



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 01:15 PM EDT

PDB ID : 5U2V  
Title : Structure of human MR1-HMB in complex with human MAIT A-F7 TCR  
Authors : Keller, A.N.; Rossjohn, J.  
Deposited on : 2016-12-01  
Resolution : 2.20 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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

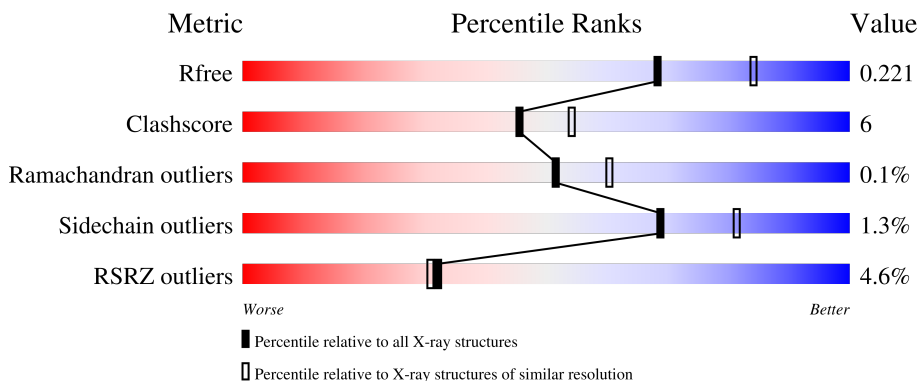
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



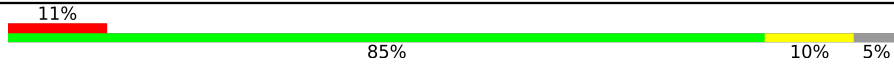

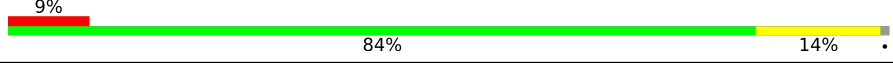
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	271	
1	C	271	
2	B	99	
2	D	99	
3	E	203	

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Mol	Chain	Length	Quality of chain
3	G	203	 11% 85% 10% 5%
4	F	245	 % 86% 12% .
4	H	245	 9% 84% 14% .

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13887 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	Total	C	N	O	S	0	0	0
			2163	1387	373	392	11			
1	C	262	Total	C	N	O	S	0	0	0
			2159	1378	372	398	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	conflict	UNP Q95460

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	Total	C	N	O	S	0	0	0
			816	519	137	157	3			
2	D	96	Total	C	N	O	S	0	0	0
			789	504	131	152	2			

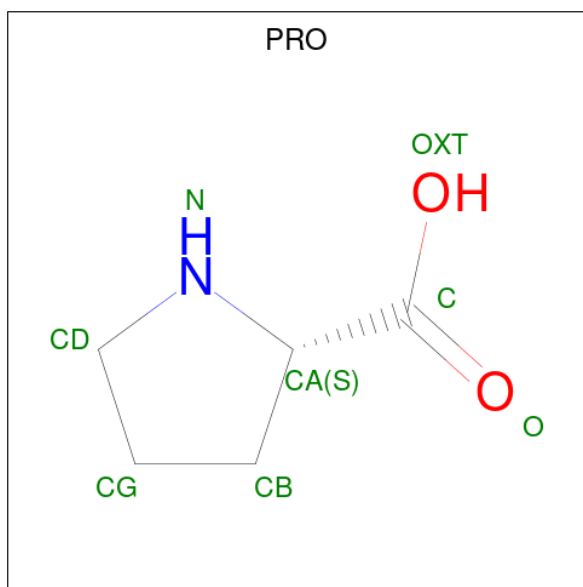
- Molecule 3 is a protein called MAIT T-cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	193	Total	C	N	O	S	0	0	0
			1493	947	241	296	9			
3	E	200	Total	C	N	O	S	0	0	0
			1546	976	249	312	9			

- Molecule 4 is a protein called MAIT T-cell receptor beta chain.

