



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:05 PM UTC

PDB ID : 7SZO / pdb_00007szo
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

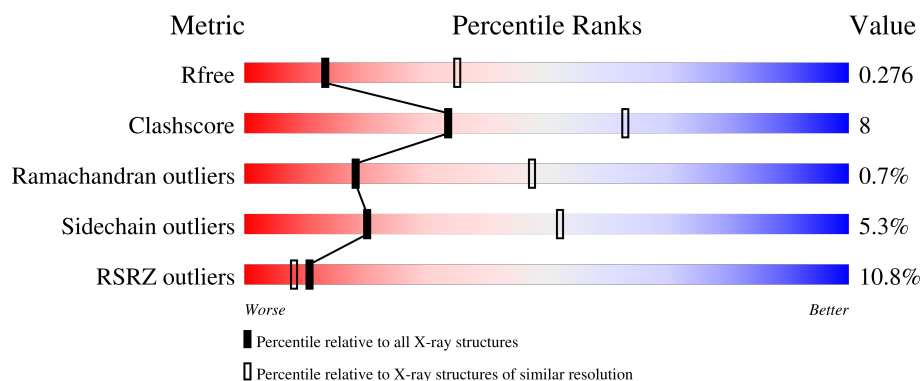
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



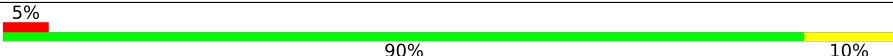
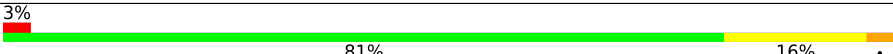
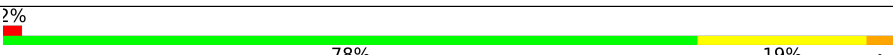
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	17% 83% 13% .
1	I	205	9% 84% 12% ..
2	E	154	34% 75% 23% ..
2	F	154	10% 80% 19% .
2	K	154	24% 74% 23% ..

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Mol	Chain	Length	Quality of chain
2	L	154	 6%82%18%
3	G	144	 7%85%14%.
3	M	144	 5%90%10%.
4	H	279	 3%81%16%.
4	N	279	 2%78%19%.

2 Entry composition

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			

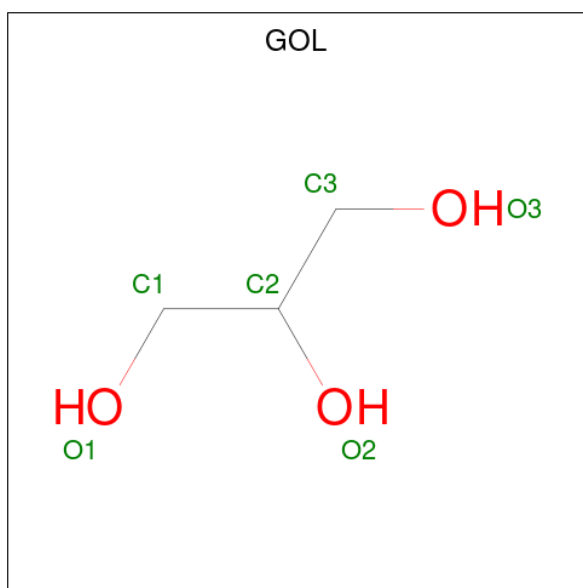
- Molecule 3 is a protein called FimG.

