



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:18 am BST

PDB ID : 4A1X  
Title : Co-Complex structure of NS3-4A protease with the inhibitory peptide CP5-46-A (Synchrotron data)  
Authors : Schmelz, S.; Kuegler, J.; Collins, J.; Heinz, D.  
Deposited on : 2011-09-20  
Resolution : 1.90 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

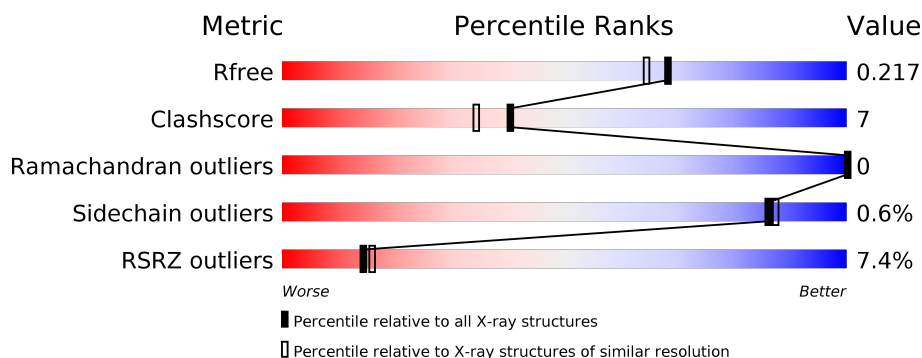
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	203	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>
1	B	203	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>•</div> </div> </div>
2	C	21	<div> <div>24%</div> <div> <div></div> <div>71%</div> <div>10%</div> <div>19%</div> </div> </div>
2	D	21	<div> <div>14%</div> <div> <div></div> <div>67%</div> <div>5%</div> <div>29%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3397 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 NONSTRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	10	0
			1461	908	263	277	13			
1	B	194	Total	C	N	O	S	0	10	0
			1479	917	269	281	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	LYS	-	linker	UNP P26662
A	0	GLY	-	linker	UNP P26662
A	1	GLY	-	linker	UNP P26662
A	181	GLY	-	expression tag	UNP P26662
A	182	SER	-	expression tag	UNP P26662
A	183	HIS	-	expression tag	UNP P26662
A	184	HIS	-	expression tag	UNP P26662
A	185	HIS	-	expression tag	UNP P26662
A	186	HIS	-	expression tag	UNP P26662
A	187	HIS	-	expression tag	UNP P26662
A	188	HIS	-	expression tag	UNP P26662
A	26	ARG	LYS	SEE REMARK 999	UNP P26662
A	30	GLU	ASP	SEE REMARK 999	UNP P26662
A	36	VAL	LEU	SEE REMARK 999	UNP P26662
A	86	GLN	PRO	SEE REMARK 999	UNP P26662
A	94	LEU	MET	SEE REMARK 999	UNP P26662
A	114	ILE	VAL	variant	UNP P26662
A	132	VAL	ILE	variant	UNP P26662
A	150	ALA	VAL	SEE REMARK 999	UNP P26662
A	170	VAL	ILE	SEE REMARK 999	UNP P26662
B	-1	LYS	-	linker	UNP P26662
B	0	GLY	-	linker	UNP P26662
B	1	GLY	-	linker	UNP P26662
B	181	GLY	-	expression tag	UNP P26662

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Chain	Residue	Modelled	Actual	Comment	Reference
B	182	SER	-	expression tag	UNP P26662
B	183	HIS	-	expression tag	UNP P26662
B	184	HIS	-	expression tag	UNP P26662
B	185	HIS	-	expression tag	UNP P26662
B	186	HIS	-	expression tag	UNP P26662
B	187	HIS	-	expression tag	UNP P26662
B	188	HIS	-	expression tag	UNP P26662
B	26	ARG	LYS	SEE REMARK 999	UNP P26662
B	30	GLU	ASP	SEE REMARK 999	UNP P26662
B	36	VAL	LEU	SEE REMARK 999	UNP P26662
B	86	GLN	PRO	SEE REMARK 999	UNP P26662
B	94	LEU	MET	SEE REMARK 999	UNP P26662
B	114	ILE	VAL	SEE REMARK 999	UNP P26662
B	132	VAL	ILE	variant	UNP P26662
B	150	ALA	VAL	SEE REMARK 999	UNP P26662
B	170	VAL	ILE	SEE REMARK 999	UNP P26662

