



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2020 – 10:07 PM EST

PDB ID : 6VBE  
Title : Crystal structure of recombinant mutant H180R of human fumarase  
Authors : Ajalla, M.A.A.; Nonato, M.C.  
Deposited on : 2019-12-18  
Resolution : 1.90 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.

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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 : 2.15.1  
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) : 2.15.1

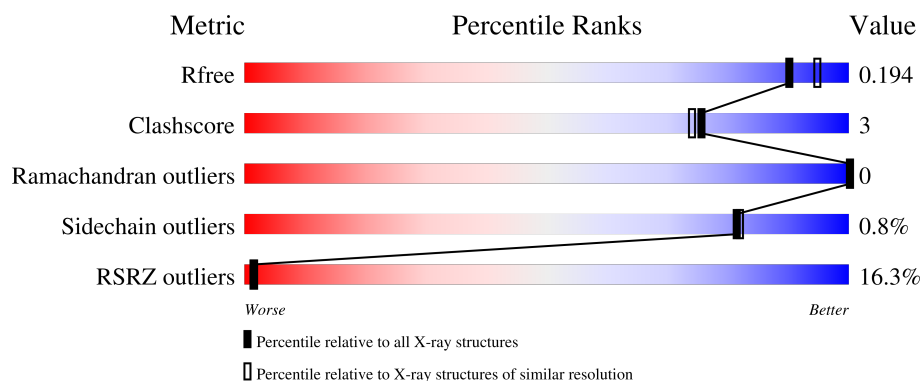
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	466	<div> <div>15%</div> <div>92%</div> <div>6%</div> </div>
1	B	466	<div> <div>18%</div> <div>91%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7582 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 Fumarate hydratase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	5	0
			3487	2202	602	659	24			
1	B	462	Total	C	N	O	S	0	6	0
			3488	2200	606	659	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	ARG	HIS	engineered mutation	UNP P07954
B	180	ARG	HIS	engineered mutation	UNP P07954

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



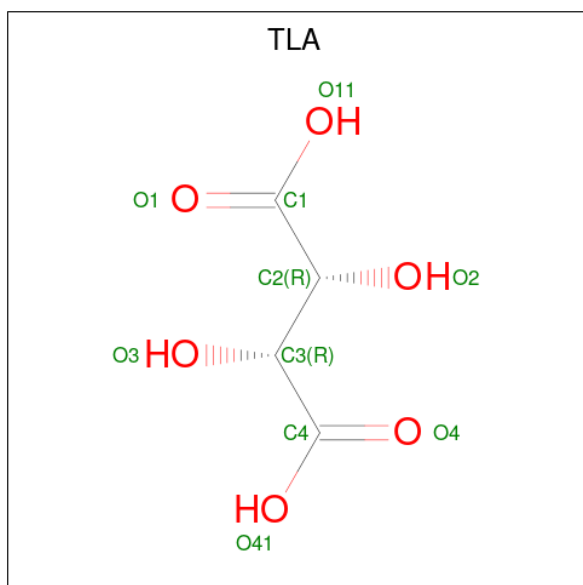
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	4	6		

