



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:44 PM UTC

PDB ID : 4FMA / pdb_00004fma
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

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

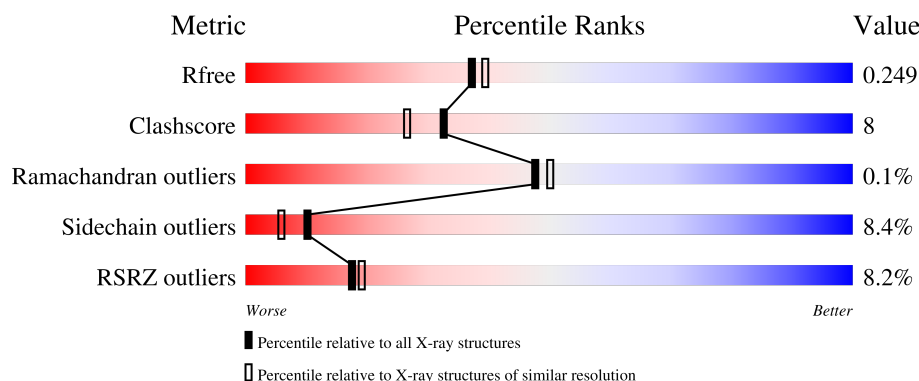
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 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	A	351	3% 85% 12% .
1	B	351	7% 87% 11% .
1	C	351	7% 82% 14% ..
1	D	351	8% 80% 16% ..
1	E	351	5% 80% 16% ..

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Mol	Chain	Length	Quality of chain
1	F	351	6% 76% 18%
1	G	351	10% 78% 17%
1	H	351	9% 80% 15%
1	I	351	14% 80% 16%
1	J	351	11% 75% 18%
1	K	351	9% 79% 16%
1	L	351	8% 78% 17%

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 (CCD ID: MG) (formula: Mg).

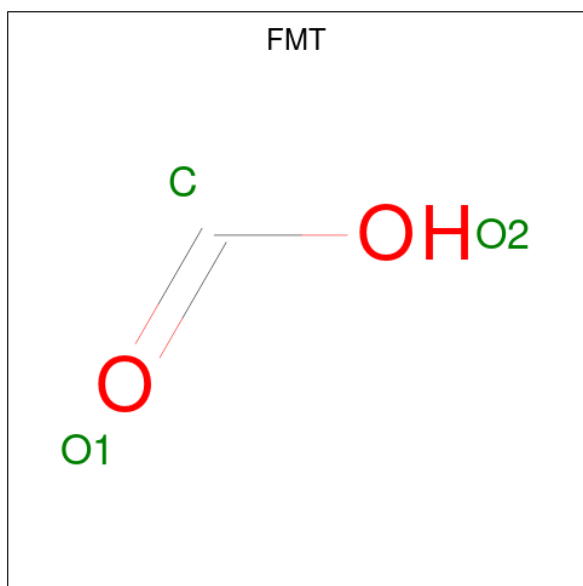
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	1	Total	Mg	0	0
			1	1		

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

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



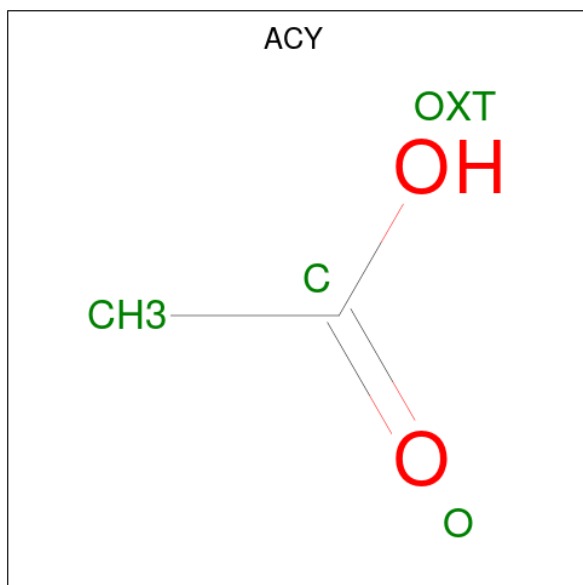
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 3	C 1	O 2	0	0
3	A	1	Total 3	C 1	O 2	0	0
3	B	1	Total 3	C 1	O 2	0	0

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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 (CCD ID: ACY) (formula: C₂H₄O₂).



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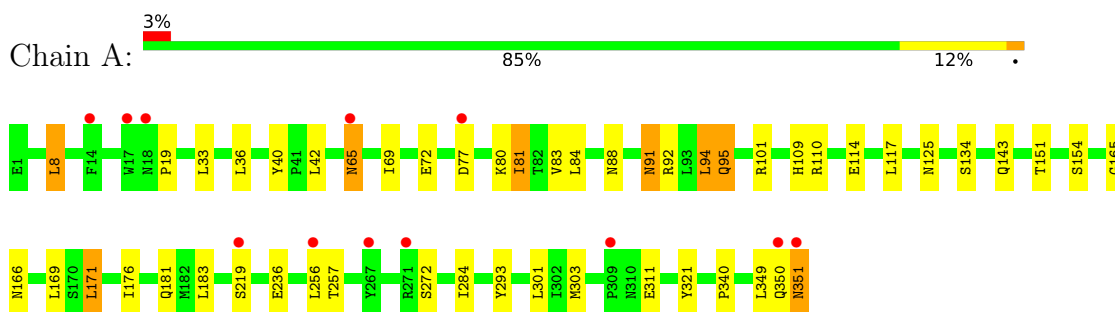
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	240	Total 240	O 240	0	0
5	G	164	Total 164	O 164	0	0
5	H	196	Total 196	O 196	0	0
5	I	153	Total 153	O 153	0	0
5	J	152	Total 152	O 152	0	0
5	K	184	Total 184	O 184	0	0
5	L	227	Total 227	O 227	0	0

