



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:44 pm BST

PDB ID : 4FMA  
Title : EspG structure  
Authors : Shao, F.; Zhu, Y.; Hu, L.  
Deposited on : 2012-06-16  
Resolution : 2.15 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

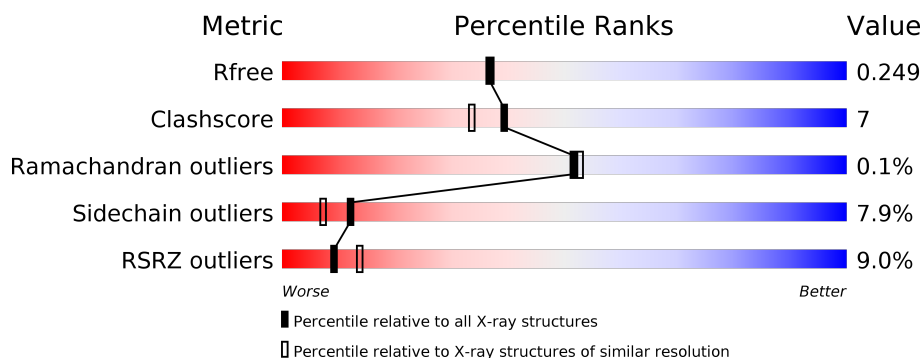
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	A	351	<div> <div>5%</div> <div>86%</div> <div>12%</div> <div>•</div> </div>
1	B	351	<div> <div>5%</div> <div>87%</div> <div>10%</div> <div>•</div> </div>
1	C	351	<div> <div>8%</div> <div>82%</div> <div>14%</div> <div>• •</div> </div>
1	D	351	<div> <div>9%</div> <div>81%</div> <div>15%</div> <div>• •</div> </div>
1	E	351	<div> <div>9%</div> <div>81%</div> <div>16%</div> <div>• •</div> </div>
1	F	351	<div> <div>7%</div> <div>79%</div> <div>16%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	351	<div><div></div><div>10%</div><div>79%</div><div>15%</div><div></div><div></div></div>
1	H	351	<div><div></div><div>13%</div><div>81%</div><div>14%</div><div></div><div></div></div>
1	I	351	<div><div></div><div>10%</div><div>81%</div><div>15%</div><div></div><div></div></div>
1	J	351	<div><div></div><div>10%</div><div>77%</div><div>17%</div><div></div><div></div></div>
1	K	351	<div><div></div><div>11%</div><div>82%</div><div>13%</div><div></div><div></div></div>
1	L	351	<div><div></div><div>9%</div><div>78%</div><div>18%</div><div></div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34644 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 EspG protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2719	1679	477	547	16			
1	B	351	Total	C	N	O	S	0	0	0
			2719	1679	477	547	16			
1	C	346	Total	C	N	O	S	0	0	0
			2671	1653	470	532	16			
1	D	341	Total	C	N	O	S	0	0	0
			2636	1632	459	529	16			
1	E	349	Total	C	N	O	S	0	0	0
			2696	1666	475	539	16			
1	F	344	Total	C	N	O	S	0	0	0
			2658	1645	467	530	16			
1	G	343	Total	C	N	O	S	0	0	0
			2627	1630	464	517	16			
1	H	347	Total	C	N	O	S	0	0	0
			2678	1657	472	533	16			
1	I	348	Total	C	N	O	S	0	0	0
			2658	1644	466	532	16			
1	J	341	Total	C	N	O	S	0	0	0
			2624	1626	459	523	16			
1	K	344	Total	C	N	O	S	0	0	0
			2639	1635	464	524	16			
1	L	348	Total	C	N	O	S	0	0	0
			2673	1655	470	532	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	2	Total	Mg	0	0
			2	2		
2	D	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	I	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	L	3	Total	Mg	0	0
			3	3		
2	F	2	Total	Mg	0	0
			2	2		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



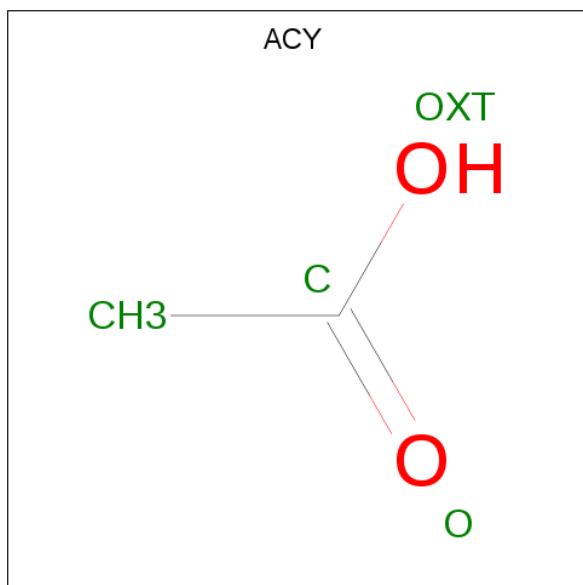
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		

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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	281	Total	O	0	0
			281	281		
5	B	287	Total	O	0	0
			287	287		
5	C	251	Total	O	0	0
			251	251		
5	D	227	Total	O	0	0
			227	227		
5	E	243	Total	O	0	0
			243	243		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	240	Total 240	O 240	0	0
5	G	164	Total 164	O 164	0	0
5	H	196	Total 196	O 196	0	0
5	I	153	Total 153	O 153	0	0
5	J	152	Total 152	O 152	0	0
5	K	184	Total 184	O 184	0	0
5	L	227	Total 227	O 227	0	0

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.

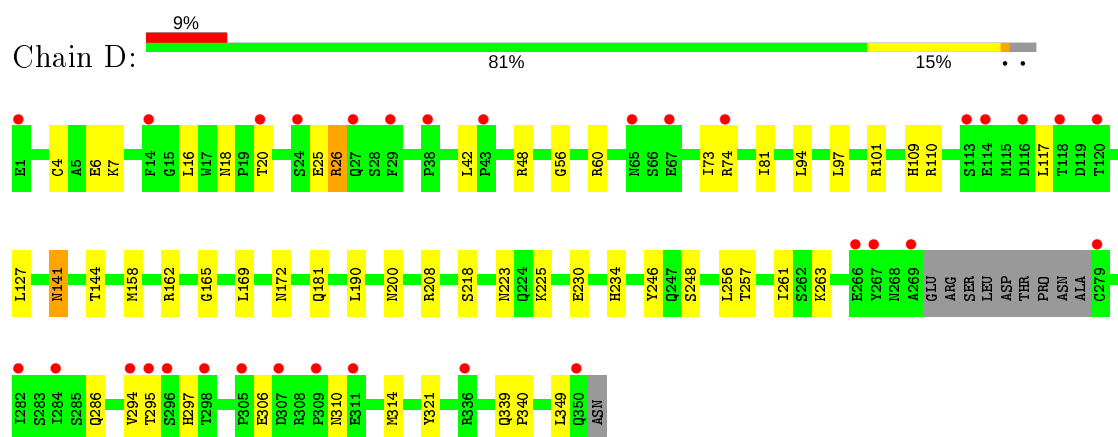
- Chain A:
- 
- | Category | Percentage |
|----------|------------|
| Green    | 86%        |
| Yellow   | 12%        |
| Red      | 5%         |

- Chain B:
- 
- | Category | Percentage |
|----------|------------|
| E1       | 5%         |
| F14      |            |
| M18      |            |
| P19      |            |
| T20      |            |
| Y21      |            |
| R22      |            |
| S23      |            |
| Q27      |            |
| S28      |            |
| F29      |            |
| P38      |            |
| M44      |            |
| T64      |            |
| M65      |            |
| S66      |            |
| P67      |            |
| S68      |            |
| L69      |            |
| I73      |            |
| R74      |            |
| T75      |            |
| F76      |            |
| D77      |            |
| M78      |            |
| N88      |            |
| P89      |            |
| Q90      |            |
| N91      |            |
| R92      |            |
| L93      |            |
| L94      |            |
| R101     |            |
| E114     |            |
| L117     |            |
| L126     |            |
| L127     |            |
| T130     |            |
| S131     |            |
| T151     |            |
| S154     |            |
| M158     |            |
| C165     |            |

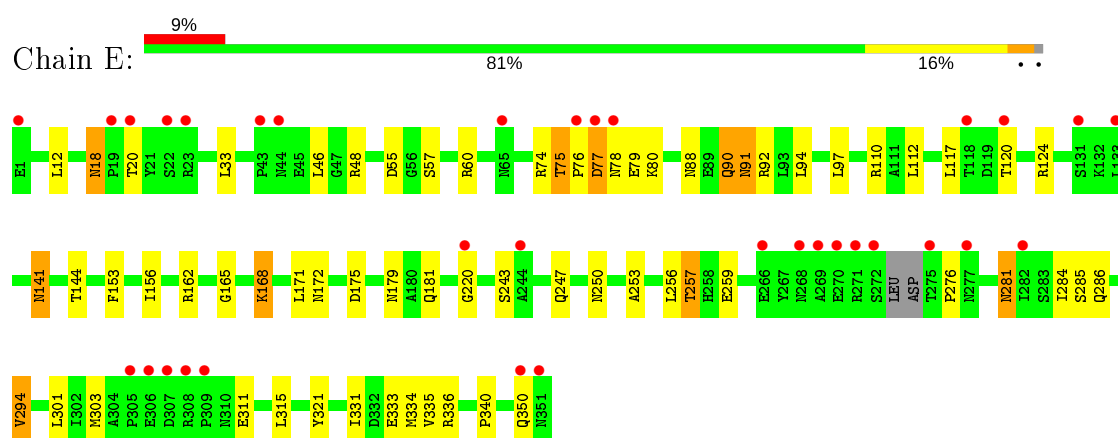
- Chain C:
- 
- 8% 82% 14%
- 
- E1 M2 M18 P19 T20 R23 Q27 Q30 L33 L36 P43 S57 R60 S66 I69 T75 P76 D77 E78 E79 K80 L85 N88 E89 Q90 N91 R92 L93 L94 S96 L97 R101 R109 R110 L117 T120 S134 L137 T138 M141 Q142 Q143 T144 G165 L169 Q181 M182 L183 L184 R185 L190 T193 R208 S218 M223 Q224 K225 E230 H234 S243 A253 L256 T257 H258 K263 E266 A269 E270 R271 SER LEU ASP THR P276 M277 M303 E306 D307 R308 R320 M310 E311 L315 Y321 K328 D332 E333 M334 V335 R336 P340 R341 Q350 ASN