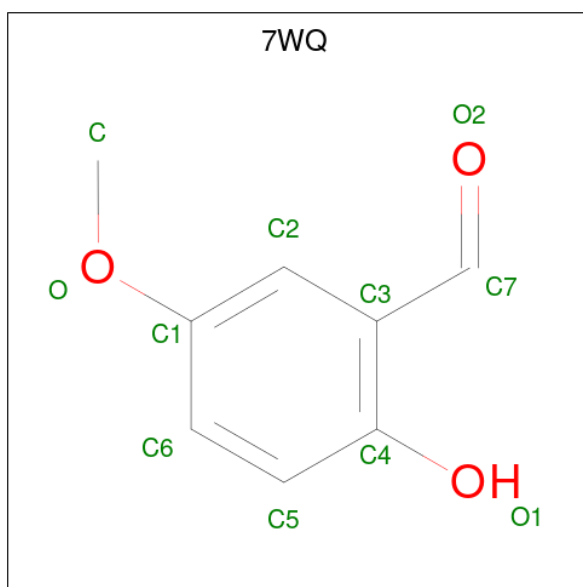
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	242	Total	C	N	O	S	0	0	0
			1907	1200	331	367	9			
4	F	242	Total	C	N	O	S	0	0	0
			1907	1200	331	367	9			

- Molecule 5 is PROLINE (three-letter code: PRO) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 6 is 2-hydroxy-5-methoxybenzaldehyde (three-letter code: 7WQ) (formula: C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	8	2		
6	C	1	Total	C	O	0	0
			10	8	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

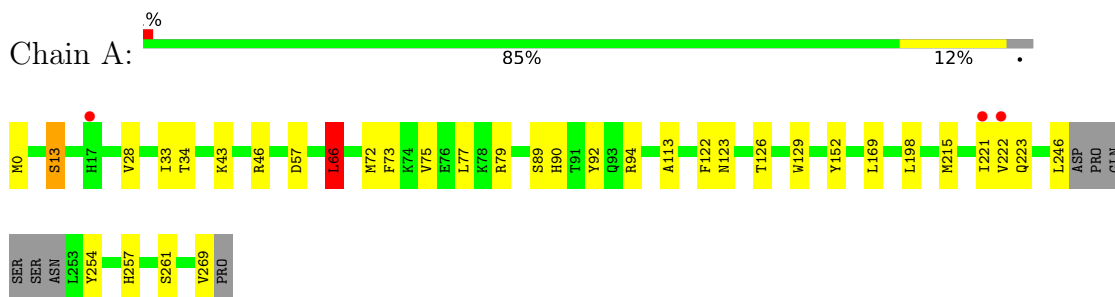
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	183	Total 183	O 183	0	0
8	B	86	Total 86	O 86	0	0
8	G	93	Total 93	O 93	0	0
8	H	97	Total 97	O 97	0	0
8	C	187	Total 187	O 187	0	0
8	D	56	Total 56	O 56	0	0
8	E	163	Total 163	O 163	0	0
8	F	203	Total 203	O 203	0	0

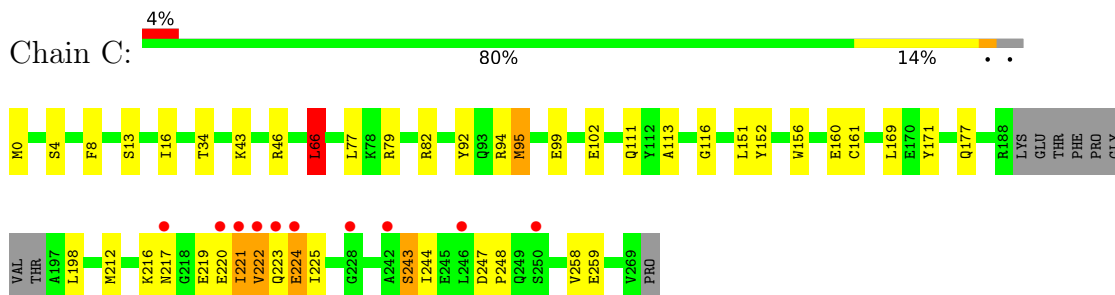
### 3 Residue-property plots [i](#)

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.

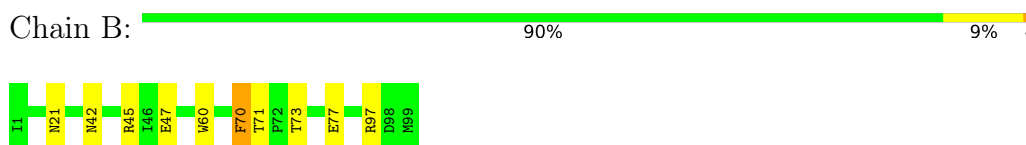
- Molecule 1: Major histocompatibility complex class I-related gene protein



