



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 05:39 PM EDT

PDB ID : 6Q9R  
Title : Crystal structure of the pathological N184K variant of calcium-free human gelsolin  
Authors : Scalone, E.; Boni, F.; Milani, M.; Eloise, M.; de Rosa, M.  
Deposited on : 2018-12-18  
Resolution : 2.73 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](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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

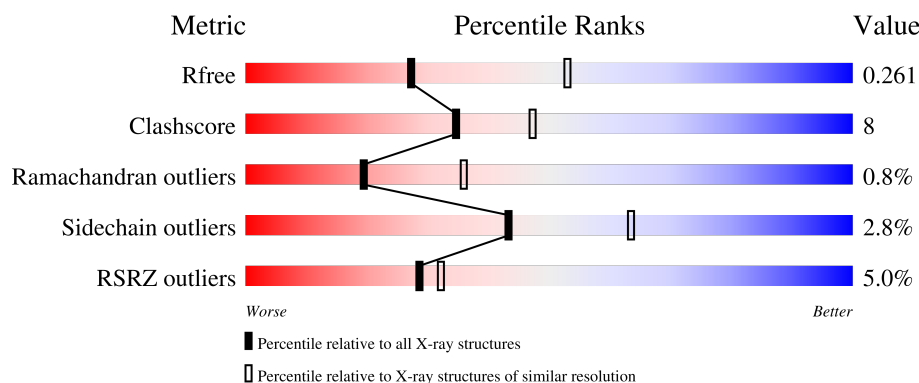
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	778	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 8%</div> </div> </div>
1	B	778	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 8%</div> </div> </div>

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	GOL	A	809	-	-	X	-
3	GOL	B	810	-	-	-	X
3	GOL	B	811	-	-	-	X
3	GOL	B	812	-	-	-	X
5	TRS	B	813	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11503 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 Gelsolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5578	3520	975	1067	16			
1	B	713	Total	C	N	O	S	0	0	0
			5564	3512	972	1064	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P06396
A	-21	GLY	-	expression tag	UNP P06396
A	-20	SER	-	expression tag	UNP P06396
A	-19	SER	-	expression tag	UNP P06396
A	-18	HIS	-	expression tag	UNP P06396
A	-17	HIS	-	expression tag	UNP P06396
A	-16	HIS	-	expression tag	UNP P06396
A	-15	HIS	-	expression tag	UNP P06396
A	-14	HIS	-	expression tag	UNP P06396
A	-13	HIS	-	expression tag	UNP P06396
A	-12	SER	-	expression tag	UNP P06396
A	-11	SER	-	expression tag	UNP P06396
A	-10	GLY	-	expression tag	UNP P06396
A	-9	LEU	-	expression tag	UNP P06396
A	-8	VAL	-	expression tag	UNP P06396
A	-7	PRO	-	expression tag	UNP P06396
A	-6	ARG	-	expression tag	UNP P06396
A	-5	GLY	-	expression tag	UNP P06396
A	-4	SER	-	expression tag	UNP P06396
A	-3	HIS	-	expression tag	UNP P06396
A	-2	MET	-	expression tag	UNP P06396
A	-1	ALA	-	expression tag	UNP P06396
A	0	SER	-	expression tag	UNP P06396
A	184	LYS	ASN	engineered mutation	UNP P06396
B	-22	MET	-	initiating methionine	UNP P06396

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	GLY	-	expression tag	UNP P06396
B	-20	SER	-	expression tag	UNP P06396
B	-19	SER	-	expression tag	UNP P06396
B	-18	HIS	-	expression tag	UNP P06396
B	-17	HIS	-	expression tag	UNP P06396
B	-16	HIS	-	expression tag	UNP P06396
B	-15	HIS	-	expression tag	UNP P06396
B	-14	HIS	-	expression tag	UNP P06396
B	-13	HIS	-	expression tag	UNP P06396
B	-12	SER	-	expression tag	UNP P06396
B	-11	SER	-	expression tag	UNP P06396
B	-10	GLY	-	expression tag	UNP P06396
B	-9	LEU	-	expression tag	UNP P06396
B	-8	VAL	-	expression tag	UNP P06396
B	-7	PRO	-	expression tag	UNP P06396
B	-6	ARG	-	expression tag	UNP P06396
B	-5	GLY	-	expression tag	UNP P06396
B	-4	SER	-	expression tag	UNP P06396
B	-3	HIS	-	expression tag	UNP P06396
B	-2	MET	-	expression tag	UNP P06396
B	-1	ALA	-	expression tag	UNP P06396
B	0	SER	-	expression tag	UNP P06396
B	184	LYS	ASN	engineered mutation	UNP P06396

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Cl 6 6	0	0
2	B	3	Total Cl 3 3	0	0