- 
- WORLD WIDE  
PDB  
PROTEIN DATA BANK

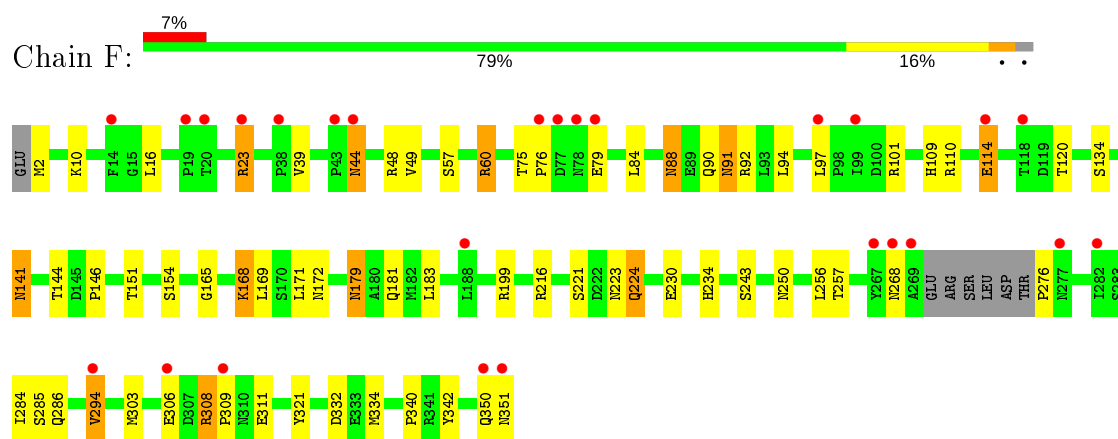




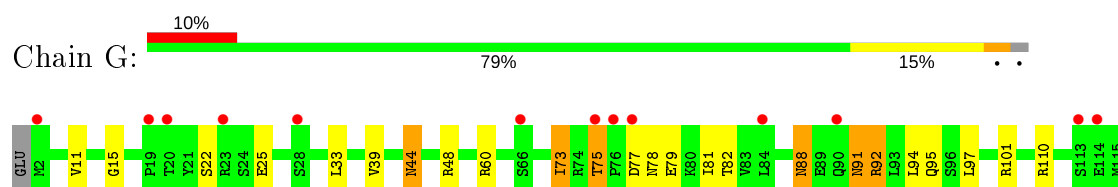
- Molecule 1: EspG protein

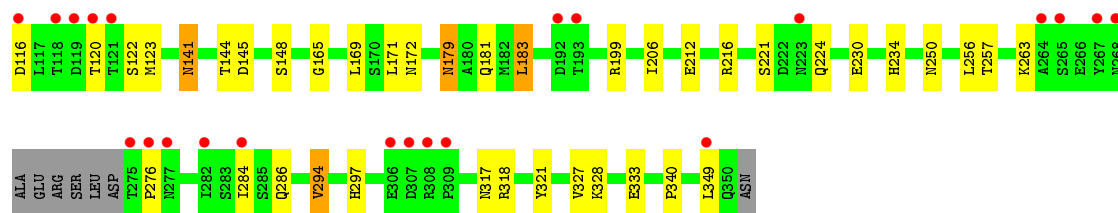


- Molecule 1: EspG protein

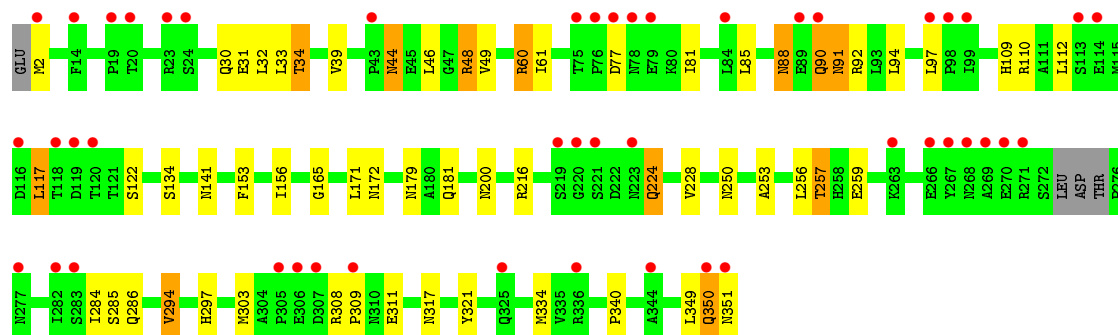
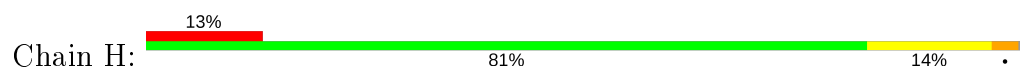


- Molecule 1: EspG protein

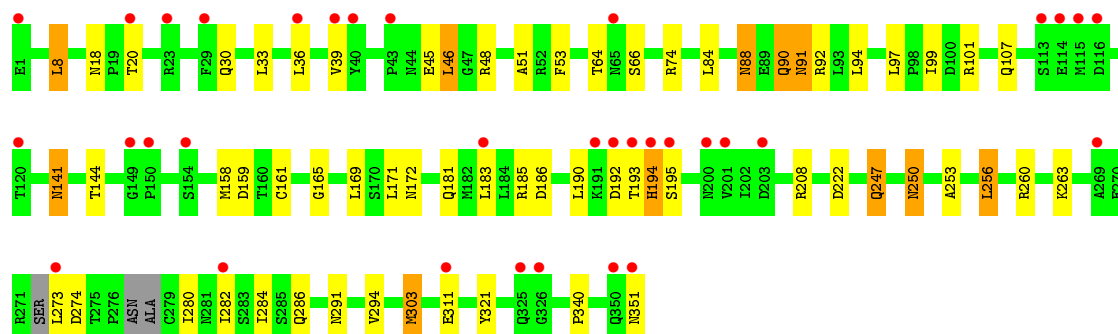
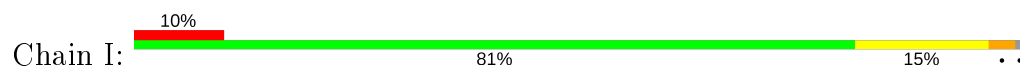




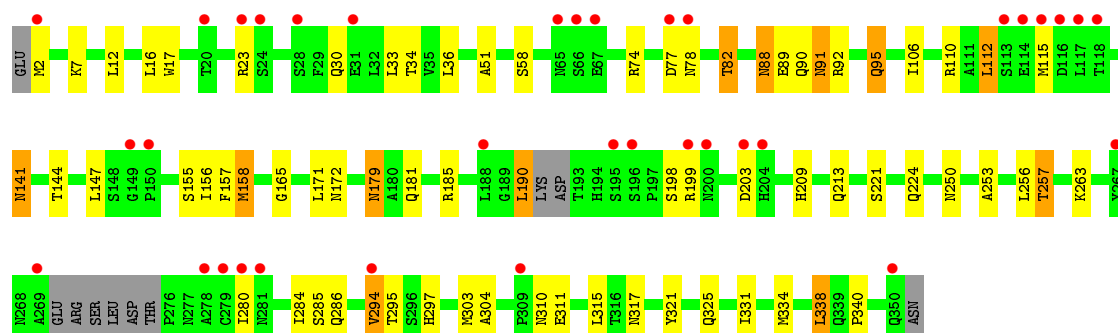
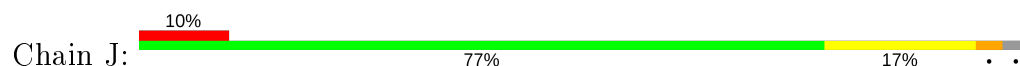
• Molecule 1: EspG protein



