



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:04 am BST

PDB ID : 3JWN  
Title : Complex of FimC, FimF, FimG and FimH  
Authors : Le Trong, I.; Aprikian, P.; Stenkamp, R.E.; Sokurenko, E.V.  
Deposited on : 2009-09-18  
Resolution : 2.69 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 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 : 2.11  
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) : 2.11

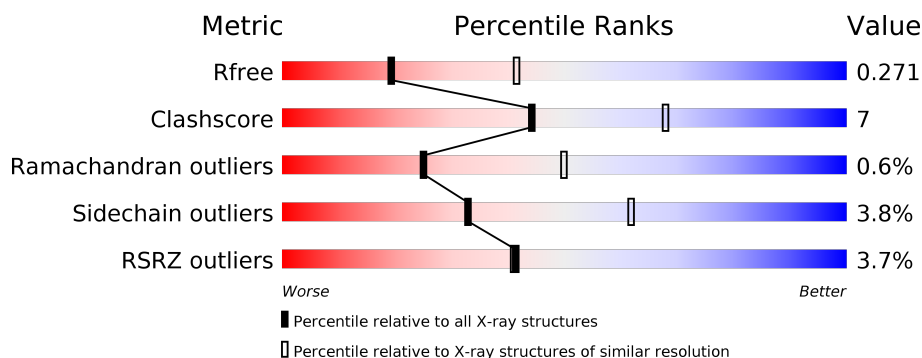
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	C	205	<div> <div>11%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> </div>
1	I	205	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> </div>
2	E	154	<div> <div>13%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div></div> </div> </div>
2	F	154	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>21%</div> <div></div> </div> </div>
2	K	154	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div></div> </div> </div>
2	L	154	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>14%</div> <div></div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	144	<div><div>%</div><div><div></div></div><div>88%12%</div><div></div></div>
3	M	144	<div><div></div><div>92%8%</div><div></div></div>
4	H	279	<div><div></div><div>78%18%</div><div></div></div>
4	N	279	<div><div></div><div>81%18%</div><div></div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13908 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 Chaperone protein fimC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	199	Total	C	N	O	S	0	1	0
			1556	985	268	296	7			
1	I	198	Total	C	N	O	S	1	1	0
			1548	980	267	295	6			

- Molecule 2 is a protein called Protein fimF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	154	Total	C	N	O	S	0	0	0
			1136	711	196	225	4			
2	F	154	Total	C	N	O	S	0	1	0
			1136	711	196	225	4			
2	K	154	Total	C	N	O	S	0	0	0
			1136	711	196	225	4			
2	L	154	Total	C	N	O	S	0	1	0
			1142	715	198	225	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	89	ALA	SER	CONFLICT	UNP P08189
F	89	ALA	SER	CONFLICT	UNP P08189
K	89	ALA	SER	CONFLICT	UNP P08189
L	89	ALA	SER	CONFLICT	UNP P08189

- Molecule 3 is a protein called Protein fimG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	144	Total	C	N	O	S	0	1	0
			1043	640	176	224	3			
3	M	144	Total	C	N	O	S	0	3	0
			1056	651	178	224	3			

- Molecule 4 is a protein called FimH protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	279	Total	C	N	O	S	0	2	0
			2061	1302	346	409	4			
4	N	279	Total	C	N	O	S	0	1	0
			2054	1298	342	410	4			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	N	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	3	Total	O	0	0
			3	3		
6	E	1	Total	O	0	0
			1	1		
6	H	3	Total	O	0	0
			3	3		
6	I	2	Total	O	0	0
			2	2		
6	L	1	Total	O	0	0
			1	1		

*Continued on next page...*

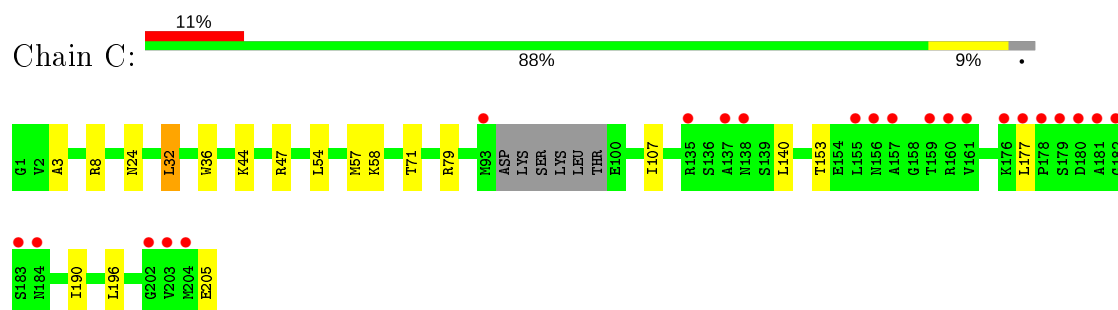
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	2	Total	O	0	0
			2	2		
6	N	16	Total	O	0	0
			16	16		

