wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2024 – 09:42 am BST

PDB ID	:	1W79
Title	:	Crystal structure of the DD-transpeptidase-carboxypeptidase from Actinomadura R39
Authors	:	Sauvage, E.; Herman, R.; Petrella, S.; Duez, C.; Frere, J.M.; Charlier, P.
Deposited on	:	2004-08-31
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

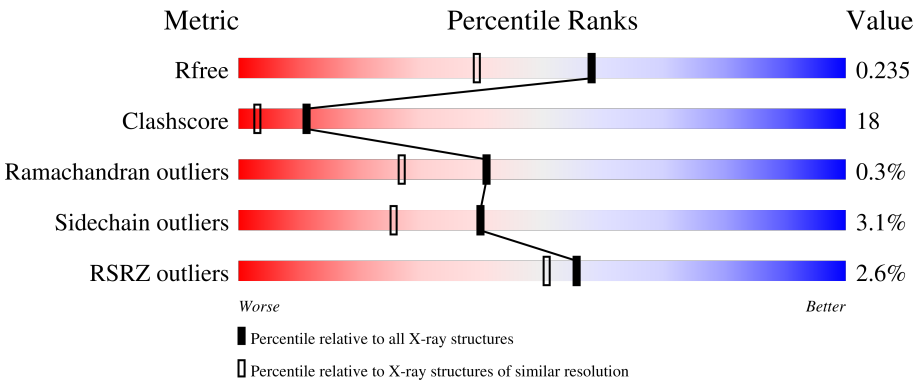
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 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	489	2%, 72%, 22%, • •
1	B	489	3%, 72%, 22%, • 5%
1	C	489	3%, 69%, 25%, • 5%
1	D	489	2%, 74%, 21%, • •

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	510	-	-	-	X
3	MG	D	511	-	-	-	X

2 Entry composition (i)

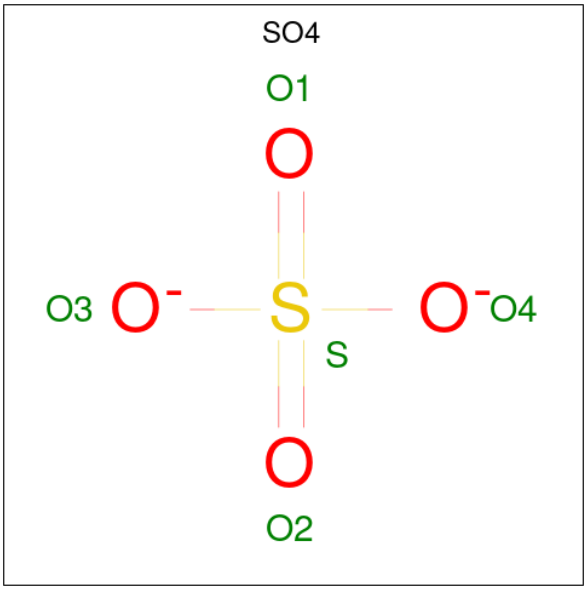
There are 4 unique types of molecules in this entry. The entry contains 15239 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-alanyl-D-alanine carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	467	3353	2076	565	706	6	0	0	1
1	B	466	3344	2071	564	703	6	0	0	1
1	C	466	3344	2071	564	703	6	0	0	1
1	D	467	3353	2076	565	706	6	0	0	1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	438	Total O 438 438	0	0
4	B	461	Total O 461 461	0	0
4	C	464	Total O 464 464	0	0
4	D	418	Total O 418 418	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: D-alanyl-D-alanine carboxypeptidase

Chain A: 2% 72% 22% • •

R1 L2 R6 L13 V25 V26 V27 A31 L36 G41 L60 F69 R81 R82 V85 Q86 D87 L88 V91 G94 D95 P96 T97 L98 E101 D102 V110 V115 R116 T117 V118 R119 G120 D121 L122 Y123 A124 D125 W128 F129 D130 S131 E132

V135 W138 W139 P140 E141 A146 Y147 Q150 A153 L154 T155 V156 A157 H158 D163 V169 T172 P173 A174 A175 E178 V182 D183 L184 Y190 L193 D194 N195 R196 A197 V198 T199 S204 L208 V221 T222 P226 A229 E240 A243 L244 A245

G246 H247 L248 F249 E250 L253 K261 G267 G268 V269 P270 A271 D272 W273 Q274 D275 A276 E277 V278 L279 A280 L287 S288 E289 I290 L291 N299 A303 E304 M305 L306 V307 Q312 T319 W320 L324 V325 E329 L334 L341 G346 L349 L354 V355

D358 T359 L364 A367 A370 P371 W376 L380 R397 L431 H440 Q449 V454 R455 E458 G467 ALA ARG MET MET ARG GLY PRO VAL GLN GLY SER GLY GLU LEU GLU CYS SER TRP VAL GLN ALA CYS

