Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 03:34 pm GMT

PDB ID	:	8CLN
Title	:	Zearalenone lactonase from Streptomyces coelicoflavus, SeMet derivative for SAD phasing
Authors	:	Puehringer, D.; Grishkovskaya, I.; Mlynek, G.; Kostan, J.
Deposited on	:	2023-02-17
Resolution	:	2.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

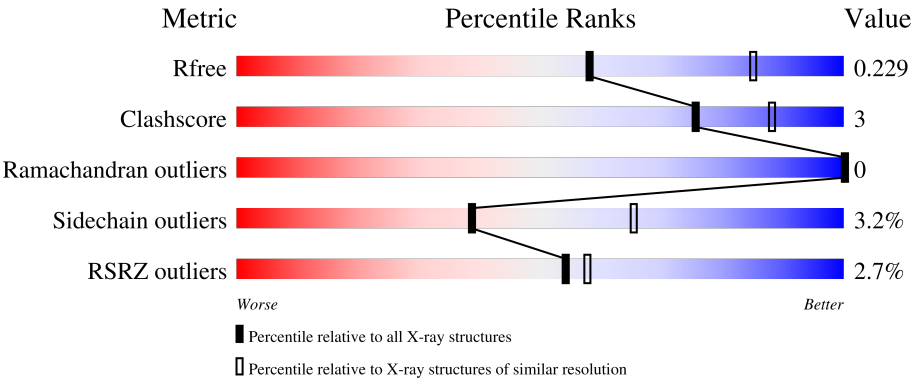
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	315	3% 89% 7% •
1	B	315	4% 87% 10% •
1	C	315	% 88% 7% • 5%
1	D	315	3% 83% 11% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18378 atoms, of which 8957 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 Hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	305	Total	C	H	N	O	S	0	1	0
			4638	1503	2265	417	441	12			
1	B	304	Total	C	H	N	O	S	0	0	0
			4615	1496	2255	416	436	12			
1	C	299	Total	C	H	N	O	S	0	1	0
			4538	1473	2214	408	431	12			
1	D	299	Total	C	H	N	O	S	0	1	0
			4549	1476	2223	408	429	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	HIS	-	expression tag	UNP H1Q8U7
A	311	HIS	-	expression tag	UNP H1Q8U7
A	312	HIS	-	expression tag	UNP H1Q8U7
A	313	HIS	-	expression tag	UNP H1Q8U7
A	314	HIS	-	expression tag	UNP H1Q8U7
A	315	HIS	-	expression tag	UNP H1Q8U7
B	310	HIS	-	expression tag	UNP H1Q8U7
B	311	HIS	-	expression tag	UNP H1Q8U7
B	312	HIS	-	expression tag	UNP H1Q8U7
B	313	HIS	-	expression tag	UNP H1Q8U7
B	314	HIS	-	expression tag	UNP H1Q8U7
B	315	HIS	-	expression tag	UNP H1Q8U7
C	310	HIS	-	expression tag	UNP H1Q8U7
C	311	HIS	-	expression tag	UNP H1Q8U7
C	312	HIS	-	expression tag	UNP H1Q8U7
C	313	HIS	-	expression tag	UNP H1Q8U7
C	314	HIS	-	expression tag	UNP H1Q8U7
C	315	HIS	-	expression tag	UNP H1Q8U7
D	310	HIS	-	expression tag	UNP H1Q8U7
D	311	HIS	-	expression tag	UNP H1Q8U7
D	312	HIS	-	expression tag	UNP H1Q8U7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	313	HIS	-	expression tag	UNP H1Q8U7
D	314	HIS	-	expression tag	UNP H1Q8U7
D	315	HIS	-	expression tag	UNP H1Q8U7

- Molecule 2 is water.

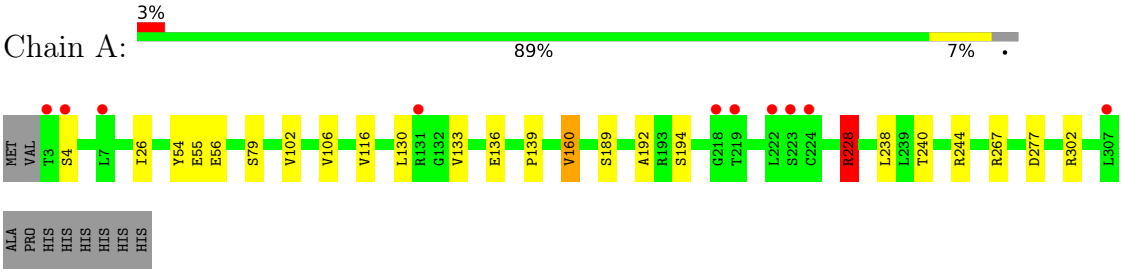
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	10	Total O 10 10	0	0
2	C	9	Total O 9 9	0	0
2	D	5	Total O 5 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