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 (CCD ID: 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		

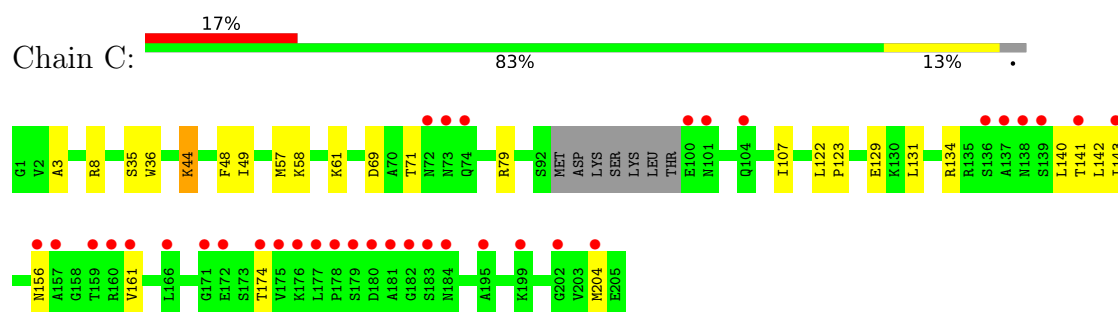
- Molecule 6 is water.

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

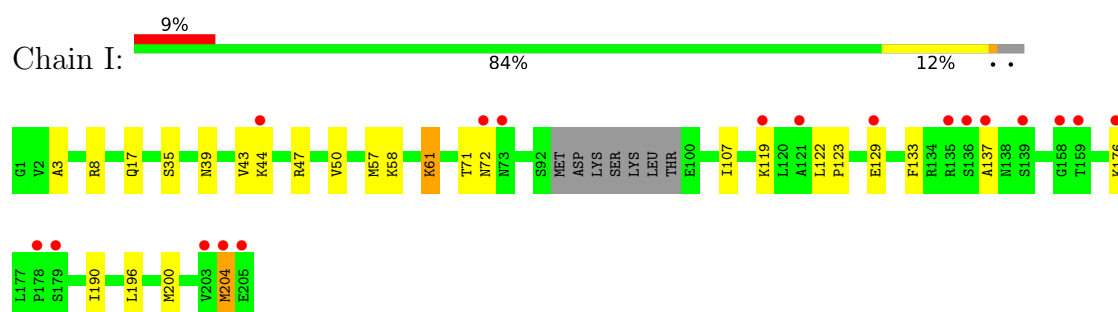
3 Residue-property plots [i](#)

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.

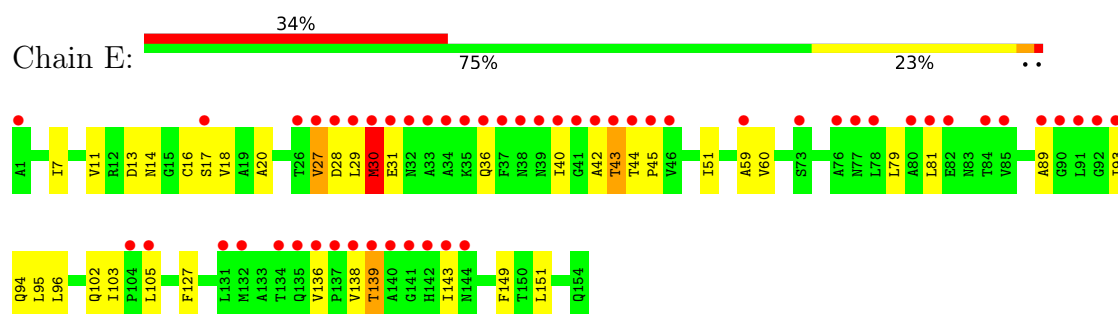
- Molecule 1: Chaperone protein FimC



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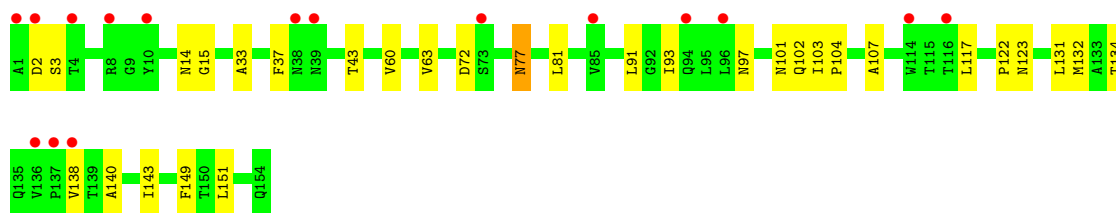