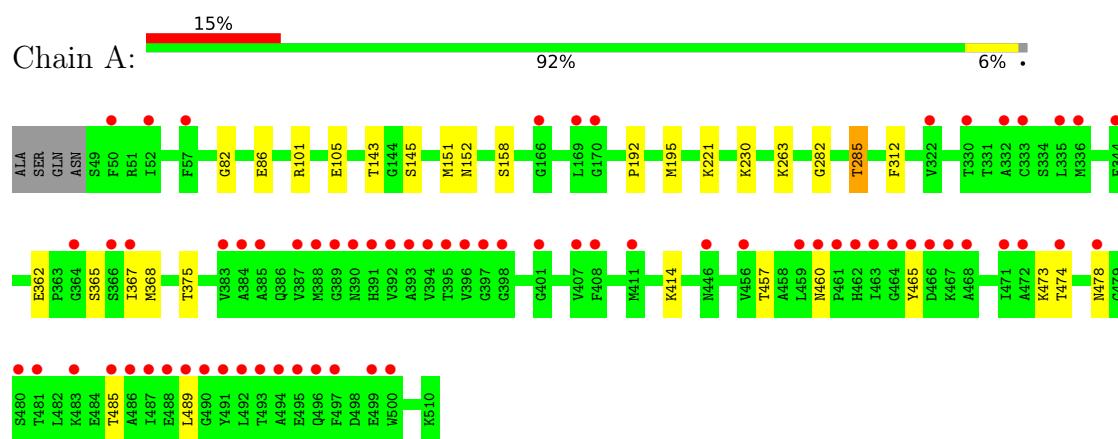
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	286	Total	O	0	0
			286	286		
4	B	293	Total	O	0	0
			293	293		

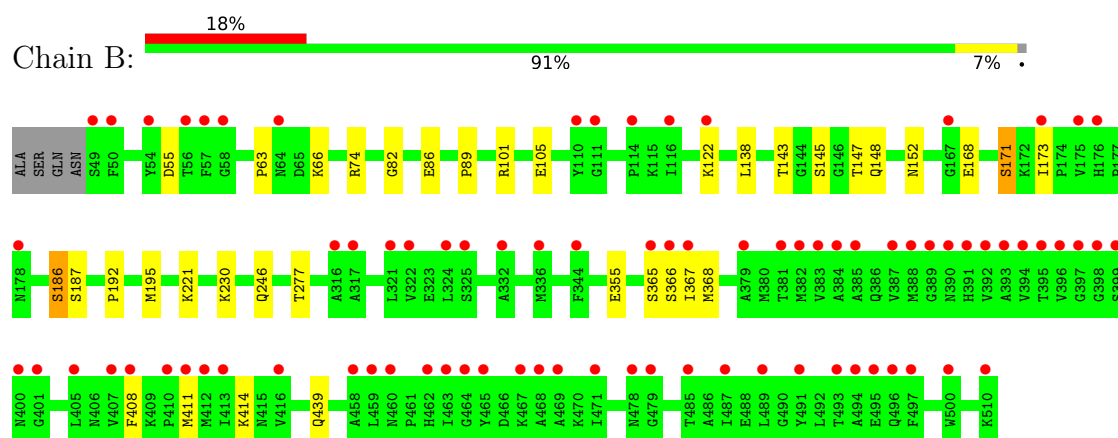
### 3 Residue-property plots [i](#)

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: Fumarate hydratase, mitochondrial



- Molecule 1: Fumarate hydratase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.88Å 189.88Å 115.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.30 – 1.90 49.30 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.30-1.90) 99.5 (49.30-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.165 , 0.193 0.165 , 0.194	Depositor DCC
$R_{free}$ test set	4789 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.0	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	0.97	EDS
Total number of atoms	7582	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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

### 5.1 Standard geometry

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

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	0/3555	0.54	1/4818 (0.0%)
1	B	0.41	0/3556	0.54	0/4821
All	All	0.41	0/7111	0.54	1/9639 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	LYS	CD-CE-NZ	-5.07	100.04	111.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	3487	0	3498	18	1
1	B	3488	0	3495	24	1
2	A	12	0	16	0	0
2	B	6	0	7	1	0
3	B	10	0	4	2	0
4	A	286	0	0	5	5
4	B	293	0	0	5	5
All	All	7582	0	7020	43	10

