



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:56 PM GMT

PDB ID : 3AXF  
Title : Perrhenate binding to A11C/R153C ModA mutant  
Authors : He, C.; Aryal, B.P.; Brugarolas, P.  
Deposited on : 2011-04-04  
Resolution : 2.00 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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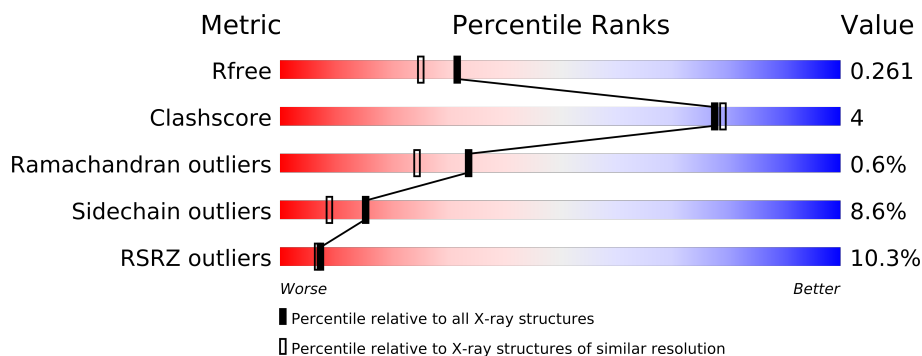
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	237	
1	B	237	
1	C	237	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5492 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.

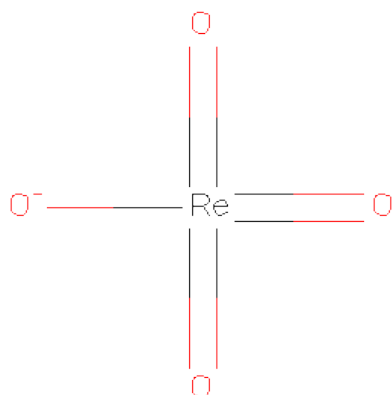
- Molecule 1 is a protein called Molybdate-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	8	0
			1804	1153	302	345	4			
1	B	231	Total	C	N	O	S	0	1	0
			1742	1111	291	336	4			
1	C	231	Total	C	N	O	S	0	7	0
			1785	1136	299	345	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P37329
A	-2	SER	-	EXPRESSION TAG	UNP P37329
A	-1	HIS	-	EXPRESSION TAG	UNP P37329
A	0	MET	-	EXPRESSION TAG	UNP P37329
A	11	CYS	ALA	ENGINEERED MUTATION	UNP P37329
A	153	CYS	ARG	ENGINEERED MUTATION	UNP P37329
B	-3	GLY	-	EXPRESSION TAG	UNP P37329
B	-2	SER	-	EXPRESSION TAG	UNP P37329
B	-1	HIS	-	EXPRESSION TAG	UNP P37329
B	0	MET	-	EXPRESSION TAG	UNP P37329
B	11	CYS	ALA	ENGINEERED MUTATION	UNP P37329
B	153	CYS	ARG	ENGINEERED MUTATION	UNP P37329
C	-3	GLY	-	EXPRESSION TAG	UNP P37329
C	-2	SER	-	EXPRESSION TAG	UNP P37329
C	-1	HIS	-	EXPRESSION TAG	UNP P37329
C	0	MET	-	EXPRESSION TAG	UNP P37329
C	11	CYS	ALA	ENGINEERED MUTATION	UNP P37329
C	153	CYS	ARG	ENGINEERED MUTATION	UNP P37329

- Molecule 2 is PERRHENATE (three-letter code: REO) (formula: O<sub>4</sub>Re).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	Re	0	0
			5	4	1		
2	B	1	Total	O	Re	0	0
			5	4	1		
2	C	1	Total	O	Re	0	0
			5	4	1		

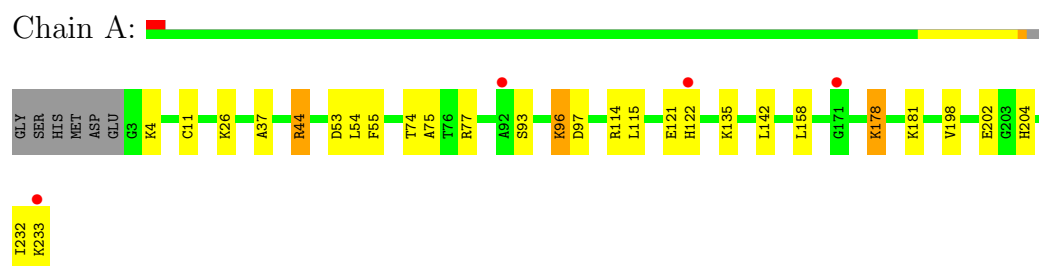
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	90	Total	O	0	0
			90	90		

