



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:26 AM GMT

PDB ID : 2H5X  
Title : RuvA from Mycobacterium tuberculosis  
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L.W.; Yu, M.; Bursey, E.; Muniyappa, K.; Chandra, N.R.; Vijayan, M.  
Deposited on : 2006-05-28  
Resolution : 2.70 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

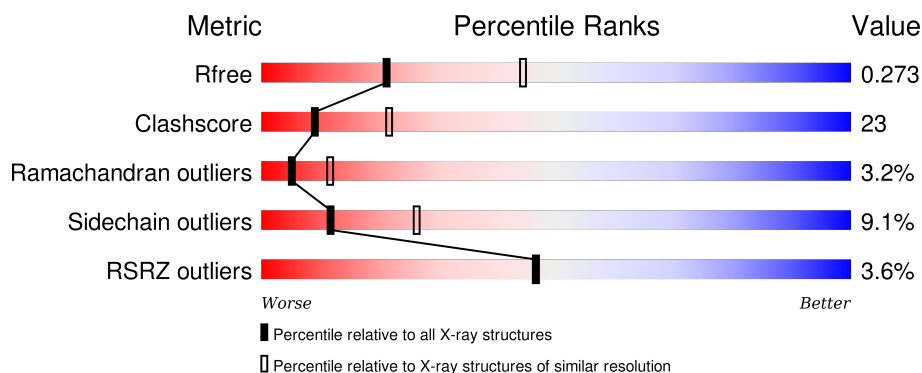
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	196	<div> <div>5%</div> <div> <div></div> <div>56%</div> <div>31%</div> <div>6% • 7%</div> </div> </div>
1	B	196	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>• • 7%</div> </div> </div>
1	C	196	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>30%</div> <div>6% • 7%</div> </div> </div>
1	D	196	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>29%</div> <div>6% • 7%</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
2	GOL	A	501	-	X	-	X
2	GOL	B	502	-	X	-	-
2	GOL	C	503	-	X	-	-
2	GOL	D	504	-	X	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5559 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 Holliday junction ATP-dependent DNA helicase ruvA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1317	825	239	248	5			
1	B	183	Total	C	N	O	S	0	0	0
			1318	823	239	251	5			
1	C	182	Total	C	N	O	S	0	0	0
			1316	822	238	251	5			
1	D	182	Total	C	N	O	S	0	0	0
			1314	820	238	251	5			

- 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		
2	B	1	Total	C	O	0	0
			6	3	3		

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

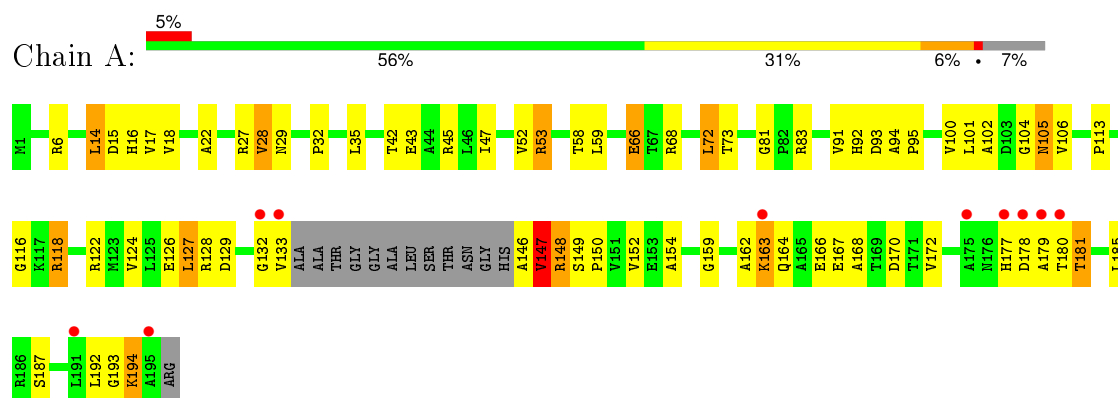
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total	O	0	0
			64	64		
3	B	74	Total	O	0	0
			74	74		
3	C	61	Total	O	0	0
			61	61		
3	D	71	Total	O	0	0
			71	71		