- Molecule 2: FimF protein

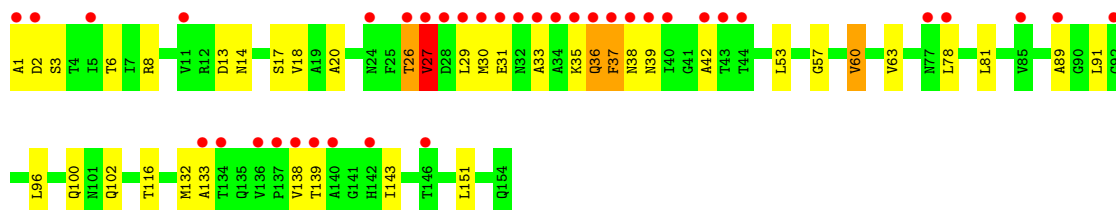
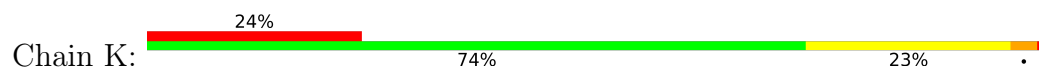


- Molecule 2: FimF protein

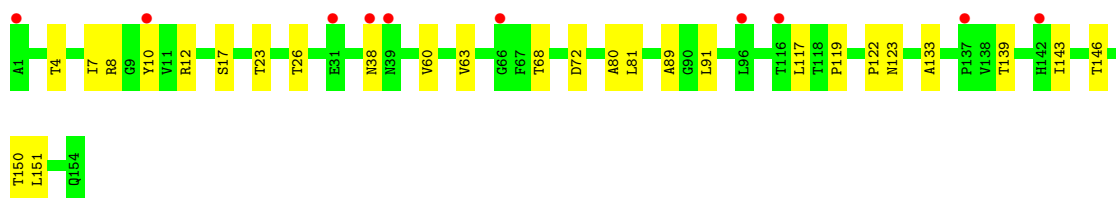
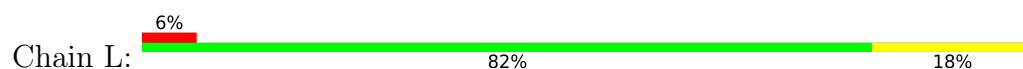




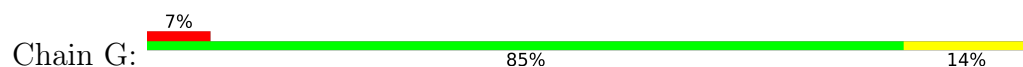
• Molecule 2: FimF protein



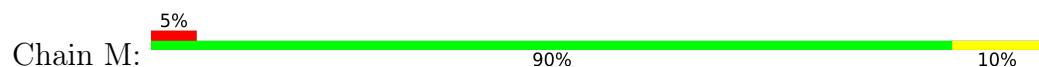
• Molecule 2: FimF protein



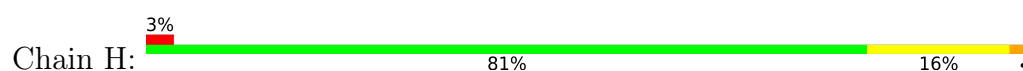
• Molecule 3: FimG

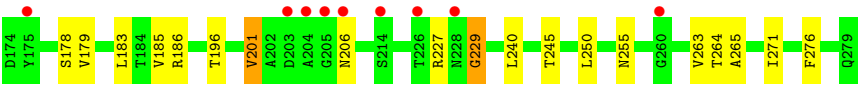


• Molecule 3: FimG

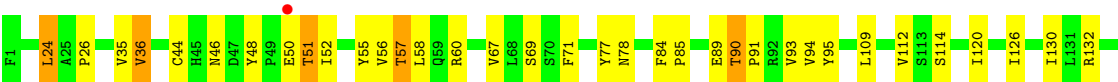
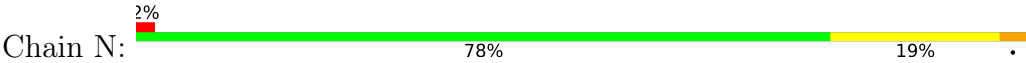