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



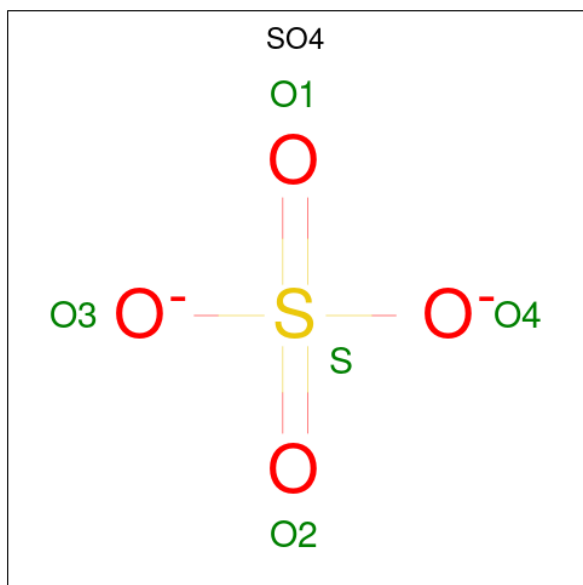
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

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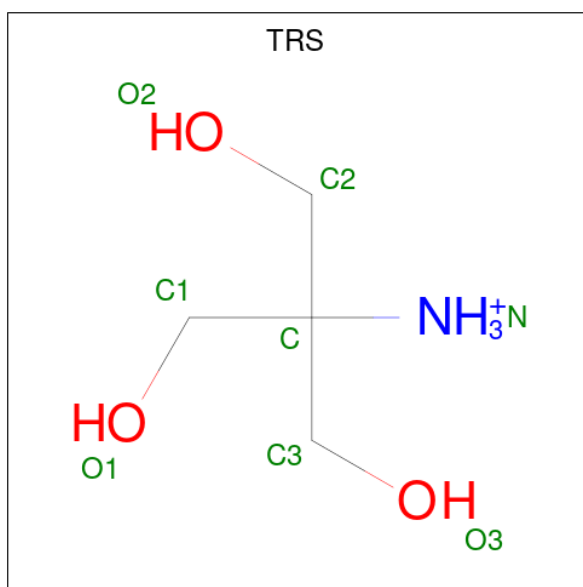
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is water.

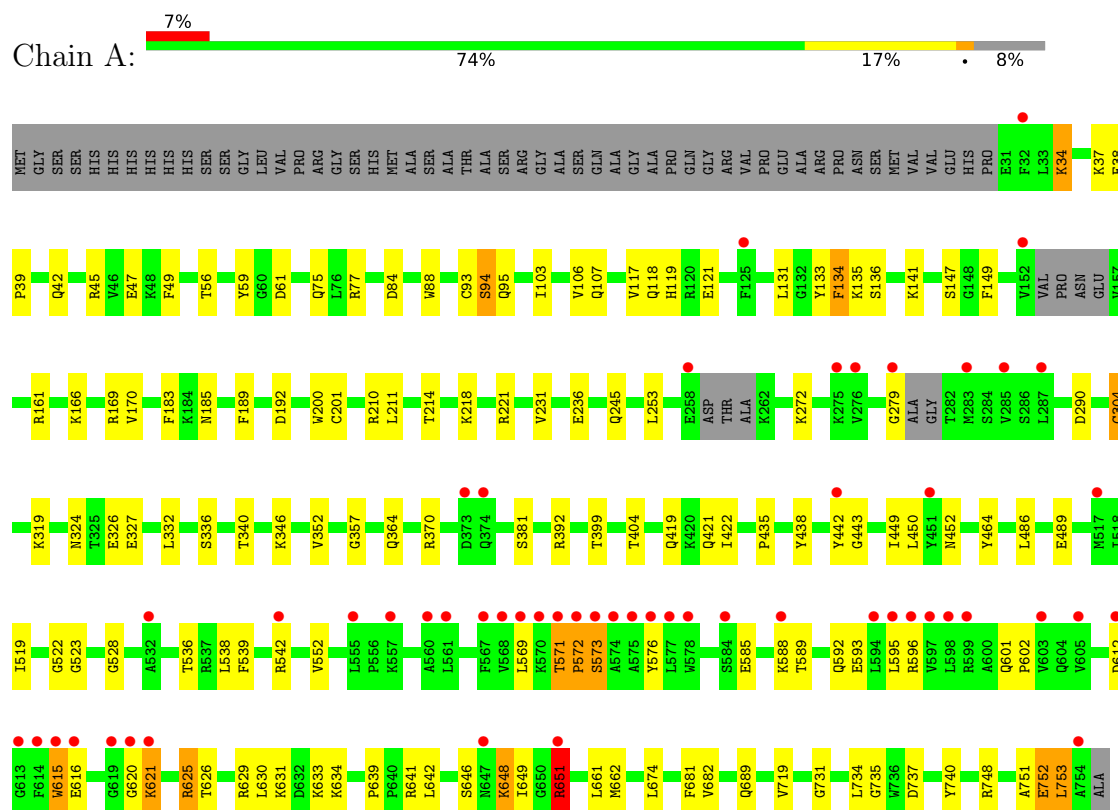
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	110	Total	O	0	0
			110	110		
6	B	122	Total	O	0	0
			122	122		