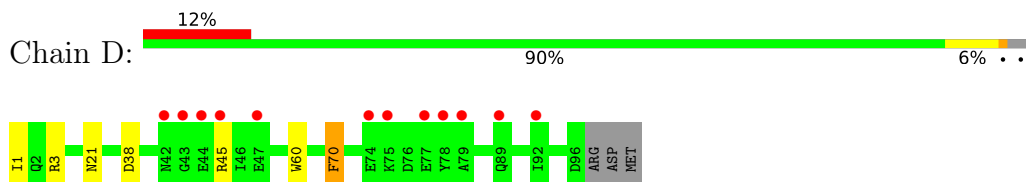
- Molecule 1: Major histocompatibility complex class I-related gene protein



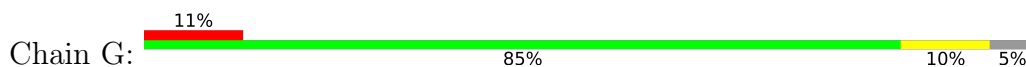
- Molecule 2: Beta-2-microglobulin



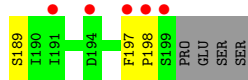
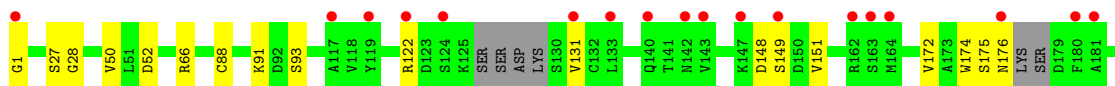
- Molecule 2: Beta-2-microglobulin



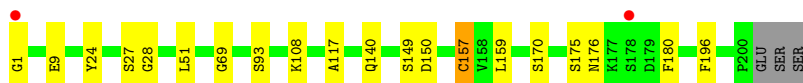
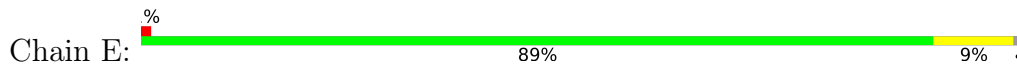
- Molecule 3: MAIT T-cell receptor alpha chain



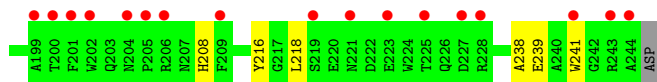
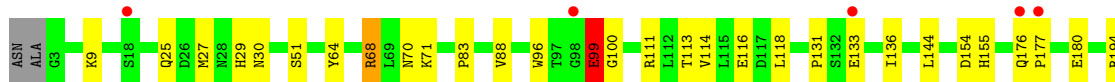
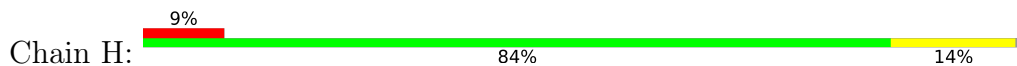




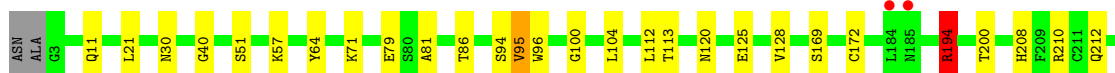
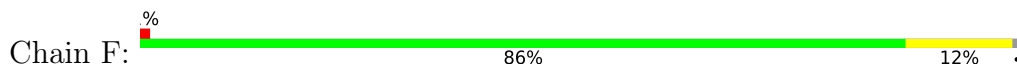
- Molecule 3: MAIT T-cell receptor alpha chain