• Molecule 4: FimH,F1C putative fimbrial adhesin fusion





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4 Data and refinement statistics

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 – 2.80 176.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (176.78-2.80) 94.4 (176.78-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.72%)	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 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.45	0/1579	0.64	0/2146
1	I	0.54	1/1579 (0.1%)	0.75	1/2146 (0.0%)
2	E	0.49	0/1155	0.63	0/1581
2	F	0.43	0/1156	0.65	0/1583
2	K	0.49	0/1154	0.64	0/1579
2	L	0.42	0/1167	0.63	0/1598
3	G	0.41	0/1066	0.60	0/1457
3	M	0.41	0/1080	0.60	0/1476
4	H	0.44	0/2097	0.65	1/2882 (0.0%)
4	N	0.43	0/2097	0.65	0/2882
All	All	0.45	1/14130 (0.0%)	0.65	2/19330 (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	-11.80	1.14	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	58	LYS	CD-CE-NZ	18.31	170.50	111.90
4	H	126	ILE	CB-CA-C	-5.33	106.31	111.05

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	12	0
1	I	1548	0	1582	13	0
2	E	1135	0	1126	35	0
2	F	1136	0	1124	26	0
2	K	1134	0	1126	26	0
2	L	1142	0	1129	20	0
3	G	1048	0	1013	14	0
3	M	1056	0	1013	14	0
4	H	2050	0	2004	36	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	212	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (212) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:14:ASN:C	2:F:60:VAL:HG12	2.15	0.70
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:57:MET:HE2	1:I:61:LYS:HB3	1.75	0.68
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: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
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
4:N:158:THR:O	4:N:158:THR:HG22	1.99	0.61
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
3:G:139:ILE:C	3:G:139:ILE:HD13	2.29	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:30:MET:HE3	2:K:30:MET:O	2.08	0.53
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
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
4:N:84:PHE:HA	4:N:85:PRO:C	2.36	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
2:E:30:MET:HE2	2:E:45:PRO:HG3	1.91	0.51
4:H:185:VAL:CG2	4:H:250:LEU:HD21	2.41	0.51
1:I:133:PHE:O	1:I:204:MET:HE3	2.11	0.51
2:L:63:VAL:CG2	2:L:117:LEU:CD1	2.85	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:MET:HE1	1:C:61:LYS:O	2.10	0.50
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
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
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
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
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
1:C:69:ASP:OD1	1:C:71:THR:HG23	2.15	0.47
4:H:84:PHE:HA	4:H:85:PRO:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:I:129:GLU:HG2	1:I:200[B]:MET:HE1	2.00	0.44
2:L:89:ALA:HB3	2:L:139:THR:OG1	2.17	0.44
2:E:30:MET:HE3	2:E:31:GLU:HG2	1.98	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
2:F:122:PRO:C	2:F:123:ASN:HD22	2.25	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:66:GLY:O	4:H:69:SER:OG	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:122:PRO:C	2:L:123:ASN:HD22	2.27	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:K:36:GLN:O	2:K:37:PHE:C	2.63	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
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
4:H:227:ARG:O	4:H:229:GLY:N	2.52	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
2:K:30:MET:HE3	2:K:33:ALA:HB3	2.04	0.40
2:F:43:THR:CG2	2:F:132:MET:HE2	2.51	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	195/205 (95%)	187 (96%)	8 (4%)	0	100	100
1	I	195/205 (95%)	188 (96%)	6 (3%)	1 (0%)	24	55
2	E	152/154 (99%)	131 (86%)	17 (11%)	4 (3%)	4	15
2	F	152/154 (99%)	150 (99%)	2 (1%)	0	100	100
2	K	152/154 (99%)	138 (91%)	8 (5%)	6 (4%)	2	8
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%)	30	60
4	N	278/279 (100%)	263 (95%)	14 (5%)	1 (0%)	30	60
All	All	1842/1872 (98%)	1753 (95%)	76 (4%)	13 (1%)	18	47

