



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 06:55 PM GMT

PDB ID : 2A79  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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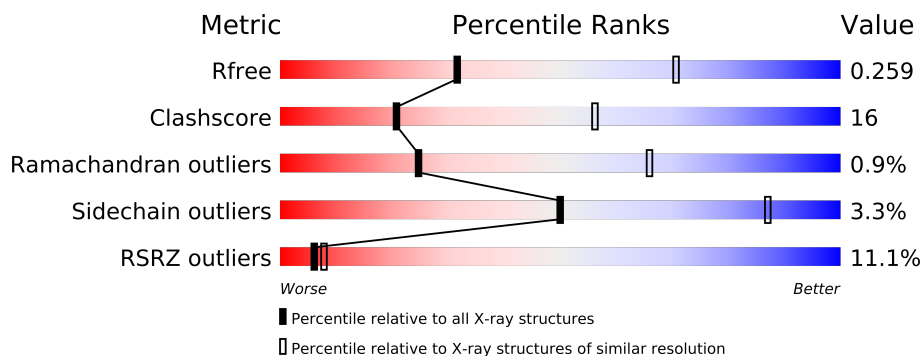
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	333	
2	B	499	
3	C	52	
4	D	21	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4997 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

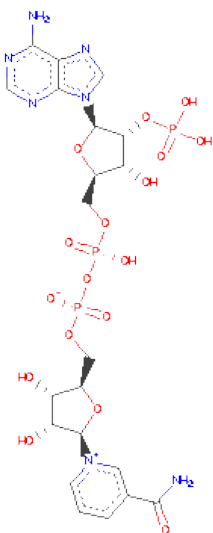
- Molecule 4 is a protein called poly-unknown chain.

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 6 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

- 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		



PRO	SER	SER	PRO	PRO	ASP	LEU	LYS	LYS	SER	ARG	SER	ALA	SER	THR	ILE	SER	LYS	SER	ASP	TYR	MET	GLU	ILE	GLN	GLY	GLY	VAL	ASN	ASN	SER	ASN	GLU	ASP	PHE	ARG	GLU	GLU	ASN	LEU	LYS	THR	ALA	ASN	CYS	THR	LEU	ALA	ASN	THR	ASN	TYR	VAL	ASN	ILE	THR	LYS	MET	LEU	THR	ASP
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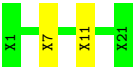
- Molecule 3: poly-unknown chain

Chain C:



- Molecule 4: poly-unknown chain

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.61Å 113.61Å 260.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.90 30.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.48-2.90) 89.9 (30.63-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.252 0.234 , 0.259	Depositor DCC
$R_{free}$ test set	1776 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.9	EDS
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 36329 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.75	0/2608	0.75	1/3524 (0.0%)
2	B	0.51	0/2021	0.58	0/2748
All	All	0.66	0/4629	0.68	1/6272 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ALA	N-CA-C	-5.36	96.52	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2556	0	2582	74	0
2	B	1972	0	1846	71	0
3	C	227	0	23	7	0
4	D	105	0	23	1	0
5	B	6	0	0	0	0
6	A	48	0	25	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	67	0	0	7	0
7	B	16	0	0	2	0
All	All	4997	0	4499	147	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (147) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:404:LEU:HB2	2:B:405:PRO:HD3	1.49	0.95
2:B:131:GLY:C	3:C:1:UNK:N	2.22	0.93
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
2:B:406:VAL:HB	2:B:407:PRO:HD3	1.65	0.77
1:A:258:GLY:O	1:A:260:PRO:HD3	1.84	0.77
2:B:404:LEU:O	2:B:407:PRO:HD2	1.89	0.73
2:B:336:PHE:O	2:B:340:ILE:HG12	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:320:THR:HG21	2:B:413:PHE:HA	1.77	0.66
1:A:288:LYS:HG2	1:A:354:ILE:HD12	1.77	0.66
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.79	0.65
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
2:B:131:GLY:C	3:C:1:UNK:H	2.01	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: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
2:B:131:GLY:CA	3:C:1:UNK:N	2.65	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:B:316:ILE:O	2:B:320:THR:HG23	2.09	0.53
1:A:254:LYS:HE3	7:A:547:HOH:O	2.08	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:302:THR:OG1	1:A:304:PRO:HD2	2.11	0.51
1:A:225:VAL:HG23	7:A:524:HOH:O	2.10	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:N	2:B:361:ILE:HD12	2.27	0.50
1:A:354:ILE:HD12	1:A:354:ILE:O	2.12	0.50
1:A:310:TRP:CE2	1:A:313:ARG:NH1	2.79	0.50
1:A:153:ASP:O	1:A:183:MET:HB2	2.11	0.50
4:D:7:UNK:O	4:D:11:UNK:CB	2.59	0.50
2:B:365:PHE:O	2:B:369:VAL:HG23	2.12	0.50
2:B:331:LEU:HB2	2:B:405:PRO:HG2	1.93	0.50
1:A:156:PHE:HA	1:A:186:GLY:O	2.12	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: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:245:PRO:HG3	1:A:320:VAL:CG1	2.43	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:232:TRP:CE3	2:B:232:TRP:HA	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
2:B:109:PHE:O	2:B:113:ILE:HG13	2.15	0.47
1:A:98:VAL:O	1:A:102: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:166:MET:HE3	1:A:170:VAL:HG23	1.97	0.46
2:B:131:GLY:CA	3:C:1:UNK:H	2.28	0.46
2:B:308:SER:HA	2:B:314:LEU:HD22	1.97	0.46
2:B:232:TRP:HA	2:B:232:TRP:HE3	1.80	0.46
1:A:314:ASN:HB2	7:A:579:HOH:O	2.15	0.46
2:B:70:ASP:OD1	2:B:70:ASP:C	2.54	0.46
2:B:398:GLY:O	2:B:402:ILE:HG13	2.16	0.46
1:A:244:SER:H	6:A:1001:NAP:H51N	1.80	0.45
1:A:323:GLY:HA3	6:A:1001:NAP:H51A	1.99	0.45
2:B:127:ARG:HG2	2:B:127:ARG:HH11	1.80	0.45
1:A:173:MET:HG3	1:A:185:TRP:CD2	2.52	0.45
2:B:58:LEU:C	2:B:58:LEU:HD23	2.36	0.45
1:A:56:THR:HB	1:A:60:PHE:HB2	1.98	0.45
2:B:120:GLU:HA	2:B:123:MET:HB3	1.99	0.44
1:A:187:THR:O	1:A:213:GLU:HA	2.16	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
2:B:109:PHE:CE2	2:B:113:ILE:HD11	2.52	0.43
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.54	0.43
1:A:246:LEU:O	1:A:247:ALA:C	2.56	0.43
1:A:174:THR:HG23	1:A:208:ILE:HD12	2.00	0.43
1:A:147:LEU:O	1:A:148:GLN:HB2	2.19	0.43
1:A:51:CYS:HB2	1:A:312:LEU:HD22	2.01	0.43
1:A:171:ARG:HD3	7:A:570:HOH:O	2.18	0.43
2:B:311:SER:CB	2:B:314:LEU:HD13	2.47	0.43
1:A:271:GLN:HG3	1:A:275:ASP:OD2	2.18	0.43
1:A:152:VAL:O	1:A:182:ALA:HA	2.19	0.43
2:B:57:THR:HG22	2:B:118:LEU:HA	2.01	0.42
1:A:70:GLU:HA	1:A:102:ILE:HD13	2.01	0.42
1:A:307:ALA:O	1:A:310:TRP:HB3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:144:LEU:HA	1:A:144:LEU:HD23	1.86	0.42
1:A:40:ARG:NH1	7:A:545:HOH:O	2.52	0.42
1:A:245:PRO:CG	1:A:320:VAL:CG1	2.98	0.42
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.88	0.42
2:B:329:GLY:HA2	2:B:332:ILE:HD11	2.01	0.42
2:B:99:ARG:HG2	2:B:99:ARG:HH11	1.85	0.42
2:B:100:ARG:HD3	2:B:106:LEU:HD12	2.02	0.42
1:A:160:PRO:HG3	1:A:190:TRP:CD1	2.55	0.42
2:B:406:VAL:HB	2:B:407:PRO:CD	2.43	0.42
2:B:324:SER:HB2	2:B:327:GLU:CG	2.49	0.42
1:A:86:THR:HG23	1:A:87:ALA:N	2.35	0.42
1:A:323:GLY:HA2	7:A:531:HOH:O	2.19	0.41
1:A:37:GLN:HE21	1:A:37:GLN:CA	2.32	0.41
2:B:325:MET:HG3	2:B:326:ARG:N	2.35	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
1:A:303:LEU:N	1:A:304:PRO:CD	2.83	0.41
2:B:358:PHE:N	2:B:359:PRO:CD	2.82	0.41
2:B:131:GLY:HA2	3:C:1:UNK:H	1.85	0.41
1:A:333:ASN:ND2	6:A:1001:NAP:H61A	2.17	0.41
2:B:131:GLY:HA2	3:C:1:UNK:N	2.35	0.41
2:B:370:VAL:HG12	2:B:370:VAL:O	2.21	0.41
2:B:56:GLU:HB2	7:B:569:HOH:O	2.20	0.41
2:B:330:LEU:HD22	2:B:334:PHE:HE1	1.86	0.41
1:A:135:HIS:O	1:A:139:GLY:N	2.47	0.40
2:B:400:LEU:O	2:B:404:LEU:HG	2.22	0.40
1:A:333:ASN:HD21	6:A:1001:NAP:H61A	1.68	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

### 5.3.1 Protein backbone ⓘ

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%)	33	76
2	B	253/499 (51%)	232 (92%)	18 (7%)	3 (1%)	19	57
All	All	577/832 (69%)	539 (93%)	33 (6%)	5 (1%)	25	66

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%)	265 (97%)	8 (3%)	55	89
2	B	188/441 (43%)	181 (96%)	7 (4%)	45	84
All	All	461/721 (64%)	446 (97%)	15 (3%)	50	87

