



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:34 PM GMT

PDB ID : 4PA6
Title : Structure of NavMS pore and C-terminal domain crystallised in the presence of channel blocking compound
Authors : Naylor, C.E.; Bagneris, C.; Wallace, B.A.
Deposited on : 2014-04-07
Resolution : 3.36 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtrriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

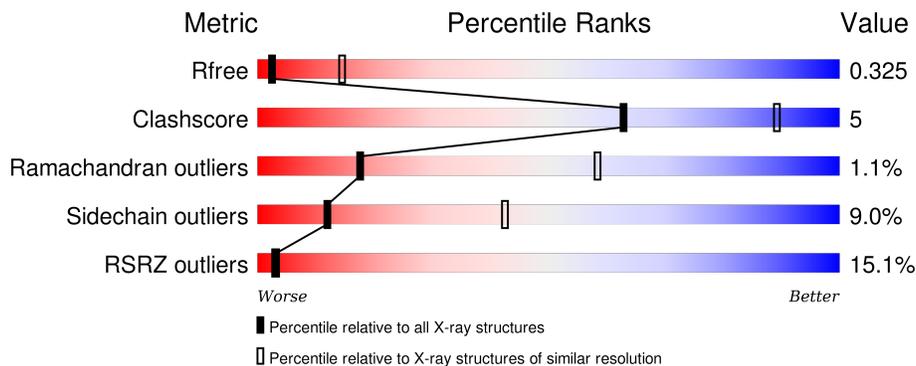
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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. 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	149	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">11%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 11%, orange 11%, yellow 14%, green 48%, grey 48%);"></div> <div style="text-align: left;">48%</div> </div>
1	B	149	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">10%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 10%, orange 10%, yellow 17%, green 44%, grey 44%);"></div> <div style="text-align: left;">44%</div> </div>
1	C	149	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">8%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 8%, orange 8%, yellow 10%, green 50%, grey 50%);"></div> <div style="text-align: left;">50%</div> </div>
1	D	149	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">7%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 7%, orange 7%, yellow 11%, green 49%, grey 49%);"></div> <div style="text-align: left;">49%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	12P	A	302	-	-	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 2950 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	92	Total 718	C 488	N 106	O 119	S 5	0	0	0
1	B	90	Total 711	C 483	N 104	O 119	S 5	0	0	0
1	C	91	Total 715	C 485	N 105	O 120	S 5	0	0	0
1	D	91	Total 712	C 482	N 105	O 120	S 5	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	GLY	-	expression tag	UNP A0L5S6
A	127	SER	-	expression tag	UNP A0L5S6
A	128	HIS	-	expression tag	UNP A0L5S6
A	129	MET	-	expression tag	UNP A0L5S6
B	126	GLY	-	expression tag	UNP A0L5S6
B	127	SER	-	expression tag	UNP A0L5S6
B	128	HIS	-	expression tag	UNP A0L5S6
B	129	MET	-	expression tag	UNP A0L5S6
C	126	GLY	-	expression tag	UNP A0L5S6
C	127	SER	-	expression tag	UNP A0L5S6
C	128	HIS	-	expression tag	UNP A0L5S6
C	129	MET	-	expression tag	UNP A0L5S6
D	126	GLY	-	expression tag	UNP A0L5S6
D	127	SER	-	expression tag	UNP A0L5S6
D	128	HIS	-	expression tag	UNP A0L5S6
D	129	MET	-	expression tag	UNP A0L5S6

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			16	10 6		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		
4	C	2	Total	Na	0	0
			2	2		

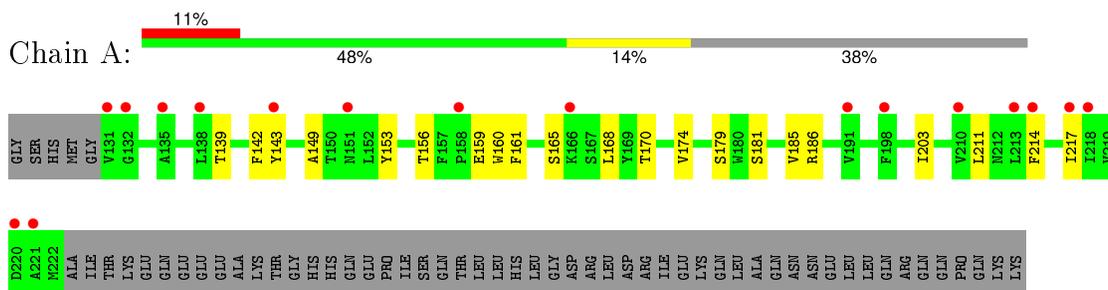
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	2	Total	O	0	0
			2	2		
5	C	5	Total	O	0	0
			5	5		
5	D	6	Total	O	0	0
			6	6		