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 (43) 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:101:ARG:NH1	1:B:105:GLU:OE1	2.08	0.86
1:B:147[B]:THR:HG22	1:B:187:SER:HB3	1.62	0.81
1:B:122:LYS:NZ	4:B:702:HOH:O	2.26	0.67
3:B:602:TLA:O41	4:B:701:HOH:O	2.14	0.65
1:A:367:ILE:HG23	1:A:368:MET:HG2	1.78	0.64
4:A:706:HOH:O	3:B:602:TLA:C4	2.46	0.64
1:A:151:MET:HE3	4:A:716:HOH:O	2.00	0.62
1:A:101:ARG:NH1	1:A:105:GLU:OE1	2.21	0.61
1:B:230:LYS:HD2	1:B:355:GLU:OE1	2.03	0.59
1:B:145:SER:OG	1:B:147[B]:THR:HG23	2.02	0.58
1:B:89:PRO:HB3	2:B:601:GOL:H12	1.87	0.56
1:B:168:GLU:O	1:B:171:SER:HB3	2.08	0.54
1:B:368:MET:HG3	4:B:991:HOH:O	2.07	0.54
1:B:439:GLN:NE2	4:B:709:HOH:O	2.42	0.53
1:A:485:THR:O	1:A:489:LEU:HG	2.09	0.53
1:B:138:LEU:HD13	1:B:148:GLN:HB3	1.90	0.52
1:B:143[A]:THR:HG22	1:B:145:SER:H	1.75	0.51
4:A:905:HOH:O	1:B:147[B]:THR:HG21	2.09	0.51
1:A:465:TYR:C	1:A:465:TYR:CD1	2.85	0.50
1:B:171:SER:OG	1:B:173:ILE:HB	2.12	0.49
1:A:282:GLY:O	1:A:285:THR:HG22	2.12	0.49
1:A:143[A]:THR:HG22	1:A:145:SER:H	1.78	0.48
1:A:457:THR:HA	1:A:460:ASN:OD1	2.16	0.46
1:B:82:GLY:HA3	1:B:86:GLU:HG3	1.97	0.46
1:A:221:LYS:HD3	1:A:221:LYS:HA	1.73	0.46
1:A:82:GLY:HA3	1:A:86:GLU:HG3	1.97	0.45
1:B:367:ILE:HG23	1:B:368:MET:HG2	1.98	0.45
1:A:414:LYS:HE2	4:A:943:HOH:O	2.16	0.45
1:B:55:ASP:CG	1:B:74:ARG:HH21	2.19	0.44
1:B:414:LYS:HE2	4:B:940:HOH:O	2.17	0.44
1:A:362:GLU:HG3	1:A:375:THR:HG21	1.99	0.44
1:B:186:SER:HB3	1:B:277:THR:HA	2.00	0.43
1:A:365:SER:OG	1:A:367:ILE:HG22	2.18	0.43
1:A:474:THR:HG22	1:A:478:ASN:OD1	2.19	0.43
1:A:473:LYS:HA	1:A:473:LYS:HD3	1.90	0.43
1:A:263:LYS:NZ	4:A:703:HOH:O	2.29	0.43
1:A:192:PRO:HA	1:A:195:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:PRO:HB2	1:B:66:LYS:HG2	2.03	0.41
1:B:408:PHE:O	1:B:411[B]:MET:HG3	2.21	0.41
1:B:192:PRO:HA	1:B:195:MET:HE3	2.03	0.41
1:B:365:SER:OG	1:B:367:ILE:HG22	2.20	0.41
1:A:312:PHE:CZ	1:B:246:GLN:HB3	2.56	0.40
1:B:221:LYS:HD3	1:B:221:LYS:HA	1.94	0.40

All (10) 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:465:TYR:OH	1:B:366:SER:OG[12_544]	1.72	0.48
4:A:933:HOH:O	4:A:933:HOH:O[12_544]	1.91	0.29
4:B:758:HOH:O	4:B:943:HOH:O[12_544]	1.96	0.24
4:B:943:HOH:O	4:B:943:HOH:O[12_544]	1.97	0.23
4:A:882:HOH:O	4:A:943:HOH:O[12_544]	2.03	0.17
4:A:705:HOH:O	4:A:750:HOH:O[12_544]	2.09	0.11
4:B:960:HOH:O	4:B:970:HOH:O[9_555]	2.14	0.06
4:A:714:HOH:O	4:A:933:HOH:O[12_544]	2.16	0.04
4:B:856:HOH:O	4:B:940:HOH:O[12_544]	2.17	0.03
4:A:942:HOH:O	4:B:934:HOH:O[12_544]	2.17	0.03