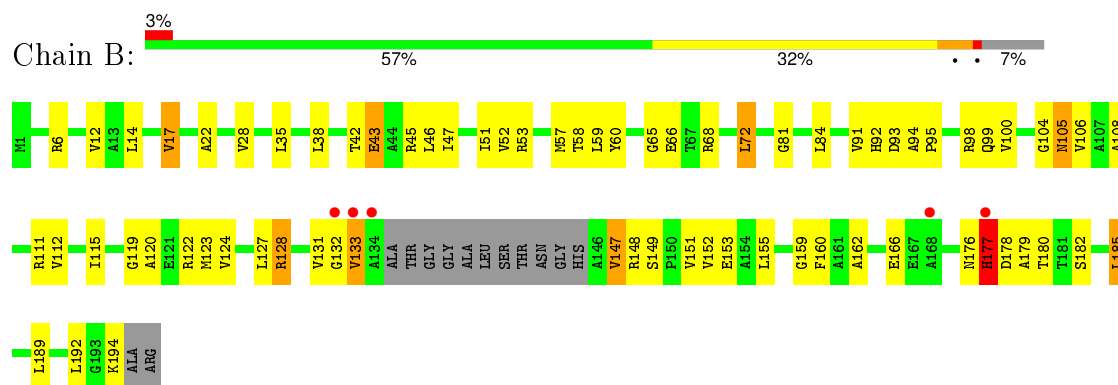
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

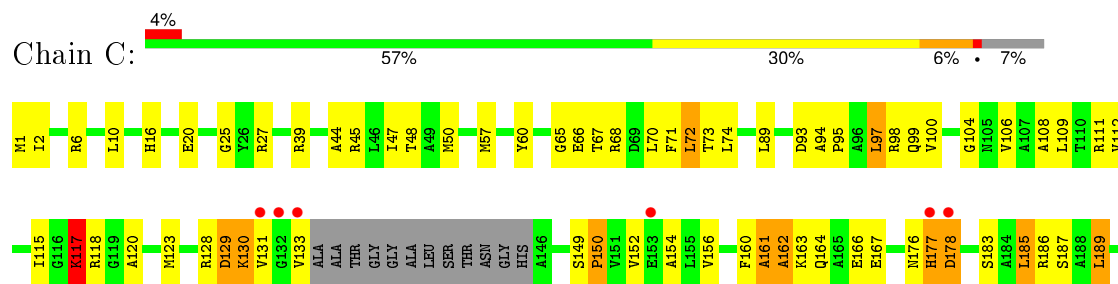
- Molecule 1: Holliday junction ATP-dependent DNA helicase ruvA



- Molecule 1: Holliday junction ATP-dependent DNA helicase ruvA



- Molecule 1: Holliday junction ATP-dependent DNA helicase ruvA





● Molecule 1: Holliday junction ATP-dependent DNA helicase ruvA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.64Å 137.64Å 88.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.49 – 2.70 44.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.49-2.70) 99.9 (44.48-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.272 0.233 , 0.273	Depositor DCC
$R_{free}$ test set	1157 reflections (4.84%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	4 of 23897 reflections (0.017%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5559	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	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 42.40 % 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 2.0508e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.33	0/1329	0.62	0/1806
1	B	0.34	0/1330	0.61	0/1808
1	C	0.33	0/1328	0.62	0/1805
1	D	0.35	0/1326	0.63	1/1802 (0.1%)
All	All	0.34	0/5313	0.62	1/7221 (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	D	176	ASN	N-CA-C	-5.58	95.92	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	1317	0	1367	67	0
1	B	1318	0	1357	57	0
1	C	1316	0	1356	72	0
1	D	1314	0	1352	70	0
2	A	6	0	4	2	0
2	B	6	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	0	4	0	0
2	D	6	0	4	1	0
3	A	64	0	0	2	0
3	B	74	0	0	0	0
3	C	61	0	0	1	0
3	D	71	0	0	3	0
All	All	5559	0	5448	248	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 23.