- Molecule 2 is a protein called CP5-46-A PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	S	0	0	0
			132	86	22	23	1			
2	D	15	Total	C	N	O	S	0	0	0
			117	78	17	21	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total	Cl	0	0
			6	6		
4	A	7	Total	Cl	0	0
			7	7		

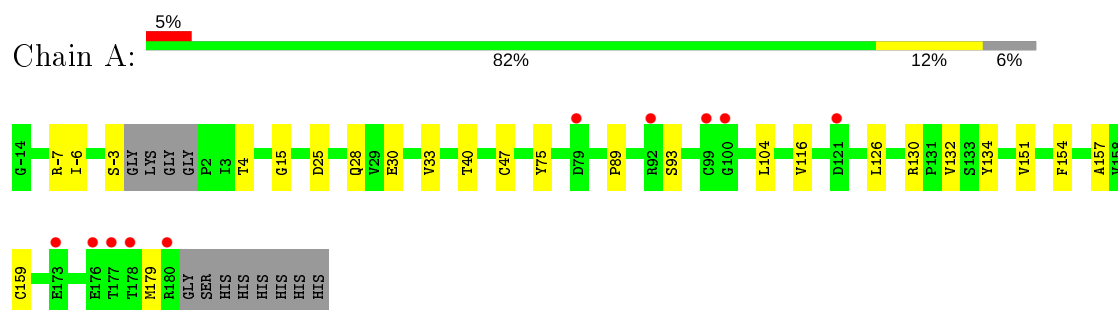
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total 87	O 87	0	0
5	B	95	Total 95	O 95	0	0
5	C	8	Total 8	O 8	0	0
5	D	3	Total 3	O 3	0	0

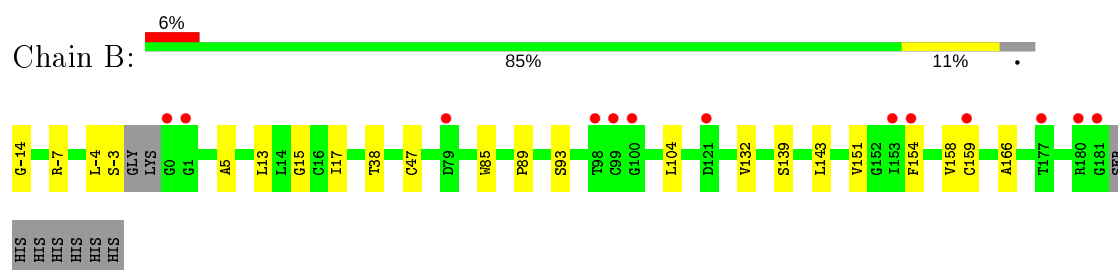
### 3 Residue-property plots [i](#)

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

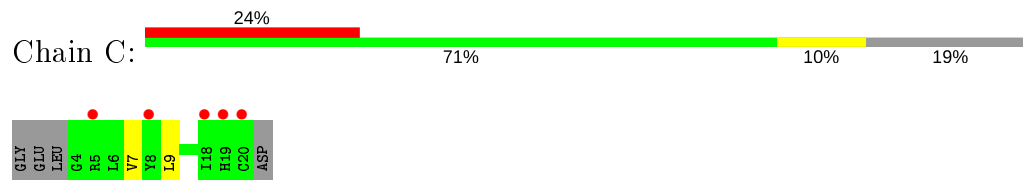
- Molecule 1: NONSTRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3



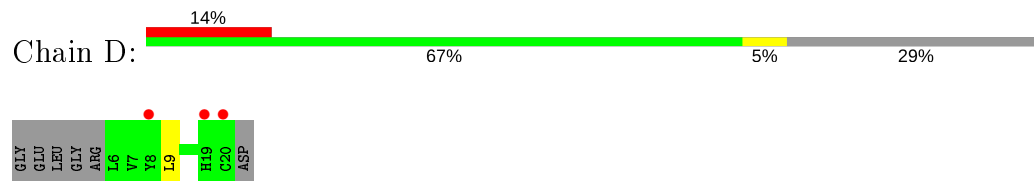
- Molecule 1: NONSTRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3



