Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 02:53 AM EDT

PDB ID	:	7SZO
Title	:	Structure of a bacterial fimbrial tip containing FocH
Authors	:	Stenkamp, R.E.; Le Trong, I.; Aprikian, P.; Sokurenko, E.V.
Deposited on	:	2021-11-29
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

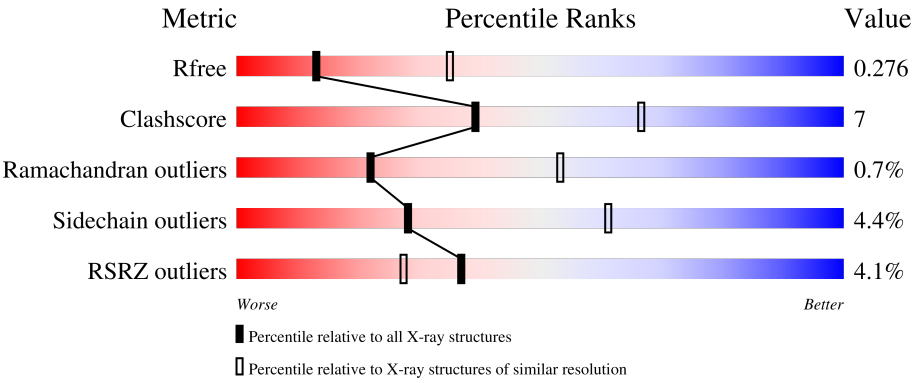
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	12% 85% 12%
1	I	205	5% 85% 11%
2	E	154	12% 75% 23%
2	F	154	81% 18%
2	K	154	12% 74% 23%

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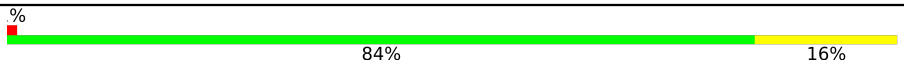
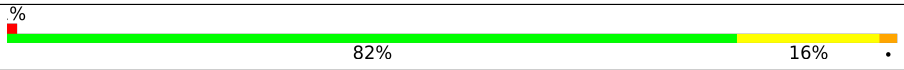
Mol	Chain	Length	Quality of chain
2	L	154	
3	G	144	
3	M	144	
4	H	279	
4	N	279	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13894 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	198	Total	C	N	O	S	0	1	0
			1548	980	267	295	6			
1	I	198	Total	C	N	O	S	1	1	0
			1548	980	267	295	6			

- Molecule 2 is a protein called FimF protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	154	Total	C	N	O	S	0	0	0
			1135	711	196	224	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
			1134	711	196	223	4			
2	L	154	Total	C	N	O	S	0	1	0
			1142	715	198	225	4			

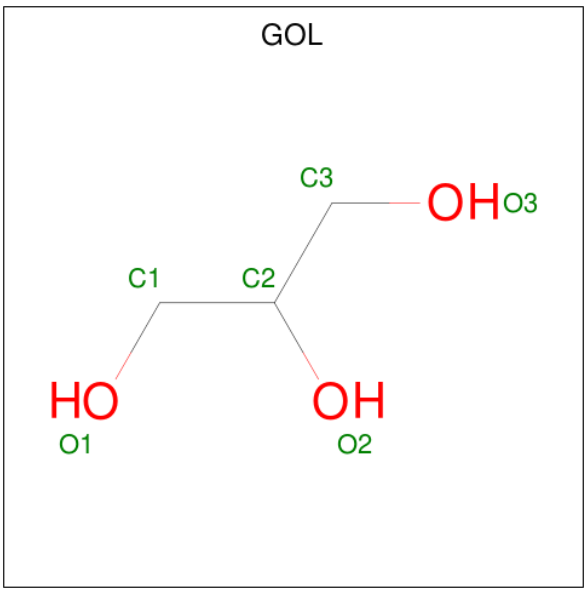
- Molecule 3 is a protein called FimG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	144	Total	C	N	O	S	0	1	0
			1048	643	177	225	3			
3	M	144	Total	C	N	O	S	0	3	0
			1056	651	178	224	3			

- Molecule 4 is a protein called FimH,F1C putative fimbrial adhesin fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	279	Total	C	N	O	S	0	1	0
			2050	1290	345	411	4			
4	N	279	Total	C	N	O	S	0	1	0
			2050	1290	344	412	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 6 3 3	0	0
5	N	1	Total C O 6 3 3	0	0

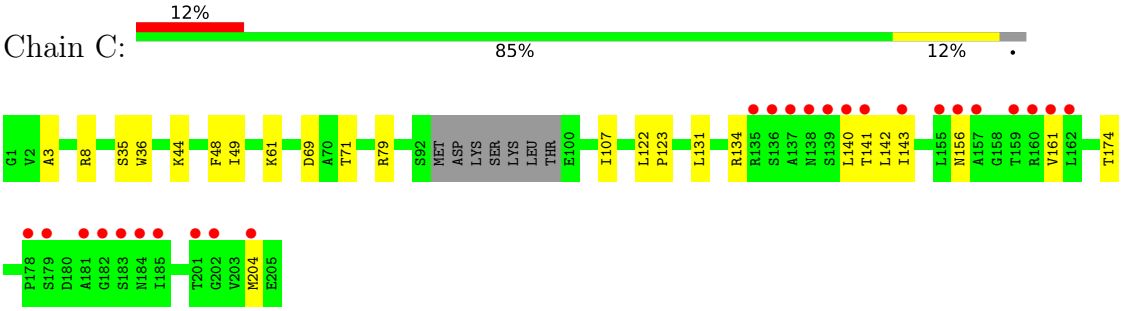
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	3	Total O 3 3	0	0
6	E	3	Total O 3 3	0	0
6	H	8	Total O 8 8	0	0
6	I	1	Total O 1 1	0	0
6	K	1	Total O 1 1	0	0
6	M	1	Total O 1 1	0	0
6	N	18	Total O 18 18	0	0