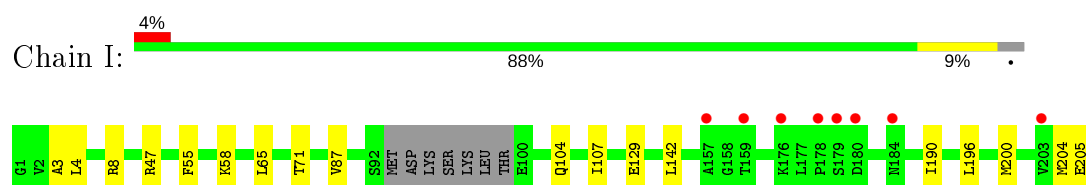
### 3 Residue-property plots [i](#)

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

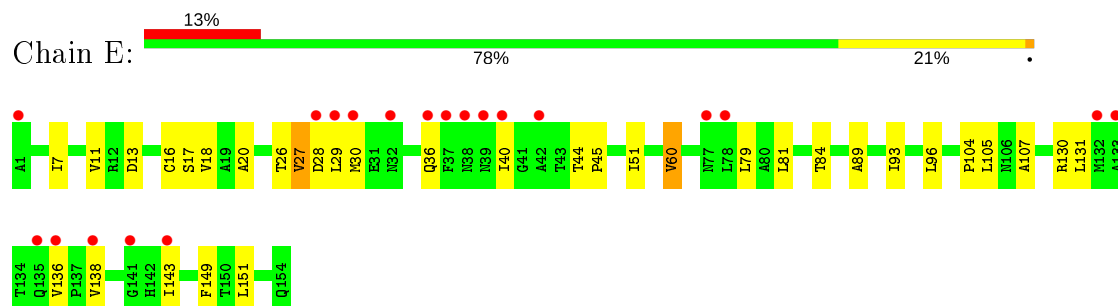
- Molecule 1: Chaperone protein fimC



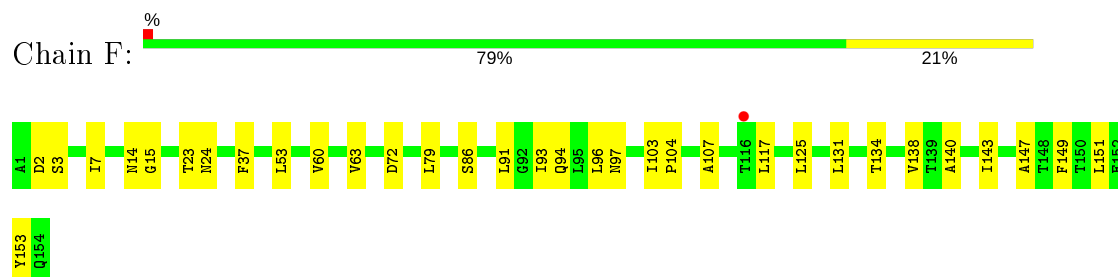
- Molecule 1: Chaperone protein fimC



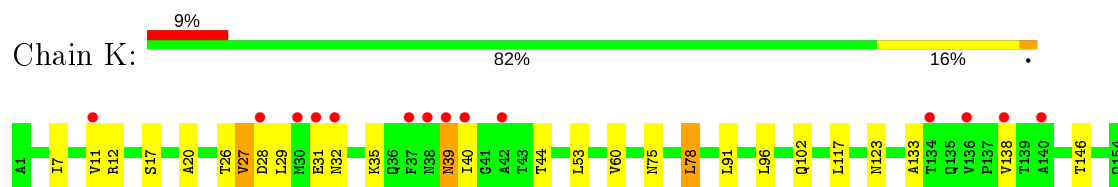
- Molecule 2: Protein fimF



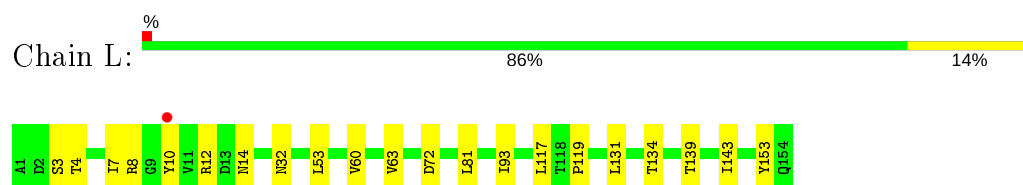
- Molecule 2: Protein fimF



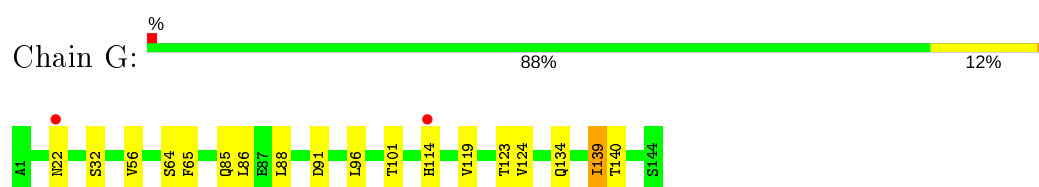
- Molecule 2: Protein fimF



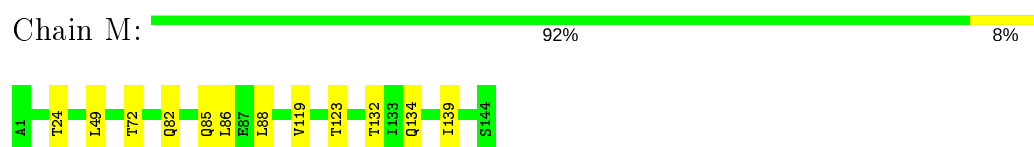
- Molecule 2: Protein fimF



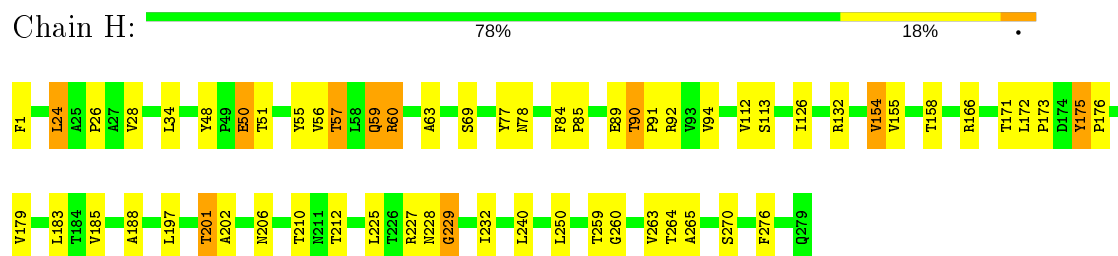
- Molecule 3: Protein fimG



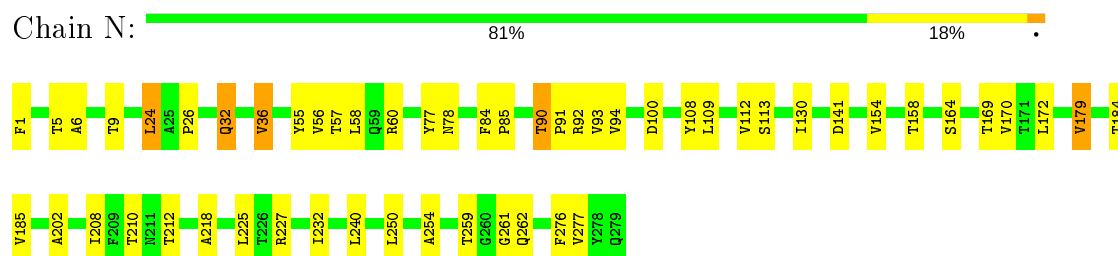
- Molecule 3: Protein fimG



- Molecule 4: FimH protein



- Molecule 4: FimH protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	216.03Å 216.03Å 532.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.34 – 2.69 48.34 – 2.69	Depositor EDS
% Data completeness (in resolution range)	90.5 (48.34-2.69) 90.5 (48.34-2.69)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0096	Depositor
R, $R_{free}$	0.244 , 0.272 0.244 , 0.271	Depositor DCC