All (248) 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:D:118:ARG:HD2	1:D:119:GLY:H	1.19	1.03
1:C:117:LYS:HD3	1:C:118:ARG:HG2	1.41	0.99
1:D:118:ARG:HD2	1:D:119:GLY:N	1.75	0.99
1:A:100:VAL:HG13	1:A:105:ASN:HB3	1.42	0.98
1:B:14:LEU:HG	1:C:185:LEU:HD12	1.49	0.93
1:B:100:VAL:HG13	1:B:105:ASN:HB3	1.55	0.87
1:C:163:LYS:O	1:C:167:GLU:HG3	1.74	0.87
1:B:180:THR:HG22	1:B:182:SER:H	1.42	0.84
1:B:6:ARG:HG3	1:B:45:ARG:HB2	1.60	0.82
1:A:118:ARG:HD2	1:A:118:ARG:H	1.45	0.81
1:A:124:VAL:O	1:A:128:ARG:HG3	1.79	0.81
1:C:2:ILE:HB	1:C:50:MET:HE3	1.62	0.81
1:C:162:ALA:O	1:C:166:GLU:HG3	1.80	0.81
1:A:94:ALA:HB3	1:A:95:PRO:HD3	1.64	0.80
1:D:96:ALA:O	1:D:99:GLN:HG2	1.83	0.79
1:D:118:ARG:HG3	3:D:633:HOH:O	1.81	0.79
1:A:91:VAL:HG12	1:A:92:HIS:CD2	2.19	0.77
1:D:191:LEU:O	1:D:194:LYS:HB3	1.85	0.76
1:B:28:VAL:HG21	1:B:46:LEU:HD23	1.68	0.76
1:A:116:GLY:HA3	1:A:118:ARG:NH1	2.02	0.75
1:D:149:SER:HB2	1:D:150:PRO:HD3	1.70	0.74
1:B:177:HIS:CD2	1:B:177:HIS:N	2.57	0.73
1:B:120:ALA:O	1:B:124:VAL:HG23	1.89	0.72
1:B:91:VAL:HG12	1:B:92:HIS:HD2	1.54	0.72
1:A:91:VAL:HG12	1:A:92:HIS:HD2	1.53	0.72
1:A:73:THR:HG22	1:A:127:LEU:HD22	1.71	0.72
1:D:94:ALA:HB3	1:D:95:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HG12	1:B:92:HIS:CD2	2.26	0.69
1:D:168:ALA:O	1:D:172:VAL:HG23	1.92	0.69
1:D:100:VAL:HG13	1:D:105:ASN:HB3	1.75	0.69
1:A:159:GLY:O	1:D:113:PRO:HB3	1.91	0.68
1:D:194:LYS:HG2	1:D:195:ALA:N	2.08	0.68
1:A:14:LEU:HG	1:B:185:LEU:HD12	1.75	0.67
1:A:124:VAL:HG12	1:A:128:ARG:HD3	1.76	0.67
1:C:117:LYS:CD	1:C:118:ARG:H	2.06	0.67
1:D:117:LYS:O	1:D:121:GLU:HG3	1.93	0.67
1:B:94:ALA:HB3	1:B:95:PRO:HD3	1.76	0.66
1:A:113:PRO:HB3	1:B:159:GLY:O	1.95	0.66
1:C:183:SER:O	1:C:187:SER:HB2	1.95	0.66
1:D:124:VAL:O	1:D:128:ARG:HB2	1.95	0.66
1:A:118:ARG:HD2	1:A:118:ARG:N	2.11	0.66
1:D:6:ARG:HG3	1:D:45:ARG:HB2	1.78	0.66
1:C:10:LEU:HD11	1:C:20:GLU:HB2	1.78	0.65
1:C:117:LYS:HD3	1:C:118:ARG:H	1.61	0.65
1:C:70:LEU:O	1:C:74:LEU:HD22	1.96	0.65
1:A:101:LEU:O	1:A:128:ARG:HG2	1.98	0.64
1:B:180:THR:HG22	1:B:182:SER:N	2.13	0.63
1:A:181:THR:HG23	1:D:14:LEU:HD11	1.80	0.63
1:A:194:LYS:HB2	1:D:111:ARG:HD3	1.80	0.63
1:C:104:GLY:HA3	1:C:128:ARG:HH21	1.63	0.63
1:D:176:ASN:ND2	1:D:179:ALA:HB2	2.14	0.63
1:C:68:ARG:HD2	1:C:72:LEU:HD22	1.82	0.62
1:B:17:VAL:HG11	1:B:38:LEU:HD23	1.80	0.61
1:C:67:THR:HG23	1:C:94:ALA:HB2	1.82	0.61
1:A:15:ASP:OD1	1:A:16:HIS:HD2	1.84	0.61
1:A:118:ARG:CD	1:A:118:ARG:H	2.03	0.61
1:C:104:GLY:HA3	1:C:128:ARG:NH2	2.15	0.60
1:A:185:LEU:HD12	1:D:14:LEU:HG	1.83	0.60
1:C:185:LEU:HD22	1:C:189:LEU:HD22	1.82	0.60
1:C:176:ASN:O	1:C:177:HIS:C	2.40	0.60
1:A:6:ARG:HG3	1:A:45:ARG:HB2	1.84	0.59
1:D:148:ARG:O	1:D:152:VAL:HG13	2.01	0.59
1:B:177:HIS:HD2	1:B:177:HIS:N	2.00	0.59