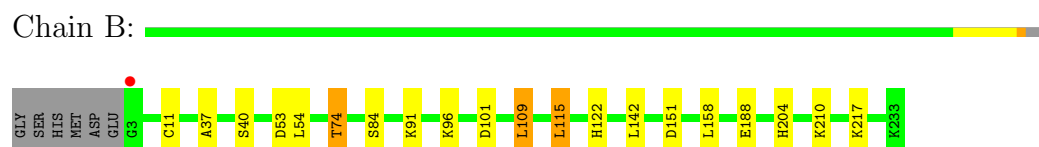
### 3 Residue-property plots

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.

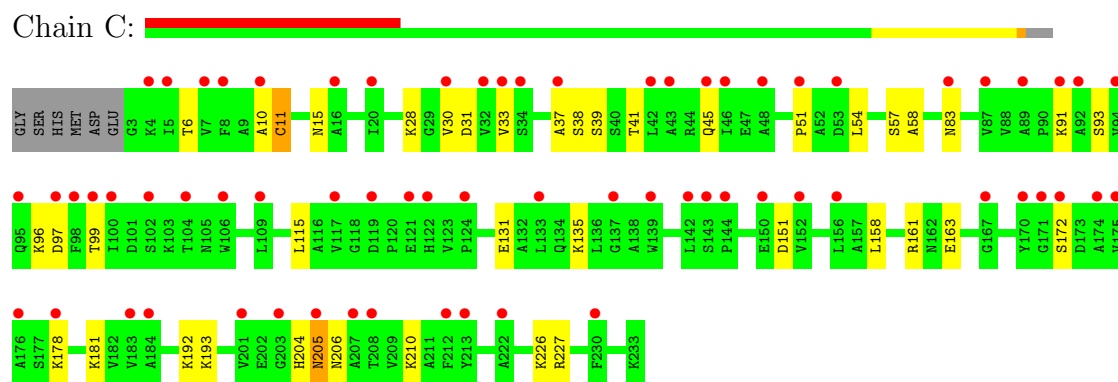
- Molecule 1: Molybdate-binding periplasmic protein



- Molecule 1: Molybdate-binding periplasmic protein



- Molecule 1: Molybdate-binding periplasmic protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.75Å 77.46Å 163.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 40.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.00) 100.0 (40.76-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.204 , 0.258 0.209 , 0.261	Depositor DCC
$R_{free}$ test set	2322 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46020 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5492	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: REO

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	1.22	8/1845 (0.4%)	0.95	3/2497 (0.1%)
1	B	1.28	5/1779 (0.3%)	1.00	5/2414 (0.2%)
1	C	0.79	0/1826	0.78	0/2479
All	All	1.12	13/5450 (0.2%)	0.91	8/7390 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	CYS	CB-SG	-22.15	1.44	1.82
1	B	188	GLU	CG-CD	7.11	1.62	1.51
1	A	96[A]	LYS	CE-NZ	6.58	1.65	1.49
1	A	96[B]	LYS	CE-NZ	6.58	1.65	1.49
1	B	37	ALA	CA-CB	6.33	1.65	1.52
1	B	188	GLU	CD-OE2	6.15	1.32	1.25
1	A	198	VAL	CB-CG1	5.74	1.64	1.52
1	A	55	PHE	CE2-CZ	5.46	1.47	1.37
1	B	11	CYS	CB-SG	-5.43	1.73	1.81
1	A	37	ALA	CA-CB	5.35	1.63	1.52
1	A	202	GLU	CD-OE2	-5.25	1.19	1.25
1	A	75	ALA	CA-CB	5.07	1.63	1.52
1	B	84	SER	CA-CB	5.04	1.60	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	LEU	CB-CG-CD2	7.02	122.93	111.00
1	A	44	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	101	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	11	CYS	CB-CA-C	-5.41	99.58	110.40
1	B	217	LYS	CD-CE-NZ	5.38	124.07	111.70
1	A	114	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	109	LEU	CB-CG-CD1	5.10	119.67	111.00
1	B	151	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	ILE	Peptide

## 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	1804	0	0	8	0
1	B	1742	0	0	3	0
1	C	1785	0	0	9	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	56	0	0	2	0
3	B	90	0	0	1	0
All	All	5492	0	0	20	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 4.