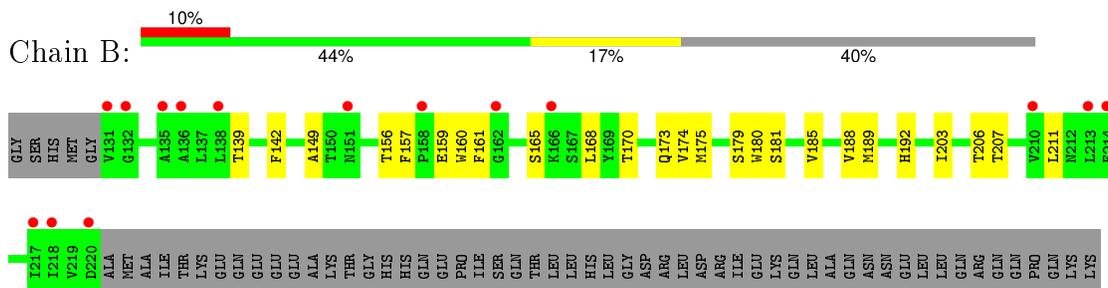
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

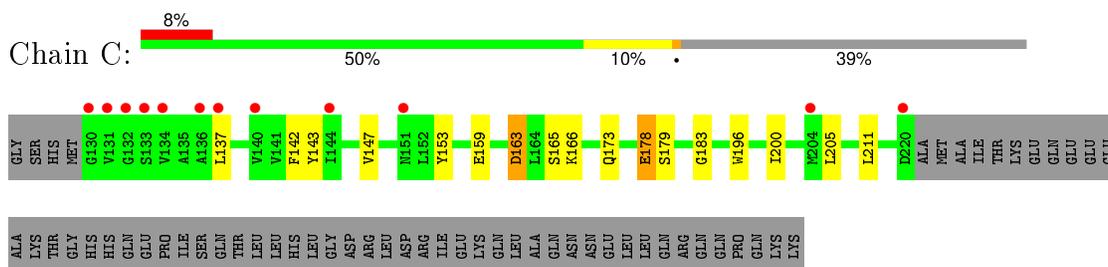
- Molecule 1: Ion transport protein



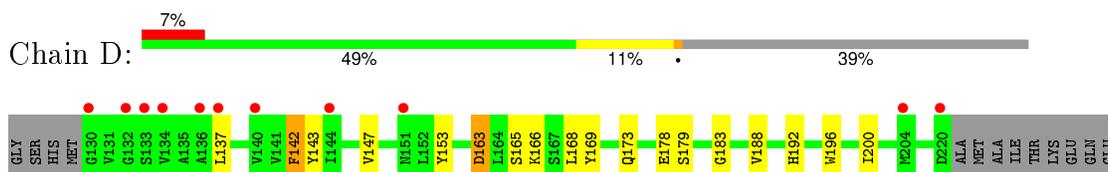
- Molecule 1: Ion transport protein



- Molecule 1: Ion transport protein



- Molecule 1: Ion transport protein



GLU
GLU
ALA
LYS
THR
GLY
HIS
HIS
GLN
GLU
PRO
ILE
SER
GLN
THR
LEU
LEU
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ASP
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ASP
ARG
ILE
GLU
LYS
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LEU
ALA
GLN
ASN
ASN
GLU
LEU
LEU
GLN
ARG
GLN
GLN
PRO
GLN
LYS
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.93Å 324.57Å 79.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.77 – 3.36 44.77 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.77-3.36) 99.8 (44.77-3.36)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.32Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.302 , 0.342 0.294 , 0.325	Depositor DCC
R_{free} test set	792 reflections (5.48%)	DCC
Wilson B-factor (Å ²)	54.9	Xtrriage
Anisotropy	1.310	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 81.2	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.27$	Xtrriage
Outliers	3 of 15246 reflections (0.020%)	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	2950	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.24 % 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 1.3499e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 12P, 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	0.49	0/740	0.68	0/1015
1	B	0.49	0/733	0.67	0/1005
1	C	0.52	0/737	0.67	0/1010
1	D	0.52	0/734	0.67	0/1006
All	All	0.51	0/2944	0.67	0/4036

There are no bond length outliers.

There are no bond angle outliers.