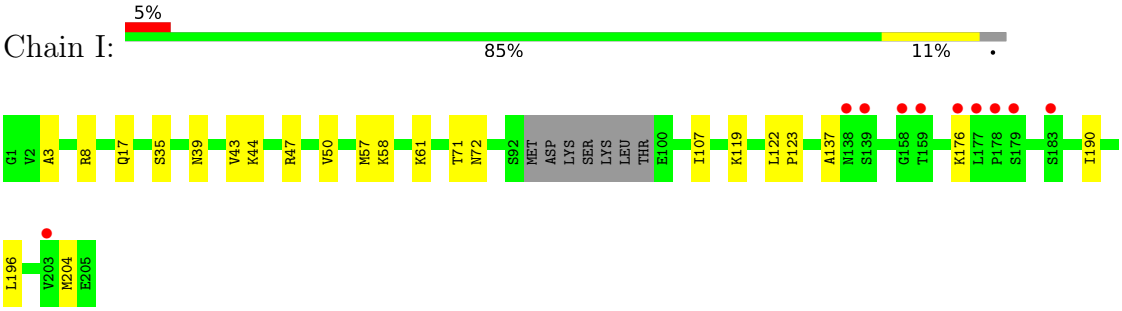
3 Residue-property plots (i)

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.

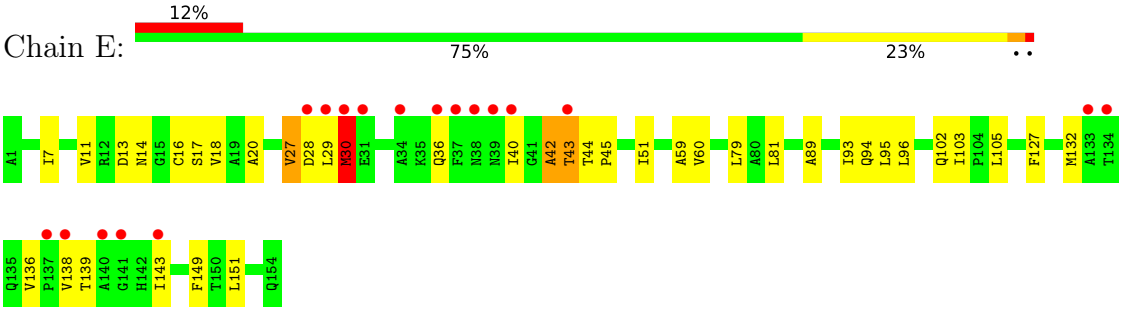
• Molecule 1: Chaperone protein FimC



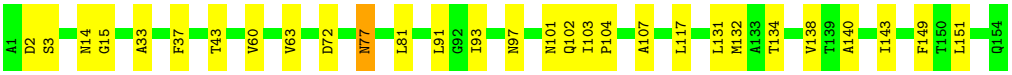
• Molecule 1: Chaperone protein FimC



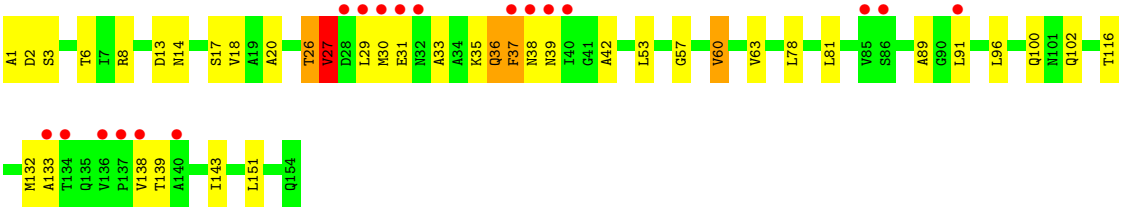
• Molecule 2: FimF protein



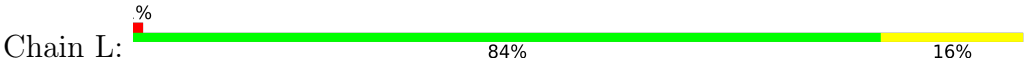
• Molecule 2: FimF protein

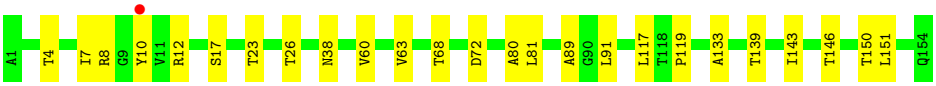


• Molecule 2: FimF protein

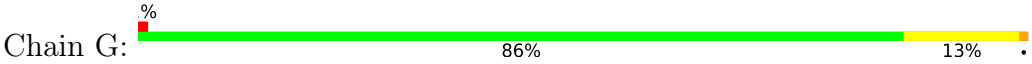


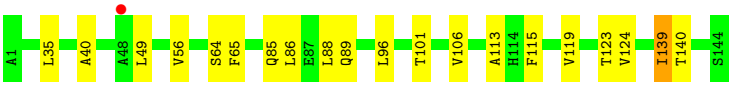
• Molecule 2: FimF protein



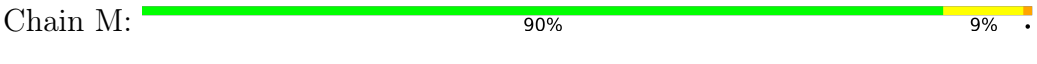


• Molecule 3: FimG

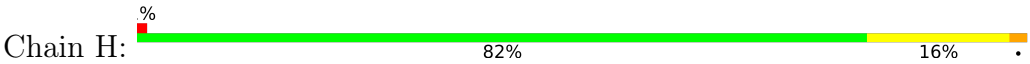


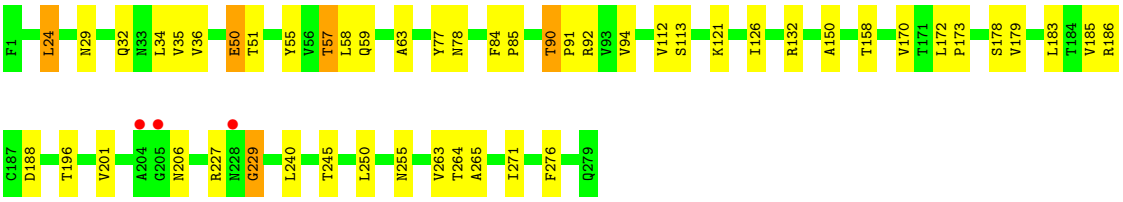


• Molecule 3: FimG

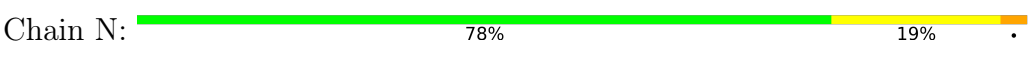


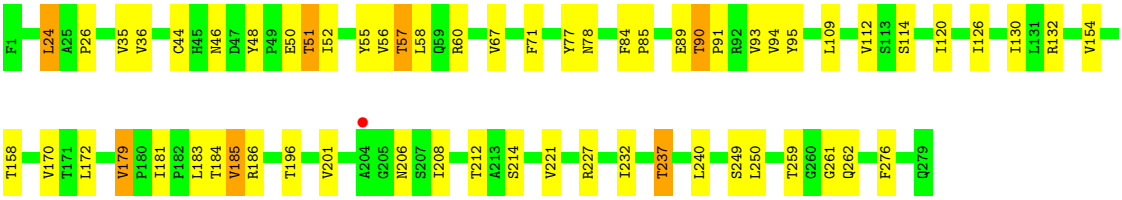
• Molecule 4: FimH,F1C putative fimbrial adhesin fusion





• Molecule 4: FimH,F1C putative fimbrial adhesin fusion




F1
L24
A25
P26
V35
V36
C44
H45
N46
D47
Y48
P49
E50
T51
I52
Y55
V56
T57
L58
Q59
R60
V67
F71
Y77
N78
F84
P85
E89
T90
P91
R92
V93
V94
Y95
L109
V112
S113
S114
I120
I126
I130
L131
R132
V154
T158
V170
T171
L172
V179
P180
I181
P182
L183
T184
V185
R186
T196
V201
A204
G205
N206
S207
I208
T212
A213
S214
V221
R227
I232
T237
L240
S249
L250
T259
G260
G261
Q262
F276
Q279