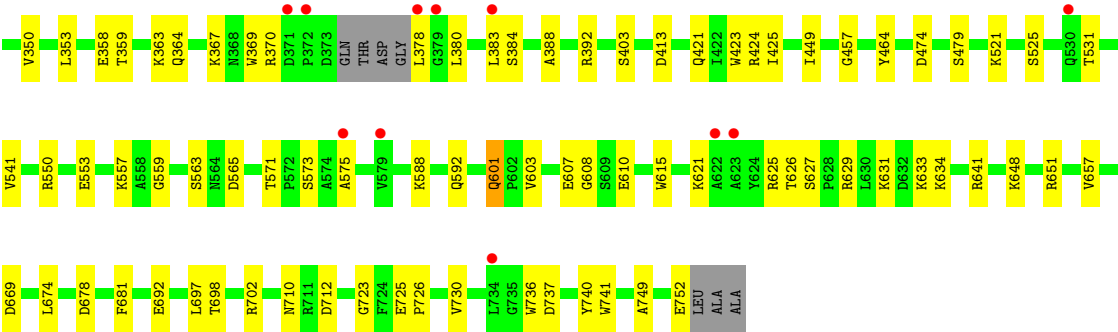


### 3 Residue-property plots

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: Gelsolin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.85Å 169.85Å 150.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.26 – 2.73 75.26 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.26-2.73) 99.9 (75.26-2.73)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???), REFMAC	Depositor
R, $R_{free}$	0.213 , 0.260 0.214 , 0.261	Depositor DCC
$R_{free}$ test set	1999 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: GOL, TRS, SO4, 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	0.30	0/5702	0.48	1/7717 (0.0%)
1	B	0.29	0/5689	0.46	0/7702
All	All	0.29	0/11391	0.47	1/15419 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	571	THR	CB-CA-C	-6.50	94.06	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	651	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	5578	0	5439	87	2
1	B	5564	0	5421	98	2
2	A	6	0	0	0	0
2	B	3	0	0	1	0
3	A	48	0	64	5	0
3	B	54	0	72	9	0
4	A	10	0	0	1	0
5	B	8	0	12	0	0
6	A	110	0	0	1	1
6	B	122	0	0	4	1
All	All	11503	0	11008	184	3

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 8.

