



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 03:38 AM GMT

PDB ID : 2GWG  
Title : Crystal Structure of 4-Oxalomesaconate Hydratase, LigJ, from *Rhodopseudomonas palustris*, Northeast Structural Genomics Target RpR66.  
Authors : Forouhar, F.; Abashidze, M.; Jayaraman, S.; Cunningham, K.; Cio, M.; Ma, L.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2006-05-04  
Resolution : 1.80 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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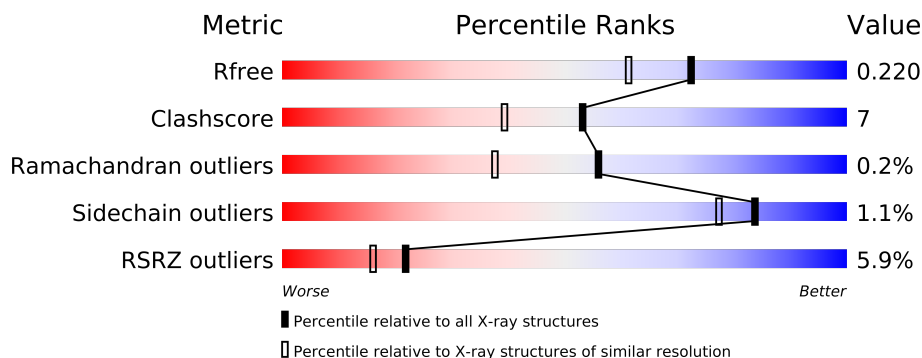
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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	350	
1	B	350	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5836 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 4-oxalomesaconate hydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	Se	0	0	0
			2607	1670	439	483	6	9			
1	B	326	Total	C	N	O	S	Se	0	0	0
			2582	1654	433	480	6	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
A	33	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
A	58	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
A	75	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
A	112	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
A	168	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
A	176	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
A	203	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
A	242	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
A	285	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
A	343	LEU	-	CLONING ARTIFACT	UNP Q6N0R4
A	344	GLU	-	CLONING ARTIFACT	UNP Q6N0R4
A	345	HIS	-	EXPRESSION TAG	UNP Q6N0R4
A	346	HIS	-	EXPRESSION TAG	UNP Q6N0R4
A	347	HIS	-	EXPRESSION TAG	UNP Q6N0R4
A	348	HIS	-	EXPRESSION TAG	UNP Q6N0R4
A	349	HIS	-	EXPRESSION TAG	UNP Q6N0R4
A	350	HIS	-	EXPRESSION TAG	UNP Q6N0R4
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
B	33	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
B	58	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
B	75	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
B	112	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
B	168	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
B	176	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	203	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
B	242	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
B	285	MSE	MET	MODIFIED RESIDUE	UNP Q6N0R4
B	343	LEU	-	CLONING ARTIFACT	UNP Q6N0R4
B	344	GLU	-	CLONING ARTIFACT	UNP Q6N0R4
B	345	HIS	-	EXPRESSION TAG	UNP Q6N0R4
B	346	HIS	-	EXPRESSION TAG	UNP Q6N0R4
B	347	HIS	-	EXPRESSION TAG	UNP Q6N0R4
B	348	HIS	-	EXPRESSION TAG	UNP Q6N0R4
B	349	HIS	-	EXPRESSION TAG	UNP Q6N0R4
B	350	HIS	-	EXPRESSION TAG	UNP Q6N0R4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