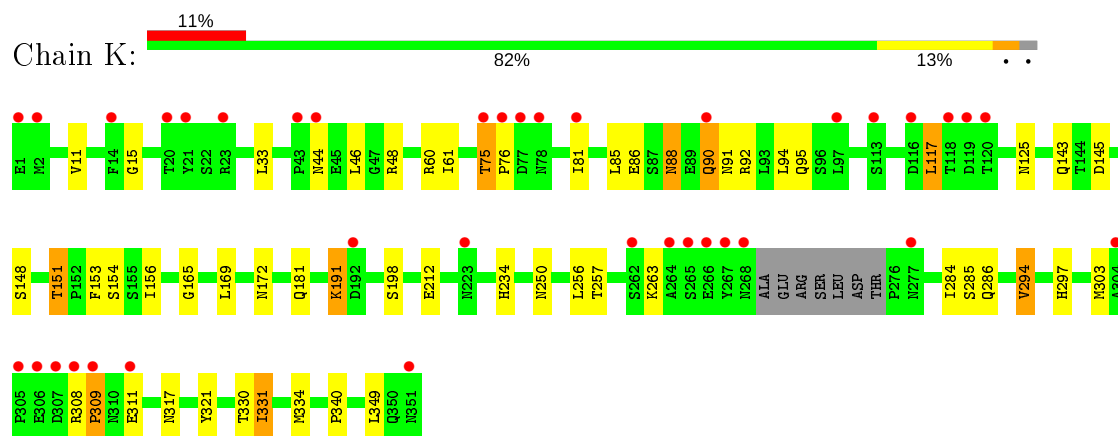
• Molecule 1: EspG protein



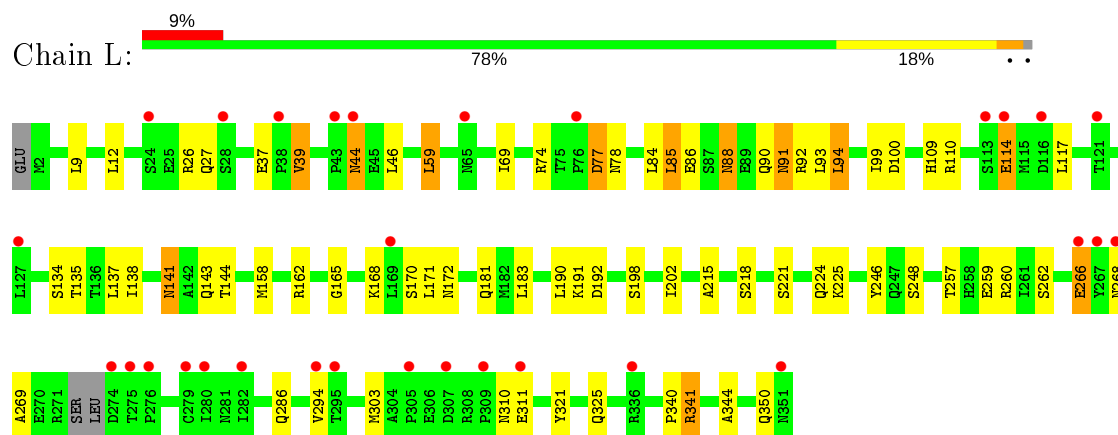
• Molecule 1: EspG protein



- Molecule 1: EspG protein



- Molecule 1: EspG protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.61Å 167.74Å 361.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 35.94 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.15) 99.8 (35.94-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.10 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.200 , 0.239 0.214 , 0.249	Depositor DCC
$R_{free}$ test set	15668 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	34644	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.67% 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: ACY, MG, FMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.43	0/2767	0.59	0/3758
1	B	0.42	0/2767	0.58	0/3758
1	C	0.39	0/2718	0.59	1/3689 (0.0%)
1	D	0.42	0/2682	0.59	0/3641
1	E	0.39	0/2743	0.57	0/3724
1	F	0.43	0/2705	0.62	0/3672
1	G	0.37	0/2674	0.57	0/3633
1	H	0.39	0/2725	0.58	1/3699 (0.0%)
1	I	0.38	0/2703	0.61	0/3673
1	J	0.37	0/2669	0.56	0/3623
1	K	0.37	0/2686	0.56	0/3649
1	L	0.43	0/2720	0.60	0/3695
All	All	0.40	0/32559	0.58	2/44214 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	46	LEU	CA-CB-CG	5.89	128.86	115.30
1	C	80	LYS	N-CA-C	5.31	125.35	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2719	0	2674	26	0
1	B	2719	0	2674	33	0
1	C	2671	0	2629	36	0
1	D	2636	0	2592	34	0
1	E	2696	0	2646	40	0
1	F	2658	0	2617	48	0
1	G	2627	0	2574	41	0
1	H	2678	0	2629	40	0
1	I	2658	0	2587	51	0
1	J	2624	0	2576	48	0
1	K	2639	0	2588	33	0
1	L	2673	0	2621	51	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
2	H	1	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	L	3	0	0	0	0
3	A	6	0	2	0	0
3	B	3	0	1	0	0
3	D	3	0	1	0	0
3	L	6	0	2	1	0
4	J	4	0	3	0	0
5	A	281	0	0	3	0
5	B	287	0	0	0	0
5	C	251	0	0	3	0
5	D	227	0	0	3	0
5	E	243	0	0	1	0
5	F	240	0	0	3	0
5	G	164	0	0	2	0
5	H	196	0	0	3	0
5	I	153	0	0	2	0
5	J	152	0	0	1	0
5	K	184	0	0	0	0
5	L	227	0	0	3	0
All	All	34644	0	31416	470	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 (470) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:172:ASN:HD21	1:J:286:GLN:H	1.10	0.99
1:F:23:ARG:HG2	1:F:23:ARG:HH11	1.31	0.95
1:D:172:ASN:HD21	1:D:286:GLN:H	1.11	0.94
1:E:172:ASN:HD21	1:E:286:GLN:H	1.16	0.92
1:G:297:HIS:HE1	1:G:318:ARG:HE	1.10	0.91
1:L:46:LEU:HD13	1:L:99:ILE:HG23	1.53	0.89
1:H:44:ASN:H	1:H:44:ASN:HD22	1.20	0.89
1:L:221:SER:H	1:L:224:GLN:HE21	1.19	0.89
1:G:48:ARG:NH1	1:G:60:ARG:HD3	1.90	0.86
1:H:172:ASN:HD21	1:H:286:GLN:H	1.20	0.86
1:J:16:LEU:HD21	1:J:33:LEU:HD21	1.54	0.86
1:L:172:ASN:HD21	1:L:286:GLN:H	1.19	0.86
1:F:350:GLN:OE1	1:F:350:GLN:HA	1.73	0.85
1:I:260:ARG:HE	1:K:143:GLN:HE21	1.25	0.84
1:J:106:ILE:HD11	1:J:256:LEU:HD21	1.60	0.84
1:I:193:THR:CG2	1:I:194:HIS:N	2.40	0.83
1:F:172:ASN:HD21	1:F:286:GLN:H	1.25	0.83
1:E:75:THR:HG22	1:E:76:PRO:HD2	1.59	0.83
1:G:297:HIS:CE1	1:G:318:ARG:HE	1.95	0.82
1:K:153:PHE:O	1:K:156:ILE:HG13	1.80	0.81
1:J:77:ASP:N	1:J:78:ASN:HA	1.93	0.80
1:L:77:ASP:CG	1:L:77:ASP:O	2.19	0.80
1:B:166:ASN:HB3	5:D:629:HOH:O	1.82	0.79
1:F:350:GLN:OE1	1:F:350:GLN:CA	2.30	0.79
1:F:60:ARG:HG2	1:F:60:ARG:HH11	1.45	0.79
1:E:120:THR:HG22	1:E:276:PRO:HD3	1.64	0.77
1:B:263:LYS:HD2	1:B:303:MET:CE	2.15	0.76
1:I:263:LYS:HG3	1:I:303:MET:HG2	1.65	0.76
1:J:77:ASP:H	1:J:78:ASN:HA	1.52	0.74
1:J:331:ILE:HA	1:J:334:MET:HE3	1.70	0.73
1:G:172:ASN:HD21	1:G:286:GLN:H	1.37	0.73
1:F:2:MET:SD	1:F:10:LYS:HE3	2.29	0.73
1:I:158:MET:HE1	1:I:193:THR:HG23	1.71	0.72
1:G:22:SER:H	1:G:25:GLU:HG3	1.55	0.72
1:G:48:ARG:HH11	1:G:60:ARG:HD3	1.53	0.72
1:H:60:ARG:CG	1:H:60:ARG:HH21	2.03	0.72
1:K:172:ASN:HD21	1:K:286:GLN:H	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:69:ILE:HD11	1:L:94:LEU:HD22	1.70	0.72
1:I:158:MET:HE1	1:I:193:THR:CG2	2.20	0.72
1:D:172:ASN:ND2	1:D:286:GLN:H	1.88	0.71
1:L:46:LEU:CD1	1:L:99:ILE:HG23	2.20	0.71
1:L:46:LEU:HD13	1:L:99:ILE:CG2	2.18	0.71
1:F:60:ARG:HH11	1:F:60:ARG:CG	2.03	0.71
1:G:44:ASN:H	1:G:44:ASN:HD22	1.36	0.71
1:F:243:SER:HB3	1:F:334:MET:CE	2.20	0.71
1:I:193:THR:HG22	1:I:194:HIS:N	2.06	0.71
1:L:262:SER:O	1:L:266:GLU:HG3	1.90	0.71
1:B:303:MET:HG3	1:B:311:GLU:O	1.91	0.71
1:I:172:ASN:HD21	1:I:286:GLN:H	1.38	0.71
1:L:172:ASN:ND2	1:L:286:GLN:H	1.89	0.70
1:D:18:ASN:HD22	1:D:20:THR:H	1.39	0.70
1:J:172:ASN:ND2	1:J:286:GLN:H	1.86	0.70
1:G:297:HIS:HE1	1:G:318:ARG:NE	1.87	0.69
1:G:120:THR:HG22	1:G:276:PRO:HD3	1.73	0.69
1:I:165:GLY:H	1:I:181:GLN:NE2	1.91	0.69
1:K:75:THR:HG22	1:K:76:PRO:HD2	1.73	0.69
1:F:44:ASN:H	1:F:44:ASN:HD22	1.37	0.69
1:G:116:ASP:HA	1:G:349:LEU:HD21	1.74	0.69
1:H:60:ARG:HG3	1:H:60:ARG:HH21	1.58	0.68
1:K:151:THR:O	1:K:151:THR:CG2	2.40	0.68
1:A:95:GLN:H	1:A:95:GLN:HE21	1.42	0.68
1:E:162:ARG:HE	1:E:247:GLN:HE22	1.40	0.68
1:I:39:VAL:HG23	1:I:48:ARG:HG3	1.75	0.68
1:E:110:ARG:HD2	1:E:350:GLN:HE21	1.59	0.67
1:E:57:SER:HB3	1:E:76:PRO:HD3	1.76	0.67
1:H:60:ARG:HB2	1:H:60:ARG:HH21	1.60	0.67
1:I:193:THR:O	1:I:194:HIS:C	2.30	0.66
1:K:308:ARG:HB3	1:K:309:PRO:HD2	1.77	0.66
1:H:200:ASN:CG	1:J:78:ASN:HB2	2.15	0.66
1:I:260:ARG:HE	1:K:143:GLN:NE2	1.91	0.66
1:C:165:GLY:H	1:C:181:GLN:NE2	1.94	0.66
1:G:284:ILE:HG12	1:G:294:VAL:HB	1.78	0.65
1:F:221:SER:OG	1:F:224:GLN:HG2	1.97	0.65
1:K:165:GLY:H	1:K:181:GLN:NE2	1.94	0.65
1:C:18:ASN:HD22	1:C:20:THR:H	1.44	0.65
1:A:165:GLY:H	1:A:181:GLN:HE21	1.44	0.65
1:E:165:GLY:H	1:E:181:GLN:NE2	1.95	0.65
1:H:253:ALA:O	1:H:257:THR:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ARG:HH12	1:D:310:ASN:HD21	1.45	0.64
1:H:350:GLN:O	1:H:351:ASN:CB	2.45	0.64
1:F:88:ASN:H	1:F:91:ASN:HD21	1.46	0.64
1:K:48:ARG:NH1	1:K:60:ARG:HD2	2.13	0.64
1:F:165:GLY:H	1:F:181:GLN:NE2	1.96	0.64
1:G:11:VAL:O	1:G:15:GLY:HA2	1.97	0.63
1:H:91:ASN:HD22	1:H:92:ARG:N	1.96	0.63
1:H:34:THR:HG22	5:H:673:HOH:O	1.98	0.63
1:B:73:ILE:CD1	1:B:75:THR:HG23	2.28	0.63
1:C:243:SER:HB3	1:C:334:MET:CE	2.29	0.63
1:J:321:TYR:HB3	1:J:340:PRO:HA	1.80	0.63
1:D:208:ARG:HE	1:K:151:THR:HG21	1.62	0.63
1:L:165:GLY:H	1:L:181:GLN:HE21	1.47	0.63
1:F:23:ARG:HH11	1:F:23:ARG:CG	2.10	0.62
1:I:165:GLY:H	1:I:181:GLN:HE21	1.45	0.62
1:D:110:ARG:NH1	1:D:310:ASN:HD21	1.96	0.62
1:J:165:GLY:H	1:J:181:GLN:NE2	1.97	0.62
1:I:193:THR:HG23	1:I:194:HIS:N	2.12	0.62
1:H:165:GLY:H	1:H:181:GLN:NE2	1.97	0.62
1:L:77:ASP:OD2	1:L:77:ASP:O	2.18	0.62
1:J:106:ILE:CD1	1:J:256:LEU:HD21	2.30	0.61
1:J:2:MET:HG2	1:J:7:LYS:HG3	1.83	0.61
1:K:11:VAL:O	1:K:15:GLY:HA2	2.00	0.61
1:G:88:ASN:ND2	1:G:91:ASN:H	1.99	0.61
1:B:165:GLY:H	1:B:181:GLN:NE2	1.99	0.61
1:L:165:GLY:H	1:L:181:GLN:NE2	1.98	0.61
1:B:263:LYS:HD2	1:B:303:MET:HE2	1.82	0.61
1:C:91:ASN:HD22	1:C:92:ARG:N	1.98	0.60
1:E:165:GLY:H	1:E:181:GLN:HE21	1.46	0.60
1:L:192:ASP:HB2	3:L:405:FMT:H	1.83	0.60
1:I:284:ILE:HG12	1:I:294:VAL:HB	1.84	0.60
1:A:165:GLY:H	1:A:181:GLN:NE2	2.00	0.60
1:F:60:ARG:HG2	1:F:60:ARG:NH1	2.17	0.60
1:K:321:TYR:HB3	1:K:340:PRO:HA	1.84	0.60
1:B:165:GLY:H	1:B:181:GLN:HE21	1.50	0.59
1:H:88:ASN:ND2	1:H:90:GLN:HG2	2.17	0.59
1:E:74:ARG:HG2	1:E:80:LYS:HG2	1.83	0.59
1:G:165:GLY:H	1:G:181:GLN:NE2	2.01	0.59
1:J:253:ALA:O	1:J:257:THR:HG23	2.01	0.59
1:K:156:ILE:HG12	1:K:334:MET:HE1	1.84	0.59
1:I:321:TYR:HB3	1:I:340:PRO:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:284:ILE:HG12	1:H:294:VAL:HB	1.82	0.59
1:H:60:ARG:CB	1:H:60:ARG:HH21	2.14	0.59
1:G:92:ARG:NH1	1:G:95:GLN:HE22	2.00	0.59
1:J:58:SER:HB3	1:J:74:ARG:HB2	1.85	0.59
1:A:91:ASN:HD22	1:A:92:ARG:N	2.01	0.59
1:E:88:ASN:H	1:E:91:ASN:HD21	1.51	0.59
1:K:284:ILE:HG12	1:K:294:VAL:HB	1.84	0.59
1:F:88:ASN:HD22	1:F:90:GLN:H	1.52	0.58
1:B:263:LYS:HD2	1:B:303:MET:HE3	1.82	0.58
1:G:88:ASN:H	1:G:91:ASN:HD21	1.52	0.58
1:D:165:GLY:H	1:D:181:GLN:HE21	1.51	0.58
1:F:165:GLY:H	1:F:181:GLN:HE21	1.51	0.58
1:K:303:MET:HB2	1:K:311:GLU:O	2.04	0.58
1:B:130:THR:HG21	1:B:316:THR:OG1	2.03	0.58
