



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:35 PM UTC

PDB ID : 2A79 / pdb_00002a79
Title : Mammalian Shaker Kv1.2 potassium channel- beta subunit complex
Authors : Long, S.B.; Campbell, E.B.; MacKinnon, R.
Deposited on : 2005-07-05
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

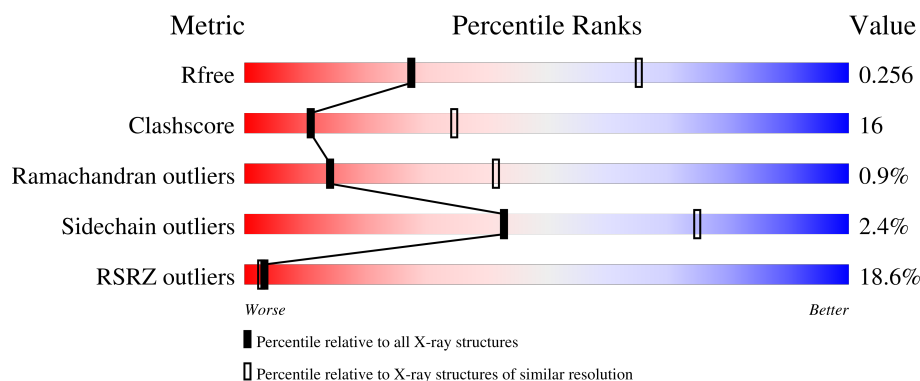
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	4% 65% 32% ..
2	B	499	19% 34% 17% 48% .
3	C	52	96% .
4	D	21	90% 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4997 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 beta-2 subunit.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	cloning artifact	UNP P62483

- Molecule 2 is a protein called Potassium voltage-gated channel subfamily A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			1972	1298	322	345	7			

- Molecule 3 is a protein called poly-unknown chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	52	Total	C	N	O	0	0	0
			227	123	52	52			

- Molecule 4 is a protein called poly-unknown chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	21	Total	C	N	O	0	0	0
			105	63	21	21			

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	6	Total	K	0	0
			6	6		

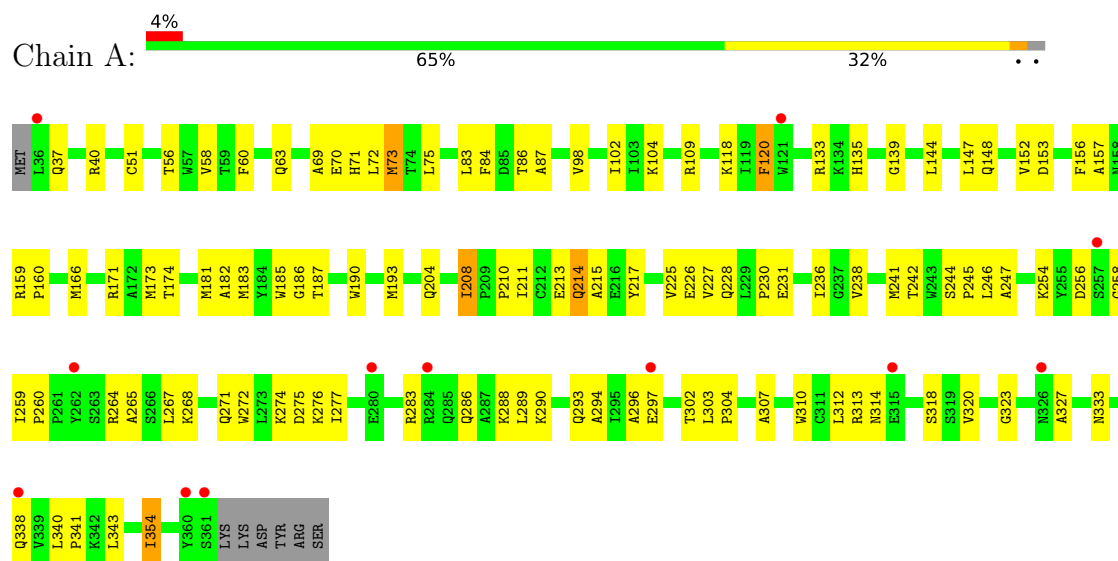
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	67	Total	O	0	0
			67	67		
7	B	16	Total	O	0	0
			16	16		