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	214.78Å 214.78Å 532.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	176.78 – 2.80 46.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (176.78-2.80) 94.4 (46.42-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0047	Depositor
R, R_{free}	0.245 , 0.274 0.246 , 0.276	Depositor DCC
R_{free} test set	5492 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	58.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.009 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 0.003 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	0.91	EDS
Total number of atoms	13894	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	C	0.33	0/1579	0.52	0/2146
1	I	0.48	1/1579 (0.1%)	0.74	1/2146 (0.0%)
2	E	0.35	0/1155	0.50	0/1581
2	F	0.31	0/1156	0.50	0/1583
2	K	0.34	0/1154	0.50	0/1579
2	L	0.31	0/1167	0.50	0/1598
3	G	0.30	0/1066	0.45	0/1457
3	M	0.29	0/1080	0.47	0/1476
4	H	0.33	0/2097	0.52	0/2882
4	N	0.33	0/2097	0.52	0/2882
All	All	0.34	1/14130 (0.0%)	0.53	1/19330 (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	-14.04	1.14	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	58	LYS	CD-CE-NZ	25.56	170.50	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1548	0	1582	11	0
1	I	1548	0	1582	11	0
2	E	1135	0	1126	34	0
2	F	1136	0	1124	25	0
2	K	1134	0	1126	25	0
2	L	1142	0	1129	19	0
3	G	1048	0	1013	14	0
3	M	1056	0	1013	14	0
4	H	2050	0	2004	35	0
4	N	2050	0	2002	39	0
5	N	12	0	16	0	0
6	C	3	0	0	0	0
6	E	3	0	0	0	0
6	H	8	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
6	M	1	0	0	0	0
6	N	18	0	0	1	0
All	All	13894	0	13717	204	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 (204) 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)
2:F:63:VAL:HG23	2:F:117:LEU:HD11	1.47	0.96
1:C:107:ILE:HD11	2:E:20:ALA:HB2	1.48	0.94
2:F:63:VAL:CG2	2:F:117:LEU:HD11	2.01	0.91
4:H:50:GLU:OE1	4:H:51:THR:HG23	1.78	0.84
2:L:63:VAL:CG2	2:L:117:LEU:HD11	2.08	0.83
4:N:90:THR:HG23	4:N:91:PRO:O	1.80	0.82
4:N:57:THR:HG21	4:N:89:GLU:OE2	1.81	0.81
4:H:240:LEU:HD11	4:H:250:LEU:HD22	1.62	0.81
3:M:49:LEU:HD13	3:M:139:ILE:HD13	1.69	0.75
4:N:57:THR:HG22	4:N:132:ARG:HB3	1.67	0.74
4:H:57:THR:HG22	4:H:132:ARG:HB3	1.70	0.74
4:N:240:LEU:HD11	4:N:250:LEU:HD22	1.69	0.74
1:I:47:ARG:HB3	1:I:71:THR:HG22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:24:LEU:HD21	4:H:126:ILE:CD1	2.20	0.72
4:N:50[B]:GLU:OE2	4:N:51:THR:HG22	1.89	0.72
4:N:172:LEU:HD23	4:N:179:VAL:HG22	1.71	0.72
4:H:113:SER:OG	4:H:158:THR:HG22	1.90	0.71
4:H:90:THR:HG23	4:H:91:PRO:O	1.90	0.71
2:K:81:LEU:HD21	2:K:143:ILE:HG23	1.73	0.69
4:H:201:VAL:HG11	4:H:206:ASN:HA	1.75	0.69
1:I:3:ALA:HB2	2:K:17:SER:HA	1.75	0.67
2:L:63:VAL:HG21	2:L:117:LEU:HD11	1.75	0.67
4:H:58:LEU:H	4:H:90:THR:HG22	1.61	0.66