1:B:88:ASN:H	1:B:91:ASN:HD21	1.52	0.57
1:J:91:ASN:HD22	1:J:92:ARG:N	2.01	0.57
1:L:100:ASP:OD2	1:L:135:THR:OG1	2.21	0.57
1:I:192:ASP:O	1:I:193:THR:C	2.40	0.57
1:K:156:ILE:HG12	1:K:334:MET:CE	2.33	0.57
1:A:166:ASN:ND2	5:A:671:HOH:O	2.36	0.57
1:B:130:THR:CG2	1:B:316:THR:OG1	2.52	0.57
1:C:185:ARG:HD3	1:C:190:LEU:O	2.05	0.57
1:L:37:GLU:OE2	1:L:170:SER:OG	2.22	0.57
1:L:141:ASN:ND2	1:L:144:THR:H	2.02	0.56
1:D:6:GLU:HG3	1:D:73:ILE:HD11	1.86	0.56
1:F:39:VAL:HG23	1:F:48:ARG:HG3	1.85	0.56
1:F:91:ASN:HD22	1:F:92:ARG:N	2.03	0.56
1:D:257:THR:O	1:D:261:ILE:HG12	2.05	0.56
1:L:110:ARG:NH1	1:L:310:ASN:OD1	2.39	0.56
1:J:155:SER:O	1:J:158:MET:HG2	2.06	0.56
1:D:321:TYR:HB3	1:D:340:PRO:HA	1.88	0.56
1:G:91:ASN:HD22	1:G:92:ARG:N	2.03	0.56
1:I:88:ASN:H	1:I:91:ASN:HD21	1.54	0.56
1:A:88:ASN:H	1:A:91:ASN:HD21	1.53	0.56
1:A:65:ASN:HB3	5:A:701:HOH:O	2.06	0.56
1:H:44:ASN:H	1:H:44:ASN:ND2	1.96	0.55
1:I:161:CYS:SG	1:I:185:ARG:NH1	2.79	0.55
1:I:193:THR:HG22	1:I:194:HIS:H	1.70	0.55
1:B:127:LEU:HD12	1:B:130:THR:HG22	1.88	0.55
1:K:117:LEU:HB2	1:K:349:LEU:HD11	1.88	0.55
1:L:260:ARG:HD2	5:L:679:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:ALA:O	1:E:257:THR:HG23	2.07	0.55
1:G:321:TYR:HB3	1:G:340:PRO:HA	1.87	0.55
1:E:303:MET:HB2	1:E:311:GLU:O	2.07	0.55
1:L:137:LEU:HD21	1:L:341:ARG:HD3	1.89	0.55
1:B:91:ASN:HD22	1:B:92:ARG:N	2.05	0.54
1:C:109:HIS:HD2	5:C:646:HOH:O	1.89	0.54
1:H:117:LEU:HD22	1:H:349:LEU:HD11	1.89	0.54
1:K:165:GLY:H	1:K:181:GLN:HE21	1.53	0.54
1:H:172:ASN:ND2	1:H:286:GLN:H	1.99	0.54
1:L:141:ASN:C	1:L:141:ASN:HD22	2.11	0.54
1:E:321:TYR:HB3	1:E:340:PRO:HA	1.90	0.54
1:F:114:GLU:H	1:F:114:GLU:CD	2.10	0.54
1:J:88:ASN:H	1:J:91:ASN:HD21	1.54	0.54
1:E:172:ASN:ND2	1:E:286:GLN:H	1.96	0.54
1:H:88:ASN:H	1:H:91:ASN:HD21	1.56	0.54
1:L:44:ASN:H	1:L:44:ASN:ND2	2.03	0.54
1:I:193:THR:O	1:I:195:SER:N	2.41	0.54
1:L:26:ARG:HH11	1:L:114:GLU:HG3	1.74	0.54
1:E:141:ASN:ND2	1:E:144:THR:H	2.06	0.53
1:A:109:HIS:HD2	5:A:529:HOH:O	1.90	0.53
1:C:165:GLY:H	1:C:181:GLN:HE21	1.55	0.53
1:F:109:HIS:HE1	1:F:134:SER:O	1.91	0.53
1:H:321:TYR:HB3	1:H:340:PRO:HA	1.89	0.53
1:I:39:VAL:CG2	1:I:48:ARG:HG3	2.37	0.53
1:C:141:ASN:HD22	1:C:141:ASN:C	2.12	0.53
1:J:284:ILE:HG12	1:J:294:VAL:HB	1.89	0.53
1:F:172:ASN:ND2	1:F:286:GLN:H	2.01	0.53
1:K:151:THR:HG22	1:K:151:THR:O	2.08	0.53
1:J:158:MET:N	1:J:158:MET:SD	2.81	0.52
1:L:88:ASN:HD22	1:L:90:GLN:H	1.58	0.52
1:C:75:THR:OG1	1:C:78:ASN:CB	2.57	0.52
1:J:156:ILE:HG21	1:J:334:MET:CE	2.39	0.52
1:D:165:GLY:H	1:D:181:GLN:NE2	2.06	0.52
1:C:78:ASN:CB	1:C:79:GLU:HA	2.38	0.52
1:I:141:ASN:ND2	1:I:144:THR:HB	2.24	0.52
1:E:88:ASN:OD1	1:E:90:GLN:HG2	2.10	0.52
1:H:224:GLN:O	1:H:228:VAL:HG23	2.10	0.52
1:F:332:ASP:HB2	5:F:634:HOH:O	2.09	0.52
1:J:92:ARG:HB3	1:J:95:GLN:HG2	1.92	0.52
1:D:127:LEU:HA	1:D:314:MET:CE	2.40	0.51
1:E:284:ILE:HG12	1:E:294:VAL:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:243:SER:HB3	1:F:334:MET:HE3	1.91	0.51
1:G:141:ASN:ND2	1:G:144:THR:H	2.07	0.51
1:J:165:GLY:H	1:J:181:GLN:HE21	1.58	0.51
1:A:303:MET:HA	1:A:311:GLU:O	2.10	0.51
1:E:168:LYS:HE3	1:E:175:ASP:OD1	2.10	0.51
1:A:95:GLN:N	1:A:95:GLN:HE21	2.08	0.51
1:C:138:ILE:HD13	1:C:256:LEU:HD23	1.91	0.51
1:K:330:THR:O	1:K:334:MET:HG3	2.10	0.51
1:J:172:ASN:HD22	1:J:285:SER:HA	1.75	0.51
1:A:321:TYR:HB3	1:A:340:PRO:HA	1.92	0.51
1:E:141:ASN:HD22	1:E:144:THR:H	1.59	0.51
1:F:141:ASN:HD22	1:F:141:ASN:C	2.14	0.51
1:J:36:LEU:HD23	1:J:51:ALA:HB2	1.93	0.51
1:L:88:ASN:H	1:L:91:ASN:HD21	1.59	0.51
1:L:141:ASN:HD21	1:L:143:GLN:HB3	1.76	0.50
1:C:257:THR:HG21	1:C:315:LEU:HD13	1.94	0.50
1:H:60:ARG:HB2	1:H:60:ARG:NH2	2.26	0.50
1:E:75:THR:CG2	1:E:76:PRO:HD2	2.37	0.50
1:E:92:ARG:HD2	5:E:711:HOH:O	2.11	0.50
1:G:141:ASN:HD21	1:G:144:THR:HG23	1.76	0.50
1:I:253:ALA:HA	1:I:256:LEU:HD23	1.94	0.50
1:B:76:PRO:C	1:B:78:ASN:H	2.14	0.49
1:J:331:ILE:HA	1:J:334:MET:CE	2.42	0.49
1:A:8:LEU:HD21	1:A:33:LEU:HD12	1.94	0.49
1:C:75:THR:HB	1:C:76:PRO:HD2	1.93	0.49
1:C:88:ASN:H	1:C:91:ASN:HD21	1.61	0.49
1:E:243:SER:HB3	1:E:334:MET:CE	2.42	0.49
1:E:91:ASN:HD22	1:E:92:ARG:N	2.10	0.49
1:G:327:VAL:HG13	1:G:333:GLU:HG3	1.94	0.49
1:I:286:GLN:HA	1:I:291:ASN:O	2.12	0.49
1:I:192:ASP:CB	1:I:194:HIS:CD2	2.95	0.49
1:K:88:ASN:ND2	1:K:91:ASN:H	2.10	0.49
1:B:117:LEU:HD22	1:B:301:LEU:HD11	1.94	0.49
1:D:109:HIS:HD2	5:D:618:HOH:O	1.94	0.49
1:L:92:ARG:HH12	1:L:109:HIS:HD2	1.60	0.49
1:F:109:HIS:HD2	5:F:542:HOH:O	1.94	0.49
1:F:243:SER:HB3	1:F:334:MET:HE1	1.94	0.49
5:D:630:HOH:O	1:K:191:LYS:HE2	2.12	0.49
1:E:141:ASN:HD21	1:E:144:THR:HG23	1.77	0.49
1:D:246:TYR:CZ	1:D:248:SER:HB2	2.48	0.49
1:H:317:ASN:ND2	5:H:517:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:ASN:HD22	1:I:141:ASN:C	2.16	0.49
1:L:303:MET:HG3	1:L:311:GLU:O	2.12	0.49
1:F:120:THR:HB	1:F:276:PRO:HD3	1.95	0.49
1:C:75:THR:O	1:C:76:PRO:C	2.50	0.49
1:E:18:ASN:HD22	1:E:20:THR:H	1.59	0.49
1:H:49:VAL:CG1	1:H:61:ILE:HB	2.42	0.49
1:E:141:ASN:HD22	1:E:141:ASN:C	2.17	0.48
1:H:60:ARG:NH2	1:H:60:ARG:HG3	2.27	0.48
1:J:172:ASN:HD21	1:J:286:GLN:N	1.93	0.48
1:B:69:ILE:HD11	1:B:94:LEU:HD13	1.95	0.48
1:C:88:ASN:OD1	1:C:90:GLN:HG2	2.13	0.48
1:F:23:ARG:NH1	1:F:23:ARG:HG2	2.12	0.48
1:F:308:ARG:HG3	1:F:309:PRO:HD2	1.96	0.48
1:D:48:ARG:NH2	1:D:60:ARG:HD2	2.29	0.48
1:E:77:ASP:N	1:E:77:ASP:OD2	2.47	0.48
1:G:75:THR:HG22	1:G:79:GLU:H	1.78	0.48
1:H:109:HIS:HD2	5:H:557:HOH:O	1.96	0.48
1:L:137:LEU:CD2	1:L:341:ARG:HD3	2.43	0.48
1:L:91:ASN:HD22	1:L:92:ARG:N	2.11	0.48
1:E:77:ASP:O	1:E:78:ASN:HB2	2.13	0.48
1:G:145:ASP:HB3	1:G:148:SER:HB3	1.95	0.48
1:A:151:THR:HB	1:A:154:SER:HB3	1.95	0.48
1:A:69:ILE:HD11	1:A:94:LEU:HD13	1.96	0.48
1:E:48:ARG:NH1	1:E:60:ARG:HD2	2.29	0.48
1:A:88:ASN:H	1:A:91:ASN:ND2	2.11	0.48
1:B:230:GLU:O	1:B:234:HIS:HD2	1.97	0.48
1:G:165:GLY:H	1:G:181:GLN:HE21	1.62	0.48
1:L:109:HIS:HE1	1:L:134:SER:O	1.95	0.48
1:I:161:CYS:SG	1:I:193:THR:HA	2.54	0.47
1:L:77:ASP:OD2	1:L:77:ASP:C	2.51	0.47
1:A:19:PRO:HG3	1:G:216:ARG:HD3	1.96	0.47
1:F:88:ASN:H	1:F:91:ASN:ND2	2.12	0.47
1:I:36:LEU:HD23	1:I:51:ALA:HB2	1.97	0.47
1:F:321:TYR:HB3	1:F:340:PRO:HA	1.97	0.47
1:I:159:ASP:CG	1:I:247:GLN:HG3	2.35	0.47
1:D:141:ASN:C	1:D:141:ASN:HD22	2.18	0.47
1:H:153:PHE:O	1:H:156:ILE:HG12	2.14	0.47
1:I:8:LEU:HD12	1:I:53:PHE:HZ	1.80	0.47
1:I:91:ASN:HD22	1:I:92:ARG:N	2.11	0.47
1:C:109:HIS:HE1	1:C:134:SER:O	1.97	0.47
1:E:153:PHE:O	1:E:156:ILE:HG12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:221:SER:N	1:L:224:GLN:HE21	2.00	0.47
1:B:88:ASN:HD22	1:B:90:GLN:H	1.62	0.47
1:H:109:HIS:HE1	1:H:134:SER:O	1.98	0.47
1:L:215:ALA:O	1:L:225:LYS:HD2	2.14	0.47
1:L:341:ARG:NH1	5:L:550:HOH:O	2.44	0.47
1:C:18:ASN:ND2	1:C:20:THR:H	2.12	0.47
1:L:74:ARG:NH1	1:L:78:ASN:OD1	2.47	0.47
1:D:141:ASN:ND2	1:D:144:THR:H	2.13	0.46
1:K:44:ASN:H	1:K:44:ASN:ND2	2.13	0.46
1:K:151:THR:HG23	1:K:154:SER:HB3	1.97	0.46
1:F:75:THR:OG1	1:F:76:PRO:HD2	2.15	0.46
1:I:303:MET:HB2	1:I:311:GLU:O	2.15	0.46
1:D:127:LEU:HA	1:D:314:MET:HE1	1.98	0.46
1:H:39:VAL:HG23	1:H:48:ARG:HG3	1.98	0.46
1:I:88:ASN:H	1:I:91:ASN:ND2	2.12	0.46
1:E:117:LEU:HD13	1:E:301:LEU:HD22	1.96	0.46
1:I:88:ASN:ND2	1:I:90:GLN:HG2	2.30	0.46
1:K:151:THR:HG23	1:K:151:THR:O	2.14	0.46
1:B:166:ASN:OD1	1:D:162:ARG:NH1	2.49	0.46
1:G:141:ASN:HD22	1:G:144:THR:H	1.62	0.46
1:C:303:MET:HA	1:C:311:GLU:O	2.16	0.46
1:F:57:SER:HB3	1:F:76:PRO:HD3	1.96	0.46
1:C:230:GLU:O	1:C:234:HIS:HD2	1.99	0.46
1:D:16:LEU:O	1:D:26:ARG:NH1	2.49	0.46
1:A:81:ILE:HD12	1:A:83:VAL:HG23	1.98	0.45
1:D:230:GLU:O	1:D:234:HIS:CD2	2.69	0.45
1:D:4:CYS:HA	1:D:7:LYS:HE3	1.98	0.45
1:L:46:LEU:CD1	1:L:99:ILE:CG2	2.86	0.45
1:A:117:LEU:HD13	1:A:301:LEU:HD22	1.98	0.45
1:E:172:ASN:ND2	1:E:285:SER:HA	2.32	0.45
1:I:88:ASN:ND2	1:I:91:ASN:H	2.14	0.45
1:L:218:SER:O	1:L:225:LYS:HE2	2.17	0.45
1:B:88:ASN:H	1:B:91:ASN:ND2	2.12	0.45
1:J:257:THR:HG21	1:J:315:LEU:HD13	1.98	0.45
1:J:88:ASN:H	1:J:91:ASN:ND2	2.15	0.45
1:D:117:LEU:HB2	1:D:349:LEU:HD11	1.99	0.45