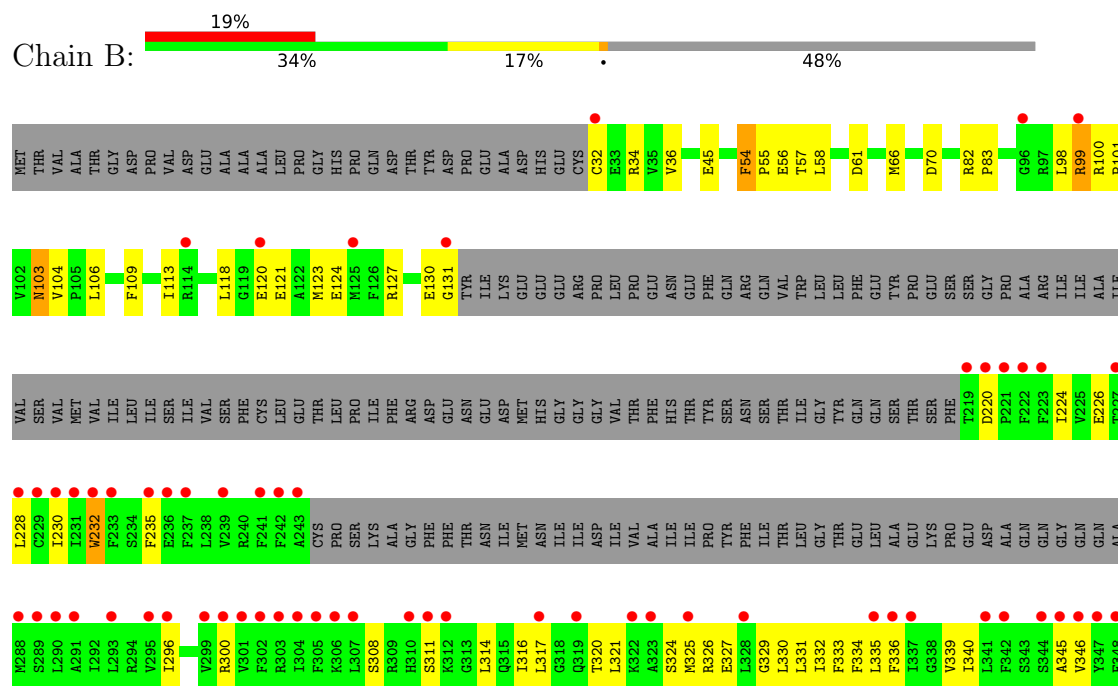
3 Residue-property plots [i](#)

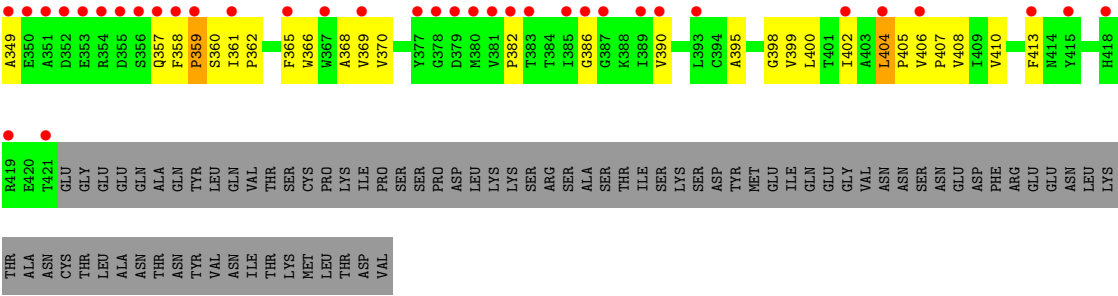
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 beta-2 subunit



- Molecule 2: Potassium voltage-gated channel subfamily A member 2

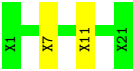
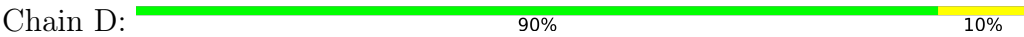




● Molecule 3: poly-unknown chain



● Molecule 4: poly-unknown chain



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	113.61Å 113.61Å 260.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.90 29.48 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.48-2.90) 91.5 (29.48-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.252 0.224 , 0.256	Depositor DCC
R_{free} test set	1952 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4997	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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, 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	0.88	1/2608 (0.0%)	1.09	8/3524 (0.2%)
2	B	0.58	0/2021	0.92	5/2748 (0.2%)
All	All	0.77	1/4629 (0.0%)	1.02	13/6272 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	MET	SD-CE	6.00	1.94	1.79