- Molecule 4: MAIT T-cell receptor beta chain



- Molecule 4: MAIT T-cell receptor beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	216.23Å 69.73Å 142.40Å 90.00° 104.36° 90.00°	Depositor
Resolution (Å)	52.37 – 2.20 52.37 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (52.37-2.20) 99.7 (52.37-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.179 , 0.221 0.179 , 0.221	Depositor DCC
$R_{free}$ test set	5208 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtrriage
Anisotropy	0.285	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: 7WQ, 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	0.53	0/2229	0.63	1/3031 (0.0%)
1	C	0.56	0/2224	0.66	2/3023 (0.1%)
2	B	0.48	0/839	0.58	0/1140
2	D	0.46	0/812	0.55	0/1105
3	E	0.54	0/1581	0.65	1/2146 (0.0%)
3	G	0.52	1/1525 (0.1%)	0.61	0/2067
4	F	0.57	0/1958	0.68	2/2664 (0.1%)
4	H	0.50	0/1958	0.68	2/2664 (0.1%)
All	All	0.53	1/13126 (0.0%)	0.64	8/17840 (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
3	G	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	88	CYS	CB-SG	-5.33	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	99	GLU	N-CA-C	-8.43	88.24	111.00
4	F	194	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	A	66	LEU	CA-CB-CG	-6.56	100.20	115.30
1	C	66	LEU	CA-CB-CG	-6.13	101.21	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	MET	CG-SD-CE	-5.92	90.73	100.20
4	F	194	ARG	NE-CZ-NH1	-5.80	117.40	120.30
4	H	68	ARG	NE-CZ-NH1	-5.64	117.48	120.30
3	E	157	CYS	CA-CB-SG	5.05	123.09	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	149	SER	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	2163	0	2045	29	0
1	C	2159	0	2033	36	0
2	B	816	0	761	7	0
2	D	789	0	735	6	0
3	E	1546	0	1450	16	0
3	G	1493	0	1403	15	0
4	F	1907	0	1799	31	0
4	H	1907	0	1799	34	0
5	A	7	0	7	1	0
6	A	10	0	0	1	0
6	C	10	0	0	1	0
7	A	6	0	8	1	0
7	C	6	0	8	2	0
8	A	183	0	0	3	1
8	B	86	0	0	4	1
8	C	187	0	0	12	2
8	D	56	0	0	2	0
8	E	163	0	0	4	2
8	F	203	0	0	11	0
8	G	93	0	0	3	1
8	H	97	0	0	8	0
All	All	13887	0	12048	158	4

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 6.