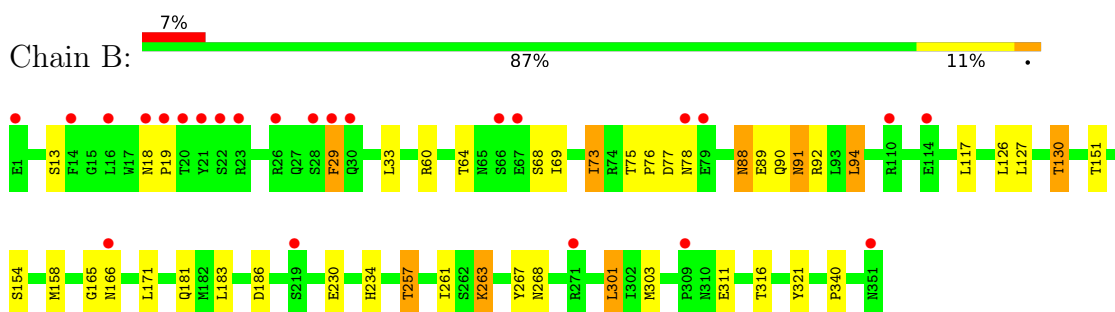
3 Residue-property plots [i](#)

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.

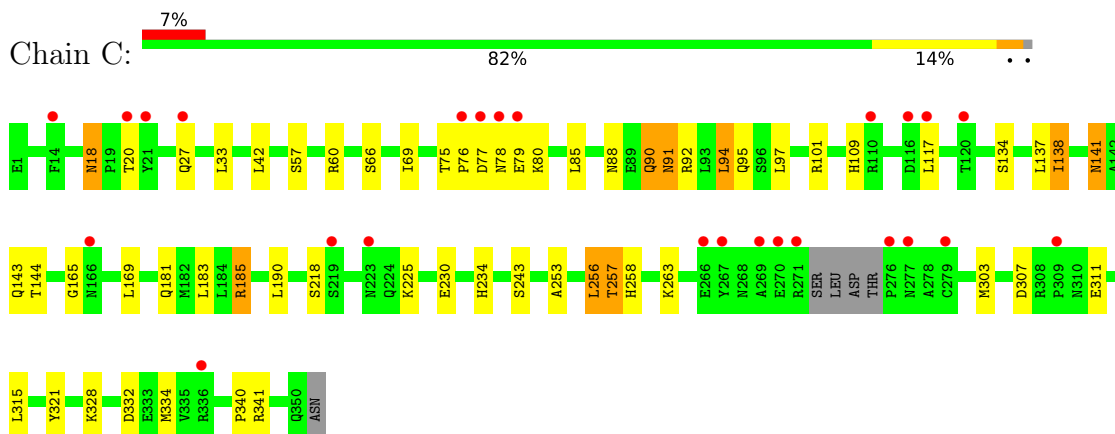
- Molecule 1: EspG protein



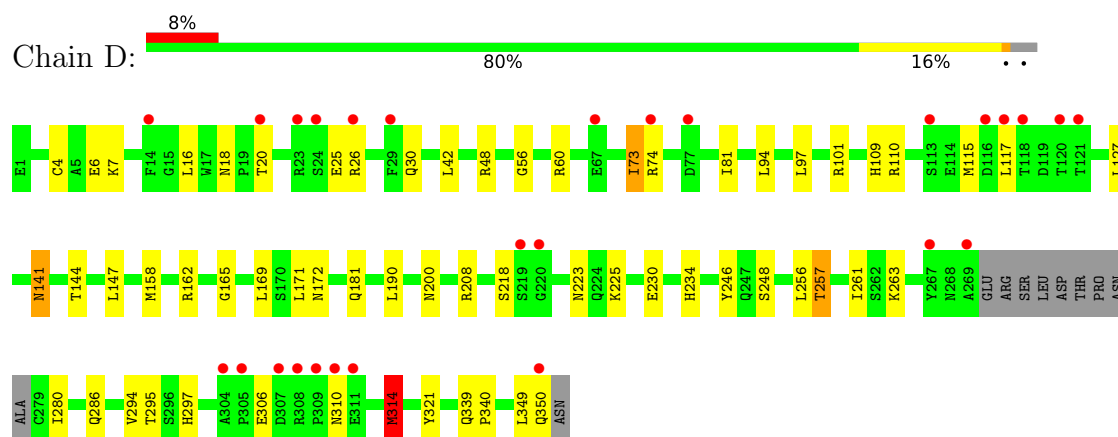
- Molecule 1: EspG protein



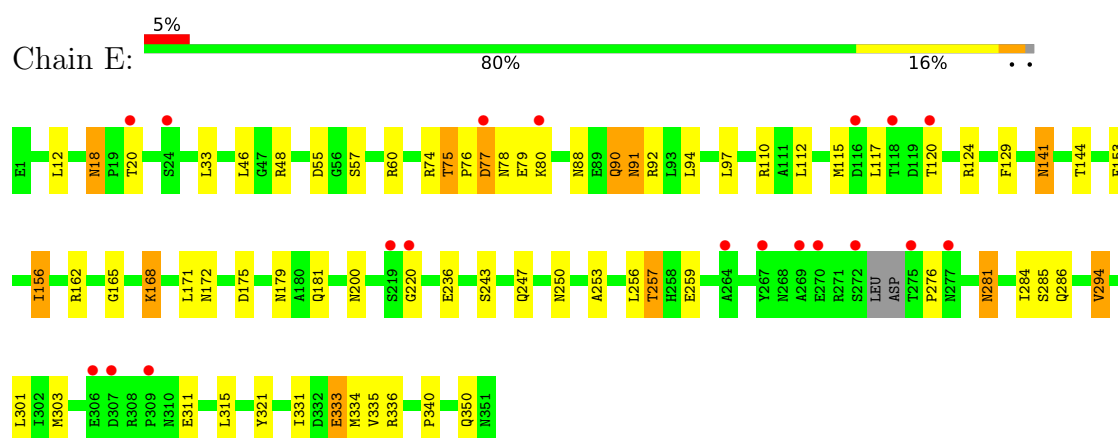