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	GLN	N-CA-C	9.28	121.16	111.14
1	A	157	ALA	N-CA-C	-8.32	96.52	109.25
2	B	54	PHE	CA-C-N	7.66	129.42	119.84
2	B	54	PHE	C-N-CA	7.66	129.42	119.84
1	A	208	ILE	N-CA-C	6.03	113.86	107.76
1	A	226	GLU	CA-C-N	-5.97	117.12	122.97
1	A	226	GLU	C-N-CA	-5.97	117.12	122.97
2	B	61	ASP	CA-C-N	5.52	124.98	119.24
2	B	61	ASP	C-N-CA	5.52	124.98	119.24
1	A	69	ALA	N-CA-C	-5.25	105.45	111.07
1	A	181	MET	N-CA-C	-5.14	107.06	113.38
1	A	211	ILE	CB-CA-C	-5.06	104.52	110.84
2	B	34	ARG	N-CA-C	5.03	118.22	110.42

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	79	0
2	B	1972	0	1846	75	0
3	C	227	0	23	7	0
4	D	105	0	23	1	0
5	A	48	0	25	5	0
6	B	6	0	0	0	0
7	A	67	0	0	7	0
7	B	16	0	0	2	0
All	All	4997	0	4499	155	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 16.

All (155) 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:131:GLY:C	3:C:1:UNK:N	2.22	0.98
2:B:404:LEU:HB2	2:B:405:PRO:HD3	1.49	0.95
2:B:113:ILE:HG23	2:B:118:LEU:HD12	1.60	0.82
1:A:286:GLN:HA	1:A:289:LEU:HD12	1.62	0.82
2:B:32:CYS:HB3	7:B:561:HOH:O	1.80	0.81
1:A:258:GLY:O	1:A:260:PRO:HD3	1.84	0.77
2:B:406:VAL:HB	2:B:407:PRO:HD3	1.65	0.77
2:B:336:PHE:O	2:B:340:ILE:HG12	1.89	0.73
2:B:404:LEU:O	2:B:407:PRO:HD2	1.89	0.73
2:B:103:ASN:H	2:B:103:ASN:HD22	1.38	0.71
1:A:40:ARG:HD2	1:A:318:SER:O	1.93	0.69
1:A:338:GLN:O	1:A:341:PRO:HD2	1.95	0.67
1:A:217:TYR:HB2	1:A:225:VAL:HG21	1.77	0.66
2:B:131:GLY:C	3:C:1:UNK:H	2.01	0.66
1:A:288:LYS:HG2	1:A:354:ILE:HD12	1.77	0.66
2:B:320:THR:HG21	2:B:413:PHE:HA	1.77	0.66
1:A:166:MET:HE1	1:A:190:TRP:HH2	1.58	0.65
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.79	0.65
1:A:166:MET:HE1	1:A:190:TRP:CH2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:PHE:N	2:B:359:PRO:HD3	2.12	0.65
1:A:294:ALA:O	1:A:297:GLU:HG2	1.97	0.63
1:A:245:PRO:HG3	1:A:320:VAL:HG13	1.80	0.63
1:A:289:LEU:HD22	1:A:303:LEU:HD21	1.81	0.62
2:B:339:VAL:HG13	2:B:368:ALA:HB3	1.81	0.62
2:B:366:TRP:O	2:B:370:VAL:HG23	2.00	0.62
1:A:185:TRP:CZ2	1:A:210:PRO:HG3	2.34	0.61
1:A:83:LEU:HD21	1:A:241:MET:HE2	1.83	0.60
1:A:63:GLN:NE2	1:A:267:LEU:HD11	2.18	0.59
1:A:256:ASP:OD2	1:A:290:LYS:HD3	2.02	0.59
1:A:244:SER:N	1:A:245:PRO:HD3	2.17	0.59
1:A:173:MET:HG3	1:A:185:TRP:CE3	2.38	0.58
2:B:98:LEU:HD21	2:B:113:ILE:HD13	1.86	0.58
2:B:131:GLY:CA	3:C:1:UNK:N	2.65	0.58
2:B:311:SER:HB2	2:B:314:LEU:HD13	1.85	0.57
1:A:236:ILE:HG13	1:A:238:VAL:HG23	1.86	0.57
2:B:317:LEU:O	2:B:321:LEU:HG	2.06	0.56
2:B:54:PHE:N	2:B:55:PRO:HD3	2.21	0.55
1:A:109:ARG:HH11	1:A:109:ARG:HG3	1.71	0.55
2:B:103:ASN:H	2:B:103:ASN:ND2	2.03	0.55
2:B:232:TRP:HZ3	2:B:235:PHE:HD2	1.55	0.55
