



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2022 – 12:10 PM JST

PDB ID : 7CM2
Title : The Crystal Structure of human USP7 USP domain from Biortus
Authors : Wang, F.; Cheng, W.; Lv, Z.; Lin, D.; Zhu, B.; Miao, Q.; Bao, X.; Shang, H.
Deposited on : 2020-07-24
Resolution : 2.25 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.27
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) : 2.27

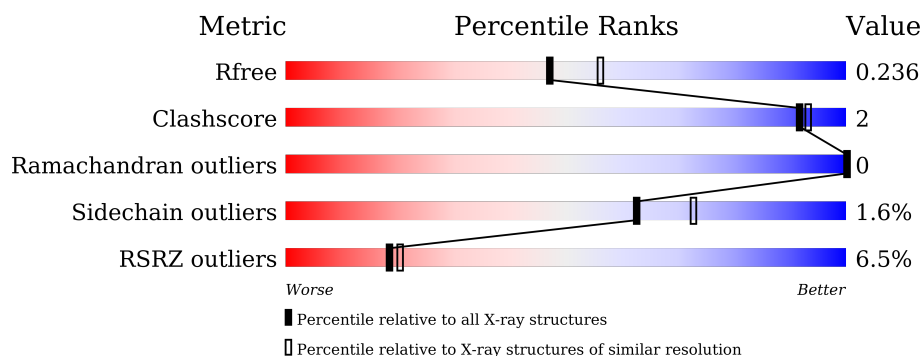
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 $\leq 5\%$. 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	370	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>9%</div> </div> </div>
1	B	370	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5807 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	1	0
			2743	1737	467	522	17			
1	B	340	Total	C	N	O	S	0	0	0
			2764	1749	472	527	16			

There are 34 discrepancies between the modelled and reference sequences:

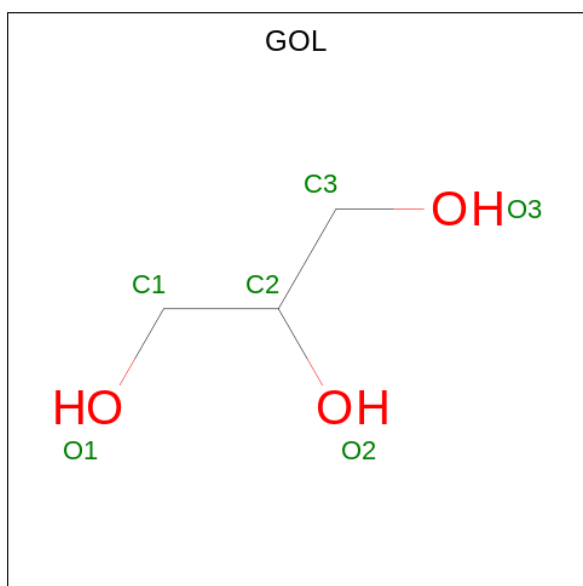
Chain	Residue	Modelled	Actual	Comment	Reference
A	191	MET	-	initiating methionine	UNP Q93009
A	192	GLY	-	expression tag	UNP Q93009
A	193	GLY	-	expression tag	UNP Q93009
A	194	SER	-	expression tag	UNP Q93009
A	195	HIS	-	expression tag	UNP Q93009
A	196	HIS	-	expression tag	UNP Q93009
A	197	HIS	-	expression tag	UNP Q93009
A	198	HIS	-	expression tag	UNP Q93009
A	199	HIS	-	expression tag	UNP Q93009
A	200	HIS	-	expression tag	UNP Q93009
A	201	GLU	-	expression tag	UNP Q93009
A	202	ASN	-	expression tag	UNP Q93009
A	203	LEU	-	expression tag	UNP Q93009
A	204	TYR	-	expression tag	UNP Q93009
A	205	PHE	-	expression tag	UNP Q93009
A	206	GLN	-	expression tag	UNP Q93009
A	207	GLY	-	expression tag	UNP Q93009
B	191	MET	-	initiating methionine	UNP Q93009
B	192	GLY	-	expression tag	UNP Q93009
B	193	GLY	-	expression tag	UNP Q93009
B	194	SER	-	expression tag	UNP Q93009
B	195	HIS	-	expression tag	UNP Q93009
B	196	HIS	-	expression tag	UNP Q93009
B	197	HIS	-	expression tag	UNP Q93009
B	198	HIS	-	expression tag	UNP Q93009

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Chain	Residue	Modelled	Actual	Comment	Reference
B	199	HIS	-	expression tag	UNP Q93009
B	200	HIS	-	expression tag	UNP Q93009
B	201	GLU	-	expression tag	UNP Q93009
B	202	ASN	-	expression tag	UNP Q93009
B	203	LEU	-	expression tag	UNP Q93009
B	204	TYR	-	expression tag	UNP Q93009
B	205	PHE	-	expression tag	UNP Q93009
B	206	GLN	-	expression tag	UNP Q93009
B	207	GLY	-	expression tag	UNP Q93009