1:H:30:GLN:O	1:H:34:THR:OG1	2.33	0.45
1:G:297:HIS:HA	1:G:317:ASN:O	2.17	0.45
1:I:74:ARG:NH1	5:I:557:HOH:O	2.50	0.45
1:I:88:ASN:HD22	1:I:90:GLN:H	1.65	0.45
1:C:91:ASN:HD22	1:C:91:ASN:C	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:88:ASN:ND2	1:J:91:ASN:H	2.14	0.45
1:D:295:THR:HG22	1:D:297:HIS:CE1	2.51	0.45
1:F:216:ARG:HE	1:J:90:GLN:NE2	2.14	0.45
1:G:73:ILE:HG23	1:G:81:ILE:HG13	1.99	0.45
1:G:88:ASN:HD21	1:G:91:ASN:H	1.64	0.45
1:I:30:GLN:HA	1:I:33:LEU:HD12	1.99	0.45
1:F:151:THR:HB	1:F:154:SER:HB2	1.99	0.44
1:L:321:TYR:HB3	1:L:340:PRO:HA	1.99	0.44
1:H:31:GLU:HG3	1:H:32:LEU:HD12	1.99	0.44
1:C:321:TYR:HB3	1:C:340:PRO:HA	1.99	0.44
1:F:284:ILE:HG12	1:F:294:VAL:HB	1.98	0.44
1:I:273:LEU:HA	1:I:274:ASP:HA	1.80	0.44
1:L:221:SER:O	1:L:225:LYS:HG2	2.18	0.44
1:E:333:GLU:OE1	1:E:336:ARG:NH2	2.48	0.44
1:I:193:THR:O	1:I:195:SER:CB	2.65	0.44
1:J:209:HIS:O	1:J:213:GLN:HG2	2.17	0.44
1:F:39:VAL:CG2	1:F:48:ARG:HG3	2.48	0.44
1:F:75:THR:HG22	1:F:79:GLU:O	2.17	0.44
1:H:39:VAL:CG2	1:H:48:ARG:HG3	2.46	0.44
1:J:30:GLN:O	1:J:34:THR:HG23	2.17	0.44
1:J:82:THR:HG22	5:J:587:HOH:O	2.17	0.44
1:A:171:LEU:HD22	1:A:176:ILE:HG13	2.00	0.44
1:F:172:ASN:ND2	1:F:285:SER:HA	2.33	0.44
1:F:306:GLU:CD	1:F:306:GLU:H	2.20	0.44
1:G:230:GLU:O	1:G:234:HIS:HD2	1.99	0.44
1:G:328:LYS:N	1:G:333:GLU:HG2	2.33	0.44
1:J:112:LEU:H	1:J:115:MET:HE2	1.83	0.44
1:J:303:MET:HA	1:J:311:GLU:O	2.18	0.44
1:F:230:GLU:O	1:F:234:HIS:HD2	2.00	0.44
1:L:141:ASN:ND2	1:L:143:GLN:HB3	2.32	0.44
1:L:88:ASN:H	1:L:91:ASN:ND2	2.15	0.44
1:C:57:SER:HB3	1:C:76:PRO:HD3	1.99	0.44
1:I:192:ASP:O	1:I:194:HIS:O	2.35	0.44
1:B:321:TYR:HB3	1:B:340:PRO:HA	1.98	0.43
1:C:75:THR:HG1	1:C:79:GLU:HA	1.83	0.43
1:F:141:ASN:ND2	1:F:144:THR:H	2.15	0.43
1:J:156:ILE:HG21	1:J:334:MET:HE1	2.00	0.43
1:C:75:THR:OG1	1:C:79:GLU:HA	2.18	0.43
1:G:297:HIS:CE1	1:G:318:ARG:NE	2.74	0.43
1:H:88:ASN:ND2	1:H:91:ASN:H	2.16	0.43
1:G:179:ASN:O	1:G:183:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:ASP:HA	1:G:78:ASN:HA	1.80	0.43
1:H:308:ARG:HB3	1:H:309:PRO:HD2	2.00	0.43
1:C:258:HIS:HD2	5:C:550:HOH:O	2.01	0.43
1:J:179:ASN:H	1:J:179:ASN:HD22	1.66	0.43
1:B:88:ASN:ND2	1:B:91:ASN:H	2.16	0.43
1:I:190:LEU:HD22	1:I:195:SER:CB	2.48	0.43
1:K:145:ASP:HB3	1:K:148:SER:HB3	2.00	0.43
1:A:171:LEU:HD12	1:A:284:ILE:HB	1.99	0.43
1:B:151:THR:HB	1:B:154:SER:HB3	2.00	0.43
1:E:88:ASN:H	1:E:91:ASN:ND2	2.15	0.43
1:H:165:GLY:H	1:H:181:GLN:HE21	1.65	0.43
1:I:192:ASP:CB	1:I:194:HIS:HD2	2.31	0.43
1:J:141:ASN:C	1:J:141:ASN:HD22	2.22	0.43
1:J:334:MET:O	1:J:338:LEU:HB2	2.19	0.43
1:B:29:PHE:C	1:B:29:PHE:CD1	2.92	0.43
1:D:74:ARG:NH2	1:K:198:SER:HB2	2.34	0.43
1:K:172:ASN:ND2	1:K:285:SER:HA	2.33	0.43
1:C:69:ILE:HD11	1:C:94:LEU:HD13	2.01	0.43
1:K:88:ASN:ND2	1:K:90:GLN:HB3	2.34	0.43
1:B:130:THR:HG23	1:B:316:THR:HG21	1.99	0.42
1:F:146:PRO:HG2	1:F:342:TYR:CZ	2.54	0.42
1:I:107:GLN:NE2	5:I:584:HOH:O	2.36	0.42
1:J:17:TRP:HB3	1:J:110:ARG:HH21	1.84	0.42
1:L:110:ARG:HD2	1:L:350:GLN:HG2	2.00	0.42
1:I:250:ASN:HD22	1:I:250:ASN:H	1.68	0.42
1:L:138:ILE:HD11	1:L:344:ALA:HB3	2.01	0.42
1:L:88:ASN:ND2	1:L:91:ASN:H	2.18	0.42
1:H:156:ILE:HD13	1:H:334:MET:CE	2.49	0.42
1:I:159:ASP:OD1	1:I:247:GLN:HG3	2.20	0.42
1:K:92:ARG:HH21	1:K:95:GLN:HE22	1.67	0.42
1:G:44:ASN:H	1:G:44:ASN:ND2	2.10	0.42
1:I:280:ILE:HD11	1:I:282:ILE:HD11	2.00	0.42
1:C:141:ASN:ND2	1:C:144:THR:H	2.17	0.42
1:B:117:LEU:HD21	1:B:126:LEU:HD23	2.02	0.42
1:D:6:GLU:CG	1:D:73:ILE:HD11	2.48	0.42
1:E:55:ASP:O	1:E:76:PRO:HB3	2.20	0.42
1:F:179:ASN:HD22	1:F:179:ASN:H	1.68	0.42
1:H:253:ALA:O	1:H:257:THR:CG2	2.67	0.42
1:H:297:HIS:HA	1:H:317:ASN:O	2.20	0.42
1:C:141:ASN:HD22	1:C:143:GLN:H	1.67	0.42
1:B:158:MET:HG3	1:D:158:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:SER:O	1:D:225:LYS:NZ	2.52	0.42
1:I:45:GLU:HA	1:I:64:THR:HA	2.01	0.42
1:L:9:LEU:HD13	1:L:59:LEU:HD21	2.01	0.42
1:B:268:ASN:HD21	1:B:301:LEU:HD23	1.84	0.42
1:B:303:MET:HA	1:B:311:GLU:O	2.20	0.42
1:C:332:ASP:HB2	5:C:642:HOH:O	2.19	0.42
1:D:127:LEU:N	1:D:314:MET:HE1	2.35	0.42
1:G:60:ARG:NH2	5:G:541:HOH:O	2.51	0.42
1:F:168:LYS:HG3	5:F:700:HOH:O	2.20	0.41
1:I:46:LEU:HD12	1:I:46:LEU:C	2.40	0.41
1:L:198:SER:O	1:L:202:ILE:HG12	2.20	0.41
1:H:303:MET:HA	1:H:311:GLU:O	2.20	0.41
1:A:72:GLU:OE2	1:A:80:LYS:HE2	2.20	0.41
1:F:23:ARG:NH1	1:F:23:ARG:CG	2.77	0.41
1:B:257:THR:O	1:B:261:ILE:HG12	2.21	0.41
1:B:64:THR:OG1	1:B:68:SER:HB3	2.20	0.41
1:C:218:SER:C	1:C:225:LYS:HZ1	2.24	0.41
1:C:243:SER:HB3	1:C:334:MET:HE1	2.02	0.41
1:G:120:THR:HG22	1:G:276:PRO:CD	2.47	0.41
1:I:303:MET:HA	1:I:311:GLU:O	2.20	0.41
1:G:141:ASN:C	1:G:141:ASN:HD22	2.24	0.41
1:I:159:ASP:OD2	1:I:247:GLN:HG3	2.21	0.41
1:A:109:HIS:HE1	1:A:134:SER:O	2.03	0.41
1:B:130:THR:HG23	1:B:316:THR:OG1	2.20	0.41
1:C:92:ARG:NH2	1:C:95:GLN:OE1	2.54	0.41
1:D:127:LEU:CA	1:D:314:MET:HE1	2.50	0.41
1:D:223:ASN:HD21	1:K:331:ILE:H	1.68	0.41
1:E:331:ILE:O	1:E:335:VAL:HG23	2.21	0.41
1:F:303:MET:HA	1:F:311:GLU:O	2.20	0.41
1:G:92:ARG:HD2	5:G:488:HOH:O	2.19	0.41
1:K:234:HIS:CE1	1:K:286:GLN:HE22	2.38	0.41
1:L:246:TYR:CZ	1:L:248:SER:HB2	2.55	0.41
1:L:85:LEU:HB3	1:L:93:LEU:HD21	2.02	0.41
1:G:221:SER:OG	1:G:224:GLN:HG2	2.21	0.41
1:G:328:LYS:H	1:G:333:GLU:HG2	1.85	0.41
1:J:88:ASN:HD22	1:J:90:GLN:H	1.69	0.41
1:K:297:HIS:HA	1:K:317:ASN:O	2.20	0.41
1:C:92:ARG:CZ	1:C:95:GLN:OE1	2.69	0.41
1:H:172:ASN:ND2	1:H:285:SER:HA	2.35	0.41
1:L:39:VAL:HG13	5:L:534:HOH:O	2.21	0.41
1:D:110:ARG:NH2	1:D:349:LEU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:SER:HB3	1:E:334:MET:HE1	2.03	0.41
1:J:295:THR:HG22	1:J:297:HIS:CE1	2.56	0.41
1:L:88:ASN:HD22	1:L:90:GLN:N	2.17	0.41
1:D:18:ASN:ND2	1:D:20:THR:H	2.14	0.41
1:J:156:ILE:HG21	1:J:334:MET:HE2	2.03	0.41
1:J:157:PHE:HB3	1:J:190:LEU:HD11	2.03	0.40
1:F:60:ARG:HH11	1:F:60:ARG:CB	2.34	0.40
1:J:221:SER:OG	1:J:224:GLN:HG2	2.22	0.40
1:L:266:GLU:HA	1:L:269:ALA:HB2	2.03	0.40
1:A:143:GLN:CD	1:E:259:GLU:HB2	2.42	0.40
1:A:91:ASN:C	1:A:91:ASN:HD22	2.24	0.40
1:C:137:LEU:HD21	1:C:341:ARG:HD2	2.04	0.40
1:C:253:ALA:O	1:C:257:THR:CG2	2.69	0.40
1:D:56:GLY:O	1:D:74:ARG:NH1	2.54	0.40
1:E:243:SER:HB3	1:E:334:MET:HE3	2.03	0.40
1:J:141:ASN:HD22	1:J:144:THR:H	1.70	0.40
1:J:297:HIS:HA	1:J:317:ASN:O	2.22	0.40
1:J:304:ALA:HB3	1:J:310:ASN:O	2.22	0.40
1:A:40:TYR:HB2	1:A:293:TYR:HB2	2.03	0.40
1:A:8:LEU:HD11	1:A:36:LEU:HG	2.03	0.40
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.88	0.40
1:E:281:ASN:C	1:E:281:ASN:HD22	2.25	0.40
1:H:253:ALA:HB2	1:H:317:ASN:HD22	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/351 (99%)	343 (98%)	6 (2%)	0	100	100
1	B	349/351 (99%)	344 (99%)	4 (1%)	1 (0%)	41	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	342/351 (97%)	333 (97%)	9 (3%)	0	100	100
1	D	337/351 (96%)	325 (96%)	12 (4%)	0	100	100
1	E	345/351 (98%)	338 (98%)	6 (2%)	1 (0%)	41	37
1	F	340/351 (97%)	334 (98%)	6 (2%)	0	100	100
1	G	339/351 (97%)	333 (98%)	6 (2%)	0	100	100
1	H	343/351 (98%)	337 (98%)	6 (2%)	0	100	100
1	I	342/351 (97%)	340 (99%)	2 (1%)	0	100	100
1	J	335/351 (95%)	327 (98%)	8 (2%)	0	100	100
1	K	340/351 (97%)	330 (97%)	9 (3%)	1 (0%)	41	37
1	L	344/351 (98%)	333 (97%)	11 (3%)	0	100	100
All	All	4105/4212 (98%)	4017 (98%)	85 (2%)	3 (0%)	51	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	ASP
1	E	220	GLY
1	K	309	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/312 (100%)	290 (93%)	22 (7%)	14	9
1	B	312/312 (100%)	298 (96%)	14 (4%)	27	24
1	C	304/312 (97%)	280 (92%)	24 (8%)	12	7
1	D	302/312 (97%)	286 (95%)	16 (5%)	22	19
1	E	307/312 (98%)	284 (92%)	23 (8%)	13	8
1	F	304/312 (97%)	275 (90%)	29 (10%)	8	4
1	G	295/312 (95%)	267 (90%)	28 (10%)	8	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	304/312 (97%)	275 (90%)	29 (10%)	8	4
1	I	299/312 (96%)	273 (91%)	26 (9%)	10	6
1	J	298/312 (96%)	273 (92%)	25 (8%)	11	6
1	K	299/312 (96%)	277 (93%)	22 (7%)	13	9
1	L	303/312 (97%)	274 (90%)	29 (10%)	8	4
All	All	3639/3744 (97%)	3352 (92%)	287 (8%)	12	7