2:F:14:ASN:C	2:F:60:VAL:HG12	2.15	0.66
2:F:63:VAL:HG23	2:F:117:LEU:CD1	2.25	0.65
4:N:196:THR:HG22	4:N:237:THR:HA	1.79	0.65
1:I:107:ILE:HD11	2:K:20:ALA:HB2	1.79	0.64
4:H:185:VAL:HG23	4:H:250:LEU:HD21	1.79	0.63
4:H:126:ILE:HD11	4:H:150:ALA:HB2	1.78	0.63
2:E:7:ILE:HG21	2:F:93:ILE:HD13	1.79	0.63
4:H:24:LEU:HD21	4:H:126:ILE:HD13	1.80	0.63
4:H:112:VAL:HG22	4:H:158:THR:HG23	1.81	0.63
4:H:172:LEU:HD23	4:H:179:VAL:HG22	1.81	0.63
4:H:185:VAL:HG21	4:H:276:PHE:CE2	2.35	0.62
4:N:58:LEU:H	4:N:90:THR:HG22	1.64	0.62
4:N:158:THR:O	4:N:158:THR:HG22	1.99	0.62
2:L:81:LEU:HD22	2:L:143:ILE:HG23	1.82	0.62
2:E:89:ALA:O	2:E:138:VAL:HG13	2.00	0.62
3:M:49:LEU:CD1	3:M:139:ILE:HD13	2.32	0.60
2:E:81:LEU:HD23	2:E:93:ILE:HG13	1.84	0.59
2:F:15:GLY:N	2:F:60:VAL:HG12	2.17	0.59
3:G:65:PHE:CE2	3:G:96:LEU:HD13	2.38	0.59
4:H:24:LEU:HD21	4:H:126:ILE:HD11	1.84	0.59
4:N:24:LEU:HD13	4:N:126:ILE:HD13	1.84	0.59
2:F:81:LEU:HD22	2:F:143:ILE:HG23	1.83	0.59
4:N:48:TYR:HB3	4:N:51:THR:HG23	1.84	0.59
4:N:48:TYR:HB3	4:N:51:THR:CG2	2.34	0.57
2:E:51:ILE:HD13	2:E:149:PHE:CE1	2.40	0.57
1:C:122:LEU:HD12	1:C:123:PRO:HD2	1.86	0.57
2:F:72:ASP:OD2	2:F:134:THR:HG21	2.04	0.57
1:I:190:ILE:HD13	1:I:196:LEU:HD23	1.86	0.57
2:L:63:VAL:HG23	2:L:117:LEU:HD11	1.85	0.57
2:K:96:LEU:HD23	2:K:102:GLN:HA	1.86	0.56
2:E:11:VAL:HG23	2:F:143:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:60:VAL:HG22	2:L:119:PRO:HA	1.87	0.56
2:K:27:VAL:HG22	2:K:31:GLU:HB2	1.87	0.55
4:N:57:THR:CG2	4:N:132:ARG:HB3	2.34	0.55
2:F:3:SER:HB3	3:G:139:ILE:HG23	1.89	0.54
3:M:139:ILE:HD11	3:M:141:TYR:CZ	2.42	0.54
3:G:64:SER:HA	3:G:101:THR:HG22	1.89	0.54
3:G:88:LEU:HD13	3:G:119:VAL:HG22	1.90	0.54
1:C:36:TRP:CD1	1:C:44:LYS:HD3	2.43	0.54
2:E:96:LEU:HD23	2:E:102:GLN:HA	1.90	0.53
2:F:104:PRO:HB2	2:F:107:ALA:HB2	1.90	0.53
3:G:139:ILE:C	3:G:139:ILE:HD13	2.29	0.53
2:F:37:PHE:CD1	2:F:138:VAL:HG21	2.43	0.53
1:I:107:ILE:HG21	2:K:18:VAL:HG11	1.89	0.53
2:E:13:ASP:HB3	2:E:59:ALA:HB2	1.91	0.53
2:E:36:GLN:HG3	2:E:136:VAL:HG11	1.91	0.53
2:F:77:ASN:N	2:F:77:ASN:HD22	2.07	0.53
1:C:3:ALA:HB2	2:E:17:SER:HA	1.91	0.53
2:K:60:VAL:HG23	2:K:60:VAL:O	2.09	0.53
3:M:49:LEU:HD13	3:M:139:ILE:CD1	2.39	0.52
2:L:63:VAL:HG23	2:L:117:LEU:CD1	2.40	0.52
2:E:44:THR:CG2	2:E:45:PRO:HD2	2.40	0.52
4:N:227:ARG:HB3	4:N:232:ILE:HD11	1.90	0.52
2:K:36:GLN:O	2:K:38:ASN:N	2.42	0.52
2:E:27:VAL:HG12	2:E:28:ASP:N	2.25	0.52
1:I:107:ILE:HD11	2:K:20:ALA:CB	2.39	0.51
3:G:56:VAL:CG1	4:H:263:VAL:HG21	2.39	0.51
4:N:26:PRO:CD	4:N:154:VAL:HG21	2.41	0.51
2:E:27:VAL:HG13	2:E:30:MET:HB2	1.91	0.51
1:I:3:ALA:HB2	2:K:17:SER:CA	2.38	0.51
2:K:35:LYS:O	2:K:37:PHE:N	2.44	0.51
4:H:185:VAL:CG2	4:H:250:LEU:HD21	2.41	0.51
2:L:63:VAL:CG2	2:L:117:LEU:CD1	2.85	0.51
4:H:77:TYR:CZ	4:H:90:THR:HG21	2.47	0.50
3:G:85:GLN:OE1	3:G:124:VAL:HG23	2.12	0.50