- Molecule 1: EspG protein



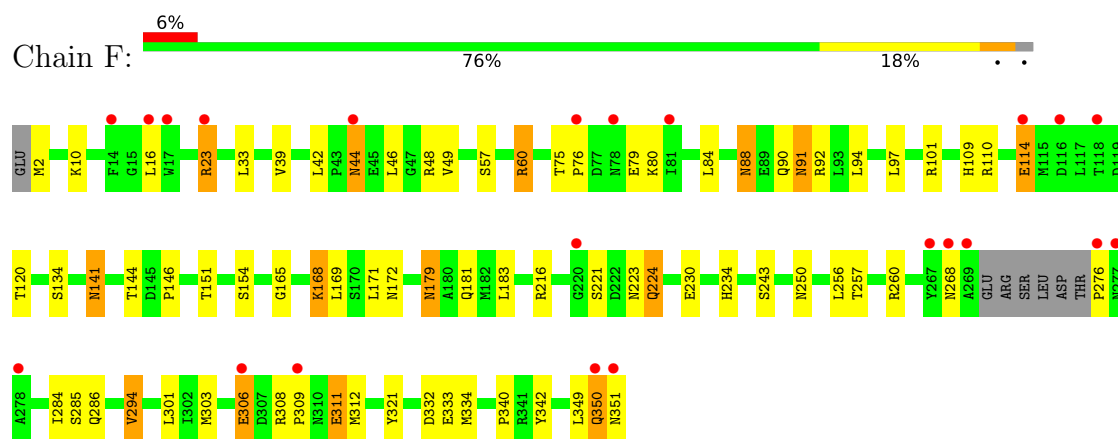
- Molecule 1: EspG protein



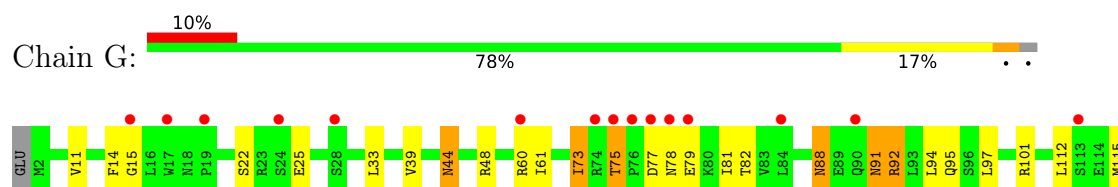
• Molecule 1: EspG protein

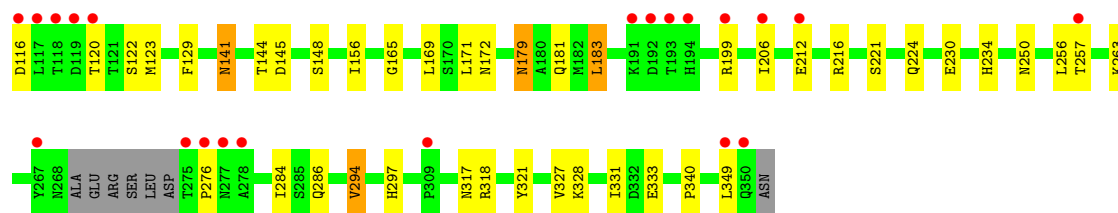


• Molecule 1: EspG protein

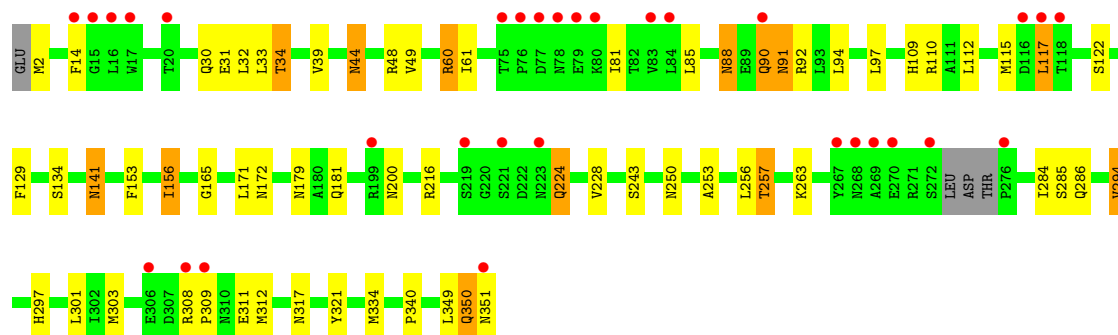
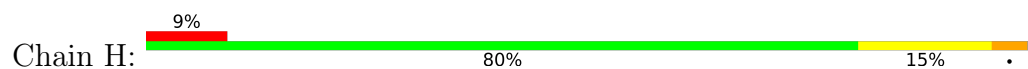