1:A:215:ALA:O	1:A:242:THR:HA	2.07	0.54
2:B:346:VAL:HG22	2:B:390:VAL:HB	1.89	0.54
1:A:133:ARG:HD2	7:A:503:HOH:O	2.08	0.54
1:A:259:ILE:HG13	1:A:274:LYS:HE3	1.89	0.54
2:B:296:ILE:O	2:B:300:ARG:HB2	2.08	0.53
1:A:254:LYS:HE3	7:A:547:HOH:O	2.08	0.53
2:B:316:ILE:O	2:B:320:THR:HG23	2.09	0.53
2:B:345:ALA:HB3	2:B:390:VAL:HG11	1.91	0.53
2:B:314:LEU:N	2:B:314:LEU:HD12	2.24	0.52
2:B:220:ASP:O	2:B:224:ILE:HG12	2.09	0.52
1:A:144:LEU:HD21	1:A:152:VAL:HG13	1.89	0.52
1:A:293:GLN:O	1:A:296:ALA:HB3	2.09	0.52
1:A:290:LYS:O	1:A:293:GLN:HB3	2.10	0.51
1:A:286:GLN:O	1:A:289:LEU:HB2	2.10	0.51
1:A:225:VAL:HG23	7:A:524:HOH:O	2.10	0.51
1:A:302:THR:OG1	1:A:304:PRO:HD2	2.11	0.51
2:B:82:ARG:HB2	2:B:83:PRO:HD3	1.92	0.50
3:C:1:UNK:O	3:C:2:UNK:C	2.59	0.50
2:B:361:ILE:HD12	2:B:361:ILE:N	2.27	0.50
1:A:153:ASP:O	1:A:183:MET:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:TRP:CE2	1:A:313:ARG:NH1	2.79	0.50
1:A:354:ILE:HD12	1:A:354:ILE:O	2.12	0.50
2:B:365:PHE:O	2:B:369:VAL:HG23	2.12	0.50
4:D:7:UNK:O	4:D:11:UNK:CB	2.59	0.50
1:A:156:PHE:HA	1:A:186:GLY:O	2.12	0.50
2:B:70:ASP:OD1	2:B:70:ASP:C	2.54	0.50
2:B:331:LEU:HB2	2:B:405:PRO:HG2	1.93	0.50
2:B:314:LEU:HD12	2:B:314:LEU:H	1.76	0.50
1:A:71:HIS:CE1	1:A:75:LEU:HD11	2.47	0.49
1:A:265:ALA:HB2	1:A:277:ILE:HD12	1.94	0.49
2:B:224:ILE:O	2:B:228:LEU:HG	2.12	0.49
2:B:58:LEU:C	2:B:58:LEU:HD23	2.36	0.49
2:B:226:GLU:O	2:B:230:ILE:HG13	2.11	0.49
2:B:332:ILE:HG13	2:B:333:PHE:N	2.27	0.49
2:B:361:ILE:HD12	2:B:361:ILE:H	1.77	0.49
1:A:214:GLN:HA	1:A:241:MET:O	2.13	0.49
2:B:349:ALA:HB1	2:B:386:GLY:HA3	1.95	0.48
1:A:302:THR:CB	1:A:304:PRO:HD2	2.44	0.48
2:B:232:TRP:CZ3	2:B:235:PHE:HD2	2.31	0.48
1:A:246:LEU:O	1:A:247:ALA:C	2.56	0.48
1:A:245:PRO:HG3	1:A:320:VAL:CG1	2.43	0.47
2:B:232:TRP:HA	2:B:232:TRP:CE3	2.49	0.47
2:B:106:LEU:HD11	2:B:130:GLU:HG2	1.97	0.47
2:B:361:ILE:N	2:B:362:PRO:CD	2.78	0.47
1:A:98:VAL:O	1:A:102:ILE:HG13	2.15	0.47
2:B:109:PHE:O	2:B:113:ILE:HG13	2.15	0.47
2:B:360:SER:HB2	2:B:362:PRO:HD2	1.97	0.47
1:A:227:VAL:O	1:A:230:PRO:HD2	2.15	0.46
1:A:264:ARG:HA	1:A:267:LEU:HG	1.98	0.46
1:A:314:ASN:HB2	7:A:579:HOH:O	2.15	0.46
2:B:131:GLY:CA	3:C:1:UNK:H	2.28	0.46
2:B:232:TRP:HA	2:B:232:TRP:HE3	1.80	0.46
2:B:308:SER:HA	2:B:314:LEU:HD22	1.97	0.46
2:B:398:GLY:O	2:B:402:ILE:HG13	2.16	0.46
1:A:244:SER:H	5:A:1001:NAP:H51N	1.80	0.45
1:A:323:GLY:HA3	5:A:1001:NAP:H51A	1.99	0.45
2:B:127:ARG:HH11	2:B:127:ARG:HG2	1.80	0.45
1:A:173:MET:HG3	1:A:185:TRP:CD2	2.52	0.45
1:A:244:SER:OG	5:A:1001:NAP:O2N	2.29	0.45
1:A:56:THR:HB	1:A:60:PHE:HB2	1.98	0.45
2:B:357:GLN:C	2:B:359:PRO:HD3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:THR:O	1:A:213:GLU:HA	2.16	0.44
