



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:26 AM UTC

PDB ID : 3SS3 / pdb\_00003ss3  
Title : Crystal structure of mouse Glutaminase C, ligand-free form  
Authors : Ambrosio, A.L.B.; Dias, S.M.G.; Cerione, R.A.  
Deposited on : 2011-07-07  
Resolution : 2.42 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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

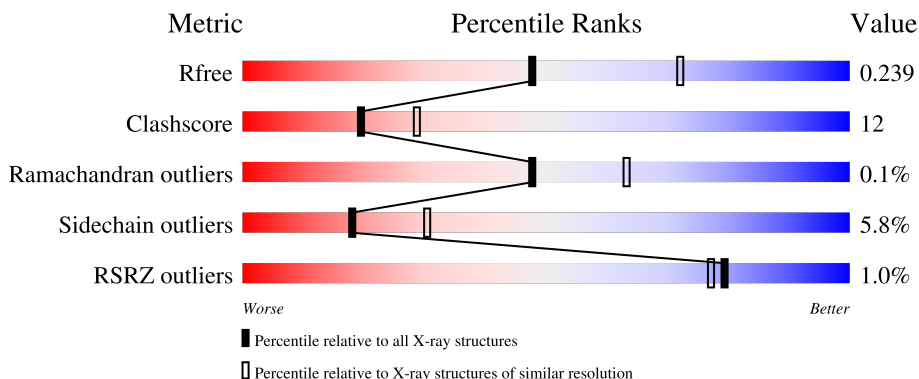
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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))
$R_{free}$	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	479	 64% 16% 18%
1	B	479	 64% 16% 19%
1	C	479	 59% 18% 20%
1	D	479	 61% 18% 20%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13253 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 Glutaminase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	Total 3083	C 1970	N 519	O 566	S 28	3	0	0
1	B	390	Total 3050	C 1948	N 515	O 559	S 28	1	0	0
1	C	383	Total 2996	C 1912	N 506	O 550	S 28	1	0	0
1	D	385	Total 3015	C 1925	N 509	O 553	S 28	1	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLY	-	expression tag	UNP Q69ZX9
A	126	SER	-	expression tag	UNP Q69ZX9
A	127	HIS	-	expression tag	UNP Q69ZX9
B	125	GLY	-	expression tag	UNP Q69ZX9
B	126	SER	-	expression tag	UNP Q69ZX9
B	127	HIS	-	expression tag	UNP Q69ZX9
C	125	GLY	-	expression tag	UNP Q69ZX9
C	126	SER	-	expression tag	UNP Q69ZX9
C	127	HIS	-	expression tag	UNP Q69ZX9
D	125	GLY	-	expression tag	UNP Q69ZX9
D	126	SER	-	expression tag	UNP Q69ZX9
D	127	HIS	-	expression tag	UNP Q69ZX9

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Cl 1	0	0
2	D	1	Total 1	Cl 1	0	0

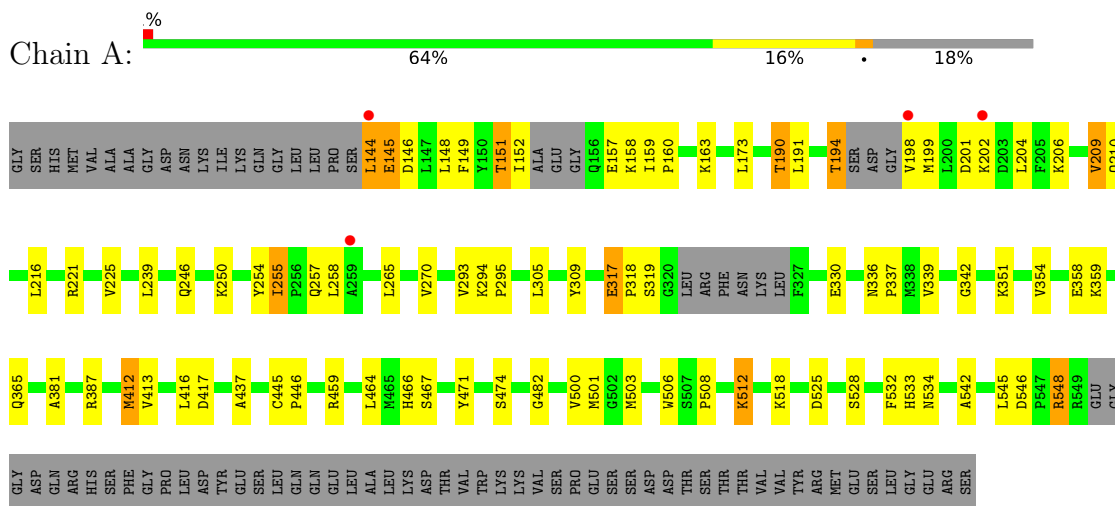
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	270	Total 270	O 270	0	0
3	B	267	Total 267	O 267	0	0
3	C	279	Total 279	O 279	0	0
3	D	289	Total 289	O 289	0	0