- Molecule 2: CP5-46-A PEPTIDE



- Molecule 2: CP5-46-A PEPTIDE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.32Å 93.32Å 82.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.82 – 1.90 19.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	80.8 (80.82-1.90) 99.7 (19.96-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.182 , 0.182 0.181 , 0.217	Depositor DCC
$R_{free}$ test set	1619 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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: ZN, CL

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	0.50	0/1487	0.66	0/2023
1	B	0.51	1/1505 (0.1%)	0.67	0/2046
2	C	0.58	0/136	0.62	0/185
2	D	0.56	0/121	0.63	0/166
All	All	0.51	1/3249 (0.0%)	0.66	0/4420

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	TRP	CD2-CE2	5.13	1.47	1.41

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	1461	0	1466	26	0
1	B	1479	0	1490	20	0
2	C	132	0	126	7	0
2	D	117	0	110	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	7	0	0	3	0
4	B	6	0	0	4	0
5	A	87	0	0	2	0
5	B	95	0	0	2	0
5	C	8	0	0	0	0
5	D	3	0	0	0	0
All	All	3397	0	3192	46	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 7.

All (46) 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)
1:B:89[B]:PRO:O	5:B:2040:HOH:O	1.66	1.12
1:A:89[B]:PRO:O	5:A:2035:HOH:O	2.04	0.74
1:B:154:PHE:CZ	2:D:9:LEU:HD13	2.22	0.74
1:B:154:PHE:CZ	2:D:9:LEU:CD1	2.71	0.73
1:A:132:VAL:CG1	1:A:159[A]:CYS:SG	2.82	0.67
1:A:132:VAL:HG11	1:A:159[A]:CYS:SG	2.37	0.65
1:A:132:VAL:HG22	4:A:1188:CL:CL	2.35	0.64
1:B:132:VAL:HG11	1:B:159:CYS:SG	2.38	0.64
1:B:154:PHE:CE2	2:D:9:LEU:HD13	2.36	0.61
1:A:25:ASP:OD2	5:A:2007:HOH:O	2.16	0.60
1:A:132:VAL:HG12	1:A:159[A]:CYS:SG	2.43	0.58
1:A:154:PHE:CZ	2:C:9:LEU:CD1	2.87	0.58
1:B:-4:LEU:O	1:B:-3:SER:HB2	2.04	0.57
1:B:47[B]:CYS:HG	1:B:93:SER:HG	1.50	0.56
1:A:130:ARG:HD2	1:A:134:TYR:CE2	2.41	0.56
1:B:139[B]:SER:OG	5:B:2053:HOH:O	2.17	0.55
1:A:157:ALA:HB2	2:C:9:LEU:HD11	1.89	0.53
1:A:159[B]:CYS:SG	2:C:7:VAL:CG2	2.98	0.52
1:B:132:VAL:HG22	4:B:1184:CL:CL	2.46	0.52
1:A:104:LEU:HD22	1:A:151[A]:VAL:HG21	1.92	0.51
1:A:104:LEU:HD22	1:A:151[B]:VAL:HG11	1.92	0.51
1:B:154:PHE:HZ	2:D:9:LEU:CD1	2.24	0.49
1:B:-14:GLY:HA2	4:B:1186:CL:CL	2.49	0.49
1:B:104:LEU:HD22	1:B:151[A]:VAL:HG21	1.95	0.49
1:A:28:GLN:NE2	1:A:30:GLU:OE2	2.46	0.48
1:B:13:LEU:O	1:B:17:ILE:HG12	2.12	0.48
1:A:159[B]:CYS:SG	2:C:7:VAL:HG21	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:OG1	4:A:1182:CL:CL	2.69	0.47
1:A:154:PHE:CZ	2:C:9:LEU:HD12	2.49	0.47
1:B:143:LEU:HB3	1:B:151[B]:VAL:HG12	1.97	0.47
1:B:132:VAL:CG1	1:B:159:CYS:SG	3.04	0.46
1:A:154:PHE:HZ	2:C:9:LEU:CD1	2.30	0.45
1:A:-3:SER:HB3	1:A:4:THR:OG1	2.16	0.45
1:A:75:TYR:CZ	1:A:179:MET:HG2	2.52	0.44
1:A:151[B]:VAL:HG22	1:A:151[B]:VAL:O	2.18	0.43