$R_{free}$ test set	6018 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for $-1/3^*h+1/3^*k+1/3^*l, -k, 8/3^*h+4/3^*k+1/3^*l$ 0.003 for $-2/3^*h-1/3^*k-1/3^*l, -1/3^*h-2/3^*k+1/3^*l, -4/3^*h+4/3^*k+1/3^*l$ 0.001 for $-h, 1/3^*h-1/3^*k-1/3^*l, -4/3^*h-8/3^*k+1/3^*l$	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13908	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: 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	C	0.32	0/1587	0.49	0/2156
1	I	0.50	1/1579 (0.1%)	0.68	1/2146 (0.0%)
2	E	0.34	0/1156	0.50	0/1583
2	F	0.30	0/1156	0.48	0/1583
2	K	0.33	0/1156	0.52	0/1583
2	L	0.31	0/1167	0.49	0/1598
3	G	0.30	0/1057	0.45	0/1445
3	M	0.30	0/1080	0.46	0/1476
4	H	0.32	0/2114	0.50	0/2904
4	N	0.32	0/2103	0.51	0/2890
All	All	0.34	1/14155 (0.0%)	0.52	1/19364 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	58	LYS	CE-NZ	-15.18	1.11	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	58	LYS	CD-CE-NZ	21.42	160.96	111.70

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	C	1556	0	1591	10	0
1	I	1548	0	1582	11	0
2	E	1136	0	1126	25	0
2	F	1136	0	1124	24	0
2	K	1136	0	1126	19	0
2	L	1142	0	1129	15	0
3	G	1043	0	1007	11	0
3	M	1056	0	1013	10	0
4	H	2061	0	2016	42	0
4	N	2054	0	2005	33	0
5	N	12	0	16	0	0
6	C	3	0	0	0	0
6	E	1	0	0	0	0
6	H	3	0	0	2	0
6	I	2	0	0	0	0
6	L	1	0	0	0	0
6	M	2	0	0	0	0
6	N	16	0	0	0	0
All	All	13908	0	13735	181	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 7.