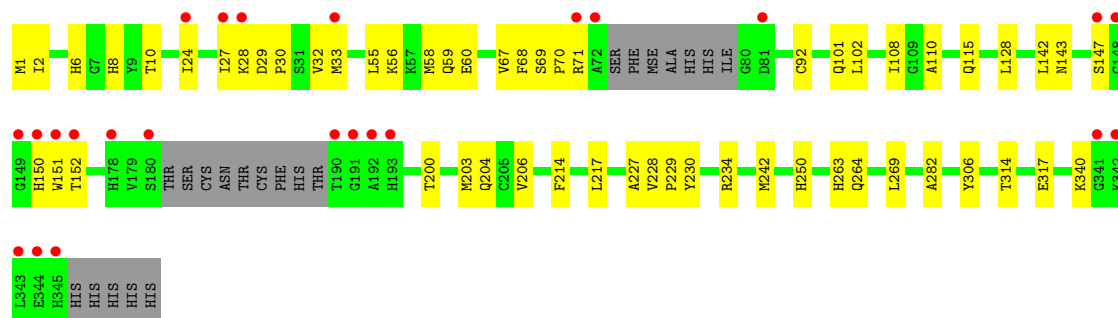
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	287	Total	O	0	0
			287	287		
3	B	358	Total	O	0	0
			358	358		

### 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.

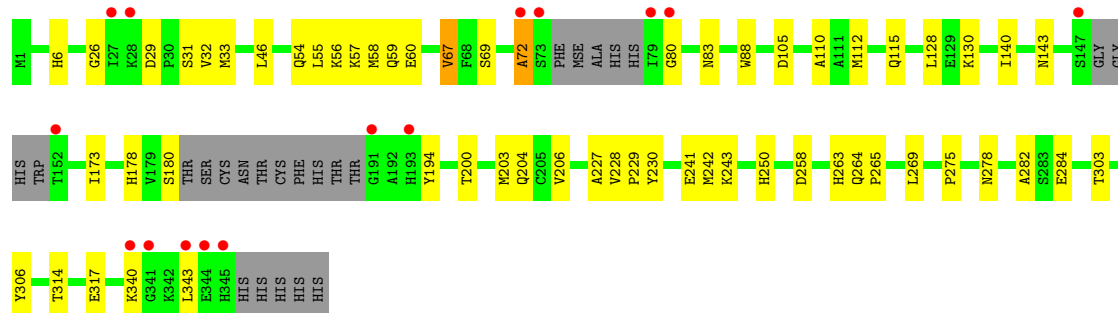
- Molecule 1: 4-oxalomesaconate hydratase

Chain A: 



- Molecule 1: 4-oxalomesaconate hydratase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.09Å 55.34Å 97.17Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	22.79 – 1.80 28.55 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.5 (22.79-1.80) 98.6 (28.55-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.181 , 0.208 0.194 , 0.220	Depositor DCC
$R_{free}$ test set	6815 reflections (9.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.8	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.0	EDS
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 136508 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: ZN

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	0.29	0/2667	0.56	1/3609 (0.0%)
1	B	0.31	0/2638	0.59	1/3567 (0.0%)
All	All	0.30	0/5305	0.57	2/7176 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	SER	CB-CA-C	5.77	121.06	110.10
1	B	67	VAL	N-CA-C	-5.25	96.82	111.00

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	2607	0	2565	35	0
1	B	2582	0	2550	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	287	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	358	0	0	8	0
All	All	5836	0	5115	72	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 7.