1:D:37:THR:HG23	1:D:38:LEU:HD13	1.83	0.59
1:B:51:ILE:HD13	1:B:60:TYR:CD1	2.37	0.59
1:D:99:GLN:O	1:D:103:ASP:HB2	2.03	0.58
1:C:106:VAL:HG23	1:C:120:ALA:HB3	1.85	0.58
1:C:100:VAL:CG1	1:C:109:LEU:HG	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:SER:O	1:A:152:VAL:HG22	2.03	0.58
1:D:89:LEU:HD23	1:D:97:LEU:HD12	1.83	0.58
1:B:81:GLY:HA3	2:B:502:GOL:H12	1.86	0.58
1:A:47:ILE:N	1:A:47:ILE:HD12	2.18	0.58
1:A:163:LYS:O	1:A:167:GLU:HG3	2.04	0.58
1:D:176:ASN:HD21	1:D:179:ALA:HB2	1.67	0.58
1:A:83:ARG:H	2:A:501:GOL:H11	1.67	0.58
1:A:177:HIS:O	1:A:179:ALA:N	2.37	0.58
1:B:119:GLY:HA2	1:B:122:ARG:NH1	2.20	0.57
1:D:101:LEU:CD1	1:D:109:LEU:HD11	2.33	0.57
1:D:101:LEU:HD12	1:D:109:LEU:HD11	1.87	0.57
1:B:194:LYS:HD3	1:B:194:LYS:O	2.04	0.57
1:A:124:VAL:CG1	1:A:128:ARG:HD3	2.35	0.57
1:C:104:GLY:CA	1:C:128:ARG:HH21	2.18	0.56
1:B:176:ASN:O	1:B:177:HIS:C	2.43	0.56
1:C:99:GLN:HA	1:C:99:GLN:OE1	2.05	0.56
1:D:115:ILE:HG23	1:D:123:MET:HE3	1.87	0.56
1:C:176:ASN:O	1:C:178:ASP:N	2.39	0.56
1:A:17:VAL:CG1	1:A:28:VAL:HG13	2.36	0.56
1:C:156:VAL:HG22	1:C:161:ALA:O	2.06	0.56
1:D:194:LYS:HG2	1:D:195:ALA:H	1.68	0.56
1:A:22:ALA:HB1	1:B:22:ALA:HB2	1.87	0.56
1:C:164:GLN:HG3	1:C:192:LEU:HD21	1.87	0.56
1:B:112:VAL:HB	1:B:115:ILE:HD12	1.86	0.55
1:A:168:ALA:O	1:A:172:VAL:HG23	2.06	0.55
1:D:194:LYS:CG	1:D:195:ALA:N	2.68	0.55
1:C:177:HIS:O	1:C:178:ASP:HB2	2.07	0.55
1:C:104:GLY:N	1:C:128:ARG:HH21	2.05	0.55
1:D:15:ASP:OD1	1:D:16:HIS:HD2	1.90	0.55
1:C:89:LEU:HD23	1:C:97:LEU:HD12	1.89	0.54
1:C:98:ARG:HD3	1:C:131:VAL:O	2.06	0.54
1:B:94:ALA:O	1:B:98:ARG:HG3	2.08	0.54
1:D:17:VAL:HG21	1:D:38:LEU:HD23	1.89	0.53
1:C:156:VAL:HA	1:C:160:PHE:O	2.09	0.53
1:B:6:ARG:HG3	1:B:45:ARG:CB	2.35	0.53
1:B:162:ALA:O	1:B:166:GLU:HG3	2.09	0.53
1:A:181:THR:HG23	1:D:14:LEU:CD1	2.39	0.52
1:A:177:HIS:C	1:A:179:ALA:H	2.13	0.52
1:C:48:THR:HA	1:C:60:TYR:O	2.09	0.52
1:C:71:PHE:HA	1:C:74:LEU:HD23	1.90	0.52
1:C:149:SER:HB2	1:C:150:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LEU:C	1:D:39:ARG:HD2	2.30	0.52
1:B:147:VAL:O	1:B:151:VAL:HG23	2.09	0.52
1:D:83:ARG:H	2:D:504:GOL:H11	1.75	0.52
1:D:66:GLU:CD	1:D:66:GLU:H	2.13	0.52
1:B:47:ILE:HG22	1:B:68:ARG:NH1	2.25	0.52
1:B:68:ARG:HD2	1:B:72:LEU:HD22	1.93	0.51
1:A:163:LYS:HE3	1:A:166:GLU:OE2	2.11	0.51
1:D:42:THR:HG22	1:D:43:GLU:N	2.25	0.51
1:C:94:ALA:HB3	1:C:95:PRO:HD3	1.93	0.51
1:B:127:LEU:O	1:B:128:ARG:HB2	2.11	0.50
1:C:70:LEU:O	1:C:73:THR:HB	2.10	0.50
1:B:131:VAL:O	1:B:133:VAL:N	2.41	0.50
1:A:27:ARG:HE	1:A:29:ASN:HD21	1.58	0.50
1:D:97:LEU:HD22	1:D:101:LEU:HD22	1.92	0.50
1:D:39:ARG:HG3	1:D:39:ARG:HH11	1.76	0.50
1:D:17:VAL:HG12	1:D:18:VAL:N	2.26	0.50
1:C:57:MET:O	1:D:1:MET:HB2	2.12	0.49
