



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3GOV / pdb_00003gov
Title : Crystal structure of the catalytic region of human MASP-1
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Deposited on : 2009-03-20
Resolution : 2.55 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 types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

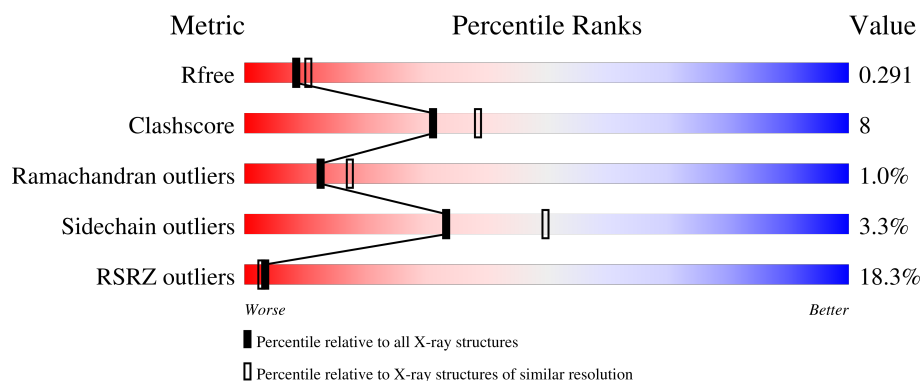
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	155	25% 85% 9% 5%
2	B	251	14% 83% 14% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3196 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 MASP-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	4	0
			1163	744	189	218	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	ALA	-	expression tag	UNP P48740
A	295	SER	-	expression tag	UNP P48740
A	296	MET	-	expression tag	UNP P48740
A	297	THR	-	expression tag	UNP P48740

- Molecule 2 is a protein called MASP-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	251	Total	C	N	O	S	0	1	0
			1931	1226	332	360	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	499	LYS	GLU	SEE REMARK 999	UNP P48740

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

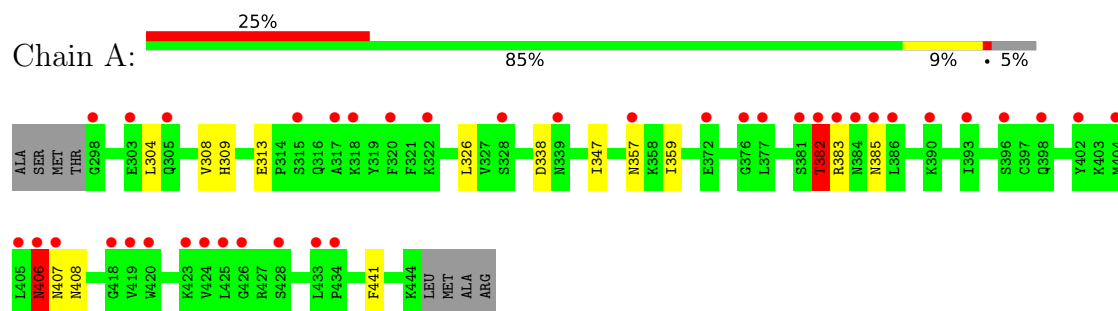
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	57	Total	O	0	0
			57	57		

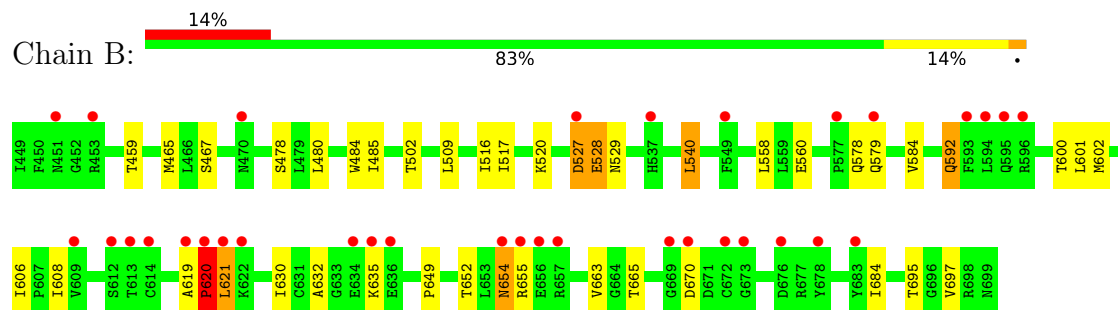
3 Residue-property plots [i](#)

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: MASP-1



• Molecule 2: MASP-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.42Å 70.41Å 121.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.98 – 2.55 45.98 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.9 (45.98-2.55) 97.9 (45.98-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.278 0.246 , 0.291	Depositor DCC
R_{free} test set	989 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3196	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.47	0/1202	0.72	1/1628 (0.1%)
2	B	0.48	0/1986	0.77	2/2701 (0.1%)
All	All	0.48	0/3188	0.75	3/4329 (0.1%)