• Molecule 1: D-alanyl-D-alanine carboxypeptidase

Chain B: 3% 72% 22% • 5%

R1 L2 T3 E4 E7 D8 I12 P16 A17 L18 E19 V27 T30 L36 K52 T55 A58 A59 L60 E61 G64 A74 Q86 D87 L88 Y89 L90 L98 A107 V115 R116 R119 R133 L134 V135 D136 D137 W138 E143 Q150

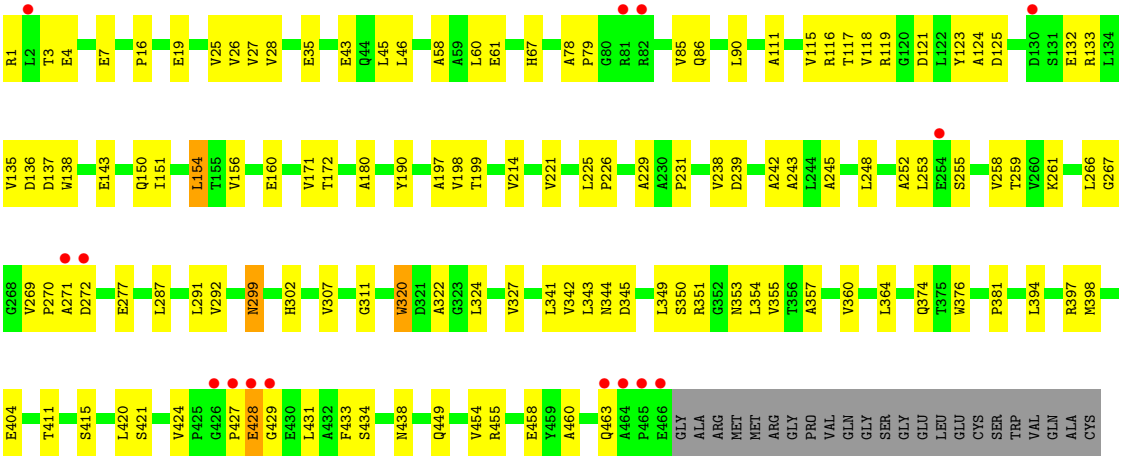
L154 T155 V156 A157 H158 R161 F162 D163 T164 A175 E178 A197 V209 I210 D211 R212 P213 V214 I219 A220 V221 A234 V238 D239 E240 P241 A242 A245 G246 H247 L248 E251 A252 L253 V260 K261 P270 A271 D272 W273 Q274 D275 A276 L279 L287

V292 P293 K296 F297 S298 N299 H302 A303 E304 V307 I310 W320 L324 L341 V342 L343 G346 S347 G348 L349 S350 R351 G352 N353 L354 T359 A373 Q374 T375 W376 G392 T393 R397 G412 S415 S418 A419 L420 G426 P427 E428 G429 E430 L431

N437 N438 P445 Q449 I452 A453 V454 A457 E458 Y459 A460 G461 H462 Q463 A464 P465 E466 GLY ALA ARG MET MET ARG GLY PRO VAL GLN GLY SER GLY GLU LEU GLU CYS SER TRP VAL GLN ALA CYS

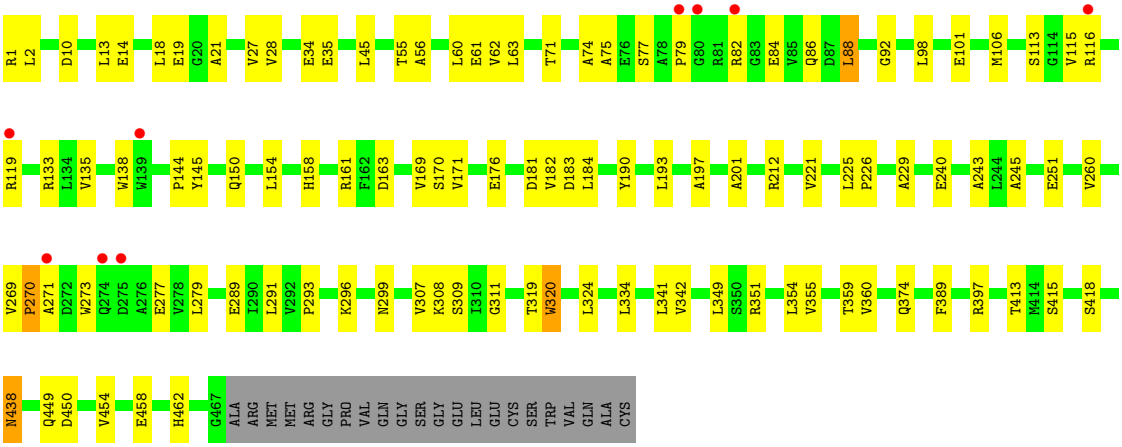
• Molecule 1: D-alanyl-D-alanine carboxypeptidase