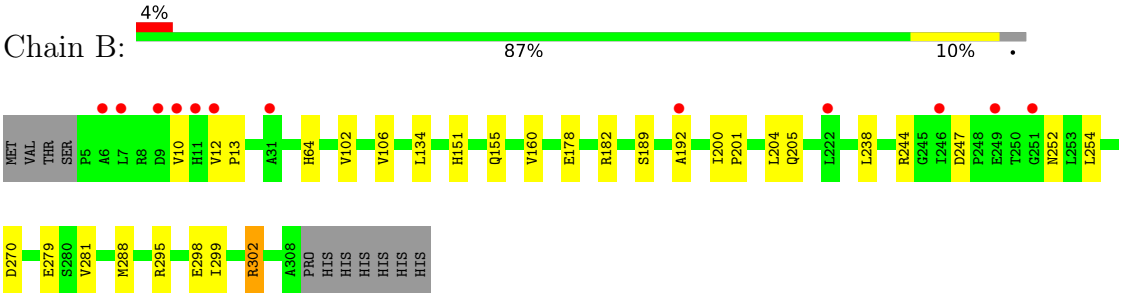
• Molecule 1: Hydrolase

Chain A:



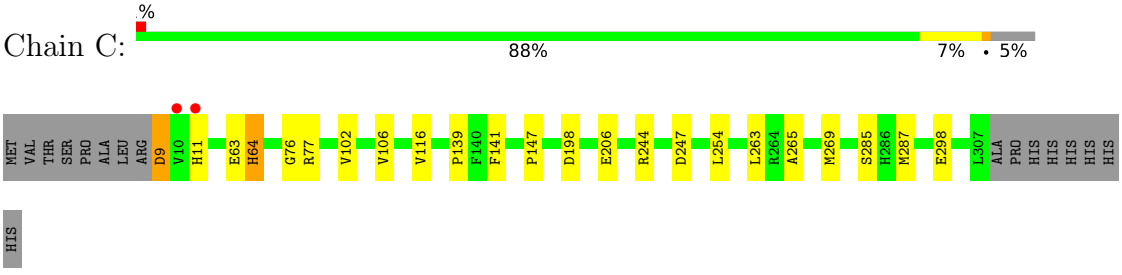
• Molecule 1: Hydrolase

Chain B:



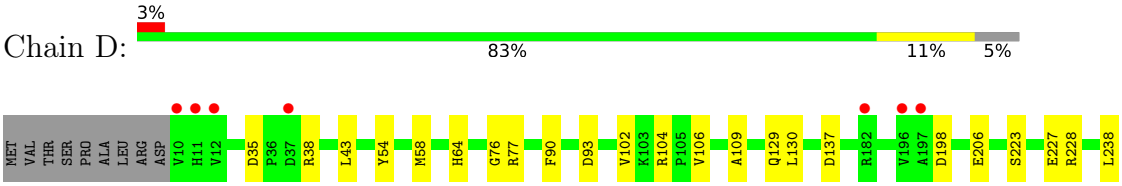
• Molecule 1: Hydrolase

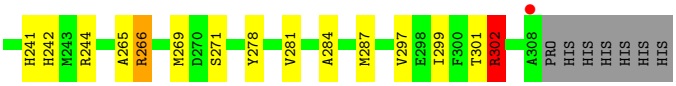
Chain C:



• Molecule 1: Hydrolase

Chain D:




H241
H242
M243
R244
A265
R266
M269
D270
S271
Y278
V281
A284
M287
V297
E298
I299
F300
T301
R302
A308
PRO
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	75.39Å 75.39Å 404.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.91 – 2.50 46.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.91-2.50) 97.5 (46.91-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1-4489	Depositor
R, R_{free}	0.183 , 0.232 0.182 , 0.229	Depositor DCC
R_{free} test set	2002 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18378	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.30	0/2446	0.56	0/3336
1	B	0.29	0/2430	0.55	0/3313
1	C	0.29	0/2402	0.56	0/3275
1	D	0.28	0/2398	0.55	0/3269
All	All	0.29	0/9676	0.56	0/13193