All (158) 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)
4:H:111:ARG:NH1	4:H:113:THR:OG1	1.98	0.95
3:G:122:ARG:NH1	8:G:303:HOH:O	2.05	0.89
3:G:52:ASP:OD2	8:G:301:HOH:O	1.90	0.87
2:D:45:ARG:NH1	8:D:101:HOH:O	2.07	0.86
4:F:79:GLU:OE1	8:F:301:HOH:O	1.95	0.85
1:C:94:ARG:HH22	7:C:302:GOL:H11	1.45	0.82
1:A:0:MET:HE1	1:A:169:LEU:HD13	1.61	0.81
2:B:71:THR:O	8:B:101:HOH:O	2.01	0.79
1:C:13:SER:O	8:C:402:HOH:O	2.01	0.78
3:E:9:GLU:OE1	8:E:301:HOH:O	2.01	0.78
4:H:25:GLN:HE21	4:H:27:MET:H	1.29	0.77
4:H:111:ARG:HH12	4:H:113:THR:HG1	1.30	0.77
1:C:217:ASN:OD1	8:C:403:HOH:O	2.04	0.75
3:G:122:ARG:NH2	8:G:304:HOH:O	2.19	0.75
1:A:152:TYR:CD1	4:H:100:GLY:HA3	2.20	0.74
1:C:224:GLU:N	8:C:401:HOH:O	1.90	0.74
2:D:38:ASP:OD1	2:D:45:ARG:NH1	2.21	0.74
3:E:1:GLY:HA2	3:E:27:SER:H	1.53	0.74
4:H:64:TYR:O	8:H:301:HOH:O	2.08	0.71
3:E:157:CYS:HB3	4:F:194:ARG:NH1	2.05	0.71
1:C:0:MET:HE2	1:C:169:LEU:HD13	1.73	0.70
3:E:170:SER:OG	4:F:194:ARG:NE	2.23	0.69
4:H:25:GLN:NE2	4:H:29:HIS:H	1.90	0.69
1:C:79:ARG:NH1	8:C:407:HOH:O	2.20	0.67
2:D:21:ASN:HB3	2:D:70:PHE:CE2	2.29	0.67
1:A:222:VAL:HA	4:F:200:THR:HG21	1.77	0.66
4:F:81:ALA:O	8:F:303:HOH:O	2.13	0.66
1:C:223:GLN:N	8:C:401:HOH:O	2.29	0.66
2:D:1:ILE:N	8:D:102:HOH:O	2.23	0.66
1:C:160:GLU:OE2	8:C:404:HOH:O	2.14	0.65
1:A:34:THR:HB	1:A:43:LYS:HE2	1.79	0.64
1:C:111:GLN:NE2	8:C:408:HOH:O	2.30	0.64
3:E:149:SER:O	8:E:302:HOH:O	2.15	0.64
2:B:77:GLU:OE1	8:B:102:HOH:O	2.15	0.64
3:G:175:SER:OG	3:G:176:ASN:N	2.31	0.64
3:E:28:GLY:HA3	3:E:93:SER:OG	1.97	0.64
4:F:244:ALA:O	8:F:304:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:O	1:C:243:SER:HA	1.98	0.63
3:G:1:GLY:HA2	3:G:27:SER:H	1.63	0.63
4:H:180:GLU:OE2	8:H:303:HOH:O	2.14	0.63
8:C:426:HOH:O	4:F:57:LYS:HE2	1.98	0.63
3:G:172:VAL:HG23	4:H:194:ARG:HH11	1.64	0.62
4:H:116:GLU:OE1	8:H:304:HOH:O	2.16	0.62
4:F:120:ASN:OD1	8:F:305:HOH:O	2.16	0.62
1:C:220:GLU:HG2	1:C:221:ILE:H	1.65	0.61
4:F:210:ARG:NH1	4:F:212:GLN:OE1	2.25	0.61
1:C:259:GLU:OE2	8:C:406:HOH:O	2.16	0.61
3:E:159:LEU:HB3	4:F:172:CYS:HB2	1.82	0.61
1:C:113:ALA:HB2	2:D:60:TRP:CE2	2.36	0.60
4:H:25:GLN:NE2	4:H:27:MET:H	1.98	0.60
2:B:42:ASN:OD1	8:B:102:HOH:O	2.16	0.60
4:H:155:HIS:HB3	4:H:216:TYR:HB2	1.84	0.59
3:G:176:ASN:N	3:G:176:ASN:OD1	2.35	0.59
4:H:9:LYS:NZ	8:H:307:HOH:O	2.36	0.58
3:G:91:LYS:HE2	8:H:354:HOH:O	2.04	0.58
1:C:43:LYS:HD3	1:C:66:LEU:HD13	1.86	0.58
1:C:77:LEU:HD13	1:C:92:TYR:HB2	1.86	0.57
1:A:46:ARG:HD2	8:B:174:HOH:O	2.05	0.57
4:H:180:GLU:OE1	8:H:305:HOH:O	2.18	0.57
4:H:208:HIS:NE2	4:H:239:GLU:OE1	2.23	0.57
1:A:113:ALA:HB2	2:B:60:TRP:CE2	2.39	0.56
3:G:172:VAL:HG23	4:H:194:ARG:NH1	2.21	0.55
8:A:406:HOH:O	4:F:200:THR:HG22	2.06	0.54
1:A:94:ARG:HH12	7:A:303:GOL:C1	2.20	0.54
1:C:94:ARG:HH22	7:C:302:GOL:C1	2.19	0.53
1:A:221:ILE:CG2	1:A:223:GLN:H	2.22	0.52
1:A:43:LYS:HD3	1:A:66:LEU:CD1	2.39	0.52
1:A:79:ARG:NH1	8:A:401:HOH:O	2.14	0.52
4:F:169:SER:O	8:F:306:HOH:O	2.18	0.52
4:H:25:GLN:HE22	4:H:29:HIS:H	1.56	0.52
1:A:215:MET:HG3	1:A:257:HIS:CD2	2.45	0.51
2:B:45:ARG:NH1	2:B:47:GLU:OE1	2.44	0.51
4:H:68:ARG:HH12	4:H:71:LYS:C	2.14	0.51
4:F:200:THR:HG23	8:F:419:HOH:O	2.11	0.51
4:F:79:GLU:HG2	8:F:426:HOH:O	2.11	0.50
3:E:170:SER:O	4:F:194:ARG:NH1	2.44	0.50
4:F:125:GLU:OE2	8:F:307:HOH:O	2.20	0.50
4:H:133:GLU:HG3	4:H:136:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PHE:HB2	1:A:129:TRP:CZ3	2.47	0.49