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 ⓘ

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%)	163 (96%)	7 (4%)	27	62
1	I	170/176 (97%)	162 (95%)	8 (5%)	23	57
2	E	123/123 (100%)	120 (98%)	3 (2%)	43	77
2	F	123/123 (100%)	120 (98%)	3 (2%)	43	77
2	K	123/123 (100%)	114 (93%)	9 (7%)	13	38
2	L	124/123 (101%)	118 (95%)	6 (5%)	23	56
3	G	116/115 (101%)	114 (98%)	2 (2%)	53	83
3	M	117/115 (102%)	113 (97%)	4 (3%)	32	68
4	H	228/227 (100%)	208 (91%)	20 (9%)	9	29
4	N	228/227 (100%)	209 (92%)	19 (8%)	10	32
All	All	1522/1528 (100%)	1441 (95%)	81 (5%)	20	52

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	ARG
1	C	35	SER
1	C	44	LYS
1	C	58	LYS
1	C	79	ARG
1	C	129	GLU
1	C	204	MET
2	E	29	LEU
2	E	30	MET
2	E	139	THR
2	F	2	ASP
2	F	77	ASN
2	F	102	GLN
3	G	32	SER
3	G	139	ILE
4	H	24	LEU

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Mol	Chain	Res	Type
4	H	34	LEU
4	H	36	VAL
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	99	THR
4	H	109	LEU
4	H	154	VAL
4	H	158	THR
4	H	170	VAL
4	H	183	LEU
4	H	186	ARG
4	H	196	THR
4	H	201	VAL
4	H	245	THR
1	I	8	ARG
1	I	17	GLN
1	I	44	LYS
1	I	61	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

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Mol	Chain	Res	Type
3	M	24	THR
3	M	82	GLN
3	M	134	GLN
3	M	139	ILE
4	N	24	LEU
4	N	36	VAL
4	N	51	THR
4	N	56	VAL
4	N	57	THR
4	N	60	ARG
4	N	69	SER
4	N	90	THR
4	N	114	SER
4	N	179	VAL
4	N	183	LEU
4	N	185	VAL
4	N	191	GLN
4	N	212	THR
4	N	214	SER
4	N	221	VAL
4	N	237	THR
4	N	250	LEU
4	N	262	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	17	GLN
1	C	24	ASN
1	C	73	ASN
1	C	126	GLN
2	E	94	GLN
2	E	135	GLN
2	F	77	ASN
2	F	102	GLN
4	H	32	GLN
4	H	45	HIS
4	H	224	GLN
4	H	267	ASN
1	I	24	ASN
2	K	144	ASN
2	L	135	GLN

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Mol	Chain	Res	Type
3	M	82	GLN
4	N	19	ASN
4	N	235	ASN
4	N	262	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	N	5002	-	5,5,5	0.42	0	5,5,5	0.17	0
5	GOL	N	5001	-	5,5,5	0.37	0	5,5,5	0.50	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	5002	-	-	4/4/4/4	-
5	GOL	N	5001	-	-	2/4/4/4	-