1:I:122:LEU:HD12	1:I:123:PRO:HD2	1.93	0.50
2:K:1:ALA:HB3	2:L:150:THR:HG22	1.93	0.50
4:H:173:PRO:HD3	4:H:179:VAL:HG13	1.94	0.50
2:K:3:SER:HB3	2:L:23:THR:O	2.11	0.50
2:K:89:ALA:HB3	2:K:139:THR:OG1	2.11	0.50
2:L:7:ILE:CD1	3:M:119:VAL:HG11	2.42	0.50
4:N:35:VAL:HG12	4:N:36:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:91:LEU:HD23	2:L:133:ALA:HA	1.92	0.50
2:L:7:ILE:HD13	3:M:119:VAL:HG11	1.93	0.49
2:F:43:THR:CG2	2:F:132:MET:HE2	2.43	0.49
3:G:86:LEU:N	3:G:86:LEU:HD22	2.27	0.49
4:H:24:LEU:N	4:H:24:LEU:HD12	2.27	0.49
2:E:11:VAL:O	2:F:140:ALA:HB1	2.13	0.49
2:K:30:MET:HE3	2:K:33:ALA:HB3	1.95	0.49
4:H:77:TYR:CE2	4:H:90:THR:HG21	2.47	0.49
4:N:158:THR:O	4:N:158:THR:CG2	2.60	0.49
4:N:179:VAL:HG13	6:N:5108:HOH:O	2.13	0.49
2:K:8:ARG:HD3	2:L:26:THR:HG21	1.95	0.49
4:N:184:THR:HG22	4:N:249:SER:HA	1.94	0.48
2:K:6:THR:HG23	2:L:146:THR:HG22	1.95	0.48
2:K:30:MET:HE3	2:K:30:MET:O	2.13	0.48
4:H:63:ALA:HB2	4:H:85:PRO:HB3	1.95	0.48
3:M:49:LEU:HB2	3:M:115:PHE:HB2	1.96	0.48
3:M:123:THR:HG23	3:M:123:THR:O	2.13	0.48
2:E:51:ILE:HD13	2:E:149:PHE:CD1	2.49	0.48
4:N:201:VAL:HG21	4:N:206:ASN:OD1	2.14	0.47
2:E:7:ILE:HD13	2:F:93:ILE:HG21	1.96	0.47
4:N:55:TYR:CD2	4:N:94:VAL:HG12	2.49	0.47
2:E:44:THR:HG23	2:E:45:PRO:HD2	1.96	0.47
4:N:185:VAL:HG21	4:N:276:PHE:CE2	2.49	0.47
4:H:24:LEU:HD11	4:H:150:ALA:CB	2.45	0.47
4:N:84:PHE:HA	4:N:85:PRO:C	2.36	0.47
1:C:69:ASP:OD1	1:C:71:THR:HG23	2.15	0.47
2:L:10:TYR:CE1	3:M:132:THR:HG22	2.49	0.47
2:F:97:ASN:HD21	2:F:101:ASN:HB2	1.79	0.47
2:F:131:LEU:HD21	2:F:143:ILE:HD13	1.97	0.46
2:K:30:MET:CE	2:K:33:ALA:HB3	2.46	0.46
4:N:26:PRO:HD2	4:N:154:VAL:HG21	1.96	0.46
4:N:77:TYR:CE2	4:N:90:THR:HG21	2.50	0.46
4:H:264:THR:HG22	4:H:265:ALA:O	2.16	0.46
2:E:51:ILE:HD12	2:E:127:PHE:CE2	2.50	0.46
3:G:123:THR:O	3:G:123:THR:HG23	2.15	0.46
3:G:139:ILE:HD13	3:G:140:THR:N	2.31	0.46
4:N:58:LEU:H	4:N:90:THR:CG2	2.28	0.46
4:N:58:LEU:HD12	4:N:130:ILE:O	2.16	0.45
2:E:14:ASN:ND2	2:F:33:ALA:HB2	2.31	0.45
2:E:79:LEU:HD12	2:E:105:LEU:HD21	1.97	0.45
3:G:106:VAL:HA	3:G:113:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:THR:OG1	1:C:174:THR:HG22	2.16	0.45
4:N:55:TYR:CE2	4:N:94:VAL:HG12	2.52	0.45
4:N:78:ASN:ND2	4:N:93:VAL:HG22	2.31	0.45
1:C:131:LEU:HD12	1:C:143:ILE:O	2.16	0.45
2:E:138:VAL:HG12	2:E:139:THR:N	2.32	0.45
4:H:271:ILE:N	4:H:271:ILE:HD12	2.32	0.45
3:M:5:ILE:HG21	4:N:181:ILE:HD13	1.99	0.45
3:M:86:LEU:N	3:M:86:LEU:HD22	2.32	0.45
2:E:51:ILE:HD13	2:E:149:PHE:CZ	2.52	0.44
2:K:91:LEU:HD23	2:K:133:ALA:HA	1.99	0.44
4:N:71:PHE:CD2	4:N:109:LEU:HD11	2.53	0.44
4:H:55:TYR:CE2	4:H:94:VAL:HG12	2.52	0.44
1:C:156:ASN:OD1	1:C:161:VAL:HG22	2.17	0.44
2:L:89:ALA:HB3	2:L:139:THR:OG1	2.17	0.44
2:E:81:LEU:HD22	2:E:143:ILE:HG23	2.00	0.44
2:F:97:ASN:HB3	2:F:103:ILE:HD11	2.00	0.44
1:I:35:SER:HB2	1:I:50:VAL:HG11	1.99	0.44