• Molecule 1: EspG protein

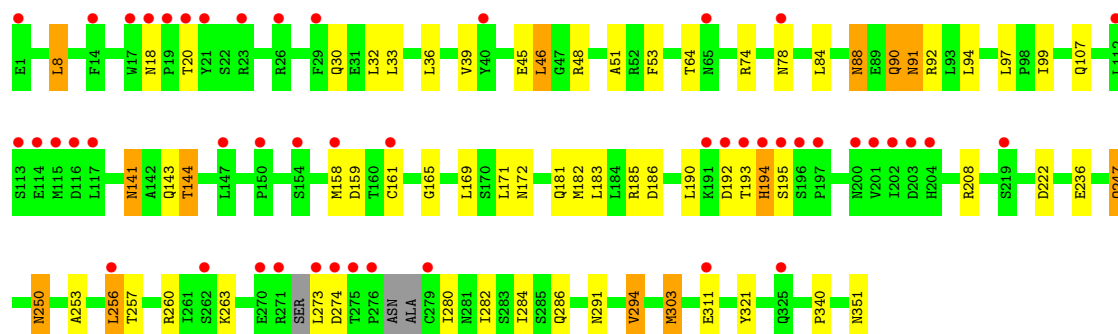




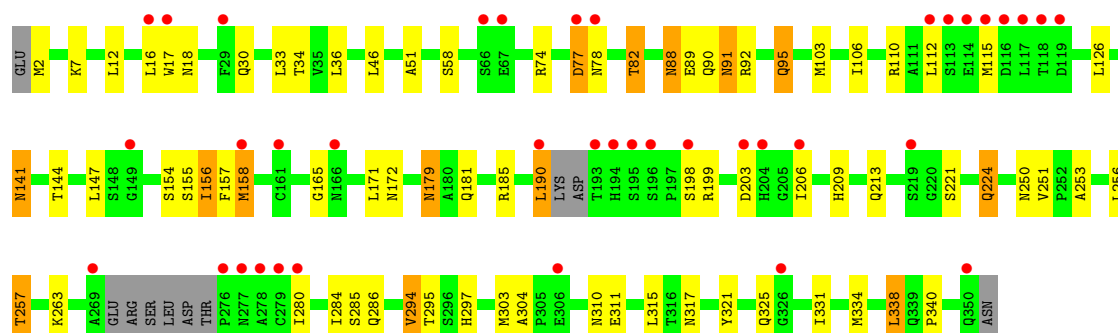
• Molecule 1: EspG protein



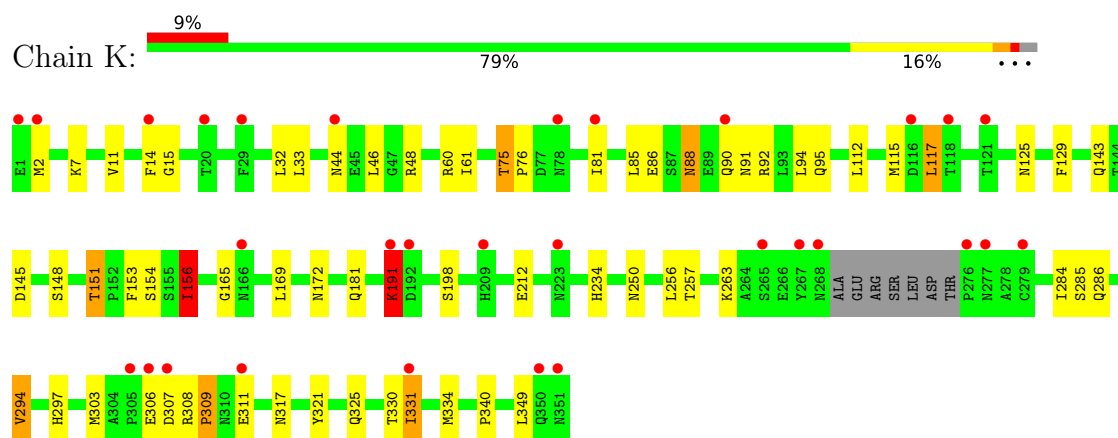
• Molecule 1: EspG protein



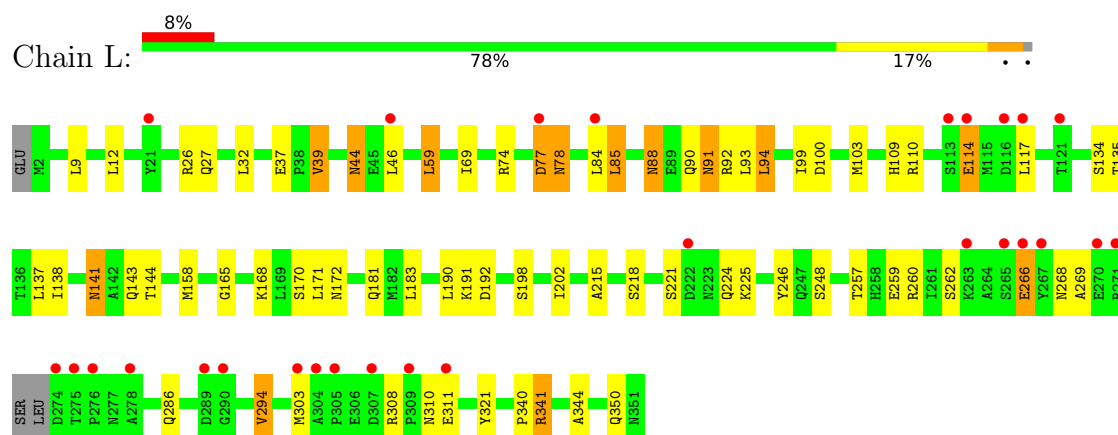
• Molecule 1: EspG protein



• 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, α , β , γ	94.61Å 167.74Å 361.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 50.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.15) 99.8 (50.00-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	29.7	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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: ACY, FMT, MG

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	0.55	0/2767	0.80	0/3758
1	B	0.54	0/2767	0.81	0/3758
1	C	0.53	0/2718	0.83	3/3689 (0.1%)
1	D	0.57	2/2682 (0.1%)	0.82	0/3641
1	E	0.51	0/2743	0.81	1/3724 (0.0%)
1	F	0.54	0/2705	0.85	4/3672 (0.1%)
1	G	0.50	0/2674	0.83	2/3633 (0.1%)
1	H	0.51	0/2725	0.81	2/3699 (0.1%)
1	I	0.51	0/2703	0.86	1/3673 (0.0%)
1	J	0.49	1/2669 (0.0%)	0.83	4/3623 (0.1%)
1	K	0.50	1/2686 (0.0%)	0.84	3/3649 (0.1%)
1	L	0.55	1/2720 (0.0%)	0.85	4/3695 (0.1%)