1:D:10:LEU:HD11	1:D:20:GLU:HB2	1.94	0.49
1:B:108:ALA:HA	1:B:111:ARG:HD2	1.93	0.49
1:D:175:ALA:HA	3:D:606:HOH:O	2.13	0.49
1:D:194:LYS:N	1:D:194:LYS:HD3	2.28	0.49
1:C:106:VAL:HG23	1:C:120:ALA:CB	2.43	0.49
1:D:193:GLY:O	1:D:194:LYS:O	2.30	0.49
1:A:194:LYS:HD2	1:D:111:ARG:HG2	1.93	0.49
1:D:115:ILE:CG2	1:D:123:MET:HE3	2.43	0.49
1:C:115:ILE:HD13	1:C:123:MET:CE	2.42	0.49
1:B:104:GLY:O	1:B:106:VAL:N	2.46	0.48
1:C:70:LEU:HG	1:C:74:LEU:HD21	1.95	0.48
1:A:53:ARG:HH21	1:D:55:ASP:HB3	1.79	0.48
1:B:57:MET:O	1:C:1:MET:HB2	2.14	0.48
1:D:47:ILE:HG21	1:D:65:GLY:HA2	1.96	0.48
1:A:47:ILE:CD1	1:A:47:ILE:N	2.76	0.48
1:C:117:LYS:N	1:C:117:LYS:HD2	2.27	0.48
1:A:17:VAL:HG22	1:A:18:VAL:N	2.29	0.48
1:C:154:ALA:HB1	1:C:185:LEU:HD11	1.95	0.47
1:C:20:GLU:HA	1:C:25:GLY:HA2	1.96	0.47
1:A:81:GLY:HA3	2:A:501:GOL:H12	1.95	0.47
1:B:115:ILE:HD13	1:B:123:MET:HE1	1.96	0.47
1:C:100:VAL:HG11	1:C:109:LEU:HG	1.97	0.47
1:B:155:LEU:O	1:B:160:PHE:HB2	2.14	0.47
1:D:5:VAL:O	1:D:45:ARG:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:VAL:O	1:C:133:VAL:HG12	2.14	0.47
1:D:17:VAL:HG22	1:D:35:LEU:CD2	2.45	0.47
1:C:164:GLN:HG3	1:C:192:LEU:CD2	2.45	0.47
1:D:68:ARG:O	1:D:68:ARG:HD2	2.15	0.47
1:B:160:PHE:CE2	1:B:192:LEU:HD13	2.50	0.46
1:C:98:ARG:NH1	1:C:98:ARG:HG3	2.29	0.46
1:C:2:ILE:CB	1:C:50:MET:HE3	2.41	0.46
1:C:108:ALA:O	1:C:111:ARG:HB2	2.15	0.46
1:A:149:SER:HB3	1:A:150:PRO:HD3	1.96	0.46
1:B:66:GLU:CD	1:B:66:GLU:H	2.18	0.46
1:C:185:LEU:CD2	1:C:189:LEU:HD22	2.46	0.46
1:D:118:ARG:HD3	3:D:702:HOH:O	2.15	0.46
1:C:100:VAL:HG12	1:C:109:LEU:HG	1.97	0.46
1:C:47:ILE:HG22	1:C:68:ARG:HG3	1.97	0.46
1:B:176:ASN:OD1	1:B:179:ALA:HB2	2.17	0.45
1:B:12:VAL:HA	1:B:17:VAL:HG12	1.98	0.45
1:B:51:ILE:N	1:B:51:ILE:HD12	2.32	0.45
1:A:104:GLY:O	1:A:106:VAL:HG23	2.17	0.45
1:C:183:SER:HA	1:C:186:ARG:HG2	1.96	0.45
1:C:16:HIS:CD2	1:C:27:ARG:NH2	2.84	0.45
1:A:91:VAL:C	1:A:92:HIS:HD2	2.19	0.45
1:A:147:VAL:O	1:A:150:PRO:HD2	2.17	0.45
1:A:185:LEU:HD23	1:A:185:LEU:O	2.17	0.45
1:A:32:PRO:HG2	1:B:189:LEU:CD1	2.46	0.45
1:D:99:GLN:HG3	1:D:100:VAL:N	2.31	0.45
1:A:17:VAL:HG13	1:A:28:VAL:HG13	1.97	0.45
1:C:2:ILE:HD12	1:C:50:MET:CE	2.47	0.45
1:B:177:HIS:CD2	1:B:177:HIS:H	2.31	0.45
1:D:127:LEU:HA	1:D:130:LYS:HB2	1.99	0.45
1:C:66:GLU:HG2	1:C:98:ARG:NH2	2.32	0.45
1:A:146:ALA:O	1:A:148:ARG:N	2.50	0.45
1:A:42:THR:HG22	1:A:43:GLU:N	2.32	0.45
1:C:50:MET:HE2	1:D:1:MET:SD	2.57	0.44
1:B:176:ASN:O	1:B:178:ASP:N	2.51	0.44
1:C:68:ARG:HD2	1:C:72:LEU:CD2	2.46	0.44
1:B:148:ARG:O	1:B:152:VAL:HG23	2.17	0.44
1:A:6:ARG:HB2	1:A:45:ARG:HG3	2.00	0.44
1:A:164:GLN:HA	1:A:167:GLU:HG3	1.99	0.44
1:D:120:ALA:O	1:D:124:VAL:HG23	2.17	0.44
1:D:127:LEU:O	1:D:128:ARG:C	2.55	0.44