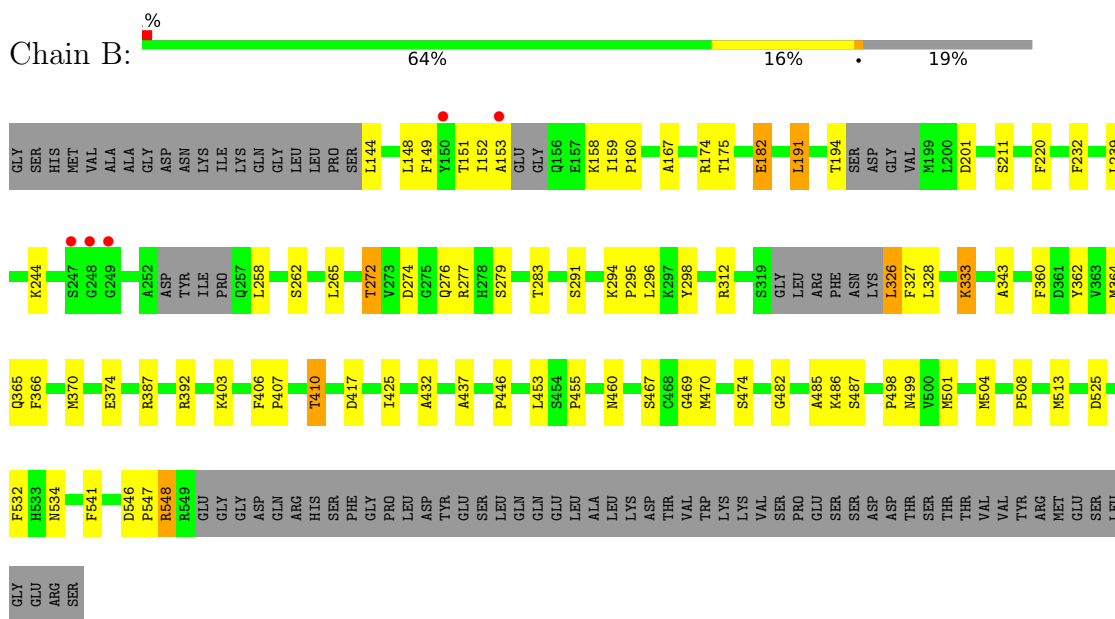
### 3 Residue-property plots

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: Glutaminase C

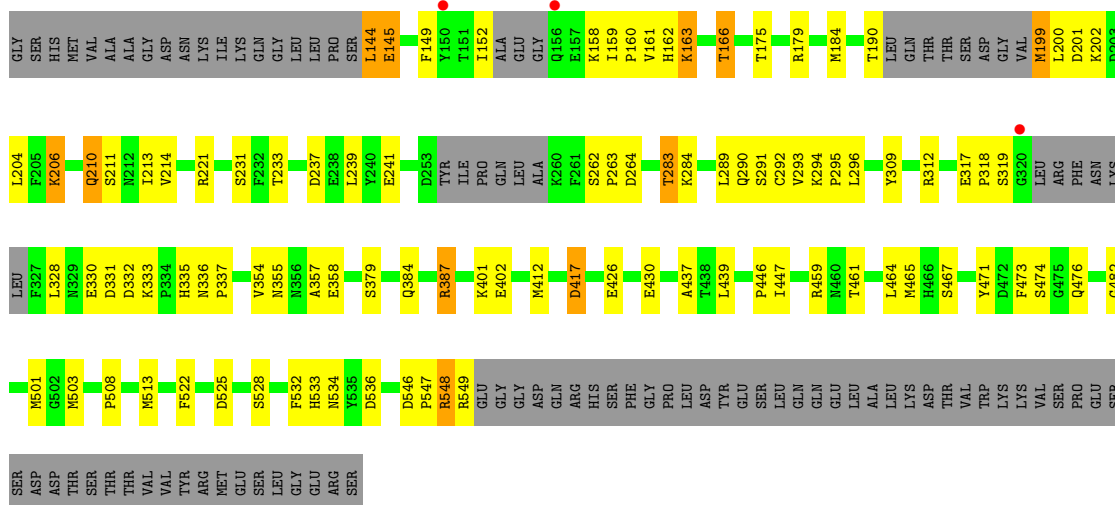


- Molecule 1: Glutaminase C

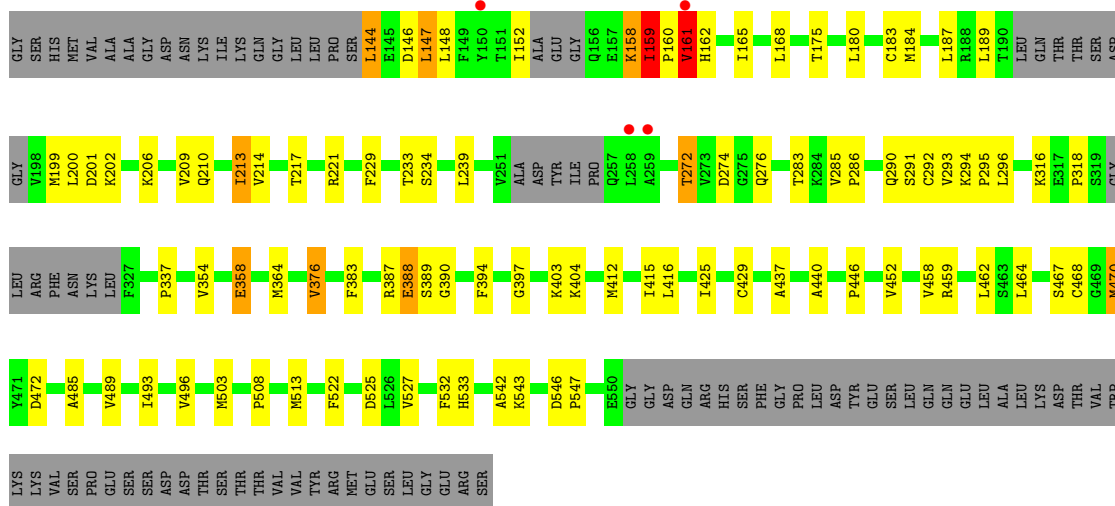


- Molecule 1: Glutaminase C





● Molecule 1: Glutaminase C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.26Å 138.81Å 179.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.42 19.93 – 2.42	Depositor EDS
% Data completeness (in resolution range)	93.7 (19.93-2.42) 93.4 (19.93-2.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.41Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.195 , 0.250 0.184 , 0.239	Depositor DCC
$R_{free}$ test set	4444 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtrriage
Anisotropy	0.195	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13253	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0229e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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:  
CL

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	0.41	0/3150	0.84	7/4249 (0.2%)
1	B	0.43	0/3114	0.81	2/4197 (0.0%)
1	C	0.43	0/3060	0.82	2/4122 (0.0%)
1	D	0.43	0/3079	0.87	8/4148 (0.2%)
All	All	0.43	0/12403	0.84	19/16716 (0.1%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	GLU	N-CA-C	7.01	116.20	108.14
1	D	159	ILE	CA-C-N	6.62	126.31	119.56
1	D	159	ILE	C-N-CA	6.62	126.31	119.56
1	C	471	TYR	CB-CA-C	-6.39	107.39	116.34
1	B	508	PRO	N-CA-C	6.11	118.15	110.70

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	3083	0	3066	64	0
1	B	3050	0	3038	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2996	0	2972	73	0
1	D	3015	0	2992	84	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	C	1	0	0	0	0
2	D	1	0	0	1	0
3	A	270	0	0	4	0
3	B	267	0	0	7	0
3	C	279	0	0	3	0
3	D	289	0	0	3	0
All	All	13253	0	12068	281	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 12.

The worst 5 of 281 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:461:THR:HG22	1:C:465:MET:HE3	1.33	1.11