3:M:139:ILE:HD11	3:M:141:TYR:CE1	2.53	0.43
4:H:58:LEU:H	4:H:90:THR:CG2	2.30	0.43
4:N:24:LEU:HB3	4:N:36:VAL:HG13	1.99	0.43
4:N:112:VAL:HG22	4:N:158:THR:HG23	1.99	0.43
4:H:113:SER:CB	4:H:158:THR:HG22	2.48	0.43
2:E:43:THR:HG23	2:E:43:THR:O	2.19	0.43
4:H:178:SER:HB3	4:H:255:ASN:ND2	2.33	0.43
2:K:26:THR:HG23	2:K:27:VAL:H	1.83	0.43
2:K:91:LEU:HD11	2:K:138:VAL:HG11	1.99	0.43
2:E:51:ILE:HD12	2:E:127:PHE:HE2	1.81	0.43
2:E:95:LEU:HB3	2:E:103:ILE:HD12	1.99	0.43
2:F:149:PHE:CE2	2:F:151:LEU:HD11	2.54	0.43
2:F:81:LEU:CD2	2:F:143:ILE:HG23	2.47	0.43
3:G:35:LEU:HD23	3:G:40:ALA:HB1	2.01	0.43
2:K:57:GLY:O	2:K:60:VAL:HG22	2.18	0.43
3:M:88:LEU:HD13	3:M:119:VAL:HG22	2.01	0.43
2:E:27:VAL:HG13	2:E:30:MET:H	1.84	0.43
3:G:49:LEU:HB2	3:G:115:PHE:HB2	2.01	0.42
2:L:81:LEU:CD2	2:L:143:ILE:HG23	2.47	0.42
2:K:42:ALA:HB2	2:K:132:MET:CB	2.50	0.42
2:E:16:CYS:SG	2:E:60:VAL:HG21	2.60	0.42
2:F:37:PHE:CZ	2:F:91:LEU:HD21	2.55	0.42
2:L:72:ASP:HA	2:L:80:ALA:HB2	2.01	0.42
4:N:46:ASN:ND2	4:N:52:ILE:O	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:84:PHE:HA	4:H:85:PRO:C	2.39	0.42
1:I:39:ASN:HD21	1:I:43:VAL:HB	1.85	0.42
4:N:67:VAL:CG2	4:N:120:ILE:HD13	2.50	0.42
1:C:142:LEU:HD12	1:C:142:LEU:N	2.35	0.41
2:E:11:VAL:HG21	2:F:91:LEU:CD1	2.50	0.41
4:H:77:TYR:CE2	4:H:90:THR:CG2	3.03	0.41
4:N:208:ILE:HG21	4:N:259:THR:HG22	2.02	0.41
2:E:42:ALA:HB2	2:E:132:MET:HE2	2.03	0.41
4:H:227:ARG:O	4:H:229:GLY:N	2.52	0.41
1:I:57:MET:HE1	1:I:61:LYS:O	2.21	0.41
2:F:91:LEU:HD22	2:F:131:LEU:HB3	2.02	0.41
2:E:18:VAL:HG21	2:E:151:LEU:CD1	2.51	0.41
2:E:94:GLN:HE21	2:E:102:GLN:HG3	1.86	0.41
2:L:151:LEU:HD12	2:L:151:LEU:N	2.36	0.41
1:C:48:PHE:O	1:C:49:ILE:HD13	2.21	0.41
1:C:134:ARG:O	1:C:140:LEU:HD12	2.21	0.41
2:E:40:ILE:HG23	2:E:40:ILE:O	2.20	0.41
2:K:63:VAL:HG11	2:K:151:LEU:HD21	2.03	0.41
4:N:44:CYS:HB2	4:N:95:TYR:CE2	2.56	0.41
4:N:112:VAL:HG22	4:N:158:THR:CG2	2.50	0.41
3:M:41:ALA:HB2	3:M:122:LEU:HB2	2.04	0.40
4:N:170:VAL:CG1	4:N:179:VAL:HG21	2.51	0.40
2:E:138:VAL:HG12	2:E:139:THR:H	1.87	0.40
3:G:88:LEU:HD12	3:G:89:GLN:N	2.37	0.40
4:H:29:ASN:HB2	4:H:32:GLN:O	2.20	0.40
4:H:35:VAL:HG12	4:H:36:VAL:HG23	2.04	0.40
4:H:55:TYR:CD2	4:H:94:VAL:HG12	2.56	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	195/205 (95%)	187 (96%)	8 (4%)	0	100 100
1	I	195/205 (95%)	188 (96%)	6 (3%)	1 (0%)	29 61
2	E	152/154 (99%)	131 (86%)	17 (11%)	4 (3%)	5 18
2	F	152/154 (99%)	150 (99%)	2 (1%)	0	100 100
2	K	152/154 (99%)	138 (91%)	8 (5%)	6 (4%)	3 10
2	L	153/154 (99%)	148 (97%)	5 (3%)	0	100 100
3	G	143/144 (99%)	140 (98%)	3 (2%)	0	100 100
3	M	144/144 (100%)	138 (96%)	6 (4%)	0	100 100
4	H	278/279 (100%)	270 (97%)	7 (2%)	1 (0%)	34 66
4	N	278/279 (100%)	263 (95%)	14 (5%)	1 (0%)	34 66
All	All	1842/1872 (98%)	1753 (95%)	76 (4%)	13 (1%)	22 53

