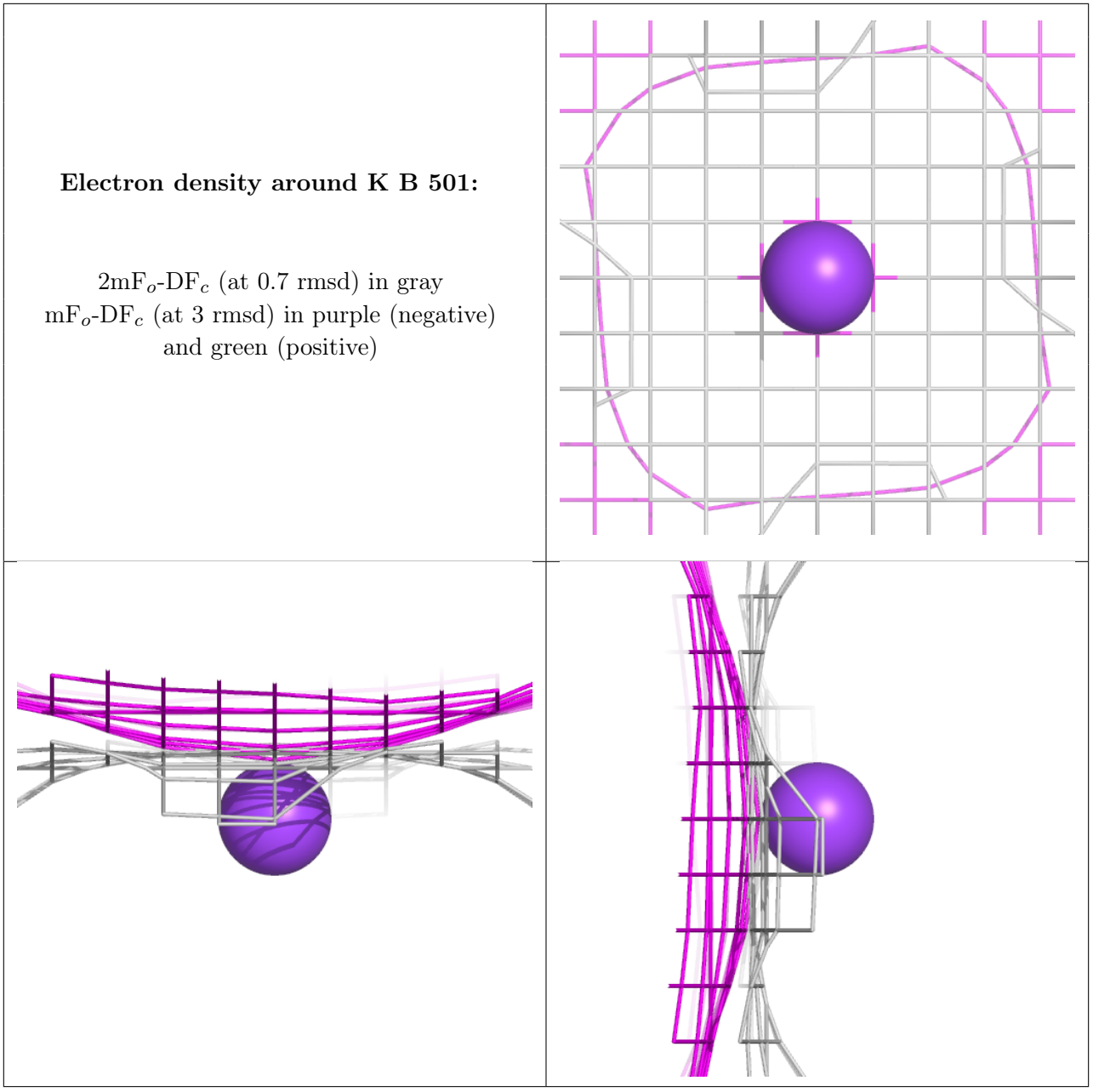






Electron density around K B 501:

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



6.5 Other polymers

There are no such residues in this entry.