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
1	B	0	1
1	D	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	ARG	Sidechain
1	B	182	ARG	Sidechain
1	D	266	ARG	Sidechain
1	D	302	ARG	Sidechain

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	2373	2265	2265	10	0
1	B	2360	2255	2255	18	0
1	C	2324	2214	2205	10	0
1	D	2326	2223	2223	19	0
2	A	14	0	0	0	0
2	B	10	0	0	0	0
2	C	9	0	0	0	0
2	D	5	0	0	0	0
All	All	9421	8957	8948	57	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 3.

All (57) 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:C:102:VAL:HG11	1:C:106:VAL:CG1	2.27	0.64
1:C:102:VAL:HG11	1:C:106:VAL:HG12	1.82	0.61
1:B:281:VAL:HG21	1:B:288:MET:CE	2.33	0.58
1:B:134:LEU:HD13	1:B:238:LEU:HG	1.86	0.58
1:B:298:GLU:OE2	1:B:302:ARG:NH2	2.37	0.58
1:C:9:ASP:N	1:C:9:ASP:OD1	2.39	0.56
1:B:102:VAL:HG11	1:B:106:VAL:CG1	2.36	0.56
1:B:178:GLU:H	1:B:178:GLU:CD	2.09	0.56
1:B:279:GLU:OE2	1:B:299:ILE:HG23	2.06	0.55
1:D:54:TYR:O	1:D:58:MET:HG3	2.07	0.54
1:D:102:VAL:HG11	1:D:106:VAL:HG22	1.88	0.54
1:D:35:ASP:HB3	1:D:38:ARG:HE	1.73	0.53
1:D:281:VAL:O	1:D:281:VAL:HG23	2.09	0.52
1:B:10:VAL:HG12	1:B:10:VAL:O	2.12	0.50
1:A:102:VAL:HG11	1:A:106:VAL:CG1	2.41	0.50
1:B:279:GLU:OE2	1:B:299:ILE:CG2	2.60	0.49
1:B:102:VAL:HG11	1:B:106:VAL:HG12	1.96	0.48
1:A:160:VAL:HG23	1:A:192:ALA:HA	1.94	0.48
1:A:238:LEU:HD13	1:A:277:ASP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:VAL:HB	1:B:13:PRO:CD	2.43	0.48
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.78	0.48
1:B:295:ARG:O	1:B:299:ILE:HG13	2.14	0.48
1:C:265:ALA:O	1:C:269:MET:HG3	2.14	0.47
1:D:281:VAL:HG23	1:D:284:ALA:HB3	1.96	0.47
1:B:200:ILE:HG22	1:B:205:GLN:HG3	1.97	0.47
1:C:63:GLU:HB3	1:C:64:HIS:CE1	2.50	0.47
1:A:116:VAL:HG23	1:A:139:PRO:HD2	1.97	0.47
1:B:247:ASP:HB2	1:B:254:LEU:HD21	1.97	0.46
1:D:104:ARG:HH11	1:D:104:ARG:HG2	1.81	0.46
1:B:160:VAL:HG22	1:B:192:ALA:HB2	1.99	0.45
1:B:155:GLN:O	1:B:252:ASN:HB3	2.15	0.45
1:C:76:GLY:HA2	1:C:206:GLU:HB3	1.97	0.45
1:D:76:GLY:HA2	1:D:206:GLU:HB3	1.99	0.44
1:D:297:VAL:O	1:D:301:THR:OG1	2.30	0.44
1:B:201:PRO:HD2	1:B:204:LEU:HD12	2.00	0.44
1:A:26:ILE:HB	1:A:79:SER:HB2	1.98	0.44
1:D:265:ALA:O	1:D:269:MET:HG3	2.18	0.44
1:D:242:HIS:CD2	1:D:242:HIS:N	2.85	0.43
1:A:136:GLU:HA	1:A:240:THR:OG1	2.18	0.43
1:A:130:LEU:HD23	1:A:133:VAL:CG1	2.49	0.42
1:D:227:GLU:HG2	1:D:228:ARG:N	2.34	0.42
1:B:281:VAL:HG21	1:B:288:MET:HE2	2.02	0.42
1:C:116:VAL:HG23	1:C:139:PRO:HD2	2.01	0.42
1:B:12:VAL:HB	1:B:13:PRO:HD3	2.01	0.42
1:C:141:PHE:O	1:C:147:PRO:HB3	2.20	0.42
1:D:104:ARG:HG2	1:D:104:ARG:NH1	2.33	0.42
1:D:266:ARG:HD2	1:D:278:TYR:CD1	2.54	0.41
1:A:54:TYR:O	1:A:55:GLU:C	2.59	0.41
1:D:129:GLN:C	1:D:130:LEU:HD12	2.41	0.41
1:A:302:ARG:HE	1:A:302:ARG:HB3	1.76	0.41
1:D:238:LEU:HD21	1:D:299:ILE:HG22	2.03	0.41
1:C:247:ASP:HB2	1:C:254:LEU:HD21	2.01	0.40
1:D:302:ARG:HD3	1:D:302:ARG:HA	1.79	0.40
1:C:77:ARG:HE	1:C:77:ARG:HB3	1.63	0.40
1:D:90:PHE:O	1:D:93:ASP:HB2	2.21	0.40
1:D:241:HIS:O	1:D:244:ARG:NH2	2.54	0.40
1:D:43:LEU:HD23	1:D:109:ALA:HB3	2.03	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	304/315 (96%)	295 (97%)	9 (3%)	0	100	100
1	B	302/315 (96%)	292 (97%)	10 (3%)	0	100	100
1	C	298/315 (95%)	288 (97%)	10 (3%)	0	100	100
1	D	298/315 (95%)	288 (97%)	10 (3%)	0	100	100
All	All	1202/1260 (95%)	1163 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	247/255 (97%)	239 (97%)	8 (3%)	39	65
1	B	244/255 (96%)	238 (98%)	6 (2%)	47	73
1	C	242/255 (95%)	233 (96%)	9 (4%)	34	60
1	D	241/255 (94%)	232 (96%)	9 (4%)	34	60
All	All	974/1020 (96%)	942 (97%)	32 (3%)	39	64