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

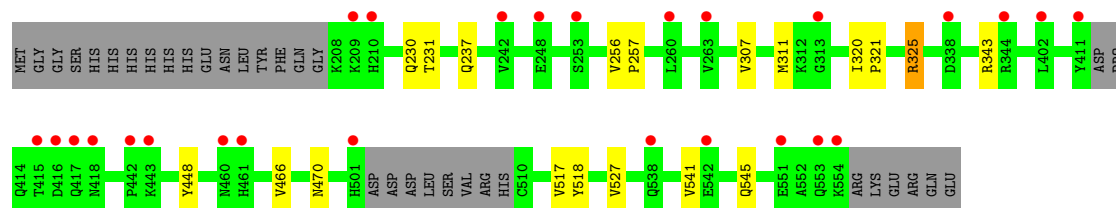
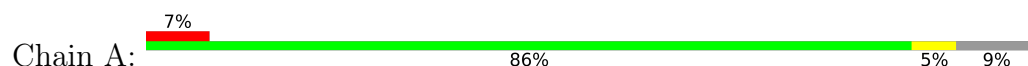
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		
3	B	135	Total	O	0	0
			135	135		

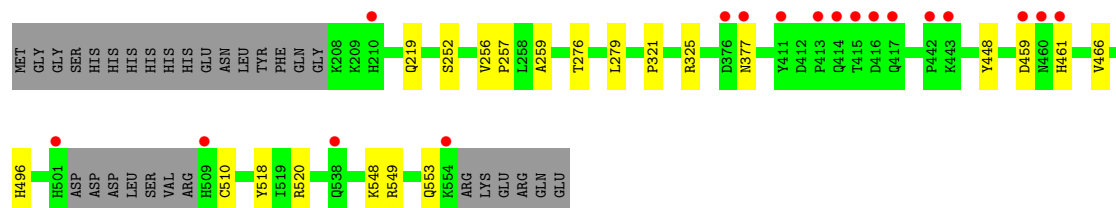
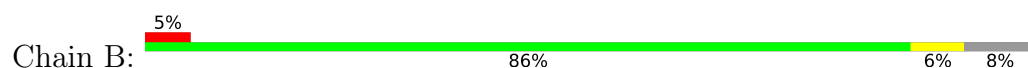
3 Residue-property plots [i](#)

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: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.05Å 69.13Å 76.86Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	19.68 – 2.25 19.68 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.68-2.25) 99.8 (19.68-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.196 , 0.236 0.202 , 0.236	Depositor DCC
R_{free} test set	1822 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5807	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.71 % 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 1.4683e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

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	0.64	0/2799	0.70	0/3771
1	B	0.63	0/2823	0.70	0/3806
All	All	0.64	0/5622	0.70	0/7577

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

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	2743	0	2687	9	0
1	B	2764	0	2703	9	0
2	A	24	0	32	0	0
2	B	24	0	32	0	0
3	A	117	0	0	0	0
3	B	135	0	0	2	0
All	All	5807	0	5454	18	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 2.

All (18) 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:219:GLN:HE22	1:B:276:THR:H	1.42	0.67
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.85	0.59
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.88	0.54
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.93	0.51
1:B:459:ASP:OD1	1:B:510:CYS:SG	2.62	0.51
1:A:321:PRO:HA	1:A:325:ARG:HB2	1.94	0.49
1:B:256:VAL:N	1:B:257:PRO:CD	2.80	0.45
1:B:259:ALA:HB1	1:B:279:LEU:HA	1.98	0.44
1:A:307:VAL:HG13	1:A:311:MET:HE3	2.00	0.44
1:A:541:VAL:O	1:A:545:GLN:HG2	2.17	0.44
1:A:256:VAL:N	1:A:257:PRO:CD	2.81	0.44
1:B:321:PRO:HA	1:B:325:ARG:HB2	2.00	0.43
1:A:256:VAL:HB	1:A:257:PRO:HD3	2.01	0.42
1:A:231:THR:CG2	1:A:517:VAL:HG21	2.50	0.42
1:B:548:LYS:NZ	3:B:710:HOH:O	2.53	0.41
1:B:549:ARG:O	1:B:553:GLN:HG2	2.20	0.41
1:A:237:GLN:HE21	1:A:527:VAL:HA	1.86	0.40
1:B:520:ARG:NH2	3:B:711:HOH:O	2.55	0.40

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	332/370 (90%)	324 (98%)	8 (2%)	0	100	100
1	B	336/370 (91%)	327 (97%)	9 (3%)	0	100	100
All	All	668/740 (90%)	651 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	304/334 (91%)	299 (98%)	5 (2%)	62	73
1	B	307/334 (92%)	302 (98%)	5 (2%)	62	73
All	All	611/668 (92%)	601 (98%)	10 (2%)	62	73

