



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:16 am 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

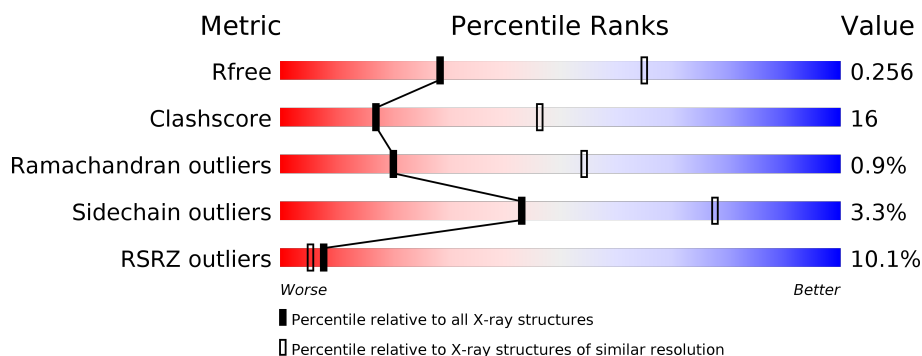
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (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. 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	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 67%; height: 10px; background-color: green;"></div> <div style="width: 30%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>67%</span> <span>30%</span> <span>• •</span> </div> </div>
2	B	499	<div> <div style="width: 11%; height: 10px; background-color: red;"></div> <div style="width: 35%; height: 10px; background-color: green;"></div> <div style="width: 16%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> <div style="width: 48%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>11%</span> <span>35%</span> <span>16%</span> <span>•</span> <span>48%</span> </div> </div>
3	C	52	<div> <div style="width: 96%; height: 10px; background-color: green;"></div> <div style="width: 4%; height: 10px; background-color: yellow;"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>96%</span> <span>•</span> </div> </div>
4	D	21	<div> <div style="width: 90%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>90%</span> <span>10%</span> </div> </div>

## 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			

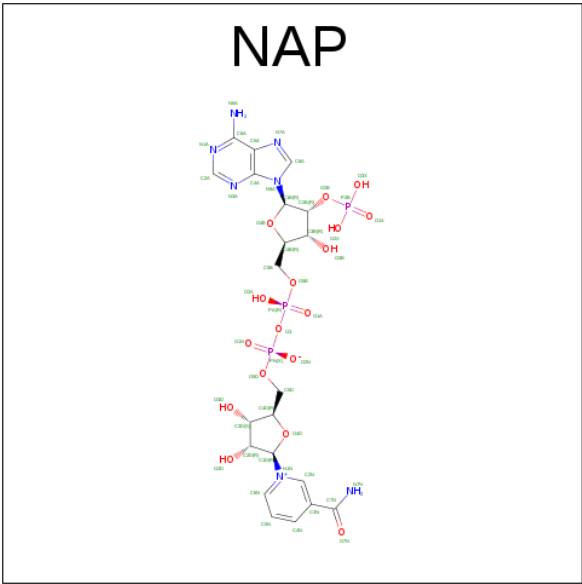
- Molecule 4 is a protein called poly-unknown chain.

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

- Molecule 5 is 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-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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		

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:

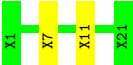
- Chain B:
- 
- 11% 35% 16% 48%
- MET THR VAL ALA THR GLY ASP PRO VAL ASP ASP GLU ALA ALA LEU PRO PRO GLY HIS PRO GLN ASP THR TYR ASP PRO PRO GLU ALA ASP HIS GLU CYS C32 V36 E45 F54 P55 E56 T57 L58 D70 R82 P83 D86 L98 R99 R100 P101 V102 N103 V104 P105 L106 I107

ASP	LEU	LYS	SER	ARG	SER	ALA	SER	THR	ILE	SER	LYS	SER	ASP	TYR	MET	GLU	ILE	GLN	GLU	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	VAL
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● 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, $\alpha$ , $\beta$ , $\gamma$	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 0.224 , 0.256	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 , 74.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <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.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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	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
7	A	67	0	0	7	0
7	B	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4997	0	4499	147	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 (147) 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: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
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
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: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	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:PHE:N	2:B:55:PRO:HD3	2.21	0.55
1:A:109:ARG:HG3	1:A:109:ARG:HH11	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:N	2:B:361:ILE:HD12	2.27	0.50
1:A:153:ASP:O	1:A:183:MET:HB2	2.11	0.50
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:331:LEU:HB2	2:B:405:PRO:HG2	1.93	0.50
2:B:314:LEU:H	2:B:314:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:PRO:HG3	1:A:320:VAL:CG1	2.43	0.47
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
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:166:MET:HE3	1:A:170:VAL:HG23	1.97	0.46
1:A:314:ASN:HB2	7:A:579:HOH:O	2.15	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:70:ASP:OD1	2:B:70:ASP:C	2.54	0.46
2:B:131:GLY:CA	3:C:1:UNK:H	2.28	0.46
2:B:398:GLY:O	2:B:402:ILE:HG13	2.16	0.46
1:A:323:GLY:HA3	6:A:1001:NAP:H51A	1.99	0.45
1:A:244:SER:H	6:A:1001:NAP:H51N	1.80	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
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: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:171:ARG:HD3	7:A:570:HOH:O	2.18	0.43
1:A:51:CYS:HB2	1:A:312:LEU:HD22	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:144:LEU:HD23	1.86	0.42
1:A:245:PRO:CG	1:A:320:VAL:CG1	2.98	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
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
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:323:GLY:HA2	7:A:531:HOH:O	2.19	0.41
1:A:37:GLN:CA	1:A:37:GLN:HE21	2.32	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: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
1:A:333:ASN:ND2	6:A:1001:NAP:H61A	2.17	0.41
2:B:131:GLY:HA2	3:C:1:UNK:H	1.85	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:131:GLY:HA2	3:C:1:UNK:N	2.35	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
1:A:333:ASN:HD21	6: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 ⓘ