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	56	GLU

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Mol	Chain	Res	Type
1	A	160	VAL
1	A	189	SER
1	A	194	SER
1	A	228	ARG
1	A	244	ARG
1	A	267	ARG
1	B	64	HIS
1	B	151	HIS
1	B	189	SER
1	B	244	ARG
1	B	270	ASP
1	B	302	ARG
1	C	9	ASP
1	C	11	HIS
1	C	64	HIS
1	C	198	ASP
1	C	244	ARG
1	C	263	LEU
1	C	285	SER
1	C	287	MET
1	C	298	GLU
1	D	64	HIS
1	D	77	ARG
1	D	137	ASP
1	D	198	ASP
1	D	223	SER
1	D	271	SER
1	D	287[A]	MET
1	D	287[B]	MET
1	D	302	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	202	GLN
1	C	151	HIS

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	305/315 (96%)	0.16	10 (3%) 46 50	32, 41, 64, 82	0
1	B	304/315 (96%)	0.24	12 (3%) 39 42	36, 50, 84, 128	0
1	C	299/315 (94%)	0.06	2 (0%) 87 89	38, 54, 76, 106	0
1	D	299/315 (94%)	0.16	8 (2%) 54 58	40, 57, 84, 107	0
All	All	1207/1260 (95%)	0.16	32 (2%) 54 58	32, 51, 79, 128	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	LEU	6.8
1	D	11	HIS	5.3
1	D	196	VAL	4.9
1	D	10	VAL	3.8
1	C	10	VAL	3.8
1	A	3	THR	3.5
1	B	11	HIS	3.3
1	B	9	ASP	3.1
1	B	249	GLU	2.9
1	B	12	VAL	2.9
1	B	6	ALA	2.9
1	C	11	HIS	2.8
1	A	223	SER	2.7
1	A	4	SER	2.6
1	D	12	VAL	2.5
1	A	218	GLY	2.3
1	B	246	ILE	2.3
1	A	219	THR	2.3
1	A	222	LEU	2.2
1	B	31	ALA	2.2
1	A	7	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	224	CYS	2.1
1	D	308	ALA	2.1
1	B	251	GLY	2.1
1	B	192	ALA	2.1
1	D	37	ASP	2.1
1	A	131	ARG	2.1
1	D	197	ALA	2.1
1	A	307	LEU	2.1
1	B	222	LEU	2.1
1	B	10	VAL	2.0
1	D	182	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.