2:B:120:GLU:HA	2:B:123:MET:HB3	1.99	0.44
1:A:272:TRP:O	1:A:276:LYS:HG3	2.17	0.44
2:B:406:VAL:O	2:B:410:VAL:HG23	2.18	0.44
2:B:395:ALA:O	2:B:399:VAL:HG23	2.18	0.44
1:A:185:TRP:CH2	1:A:210:PRO:HG3	2.52	0.44
2:B:124:GLU:O	2:B:127:ARG:HB2	2.18	0.43
1:A:71:HIS:CD2	1:A:327:ALA:HB2	2.53	0.43
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.54	0.43
2:B:109:PHE:CE2	2:B:113:ILE:HD11	2.52	0.43
1:A:174:THR:HG23	1:A:208:ILE:HD12	2.00	0.43
1:A:73:MET:HE3	1:A:84:PHE:CD2	2.54	0.43
1:A:51:CYS:HB2	1:A:312:LEU:HD22	2.01	0.43
1:A:147:LEU:O	1:A:148:GLN:HB2	2.19	0.43
1:A:171:ARG:HD3	7:A:570:HOH:O	2.18	0.43
1:A:271:GLN:HG3	1:A:275:ASP:OD2	2.18	0.43
2:B:311:SER:CB	2:B:314:LEU:HD13	2.47	0.43
1:A:152:VAL:O	1:A:182:ALA:HA	2.19	0.43
1:A:70:GLU:HA	1:A:102:ILE:HD13	2.01	0.42
2:B:57:THR:HG22	2:B:118:LEU:HA	2.01	0.42
1:A:307:ALA:O	1:A:310:TRP:HB3	2.19	0.42
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.86	0.42
1:A:40:ARG:NH1	7:A:545:HOH:O	2.52	0.42
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.88	0.42
1:A:245:PRO:CG	1:A:320:VAL:CG1	2.98	0.42
2:B:99:ARG:HG2	2:B:99:ARG:HH11	1.85	0.42
2:B:329:GLY:HA2	2:B:332:ILE:HD11	2.01	0.42
1:A:160:PRO:HG3	1:A:190:TRP:CD1	2.55	0.42
2:B:100:ARG:HD3	2:B:106:LEU:HD12	2.02	0.42
2:B:324:SER:HB2	2:B:327:GLU:CG	2.49	0.42
2:B:406:VAL:HB	2:B:407:PRO:CD	2.43	0.42
1:A:86:THR:HG23	1:A:87:ALA:N	2.35	0.42
1:A:37:GLN:CA	1:A:37:GLN:HE21	2.32	0.41
1:A:323:GLY:HA2	7:A:531:HOH:O	2.19	0.41
1:A:340:LEU:HD12	1:A:343:LEU:HD12	2.02	0.41
2:B:101:PRO:HB2	2:B:104:VAL:HG23	2.02	0.41
2:B:325:MET:HG3	2:B:326:ARG:N	2.35	0.41
1:A:231:GLU:HG2	2:B:66:MET:HE1	2.03	0.41
1:A:303:LEU:N	1:A:304:PRO:CD	2.83	0.41
2:B:327:GLU:CD	2:B:408:VAL:HG11	2.45	0.41
2:B:358:PHE:N	2:B:359:PRO:CD	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASN:ND2	5:A:1001:NAP:H61A	2.17	0.41
2:B:131:GLY:HA2	3:C:1:UNK:H	1.85	0.41
2:B:56:GLU:HB2	7:B:569:HOH:O	2.20	0.41
2:B:131:GLY:HA2	3:C:1:UNK:N	2.35	0.41
2:B:370:VAL:O	2:B:370:VAL:HG12	2.21	0.41
2:B:330:LEU:HD22	2:B:334:PHE:HE1	1.86	0.41
2:B:335:LEU:C	2:B:335:LEU:HD23	2.45	0.41
1:A:135:HIS:O	1:A:139:GLY:N	2.47	0.40
1:A:333:ASN:HD21	5:A:1001:NAP:H61A	1.68	0.40
2:B:400:LEU:O	2:B:404:LEU:HG	2.22	0.40
1:A:73:MET:HG2	1:A:84:PHE:CE2	2.57	0.40
1:A:40:ARG:HE	1:A:51:CYS:HB3	1.87	0.40
2:B:36:VAL:HG22	2:B:45:GLU:HG2	2.03	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%)	307 (95%)	15 (5%)	2 (1%)	21	51
2	B	253/499 (51%)	232 (92%)	18 (7%)	3 (1%)	10	34
All	All	577/832 (69%)	539 (93%)	33 (6%)	5 (1%)	14	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
2	B	359	PRO
2	B	121	GLU
2	B	404	LEU
1	A	58	VAL