### 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%)	28	64
2	B	253/499 (51%)	232 (92%)	18 (7%)	3 (1%)	15	46
All	All	577/832 (69%)	539 (93%)	33 (6%)	5 (1%)	20	54

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%)	48	81
2	B	188/441 (43%)	181 (96%)	7 (4%)	39	74
All	All	461/721 (64%)	446 (97%)	15 (3%)	43	77

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

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Mol	Chain	Res	Type
1	A	354	ILE
2	B	82	ARG
2	B	86	ASP
2	B	99	ARG
2	B	103	ASN
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 [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 carbohydrates 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	$\# Z  > 2$
6	NAP	A	1001	-	44,52,52	1.54	9 (20%)	51,80,80	1.27	5 (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
6	NAP	A	1001	-	-	0/27/67/67	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1001	NAP	O4D-C1D	-3.45	1.36	1.41
6	A	1001	NAP	C7N-N7N	2.23	1.37	1.33
6	A	1001	NAP	O4B-C4B	2.37	1.50	1.45
6	A	1001	NAP	P2B-O2B	2.39	1.63	1.59
6	A	1001	NAP	C6N-N1N	2.73	1.42	1.35
6	A	1001	NAP	C2A-N3A	2.91	1.37	1.32
6	A	1001	NAP	C4N-C3N	3.14	1.44	1.39
6	A	1001	NAP	C4A-N3A	3.29	1.40	1.35
6	A	1001	NAP	O4B-C1B	3.45	1.46	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	NAP	N3A-C2A-N1A	-2.77	126.45	128.86
6	A	1001	NAP	C3N-C7N-N7N	-2.13	115.35	117.77
6	A	1001	NAP	C2B-C3B-C4B	2.35	107.29	101.95
6	A	1001	NAP	O2B-C2B-C3B	2.51	120.93	111.63
6	A	1001	NAP	O7N-C7N-N7N	2.78	126.53	122.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1001	NAP	4	0

## 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<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%)	-0.23	3 (0%) 84 83	31, 50, 79, 91	0
2	B	259/499 (51%)	0.94	56 (21%) 1 1	47, 157, 164, 165	0
3	C	0/52	-	-	-	-
4	D	0/21	-	-	-	-
All	All	585/905 (64%)	0.29	59 (10%) 8 5	31, 68, 163, 165	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	386	GLY	8.1
2	B	382	PRO	7.6
2	B	356	SER	7.5
2	B	355	ASP	7.4
2	B	243	ALA	7.1
2	B	347	TYR	7.0
2	B	351	ALA	6.9
2	B	289	SER	6.9
2	B	288	MET	6.3
2	B	311	SER	5.1
2	B	242	PHE	5.0
2	B	221	PRO	5.0
2	B	353	GLU	5.0
2	B	220	ASP	4.9
2	B	385	ILE	4.8
2	B	352	ASP	4.7
2	B	387	GLY	4.5
2	B	323	ALA	4.4
2	B	219	THR	4.4
2	B	294	ARG	4.3
2	B	239	VAL	4.3
2	B	291	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	290	LEU	3.9
2	B	421	THR	3.9
2	B	32	CYS	3.8
2	B	354	ARG	3.7
2	B	389	ILE	3.7
2	B	357	GLN	3.7
1	A	361	SER	3.7
2	B	417	TYR	3.6
2	B	359	PRO	3.6
2	B	348	PHE	3.4
2	B	358	PHE	3.4
2	B	415	TYR	3.2
2	B	293	LEU	3.1
2	B	350	GLU	3.0
2	B	238	LEU	3.0
2	B	223	PHE	2.9
2	B	308	SER	2.8
2	B	325	MET	2.8
2	B	390	VAL	2.8
1	A	36	LEU	2.8
2	B	419	ARG	2.7
2	B	297	ARG	2.6
2	B	240	ARG	2.6
2	B	234	SER	2.6
2	B	384	THR	2.5
2	B	349	ALA	2.5
2	B	292	ILE	2.5
2	B	418	HIS	2.5
2	B	374	THR	2.4
2	B	222	PHE	2.3
1	A	360	TYR	2.3
2	B	324	SER	2.2
2	B	229	CYS	2.2
2	B	233	PHE	2.2
2	B	414	ASN	2.1
2	B	305	PHE	2.1
2	B	237	PHE	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 [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAP	A	1001	48/48	0.95	0.23	0.23	46,51,59,60	0
5	K	B	505	1/1	0.70	0.42	-	89,89,89,89	1
5	K	B	502	1/1	0.81	0.17	-	89,89,89,89	1
5	K	B	504	1/1	0.70	0.30	-	89,89,89,89	1
5	K	B	503	1/1	0.95	0.14	-	89,89,89,89	1
5	K	B	500	1/1	0.83	0.17	-	89,89,89,89	1
5	K	B	501	1/1	0.97	0.19	-	89,89,89,89	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.