3:E:150:ASP:OD2	8:E:303:HOH:O	2.20	0.49
1:A:122:PHE:HB2	1:A:129:TRP:CH2	2.48	0.49
1:C:79:ARG:HD2	8:C:407:HOH:O	2.12	0.49
1:C:221:ILE:HD12	1:C:244:ILE:HD11	1.93	0.49
1:A:221:ILE:HG23	1:A:223:GLN:H	1.78	0.49
4:H:30:ASN:OD1	4:H:71:LYS:NZ	2.45	0.48
1:C:8:PHE:CE2	1:C:95:MET:HG3	2.47	0.48
4:F:40:GLY:HA2	8:F:483:HOH:O	2.13	0.48
4:F:128:VAL:HG23	4:F:238:ALA:HB3	1.95	0.48
2:B:21:ASN:HB3	2:B:70:PHE:CE2	2.48	0.48
4:F:94:SER:HB3	4:F:104:LEU:HD23	1.94	0.48
1:C:171:TYR:OH	8:C:405:HOH:O	2.15	0.48
1:C:221:ILE:HD12	1:C:244:ILE:CD1	2.44	0.48
1:C:247:ASP:OD1	1:C:248:PRO:HD2	2.13	0.48
3:G:28:GLY:HA3	3:G:93:SER:OG	2.14	0.48
1:A:57:ASP:N	1:A:57:ASP:OD1	2.44	0.47
1:A:198:LEU:HD13	1:A:269:VAL:HG21	1.96	0.47
1:A:221:ILE:O	4:F:200:THR:HG21	2.14	0.47
4:H:96:TRP:HB2	4:H:99:GLU:HG3	1.95	0.47
4:H:131:PRO:HD3	4:H:144:LEU:HG	1.96	0.47
4:F:11:GLN:HB3	4:F:112:LEU:HD23	1.97	0.47
1:C:116:GLY:O	2:D:3:ARG:NH2	2.48	0.47
1:A:77:LEU:HD13	1:A:92:TYR:HB2	1.95	0.47
1:A:13:SER:HB3	1:A:90:HIS:H	1.79	0.47
1:C:4:SER:HB3	1:C:99:GLU:HG2	1.96	0.47
1:C:43:LYS:NZ	6:C:301:7WQ:O1	2.47	0.47
1:A:246:LEU:HD22	1:A:254:TYR:CE2	2.50	0.47
3:E:176:ASN:HB2	8:E:309:HOH:O	2.14	0.47
3:E:170:SER:HG	4:F:194:ARG:HE	1.57	0.47
4:H:241:TRP:NE1	8:H:302:HOH:O	2.09	0.46
1:C:46:ARG:HA	1:C:46:ARG:HD3	1.75	0.46
3:G:50:VAL:O	3:G:66:ARG:HD3	2.16	0.46
4:H:154:ASP:OD1	4:H:177:PRO:HG2	2.15	0.46
4:F:86:THR:HG23	4:F:113:THR:HA	1.96	0.46
4:H:68:ARG:NH1	4:H:70:ASN:O	2.48	0.46
4:H:30:ASN:O	4:H:51:SER:HA	2.15	0.46
1:C:222:VAL:H	1:C:225:ILE:HD12	1.80	0.46
4:F:194:ARG:NH1	8:F:320:HOH:O	2.47	0.46
3:G:148:ASP:O	3:G:151:VAL:HB	2.16	0.45
4:F:95:VAL:HG22	4:F:96:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:25:GLN:HE21	4:H:27:MET:N	2.06	0.45
3:G:131:VAL:HG22	3:G:174:TRP:HB3	1.99	0.45
3:E:117:ALA:HB2	3:E:196:PHE:HB3	1.99	0.45
4:F:208:HIS:HB2	4:F:241:TRP:CZ3	2.52	0.45
2:B:73:THR:O	2:B:97:ARG:NH2	2.50	0.45
4:F:30:ASN:O	4:F:51:SER:HA	2.17	0.45
1:A:28:VAL:HG23	1:A:33:ILE:HD13	1.99	0.44
1:A:269:VAL:C	5:A:301:PRO:N	2.70	0.44
3:E:175:SER:HB3	3:E:180:PHE:CG	2.52	0.44
4:H:118:LEU:HD13	4:H:218:LEU:HD22	1.98	0.44
4:H:88:VAL:HG22	4:H:111:ARG:HD3	1.99	0.44
3:G:197:PHE:HA	3:G:198:PRO:HD2	1.89	0.44
4:F:11:GLN:HB3	4:F:112:LEU:CD2	2.47	0.44
4:H:208:HIS:HB2	4:H:241:TRP:CZ3	2.53	0.44
3:E:108:LYS:NZ	3:E:140:GLN:HE22	2.16	0.44
1:C:156:TRP:CZ3	1:C:161:CYS:HB2	2.53	0.43
1:C:152:TYR:CD2	4:F:100:GLY:HA2	2.54	0.43
1:A:123:ASN:HD21	1:A:126:THR:HG23	1.83	0.43
4:H:83:PRO:HA	4:H:114:VAL:HB	2.00	0.43
4:F:21:LEU:HD12	4:F:21:LEU:N	2.34	0.43
1:A:72:MET:HA	4:H:96:TRP:CH2	2.54	0.43
1:C:151:LEU:HD22	3:E:51:LEU:HD12	2.01	0.43
1:A:13:SER:HB3	1:A:89:SER:HA	2.01	0.43
1:C:216:LYS:O	1:C:219:GLU:N	2.46	0.42
1:C:247:ASP:HA	1:C:248:PRO:HD3	1.90	0.42
1:C:221:ILE:HG13	1:C:225:ILE:HD11	2.01	0.41
1:A:13:SER:CB	1:A:90:HIS:H	2.33	0.41
1:C:212:MET:HG2	1:C:258:VAL:HG22	2.01	0.41
1:C:34:THR:HB	1:C:43:LYS:HE2	2.03	0.41
1:A:79:ARG:NH2	8:A:401:HOH:O	2.52	0.41
1:C:177:GLN:HG2	8:C:511:HOH:O	2.21	0.41
4:H:176:GLN:HA	4:H:177:PRO:HD3	1.89	0.41
1:A:43:LYS:NZ	6:A:302:7WQ:O1	2.54	0.41
1:A:75:VAL:O	1:A:79:ARG:HG3	2.21	0.41
3:E:24:TYR:CZ	3:E:69:GLY:HA2	2.56	0.41
4:H:111:ARG:NH1	4:H:113:THR:HG1	2.01	0.40
4:H:238:ALA:HB1	8:H:329:HOH:O	2.21	0.40
3:G:1:GLY:CA	3:G:27:SER:H	2.31	0.40
4:F:64:TYR:O	8:F:308:HOH:O	2.21	0.40