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	65	ASN
1	A	77	ASP
1	A	81	ILE
1	A	84	LEU
1	A	91	ASN
1	A	94	LEU
1	A	95	GLN
1	A	101	ARG
1	A	110	ARG
1	A	114	GLU
1	A	125	ASN
1	A	169	LEU
1	A	171	LEU
1	A	183	LEU
1	A	208	ARG
1	A	219	SER
1	A	256	LEU
1	A	257	THR
1	A	272	SER
1	A	349	LEU
1	A	351	ASN
1	B	29	PHE
1	B	73	ILE
1	B	88	ASN
1	B	91	ASN
1	B	94	LEU
1	B	101	ARG
1	B	130	THR
1	B	171	LEU

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Mol	Chain	Res	Type
1	B	183	LEU
1	B	186	ASP
1	B	200	ASN
1	B	257	THR
1	B	301	LEU
1	B	312	MET
1	C	18	ASN
1	C	33	LEU
1	C	60	ARG
1	C	66	SER
1	C	77	ASP
1	C	85	LEU
1	C	90	GLN
1	C	91	ASN
1	C	94	LEU
1	C	97	LEU
1	C	101	ARG
1	C	117	LEU
1	C	138	ILE
1	C	141	ASN
1	C	169	LEU
1	C	183	LEU
1	C	185	ARG
1	C	208	ARG
1	C	256	LEU
1	C	257	THR
1	C	263	LYS
1	C	271	ARG
1	C	307	ASP
1	C	328	LYS
1	D	25	GLU
1	D	26	ARG
1	D	42	LEU
1	D	81	ILE
1	D	94	LEU
1	D	97	LEU
1	D	101	ARG
1	D	141	ASN
1	D	169	LEU
1	D	190	LEU
1	D	200	ASN
1	D	256	LEU

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Mol	Chain	Res	Type
1	D	263	LYS
1	D	294	VAL
1	D	306	GLU
1	D	339	GLN
1	E	12	LEU
1	E	18	ASN
1	E	33	LEU
1	E	46	LEU
1	E	75	THR
1	E	77	ASP
1	E	79	GLU
1	E	90	GLN
1	E	91	ASN
1	E	94	LEU
1	E	97	LEU
1	E	112	LEU
1	E	124	ARG
1	E	141	ASN
1	E	168	LYS
1	E	171	LEU
1	E	179	ASN
1	E	250	ASN
1	E	256	LEU
1	E	257	THR
1	E	281	ASN
1	E	294	VAL
1	E	315	LEU
1	F	16	LEU
1	F	23	ARG
1	F	44	ASN
1	F	49	VAL
1	F	60	ARG
1	F	84	LEU
1	F	88	ASN
1	F	91	ASN
1	F	94	LEU
1	F	97	LEU
1	F	101	ARG
1	F	110	ARG
1	F	114	GLU
1	F	141	ASN
1	F	168	LYS

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Mol	Chain	Res	Type
1	F	169	LEU
1	F	171	LEU
1	F	179	ASN
1	F	183	LEU
1	F	199	ARG
1	F	223	ASN
1	F	224	GLN
1	F	250	ASN
1	F	256	LEU
1	F	257	THR
1	F	268	ASN
1	F	294	VAL
1	F	308	ARG
1	F	351	ASN
1	G	33	LEU
1	G	39	VAL
1	G	44	ASN
1	G	73	ILE
1	G	75	THR
1	G	82	THR
1	G	88	ASN
1	G	91	ASN
1	G	92	ARG
1	G	94	LEU
1	G	97	LEU
1	G	101	ARG
1	G	110	ARG
1	G	122	SER
1	G	123	MET
1	G	141	ASN
1	G	169	LEU
1	G	171	LEU
1	G	179	ASN
1	G	183	LEU
1	G	199	ARG
1	G	206	ILE
1	G	212	GLU
1	G	250	ASN
1	G	256	LEU
1	G	257	THR
1	G	263	LYS
1	G	294	VAL