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	325	ARG
1	A	343	ARG
1	A	466	VAL
1	A	470	ASN
1	B	252	SER
1	B	377	ASN
1	B	461	HIS
1	B	466	VAL
1	B	496	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	237	GLN
1	A	268	GLN
1	A	496	HIS
1	A	553	GLN
1	B	219	GLN
1	B	230	GLN
1	B	268	GLN
1	B	294	HIS
1	B	418	ASN
1	B	470	ASN
1	B	538	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	B	602	-	5,5,5	0.11	0	5,5,5	0.28	0
2	GOL	A	601	-	5,5,5	0.10	0	5,5,5	0.36	0
2	GOL	B	603	-	5,5,5	0.10	0	5,5,5	0.27	0
2	GOL	A	604	-	5,5,5	0.10	0	5,5,5	0.26	0
2	GOL	A	602	-	5,5,5	0.10	0	5,5,5	0.34	0
2	GOL	B	601	-	5,5,5	0.13	0	5,5,5	0.39	0
2	GOL	B	604	-	5,5,5	0.10	0	5,5,5	0.29	0
2	GOL	A	603	-	5,5,5	0.10	0	5,5,5	0.30	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	602	-	-	2/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	603	-	-	4/4/4/4	-
2	GOL	A	604	-	-	2/4/4/4	-
2	GOL	A	602	-	-	0/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	B	604	-	-	4/4/4/4	-
2	GOL	A	603	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	C1-C2-C3-O3
2	A	601	GOL	O2-C2-C3-O3
2	B	601	GOL	C1-C2-C3-O3
2	B	603	GOL	C1-C2-C3-O3
2	B	604	GOL	C1-C2-C3-O3
2	A	603	GOL	O2-C2-C3-O3
2	B	604	GOL	O2-C2-C3-O3
2	A	603	GOL	O1-C1-C2-C3
2	A	603	GOL	C1-C2-C3-O3
2	A	604	GOL	C1-C2-C3-O3
2	B	602	GOL	C1-C2-C3-O3
2	B	604	GOL	O1-C1-C2-C3
2	A	603	GOL	O1-C1-C2-O2
2	B	601	GOL	O2-C2-C3-O3
2	B	603	GOL	O2-C2-C3-O3
2	B	602	GOL	O2-C2-C3-O3
2	A	604	GOL	O2-C2-C3-O3
2	B	604	GOL	O1-C1-C2-O2
2	B	603	GOL	O1-C1-C2-C3
2	B	603	GOL	O1-C1-C2-O2

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

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, 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	337/370 (91%)	0.36	26 (7%) 13 14	31, 47, 78, 111	3 (0%)
1	B	340/370 (91%)	0.20	18 (5%) 26 29	28, 41, 76, 101	0
All	All	677/740 (91%)	0.28	44 (6%) 18 20	28, 44, 77, 111	3 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	416	ASP	4.5
1	A	501	HIS	4.4
1	A	416	ASP	4.4
1	B	413	PRO	4.3
1	A	415	THR	4.2
1	A	461	HIS	4.2
1	B	509	HIS	4.0
1	B	461	HIS	4.0
1	B	417	GLN	4.0
1	A	538	GLN	3.7
1	A	411	TYR	3.7
1	A	417	GLN	3.7
1	A	443	LYS	3.7
1	B	210	HIS	3.4
1	A	553	GLN	3.4
1	A	542	GLU	3.3
1	B	501	HIS	3.2
1	A	460	ASN	3.0
1	B	411	TYR	3.0
1	A	313	GLY	3.0
1	A	209	LYS	3.0
1	B	459	ASP	2.9
1	A	338	ASP	2.9
1	A	442	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	263	VAL	2.8
1	B	376	ASP	2.8
1	B	554	LYS	2.7
1	B	414	GLN	2.7
1	A	554	LYS	2.7
1	B	460	ASN	2.7
1	A	402	LEU	2.6
1	A	210	HIS	2.6
1	A	253	SER	2.5
1	A	551	GLU	2.4
1	B	442	PRO	2.4
1	B	377	ASN	2.3
1	B	538	GLN	2.3
1	A	260	LEU	2.3
1	A	344	ARG	2.3
1	A	248	GLU	2.2
1	A	418	ASN	2.2
1	B	415	THR	2.2
1	A	242	VAL	2.1
1	B	443	LYS	2.1

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
2	GOL	A	603	6/6	0.79	0.22	72,74,75,75	0
2	GOL	B	603	6/6	0.84	0.25	63,63,64,64	0
2	GOL	A	604	6/6	0.89	0.22	67,70,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	B	604	6/6	0.90	0.18	60,64,66,68	0
2	GOL	B	601	6/6	0.94	0.18	38,41,42,42	0
2	GOL	A	602	6/6	0.95	0.20	46,48,49,50	0
2	GOL	A	601	6/6	0.96	0.13	46,47,48,48	0
2	GOL	B	602	6/6	0.96	0.11	41,43,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.