1:C:47:ILE:HD12	1:C:47:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:VAL:HB	1:C:115:ILE:HD12	2.00	0.44
1:C:117:LYS:CD	1:C:118:ARG:N	2.76	0.44
1:C:10:LEU:CD1	1:C:20:GLU:HB2	2.47	0.44
1:D:99:GLN:CG	1:D:100:VAL:N	2.80	0.44
1:A:154:ALA:HB2	1:D:14:LEU:HD23	1.99	0.44
1:A:177:HIS:C	1:A:179:ALA:N	2.71	0.43
1:C:152:VAL:O	1:C:156:VAL:HG23	2.18	0.43
1:C:98:ARG:HG3	1:C:98:ARG:HH11	1.83	0.43
1:C:128:ARG:C	1:C:130:LYS:H	2.21	0.43
1:A:180:THR:HG23	3:A:677:HOH:O	2.18	0.43
1:B:58:THR:HG22	1:B:59:LEU:N	2.34	0.43
1:C:109:LEU:HA	1:C:109:LEU:HD23	1.71	0.43
1:B:98:ARG:HB3	1:B:131:VAL:HG11	2.01	0.43
1:C:70:LEU:HG	1:C:74:LEU:CD2	2.48	0.43
1:B:115:ILE:HD13	1:B:123:MET:CE	2.48	0.43
1:A:68:ARG:HD2	1:A:72:LEU:HD22	2.00	0.43
1:A:129:ASP:HA	1:A:133:VAL:HB	2.00	0.43
1:A:193:GLY:O	1:A:194:LYS:O	2.37	0.42
1:C:115:ILE:HD13	1:C:123:MET:HE3	2.01	0.42
1:A:6:ARG:CZ	1:D:20:GLU:OE2	2.67	0.42
1:A:172:VAL:HG11	1:A:187:SER:HB2	2.00	0.42
1:A:66:GLU:OE1	1:A:66:GLU:N	2.53	0.42
1:A:192:LEU:C	1:A:194:LYS:H	2.23	0.42
1:C:6:ARG:HG3	1:C:45:ARG:HB2	2.01	0.42
1:D:10:LEU:CD1	1:D:20:GLU:HB2	2.50	0.42
1:D:96:ALA:O	1:D:100:VAL:HG23	2.19	0.42
1:A:113:PRO:HG2	1:B:160:PHE:CD1	2.55	0.41
1:C:93:ASP:HB3	1:C:95:PRO:HD2	2.01	0.41
1:D:37:THR:O	1:D:37:THR:OG1	2.36	0.41
1:A:162:ALA:C	1:A:164:GLN:H	2.24	0.41
1:A:148:ARG:HH21	1:A:170:ASP:CG	2.23	0.41
1:D:100:VAL:HG13	1:D:108:ALA:HB3	2.01	0.41
1:D:94:ALA:O	1:D:98:ARG:HG3	2.20	0.41
1:B:124:VAL:O	1:B:128:ARG:HB2	2.20	0.41
1:A:192:LEU:C	1:A:194:LYS:N	2.74	0.41
1:A:58:THR:HG22	1:A:59:LEU:N	2.35	0.41
1:B:42:THR:HG22	1:B:43:GLU:N	2.36	0.41
1:B:52:VAL:O	1:B:52:VAL:HG23	2.20	0.41
1:B:177:HIS:HD2	1:B:177:HIS:H	1.69	0.41
1:B:119:GLY:HA2	1:B:122:ARG:HH11	1.84	0.41
1:D:189:LEU:HD23	1:D:189:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ARG:HD3	3:C:651:HOH:O	2.21	0.41
1:D:115:ILE:HG12	1:D:123:MET:HE1	2.02	0.41
1:B:115:ILE:HG21	1:B:123:MET:CE	2.51	0.41
1:A:53:ARG:HD3	3:A:772:HOH:O	2.21	0.41
1:D:98:ARG:HH11	1:D:98:ARG:HG2	1.85	0.41
1:C:47:ILE:HG21	1:C:65:GLY:HA2	2.02	0.41
1:D:147:VAL:HG23	1:D:148:ARG:N	2.35	0.41
1:D:148:ARG:NE	1:D:170:ASP:OD1	2.52	0.41
1:B:47:ILE:HG21	1:B:65:GLY:HA2	2.02	0.41
1:B:14:LEU:HA	1:B:14:LEU:HD12	1.93	0.40
1:A:102:ALA:C	1:A:104:GLY:H	2.24	0.40
1:C:6:ARG:HA	1:C:44:ALA:O	2.22	0.40
1:B:28:VAL:CG2	1:B:46:LEU:HD23	2.45	0.40
1:C:6:ARG:HB2	1:C:45:ARG:HD3	2.02	0.40
1:A:91:VAL:O	1:A:92:HIS:HD2	2.04	0.40
1:D:152:VAL:CG2	1:D:153:GLU:N	2.84	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	179/196 (91%)	165 (92%)	7 (4%)	7 (4%)	4	8
1	B	179/196 (91%)	160 (89%)	14 (8%)	5 (3%)	6	15
1	C	178/196 (91%)	159 (89%)	11 (6%)	8 (4%)	3	6
1	D	178/196 (91%)	167 (94%)	8 (4%)	3 (2%)	11	29
All	All	714/784 (91%)	651 (91%)	40 (6%)	23 (3%)	5	12