All	All	0.52	5/32559 (0.0%)	0.83	24/44214 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	314	MET	SD-CE	-8.00	1.59	1.79
1	L	294	VAL	C-O	-6.48	1.17	1.24
1	J	251	VAL	CA-CB	6.01	1.57	1.54
1	D	314	MET	C-O	-5.56	1.17	1.24
1	K	14	PHE	C-O	-5.28	1.17	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	LYS	N-CA-C	10.37	125.35	108.34
1	K	14	PHE	N-CA-C	8.67	121.98	111.40
1	G	14	PHE	N-CA-C	7.76	123.22	112.04
1	J	156	ILE	N-CA-C	7.14	117.28	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	350	GLN	N-CA-C	6.91	120.25	110.23
1	K	156	ILE	N-CA-C	6.87	117.63	110.62
1	L	308	ARG	CA-C-N	6.37	127.80	119.84
1	L	308	ARG	C-N-CA	6.37	127.80	119.84
1	F	349	LEU	CA-C-N	6.34	129.71	120.71
1	F	349	LEU	C-N-CA	6.34	129.71	120.71
1	H	14	PHE	N-CA-C	6.17	118.93	111.40
1	L	294	VAL	N-CA-C	6.11	117.28	108.48
1	K	191	LYS	N-CA-C	5.84	117.32	111.07
1	E	156	ILE	N-CA-C	5.81	116.55	110.62
1	G	156	ILE	N-CA-C	5.72	115.92	110.42
1	H	156	ILE	N-CA-C	5.60	116.33	110.62
1	C	42	LEU	CA-C-N	5.56	125.66	119.32
1	C	42	LEU	C-N-CA	5.56	125.66	119.32
1	F	350	GLN	CB-CA-C	-5.56	100.49	109.72
1	L	78	ASN	N-CA-CB	-5.47	107.93	114.17
1	J	77	ASP	N-CA-C	5.36	121.57	114.12
1	I	194	HIS	N-CA-C	-5.27	102.40	110.30
1	J	18	ASN	CA-C-N	5.04	125.31	119.47
1	J	18	ASN	C-N-CA	5.04	125.31	119.47