1:B:406:PHE:HB3	1:B:410:THR:HG21	1.37	1.01
1:C:295:PRO:HB2	1:C:465:MET:HE2	1.41	0.99
1:D:159:ILE:HD13	1:D:161:VAL:H	1.25	0.99
1:C:145:GLU:HG3	1:C:206:LYS:HG3	1.41	0.98

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	386/479 (81%)	380 (98%)	6 (2%)	0	100	100
1	B	380/479 (79%)	376 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	373/479 (78%)	365 (98%)	8 (2%)	0	100	100
1	D	375/479 (78%)	367 (98%)	7 (2%)	1 (0%)	36	49
All	All	1514/1916 (79%)	1488 (98%)	25 (2%)	1 (0%)	48	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	VAL

### 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	343/415 (83%)	321 (94%)	22 (6%)	16	26
1	B	339/415 (82%)	323 (95%)	16 (5%)	23	39
1	C	333/415 (80%)	309 (93%)	24 (7%)	13	21
1	D	335/415 (81%)	319 (95%)	16 (5%)	23	38
All	All	1350/1660 (81%)	1272 (94%)	78 (6%)	18	30

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	417	ASP
1	D	296	LEU
1	C	528	SER
1	D	159	ILE
1	D	388	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	156	GLN

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Mol	Chain	Res	Type
1	C	355	ASN
1	D	421	GLN
1	D	352	GLN
1	D	355	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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.

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, 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	394/479 (82%)	-0.53	4 (1%) 79 77	16, 26, 55, 73	4 (1%)
1	B	390/479 (81%)	-0.49	5 (1%) 75 72	15, 26, 55, 73	2 (0%)
1	C	383/479 (79%)	-0.56	3 (0%) 82 80	15, 26, 56, 83	2 (0%)
1	D	385/479 (80%)	-0.49	4 (1%) 79 77	13, 26, 56, 91	4 (1%)
All	All	1552/1916 (81%)	-0.52	16 (1%) 79 77	13, 26, 56, 91	12 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	SER	4.3
1	B	248	GLY	3.0
1	D	258	LEU	2.6
1	B	249	GLY	2.4
1	B	150	TYR	2.3

### 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 oligosaccharides 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
2	CL	A	1	1/1	0.99	0.05	27,27,27,27	0
2	CL	B	2	1/1	0.99	0.04	36,36,36,36	0
2	CL	C	3	1/1	0.99	0.05	25,25,25,25	0
2	CL	D	4	1/1	0.99	0.04	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.