Chain C: 3% 69% 25% • 5%



- Molecule 1: D-alanyl-D-alanine carboxypeptidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.19Å 93.37Å 107.27Å 90.00° 94.25° 90.00°	Depositor
Resolution (Å)	19.95 – 1.80 106.98 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.95-1.80) 94.7 (106.98-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.240 0.209 , 0.235	Depositor DCC
R_{free} test set	10665 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15239	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.29% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4

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	0/3412	0.59	0/4668
1	B	0.30	0/3403	0.60	0/4656
1	C	0.29	0/3403	0.59	0/4656
1	D	0.29	0/3412	0.60	0/4668
All	All	0.29	0/13630	0.60	0/18648

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	3353	0	3201	115	0
1	B	3344	0	3195	125	0
1	C	3344	0	3195	136	0
1	D	3353	0	3201	93	1
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2	0	0	0	0
4	A	438	0	0	79	0
4	B	461	0	0	92	0
4	C	464	0	0	92	0
4	D	418	0	0	52	1
All	All	15239	0	12792	469	1

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 18.

The worst 5 of 469 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:12:ILE:HG21	4:B:2447:HOH:O	1.46	1.16
1:A:184:LEU:HA	4:A:2195:HOH:O	1.60	1.01
1:C:151:ILE:HB	4:C:2135:HOH:O	1.63	0.98
1:A:221:VAL:HG12	4:A:2240:HOH:O	1.65	0.97
1:C:434:SER:HB3	4:C:2377:HOH:O	1.64	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:HIS:ND1	4:D:2189:HOH:O[2_645]	2.14	0.06

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	465/489 (95%)	448 (96%)	16 (3%)	1 (0%)	47 33
1	B	464/489 (95%)	449 (97%)	14 (3%)	1 (0%)	47 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	464/489 (95%)	450 (97%)	13 (3%)	1 (0%)	47	33
1	D	465/489 (95%)	448 (96%)	15 (3%)	2 (0%)	34	21
All	All	1858/1956 (95%)	1795 (97%)	58 (3%)	5 (0%)	41	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	D	86	GLN
1	C	428	GLU
1	D	270	PRO
1	B	270	PRO

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	339/356 (95%)	328 (97%)	11 (3%)	39	25
1	B	338/356 (95%)	324 (96%)	14 (4%)	30	16
1	C	338/356 (95%)	330 (98%)	8 (2%)	49	36
1	D	339/356 (95%)	330 (97%)	9 (3%)	44	31
All	All	1354/1424 (95%)	1312 (97%)	42 (3%)	40	25

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	320	TRP
1	D	88	LEU
1	C	349	LEU
1	C	463	GLN
1	D	289	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	396	ASN
1	D	299	ASN
1	B	463	GLN
1	D	449	GLN
1	D	50	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	SO4	A	501	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	C	502	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	D	502	-	4,4,4	0.26	0	6,6,6	0.04	0
2	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	A	502	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	B	501	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	C	500	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	D	500	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	B	500	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	500	-	4,4,4	0.22	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	C	501	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	B	502	-	4,4,4	0.24	0	6,6,6	0.04	0

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	467/489 (95%)	0.05	12 (2%)	56	51	10, 21, 37, 49	0
1	B	466/489 (95%)	-0.01	13 (2%)	53	47	11, 20, 35, 44	0
1	C	466/489 (95%)	0.03	15 (3%)	47	41	11, 20, 34, 46	0
1	D	467/489 (95%)	-0.04	9 (1%)	66	63	10, 19, 35, 47	0
All	All	1866/1956 (95%)	0.01	49 (2%)	56	51	10, 20, 36, 49	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	429	GLY	9.4
1	C	429	GLY	9.3
1	B	427	PRO	8.2
1	C	427	PRO	6.8
1	B	428	GLU	6.6

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)

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, 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	B-factors(Å^2)	Q<0.9
3	MG	D	510	1/1	0.54	0.70	54,54,54,54	0
3	MG	D	511	1/1	0.54	0.51	51,51,51,51	0
2	SO4	A	502	5/5	0.90	0.20	51,52,52,53	0
2	SO4	B	501	5/5	0.93	0.15	37,38,38,40	0
2	SO4	D	502	5/5	0.94	0.15	50,51,52,52	0
2	SO4	C	502	5/5	0.95	0.10	46,46,47,47	0
2	SO4	A	501	5/5	0.95	0.09	36,37,38,38	0
3	MG	A	510	1/1	0.97	0.27	5,5,5,5	0
2	SO4	B	502	5/5	0.97	0.12	48,49,49,50	0
2	SO4	C	501	5/5	0.97	0.08	34,35,36,36	0
2	SO4	D	501	5/5	0.98	0.09	29,29,31,32	0
2	SO4	A	500	5/5	0.99	0.11	14,14,17,19	0
2	SO4	B	500	5/5	0.99	0.09	16,17,19,20	0
3	MG	A	511	1/1	0.99	0.27	1,1,1,1	0
2	SO4	D	500	5/5	0.99	0.07	13,14,15,16	0
2	SO4	C	500	5/5	0.99	0.09	17,17,20,21	0

6.5 Other polymers (i)

There are no such residues in this entry.