All (181) 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:60[A]:ARG:HD2	6:H:527:HOH:O	1.50	1.09
2:L:63:VAL:HG13	2:L:117:LEU:HD11	1.41	0.98
2:F:63:VAL:HG23	2:F:117:LEU:HD11	1.43	0.98
1:I:107:ILE:HD11	2:K:20:ALA:HB2	1.54	0.88
4:N:90:THR:HG23	4:N:91:PRO:O	1.74	0.87
4:H:57:THR:HG21	4:H:89:GLU:OE2	1.77	0.85
4:N:202:ALA:HB2	4:N:210:THR:HG22	1.63	0.80
2:F:63:VAL:CG2	2:F:117:LEU:HD11	2.11	0.79
2:F:63:VAL:HG23	2:F:117:LEU:CD1	2.15	0.77
2:L:63:VAL:CG1	2:L:117:LEU:HD11	2.16	0.76
4:H:202:ALA:HB2	4:H:210:THR:HG22	1.70	0.73
1:I:3:ALA:HB2	2:K:17:SER:HA	1.74	0.70
2:K:7:ILE:HG21	2:L:93:ILE:HD13	1.75	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:112:VAL:HG22	4:H:158:THR:HG23	1.77	0.67
4:N:172:LEU:HD23	4:N:179:VAL:HG22	1.76	0.67
4:H:24:LEU:HD21	4:H:126:ILE:HD11	1.76	0.67
2:E:18:VAL:HG21	2:E:151:LEU:HD12	1.76	0.67
4:H:24:LEU:HD21	4:H:126:ILE:CD1	2.25	0.66
4:H:50:GLU:OE1	4:H:51:THR:HG23	1.95	0.65
2:E:36:GLN:HG3	2:E:136:VAL:HG13	1.79	0.65
1:C:107:ILE:HD11	2:E:20:ALA:HB2	1.78	0.64
4:H:57:THR:HG22	4:H:132:ARG:HB3	1.78	0.64
1:I:190:ILE:HD13	1:I:196:LEU:HD23	1.78	0.64
2:L:63:VAL:HG12	2:L:153:TYR:CD2	2.31	0.64
2:E:131:LEU:HD13	2:E:143:ILE:HD13	1.80	0.64
4:N:185:VAL:HG21	4:N:276:PHE:CE2	2.33	0.63
4:H:185:VAL:HG21	4:H:276:PHE:CE2	2.34	0.63
1:I:47:ARG:HB3	1:I:71:THR:HG22	1.81	0.62
2:F:14:ASN:C	2:F:60:VAL:HG12	2.18	0.62
4:N:164:SER:HB3	4:N:184:THR:HG22	1.79	0.62
3:G:139:ILE:HD13	3:G:139:ILE:C	2.20	0.62
4:H:113:SER:OG	4:H:158:THR:HG22	2.00	0.62
2:E:7:ILE:HG21	2:F:93:ILE:HD13	1.83	0.61
3:G:65:PHE:CE2	3:G:96:LEU:HD13	2.36	0.61
2:E:81:LEU:HD22	2:E:143:ILE:HG23	1.83	0.60
4:H:90:THR:HG23	4:H:91:PRO:O	2.02	0.60
2:F:3:SER:HB3	3:G:139:ILE:HG23	1.84	0.60
2:E:79:LEU:HD12	2:E:105:LEU:HD21	1.83	0.60
4:H:63:ALA:HB2	4:H:85:PRO:HB3	1.84	0.59
4:N:58:LEU:H	4:N:90:THR:HG22	1.66	0.59
4:N:240:LEU:HD11	4:N:250:LEU:HD22	1.85	0.58
1:C:36:TRP:CD1	1:C:44:LYS:HD3	2.38	0.58
4:N:208:ILE:HG21	4:N:259:THR:HG22	1.86	0.57
2:F:94:GLN:OE1	2:F:96:LEU:HD21	2.04	0.57
2:L:63:VAL:HG13	2:L:117:LEU:CD1	2.25	0.57
4:N:24:LEU:HB3	4:N:36:VAL:HG13	1.86	0.57
2:F:97:ASN:HB3	2:F:103:ILE:HD11	1.87	0.56
2:K:91:LEU:HD23	2:K:133:ALA:HA	1.87	0.56
1:C:32:LEU:HD22	1:C:54:LEU:HD11	1.86	0.56
4:H:59[B]:GLN:HG3	6:H:527:HOH:O	2.04	0.56
3:G:85:GLN:OE1	3:G:124:VAL:HG23	2.06	0.56
4:H:185:VAL:CG2	4:H:250:LEU:HD21	2.36	0.55
2:K:27:VAL:HG13	2:K:28:ASP:H	1.70	0.55
4:N:227:ARG:HB3	4:N:232:ILE:HD11	1.89	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:158:THR:CG2	4:N:158:THR:O	2.54	0.54
4:N:5:THR:HG22	4:N:6:ALA:N	2.22	0.54
2:F:72:ASP:OD2	2:F:134:THR:HG21	2.08	0.54
4:H:69:SER:HB2	4:N:130:ILE:HD11	1.88	0.54
1:C:107:ILE:HD11	2:E:20:ALA:CB	2.37	0.53
3:M:49:LEU:HD13	3:M:139:ILE:CD1	2.37	0.53
4:H:172:LEU:HD23	4:H:179:VAL:HG22	1.89	0.53
2:F:37:PHE:CD1	2:F:138:VAL:HG21	2.43	0.53
4:N:164:SER:CB	4:N:184:THR:HG22	2.38	0.53
4:H:28:VAL:HG12	4:H:188:ALA:HB2	1.92	0.52
4:H:201:THR:HG21	4:H:206:ASN:CG	2.29	0.52