## 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	465/466 (100%)	456 (98%)	9 (2%)	0	100	100
1	B	466/466 (100%)	454 (97%)	12 (3%)	0	100	100
All	All	931/932 (100%)	910 (98%)	21 (2%)	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	366/374 (98%)	363 (99%)	3 (1%)	81	82
1	B	366/374 (98%)	363 (99%)	3 (1%)	81	82
All	All	732/748 (98%)	726 (99%)	6 (1%)	81	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	158	SER
1	A	285	THR
1	B	152	ASN
1	B	171	SER
1	B	186	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

4 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	GOL	A	601	-	5,5,5	1.14	1 (20%)	5,5,5	1.01	0
2	GOL	A	602	-	5,5,5	0.23	0	5,5,5	0.47	0
3	TLA	B	602	-	3,9,9	0.94	0	6,12,12	1.11	1 (16%)
2	GOL	B	601	-	5,5,5	1.21	1 (20%)	5,5,5	0.82	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
2	GOL	A	601	-	-	0/4/4/4	-
2	GOL	A	602	-	-	4/4/4/4	-
3	TLA	B	602	-	-	4/4/12/12	-
2	GOL	B	601	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GOL	O2-C2	-2.43	1.36	1.43
2	A	601	GOL	O2-C2	-2.11	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TLA	C1-C2-C3	-2.34	108.06	113.11