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	2
2	B	0	2
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	621	LEU	N-CA-C	-12.28	96.45	112.41
2	B	528	GLU	N-CA-C	6.58	124.82	110.80
1	A	406	ASN	N-CA-C	-6.42	98.72	108.67

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	THR	Peptide
1	A	406	ASN	Peptide
2	B	527	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	B	620	PRO	Peptide

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	1163	0	1141	11	0
2	B	1931	0	1837	40	0
3	A	6	0	8	2	0
3	B	6	0	8	0	0
4	A	33	0	0	0	0
4	B	57	0	0	0	0
All	All	3196	0	2994	50	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 8.

All (50) 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:A:304:LEU:HD22	1:A:359:ILE:HD11	1.21	1.10
2:B:695:THR:CG2	2:B:697:VAL:HG23	1.95	0.96
2:B:695:THR:HG22	2:B:697:VAL:HG23	1.50	0.94
2:B:485:ILE:CD1	2:B:516:ILE:HG21	2.01	0.91
2:B:619:ALA:HA	2:B:620:PRO:C	1.99	0.88
2:B:465:MET:HE2	2:B:517:ILE:HD12	1.55	0.86
2:B:465:MET:HE3	2:B:467:SER:OG	1.78	0.84
2:B:584:VAL:HG12	2:B:652:THR:CG2	2.10	0.81
2:B:485:ILE:HD13	2:B:516:ILE:HG21	1.62	0.80
2:B:527:ASP:HB3	2:B:529:ASN:H	1.51	0.74
2:B:620:PRO:HB2	2:B:621:LEU:HG	1.76	0.67
2:B:484:TRP:CD1	2:B:695:THR:HG23	2.31	0.65
2:B:485:ILE:HD11	2:B:516:ILE:HG21	1.79	0.64
2:B:608:ILE:HD13	2:B:630:ILE:HD11	1.80	0.64
2:B:527:ASP:HB3	2:B:529:ASN:N	2.13	0.63
2:B:695:THR:HG21	2:B:697:VAL:HG23	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:MET:CE	2:B:517:ILE:HD12	2.27	0.63
2:B:695:THR:CG2	2:B:697:VAL:CG2	2.75	0.63
2:B:695:THR:HG21	2:B:697:VAL:CG2	2.30	0.61
1:A:304:LEU:CD2	1:A:359:ILE:HD11	2.15	0.61
2:B:584:VAL:HG12	2:B:652:THR:HG23	1.82	0.61
2:B:654:ASN:HD22	2:B:655:ARG:N	2.00	0.59
2:B:619:ALA:HA	2:B:621:LEU:N	2.18	0.57
2:B:579:GLN:CD	2:B:579:GLN:H	2.15	0.55
2:B:619:ALA:CA	2:B:620:PRO:C	2.77	0.55
1:A:304:LEU:HD22	1:A:359:ILE:CD1	2.15	0.54
2:B:578:GLN:HG3	2:B:663:VAL:CG1	2.38	0.53
2:B:592:GLN:HE22	2:B:602:MET:HE2	1.72	0.53
2:B:665:THR:HG23	2:B:684:ILE:HD11	1.91	0.52
2:B:578:GLN:HG3	2:B:663:VAL:HG11	1.92	0.51
2:B:485:ILE:HD13	2:B:516:ILE:CG2	2.39	0.49
2:B:620:PRO:HB2	2:B:621:LEU:CG	2.42	0.49
1:A:313:GLU:HB2	3:A:1:GOL:H32	1.94	0.49
2:B:485:ILE:HD12	2:B:558:LEU:HD21	1.94	0.48
2:B:540:LEU:HD23	2:B:540:LEU:N	2.27	0.48
1:A:441:PHE:O	2:B:459:THR:HG22	2.15	0.47
2:B:606:ILE:HD12	2:B:632:ALA:HB1	1.98	0.46
2:B:478:SER:OG	2:B:649:PRO:HB3	2.17	0.45
2:B:592:GLN:NE2	2:B:602:MET:HE2	2.32	0.45
1:A:406:ASN:ND2	1:A:408:ASN:O	2.51	0.44
2:B:620:PRO:HB2	2:B:621:LEU:CA	2.48	0.44
2:B:584:VAL:HA	2:B:652:THR:HG22	2.01	0.43
2:B:465:MET:HE1	2:B:520:LYS:HE2	2.00	0.43
2:B:600:THR:HG22	2:B:601:LEU:O	2.19	0.43
1:A:326:LEU:HB2	3:A:1:GOL:H31	2.02	0.41
1:A:347:ILE:HG22	1:A:357:ASN:HB2	2.01	0.41
1:A:382:THR:HG22	1:A:383:ARG:H	1.84	0.41
1:A:382:THR:HG22	1:A:383:ARG:N	2.36	0.41
1:A:308:VAL:HG12	1:A:309:HIS:CD2	2.55	0.40
2:B:600:THR:HG22	2:B:601:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	149/155 (96%)	142 (95%)	6 (4%)	1 (1%)	18	25
2	B	250/251 (100%)	237 (95%)	10 (4%)	3 (1%)	10	13
All	All	399/406 (98%)	379 (95%)	16 (4%)	4 (1%)	12	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	407	ASN
2	B	528	GLU
2	B	620	PRO
2	B	670	ASP

