



Full wwPDB X-ray Structure Validation Report

Jun 20, 2014 – 07:48 AM EDT

PDB ID : 4CBC
Title : Open-form NavMS Sodium Channel Pore (with C-terminal Domain) after thallium soak
Authors : Bagneris, C.; Naylor, C.E.; Wallace, B.A.
Deposited on : 2013-10-12
Resolution : 2.66 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

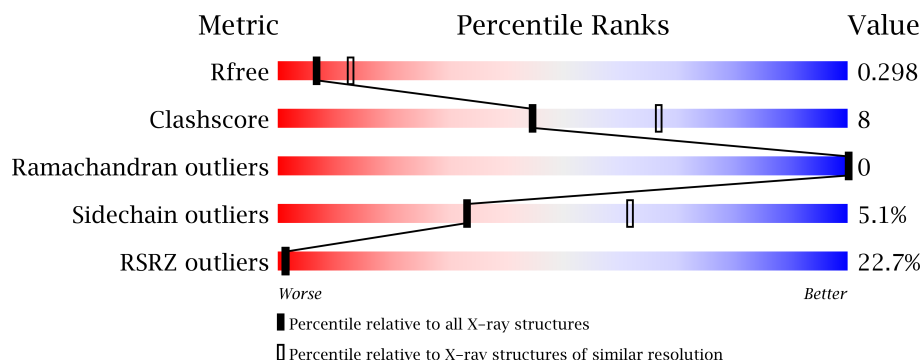
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
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) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.66 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	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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 ≥ 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	149	
1	B	149	
1	C	149	
1	D	149	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	2CV	B	1202	-	X
3	NA	A	1301	-	X
3	NA	A	1302	-	X
3	NA	A	1303	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	NA	C	1301	-	X
3	NA	C	1302	-	X
3	NA	C	1303	-	X

2 Entry composition i

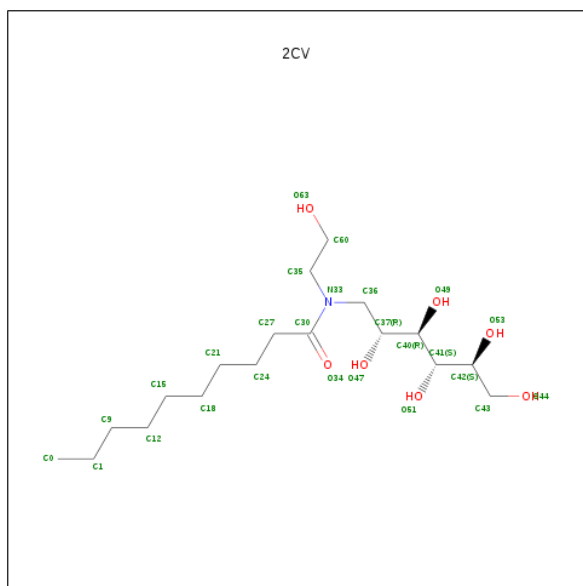
There are 4 unique types of molecules in this entry. The entry contains 3125 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ION TRANSPORT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	S	0	0	0
			728	493	107	122	6			
1	B	93	Total	C	N	O	S	0	0	0
			728	493	107	122	6			
1	C	93	Total	C	N	O	S	0	0	0
			728	493	107	122	6			
1	D	93	Total	C	N	O	S	0	0	0
			728	493	107	122	6			

- Molecule 2 is HEGA-10 (three-letter code: 2CV) (formula: C₁₈H₃₇NO₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	18	1	7		
2	A	1	Total	C	N	O	0	0
			13	11	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			26	18	1	7		
2	B	1	Total	C	N	O	0	0
			16	13	1	2		
2	C	1	Total	C	N	O	0	0
			18	13	1	4		
2	D	1	Total	C	N	O	0	0
			20	15	1	4		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		
3	C	3	Total	Na	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	21	Total	O	0	0
			21	21		
4	C	22	Total	O	0	0
			22	22		
4	D	23	Total	O	0	0
			23	23		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.90Å 331.70Å 79.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.47 – 2.66 45.47 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.47-2.66) 89.6 (45.47-2.66)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.276 , 0.299 0.272 , 0.298	Depositor DCC
R_{free} test set	1432 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	1.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 30842 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	3125	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.33 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.7424e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities 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: NA, 2CV

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	0.28	0/750	0.46	0/1027
1	B	0.28	0/750	0.48	0/1027
1	C	0.28	0/750	0.48	0/1027
1	D	0.28	0/750	0.49	0/1027
All	All	0.28	0/3000	0.48	0/4108

There are no bond length outliers.