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	602	GOL	C1-C2-C3-O3
3	B	602	TLA	C1-C2-C3-C4
2	A	602	GOL	O1-C1-C2-O2
2	A	602	GOL	O2-C2-C3-O3
3	B	602	TLA	O2-C2-C3-O3
2	B	601	GOL	C1-C2-C3-O3
3	B	602	TLA	O2-C2-C3-C4
3	B	602	TLA	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	TLA	2	0
2	B	601	GOL	1	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	462/466 (99%)	0.69	69 (14%) <b>2</b> <b>2</b>	26, 40, 73, 85	5 (1%)
1	B	462/466 (99%)	0.67	82 (17%) <b>1</b> <b>1</b>	26, 38, 72, 83	3 (0%)
All	All	924/932 (99%)	0.68	151 (16%) <b>1</b> <b>1</b>	26, 39, 73, 85	8 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	468	ALA	6.3
1	A	489	LEU	6.0
1	A	490	GLY	5.9
1	A	463	ILE	5.8
1	A	487	ILE	5.5
1	A	493	THR	5.5
1	A	491	TYR	5.3
1	A	500	TRP	5.2
1	A	50	PHE	5.2
1	A	364	GLY	5.2
1	B	468	ALA	5.0
1	A	392	VAL	4.9
1	A	464	GLY	4.8
1	B	394	VAL	4.7
1	A	465	TYR	4.6
1	A	396	VAL	4.6
1	A	497	PHE	4.4
1	B	396	VAL	4.4
1	B	392	VAL	4.4
1	B	407	VAL	4.4
1	B	385	ALA	4.3
1	B	487	ILE	4.3
1	B	493	THR	4.3
1	A	385	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	365	SER	4.1
1	A	486	ALA	4.1
1	A	394	VAL	4.1
1	A	499	GLU	4.1
1	A	397	GLY	4.1
1	A	492	LEU	4.0
1	B	395	THR	3.9
1	B	491	TYR	3.9
1	B	56	THR	3.9
1	A	333	CYS	3.8
1	B	465	TYR	3.8
1	B	408	PHE	3.8
1	B	393	ALA	3.7
1	B	500	TRP	3.7
1	A	495	GLU	3.7
1	B	178	ASN	3.6
1	A	467	LYS	3.6
1	A	387	VAL	3.6
1	A	393	ALA	3.5
1	B	471	ILE	3.5
1	B	397	GLY	3.5
1	A	461	PRO	3.5
1	A	496	GLN	3.5
1	B	464	GLY	3.5
1	B	173	ILE	3.4
1	A	388	MET	3.4
1	A	170	GLY	3.4
1	A	332	ALA	3.4
1	B	322	VAL	3.3
1	B	489	LEU	3.3
1	A	460	ASN	3.3
1	B	388	MET	3.3
1	B	50	PHE	3.3
1	A	459	LEU	3.2
1	A	472	ALA	3.2
1	A	456	VAL	3.2
1	A	462	HIS	3.1
1	B	366	SER	3.1
1	B	54	TYR	3.1
1	B	462	HIS	3.0
1	B	317	ALA	3.0
1	B	332	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	483	LYS	3.0
1	A	52	ILE	3.0
1	B	367	ILE	3.0
1	B	497	PHE	3.0
1	B	412	MET	3.0
1	A	389	GLY	2.9
1	A	471	ILE	2.9
1	B	387	VAL	2.9
1	A	330	THR	2.9
1	B	463	ILE	2.9
1	B	176	HIS	2.9
1	A	411[A]	MET	2.9
1	B	460	ASN	2.9
1	A	166	GLY	2.8
1	B	58	GLY	2.8
1	A	395	THR	2.8
1	A	366	SER	2.8
1	B	478	ASN	2.8
1	B	405	LEU	2.8
1	A	494	ALA	2.8
1	A	367	ILE	2.8
1	B	398	GLY	2.8
1	B	316	ALA	2.8
1	B	411[A]	MET	2.8
1	B	175	VAL	2.8
1	A	391	HIS	2.7
1	B	49	SER	2.7
1	B	111	GLY	2.7
1	B	321	LEU	2.7
1	B	479	GLY	2.7
1	A	478	ASN	2.7
1	A	169	LEU	2.7
1	B	390	ASN	2.6
1	B	383	VAL	2.6
1	B	510	LYS	2.6
1	A	474	THR	2.6
1	A	408	PHE	2.5
1	B	413	ILE	2.5
1	A	407	VAL	2.5
1	A	322	VAL	2.5
1	A	446	ASN	2.5
1	B	384	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	481	THR	2.5
1	B	399	SER	2.5
1	B	416	VAL	2.4
1	A	336	MET	2.4
1	B	496	GLN	2.4
1	A	466	ASP	2.4
1	B	167	GLY	2.4
1	B	389	GLY	2.4
1	B	467	LYS	2.4
1	B	485	THR	2.4
1	A	485	THR	2.4
1	B	57	PHE	2.3
1	B	336	MET	2.3
1	B	114	PRO	2.3
1	A	344	PHE	2.3
1	B	381	THR	2.3
1	B	494	ALA	2.3
1	B	324	LEU	2.3
1	B	110	TYR	2.2
1	A	57	PHE	2.2
1	A	398	GLY	2.2
1	B	458	ALA	2.2
1	B	459	LEU	2.2
1	A	488	GLU	2.2
1	B	116	ILE	2.2
1	A	480	SER	2.2
1	A	384	ALA	2.2
1	B	344	PHE	2.2
1	A	383	VAL	2.2
1	B	495	GLU	2.1
1	A	390	ASN	2.1
1	B	382	MET	2.1
1	B	64	ASN	2.1
1	B	401	GLY	2.1
1	B	400	ASN	2.1
1	B	469	ALA	2.1
1	B	391	HIS	2.1
1	A	401	GLY	2.1
1	B	379	ALA	2.1
1	B	410	PRO	2.0
1	A	335	LEU	2.0
1	B	122	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	325	SER	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( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	602	6/6	0.83	0.16	48,51,61,63	0
3	TLA	B	602	10/10	0.83	0.13	50,59,63,63	10
2	GOL	B	601	6/6	0.91	0.12	42,50,53,55	0
2	GOL	A	601	6/6	0.97	0.09	42,47,50,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.