All (184) 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:557:LYS:HD3	1:B:559:GLY:H	1.27	0.99
1:B:264:ASP:HB2	1:B:651:ARG:HH21	1.39	0.86
1:A:648:LYS:NZ	1:A:651:ARG:HG3	1.98	0.79
1:A:625:ARG:HE	1:A:626:THR:H	1.33	0.76
1:B:293:PRO:HB2	1:B:367:LYS:HG2	1.69	0.75
1:A:648:LYS:HZ3	1:A:651:ARG:HG3	1.52	0.73
1:B:323:ALA:O	1:B:328:ARG:NH1	2.23	0.70
1:A:595:LEU:HD13	1:A:602:PRO:HB3	1.74	0.70
1:A:536:THR:HG22	1:A:571:THR:HA	1.75	0.69
1:A:131:LEU:HD13	1:A:170:VAL:HG11	1.73	0.68
1:B:264:ASP:O	1:B:266:ALA:N	2.27	0.66
1:A:419:GLN:HB2	1:A:452:ASN:HD22	1.60	0.66
1:A:449:ILE:HB	1:A:464:TYR:HB2	1.77	0.66
1:A:630:LEU:HD23	1:A:634:LYS:HA	1.77	0.66
1:B:166:LYS:HE3	1:B:258:GLU:HB2	1.76	0.66
1:A:94:SER:OG	1:A:95:GLN:N	2.27	0.65
1:A:519:ILE:HD12	1:A:552:VAL:HG22	1.78	0.65
1:A:218:LYS:HE2	1:A:221:ARG:HH22	1.62	0.65
1:B:557:LYS:HD3	1:B:559:GLY:N	2.07	0.64
1:B:702:ARG:NH2	6:B:906:HOH:O	2.31	0.64
1:B:169:ARG:HD2	1:B:657:VAL:HG22	1.81	0.62
1:A:751:ALA:O	1:A:753:LEU:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:LYS:HG3	1:B:322:GLN:HG2	1.82	0.62
1:B:341:LYS:NZ	6:B:907:HOH:O	2.33	0.62
1:B:741:TRP:HB2	3:B:812:GOL:H32	1.83	0.61
1:A:737:ASP:HB3	1:A:740:TYR:HB2	1.81	0.61
1:B:588:LYS:O	1:B:592:GLN:HG3	2.00	0.61
1:B:120:ARG:HH22	1:B:346:LYS:HE3	1.66	0.61
1:A:625:ARG:HE	1:A:626:THR:N	2.00	0.60
1:B:737:ASP:HB3	1:B:740:TYR:HB2	1.83	0.59
1:A:37:LYS:HG3	1:A:42:GLN:HE22	1.66	0.59
1:A:542:ARG:HG3	1:A:629:ARG:HH21	1.68	0.59
1:B:625:ARG:HE	1:B:627:SER:H	1.50	0.59
1:A:75:GLN:NE2	6:A:901:HOH:O	2.36	0.58
1:A:682:VAL:HG13	1:A:719:VAL:HA	1.86	0.58
1:B:45:ARG:NH2	1:B:149:PHE:O	2.37	0.58
1:B:35:ALA:HA	1:B:42:GLN:HE22	1.70	0.57
1:A:641:ARG:NH2	4:A:815:SO4:O3	2.31	0.57
1:B:563:SER:OG	1:B:607:GLU:OE2	2.20	0.56
1:B:353:LEU:HD23	1:B:358:GLU:HA	1.86	0.56
1:B:425:ILE:HG13	1:B:479:SER:HB3	1.87	0.56
1:A:641:ARG:HE	3:A:809:GOL:H11	1.71	0.56
1:A:45:ARG:NH1	1:A:47:GLU:OE2	2.39	0.56
1:B:168:ARG:NH2	1:B:669:ASP:OD1	2.38	0.55
1:A:340:THR:HG22	1:A:346:LYS:HE2	1.87	0.55
1:B:565:ASP:OD2	1:B:629:ARG:NH2	2.39	0.55
1:A:200:TRP:CZ2	1:A:236:GLU:HG2	2.42	0.55
1:A:734:LEU:HG	1:A:735:GLY:N	2.22	0.54
1:B:31:GLU:OE2	1:B:32:PHE:N	2.29	0.54
1:A:662:MET:HA	1:A:734:LEU:CD2	2.37	0.54
1:A:629:ARG:NH1	3:A:807:GOL:O2	2.41	0.54
1:A:734:LEU:HD23	1:A:734:LEU:N	2.23	0.54
1:B:264:ASP:OD1	1:B:651:ARG:HB3	2.08	0.54
1:B:521:LYS:HB2	1:B:553:GLU:HG2	1.90	0.53
1:B:424:ARG:NH1	1:B:525:SER:OG	2.41	0.53
1:A:585:GLU:HG2	1:A:588:LYS:HE2	1.91	0.53
1:A:601:GLN:HG3	1:A:602:PRO:HD2	1.90	0.53
1:A:201:CYS:HB3	1:A:210:ARG:HD3	1.91	0.53
1:B:641:ARG:HH21	3:B:807:GOL:H32	1.74	0.52
1:A:45:ARG:NH2	1:A:149:PHE:O	2.42	0.52
1:A:218:LYS:HE2	1:A:221:ARG:NH2	2.24	0.52