All (20) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:121:GLU:O	1:A:122[B]:HIS:CG	2.38	0.76
1:C:204:HIS:O	1:C:205[B]:ASN:CB	2.37	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:SER:O	1:A:181:LYS:NZ	2.27	0.67
1:B:53:ASP:OD1	1:B:204:HIS:CD2	2.50	0.63
1:A:44:ARG:NH2	3:A:421:HOH:O	2.34	0.60
1:C:83:ASN:ND2	1:C:172:SER:OG	2.41	0.53
1:A:53:ASP:OD1	1:A:204:HIS:CD2	2.61	0.53
1:C:11[B]:CYS:SG	1:C:151:ASP:OD2	2.68	0.52
1:B:74:THR:CG2	3:B:482:HOH:O	2.60	0.50
1:C:11[B]:CYS:SG	1:C:37:ALA:CA	3.00	0.49
1:A:178:LYS:N	1:A:178:LYS:CD	2.78	0.47
1:C:93:SER:O	1:C:181:LYS:NZ	2.49	0.46
1:B:40:SER:OG	1:B:122:HIS:ND1	2.50	0.45
1:A:204:HIS:CE1	3:A:449:HOH:O	2.70	0.45
1:A:121:GLU:O	1:A:122[B]:HIS:CD2	2.71	0.44
1:C:131:GLU:OE1	1:C:192:LYS:N	2.51	0.43
1:C:161:ARG:NE	1:C:163:GLU:OE2	2.51	0.43
1:C:39:SER:OG	1:C:58:ALA:N	2.52	0.42
1:A:121:GLU:C	1:A:122[B]:HIS:CG	2.93	0.41
1:C:37:ALA:O	1:C:38:SER:C	2.58	0.41

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	236/237 (100%)	229 (97%)	7 (3%)	0	100	100
1	B	230/237 (97%)	228 (99%)	2 (1%)	0	100	100
1	C	236/237 (100%)	214 (91%)	17 (7%)	5 (2%)	11	3
All	All	702/711 (99%)	671 (96%)	26 (4%)	5 (1%)	33	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	205[A]	ASN

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Mol	Chain	Res	Type
1	C	205[B]	ASN
1	C	10	ALA
1	C	97	ASP
1	C	51	PRO

### 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	190/187 (102%)	172 (90%)	18 (10%)	12	7
1	B	183/187 (98%)	174 (95%)	9 (5%)	35	28
1	C	189/187 (101%)	164 (87%)	25 (13%)	6	3
All	All	562/561 (100%)	510 (91%)	52 (9%)	15	7

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	26	LYS
1	A	54[A]	LEU
1	A	54[B]	LEU
1	A	74	THR
1	A	77	ARG
1	A	96[A]	LYS
1	A	96[B]	LYS
1	A	97	ASP
1	A	115	LEU
1	A	135	LYS
1	A	142	LEU
1	A	158	LEU
1	A	178	LYS
1	A	210	LYS
1	A	223	GLU
1	A	233[A]	LYS
1	A	233[B]	LYS
1	B	54	LEU

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Mol	Chain	Res	Type
1	B	74	THR
1	B	91	LYS
1	B	96	LYS
1	B	109	LEU
1	B	115	LEU
1	B	142	LEU
1	B	158	LEU
1	B	210	LYS
1	C	6	THR
1	C	11[A]	CYS
1	C	11[B]	CYS
1	C	15	ASN
1	C	28	LYS
1	C	30	VAL
1	C	31	ASP
1	C	33	VAL
1	C	41	THR
1	C	45	GLN
1	C	54[A]	LEU
1	C	54[B]	LEU
1	C	57	SER
1	C	91	LYS
1	C	96	LYS
1	C	99	THR
1	C	115	LEU
1	C	135	LYS
1	C	158	LEU
1	C	178	LYS
1	C	193	LYS
1	C	206	ASN
1	C	210	LYS
1	C	226	LYS
1	C	227	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 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 ⓘ

3 ligands are modelled in this entry.