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	27	VAL
2	E	43	THR
2	K	29	LEU
2	K	36	GLN
2	K	37	PHE
2	E	42	ALA
2	K	2	ASP
1	I	137	ALA
2	E	30	MET
4	H	229	GLY
4	N	261	GLY
2	K	60	VAL
2	K	27	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	C	170/176 (97%)	165 (97%)	5 (3%)	42 76
1	I	170/176 (97%)	163 (96%)	7 (4%)	30 64
2	E	123/123 (100%)	121 (98%)	2 (2%)	62 88
2	F	123/123 (100%)	120 (98%)	3 (2%)	49 81
2	K	123/123 (100%)	114 (93%)	9 (7%)	14 38
2	L	124/123 (101%)	118 (95%)	6 (5%)	25 58
3	G	116/115 (101%)	115 (99%)	1 (1%)	78 94
3	M	117/115 (102%)	114 (97%)	3 (3%)	46 79
4	H	228/227 (100%)	212 (93%)	16 (7%)	15 40
4	N	228/227 (100%)	212 (93%)	16 (7%)	15 40
All	All	1522/1528 (100%)	1454 (96%)	68 (4%)	28 60

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	ARG
1	C	35	SER
1	C	61	LYS
1	C	79	ARG
1	C	204	MET
2	E	29	LEU
2	E	30	MET
2	F	2	ASP
2	F	77	ASN
2	F	102	GLN
3	G	139	ILE
4	H	24	LEU
4	H	34	LEU
4	H	50	GLU
4	H	57	THR
4	H	59[A]	GLN
4	H	59[B]	GLN
4	H	78	ASN
4	H	90	THR
4	H	92	ARG
4	H	121	LYS
4	H	170	VAL
4	H	183	LEU
4	H	186	ARG