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%)	266 (97%)	7 (3%)	40	73
2	B	188/441 (43%)	184 (98%)	4 (2%)	47	77
All	All	461/721 (64%)	450 (98%)	11 (2%)	43	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	MET
1	A	104	LYS
1	A	204	GLN
1	A	214	GLN
1	A	268	LYS
1	A	283	ARG
1	A	354	ILE
2	B	99	ARG
2	B	103	ASN
2	B	232	TRP
2	B	382	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	71	HIS
1	A	163	ASN
1	A	234	HIS
1	A	326	ASN
1	A	333	ASN
2	B	53	GLN
2	B	103	ASN
2	B	412	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z > 2$
5	NAP	A	1001	-	50,52,52	1.52	9 (18%)	71,80,80	1.25	7 (9%)

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
5	NAP	A	1001	-	-	7/35/67/67	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	NAP	O4D-C1D	-3.35	1.36	1.40
5	A	1001	NAP	C4N-C3N	3.35	1.44	1.39
5	A	1001	NAP	C4A-N3A	3.20	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	NAP	C6N-N1N	3.15	1.42	1.35
5	A	1001	NAP	C5A-N7A	-3.02	1.33	1.39
5	A	1001	NAP	O4B-C4B	2.42	1.50	1.45
5	A	1001	NAP	P2B-O2B	2.41	1.63	1.59
5	A	1001	NAP	PN-O3	-2.38	1.56	1.59
5	A	1001	NAP	C7N-N7N	2.38	1.37	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	NAP	P2B-O2B-C2B	3.61	133.07	123.43
5	A	1001	NAP	C2B-C1B-N9A	-3.26	108.39	113.75
5	A	1001	NAP	O7N-C7N-N7N	2.71	126.53	122.62
5	A	1001	NAP	O2B-C2B-C3B	2.58	120.93	111.68
5	A	1001	NAP	C2B-C3B-C4B	2.47	107.29	101.99
5	A	1001	NAP	C2A-N1A-C6A	2.13	122.23	118.73
5	A	1001	NAP	O4B-C1B-N9A	2.01	111.96	108.09

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	NAP	O4D-C1D-N1N-C6N
5	A	1001	NAP	O4D-C4D-C5D-O5D
5	A	1001	NAP	C1B-C2B-O2B-P2B
5	A	1001	NAP	C3D-C4D-C5D-O5D
5	A	1001	NAP	PN-O3-PA-O5B
5	A	1001	NAP	C3B-C2B-O2B-P2B
5	A	1001	NAP	O4D-C1D-N1N-C2N