2:K:117:LEU:HD22	2:K:123:ASN:CB	2.41	0.51
2:L:10:TYR:CE1	3:M:132:THR:HG22	2.45	0.51
2:L:60:VAL:HG22	2:L:119:PRO:HA	1.92	0.51
2:F:23:THR:HG22	2:F:24:ASN:ND2	2.26	0.51
4:H:240:LEU:HD11	4:H:250:LEU:HD22	1.91	0.51
1:I:104:GLN:HB3	2:K:146:THR:HG22	1.92	0.50
4:H:185:VAL:HG23	4:H:250:LEU:HD21	1.93	0.50
4:N:170:VAL:CG1	4:N:179:VAL:HG21	2.41	0.50
4:N:1:PHE:CZ	4:N:56:VAL:HG21	2.45	0.50
2:E:18:VAL:HG21	2:E:151:LEU:CD1	2.41	0.50
4:H:55:TYR:CD2	4:H:94:VAL:HG12	2.46	0.50
1:C:24:ASN:H	1:C:57:MET:HE1	1.75	0.50
2:E:16:CYS:SG	2:E:60:VAL:HG21	2.52	0.50
2:K:60:VAL:HG23	2:K:60:VAL:O	2.11	0.50
4:H:24:LEU:HD12	4:H:24:LEU:N	2.27	0.50
2:E:11:VAL:O	2:F:140:ALA:HB1	2.12	0.49
1:I:3:ALA:HB2	2:K:17:SER:CA	2.40	0.49
3:G:123:THR:O	3:G:123:THR:HG23	2.13	0.49
4:H:227:ARG:O	4:H:229:GLY:N	2.46	0.49
2:E:40:ILE:HG23	2:E:40:ILE:O	2.12	0.49
2:F:104:PRO:HB2	2:F:107:ALA:HB2	1.93	0.49
2:K:40:ILE:HG23	2:K:40:ILE:O	2.13	0.49
2:E:26:THR:O	2:E:28:ASP:N	2.44	0.49
2:F:149:PHE:CE2	2:F:151:LEU:HD11	2.48	0.49
2:K:11:VAL:O	2:L:32:ASN:O	2.31	0.48
4:N:185:VAL:HG21	4:N:276:PHE:CZ	2.48	0.48
2:F:151:LEU:HD12	2:F:151:LEU:N	2.29	0.48
3:G:86:LEU:N	3:G:86:LEU:HD22	2.28	0.48
4:N:57:THR:HG22	4:N:92:ARG:HA	1.95	0.48
2:F:63:VAL:HG22	2:F:153:TYR:CD2	2.49	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1:PHE:CE1	4:H:56:VAL:HG21	2.48	0.48
2:E:11:VAL:HG21	2:F:91:LEU:CD1	2.43	0.48
2:K:32:ASN:HA	2:K:35:LYS:HB2	1.96	0.48
3:G:88:LEU:HD13	3:G:119:VAL:HG22	1.95	0.48
3:G:139:ILE:HD13	3:G:140:THR:N	2.29	0.48
2:K:39:ASN:O	2:K:133:ALA:O	2.32	0.48
4:N:158:THR:HG22	4:N:158:THR:O	2.14	0.47
3:M:49:LEU:CD1	3:M:139:ILE:CD1	2.92	0.47
4:H:173:PRO:HD3	4:H:179:VAL:HG13	1.96	0.47
4:H:24:LEU:HD11	4:H:126:ILE:HD11	1.97	0.47
3:M:88:LEU:HD13	3:M:119:VAL:HG22	1.97	0.47
2:E:51:ILE:HD13	2:E:149:PHE:CD1	2.50	0.47
4:H:55:TYR:CE2	4:H:94:VAL:HG12	2.50	0.47
2:L:7:ILE:HD13	3:M:119:VAL:HG11	1.97	0.47
3:M:49:LEU:HD13	3:M:139:ILE:HD12	1.95	0.46
4:N:84:PHE:HA	4:N:85:PRO:C	2.36	0.46
3:G:64:SER:HA	3:G:101:THR:HG22	1.96	0.46
2:K:75:ASN:HB3	2:K:78:LEU:HD22	1.97	0.46
2:L:7:ILE:CD1	3:M:119:VAL:HG11	2.46	0.46
4:H:197:LEU:HD13	4:H:225:LEU:HD12	1.98	0.46
4:H:227:ARG:HG2	4:H:232:ILE:HD11	1.97	0.46
4:N:112:VAL:HG22	4:N:158:THR:HG23	1.97	0.46
2:K:53:LEU:HD23	2:K:117:LEU:HD11	1.98	0.45
2:E:44:THR:HG23	2:E:45:PRO:HD2	1.97	0.45
2:F:91:LEU:HD11	2:F:138:VAL:HG11	1.98	0.45
4:H:171:THR:O	4:H:179:VAL:HG11	2.15	0.45
4:N:32:GLN:HG3	4:N:108:TYR:HB3	1.98	0.45
4:N:26:PRO:CD	4:N:154:VAL:HG21	2.46	0.45
4:N:78:ASN:ND2	4:N:93:VAL:HG22	2.31	0.45
4:N:26:PRO:HD2	4:N:154:VAL:HG21	1.98	0.45
1:C:47:ARG:HB3	1:C:71:THR:HG22	1.99	0.45
2:E:27:VAL:HG22	2:E:30:MET:H	1.82	0.45
4:N:58:LEU:H	4:N:90:THR:CG2	2.28	0.45
2:F:53:LEU:HD11	2:F:125:LEU:HD11	1.98	0.45
4:N:225:LEU:HD23	4:N:254:ALA:HA	1.99	0.45
3:M:72:THR:HG21	3:M:85:GLN:NE2	2.33	0.44
4:N:185:VAL:CG2	4:N:250:LEU:HD21	2.48	0.44
2:F:79:LEU:HD22	2:F:147:ALA:HB2	1.99	0.44