1:A:399:THR:HG21	1:B:457:GLY:HA3	1.91	0.52
1:A:641:ARG:NE	3:A:809:GOL:H11	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:THR:HB	1:A:572:PRO:HD2	1.92	0.52
1:B:269:LYS:HZ1	1:B:710:ASN:CG	2.13	0.52
1:B:314:LYS:NZ	6:B:917:HOH:O	2.43	0.51
1:A:538:LEU:HD12	1:A:539:PHE:H	1.75	0.51
1:B:629:ARG:NH1	2:B:802:CL:CL	2.81	0.51
1:B:120:ARG:HB3	1:B:350:VAL:HB	1.92	0.50
1:B:200:TRP:CZ2	1:B:236:GLU:HG2	2.46	0.50
1:A:648:LYS:HZ2	1:A:651:ARG:HG3	1.75	0.50
1:B:287:LEU:HD21	1:B:290:ASP:HB3	1.94	0.50
1:B:57:ASN:O	1:B:223:ASN:HB3	2.12	0.49
1:A:734:LEU:HD23	1:A:734:LEU:H	1.75	0.49
1:B:264:ASP:CG	1:B:651:ARG:HE	2.15	0.49
1:A:642:LEU:HB2	1:A:661:LEU:HD22	1.94	0.49
1:B:306:ILE:HD12	1:B:317:VAL:HG22	1.95	0.49
1:B:378:LEU:C	1:B:633:LYS:HE2	2.33	0.48
1:A:593:GLU:HA	1:A:596:ARG:HD3	1.95	0.48
1:B:571:THR:HG23	1:B:573:SER:H	1.78	0.48
1:A:364:GLN:OE1	3:A:809:GOL:O1	2.23	0.48
1:B:147:SER:HB2	1:B:149:PHE:HD1	1.78	0.48
1:A:61:ASP:HB3	1:A:141:LYS:HD2	1.96	0.48
1:B:183:PHE:HA	1:B:189:PHE:CZ	2.48	0.48
1:B:364:GLN:NE2	3:B:808:GOL:O1	2.37	0.48
1:B:723:GLY:HA3	3:B:812:GOL:H2	1.93	0.48
1:B:359:THR:O	1:B:363:LYS:HG3	2.13	0.48
1:B:413:ASP:OD1	1:B:726:PRO:HB2	2.14	0.48
1:B:425:ILE:HG13	1:B:479:SER:CB	2.43	0.48
1:B:346:LYS:NZ	6:B:922:HOH:O	2.47	0.47
1:A:38:GLU:HB2	1:A:39:PRO:HD2	1.96	0.47
1:B:363:LYS:HD2	1:B:369:TRP:CD1	2.49	0.47
1:A:117:VAL:HG23	1:A:119:HIS:CE1	2.49	0.47
1:B:239:GLU:HG3	1:B:244:LEU:HD21	1.96	0.47
1:A:279:GLY:H	1:A:327:GLU:CD	2.18	0.47
1:A:37:LYS:HG3	1:A:42:GLN:NE2	2.30	0.47
1:A:221:ARG:HD3	1:A:231:VAL:HG23	1.96	0.47
1:A:272:LYS:HG2	1:A:290:ASP:HA	1.97	0.47
1:A:748:ARG:O	1:A:752:GLU:HG2	2.15	0.47
1:B:71:LEU:HD11	1:B:83:TYR:HB3	1.95	0.47
1:B:384:SER:OG	3:B:807:GOL:H31	2.14	0.47
1:B:449:ILE:HB	1:B:464:TYR:HB2	1.96	0.47
1:A:662:MET:HA	1:A:734:LEU:HD21	1.97	0.46
1:B:678:ASP:HB2	3:B:809:GOL:H32	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:ND2	1:A:253:LEU:O	2.48	0.46
1:B:71:LEU:HD13	1:B:85:LEU:HG	1.97	0.46
1:B:603:VAL:O	1:B:603:VAL:HG23	2.16	0.46
1:A:422:ILE:HG23	1:A:449:ILE:HD13	1.98	0.46
1:B:541:VAL:O	1:B:565:ASP:HB3	2.16	0.45
1:B:674:LEU:HB3	1:B:681:PHE:HB2	1.97	0.45
1:A:585:GLU:O	1:A:589:THR:HG22	2.16	0.45
1:B:625:ARG:HE	1:B:626:THR:N	2.13	0.45
1:A:486:LEU:HA	1:A:489:GLU:HG2	1.99	0.45
1:A:56:THR:HA	1:A:59:TYR:CD1	2.51	0.45
1:B:575:ALA:O	1:B:603:VAL:HG22	2.17	0.45
1:B:641:ARG:HG3	3:B:808:GOL:H31	1.98	0.45
1:A:571:THR:HB	1:A:572:PRO:CD	2.44	0.45
1:A:118:GLN:HB2	1:A:352:VAL:HB	1.99	0.45
1:B:615:TRP:CD2	1:B:621:LYS:HB3	2.51	0.45
1:B:625:ARG:NE	1:B:627:SER:H	2.15	0.45
1:B:165:VAL:HG13	1:B:171:VAL:HG21	1.99	0.44
1:B:35:ALA:HB1	1:B:71:LEU:HD23	1.99	0.44
1:B:135:LYS:HE3	1:B:135:LYS:HB2	1.53	0.44