All (23) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	147	VAL
1	B	133	VAL
1	B	177	HIS
1	C	117	LYS
1	C	161	ALA
1	C	177	HIS
1	D	194	LYS
1	A	178	ASP
1	A	194	LYS
1	B	105	ASN
1	B	128	ARG
1	B	132	GLY
1	C	178	ASP
1	D	130	LYS
1	A	105	ASN
1	C	130	LYS
1	A	163	LYS
1	C	162	ALA
1	A	132	GLY
1	A	148	ARG
1	C	129	ASP
1	D	128	ARG
1	C	150	PRO

### 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	132/143 (92%)	118 (89%)	14 (11%)	8	19
1	B	132/143 (92%)	119 (90%)	13 (10%)	10	23
1	C	133/143 (93%)	126 (95%)	7 (5%)	28	57
1	D	132/143 (92%)	118 (89%)	14 (11%)	8	19
All	All	529/572 (92%)	481 (91%)	48 (9%)	12	26

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	28	VAL
1	A	35	LEU
1	A	52	VAL
1	A	53	ARG
1	A	66	GLU
1	A	72	LEU
1	A	93	ASP
1	A	118	ARG
1	A	122	ARG
1	A	126	GLU
1	A	127	LEU
1	A	147	VAL
1	A	181	THR
1	B	17	VAL
1	B	35	LEU
1	B	43	GLU
1	B	53	ARG
1	B	72	LEU
1	B	84	LEU
1	B	93	ASP
1	B	99	GLN
1	B	147	VAL
1	B	149	SER
1	B	153	GLU
1	B	177	HIS
1	B	185	LEU
1	C	39	ARG
1	C	72	LEU
1	C	97	LEU
1	C	117	LYS
1	C	129	ASP
1	C	185	LEU
1	C	189	LEU
1	D	14	LEU
1	D	37	THR
1	D	38	LEU
1	D	39	ARG
1	D	43	GLU
1	D	53	ARG
1	D	97	LEU
1	D	101	LEU
1	D	103	ASP