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	A	2719	0	2674	27	0
1	B	2719	0	2674	36	0
1	C	2671	0	2629	36	0
1	D	2636	0	2592	36	0
1	E	2696	0	2646	42	0
1	F	2658	0	2617	50	0
1	G	2627	0	2574	46	0
1	H	2678	0	2629	46	0
1	I	2658	0	2587	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2624	0	2576	50	0
1	K	2639	0	2588	37	0
1	L	2673	0	2621	52	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	498	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 (498) 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:J:156:ILE:HG21	1:J:334:MET:HE1	1.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:F:350:GLN:OE1	1.73	0.85
1:L:77:ASP:CG	1:L:77:ASP:O	2.19	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:B:263:LYS:HD2	1:B:303:MET:HE2	1.62	0.81
1:J:77:ASP:N	1:J:78:ASN:HA	1.93	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:D:127:LEU:HA	1:D:314:MET:HE1	1.64	0.78
1:E:120:THR:HG22	1:E:276:PRO:HD3	1.64	0.77
1:H:156:ILE:HD13	1:H:334:MET:HE1	1.67	0.77
1:B:263:LYS:HD2	1:B:303:MET:CE	2.15	0.76
1:D:127:LEU:CA	1:D:314:MET:HE1	2.14	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:G:172:ASN:HD21	1:G:286:GLN:H	1.37	0.73
1:I:158:MET:HE1	1:I:193:THR:CG2	2.19	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	0.73
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:HH21	1:H:60:ARG:CG	2.03	0.72
1:K:172:ASN:HD21	1:K:286:GLN:H	1.37	0.72
1:L:69:ILE:HD11	1:L:94:LEU:HD22	1.70	0.72
1:E:243:SER:HB3	1:E:334:MET:HE3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:ILE:HG12	1:K:334:MET:HE1	1.72	0.71
1:D:172:ASN:ND2	1:D:286:GLN:H	1.88	0.71
1:L:46:LEU:HD13	1:L:99:ILE:CG2	2.18	0.71
1:L:46:LEU:CD1	1:L:99:ILE:HG23	2.20	0.71
1:I:193:THR:O	1:I:194:HIS:C	2.30	0.71
1:F:60:ARG:HH11	1:F:60:ARG:CG	2.03	0.71
1:G:44:ASN:HD22	1:G:44:ASN:H	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:H:200:ASN:CG	1:J:78:ASN:HB2	2.15	0.70
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:HH21	1:H:60:ARG:HG3	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:57:SER:HB3	1:E:76:PRO:HD3	1.76	0.67
1:E:110:ARG:HD2	1:E:350:GLN:HE21	1.59	0.67
1:G:115:MET:HE1	1:G:129:PHE:HB2	1.76	0.67
1:H:60:ARG:HH21	1:H:60:ARG:HB2	1.60	0.67
1:H:243:SER:HB3	1:H:334:MET:HE3	1.78	0.66
1:K:308:ARG:HB3	1:K:309:PRO:HD2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:253:ALA:O	1:H:257:THR:HG23	1.97	0.65
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:243:SER:HB3	1:F:334:MET:HE3	1.79	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:D:208:ARG:HE	1:K:151:THR:HG21	1.62	0.63
1:J:321:TYR:HB3	1:J:340:PRO:HA	1.80	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:I:192:ASP:O	1:I:193:THR:C	2.40	0.62
1:H:165:GLY:H	1:H:181:GLN:NE2	1.97	0.62
1:L:77:ASP:O	1:L:77:ASP:OD2	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: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:E:115:MET:HE1	1:E:129:PHE:HB2	1.82	0.60
1:I:182:MET:HE1	1:I:185:ARG:HH21	1.66	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:F:114:GLU:CD	1:F:114:GLU:H	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:321:TYR:HB3	1:I:340:PRO:HA	1.85	0.59
1:H:60:ARG:HH21	1:H:60:ARG:CB	2.14	0.59
1:H:284:ILE:HG12	1:H:294:VAL:HB	1.82	0.59
1:L:141:ASN:C	1:L:141:ASN:HD22	2.11	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:J:157:PHE:H	1:J:158:MET:HE2	1.68	0.58
1:F:88:ASN:HD22	1:F:90:GLN:H	1.52	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:C:141:ASN:C	1:C:141:ASN:HD22	2.12	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:A:166:ASN:ND2	5:A:671:HOH:O	2.36	0.57
1:K:156:ILE:HG12	1:K:334:MET:CE	2.33	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: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:F:141:ASN:C	1:F:141:ASN:HD22	2.14	0.55
1:I:161:CYS:SG	1:I:185:ARG:NH1	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:44:ASN:H	1:H:44:ASN:ND2	1.96	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:J:154:SER:O	1:J:158:MET:HE3	2.07	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:E:321:TYR:HB3	1:E:340:PRO:HA	1.90	0.54
1:B:76:PRO:C	1:B:78:ASN:H	2.14	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:75:THR:O	1:C:76:PRO:C	2.50	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:E:141:ASN:C	1:E:141:ASN:HD22	2.17	0.53
1:J:284:ILE:HG12	1:J:294:VAL:HB	1.89	0.53
1:E:156:ILE:HD13	1:E:334:MET:HE1	1.91	0.53
1:I:141:ASN:C	1:I:141:ASN:HD22	2.16	0.53
1:F:172:ASN:ND2	1:F:286:GLN:H	2.01	0.53
1:K:151:THR:O	1:K:151:THR:HG22	2.08	0.53
1:H:263:LYS:HG3	1:H:303:MET:HE2	1.90	0.53
1:J:158:MET:SD	1:J:158:MET:N	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:L:77:ASP:OD2	1:L:77:ASP:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:159:ASP:CG	1:I:247:GLN:HG3	2.35	0.52
1:D:141:ASN:C	1:D:141:ASN:HD22	2.18	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:E:284:ILE:HG12	1:E:294:VAL:HB	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:HE21	1:A:95:GLN:N	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: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:J:331:ILE:HA	1:J:334:MET:HE2	1.93	0.50
1:L:141:ASN:HD21	1:L:143:GLN:HB3	1.76	0.50
1:C:243:SER:HB3	1:C:334:MET:HE3	1.93	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: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: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:C:91:ASN:HD22	1:C:91:ASN:C	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:GLU:OE2	1:L:170:SER:OG	2.22	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
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:H:115:MET:HE1	1:H:129:PHE:HB2	1.93	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
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: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:B:267:TYR:HB2	1:B:303:MET:HE1	1.95	0.48