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	198/205 (96%)	0.88	35 (17%) 4 3	34, 55, 92, 97	1 (0%)
1	I	198/205 (96%)	0.68	18 (9%) 15 11	39, 56, 83, 88	2 (1%)
2	E	154/154 (100%)	1.94	53 (34%) 1 1	47, 66, 102, 104	0
2	F	154/154 (100%)	0.93	16 (10%) 11 8	49, 62, 72, 76	2 (1%)
2	K	154/154 (100%)	1.64	37 (24%) 2 1	51, 69, 99, 102	0
2	L	154/154 (100%)	0.52	10 (6%) 25 18	32, 53, 66, 69	4 (2%)
3	G	144/144 (100%)	0.89	10 (6%) 23 16	42, 68, 76, 77	3 (2%)
3	M	144/144 (100%)	0.47	7 (4%) 35 27	36, 58, 67, 70	3 (2%)
4	H	279/279 (100%)	0.22	9 (3%) 50 40	21, 39, 67, 74	2 (0%)
4	N	279/279 (100%)	0.05	6 (2%) 62 52	23, 40, 58, 65	1 (0%)
All	All	1858/1872 (99%)	0.73	201 (10%) 11 8	21, 58, 83, 104	18 (0%)

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	37	PHE	9.5
2	E	40	ILE	9.4
2	K	29	LEU	9.0
2	E	29	LEU	8.2
2	K	40	ILE	7.6
2	E	39	ASN	7.3
3	G	114	HIS	6.7
2	E	43	THR	6.7
2	K	32	ASN	6.6
2	E	33	ALA	6.4
1	C	137	ALA	6.1
2	K	39	ASN	6.1
3	M	33[A]	PHE	5.9