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Mol	Chain	Res	Type
4	H	188	ASP
4	H	196	THR
4	H	245	THR
1	I	8	ARG
1	I	17	GLN
1	I	44	LYS
1	I	72	ASN
1	I	119	LYS
1	I	176	LYS
1	I	204	MET
2	K	13	ASP
2	K	14	ASN
2	K	26	THR
2	K	27	VAL
2	K	39	ASN
2	K	53	LEU
2	K	78	LEU
2	K	100	GLN
2	K	116	THR
2	L	4	THR
2	L	8	ARG
2	L	12	ARG
2	L	17	SER
2	L	38	ASN
2	L	68	THR
3	M	82	GLN
3	M	134	GLN
3	M	139	ILE
4	N	24	LEU
4	N	51	THR
4	N	56	VAL
4	N	57	THR
4	N	60	ARG
4	N	90	THR
4	N	114	SER
4	N	179	VAL
4	N	183	LEU
4	N	185	VAL
4	N	186	ARG
4	N	212	THR
4	N	214	SER
4	N	221	VAL

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Mol	Chain	Res	Type
4	N	237	THR
4	N	262	GLN

Sometimes 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	E	94	GLN
2	F	135	GLN
4	N	32	GLN
4	N	235	ASN
4	N	262	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	5001	-	5,5,5	0.37	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	N	5002	-	5,5,5	0.42	0	5,5,5	0.17	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	5001	-	-	2/4/4/4	-
5	GOL	N	5002	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	5002	GOL	O1-C1-C2-C3
5	N	5001	GOL	O1-C1-C2-C3
5	N	5002	GOL	C1-C2-C3-O3
5	N	5002	GOL	O1-C1-C2-O2
5	N	5002	GOL	O2-C2-C3-O3
5	N	5001	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	C	198/205 (96%)	0.54	25 (12%) 3 2	34, 55, 92, 97	0
1	I	198/205 (96%)	0.27	10 (5%) 28 19	39, 57, 83, 88	1 (0%)
2	E	154/154 (100%)	0.51	18 (11%) 4 2	47, 66, 102, 104	0
2	F	154/154 (100%)	0.21	0 100 100	49, 63, 72, 76	2 (1%)
2	K	154/154 (100%)	0.65	18 (11%) 4 2	51, 69, 99, 102	0
2	L	154/154 (100%)	0.04	1 (0%) 89 86	42, 53, 66, 69	3 (1%)
3	G	144/144 (100%)	0.22	1 (0%) 87 84	50, 68, 76, 77	2 (1%)
3	M	144/144 (100%)	-0.07	0 100 100	41, 59, 67, 70	1 (0%)
4	H	279/279 (100%)	-0.05	3 (1%) 80 75	25, 39, 67, 74	1 (0%)
4	N	279/279 (100%)	-0.18	1 (0%) 92 91	28, 40, 58, 65	0
All	All	1858/1872 (99%)	0.18	77 (4%) 37 27	25, 58, 83, 104	10 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	32	ASN	6.3
2	E	39	ASN	5.6
2	K	39	ASN	5.4
2	K	40	ILE	5.1
1	C	181	ALA	4.8
1	C	178	PRO	4.6
2	E	30	MET	4.6
2	E	40	ILE	4.4
1	C	159	THR	4.1
1	C	184	ASN	3.8
1	C	138	ASN	3.8
2	E	37	PHE	3.6
2	K	28	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	K	38	ASN	3.5
1	C	160	ARG	3.5
2	E	29	LEU	3.3
2	K	31	GLU	3.3
2	K	136	VAL	3.3
4	H	228	ASN	3.1
1	C	179	SER	3.0
1	C	143	ILE	3.0
1	C	139	SER	3.0
1	I	158	GLY	3.0
1	I	178	PRO	2.9
2	K	138	VAL	2.9
1	C	204	MET	2.9
1	C	157	ALA	2.8
4	N	204	ALA	2.8
2	L	10	TYR	2.8
1	C	182	GLY	2.8
1	C	156	ASN	2.7
1	C	161	VAL	2.7
2	K	85	VAL	2.7
2	K	91	LEU	2.7
2	K	137	PRO	2.7
2	K	140	ALA	2.7
2	E	137	PRO	2.6
1	C	183	SER	2.6
1	C	155	LEU	2.6
2	E	38	ASN	2.6
1	I	138	ASN	2.6
1	C	201	THR	2.6
1	C	135	ARG	2.5
3	G	48	ALA	2.5
1	C	185	ILE	2.5
1	I	179	SER	2.5
4	H	205	GLY	2.5
2	K	30	MET	2.4
1	C	136	SER	2.4
2	E	143	ILE	2.4
2	E	28	ASP	2.4
1	I	176	LYS	2.4
1	I	159	THR	2.4
4	H	204	ALA	2.4
1	C	140	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	134	THR	2.3
2	K	86	SER	2.3
1	C	137	ALA	2.3
2	K	29	LEU	2.3
2	E	31	GLU	2.3
1	I	203	VAL	2.2
1	C	162	LEU	2.2
2	K	37	PHE	2.2
1	I	183	SER	2.2
1	C	141	THR	2.2
2	E	36	GLN	2.2
1	I	139	SER	2.1
2	E	138	VAL	2.1
1	I	177	LEU	2.1
2	E	133	ALA	2.1
2	E	43	THR	2.1
2	E	134	THR	2.1
2	E	34	ALA	2.1
2	E	140	ALA	2.1
2	E	141	GLY	2.0
1	C	202	GLY	2.0
2	K	133	ALA	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	N	5001	6/6	0.89	0.28	47,47,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	N	5002	6/6	0.91	0.32	50,51,52,53	0

6.5 Other polymers (i)

There are no such residues in this entry.