1:F:306:GLU:H	1:F:306:GLU:CD	2.20	0.48
1:H:60:ARG:HG3	1:H:60:ARG:NH2	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:HG2	1:F:23:ARG:NH1	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:OD2	1:E:77:ASP:N	2.47	0.48
1:G:75:THR:HG22	1:G:79:GLU:H	1.78	0.48
1:K:2:MET:HE3	1:K:7:LYS:HA	1.96	0.48
1:D:127:LEU:HA	1:D:314:MET:CE	2.40	0.48
1:H:109:HIS:HD2	5:H:557:HOH:O	1.96	0.48
1:L:91:ASN:HD22	1:L:92:ARG:N	2.11	0.48
1:L:137:LEU:CD2	1:L:341:ARG:HD3	2.43	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:69:ILE:HD11	1:A:94:LEU:HD13	1.96	0.48
1:A:151:THR:HB	1:A:154:SER:HB3	1.95	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:J:141:ASN:HD22	1:J:141:ASN:C	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:29:PHE:CD1	1:B:29:PHE:C	2.92	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
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:H:39:VAL:HG23	1:H:48:ARG:HG3	1.98	0.46
1:I:46:LEU:C	1:I:46:LEU:HD12	2.40	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:O	1:K:151:THR:HG23	2.14	0.46
1:G:141:ASN:C	1:G:141:ASN:HD22	2.24	0.46
1:J:157:PHE:N	1:J:158:MET:HE2	2.30	0.46
1:B:166:ASN:OD1	1:D:162:ARG:NH1	2.49	0.46
1:C:75:THR:HG1	1:C:79:GLU:HA	1.80	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:4:CYS:HA	1:D:7:LYS:HE3	1.98	0.45
1:D:230:GLU:O	1:D:234:HIS:CD2	2.69	0.45
1:L:46:LEU:CD1	1:L:99:ILE:CG2	2.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:243:SER:HB3	1:E:334:MET:CE	2.42	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:A:91:ASN:HD22	1:A:91:ASN:C	2.24	0.45
1:A:143:GLN:CD	1:E:259:GLU:HB2	2.42	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:B:158:MET:HG2	1:D:158:MET:HE1	1.98	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:J:88:ASN:ND2	1:J:91:ASN:H	2.14	0.45
1:K:112:LEU:HD12	1:K:115:MET:HE3	1.98	0.45
1:C:218:SER:C	1:C:225:LYS:HZ1	2.24	0.45
1:D:295:THR:HG22	1:D:297:HIS:CE1	2.51	0.45
1:E:281:ASN:C	1:E:281:ASN:HD22	2.25	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:K:306:GLU:HA	1:K:307:ASP:C	2.42	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:91:ASN:HD22	1:J:91:ASN:C	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:30:GLN:HE22	1:D:115:MET:HE3	1.81	0.44
1:F:172:ASN:ND2	1:F:285:SER:HA	2.33	0.44
1:G:115:MET:HE1	1:G:129:PHE:CB	2.47	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: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:88:ASN:H	1:L:91:ASN:ND2	2.15	0.44
1:L:141:ASN:ND2	1:L:143:GLN:HB3	2.32	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:E:200:ASN:CG	1:I:78:ASN:HA	2.43	0.43
1:F:141:ASN:ND2	1:F:144:THR:H	2.15	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:77:ASP:HA	1:G:78:ASN:HA	1.80	0.43
1:G:179:ASN:O	1:G:183:LEU:HD22	2.18	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:H:88:ASN:C	1:H:88:ASN:HD22	2.27	0.43
1:J:179:ASN:H	1:J:179:ASN:HD22	1.66	0.43
1:D:127:LEU:N	1:D:314:MET:HE1	2.33	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:G:112:LEU:HD12	1:G:115:MET:HE3	2.01	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:334:MET:O	1:J:338:LEU:HB2	2.19	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:A:350:GLN:O	1:A:351:ASN:C	2.62	0.43
1:K:88:ASN:ND2	1:K:90:GLN:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:115:MET:HE1	1:K:129:PHE:HB2	2.01	0.43
1:L:91:ASN:HD22	1:L:91:ASN:C	2.26	0.42
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:G:91:ASN:HD22	1:G:91:ASN:C	2.28	0.42
1:I:250:ASN:H	1:I:250:ASN:HD22	1.68	0.42
1:L:88:ASN:ND2	1:L:91:ASN:H	2.18	0.42
1:L:138:ILE:HD11	1:L:344:ALA:HB3	2.01	0.42
1:I:159:ASP:OD1	1:I:247:GLN:HG3	2.20	0.42
1:J:115:MET:HE3	1:J:126:LEU:HD13	2.01	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:H:141:ASN:C	1:H:141:ASN:HD22	2.26	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:91:ASN:HD22	1:F:91:ASN:C	2.27	0.42
1:F:114:GLU:CD	1:F:114:GLU:N	2.77	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: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:G:60:ARG:NH2	5:G:541:HOH:O	2.51	0.42
1:H:301:LEU:HB3	1:H:312:MET:HE3	2.02	0.42
1:F:168:LYS:HG3	5:F:700:HOH:O	2.20	0.41
1:L:198:SER:O	1:L:202:ILE:HG12	2.20	0.41
1:G:88:ASN:HD22	1:G:88:ASN:C	2.27	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:CG	1:F:23:ARG:NH1	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:THR:OG1	1:B:68:SER:HB3	2.20	0.41
1:B:257:THR:O	1:B:261:ILE:HG12	2.21	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:B:76:PRO:C	1:B:78:ASN:N	2.79	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: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:85:LEU:HB3	1:L:93:LEU:HD21	2.02	0.41
1:L:246:TYR:CZ	1:L:248:SER:HB2	2.55	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:B:60:ARG:HD2	1:B:60:ARG:C	2.45	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
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:B:158:MET:CG	1:D:158:MET:HE1	2.51	0.40
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:F:301:LEU:HD13	1:F:312:MET:HE2	2.03	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: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: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:8:LEU:HD11	1:A:36:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TYR:HB2	1:A:293:TYR:HB2	2.03	0.40
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.88	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%)	36	34
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%)	36	34
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%)	36	34
1	L	344/351 (98%)	333 (97%)	11 (3%)	0	100	100
All	All	4105/4212 (98%)	4017 (98%)	85 (2%)	3 (0%)	48	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	ASP