1:A:130:ARG:HD2	1:A:134:TYR:CD2	2.53	0.43
1:A:-6:ILE:HB	1:A:33:VAL:HB	2.00	0.43
1:B:158:VAL:HB	1:B:166:ALA:HB3	2.00	0.43
1:A:116:VAL:HG22	1:A:126:LEU:HD23	2.01	0.42
1:A:159[B]:CYS:SG	2:C:7:VAL:HG23	2.59	0.42
1:B:15:GLY:HA3	4:B:1188:CL:CL	2.57	0.41
1:A:15:GLY:HA3	4:A:1183:CL:CL	2.58	0.41
1:B:-4:LEU:HD23	1:B:5:ALA:HB2	2.02	0.41
1:B:38:THR:HB	4:B:1185:CL:CL	2.57	0.40
1:A:47[B]:CYS:SG	1:A:93:SER:OG	2.67	0.40
1:B:-4:LEU:O	1:B:-3:SER:CB	2.70	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	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
1	B	200/203 (98%)	197 (98%)	3 (2%)	0	100	100
2	C	15/21 (71%)	14 (93%)	1 (7%)	0	100	100
2	D	13/21 (62%)	12 (92%)	1 (8%)	0	100	100
All	All	425/448 (95%)	418 (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	164/164 (100%)	163 (99%)	1 (1%)	86	87
1	B	165/164 (101%)	164 (99%)	1 (1%)	86	87
2	C	14/17 (82%)	14 (100%)	0	100	100
2	D	13/17 (76%)	13 (100%)	0	100	100
All	All	356/362 (98%)	354 (99%)	2 (1%)	86	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-7	ARG
1	B	-7	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	191/203 (94%)	0.21	10 (5%) 27 30	11, 24, 42, 60	0
1	B	194/203 (95%)	0.31	13 (6%) 17 20	12, 26, 49, 67	0
2	C	17/21 (80%)	1.20	5 (29%) 0 0	16, 32, 66, 72	0
2	D	15/21 (71%)	0.97	3 (20%) 1 1	17, 30, 64, 76	0
All	All	417/448 (93%)	0.32	31 (7%) 14 16	11, 26, 49, 76	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	ARG	5.1
2	D	20	CYS	4.9
2	C	19	HIS	4.7
1	B	181	GLY	4.5
1	B	99	CYS	4.2
2	C	20	CYS	4.2
1	B	0	GLY	4.0
1	A	79	ASP	3.8
1	A	177	THR	3.6
1	A	99	CYS	3.5
1	B	1	GLY	3.3
2	C	18	ILE	3.2
1	B	121	ASP	3.2
2	D	19	HIS	3.1
1	B	100	GLY	3.0
1	B	98	THR	2.9
1	B	177	THR	2.9
1	B	79	ASP	2.7
1	A	180	ARG	2.7
1	A	178	THR	2.7
2	C	5	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	8	TYR	2.3
1	A	173	GLU	2.2
1	B	159	CYS	2.2
1	A	100	GLY	2.2
1	A	121	ASP	2.2
1	B	153	ILE	2.1
1	A	92	ARG	2.1
2	D	8	TYR	2.0
1	B	154	PHE	2.0
1	A	176	GLU	2.0

## 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 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	A	1188	1/1	0.91	0.28	57,57,57,57	0
4	CL	B	1185	1/1	0.92	0.17	51,51,51,51	0
4	CL	B	1184	1/1	0.93	0.21	52,52,52,52	0
4	CL	B	1187	1/1	0.94	0.21	55,55,55,55	0
4	CL	A	1185	1/1	0.95	0.06	52,52,52,52	0
3	ZN	B	1182	1/1	0.95	0.13	62,62,62,62	0
3	ZN	A	1181	1/1	0.97	0.05	42,42,42,42	0
4	CL	B	1183	1/1	0.98	0.04	33,33,33,33	0
4	CL	A	1184	1/1	0.98	0.07	31,31,31,31	0
4	CL	A	1182	1/1	0.98	0.13	55,55,55,55	0
4	CL	A	1186	1/1	0.99	0.05	32,32,32,32	0
4	CL	A	1183	1/1	0.99	0.04	24,24,24,24	0
4	CL	B	1188	1/1	0.99	0.04	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	A	1187	1/1	0.99	0.12	45,45,45,45	0
4	CL	B	1186	1/1	0.99	0.04	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.