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Mol	Chain	Res	Type	RSRZ
2	E	30	MET	5.8
2	K	30	MET	5.8
2	E	41	GLY	5.5
4	N	204	ALA	5.2
2	K	37	PHE	5.2
2	E	32	ASN	5.1
2	K	31	GLU	5.1
2	K	2	ASP	5.1
2	E	35	LYS	5.0
2	K	33	ALA	4.9
1	C	204	MET	4.9
2	E	44	THR	4.8
2	E	137	PRO	4.8
1	C	178	PRO	4.8
2	K	27	VAL	4.8
2	E	42	ALA	4.8
2	K	28	ASP	4.7
2	K	43	THR	4.6
2	E	131	LEU	4.6
4	H	205	GLY	4.6
2	E	1	ALA	4.6
2	K	38	ASN	4.5
2	E	26	THR	4.4
1	C	159	THR	4.3
1	C	176	LYS	4.2
2	K	26	THR	4.2
2	K	1	ALA	4.1
2	K	85	VAL	4.0
4	N	50[A]	GLU	4.0
1	I	204	MET	4.0
2	E	81	LEU	3.9
2	F	136	VAL	3.9
1	C	136	SER	3.9
1	I	137	ALA	3.9
2	K	44	THR	3.9
2	E	45	PRO	3.8
3	M	114[A]	HIS	3.8
2	K	35	LYS	3.8
2	E	91	LEU	3.7
2	E	27	VAL	3.7
2	K	138	VAL	3.7
4	H	204	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	28	ASP	3.7
2	E	38	ASN	3.7
2	K	34	ALA	3.6
2	F	1	ALA	3.6
2	E	142	HIS	3.6
4	N	260	GLY	3.6
2	E	141	GLY	3.5
1	C	184	ASN	3.5
2	E	80	ALA	3.4
2	L	116	THR	3.4
2	K	137	PRO	3.3
2	K	42	ALA	3.3
2	L	1	ALA	3.3
2	E	85	VAL	3.3
2	E	76	ALA	3.3
2	E	136	VAL	3.3
2	E	84	THR	3.3
2	E	36	GLN	3.2
2	E	135	GLN	3.2
2	F	137	PRO	3.2
2	L	10	TYR	3.1
2	K	133	ALA	3.1
1	C	138	ASN	3.1
3	G	36	MET	3.1
2	K	89	ALA	3.1
1	I	121	ALA	3.0
2	F	138	VAL	3.0
2	K	36	GLN	3.0
2	F	39	ASN	3.0
4	N	206	ASN	3.0
1	C	179	SER	3.0
1	I	179	SER	3.0
2	E	31	GLU	3.0
2	E	134	THR	3.0
4	H	260	GLY	2.9
1	I	136	SER	2.9
4	N	203	ASP	2.9
2	E	140	ALA	2.9
1	C	141	THR	2.9
1	C	143	ILE	2.9
2	E	138	VAL	2.8
1	C	160	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	143	ILE	2.8
2	E	132	MET	2.8
3	G	54	CYS	2.8
1	C	139	SER	2.8
1	I	178	PRO	2.7
1	C	175	VAL	2.7
2	E	34	ALA	2.7
1	C	73	ASN	2.7
1	C	101	ASN	2.7
3	M	22	ASN	2.7
4	H	206	ASN	2.7
1	I	203	VAL	2.7
3	M	139	ILE	2.6
4	H	214	SER	2.7
2	F	2	ASP	2.6
1	C	199	LYS	2.6
2	F	94	GLN	2.6
2	E	90	GLY	2.6
1	C	177	LEU	2.6
2	E	82	GLU	2.6
3	M	52	THR	2.5
1	C	181	ALA	2.5
4	N	205	GLY	2.5
4	H	175	TYR	2.5
2	K	140	ALA	2.5
1	I	176	LYS	2.5
1	C	174	THR	2.5
2	E	139	THR	2.5
2	K	134	THR	2.5
1	I	44	LYS	2.5
2	E	77	ASN	2.5
4	H	228	ASN	2.5
1	C	171	GLY	2.5
2	E	59	ALA	2.5
3	G	105	GLN	2.5
1	I	72	ASN	2.5
2	E	144	ASN	2.5
1	C	183	SER	2.4
3	G	33	PHE	2.4
3	G	134[A]	GLN	2.4
2	E	105	LEU	2.4
1	I	135	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	205	GLU	2.4
2	K	146	THR	2.4
2	K	24	ASN	2.4
1	C	172	GLU	2.4
2	L	38	ASN	2.4
2	K	11	VAL	2.4
1	C	157	ALA	2.4
2	L	39	ASN	2.3
1	C	72	ASN	2.3
3	M	36	MET	2.3
1	I	159	THR	2.3
2	F	116	THR	2.3
1	I	129	GLU	2.3
1	I	139	SER	2.3
2	F	10	TYR	2.3
2	K	136	VAL	2.3
2	F	38	ASN	2.3
2	F	114	TRP	2.3
4	H	226	THR	2.3
1	C	156	ASN	2.2
1	C	195	ALA	2.2
1	I	73	ASN	2.2
2	L	31	GLU	2.2
2	L	96	LEU	2.2
2	F	8	ARG	2.2
2	K	142	HIS	2.2
3	G	32	SER	2.2
3	G	22	ASN	2.2
1	C	74	GLN	2.2
2	E	104	PRO	2.2
1	I	119	LYS	2.2
1	C	202	GLY	2.2
2	E	93	ILE	2.1
4	H	203	ASP	2.1
1	I	158	GLY	2.1
2	E	92	GLY	2.1
2	E	89	ALA	2.1
2	K	77	ASN	2.1
2	E	46	VAL	2.1
2	E	17	SER	2.1
3	M	19	SER	2.1
3	G	111	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	166	LEU	2.1
2	E	78	LEU	2.1
2	L	66	GLY	2.1
1	C	180	ASP	2.1
2	F	4	THR	2.1
1	C	100	GLU	2.1
2	F	73	SER	2.0
1	C	104	GLN	2.0
2	L	142[A]	HIS	2.0
2	F	96	LEU	2.0
2	K	5	ILE	2.0
2	E	73	SER	2.0
3	G	25	VAL	2.0
2	L	137	PRO	2.0
2	K	78	LEU	2.0
1	C	182	GLY	2.0
2	K	92	GLY	2.0
2	K	139	THR	2.0
1	C	161	VAL	2.0
2	F	85	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	N	5001	6/6	0.84	0.23	47,47,48,48	0
5	GOL	N	5002	6/6	0.93	0.15	50,51,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.