All (72) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:227:ALA:HB2	1:B:227:ALA:HB2	1.51	0.92
1:B:115:GLN:HE22	1:B:143:ASN:H	1.22	0.88
1:A:115:GLN:HE22	1:A:143:ASN:H	1.24	0.82
1:A:10:THR:HA	1:A:71:ARG:HD3	1.68	0.75
1:A:69:SER:HB3	1:A:110:ALA:HB3	1.73	0.70
1:B:130:LYS:HE2	3:B:694:HOH:O	1.92	0.69
1:A:203:MSE:HE1	1:A:242:MSE:HE1	1.77	0.66
1:A:24:ILE:O	1:A:27:ILE:HG22	1.98	0.63
1:B:33:MSE:HG3	3:B:722:HOH:O	2.00	0.62
1:B:230:TYR:HA	1:B:269:LEU:HD21	1.82	0.61
1:A:228:VAL:HB	1:A:229:PRO:HD3	1.83	0.60
1:A:58:MSE:HE3	3:A:644:HOH:O	2.01	0.60
1:A:230:TYR:HA	1:A:269:LEU:HD21	1.85	0.59
1:A:101:GLN:HG2	3:A:563:HOH:O	2.03	0.58
1:A:150:HIS:HB3	1:A:152:THR:HG23	1.85	0.58
1:B:228:VAL:HB	1:B:229:PRO:HD3	1.86	0.58
1:A:67:VAL:HA	1:A:108:ILE:HG23	1.87	0.56
1:B:69:SER:HB3	1:B:110:ALA:HB3	1.88	0.55
1:A:102:LEU:HD13	3:A:642:HOH:O	2.08	0.54
1:A:214:PHE:HB3	1:A:217:LEU:HB2	1.89	0.54
1:A:2:ILE:N	1:A:2:ILE:HD12	2.24	0.53
1:A:200:THR:O	1:A:204:GLN:HG3	2.08	0.52
1:A:30:PRO:HA	1:A:33:MSE:HG3	1.92	0.52
1:A:29:ASP:O	1:A:32:VAL:HG22	2.10	0.52
1:B:88:TRP:CD1	1:B:112:MSE:HE1	2.45	0.52
1:B:80:GLY:HA2	3:B:654:HOH:O	2.11	0.51
1:B:72:ALA:HB1	1:B:180:SER:HA	1.92	0.51
1:B:241:GLU:HG3	3:B:463:HOH:O	2.12	0.50
1:B:29:ASP:OD1	1:B:31:SER:HB3	2.11	0.50
1:B:284:GLU:HG2	3:B:553:HOH:O	2.11	0.50
1:B:203:MSE:HE1	1:B:242:MSE:HE1	1.94	0.50
1:A:56:LYS:O	1:A:60:GLU:HG3	2.12	0.50
1:A:55:LEU:O	1:A:59:GLN:HG3	2.12	0.49
1:B:56:LYS:O	1:B:60:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:88:TRP:HD1	1:B:112:MSE:HE1	1.78	0.49
1:B:26:GLY:HA3	1:B:33:MSE:HG2	1.95	0.48
1:A:27:ILE:HG23	1:A:28:LYS:HG2	1.95	0.48
1:A:314:THR:OG1	1:A:317:GLU:HG3	2.13	0.47
1:B:29:ASP:O	1:B:32:VAL:HG22	2.15	0.47
1:A:10:THR:HG22	1:A:71:ARG:HG2	1.97	0.47
1:B:140:ILE:HG23	1:B:173:ILE:HD12	1.96	0.47
1:B:72:ALA:HB2	1:B:178:HIS:HE1	1.80	0.46
1:A:67:VAL:HG12	1:A:110:ALA:HB2	1.97	0.46
1:B:275:PRO:HB2	1:B:278:ASN:HD22	1.81	0.45
1:A:206:VAL:O	1:A:250:HIS:HE1	1.99	0.45
1:A:10:THR:HA	1:A:71:ARG:CD	2.43	0.45
1:A:8:HIS:HA	1:A:69:SER:O	2.17	0.45
1:B:314:THR:OG1	1:B:317:GLU:HG3	2.16	0.45
1:A:264:GLN:OE1	1:A:306:TYR:HA	2.17	0.44
1:B:105:ASP:OD2	1:B:340:LYS:HE3	2.17	0.44
1:B:128:LEU:HD23	1:B:128:LEU:C	2.38	0.44
1:B:67:VAL:HG12	1:B:110:ALA:HB2	1.98	0.44
1:B:54:GLN:O	1:B:58:MSE:HG3	2.18	0.44
1:A:340:LYS:HG2	3:A:450:HOH:O	2.18	0.43
1:B:250:HIS:HD2	3:B:488:HOH:O	2.02	0.43
1:B:206:VAL:O	1:B:250:HIS:HE1	2.01	0.43
1:B:55:LEU:O	1:B:59:GLN:HG3	2.18	0.43
1:A:70:PRO:HB3	1:A:92:CYS:HB3	2.00	0.43
1:B:83:ASN:HB2	3:B:725:HOH:O	2.18	0.43
1:B:258:ASP:C	1:B:258:ASP:OD1	2.57	0.42
1:B:241:GLU:O	1:B:243:LYS:HE2	2.19	0.42
1:B:303:THR:HA	1:B:306:TYR:CD2	2.54	0.41
1:B:6:HIS:HB3	1:B:282:ALA:HB1	2.01	0.41
1:B:57:LYS:HE3	3:B:529:HOH:O	2.20	0.41
1:A:6:HIS:HB3	1:A:282:ALA:HB1	2.02	0.41
1:B:200:THR:O	1:B:204:GLN:HG3	2.20	0.41
1:B:26:GLY:HA2	1:B:29:ASP:O	2.21	0.41
1:B:264:GLN:HB3	1:B:265:PRO:HD3	2.03	0.41
1:A:150:HIS:O	1:A:151:TRP:HB2	2.21	0.40
1:A:234:ARG:HD3	1:B:194:TYR:OH	2.21	0.40
1:A:128:LEU:C	1:A:128:LEU:HD23	2.42	0.40
1:A:1:MSE:C	1:A:2:ILE:HD12	2.41	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	323/350 (92%)	311 (96%)	12 (4%)	0	100	100
1	B	318/350 (91%)	307 (96%)	10 (3%)	1 (0%)	50	31
All	All	641/700 (92%)	618 (96%)	22 (3%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	ALA