4:H:84:PHE:HA	4:H:85:PRO:C	2.37	0.44
4:N:55:TYR:CE2	4:N:94:VAL:HG12	2.53	0.44
1:C:190:ILE:HD13	1:C:196:LEU:HD23	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:GLY:N	2:F:60:VAL:HG12	2.32	0.44
4:N:24:LEU:HD23	4:N:24:LEU:H	1.83	0.44
2:F:7:ILE:HD13	3:G:119:VAL:HG11	2.00	0.43
1:I:142:LEU:N	1:I:142:LEU:HD12	2.34	0.43
2:E:81:LEU:CD2	2:E:143:ILE:HG23	2.48	0.43
2:E:89:ALA:O	2:E:138:VAL:HG13	2.19	0.43
2:E:26:THR:HG23	2:E:27:VAL:H	1.84	0.43
1:I:129:GLU:OE2	1:I:200[B]:MET:HE2	2.19	0.43
4:N:77:TYR:CE2	4:N:90:THR:HG21	2.54	0.43
1:C:3:ALA:HB2	2:E:17:SER:HA	2.00	0.43
2:E:60:VAL:HG23	2:E:60:VAL:O	2.18	0.43
2:L:131:LEU:HD21	2:L:143:ILE:HD13	2.01	0.43
3:M:86:LEU:N	3:M:86:LEU:HD22	2.34	0.43
2:E:96:LEU:HD11	2:E:130:ARG:NE	2.34	0.43
1:I:204:MET:O	1:I:205:GLU:HB2	2.19	0.43
2:L:81:LEU:HD22	2:L:143:ILE:HG23	2.00	0.43
2:K:91:LEU:HD11	2:K:138:VAL:HG11	2.00	0.42
4:H:175:TYR:CE2	4:H:176:PRO:HB3	2.53	0.42
1:I:55:PHE:HE2	1:I:65:LEU:HD21	1.84	0.42
1:C:140:LEU:HB2	1:C:177:LEU:HD22	2.01	0.42
4:H:26:PRO:HG2	4:H:154:VAL:HG13	2.01	0.42
1:C:153:THR:HG21	1:C:196:LEU:HD21	2.02	0.42
4:H:77:TYR:CE2	4:H:90:THR:HG21	2.54	0.42
4:H:185:VAL:HG21	4:H:250:LEU:HD21	2.02	0.42
4:H:158:THR:O	4:H:158:THR:CG2	2.67	0.42
4:N:113:SER:OG	4:N:158:THR:HG22	2.20	0.42
4:N:55:TYR:CD2	4:N:94:VAL:HG12	2.55	0.41
4:H:259:THR:OG1	4:H:260:GLY:N	2.53	0.41
4:H:155:VAL:HG11	4:H:166:ARG:HD2	2.01	0.41
2:L:14:ASN:C	2:L:60:VAL:HG12	2.41	0.41
2:L:72:ASP:OD2	2:L:134:THR:HG21	2.21	0.41
3:M:123:THR:HG23	3:M:123:THR:O	2.20	0.41
2:F:149:PHE:HE2	2:F:151:LEU:HD11	1.84	0.41
4:H:264:THR:HG22	4:H:265:ALA:O	2.21	0.41
2:K:35:LYS:CE	2:K:133:ALA:HB2	2.50	0.41
2:L:63:VAL:HG12	2:L:153:TYR:CE2	2.56	0.40
2:E:104:PRO:HB2	2:E:107:ALA:HB2	2.02	0.40
2:K:96:LEU:HD13	2:K:102:GLN:HA	2.04	0.40
4:H:1:PHE:CZ	4:H:56:VAL:HG21	2.56	0.40
3:G:56:VAL:CG1	4:H:263:VAL:HG21	2.50	0.40
2:F:131:LEU:HD21	2:F:143:ILE:HD13	2.04	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:LEU:HD21	1:I:87:VAL:HG21	2.02	0.40
2:K:26:THR:O	2:K:28:ASP:N	2.54	0.40
2:E:81:LEU:HD23	2:E:93:ILE:HG13	2.04	0.40
4:H:112:VAL:CG2	4:H:158:THR:HG23	2.50	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	C	196/205 (96%)	186 (95%)	10 (5%)	0	100	100
1	I	195/205 (95%)	191 (98%)	4 (2%)	0	100	100
2	E	152/154 (99%)	135 (89%)	15 (10%)	2 (1%)	12	30
2	F	152/154 (99%)	150 (99%)	2 (1%)	0	100	100
2	K	152/154 (99%)	139 (91%)	10 (7%)	3 (2%)	7	19
2	L	153/154 (99%)	146 (95%)	7 (5%)	0	100	100
3	G	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
3	M	144/144 (100%)	140 (97%)	4 (3%)	0	100	100
4	H	279/279 (100%)	270 (97%)	6 (2%)	3 (1%)	14	34
4	N	278/279 (100%)	269 (97%)	6 (2%)	3 (1%)	14	34
All	All	1843/1872 (98%)	1763 (96%)	69 (4%)	11 (1%)	25	50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	27	VAL
4	N	261	GLY
4	N	169	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
4	H	228	ASN
2	K	12	ARG
4	N	218	ALA
2	E	27	VAL
4	H	175	TYR
4	H	229	GLY
2	K	44	THR
2	E	60	VAL