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
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	82	ARG
2	B	86	ASP
2	B	99	ARG
2	B	103	ASN

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Mol	Chain	Res	Type
2	B	123	MET
2	B	336	PHE
2	B	382	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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	47	GLN
2	B	53	GLN
2	B	103	ASN
2	B	412	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
6	NAP	A	1001	-	52,52,52	1.35	7 (13%)	80,80,80	1.43	9 (11%)

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
6	NAP	A	1001	-	-	0/35/67/67	0/3/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1001	NAP	O4D-C1D	-3.15	1.36	1.41
6	A	1001	NAP	C4A-N3A	3.14	1.40	1.35
6	A	1001	NAP	O4B-C1B	3.05	1.46	1.41
6	A	1001	NAP	C4N-C3N	3.00	1.44	1.39
6	A	1001	NAP	C6N-N1N	2.48	1.42	1.35
6	A	1001	NAP	C2A-N3A	2.45	1.37	1.32
6	A	1001	NAP	O4B-C4B	2.28	1.50	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	NAP	P2B-O2B-C2B	5.28	133.07	121.96
6	A	1001	NAP	O4B-C1B-N9A	3.78	111.96	108.44
6	A	1001	NAP	C8A-N9A-C4A	-3.42	104.29	106.90
6	A	1001	NAP	O7N-C7N-N7N	2.73	126.53	122.59
6	A	1001	NAP	N3A-C2A-N1A	-2.71	126.45	128.71
6	A	1001	NAP	O2X-P2B-O2B	-2.70	99.31	107.09
6	A	1001	NAP	O2B-C2B-C3B	2.40	120.93	111.54
6	A	1001	NAP	C2B-C3B-C4B	2.25	107.29	101.94
6	A	1001	NAP	C3N-C7N-N7N	-2.13	115.35	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	326/333 (97%)	-0.19	5 (1%) 70 79	31, 50, 79, 91	0
2	B	259/499 (51%)	1.10	61 (23%) 1 2	47, 157, 164, 165	0
3	C	0/52	-	-	-	-
4	D	0/21	-	-	-	-
All	All	585/905 (64%)	0.38	66 (11%) 6 7	31, 68, 163, 165	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	386	GLY	9.8
2	B	382	PRO	9.5
2	B	351	ALA	9.1
2	B	356	SER	8.2
2	B	355	ASP	8.2
2	B	288	MET	7.9
2	B	289	SER	7.2
2	B	347	TYR	6.8
2	B	385	ILE	6.5
2	B	352	ASP	6.1
2	B	353	GLU	5.8
2	B	243	ALA	5.7
2	B	219	THR	5.3
2	B	221	PRO	5.2
2	B	242	PHE	5.1
2	B	323	ALA	5.0
2	B	220	ASP	5.0
2	B	311	SER	5.0
2	B	389	ILE	5.0
1	A	361	SER	4.8
2	B	358	PHE	4.6
2	B	354	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	359	PRO	4.6
2	B	291	ALA	4.5
2	B	239	VAL	4.4
2	B	387	GLY	4.2
2	B	290	LEU	4.2
2	B	294	ARG	4.2
2	B	32	CYS	4.1
2	B	421	THR	4.1
2	B	415	TYR	4.1
2	B	417	TYR	4.1
2	B	357	GLN	4.0
2	B	348	PHE	3.8
2	B	350	GLU	3.6
2	B	390	VAL	3.2
2	B	419	ARG	3.1
1	A	36	LEU	3.1
2	B	349	ALA	3.0
2	B	384	THR	3.0
2	B	381	VAL	3.0
2	B	325	MET	3.0
2	B	297	ARG	3.0
2	B	229	CYS	3.0
2	B	293	LEU	2.9
2	B	240	ARG	2.8
2	B	223	PHE	2.8
2	B	308	SER	2.8
1	A	360	TYR	2.8
2	B	374	THR	2.7
2	B	237	PHE	2.6
2	B	233	PHE	2.6
2	B	238	LEU	2.6
2	B	319	GLN	2.6
2	B	305	PHE	2.4
2	B	414	ASN	2.4
2	B	383	THR	2.3
2	B	418	HIS	2.3
2	B	346	VAL	2.3
1	A	262	TYR	2.2
2	B	222	PHE	2.2
2	B	114	ARG	2.2
2	B	413	PHE	2.2
1	A	315	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	292	ILE	2.1
2	B	306	LYS	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAP	A	1001	48/48	0.23	0.34	46,51,59,60	0
5	K	B	505	1/1	0.23	-0.64	89,89,89,89	1
5	K	B	503	1/1	0.20	-1.16	89,89,89,89	1
5	K	B	500	1/1	0.12	-3.28	89,89,89,89	1
5	K	B	502	1/1	0.11	-3.76	89,89,89,89	1
5	K	B	501	1/1	0.09	-7.85	89,89,89,89	1
5	K	B	504	1/1	0.29	-	89,89,89,89	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.