There are no bond angle outliers.

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	728	0	738	15	0
1	B	728	0	738	15	0
1	C	728	0	738	8	0
1	D	728	0	738	13	0
2	A	39	0	56	5	0
2	B	42	0	61	3	0
2	C	18	0	22	2	0
2	D	20	0	29	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	C	3	0	0	0	0
4	A	22	0	0	6	0
4	B	21	0	0	4	0
4	C	22	0	0	3	0
4	D	23	0	0	3	0
All	All	3125	0	3120	52	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 8.

All (52) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:183:GLY:O	4:B:2016:HOH:O	1.93	0.85
1:D:159:GLU:OE2	4:D:2008:HOH:O	1.95	0.84
1:C:196:TRP:HE1	2:C:1201:2CV:H47	1.38	0.69
1:D:201:PRO:HA	1:D:204:MET:HE2	1.83	0.61
1:A:193:PRO:HB2	2:A:1201:2CV:H41	1.84	0.59
1:A:159:GLU:OE2	4:A:2010:HOH:O	2.17	0.58
4:B:2006:HOH:O	1:C:155:ALA:O	2.17	0.58
1:C:159:GLU:OE2	4:C:2011:HOH:O	2.16	0.57
1:C:191:VAL:O	4:C:2021:HOH:O	2.17	0.57
1:D:193:PRO:O	2:D:1201:2CV:O47	2.22	0.56
1:B:182:MET:O	4:B:2015:HOH:O	2.18	0.54
1:A:182:MET:O	4:A:2016:HOH:O	2.18	0.54
1:B:157:PHE:CZ	1:B:188:VAL:HA	2.44	0.52
1:A:142:PHE:HZ	1:A:172:PHE:HA	1.74	0.52
4:A:2008:HOH:O	1:D:155:ALA:O	2.19	0.51
2:A:1201:2CV:H212	1:B:169:TYR:HB2	1.92	0.50
1:A:157:PHE:CZ	1:A:188:VAL:HA	2.46	0.50
1:D:142:PHE:HD1	1:D:168:LEU:HD12	1.78	0.49
1:D:157:PHE:CZ	1:D:188:VAL:HA	2.48	0.49
1:B:142:PHE:HD1	1:B:168:LEU:HD12	1.76	0.49
1:A:164:LEU:HD22	1:A:168:LEU:HD22	1.96	0.48
1:B:142:PHE:HZ	1:B:172:PHE:HA	1.78	0.48
1:A:193:PRO:O	2:A:1201:2CV:O47	2.26	0.48
1:B:159:GLU:OE2	4:B:2010:HOH:O	2.20	0.47
1:A:135:ALA:O	1:A:139:THR:OG1	2.19	0.47
1:A:183:GLY:O	4:A:2017:HOH:O	2.21	0.47
1:A:142:PHE:HD1	1:A:168:LEU:HD12	1.80	0.47
1:B:135:ALA:O	1:B:139:THR:OG1	2.25	0.47
1:B:138:LEU:O	1:B:142:PHE:HB2	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:2011:HOH:O	1:D:156:THR:O	2.20	0.46
1:C:152:LEU:O	4:C:2008:HOH:O	2.21	0.45
1:D:152:LEU:O	4:D:2006:HOH:O	2.21	0.45
1:D:146:ALA:O	1:D:150:THR:OG1	2.30	0.45
1:A:187:PRO:HB3	4:A:2018:HOH:O	2.17	0.44
1:B:145:ALA:HB2	2:B:1202:2CV:H01C	2.00	0.43
1:C:196:TRP:NE1	2:C:1201:2CV:O47	2.35	0.43
2:B:1201:2CV:H352	2:B:1201:2CV:H272	1.75	0.43
1:D:164:LEU:HD22	1:D:168:LEU:HD22	2.00	0.43
1:D:187:PRO:O	4:D:2016:HOH:O	2.21	0.43