### 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	C	171/176 (97%)	166 (97%)	5 (3%)	42	71
1	I	170/176 (97%)	169 (99%)	1 (1%)	86	95
2	E	123/123 (100%)	120 (98%)	3 (2%)	49	77
2	F	123/123 (100%)	121 (98%)	2 (2%)	62	85
2	K	123/123 (100%)	119 (97%)	4 (3%)	38	67
2	L	124/123 (101%)	118 (95%)	6 (5%)	25	53
3	G	115/115 (100%)	109 (95%)	6 (5%)	23	49
3	M	117/115 (102%)	114 (97%)	3 (3%)	46	75
4	H	227/225 (101%)	210 (92%)	17 (8%)	13	31
4	N	226/225 (100%)	213 (94%)	13 (6%)	20	43
All	All	1519/1524 (100%)	1459 (96%)	60 (4%)	33	61

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	ARG
1	C	32	LEU
1	C	58	LYS
1	C	79	ARG
1	C	205	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	13	ASP
2	E	29	LEU
2	E	84	THR
2	F	2	ASP
2	F	86	SER
3	G	22	ASN
3	G	32	SER
3	G	91	ASP
3	G	114	HIS
3	G	134	GLN
3	G	139	ILE
4	H	24	LEU
4	H	34	LEU
4	H	48	TYR
4	H	50	GLU
4	H	57	THR
4	H	59[A]	GLN
4	H	59[B]	GLN
4	H	60[A]	ARG
4	H	60[B]	ARG
4	H	78	ASN
4	H	90	THR
4	H	92	ARG
4	H	154	VAL
4	H	183	LEU
4	H	201	THR
4	H	212	THR
4	H	270	SER
1	I	8	ARG
2	K	29	LEU
2	K	31	GLU
2	K	39	ASN
2	K	78	LEU
2	L	3	SER
2	L	4	THR
2	L	8	ARG
2	L	12	ARG
2	L	53	LEU
2	L	139	THR
3	M	24	THR
3	M	82	GLN
3	M	134	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	N	9	THR
4	N	24	LEU
4	N	32	GLN
4	N	36	VAL
4	N	60	ARG
4	N	90	THR
4	N	100	ASP
4	N	109	LEU
4	N	141	ASP
4	N	179	VAL
4	N	212	THR
4	N	262	GLN
4	N	277	VAL