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	718	0	726	8	0
1	B	711	0	721	12	0
1	C	715	0	724	4	0
1	D	712	0	715	7	0
2	A	15	0	16	1	0
2	B	15	0	16	0	0
2	C	15	0	16	2	0
2	D	15	0	16	0	0
3	A	16	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	5	0	0	0	0
5	D	6	0	0	0	0
All	All	2950	0	2971	31	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 5.

All (31) 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:C:301:2CV:H212	1:D:169:TYR:HB2	1.76	0.68
1:C:196:TRP:HB2	1:C:200:ILE:HD12	1.88	0.56
1:C:179:SER:HB3	1:C:183:GLY:HA3	1.89	0.55
2:C:301:2CV:O34	2:C:301:2CV:H37	2.07	0.55
1:A:160:TRP:HB3	1:A:170:THR:HG21	1.89	0.55
1:D:179:SER:HB3	1:D:183:GLY:HA3	1.88	0.54
1:D:196:TRP:HB2	1:D:200:ILE:HD12	1.88	0.54
1:B:160:TRP:HB3	1:B:170:THR:HG21	1.91	0.53
1:A:149:ALA:HB1	1:A:161:PHE:CD1	2.45	0.52
1:B:181:SER:HA	1:B:185:VAL:HB	1.96	0.47
1:B:157:PHE:CZ	1:B:188:VAL:HA	2.51	0.46
1:B:149:ALA:HB1	1:B:161:PHE:CD1	2.52	0.45
1:C:163:ASP:H	1:C:166:LYS:HD2	1.80	0.45
1:B:175:MET:HG3	1:B:206:THR:HB	1.99	0.44
1:A:174:VAL:HG13	1:A:203:ILE:HD11	1.98	0.44
1:B:175:MET:O	1:B:207:THR:HG22	2.18	0.44
1:A:165:SER:HA	1:A:168:LEU:HD12	2.00	0.43
1:B:165:SER:HA	1:B:168:LEU:HD12	2.01	0.43
1:A:214:PHE:HA	1:A:217:ILE:HD12	2.01	0.43
1:C:143:TYR:O	1:C:147:VAL:HG23	2.18	0.43
1:B:180:TRP:HE3	1:B:185:VAL:HG21	1.84	0.42
1:A:181:SER:HA	1:A:185:VAL:HB	2.01	0.42
1:A:181:SER:HB3	1:B:173:GLN:HG3	2.00	0.42
1:D:143:TYR:O	1:D:147:VAL:HG23	2.19	0.42
2:A:301:2CV:O34	2:A:301:2CV:H37	2.19	0.42
1:D:188:VAL:HG13	1:D:192:HIS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ASP:H	1:D:166:LYS:HD2	1.86	0.41
1:B:174:VAL:HG13	1:B:203:ILE:HD11	2.03	0.41
1:D:142:PHE:HD2	1:D:168:LEU:HD23	1.87	0.40
1:B:189:MET:HA	1:B:192:HIS:O	2.21	0.40
1:A:186:ARG:NH2	1:B:170:THR:HG23	2.36	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	90/149 (60%)	81 (90%)	8 (9%)	1 (1%)	17	58
1	B	88/149 (59%)	81 (92%)	6 (7%)	1 (1%)	17	58
1	C	89/149 (60%)	83 (93%)	5 (6%)	1 (1%)	17	58
1	D	89/149 (60%)	83 (93%)	5 (6%)	1 (1%)	17	58
All	All	356/596 (60%)	328 (92%)	24 (7%)	4 (1%)	17	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	SER
1	B	179	SER
1	C	178	GLU
1	D	178	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	77/129 (60%)	70 (91%)	7 (9%)	12	41
1	B	78/129 (60%)	73 (94%)	5 (6%)	22	60
1	C	78/129 (60%)	68 (87%)	10 (13%)	5	23
1	D	77/129 (60%)	71 (92%)	6 (8%)	16	51
All	All	310/516 (60%)	282 (91%)	28 (9%)	12	42

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	THR
1	A	142	PHE
1	A	143	TYR
1	A	153	TYR
1	A	156	THR
1	A	159	GLU
1	A	211	LEU
1	B	139	THR
1	B	142	PHE
1	B	156	THR
1	B	159	GLU
1	B	211	LEU
1	C	137	LEU
1	C	142	PHE
1	C	153	TYR
1	C	159	GLU
1	C	163	ASP
1	C	165	SER
1	C	173	GLN
1	C	178	GLU
1	C	205	LEU
1	C	211	LEU
1	D	137	LEU
1	D	142	PHE
1	D	153	TYR
1	D	163	ASP
1	D	165	SER
1	D	173	GLN

