



# wwPDB X-ray Structure Validation Summary Report

Dec 3, 2023 – 02:47 am GMT

PDB ID : 1OJV  
Title : Decay accelerating factor (CD55): the structure of an intact human complement regulator.  
Authors : Lukacik, P.; Roversi, P.; White, J.; Esser, D.; Smith, G.P.; Billington, J.; Williams, P.A.; Rudd, P.M.; Wormald, M.R.; Crispin, M.D.M.; Radcliffe, C.M.; Dwek, C.M.; Evans, D.J.; Morgan, B.P.; Smith, R.A.G.; Lea, S.M.  
Deposited on : 2003-07-16  
Resolution : 2.30 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
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

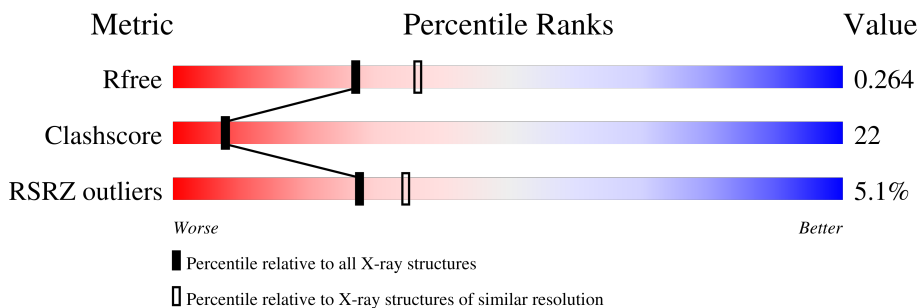
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	254	
1	B	254	

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
2	ACT	A	300	-	-	X	-
2	ACT	A	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	300	-	-	X	-
4	GOL	A	1256	-	X	X	-
4	GOL	A	1257	-	X	X	-
4	GOL	A	1258	-	X	-	-
4	GOL	B	1256	-	X	-	-
4	GOL	B	1257	-	X	-	-
4	GOL	B	1258	-	X	-	-
4	GOL	B	1259	-	X	-	-
4	GOL	B	1260	-	X	-	X
4	GOL	B	1261	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4218 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.

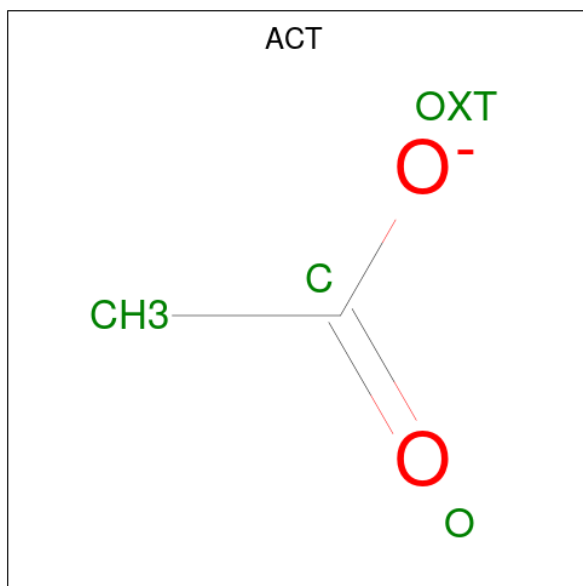
- Molecule 1 is a protein called COMPLEMENT DECAY-ACCELERATING FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	1969	1234	330	386	19	0	0	0
1	B	253	1961	1229	329	385	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ILE	THR	SEE REMARK 999	UNP P08174
B	48	ILE	THR	SEE REMARK 999	UNP P08174

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



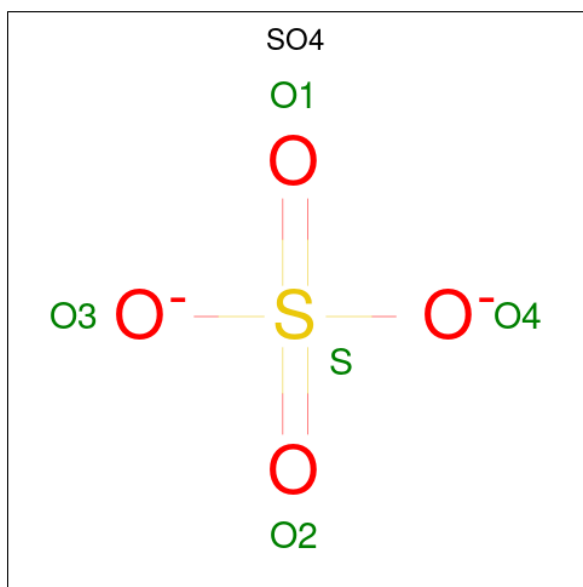
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