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

Mol	Chain	Res	Type
1	C	73	ASN
2	F	77	ASN
2	F	102	GLN
2	F	135	GLN
2	K	94	GLN
2	K	102	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](#)

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	$\# Z  > 2$
5	GOL	N	302	-	5,5,5	0.43	0	5,5,5	0.37	0
5	GOL	N	301	-	5,5,5	0.37	0	5,5,5	0.31	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	GOL	N	302	-	-	4/4/4/4	-
5	GOL	N	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	302	GOL	O1-C1-C2-C3
5	N	302	GOL	C1-C2-C3-O3
5	N	302	GOL	O1-C1-C2-O2
5	N	302	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	C	199/205 (97%)	0.69	22 (11%) 5 4	40, 62, 94, 96	0
1	I	198/205 (96%)	0.38	8 (4%) 38 37	42, 61, 83, 87	1 (0%)
2	E	154/154 (100%)	0.76	20 (12%) 3 2	53, 69, 104, 107	0
2	F	154/154 (100%)	0.32	1 (0%) 89 91	56, 67, 77, 79	2 (1%)
2	K	154/154 (100%)	0.74	14 (9%) 9 7	54, 69, 104, 108	0
2	L	154/154 (100%)	0.19	1 (0%) 89 91	52, 60, 73, 75	3 (1%)
3	G	144/144 (100%)	0.29	2 (1%) 75 77	54, 72, 80, 82	1 (0%)
3	M	144/144 (100%)	0.05	0 100 100	52, 66, 72, 76	0
4	H	279/279 (100%)	0.12	0 100 100	35, 46, 71, 75	1 (0%)
4	N	279/279 (100%)	-0.05	0 100 100	34, 47, 62, 65	0
All	All	1859/1872 (99%)	0.32	68 (3%) 41 41	34, 63, 84, 108	8 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	40	ILE	10.2
2	K	39	ASN	6.6
2	K	32	ASN	6.5
2	E	39	ASN	6.4
2	E	37	PHE	6.1
2	K	42	ALA	6.1
2	E	30	MET	5.7
2	K	40	ILE	5.0
2	K	30	MET	4.8
1	C	179	SER	4.5
2	K	37	PHE	4.3
1	C	178	PRO	4.2
2	E	42	ALA	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	E	38	ASN	4.0
1	C	157	ALA	3.9
2	K	38	ASN	3.9
1	C	138	ASN	3.7
1	C	160	ARG	3.6
2	L	10	TYR	3.5
1	C	156	ASN	3.5
2	K	31	GLU	3.5
1	C	182	GLY	3.4
2	E	143	ILE	3.3
1	C	137	ALA	3.2
2	E	1	ALA	3.2
1	I	203	VAL	3.1
1	C	161	VAL	3.1
1	C	181	ALA	3.1
1	C	203	VAL	3.0
2	E	32	ASN	3.0
1	C	159	THR	3.0
1	C	202	GLY	3.0
2	E	28	ASP	2.9
2	E	136	VAL	2.9
2	K	28	ASP	2.9
2	E	141	GLY	2.8
1	C	135	ARG	2.7
1	C	204	MET	2.7
1	I	184	ASN	2.7
2	E	133	ALA	2.7
2	K	140	ALA	2.7
2	E	77	ASN	2.7
1	I	176	LYS	2.7
1	C	184	ASN	2.6
2	E	78	LEU	2.6
1	C	180	ASP	2.6
1	I	157	ALA	2.6
1	C	155	LEU	2.6
2	F	116	THR	2.6
1	C	183	SER	2.4
2	E	36	GLN	2.4
1	I	159	THR	2.4
1	I	178	PRO	2.4
2	K	138	VAL	2.3
1	C	176	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	K	134	THR	2.3
3	G	114	HIS	2.3
1	I	180	ASP	2.3
3	G	22	ASN	2.2
1	C	177	LEU	2.2
2	E	29	LEU	2.2
2	K	136	VAL	2.2
2	E	135	GLN	2.1
2	K	11	VAL	2.1
1	I	179	SER	2.1
2	E	132	MET	2.1
2	E	138	VAL	2.0
1	C	93	MET	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 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	N	301	6/6	0.87	0.27	61,62,62,62	0
5	GOL	N	302	6/6	0.94	0.21	55,55,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.