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Mol	Chain	Res	Type
1	H	2	MET
1	H	33	LEU
1	H	34	THR
1	H	44	ASN
1	H	48	ARG
1	H	60	ARG
1	H	77	ASP
1	H	81	ILE
1	H	85	LEU
1	H	88	ASN
1	H	90	GLN
1	H	91	ASN
1	H	94	LEU
1	H	97	LEU
1	H	110	ARG
1	H	112	LEU
1	H	117	LEU
1	H	122	SER
1	H	141	ASN
1	H	171	LEU
1	H	179	ASN
1	H	216	ARG
1	H	224	GLN
1	H	250	ASN
1	H	256	LEU
1	H	257	THR
1	H	259	GLU
1	H	294	VAL
1	H	350	GLN
1	I	8	LEU
1	I	18	ASN
1	I	20	THR
1	I	46	LEU
1	I	66	SER
1	I	84	LEU
1	I	88	ASN
1	I	90	GLN
1	I	91	ASN
1	I	94	LEU
1	I	97	LEU
1	I	99	ILE
1	I	101	ARG

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Mol	Chain	Res	Type
1	I	141	ASN
1	I	169	LEU
1	I	171	LEU
1	I	183	LEU
1	I	186	ASP
1	I	194	HIS
1	I	208	ARG
1	I	222	ASP
1	I	247	GLN
1	I	250	ASN
1	I	256	LEU
1	I	303	MET
1	I	351	ASN
1	J	12	LEU
1	J	23	ARG
1	J	82	THR
1	J	88	ASN
1	J	89	GLU
1	J	91	ASN
1	J	95	GLN
1	J	112	LEU
1	J	141	ASN
1	J	147	LEU
1	J	158	MET
1	J	171	LEU
1	J	179	ASN
1	J	185	ARG
1	J	190	LEU
1	J	198	SER
1	J	199	ARG
1	J	203	ASP
1	J	250	ASN
1	J	257	THR
1	J	263	LYS
1	J	280	ILE
1	J	294	VAL
1	J	325	GLN
1	J	338	LEU
1	K	33	LEU
1	K	46	LEU
1	K	61	ILE
1	K	75	THR

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Mol	Chain	Res	Type
1	K	81	ILE
1	K	85	LEU
1	K	86	GLU
1	K	88	ASN
1	K	90	GLN
1	K	94	LEU
1	K	117	LEU
1	K	125	ASN
1	K	151	THR
1	K	169	LEU
1	K	191	LYS
1	K	212	GLU
1	K	250	ASN
1	K	256	LEU
1	K	257	THR
1	K	263	LYS
1	K	294	VAL
1	K	331	ILE
1	L	12	LEU
1	L	27	GLN
1	L	39	VAL
1	L	44	ASN
1	L	59	LEU
1	L	77	ASP
1	L	84	LEU
1	L	85	LEU
1	L	86	GLU
1	L	88	ASN
1	L	91	ASN
1	L	94	LEU
1	L	114	GLU
1	L	117	LEU
1	L	141	ASN
1	L	158	MET
1	L	162	ARG
1	L	168	LYS
1	L	171	LEU
1	L	183	LEU
1	L	190	LEU
1	L	191	LYS
1	L	257	THR
1	L	259	GLU

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Mol	Chain	Res	Type
1	L	266	GLU
1	L	268	ASN
1	L	294	VAL
1	L	325	GLN
1	L	341	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	95	GLN
1	A	102	HIS
1	A	109	HIS
1	A	166	ASN
1	A	181	GLN
1	A	209	HIS
1	A	213	GLN
1	A	224	GLN
1	A	291	ASN
1	A	317	ASN
1	B	88	ASN
1	B	91	ASN
1	B	181	GLN
1	B	224	GLN
1	B	234	HIS
1	B	317	ASN
1	C	18	ASN
1	C	90	GLN
1	C	91	ASN
1	C	109	HIS
1	C	141	ASN
1	C	181	GLN
1	C	200	ASN
1	C	213	GLN
1	C	223	ASN
1	C	234	HIS
1	C	258	HIS
1	C	317	ASN
1	D	18	ASN
1	D	27	GLN
1	D	30	GLN
1	D	109	HIS

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Mol	Chain	Res	Type
1	D	141	ASN
1	D	172	ASN
1	D	181	GLN
1	D	200	ASN
1	D	204	HIS
1	D	213	GLN
1	D	223	ASN
1	D	258	HIS
1	D	310	ASN
1	D	339	GLN
1	E	18	ASN
1	E	91	ASN
1	E	141	ASN
1	E	172	ASN
1	E	179	ASN
1	E	181	GLN
1	E	194	HIS
1	E	213	GLN
1	E	234	HIS
1	E	247	GLN
1	E	250	ASN
1	E	281	ASN
1	E	317	ASN
1	E	350	GLN
1	E	351	ASN
1	F	44	ASN
1	F	88	ASN
1	F	91	ASN
1	F	109	HIS
1	F	141	ASN
1	F	172	ASN
1	F	181	GLN
1	F	200	ASN
1	F	213	GLN
1	F	234	HIS
1	F	250	ASN
1	F	268	ASN
1	F	317	ASN
1	F	351	ASN
1	G	44	ASN
1	G	88	ASN
1	G	91	ASN

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Mol	Chain	Res	Type
1	G	95	GLN
1	G	141	ASN
1	G	172	ASN
1	G	179	ASN
1	G	181	GLN
1	G	224	GLN
1	G	234	HIS
1	G	250	ASN
1	G	258	HIS
1	G	297	HIS
1	G	317	ASN
1	H	44	ASN
1	H	88	ASN
1	H	91	ASN
1	H	109	HIS
1	H	141	ASN
1	H	172	ASN
1	H	179	ASN
1	H	181	GLN
1	H	213	GLN
1	H	223	ASN
1	H	250	ASN
1	H	317	ASN
1	H	325	GLN
1	I	18	ASN
1	I	88	ASN
1	I	91	ASN
1	I	141	ASN
1	I	172	ASN
1	I	181	GLN
1	I	194	HIS
1	I	234	HIS
1	I	250	ASN
1	I	268	ASN
1	I	317	ASN
1	I	351	ASN
1	J	88	ASN
1	J	90	GLN
1	J	91	ASN
1	J	141	ASN
1	J	172	ASN
1	J	179	ASN

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Mol	Chain	Res	Type
1	J	181	GLN
1	J	250	ASN
1	J	317	ASN
1	K	44	ASN
1	K	88	ASN
1	K	95	GLN
1	K	125	ASN
1	K	143	GLN
1	K	172	ASN
1	K	181	GLN
1	K	213	GLN
1	K	234	HIS
1	K	250	ASN
1	K	268	ASN
1	K	317	ASN
1	K	325	GLN
1	L	30	GLN
1	L	44	ASN
1	L	88	ASN
1	L	90	GLN
1	L	91	ASN
1	L	109	HIS
1	L	141	ASN
1	L	172	ASN
1	L	181	GLN
1	L	213	GLN
1	L	224	GLN
1	L	258	HIS
1	L	317	ASN
1	L	325	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 19 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z  > 2$
3	FMT	A	404	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	402	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	403	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	L	404	-	0,2,2	0.00	-	0,1,1	0.00	-
4	ACY	J	403	-	1,3,3	1.46	0	0,3,3	0.00	-
3	FMT	D	404	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	L	405	-	0,2,2	0.00	-	0,1,1	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	405	FMT	1	0

## 5.7 Other polymers [i](#)

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	A	351/351 (100%)	0.37	17 (4%) 30 39	16, 27, 50, 63	0
1	B	351/351 (100%)	0.37	19 (5%) 25 34	15, 28, 52, 90	0
1	C	346/351 (98%)	0.54	29 (8%) 11 15	19, 31, 62, 88	0
1	D	341/351 (97%)	0.59	32 (9%) 8 12	18, 32, 60, 71	0
1	E	349/351 (99%)	0.61	33 (9%) 8 12	22, 33, 61, 86	0
1	F	344/351 (98%)	0.56	26 (7%) 13 19	20, 31, 58, 75	0
1	G	343/351 (97%)	0.65	35 (10%) 6 10	24, 41, 70, 85	0
1	H	347/351 (98%)	0.75	47 (13%) 3 3	22, 38, 69, 94	0
1	I	348/351 (99%)	0.70	34 (9%) 7 11	24, 43, 74, 113	0
1	J	341/351 (97%)	0.64	35 (10%) 6 9	26, 41, 63, 80	0
1	K	344/351 (98%)	0.63	37 (10%) 5 8	25, 42, 69, 84	0
1	L	348/351 (99%)	0.54	30 (8%) 10 15	17, 31, 58, 81	0
All	All	4153/4212 (98%)	0.58	374 (9%) 9 14	15, 35, 65, 113	0