1:C:179:SER:HA	1:D:178:GLU:OE2	2.19	0.42
2:A:1201:2CV:H601	1:B:166:LYS:HG2	2.02	0.42
1:D:216:GLY:O	1:D:220:ASP:HB2	2.20	0.42
1:A:203:ILE:O	1:A:207:THR:HB	2.20	0.41
1:B:175:MET:SD	1:B:206:THR:HB	2.60	0.41
1:B:216:GLY:O	1:B:220:ASP:HB2	2.20	0.41
1:B:203:ILE:O	1:B:207:THR:HB	2.19	0.41
1:A:196:TRP:HB2	1:A:200:ILE:HD13	2.02	0.41
1:A:163:ASP:HB2	1:A:166:LYS:H	1.84	0.41
1:C:164:LEU:HD22	1:C:168:LEU:HD22	2.03	0.41
1:A:209:THR:O	1:A:213:LEU:N	2.52	0.41
2:A:1201:2CV:H181	1:B:168:LEU:HB3	2.03	0.41
2:B:1201:2CV:H361	2:B:1201:2CV:H602	1.78	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	91/149 (61%)	89 (98%)	2 (2%)	0	100	100
1	B	91/149 (61%)	88 (97%)	3 (3%)	0	100	100
1	C	91/149 (61%)	90 (99%)	1 (1%)	0	100	100
1	D	91/149 (61%)	90 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	364/596 (61%)	357 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	79/129 (61%)	75 (95%)	4 (5%)	33	62
1	B	79/129 (61%)	75 (95%)	4 (5%)	33	62
1	C	79/129 (61%)	75 (95%)	4 (5%)	33	62
1	D	79/129 (61%)	75 (95%)	4 (5%)	33	62
All	All	316/516 (61%)	300 (95%)	16 (5%)	33	62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	142	PHE
1	A	164	LEU
1	A	168	LEU
1	B	137	LEU
1	B	142	PHE
1	B	164	LEU
1	B	168	LEU
1	C	137	LEU
1	C	142	PHE
1	C	164	LEU
1	C	168	LEU
1	D	137	LEU
1	D	142	PHE
1	D	164	LEU
1	D	168	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
2	2CV	A	1201	-	25,25,25	0.17	0	30,30,30	0.45	0
2	2CV	A	1202	-	11,12,25	0.30	0	11,12,30	0.27	0
2	2CV	B	1201	-	25,25,25	0.19	0	30,30,30	0.29	0
2	2CV	B	1202	-	14,15,25	0.13	0	14,16,30	0.60	1 (7%)
2	2CV	C	1201	-	16,17,25	4.23	2 (12%)	16,19,30	0.54	0
2	2CV	D	1201	-	18,19,25	3.70	1 (5%)	18,21,30	0.33	0

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
2	2CV	A	1201	-	-	0/34/34/34	0/0/0/0
2	2CV	A	1202	-	-	0/9/11/34	0/0/0/0
2	2CV	B	1201	-	-	0/34/34/34	0/0/0/0
2	2CV	B	1202	-	-	0/16/16/34	0/0/0/0
2	2CV	C	1201	-	-	0/18/20/34	0/0/0/0
2	2CV	D	1201	-	-	0/20/22/34	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	2CV	O49-C40	15.70	1.42	1.25
2	C	1201	2CV	O49-C40	15.68	1.42	1.25
2	C	1201	2CV	C9-C12	-6.37	1.52	1.55

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	2CV	C35-N33-C30	2.06	123.16	119.39