1:B:221:ARG:NH1	1:B:222:ASP:OD1	2.48	0.44
1:B:76:LEU:C	1:B:78:ASN:H	2.20	0.44
1:B:712:ASP:HB2	3:B:806:GOL:H12	1.99	0.44
1:B:749:ALA:O	1:B:752:GLU:HB3	2.17	0.44
1:A:147:SER:HB2	1:A:149:PHE:HD2	1.83	0.43
1:A:625:ARG:NE	1:A:625:ARG:HA	2.32	0.43
1:A:37:LYS:CG	1:A:42:GLN:HE22	2.31	0.43
1:B:198:HIS:CE1	1:B:240:PRO:HG2	2.53	0.43
1:A:88:TRP:HA	1:A:121:GLU:O	2.19	0.43
1:A:304:CYS:HB3	1:A:319:LYS:HA	2.00	0.43
1:A:324:ASN:OD1	1:A:326:GLU:HB2	2.19	0.43
1:A:674:LEU:HB3	1:A:681:PHE:HB2	2.00	0.43
1:B:648:LYS:HD3	1:B:648:LYS:HA	1.73	0.43
1:A:616:GLU:HA	1:A:620:GLY:H	1.83	0.43
1:B:45:ARG:O	1:B:47:GLU:HG3	2.18	0.43
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.86	0.43
1:B:276:VAL:CG1	1:B:306:ILE:HG12	2.49	0.43
1:A:183:PHE:HA	1:A:189:PHE:CZ	2.54	0.43
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.90	0.43
1:B:608:GLY:N	1:B:610:GLU:OE2	2.52	0.42
1:A:404:THR:O	1:A:731:GLY:HA3	2.19	0.42
1:B:730:VAL:HG13	1:B:736:TRP:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:TRP:CE3	1:A:621:LYS:HB3	2.54	0.42
1:B:383:LEU:HD11	1:B:392:ARG:HH22	1.84	0.42
1:B:697:LEU:HD23	1:B:697:LEU:HA	1.86	0.42
1:A:625:ARG:NE	1:A:626:THR:H	2.10	0.42
1:A:106:VAL:HG23	1:A:332:LEU:HD12	2.01	0.42
1:B:648:LYS:NZ	1:B:692:GLU:OE2	2.52	0.42
1:A:357:GLY:HA2	1:A:381:SER:HB2	2.02	0.42
1:A:442:TYR:HD1	1:A:523:GLY:HA3	1.84	0.42
1:B:625:ARG:HE	1:B:626:THR:H	1.66	0.42
1:B:725:GLU:OE2	3:B:804:GOL:H12	2.20	0.41
1:A:103:ILE:O	1:A:107:GLN:HG3	2.21	0.41
1:B:169:ARG:HA	1:B:169:ARG:HD3	1.99	0.41
1:B:269:LYS:NZ	1:B:710:ASN:OD1	2.53	0.41
1:A:161:ARG:NH2	1:A:192:ASP:OD2	2.53	0.41
1:A:435:PRO:HA	1:A:438:TYR:CD1	2.55	0.41
1:A:34:LYS:HE2	1:A:34:LYS:H	1.85	0.41
1:A:569:LEU:HB3	1:A:576:TYR:HB2	2.03	0.41
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.91	0.41
1:A:639:PRO:O	3:A:809:GOL:H12	2.20	0.41
1:B:125:PHE:CE2	1:B:347:GLN:HG2	2.55	0.41
1:B:199:GLN:HG2	1:B:233:VAL:HG13	2.01	0.41
1:B:601:GLN:H	1:B:601:GLN:HG3	1.67	0.41
1:B:270:LEU:HD13	1:B:270:LEU:HA	1.93	0.41
1:A:443:GLY:HA3	1:A:522:GLY:H	1.86	0.41
1:A:592:GLN:O	1:A:596:ARG:HG3	2.20	0.41
1:B:76:LEU:O	1:B:78:ASN:N	2.48	0.41
1:B:421:GLN:HG2	1:B:423:TRP:CZ2	2.56	0.41
1:B:698:THR:HG22	1:B:702:ARG:HD2	2.02	0.41
1:A:93:CYS:SG	1:A:94:SER:N	2.95	0.41
1:A:211:LEU:O	1:A:214:THR:OG1	2.35	0.41
1:A:133:TYR:HB2	1:A:134:PHE:CE2	2.56	0.40
1:A:612:ASP:HA	1:A:615:TRP:HB2	2.02	0.40
1:B:474:ASP:OD1	1:B:474:ASP:N	2.50	0.40
1:B:290:ASP:OD1	1:B:290:ASP:N	2.53	0.40
1:B:383:LEU:HD21	1:B:388:ALA:HA	2.03	0.40
1:A:77:ARG:CZ	1:A:392:ARG:HG3	2.51	0.40
1:A:421:GLN:NE2	1:A:450:LEU:HD23	2.36	0.40
1:B:39:PRO:HA	1:B:73:THR:HB	2.03	0.40
1:B:88:TRP:CZ2	1:B:123:GLN:HB2	2.56	0.40