All (4) 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)
8:G:343:HOH:O	8:C:480:HOH:O[2_658]	1.95	0.25
8:B:169:HOH:O	8:C:429:HOH:O[4_548]	1.96	0.24
8:E:425:HOH:O	8:E:453:HOH:O[4_548]	2.00	0.20
8:A:562:HOH:O	8:E:312:HOH:O[4_558]	2.15	0.05

### 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	260/271 (96%)	250 (96%)	10 (4%)	0	100	100
1	C	258/271 (95%)	251 (97%)	5 (2%)	2 (1%)	19	19
2	B	97/99 (98%)	97 (100%)	0	0	100	100
2	D	94/99 (95%)	91 (97%)	3 (3%)	0	100	100
3	E	198/203 (98%)	192 (97%)	6 (3%)	0	100	100
3	G	187/203 (92%)	181 (97%)	6 (3%)	0	100	100
4	F	240/245 (98%)	237 (99%)	3 (1%)	0	100	100
4	H	240/245 (98%)	234 (98%)	6 (2%)	0	100	100
All	All	1574/1636 (96%)	1533 (97%)	39 (2%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	102	GLU
1	C	222	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	228/241 (95%)	224 (98%)	4 (2%)	59	72
1	C	230/241 (95%)	224 (97%)	6 (3%)	46	58
2	B	91/94 (97%)	90 (99%)	1 (1%)	73	85
2	D	88/94 (94%)	87 (99%)	1 (1%)	73	85
3	E	171/180 (95%)	171 (100%)	0	100	100
3	G	163/180 (91%)	162 (99%)	1 (1%)	86	93
4	F	206/211 (98%)	202 (98%)	4 (2%)	57	71
4	H	206/211 (98%)	205 (100%)	1 (0%)	88	94
All	All	1383/1452 (95%)	1365 (99%)	18 (1%)	69	81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	66	LEU
1	A	73	PHE
1	A	261	SER
2	B	70	PHE
3	G	189	SER
4	H	99	GLU
1	C	16	ILE
1	C	66	LEU
1	C	82	ARG
1	C	221	ILE
1	C	224	GLU
1	C	243	SER
2	D	70	PHE
4	F	71	LYS
4	F	95	VAL
4	F	194	ARG
4	F	219	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN

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Mol	Chain	Res	Type
1	A	177	GLN
4	H	25	GLN
1	C	153	GLN
3	E	120	GLN
3	E	140	GLN