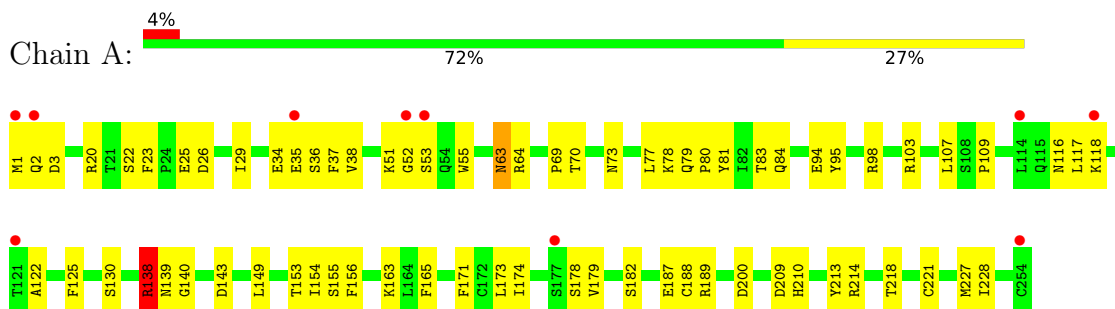
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	105	Total O 105 105	0	0
5	B	107	Total O 107 107	0	0

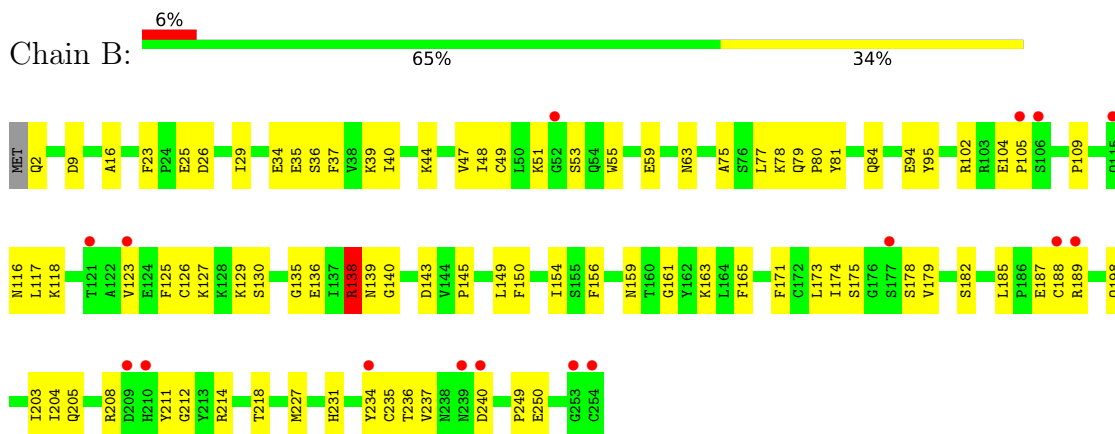
### 3 Residue-property plots [i](#)

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: COMPLEMENT DECAY-ACCELERATING FACTOR



- Molecule 1: COMPLEMENT DECAY-ACCELERATING FACTOR



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.67Å 55.08Å 61.65Å 86.47° 84.37° 64.91°	Depositor
Resolution (Å)	16.00 – 2.30 15.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.0 (16.00-2.30) 94.7 (15.99-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.95 (at 2.29Å)	Xtrriage
Refinement program	TNT 5F	Depositor
R, $R_{free}$	0.210 , (Not available) 0.219 , 0.264	Depositor DCC
$R_{free}$ test set	1197 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtrriage
Anisotropy	0.379	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.030 for -h,-h+k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% 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: SO4, ACT, GOL

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	0.37	0/2022	0.58	1/2749 (0.0%)
1	B	0.36	0/2014	0.54	1/2739 (0.0%)
All	All	0.36	0/4036	0.56	2/5488 (0.0%)

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	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	138	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	A	138	ARG	NE-CZ-NH1	-8.88	115.86	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ARG	Sidechain
1	A	63	ASN	Peptide,Mainchain
1	B	138	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	1969	0	1867	77	0
1	B	1961	0	1855	89	0
2	A	8	0	6	8	0
2	B	4	0	3	4	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	18	0	12	9	0
4	B	36	0	24	4	0
5	A	105	0	0	7	0
5	B	107	0	0	15	0
All	All	4218	0	3767	169	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 22.