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	131/140 (94%)	128 (98%)	3 (2%)	44	62
2	B	203/215 (94%)	195 (96%)	8 (4%)	28	43
All	All	334/355 (94%)	323 (97%)	11 (3%)	33	50

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	ASP
1	A	382	THR

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Mol	Chain	Res	Type
1	A	385	ASN
2	B	480	LEU
2	B	502	THR
2	B	509	LEU
2	B	540	LEU
2	B	560	GLU
2	B	592	GLN
2	B	635	LYS
2	B	654	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	HIS
1	A	316	GLN
1	A	346	GLN
1	A	375	HIS
1	A	385	ASN
2	B	543	GLN
2	B	592	GLN
2	B	654	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](#)

2 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	$\# Z > 2$
3	GOL	B	2	-	5,5,5	0.44	0	5,5,5	0.33	0
3	GOL	A	1	-	5,5,5	0.41	0	5,5,5	0.63	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	2	-	-	0/4/4/4	-
3	GOL	A	1	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	GOL	C1-C2-C3-O3
3	A	1	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	GOL	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	147/155 (94%)	1.52	39 (26%) 1 1	29, 48, 58, 65	4 (2%)
2	B	251/251 (100%)	1.05	34 (13%) 7 5	29, 49, 58, 62	1 (0%)
All	All	398/406 (98%)	1.22	73 (18%) 3 3	29, 48, 58, 65	5 (1%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	THR	4.9
1	A	407	ASN	4.4
2	B	656	GLU	4.3
2	B	594	LEU	4.1
2	B	621	LEU	4.1
1	A	398[A]	GLN	4.0
2	B	670	ASP	4.0
2	B	593	PHE	3.9
1	A	405	LEU	3.9
2	B	655	ARG	3.8
2	B	673	GLY	3.8
1	A	383	ARG	3.7
1	A	396	SER	3.3
2	B	620	PRO	3.3
2	B	579	GLN	3.2
1	A	339	ASN	3.2
2	B	596	ARG	3.1
2	B	619	ALA	3.0
2	B	676	ASP	3.0
2	B	672	CYS	2.9
2	B	451	ASN	2.9
2	B	678	TYR	2.9
2	B	634	GLU	2.8
2	B	635	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	420	TRP	2.7
2	B	612	SER	2.7
2	B	636	GLU	2.7
2	B	614	CYS	2.6
1	A	433	LEU	2.6
1	A	381	SER	2.6
2	B	470	ASN	2.6
1	A	376	GLY	2.6
1	A	419	VAL	2.6
1	A	357	ASN	2.5
2	B	683	TYR	2.5
2	B	622	LYS	2.5
1	A	404	MET	2.5
1	A	377	LEU	2.5
1	A	320	PHE	2.5
2	B	669	GLY	2.4
1	A	402	TYR	2.4
2	B	537	HIS	2.4
2	B	613	THR	2.4
1	A	385	ASN	2.4
1	A	322[A]	LYS	2.4
1	A	328	SER	2.3
1	A	386	LEU	2.3
2	B	527	ASP	2.3
1	A	423	LYS	2.3
1	A	303	GLU	2.3
2	B	577	PRO	2.3
2	B	654	ASN	2.2
2	B	609	VAL	2.2
1	A	384	ASN	2.2
1	A	305	GLN	2.2
1	A	426	GLY	2.2
1	A	315	SER	2.2
1	A	393	ILE	2.2
1	A	434	PRO	2.2
2	B	453	ARG	2.2
1	A	298	GLY	2.1
1	A	318[A]	LYS	2.1
2	B	595	GLN	2.1
1	A	317	ALA	2.1
1	A	424	VAL	2.1
2	B	657	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	428	SER	2.1
1	A	425	LEU	2.1
1	A	390	LYS	2.1
1	A	406	ASN	2.0
2	B	549	PHE	2.0
1	A	372	GLU	2.0
1	A	418	GLY	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 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, 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($\text{\AA}^2$)	Q<0.9
3	GOL	B	2	6/6	0.83	0.17	59,60,60,60	0
3	GOL	A	1	6/6	0.91	0.12	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.