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	118	THR	7.9
1	D	309	PRO	6.7
1	H	270	GLU	6.5
1	L	309	PRO	6.4
1	H	20	THR	6.1
1	C	78	ASN	6.0
1	E	309	PRO	5.9
1	G	275	THR	5.8
1	H	269	ALA	5.8
1	H	118	THR	5.6
1	E	118	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	269	ALA	5.3
1	D	24	SER	5.1
1	E	77	ASP	4.9
1	G	77	ASP	4.9
1	F	78	ASN	4.9
1	I	114	GLU	4.8
1	K	78	ASN	4.8
1	A	351	ASN	4.8
1	G	309	PRO	4.8
1	H	309	PRO	4.7
1	B	23	ARG	4.7
1	K	21	TYR	4.7
1	H	351	ASN	4.7
1	D	113	SER	4.7
1	L	274	ASP	4.6
1	I	20	THR	4.6
1	E	275	THR	4.6
1	D	305	PRO	4.5
1	C	270	GLU	4.5
1	C	20	THR	4.5
1	K	20	THR	4.5
1	C	269	ALA	4.5
1	G	76	PRO	4.4
1	F	351	ASN	4.4
1	F	309	PRO	4.4
1	B	27	GLN	4.3
1	K	118	THR	4.3
1	J	114	GLU	4.3
1	B	66	SER	4.3
1	L	305	PRO	4.3
1	K	267	TYR	4.2
1	I	113	SER	4.2
1	F	277	ASN	4.2
1	C	76	PRO	4.1
1	A	65	ASN	4.1
1	H	78	ASN	4.1
1	H	2	MET	4.0
1	H	19	PRO	4.0
1	I	116	ASP	3.9
1	C	277	ASN	3.9
1	H	79	GLU	3.9
1	H	268	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	77	ASP	3.9
1	G	20	THR	3.9
1	K	76	PRO	3.9
1	H	271	ARG	3.9
1	H	306	GLU	3.9
1	I	351	ASN	3.9
1	K	14	PHE	3.8
1	H	14	PHE	3.8
1	E	20	THR	3.8
1	E	277	ASN	3.8
1	L	307	ASP	3.7
1	C	79	GLU	3.7
1	K	266	GLU	3.7
1	I	203	ASP	3.7
1	C	271	ARG	3.6
1	F	282	ILE	3.6
1	H	77	ASP	3.6
1	B	1	GLU	3.6
1	K	265	SER	3.6
1	K	309	PRO	3.6
1	D	65	ASN	3.6
1	K	268	ASN	3.6
1	L	267	TYR	3.6
1	E	271	ARG	3.6
1	I	150	PRO	3.6
1	J	23	ARG	3.5
1	F	19	PRO	3.5
1	F	43	PRO	3.5
1	F	350	GLN	3.5
1	F	20	THR	3.5
1	G	277	ASN	3.4
1	K	223	ASN	3.4
1	E	76	PRO	3.4
1	H	267	TYR	3.4
1	C	19	PRO	3.4
1	E	307	ASP	3.4
1	C	27	GLN	3.4
1	G	2	MET	3.3
1	I	200	ASN	3.3
1	H	113	SER	3.3
1	E	351	ASN	3.3
1	K	277	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	113	SER	3.3
1	F	77	ASP	3.3
1	A	1	GLU	3.3
1	I	193	THR	3.3
1	J	118	THR	3.3
1	H	114	GLU	3.3
1	D	307	ASP	3.2
1	F	118	THR	3.2
1	F	44	ASN	3.2
1	L	268	ASN	3.2
1	I	23	ARG	3.2
1	H	282	ILE	3.2
1	H	76	PRO	3.2
1	G	90	GLN	3.2
1	A	23	ARG	3.2
1	J	67	GLU	3.2
1	D	350	GLN	3.2
1	F	76	PRO	3.1
1	E	78	ASN	3.1
1	J	116	ASP	3.1
1	K	264	ALA	3.1
1	F	23	ARG	3.1
1	B	67	GLU	3.1
1	E	1	GLU	3.1
1	G	349	LEU	3.1
1	K	351	ASN	3.1
1	J	199	ARG	3.1
1	E	43	PRO	3.1
1	J	115	MET	3.1
1	G	19	PRO	3.1
1	K	1	GLU	3.1
1	I	149	GLY	3.0
1	K	2	MET	3.0
1	D	27	GLN	3.0
1	C	276	PRO	3.0
1	H	223	ASN	3.0
1	J	200	ASN	3.0
1	A	36	LEU	3.0
1	K	23	ARG	3.0
1	K	77	ASP	3.0
1	D	282	ILE	3.0
1	H	307	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	309	PRO	3.0
1	I	194	HIS	3.0
1	J	188	LEU	3.0
1	E	306	GLU	2.9
1	J	196	SER	2.9
1	G	75	THR	2.9
1	G	121	THR	2.9
1	F	268	ASN	2.9
1	A	14	PHE	2.9
1	J	280	ILE	2.9
1	K	113	SER	2.9
1	C	1	GLU	2.9
1	F	79	GLU	2.9
1	C	36	LEU	2.9
1	H	277	ASN	2.9
1	H	120	THR	2.9
1	L	275	THR	2.9
1	D	20	THR	2.8
1	K	120	THR	2.8
1	G	28	SER	2.8
1	G	308	ARG	2.8
1	F	114	GLU	2.8
1	G	264	ALA	2.8
1	G	113	SER	2.8
1	B	309	PRO	2.8
1	C	43	PRO	2.8
1	H	116	ASP	2.8
1	D	279	CYS	2.8
1	E	120	THR	2.8
1	F	306	GLU	2.8
1	K	308	ARG	2.8
1	L	311	GLU	2.8
1	I	273	LEU	2.8
1	D	269	ALA	2.8
1	D	114	GLU	2.7
1	J	77	ASP	2.7
1	F	269	ALA	2.7
1	E	270	GLU	2.7
1	J	294	VAL	2.7
1	H	350	GLN	2.7
1	E	305	PRO	2.7
1	I	183	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	117	LEU	2.7
1	K	75	THR	2.7
1	I	29	PHE	2.7
1	E	133	LEU	2.7
1	D	296	SER	2.7
1	L	113	SER	2.7
1	J	350	GLN	2.7
1	C	120	THR	2.7
1	C	223	ASN	2.6
1	J	78	ASN	2.6
1	J	204	HIS	2.6
1	A	309	PRO	2.6
1	D	336	ARG	2.6
1	K	81	ILE	2.6
1	B	28	SER	2.6
1	J	66	SER	2.6
1	F	267	TYR	2.6
1	E	268	ASN	2.6
1	E	44	ASN	2.6
1	I	1	GLU	2.6
1	G	120	THR	2.6
1	L	282	ILE	2.6
1	K	43	PRO	2.6
1	L	114	GLU	2.6
1	G	118	THR	2.5
1	C	90	GLN	2.5
1	F	14	PHE	2.5
1	K	307	ASP	2.5
1	F	97	LEU	2.5
1	I	40	TYR	2.5
1	D	284	ILE	2.5
1	I	192	ASP	2.5
1	L	280	ILE	2.5
1	C	306	GLU	2.5
1	F	294	VAL	2.5
1	I	115	MET	2.5
1	J	267	TYR	2.5
1	B	280	ILE	2.5
1	B	282	ILE	2.5
1	G	284	ILE	2.5
1	I	39	VAL	2.5
1	D	311	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	44	ASN	2.5
1	K	304	ALA	2.5
1	E	23	ARG	2.5
1	H	266	GLU	2.5
1	B	38	PRO	2.4
1	C	23	ARG	2.4
1	D	294	VAL	2.4
1	D	266	GLU	2.4
1	K	116	ASP	2.4
1	L	28	SER	2.4
1	D	29	PHE	2.4
1	I	65	ASN	2.4
1	J	278	ALA	2.4
1	K	90	GLN	2.4
1	G	268	ASN	2.4
1	H	119	ASP	2.4
1	D	267	TYR	2.4
1	J	24	SER	2.4
1	H	84	LEU	2.4
1	H	97	LEU	2.4
1	I	36	LEU	2.4
1	J	31	GLU	2.4
1	H	98	PRO	2.4
1	J	150	PRO	2.4
1	B	114	GLU	2.4
1	H	75	THR	2.4
1	K	311	GLU	2.4
1	H	23	ARG	2.4
1	G	84	LEU	2.4
1	B	351	ASN	2.4
1	I	201	VAL	2.4
1	C	2	MET	2.4
1	I	325	GLN	2.4
1	G	267	TYR	2.4
1	J	279	CYS	2.3
1	H	263	LYS	2.3
1	G	265	SER	2.3
1	H	344	ALA	2.3
1	K	262	SER	2.3
1	C	110	ARG	2.3
1	D	74	ARG	2.3
1	I	350	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	220	GLY	2.3
1	J	2	MET	2.3
1	J	149	GLY	2.3
1	A	38	PRO	2.3
1	A	98	PRO	2.3
1	D	14	PHE	2.3
1	H	305	PRO	2.3
1	L	24	SER	2.3
1	G	223	ASN	2.3
1	J	65	ASN	2.3
1	D	1	GLU	2.3
1	B	209	HIS	2.3
1	C	307	ASP	2.3
1	J	203	ASP	2.3
1	D	38	PRO	2.3
1	H	43	PRO	2.3
1	H	283	SER	2.3
1	J	195	SER	2.3
1	G	23	ARG	2.3
1	B	29	PHE	2.3
1	D	295	THR	2.3
1	K	119	ASP	2.3
1	G	276	PRO	2.3
1	H	24	SER	2.3
1	H	90	GLN	2.3
1	L	127	LEU	2.2
1	B	14	PHE	2.2
1	G	193	THR	2.2
1	L	295	THR	2.2
1	A	271	ARG	2.2
1	E	266	GLU	2.2
1	A	18	ASN	2.2
1	L	266	GLU	2.2
1	I	154	SER	2.2
1	L	43	PRO	2.2
1	B	130	THR	2.2
1	H	325	GLN	2.2
1	F	188	LEU	2.2
1	E	19	PRO	2.2
1	E	22	SER	2.2
1	L	38	PRO	2.2
1	K	192	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	269	ALA	2.2
1	I	282	ILE	2.2
1	I	311	GLU	2.2
1	L	336	ARG	2.2
1	L	65	ASN	2.2
1	A	280	ILE	2.2
1	E	244	ALA	2.2
1	G	307	ASP	2.2
1	B	131	SER	2.2
1	E	131	SER	2.2
1	I	191	LYS	2.2
1	I	195	SER	2.2
1	A	61	ILE	2.1
1	E	350	GLN	2.1
1	F	99	ILE	2.1
1	L	76	PRO	2.1
1	J	281	ASN	2.1
1	D	116	ASP	2.1
1	L	279	CYS	2.1
1	H	219	SER	2.1
1	D	67	GLU	2.1
1	K	306	GLU	2.1
1	D	43	PRO	2.1
1	F	38	PRO	2.1
1	K	305	PRO	2.1
1	E	65	ASN	2.1
1	K	97	LEU	2.1
1	H	220	GLY	2.1
1	A	131	SER	2.1
1	B	21	TYR	2.1
1	D	120	THR	2.1
1	G	116	ASP	2.1
1	H	336	ARG	2.1
1	C	266	GLU	2.1
1	E	282	ILE	2.1
1	G	282	ILE	2.1
1	E	272	SER	2.1
1	A	39	VAL	2.1
1	D	298	THR	2.1
1	J	269	ALA	2.1
1	L	276	PRO	2.1
1	L	121	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	336	ARG	2.1
1	J	28	SER	2.1
1	A	281	ASN	2.1
1	G	114	GLU	2.1
1	L	116	ASP	2.1
1	G	66	SER	2.0
1	I	120	THR	2.0
1	L	294	VAL	2.0
1	G	306	GLU	2.0
1	H	89	GLU	2.0
1	E	308	ARG	2.0
1	G	119	ASP	2.0
1	L	351	ASN	2.0
1	I	43	PRO	2.0
1	C	97	LEU	2.0
1	J	20	THR	2.0
1	I	326	GLY	2.0
1	B	44	ASN	2.0
1	C	30	GLN	2.0
1	H	221	SER	2.0
1	K	44	ASN	2.0
1	C	309	PRO	2.0
1	A	282	ILE	2.0
1	C	193	THR	2.0
1	H	99	ILE	2.0
1	L	169	LEU	2.0
1	G	192	ASP	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(Å <sup>2</sup> )	Q<0.9
2	MG	D	402	1/1	0.70	0.19	44,44,44,44	0
2	MG	I	402	1/1	0.73	0.10	64,64,64,64	0
2	MG	H	401	1/1	0.83	0.07	63,63,63,63	0
2	MG	C	401	1/1	0.84	0.07	39,39,39,39	0
2	MG	E	401	1/1	0.85	0.07	47,47,47,47	0
2	MG	L	402	1/1	0.87	0.48	60,60,60,60	0
3	FMT	B	402	3/3	0.87	0.13	44,44,44,44	0
2	MG	F	402	1/1	0.89	0.14	46,46,46,46	0
2	MG	J	401	1/1	0.90	0.07	46,46,46,46	0
2	MG	D	401	1/1	0.90	0.06	34,34,34,34	0
4	ACY	J	403	4/4	0.90	0.21	57,57,57,57	0
2	MG	D	403	1/1	0.91	0.10	54,54,54,54	0
2	MG	L	403	1/1	0.91	0.07	49,49,49,49	0
2	MG	C	402	1/1	0.92	0.07	59,59,59,59	0
2	MG	A	401	1/1	0.92	0.13	27,27,27,27	0
3	FMT	L	405	3/3	0.92	0.21	35,35,35,35	0
2	MG	J	402	1/1	0.93	0.07	39,39,39,39	0
2	MG	L	401	1/1	0.94	0.08	34,34,34,34	0
2	MG	I	401	1/1	0.94	0.15	34,34,34,34	0
3	FMT	A	403	3/3	0.95	0.23	39,39,39,39	0
2	MG	A	402	1/1	0.96	0.07	31,31,31,31	0
2	MG	B	401	1/1	0.96	0.11	35,35,35,35	0
3	FMT	A	404	3/3	0.96	0.20	34,34,34,35	0
3	FMT	D	404	3/3	0.97	0.15	21,21,21,21	0
2	MG	F	401	1/1	0.97	0.11	30,30,30,30	0
3	FMT	L	404	3/3	0.98	0.12	21,21,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.