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, 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	93/149 (62%)	1.38	22 (23%) 1 1	38, 58, 134, 157	0
1	B	93/149 (62%)	1.37	20 (21%) 1 1	37, 56, 137, 168	0
1	C	93/149 (62%)	1.34	22 (23%) 1 1	41, 56, 143, 168	0
1	D	93/149 (62%)	1.33	18 (19%) 2 2	38, 57, 143, 169	0
All	All	372/596 (62%)	1.35	82 (22%) 1 1	37, 57, 143, 169	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	222	MET	9.4
1	D	222	MET	7.9
1	C	214	PHE	7.5
1	D	214	PHE	7.4
1	B	140	VAL	6.7
1	D	218	ILE	6.3
1	B	222	MET	6.3
1	A	222	MET	6.3
1	D	138	LEU	6.2
1	A	144	ILE	6.0
1	A	140	VAL	5.6
1	C	210	VAL	5.4
1	D	217	ILE	5.2
1	B	220	ASP	5.2
1	A	208	PHE	5.1
1	B	144	ILE	4.9
1	C	138	LEU	4.7
1	A	141	VAL	4.7
1	A	219	VAL	4.6
1	B	141	VAL	4.4
1	D	213	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	219	VAL	4.4
1	C	217	ILE	4.2
1	C	220	ASP	4.2
1	D	220	ASP	4.2
1	C	213	LEU	4.1
1	C	143	TYR	4.1
1	A	134	VAL	4.1
1	A	220	ASP	4.1
1	D	143	TYR	4.1
1	B	221	ALA	4.0
1	A	204	MET	3.9
1	D	219	VAL	3.8
1	C	218	ILE	3.8
1	B	208	PHE	3.7
1	C	219	VAL	3.5
1	B	134	VAL	3.4
1	A	209	THR	3.3
1	D	132	GLY	3.2
1	A	138	LEU	3.2
1	A	221	ALA	3.1
1	D	210	VAL	3.1
1	A	137	LEU	3.0
1	C	209	THR	3.0
1	B	204	MET	2.9
1	D	209	THR	2.8
1	D	207	THR	2.8
1	D	134	VAL	2.8
1	C	207	THR	2.8
1	D	131	VAL	2.8
1	B	138	LEU	2.7
1	B	137	LEU	2.6
1	A	160	TRP	2.6
1	B	214	PHE	2.5
1	C	135	ALA	2.5
1	B	205	LEU	2.5
1	C	211	LEU	2.5
1	C	134	VAL	2.4
1	A	216	GLY	2.3
1	C	132	GLY	2.3
1	B	209	THR	2.3
1	C	221	ALA	2.3
1	A	215	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	198	PHE	2.3
1	D	221	ALA	2.2
1	D	139	THR	2.2
1	A	205	LEU	2.2
1	B	179	SER	2.2
1	B	160	TRP	2.2
1	B	172	PHE	2.2
1	A	197	VAL	2.1
1	B	215	ILE	2.1
1	A	172	PHE	2.1
1	C	202	PHE	2.1
1	D	188	VAL	2.1
1	A	136	ALA	2.0
1	C	131	VAL	2.0
1	A	214	PHE	2.0
1	A	201	PRO	2.0
1	B	216	GLY	2.0
1	C	175	MET	2.0
1	C	181	SER	2.0

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NA	A	1303	1/1	1.67	139.65	79,79,79,79	1
3	NA	A	1302	1/1	0.85	29.14	91,91,91,91	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	A	1301	1/1	0.82	27.19	89,89,89,89	1
3	NA	C	1302	1/1	0.48	17.79	51,51,51,51	1
3	NA	C	1301	1/1	0.77	15.88	70,70,70,70	1
3	NA	C	1303	1/1	0.71	10.46	77,77,77,77	1
2	2CV	B	1202	16/26	0.49	2.88	79,83,98,103	0
2	2CV	A	1202	13/26	0.43	1.79	63,80,83,88	0
2	2CV	B	1201	26/26	0.34	1.78	55,76,98,103	0
2	2CV	A	1201	26/26	0.32	1.60	49,70,106,111	0
2	2CV	D	1201	20/26	0.22	0.49	43,75,91,100	0
2	2CV	C	1201	18/26	0.17	-0.93	40,75,94,95	0

6.5 Other polymers ⓘ

There are no such residues in this entry.