All (3) 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:A:147:SER:OG	1:B:245:GLN:OE1[5_555]	2.18	0.02
6:A:921:HOH:O	6:B:937:HOH:O[5_555]	2.18	0.02
1:A:245:GLN:OE1	1:B:147:SER:OG[5_555]	2.19	0.01

## 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	707/778 (91%)	673 (95%)	28 (4%)	6 (1%)	19	36
1	B	705/778 (91%)	669 (95%)	31 (4%)	5 (1%)	22	40
All	All	1412/1556 (91%)	1342 (95%)	59 (4%)	11 (1%)	19	36

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	GLU
1	B	531	THR
1	A	573	SER
1	A	649	ILE
1	B	135	LYS
1	B	257	THR
1	B	265	ALA
1	A	631	LYS
1	A	528	GLY
1	A	753	LEU
1	B	157	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	583/629 (93%)	561 (96%)	22 (4%)	33	54
1	B	582/629 (92%)	571 (98%)	11 (2%)	57	74
All	All	1165/1258 (93%)	1132 (97%)	33 (3%)	43	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	49	PHE
1	A	84	ASP
1	A	94	SER
1	A	134	PHE
1	A	135	LYS
1	A	136	SER
1	A	166	LYS
1	A	169	ARG
1	A	304	CYS
1	A	336	SER
1	A	370	ARG
1	A	572	PRO
1	A	573	SER
1	A	615	TRP
1	A	621	LYS
1	A	625	ARG
1	A	633	LYS
1	A	646	SER
1	A	648	LYS
1	A	651	ARG
1	A	689	GLN
1	B	49	PHE
1	B	94	SER
1	B	155	ASN
1	B	269	LYS
1	B	287	LEU
1	B	370	ARG
1	B	403	SER
1	B	550	ARG
1	B	601	GLN
1	B	631	LYS
1	B	634	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	206	ASN
1	A	421	GLN
1	A	452	ASN
1	A	455	HIS
1	B	195	ASN
1	B	204	ASN
1	B	459	GLN
1	B	647	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 29 ligands modelled in this entry, 9 are monoatomic - leaving 20 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	$\# Z  > 2$
3	GOL	A	812	-	5,5,5	0.93	0	5,5,5	0.98	0
3	GOL	A	808	-	5,5,5	0.89	0	5,5,5	1.06	0
5	TRS	B	813	-	7,7,7	0.32	0	9,9,9	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	813	-	5,5,5	0.91	0	5,5,5	0.97	0
3	GOL	B	805	-	5,5,5	0.89	0	5,5,5	1.01	0
3	GOL	B	804	-	5,5,5	0.90	0	5,5,5	1.01	0
3	GOL	B	812	-	5,5,5	0.88	0	5,5,5	0.96	0
3	GOL	B	807	-	5,5,5	0.90	0	5,5,5	0.94	0
3	GOL	A	811	-	5,5,5	0.95	0	5,5,5	0.95	0
3	GOL	B	806	-	5,5,5	0.85	0	5,5,5	1.02	0
3	GOL	B	809	-	5,5,5	0.90	0	5,5,5	0.96	0
3	GOL	B	808	-	5,5,5	0.93	0	5,5,5	0.96	0
3	GOL	B	811	-	5,5,5	0.91	0	5,5,5	0.99	0
3	GOL	B	810	-	5,5,5	0.90	0	5,5,5	0.98	0
3	GOL	A	807	-	5,5,5	0.88	0	5,5,5	0.97	0
4	SO4	A	816	-	4,4,4	0.15	0	6,6,6	0.05	0
3	GOL	A	810	-	5,5,5	0.91	0	5,5,5	1.05	0
4	SO4	A	815	-	4,4,4	0.14	0	6,6,6	0.09	0
3	GOL	A	814	-	5,5,5	0.87	0	5,5,5	0.99	0
3	GOL	A	809	-	5,5,5	0.88	0	5,5,5	1.00	0

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
3	GOL	B	812	-	-	1/4/4/4	-
3	GOL	B	807	-	-	4/4/4/4	-
3	GOL	A	811	-	-	2/4/4/4	-
3	GOL	A	807	-	-	2/4/4/4	-
3	GOL	A	808	-	-	2/4/4/4	-
3	GOL	A	812	-	-	0/4/4/4	-
3	GOL	B	805	-	-	2/4/4/4	-
3	GOL	B	810	-	-	2/4/4/4	-
3	GOL	B	806	-	-	2/4/4/4	-
3	GOL	B	809	-	-	0/4/4/4	-
3	GOL	A	810	-	-	1/4/4/4	-
3	GOL	B	804	-	-	2/4/4/4	-
3	GOL	B	808	-	-	0/4/4/4	-
5	TRS	B	813	-	-	1/9/9/9	-
3	GOL	B	811	-	-	0/4/4/4	-
3	GOL	A	813	-	-	0/4/4/4	-
3	GOL	A	814	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	809	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	807	GOL	O1-C1-C2-O2
3	A	807	GOL	O1-C1-C2-C3
3	A	808	GOL	C1-C2-C3-O3
3	A	809	GOL	O1-C1-C2-C3
3	A	814	GOL	O1-C1-C2-C3
3	A	814	GOL	C1-C2-C3-O3
3	B	805	GOL	C1-C2-C3-O3
3	B	806	GOL	C1-C2-C3-O3
3	B	807	GOL	O1-C1-C2-C3
3	B	807	GOL	C1-C2-C3-O3
3	B	810	GOL	C1-C2-C3-O3
3	B	810	GOL	O2-C2-C3-O3
3	A	811	GOL	C1-C2-C3-O3
3	A	811	GOL	O2-C2-C3-O3
3	A	814	GOL	O1-C1-C2-O2
3	A	814	GOL	O2-C2-C3-O3
3	A	808	GOL	O2-C2-C3-O3
3	B	807	GOL	O1-C1-C2-O2
3	A	809	GOL	O1-C1-C2-O2
3	B	805	GOL	O2-C2-C3-O3
3	B	806	GOL	O2-C2-C3-O3
3	B	812	GOL	O1-C1-C2-O2
3	B	804	GOL	O1-C1-C2-O2
3	B	807	GOL	O2-C2-C3-O3
3	A	810	GOL	O2-C2-C3-O3
5	B	813	TRS	C2-C-C1-O1
3	B	804	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	804	GOL	1	0
3	B	812	GOL	2	0
3	B	807	GOL	2	0
3	B	806	GOL	1	0
3	B	809	GOL	1	0
3	B	808	GOL	2	0
3	A	807	GOL	1	0
4	A	815	SO4	1	0
3	A	809	GOL	4	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