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

sidechains are listed below:

Mol	Chain	Res	Type
1	D	192	HIS

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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	301	-	14,14,25	0.20	0	14,16,30	0.75	1 (7%)
3	12P	A	302	-	15,15,36	0.17	0	14,14,35	0.11	0
2	2CV	B	301	-	14,14,25	0.20	0	14,16,30	0.58	0
2	2CV	C	301	-	14,14,25	0.23	0	14,16,30	1.29	1 (7%)
2	2CV	D	300	-	14,14,25	0.22	0	14,16,30	0.56	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	301	-	-	0/17/17/34	0/0/0/0
3	12P	A	302	-	-	0/13/13/34	0/0/0/0
2	2CV	B	301	-	-	0/17/17/34	0/0/0/0
2	2CV	C	301	-	-	0/17/17/34	0/0/0/0
2	2CV	D	300	-	-	0/17/17/34	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	2CV	C35-N33-C36	-4.27	111.30	115.45
2	A	301	2CV	C35-N33-C36	-2.10	113.40	115.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	2CV	1	0
2	C	301	2CV	2	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, 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	92/149 (61%)	0.88	17 (18%) 2 2	44, 59, 140, 214	0
1	B	90/149 (60%)	0.80	15 (16%) 2 2	45, 60, 138, 203	0
1	C	91/149 (61%)	0.82	12 (13%) 4 4	43, 62, 130, 197	0
1	D	91/149 (61%)	0.75	11 (12%) 6 5	43, 60, 134, 201	0
All	All	364/596 (61%)	0.81	55 (15%) 3 3	43, 60, 140, 214	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	133	SER	6.6
1	A	131	VAL	6.6
1	C	133	SER	6.1
1	A	132	GLY	5.6
1	C	220	ASP	5.5
1	B	131	VAL	5.5
1	B	132	GLY	4.3
1	D	220	ASP	4.3
1	A	151	ASN	3.9
1	C	134	VAL	3.7
1	A	217	ILE	3.5
1	D	204	MET	3.3
1	A	221	ALA	3.3
1	B	151	ASN	3.2
1	B	217	ILE	3.2
1	B	158	PRO	3.2
1	C	204	MET	3.1
1	B	135	ALA	3.1
1	B	214	PHE	3.0
1	C	132	GLY	3.0
1	B	210	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	158	PRO	2.9
1	D	134	VAL	2.9
1	D	137	LEU	2.9
1	D	144	ILE	2.9
1	A	213	LEU	2.9
1	B	213	LEU	2.9
1	A	135	ALA	2.8
1	D	140	VAL	2.8
1	C	130	GLY	2.8
1	A	210	VAL	2.7
1	A	220	ASP	2.7
1	D	132	GLY	2.7
1	D	130	GLY	2.6
1	B	138	LEU	2.6
1	C	140	VAL	2.5
1	C	144	ILE	2.5
1	A	191	VAL	2.4
1	B	162	GLY	2.4
1	A	198	PHE	2.4
1	C	136	ALA	2.3
1	D	136	ALA	2.3
1	A	143	TYR	2.3
1	A	214	PHE	2.3
1	C	131	VAL	2.3
1	A	218	ILE	2.2
1	B	136	ALA	2.2
1	A	166	LYS	2.2
1	B	166	LYS	2.2
1	A	138	LEU	2.2
1	C	151	ASN	2.2
1	D	151	ASN	2.2
1	B	220	ASP	2.1
1	C	137	LEU	2.0
1	B	218	ILE	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 [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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	12P	A	302	16/37	0.69	0.46	1.85	74,85,89,89	0
2	2CV	D	300	15/26	0.67	0.38	1.82	86,92,95,97	0
2	2CV	C	301	15/26	0.71	0.35	1.27	89,98,107,109	0
2	2CV	B	301	15/26	0.81	0.35	0.55	92,98,103,106	0
2	2CV	A	301	15/26	0.81	0.31	0.21	97,102,104,104	0
4	NA	C	302	1/1	0.98	0.84	-	50,50,50,50	1
4	NA	B	302	1/1	1.00	0.66	-	51,51,51,51	1
4	NA	C	303	1/1	0.97	0.66	-	54,54,54,54	1
4	NA	A	303	1/1	0.95	0.80	-	52,52,52,52	1

6.5 Other polymers [i](#)

There are no such residues in this entry.