### 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](#)

5 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	$\# Z  > 2$
5	PRO	A	301	-	5,7,8	0.59	0	7,8,10	1.34	1 (14%)
7	GOL	A	303	-	5,5,5	0.38	0	5,5,5	0.90	0
6	7WQ	C	301	1	10,10,11	0.33	0	13,13,14	0.47	0
7	GOL	C	302	-	5,5,5	0.41	0	5,5,5	0.77	0
6	7WQ	A	302	1	10,10,11	0.31	0	13,13,14	0.46	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
5	PRO	A	301	-	-	0/0/9/11	0/1/1/1
7	GOL	A	303	-	-	2/4/4/4	-
6	7WQ	C	301	1	-	0/2/2/4	0/1/1/1
7	GOL	C	302	-	-	1/4/4/4	-
6	7WQ	A	302	1	-	0/2/2/4	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301	PRO	O-C-CA	-2.39	118.51	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	303	GOL	O1-C1-C2-C3
7	A	303	GOL	O1-C1-C2-O2
7	C	302	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	PRO	1	0
7	A	303	GOL	1	0
6	C	301	7WQ	1	0
7	C	302	GOL	2	0
6	A	302	7WQ	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	264/271 (97%)	-0.06	3 (1%) 80 79	20, 29, 51, 87	1 (0%)
1	C	262/271 (96%)	0.03	10 (3%) 40 38	18, 30, 68, 96	1 (0%)
2	B	99/99 (100%)	-0.15	0 100 100	20, 32, 54, 60	0
2	D	96/99 (96%)	0.65	12 (12%) 3 3	24, 49, 77, 93	0
3	E	200/203 (98%)	-0.18	2 (1%) 82 81	19, 29, 55, 67	0
3	G	193/203 (95%)	0.49	23 (11%) 4 4	21, 40, 80, 93	0
4	F	242/245 (98%)	-0.08	2 (0%) 86 85	19, 29, 48, 79	0
4	H	242/245 (98%)	0.29	22 (9%) 9 8	24, 43, 74, 108	0
All	All	1598/1636 (97%)	0.09	74 (4%) 32 31	18, 33, 70, 108	2 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	222	VAL	7.8
3	G	162	ARG	5.6
1	A	17	HIS	5.3
4	H	205	PRO	5.2
4	H	244	ALA	4.5
1	C	223	GLN	4.1
4	H	225	THR	4.1
3	G	180	PHE	4.0
4	H	199	ALA	3.5
3	G	131	VAL	3.3
2	D	78	TYR	3.3
1	C	242	ALA	3.3
4	H	206	ARG	3.3
4	H	202	TRP	3.2
1	C	246	LEU	3.2
2	D	79	ALA	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	220	GLU	3.2
2	D	44	GLU	3.1
1	C	221	ILE	3.1
4	H	200	THR	3.1
2	D	75	LYS	3.0
2	D	77	GLU	3.0
3	G	149	SER	3.0
2	D	92	ILE	3.0
4	H	204	ASN	3.0
4	H	219	SER	2.9
3	G	181	ALA	2.9
3	G	191	ILE	2.9
2	D	43	GLY	2.9
4	H	243	ARG	2.8
3	G	194	ASP	2.8
4	H	201	PHE	2.8
3	G	163	SER	2.7
4	H	227	ASP	2.7
1	C	217	ASN	2.6
3	G	140	GLN	2.6
1	A	222	VAL	2.6
3	G	147	LYS	2.6
3	G	124	SER	2.6
2	D	42	ASN	2.6
4	F	185	ASN	2.6
2	D	47	GLU	2.6
3	G	197	PHE	2.5
3	G	119	TYR	2.5
4	H	221	ASN	2.5
4	H	223	GLU	2.5
3	E	1	GLY	2.5
3	G	117	ALA	2.4
3	G	164	MET	2.4
4	H	98	GLY	2.4
1	C	224	GLU	2.4
3	G	143	VAL	2.4
2	D	45	ARG	2.3
1	C	228	GLY	2.3
4	H	209	PHE	2.3
4	H	133	GLU	2.3
2	D	89	GLN	2.3
3	G	1	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
4	H	18	SER	2.3
3	G	176	ASN	2.3
4	H	177	PRO	2.3
4	H	228	ARG	2.1
3	G	199	SER	2.1
2	D	74	GLU	2.1
3	G	122	ARG	2.1
4	F	184	LEU	2.1
4	H	241	TRP	2.1
3	G	142	ASN	2.1
1	C	250	SER	2.1
1	A	221	ILE	2.0
4	H	176	GLN	2.0
3	G	133	LEU	2.0
3	E	178	SER	2.0
3	G	198	PRO	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
7	GOL	C	302	6/6	0.74	0.19	34,39,40,42	0
5	PRO	A	301	7/8	0.81	0.28	61,66,68,68	0
7	GOL	A	303	6/6	0.93	0.24	48,48,50,51	0
6	7WQ	A	302	10/11	0.93	0.13	25,28,33,35	0
6	7WQ	C	301	10/11	0.94	0.12	19,25,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.