### 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	715/778 (91%)	0.65	54 (7%)	13 15	40, 57, 103, 134	0
1	B	713/778 (91%)	0.45	18 (2%)	57 64	36, 55, 97, 140	0
All	All	1428/1556 (91%)	0.55	72 (5%)	28 32	36, 56, 101, 140	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	620	GLY	7.0
1	A	569	LEU	5.8
1	B	280	ALA	5.7
1	B	378	LEU	5.3
1	A	576	TYR	4.7
1	A	615	TRP	4.7
1	A	598	LEU	4.6
1	A	594	LEU	4.4
1	A	374	GLN	4.4
1	A	754	ALA	4.4
1	B	575	ALA	4.3
1	B	379	GLY	4.3
1	A	578	TRP	3.8
1	A	577	LEU	3.6
1	A	614	PHE	3.4
1	A	560	ALA	3.4
1	A	621	LYS	3.4
1	A	595	LEU	3.4
1	A	619	GLY	3.3
1	A	575	ALA	3.2
1	A	613	GLY	3.2
1	B	372	PRO	3.2
1	A	605	VAL	3.1
1	B	282	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	651	ARG	3.0
1	A	568	VAL	3.0
1	A	567	PHE	2.8
1	A	571	THR	2.8
1	A	275	LYS	2.8
1	A	647	ASN	2.8
1	A	603	VAL	2.7
1	A	258	GLU	2.7
1	B	734	LEU	2.7
1	B	257	THR	2.7
1	A	279	GLY	2.7
1	A	612	ASP	2.6
1	A	574	ALA	2.6
1	A	596	ARG	2.6
1	B	290	ASP	2.6
1	A	616	GLU	2.6
1	A	442	TYR	2.5
1	B	579	VAL	2.5
1	A	570	LYS	2.5
1	A	555	LEU	2.5
1	B	263	GLU	2.5
1	A	276	VAL	2.5
1	A	557	LYS	2.5
1	A	517	MET	2.5
1	A	572	PRO	2.4
1	A	532	ALA	2.4
1	A	287	LEU	2.4
1	A	561	LEU	2.4
1	A	283	MET	2.3
1	A	125	PHE	2.3
1	A	285	VAL	2.3
1	B	530	GLN	2.3
1	B	125	PHE	2.3
1	A	542	ARG	2.3
1	A	573	SER	2.3
1	A	373	ASP	2.3
1	B	228	ARG	2.2
1	B	622	ALA	2.2
1	B	371	ASP	2.2
1	B	383	LEU	2.1
1	A	451	TYR	2.1
1	A	597	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	32	PHE	2.1
1	A	588	LYS	2.0
1	A	152	VAL	2.0
1	B	623	ALA	2.0
1	A	584	SER	2.0
1	A	599	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](#)

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(Å <sup>2</sup> )	Q<0.9
3	GOL	B	812	6/6	0.56	0.50	91,95,99,105	0
3	GOL	A	811	6/6	0.57	0.39	77,85,86,88	0
3	GOL	B	810	6/6	0.58	0.40	79,88,89,90	0
5	TRS	B	813	8/8	0.62	0.45	111,115,118,120	0
3	GOL	B	811	6/6	0.72	0.61	78,81,83,85	0
3	GOL	A	814	6/6	0.74	0.38	84,86,87,89	0
3	GOL	B	807	6/6	0.78	0.30	61,62,66,67	0
2	CL	B	802	1/1	0.81	0.20	85,85,85,85	0
3	GOL	A	807	6/6	0.87	0.14	60,62,71,72	0
2	CL	A	806	1/1	0.87	0.17	81,81,81,81	0
3	GOL	A	808	6/6	0.88	0.37	79,81,81,83	0
2	CL	A	803	1/1	0.88	0.14	79,79,79,79	0
3	GOL	B	804	6/6	0.89	0.27	66,68,70,70	0
2	CL	A	805	1/1	0.89	0.21	82,82,82,82	0
2	CL	B	801	1/1	0.90	0.16	72,72,72,72	0
3	GOL	B	808	6/6	0.90	0.37	62,67,76,79	0
4	SO4	A	815	5/5	0.91	0.26	71,73,78,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	801	1/1	0.92	0.16	72,72,72,72	0
3	GOL	B	809	6/6	0.93	0.19	74,75,79,80	0
2	CL	A	802	1/1	0.93	0.15	74,74,74,74	0
3	GOL	A	812	6/6	0.93	0.29	70,72,76,77	0
3	GOL	A	809	6/6	0.94	0.29	56,62,70,74	0
3	GOL	A	813	6/6	0.94	0.34	52,56,59,60	0
3	GOL	A	810	6/6	0.95	0.22	50,50,51,53	0
4	SO4	A	816	5/5	0.95	0.16	76,76,77,80	0
3	GOL	B	806	6/6	0.95	0.20	38,42,46,48	0
2	CL	B	803	1/1	0.96	0.36	104,104,104,104	0
2	CL	A	804	1/1	0.97	0.12	71,71,71,71	0
3	GOL	B	805	6/6	0.98	0.26	43,44,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.