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	REO	A	301	-	4,4,4	3.91	3 (75%)	0,6,6	0.00	-
2	REO	B	301	-	4,4,4	2.13	2 (50%)	0,6,6	0.00	-
2	REO	C	301	-	4,4,4	3.46	4 (100%)	0,6,6	0.00	-

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	REO	A	301	-	-	0/0/0/0	0/0/0/0
2	REO	B	301	-	-	0/0/0/0	0/0/0/0
2	REO	C	301	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	REO	RE-O13	4.89	1.91	1.69
2	A	301	REO	RE-O15	-4.51	1.62	1.73
2	C	301	REO	RE-O15	4.35	1.84	1.73
2	A	301	REO	RE-O14	3.75	1.86	1.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	REO	RE-O13	3.68	1.86	1.69
2	C	301	REO	RE-O14	3.35	1.84	1.69
2	C	301	REO	RE-O12	3.08	1.83	1.69
2	C	301	REO	RE-O13	2.85	1.82	1.69
2	B	301	REO	RE-O12	2.10	1.79	1.69

There are no bond angle outliers.

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	231/237 (97%)	0.12	4 (1%) 67 67	19, 36, 57, 67	1 (0%)
1	B	231/237 (97%)	-0.10	1 (0%) 90 91	18, 26, 40, 52	0
1	C	231/237 (97%)	1.56	67 (29%) 1 1	45, 67, 93, 117	0
All	All	693/711 (97%)	0.52	72 (10%) 7 6	18, 39, 81, 117	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	VAL	6.8
1	C	207	ALA	6.4
1	C	51	PRO	5.7
1	C	99	THR	5.5
1	C	32	VAL	5.3
1	C	122[A]	HIS	5.2
1	C	98	PHE	5.1
1	C	48	ALA	5.1
1	C	97	ASP	4.9
1	C	175	VAL	4.8
1	C	100	ILE	4.7
1	C	183	VAL	4.5
1	C	106	TRP	4.4
1	A	233[A]	LYS	4.4
1	C	222	ALA	4.2
1	C	94	VAL	4.0
1	C	20	ILE	4.0
1	C	203	GLY	4.0
1	C	4	LYS	3.9
1	C	104	THR	3.8
1	C	87	VAL	3.6
1	C	33	VAL	3.5
1	A	171	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	92	ALA	3.4
1	C	5	ILE	3.3
1	C	201	VAL	3.2
1	A	92	ALA	3.2
1	A	122[A]	HIS	3.2
1	C	124	PRO	3.2
1	C	102	SER	3.2
1	C	144	PRO	3.1
1	C	43	ALA	3.0
1	C	139	TRP	3.0
1	C	208	THR	3.0
1	C	174	ALA	3.0
1	C	171	GLY	3.0
1	C	133	LEU	3.0
1	C	172	SER	2.8
1	C	184	ALA	2.8
1	C	178	LYS	2.7
1	C	42	LEU	2.7
1	C	170	TYR	2.7
1	C	213	TYR	2.7
1	C	205[A]	ASN	2.6
1	C	10	ALA	2.6
1	C	142	LEU	2.6
1	C	95	GLN	2.6
1	C	89	ALA	2.6
1	C	46	ILE	2.5
1	C	34[A]	SER	2.5
1	C	7	VAL	2.5
1	C	45	GLN	2.5
1	C	143	SER	2.4
1	C	176	ALA	2.4
1	C	121	GLU	2.4
1	C	83	ASN	2.4
1	C	37	ALA	2.4
1	C	119[A]	ASP	2.4
1	B	3	GLY	2.3
1	C	16	ALA	2.3
1	C	53	ASP	2.3
1	C	8	PHE	2.2
1	C	167	GLY	2.2
1	C	230	PHE	2.2
1	C	117	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	109	LEU	2.1
1	C	152	VAL	2.1
1	C	150	GLU	2.1
1	C	212	PHE	2.1
1	C	137	GLY	2.0
1	C	156	LEU	2.0
1	C	91	LYS	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, 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
2	REO	B	301	5/5	0.13	-0.21	18,20,24,26	0
2	REO	A	301	5/5	0.12	-0.31	19,20,30,36	0
2	REO	C	301	5/5	0.09	-2.22	69,69,71,74	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.