The worst 5 of 169 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)
4:A:1256:GOL:C1	4:A:1256:GOL:O1	1.63	1.46
1:A:116:ASN:HB2	1:A:118:LYS:HE3	1.35	1.05
1:B:16:ALA:HB3	5:B:2012:HOH:O	1.53	1.05
1:B:116:ASN:HB2	1:B:118:LYS:HE3	1.35	1.04
1:A:165:PHE:HD2	1:A:189:ARG:HG3	1.22	1.01

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

14 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	ACT	A	300	-	3,3,3	1.21	0	3,3,3	0.78	0
3	SO4	B	1255	-	4,4,4	0.47	0	6,6,6	0.75	0
4	GOL	A	1258	-	5,5,5	4.49	5 (100%)	5,5,5	5.75	3 (60%)
2	ACT	B	300	-	3,3,3	1.21	1 (33%)	3,3,3	0.78	0
4	GOL	B	1261	-	5,5,5	4.57	5 (100%)	5,5,5	5.75	3 (60%)
4	GOL	B	1257	-	5,5,5	4.47	5 (100%)	5,5,5	5.77	3 (60%)
4	GOL	B	1258	-	5,5,5	4.53	5 (100%)	5,5,5	5.73	3 (60%)
4	GOL	A	1257	-	5,5,5	4.51	5 (100%)	5,5,5	5.72	3 (60%)
4	GOL	B	1260	-	5,5,5	4.53	5 (100%)	5,5,5	5.73	3 (60%)
2	ACT	A	301	-	3,3,3	1.25	1 (33%)	3,3,3	0.77	0
4	GOL	B	1259	-	5,5,5	4.51	5 (100%)	5,5,5	5.73	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	1255	-	4,4,4	0.36	0	6,6,6	0.79	0
4	GOL	A	1256	-	5,5,5	4.57	5 (100%)	5,5,5	5.77	3 (60%)
4	GOL	B	1256	-	5,5,5	4.47	5 (100%)	5,5,5	5.71	3 (60%)

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
4	GOL	A	1258	-	-	3/4/4/4	-
4	GOL	B	1261	-	-	3/4/4/4	-
4	GOL	B	1257	-	-	2/4/4/4	-
4	GOL	B	1258	-	-	2/4/4/4	-
4	GOL	A	1257	-	-	2/4/4/4	-
4	GOL	B	1260	-	-	2/4/4/4	-
4	GOL	B	1259	-	-	2/4/4/4	-
4	GOL	A	1256	-	-	3/4/4/4	-
4	GOL	B	1256	-	-	2/4/4/4	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1261	GOL	C3-C2	-7.46	1.21	1.51
4	A	1256	GOL	C3-C2	-7.43	1.21	1.51
4	B	1258	GOL	C3-C2	-7.39	1.21	1.51
4	B	1260	GOL	C3-C2	-7.39	1.21	1.51
4	A	1258	GOL	C3-C2	-7.35	1.21	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1256	GOL	O3-C3-C2	10.67	161.36	110.20
4	B	1257	GOL	O3-C3-C2	10.53	160.68	110.20
4	B	1261	GOL	O3-C3-C2	10.49	160.52	110.20
4	A	1258	GOL	O3-C3-C2	10.48	160.44	110.20
4	B	1258	GOL	O3-C3-C2	10.45	160.30	110.20

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1256	GOL	C1-C2-C3-O3
4	A	1257	GOL	O1-C1-C2-C3
4	A	1257	GOL	C1-C2-C3-O3
4	A	1258	GOL	O1-C1-C2-C3
4	A	1258	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	ACT	4	0
2	B	300	ACT	4	0
4	B	1261	GOL	2	0
4	B	1257	GOL	1	0
4	A	1257	GOL	4	0
2	A	301	ACT	4	0
4	B	1259	GOL	1	0
4	A	1256	GOL	5	0

## 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, 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	254/254 (100%)	0.33	10 (3%) 39 46	16, 27, 46, 62	0
1	B	253/254 (99%)	0.35	16 (6%) 20 25	16, 27, 46, 61	0
All	All	507/508 (99%)	0.34	26 (5%) 28 35	16, 27, 46, 62	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	CYS	5.6
1	B	240	ASP	4.0
1	B	234	TYR	4.0
1	B	254	CYS	3.7
1	B	210	HIS	3.6

### 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, 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	GOL	B	1260	6/6	0.49	0.48	69,69,69,70	0
4	GOL	A	1257	6/6	0.63	0.32	70,70,70,70	0
4	GOL	A	1256	6/6	0.64	0.27	48,48,49,49	0
4	GOL	B	1256	6/6	0.73	0.28	40,40,41,41	0
4	GOL	B	1258	6/6	0.75	0.32	63,63,63,64	0
4	GOL	B	1261	6/6	0.77	0.20	48,48,49,49	0
4	GOL	B	1259	6/6	0.82	0.26	71,71,71,71	0
4	GOL	A	1258	6/6	0.83	0.29	48,48,49,49	0
4	GOL	B	1257	6/6	0.86	0.23	35,38,38,39	0
3	SO4	B	1255	5/5	0.91	0.30	61,61,61,61	0
2	ACT	A	301	4/4	0.91	0.23	38,38,38,39	0
2	ACT	A	300	4/4	0.96	0.17	33,33,33,33	0
2	ACT	B	300	4/4	0.96	0.12	29,29,29,29	0
3	SO4	A	1255	5/5	0.99	0.09	23,23,23,23	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.