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Mol	Chain	Res	Type
1	D	129	ASP
1	D	152	VAL
1	D	178	ASP
1	D	185	LEU
1	D	194	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	29	ASN
1	A	92	HIS
1	A	164	GLN
1	B	29	ASN
1	B	40	GLN
1	B	92	HIS
1	B	177	HIS
1	C	92	HIS
1	D	16	HIS
1	D	164	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 carbohydrates 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	501	-	5,5,5	4.81	5 (100%)	5,5,5	5.65	3 (60%)
2	GOL	B	502	-	5,5,5	4.80	5 (100%)	5,5,5	5.68	3 (60%)
2	GOL	C	503	-	5,5,5	4.87	5 (100%)	5,5,5	5.65	3 (60%)
2	GOL	D	504	-	5,5,5	4.73	5 (100%)	5,5,5	5.74	3 (60%)

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	501	-	-	0/4/4/4	0/0/0/0
2	GOL	B	502	-	-	0/4/4/4	0/0/0/0
2	GOL	C	503	-	-	0/4/4/4	0/0/0/0
2	GOL	D	504	-	-	0/4/4/4	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	GOL	C3-C2	-8.26	1.20	1.52
2	B	502	GOL	C3-C2	-8.20	1.21	1.52
2	A	501	GOL	C3-C2	-8.12	1.21	1.52
2	D	504	GOL	C3-C2	-8.06	1.21	1.52
2	D	504	GOL	C1-C2	-3.46	1.39	1.52
2	A	501	GOL	C1-C2	-3.36	1.39	1.52
2	B	502	GOL	C1-C2	-3.27	1.39	1.52
2	C	503	GOL	C1-C2	-3.18	1.40	1.52
2	C	503	GOL	O2-C2	-3.15	1.34	1.43
2	A	501	GOL	O2-C2	-3.06	1.34	1.43
2	B	502	GOL	O2-C2	-2.76	1.35	1.43
2	D	504	GOL	O2-C2	-2.70	1.35	1.43
2	D	504	GOL	O3-C3	3.11	1.55	1.42
2	A	501	GOL	O3-C3	3.12	1.55	1.42
2	C	503	GOL	O3-C3	3.30	1.56	1.42
2	B	502	GOL	O3-C3	3.36	1.56	1.42
2	D	504	GOL	O1-C1	4.25	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	GOL	O1-C1	4.31	1.60	1.42
2	A	501	GOL	O1-C1	4.42	1.61	1.42
2	C	503	GOL	O1-C1	4.43	1.61	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	GOL	O1-C1-C2	3.12	125.30	110.18
2	D	504	GOL	O1-C1-C2	3.13	125.35	110.18
2	A	501	GOL	O1-C1-C2	3.19	125.67	110.18
2	B	502	GOL	O1-C1-C2	3.33	126.36	110.18
2	D	504	GOL	O2-C2-C3	6.46	138.26	108.65
2	C	503	GOL	O2-C2-C3	6.55	138.70	108.65
2	A	501	GOL	O2-C2-C3	6.57	138.76	108.65
2	B	502	GOL	O2-C2-C3	6.68	139.30	108.65
2	B	502	GOL	O3-C3-C2	10.24	159.87	110.18
2	A	501	GOL	O3-C3-C2	10.28	160.03	110.18
2	C	503	GOL	O3-C3-C2	10.33	160.28	110.18
2	D	504	GOL	O3-C3-C2	10.61	161.64	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	2	0
2	B	502	GOL	1	0
2	D	504	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	183/196 (93%)	0.22	10 (5%) 29 27	18, 38, 84, 100	0
1	B	183/196 (93%)	0.20	5 (2%) 58 58	17, 40, 79, 100	0
1	C	182/196 (92%)	0.16	7 (3%) 44 44	16, 37, 79, 100	0
1	D	182/196 (92%)	0.07	4 (2%) 65 66	15, 38, 77, 100	0
All	All	730/784 (93%)	0.16	26 (3%) 46 46	15, 38, 83, 100	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	VAL	11.1
1	C	133	VAL	7.1
1	A	133	VAL	7.1
1	A	132	GLY	6.5
1	C	132	GLY	5.9
1	A	195	ALA	5.9
1	B	134	ALA	5.3
1	B	177	HIS	4.9
1	D	178	ASP	4.3
1	A	178	ASP	2.9
1	A	179	ALA	2.9
1	C	178	ASP	2.7
1	C	131	VAL	2.7
1	A	163	LYS	2.6
1	B	132	GLY	2.5
1	C	193	GLY	2.4
1	D	194	LYS	2.3
1	D	175	ALA	2.3
1	A	180	THR	2.3
1	B	168	ALA	2.3
1	A	191	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	177	HIS	2.2
1	C	153	GLU	2.2
1	A	175	ALA	2.1
1	D	195	ALA	2.1
1	A	177	HIS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	A	501	6/6	0.90	0.23	2.40	49,49,49,49	0
2	GOL	B	502	6/6	0.88	0.23	1.74	58,58,58,58	0
2	GOL	C	503	6/6	0.78	0.26	1.35	49,49,49,49	0
2	GOL	D	504	6/6	0.86	0.21	1.18	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.