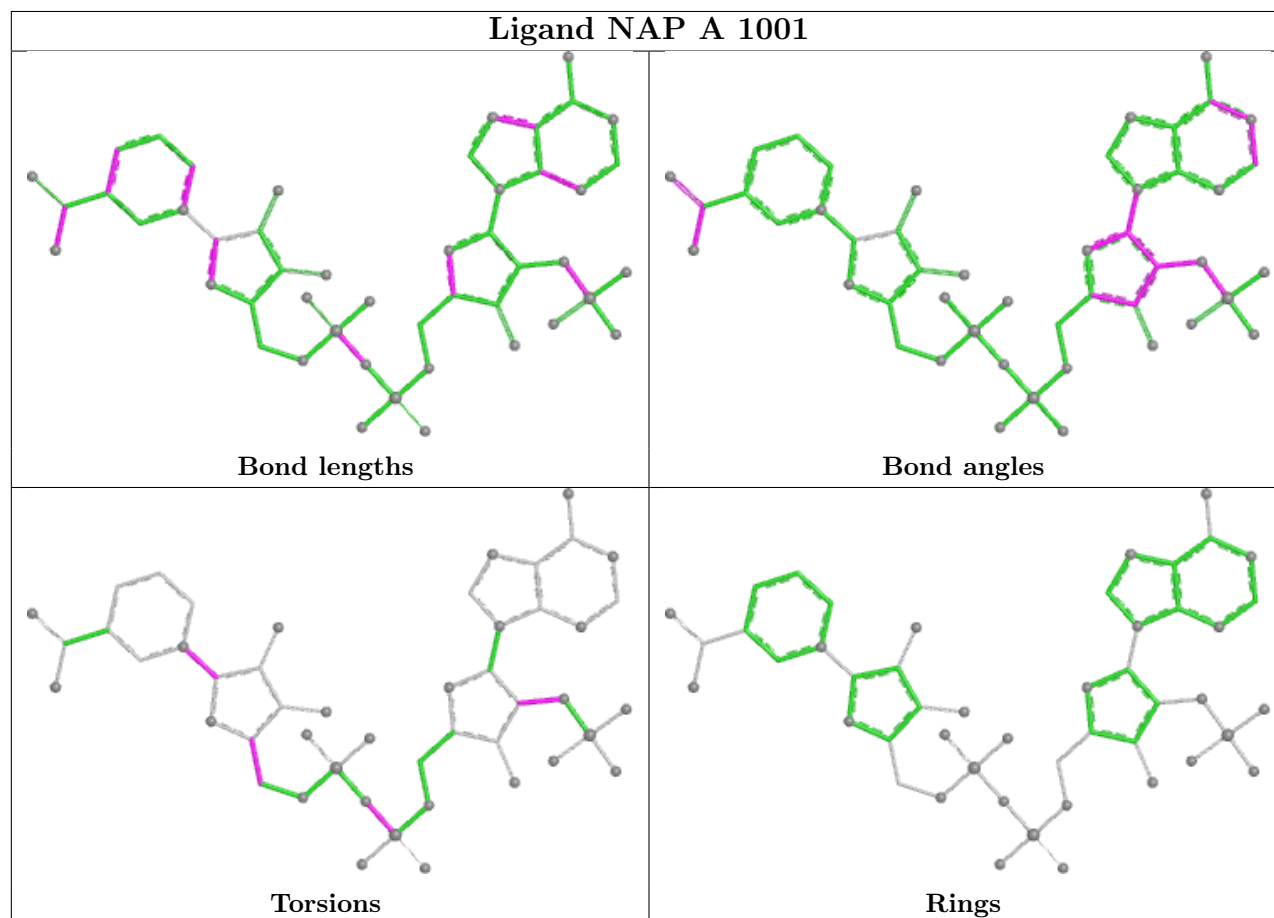
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	NAP	5	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%)	-0.10	12 (3%) 45 37	31, 50, 79, 91	0
2	B	259/499 (51%)	1.77	97 (37%) 1 0	47, 157, 164, 165	0
3	C	0/52	-	-	-	-
4	D	0/21	-	-	-	-
All	All	585/905 (64%)	0.72	109 (18%) 3 3	31, 68, 163, 165	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	380	MET	8.7
2	B	355	ASP	6.9
2	B	351	ALA	6.9
2	B	386	GLY	6.8
2	B	347	TYR	6.6
2	B	382	PRO	6.0
2	B	352	ASP	5.8
2	B	357	GLN	5.4
1	A	361	SER	5.3
2	B	381	VAL	5.0
2	B	348	PHE	4.9
2	B	293	LEU	4.8
2	B	377	TYR	4.4
2	B	232	TRP	4.3
2	B	415	TYR	4.2
2	B	220	ASP	4.2
2	B	361	ILE	4.2
2	B	305	PHE	4.2
2	B	418	HIS	4.1
2	B	378	GLY	4.1
2	B	358	PHE	4.1
2	B	222	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	389	ILE	4.0
2	B	350	GLU	4.0
2	B	289	SER	3.9
2	B	243	ALA	3.8
2	B	385	ILE	3.8
2	B	379	ASP	3.8
1	A	315	GLU	3.7
2	B	301	VAL	3.7
2	B	311	SER	3.6
2	B	242	PHE	3.6
2	B	236	GLU	3.6
2	B	356	SER	3.5
2	B	223	PHE	3.5
2	B	230	ILE	3.5
2	B	336	PHE	3.5
2	B	239	VAL	3.5
2	B	235	PHE	3.4
2	B	421	THR	3.4
2	B	349	ALA	3.3
2	B	233	PHE	3.3
2	B	219	THR	3.3
2	B	390	VAL	3.3
2	B	229	CYS	3.3
2	B	419	ARG	3.2
2	B	32	CYS	3.2
2	B	228	LEU	3.2
2	B	335	LEU	3.2
2	B	325	MET	3.2
2	B	387	GLY	3.1
2	B	296	ILE	3.1
2	B	354	ARG	3.0
2	B	359	PRO	3.0
2	B	231	ILE	2.9
2	B	221	PRO	2.9
2	B	342	PHE	2.9
2	B	306	LYS	2.8
2	B	227	THR	2.8
1	A	262	TYR	2.8
2	B	303	ARG	2.8
2	B	310	HIS	2.8
2	B	317	LEU	2.8
1	A	360	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	241	PHE	2.8
2	B	383	THR	2.8
2	B	323	ALA	2.7
2	B	304	ILE	2.7
2	B	99	ARG	2.7
2	B	237	PHE	2.7
2	B	300	ARG	2.7
2	B	346	VAL	2.6
2	B	353	GLU	2.6
1	A	284	ARG	2.6
1	A	297	GLU	2.6
2	B	96	GLY	2.5
2	B	345	ALA	2.5
2	B	299	VAL	2.5
2	B	291	ALA	2.4
2	B	402	ILE	2.4
2	B	114	ARG	2.4
2	B	312	LYS	2.4
1	A	338	GLN	2.4
2	B	131	GLY	2.4
1	A	257	SER	2.4
2	B	120	GLU	2.4
1	A	36	LEU	2.4
2	B	344	SER	2.3
2	B	288	MET	2.3
2	B	393	LEU	2.3
2	B	367	TRP	2.3
2	B	295	VAL	2.3
2	B	125	MET	2.3
2	B	307	LEU	2.3
1	A	326	ASN	2.3
2	B	328	LEU	2.3
2	B	404	LEU	2.3
2	B	337	ILE	2.2
2	B	302	PHE	2.2
2	B	365	PHE	2.2
2	B	341	LEU	2.2
2	B	406	VAL	2.2
2	B	290	LEU	2.2
2	B	369	VAL	2.1
1	A	121	TRP	2.1
1	A	280	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	322	LYS	2.1
2	B	319	GLN	2.1
2	B	413	PHE	2.1