### 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	283/293 (97%)	280 (99%)	3 (1%)	84	77
1	B	282/293 (96%)	279 (99%)	3 (1%)	84	77
All	All	565/586 (96%)	559 (99%)	6 (1%)	84	77

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	PHE
1	A	142	LEU
1	A	263	HIS
1	B	46	LEU
1	B	263	HIS
1	B	343	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	196	ASN
1	A	240	GLN
1	A	250	HIS
1	A	254	ASN
1	A	278	ASN
1	B	47	GLN
1	B	115	GLN
1	B	196	ASN
1	B	240	GLN
1	B	250	HIS
1	B	254	ASN
1	B	278	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 2 ligands modelled in this entry, 2 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.

## 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	329/350 (94%)	0.34	24 (7%) 15 10	10, 21, 40, 51	0
1	B	326/350 (93%)	-0.02	15 (4%) 31 24	9, 15, 39, 50	0
All	All	655/700 (93%)	0.16	39 (5%) 22 16	9, 18, 40, 51	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	TRP	10.2
1	B	345	HIS	9.7
1	B	343	LEU	8.1
1	A	190	THR	8.0
1	B	79	ILE	7.5
1	A	343	LEU	7.4
1	A	150	HIS	6.8
1	A	345	HIS	6.8
1	B	344	GLU	6.1
1	B	152	THR	5.8
1	A	148	GLY	5.3
1	A	27	ILE	4.9
1	B	80	GLY	4.5
1	A	72	ALA	4.4
1	A	152	THR	4.4
1	B	73	SER	4.2
1	A	149	GLY	4.1
1	A	24	ILE	4.0
1	A	147	SER	3.6
1	A	71	ARG	3.5
1	A	344	GLU	3.4
1	B	147	SER	3.3
1	A	341	GLY	3.2
1	A	191	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	33	MSE	3.1
1	B	28	LYS	2.9
1	A	342	LYS	2.8
1	A	28	LYS	2.7
1	A	193	HIS	2.6
1	A	192	ALA	2.6
1	B	27	ILE	2.6
1	B	191	GLY	2.5
1	B	193	HIS	2.3
1	A	180	SER	2.2
1	A	81	ASP	2.1
1	B	341	GLY	2.1
1	B	340	LYS	2.0
1	B	72	ALA	2.0
1	A	178	HIS	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	ZN	A	401	1/1	0.03	-2.18	20,20,20,20	0
2	ZN	B	401	1/1	0.03	-2.22	16,16,16,16	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.