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](#)

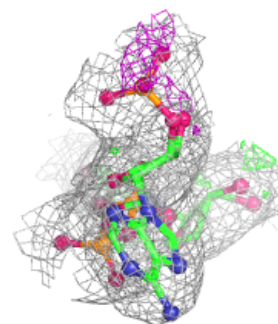
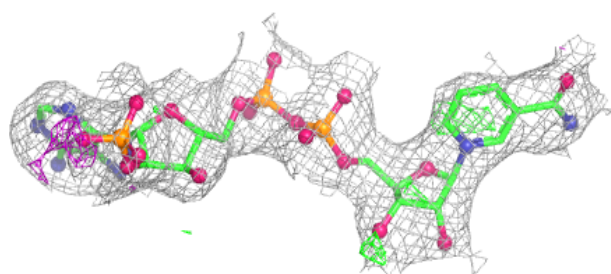
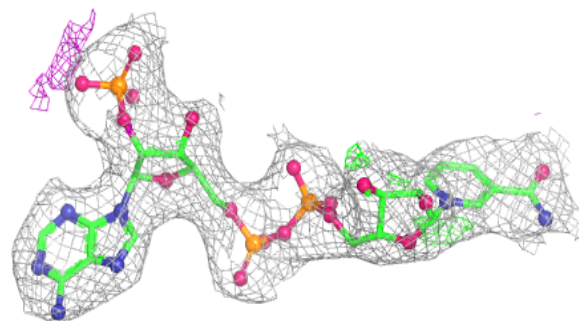
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	K	B	504	1/1	0.30	0.21	89,89,89,89	1
6	K	B	505	1/1	0.56	0.21	89,89,89,89	1
6	K	B	503	1/1	0.74	0.10	89,89,89,89	1
6	K	B	501	1/1	0.85	0.08	89,89,89,89	1
6	K	B	502	1/1	0.87	0.09	89,89,89,89	1
6	K	B	500	1/1	0.93	0.06	89,89,89,89	1
5	NAP	A	1001	48/48	0.96	0.09	46,51,59,60	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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.