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Mol	Chain	Res	Type
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%)	289 (93%)	23 (7%)	13	8
1	B	312/312 (100%)	297 (95%)	15 (5%)	23	20
1	C	304/312 (97%)	281 (92%)	23 (8%)	12	8
1	D	302/312 (97%)	280 (93%)	22 (7%)	13	8
1	E	307/312 (98%)	282 (92%)	25 (8%)	11	7
1	F	304/312 (97%)	269 (88%)	35 (12%)	5	2
1	G	295/312 (95%)	266 (90%)	29 (10%)	7	4
1	H	304/312 (97%)	278 (91%)	26 (9%)	10	5
1	I	299/312 (96%)	270 (90%)	29 (10%)	8	4
1	J	298/312 (96%)	270 (91%)	28 (9%)	8	4
1	K	299/312 (96%)	275 (92%)	24 (8%)	11	7
1	L	303/312 (97%)	275 (91%)	28 (9%)	8	4
All	All	3639/3744 (97%)	3332 (92%)	307 (8%)	10	6

All (307) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	42	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

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Mol	Chain	Res	Type
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	219	SER
1	A	236	GLU
1	A	256	LEU
1	A	257	THR
1	A	272	SER
1	A	349	LEU
1	A	351	ASN
1	B	13	SER
1	B	29	PHE
1	B	33	LEU
1	B	73	ILE
1	B	88	ASN
1	B	89	GLU
1	B	91	ASN
1	B	94	LEU
1	B	130	THR
1	B	171	LEU
1	B	183	LEU
1	B	186	ASP
1	B	257	THR
1	B	263	LYS
1	B	301	LEU
1	C	18	ASN
1	C	27	GLN
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

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Mol	Chain	Res	Type
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	256	LEU
1	C	257	THR
1	C	263	LYS
1	C	307	ASP
1	C	328	LYS
1	D	25	GLU
1	D	42	LEU
1	D	73	ILE
1	D	81	ILE
1	D	94	LEU
1	D	97	LEU
1	D	101	ARG
1	D	141	ASN
1	D	147	LEU
1	D	169	LEU
1	D	171	LEU
1	D	190	LEU
1	D	200	ASN
1	D	256	LEU
1	D	257	THR
1	D	263	LYS
1	D	280	ILE
1	D	294	VAL
1	D	306	GLU
1	D	314	MET
1	D	339	GLN
1	D	350	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

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Mol	Chain	Res	Type
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	236	GLU
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	E	333	GLU
1	F	16	LEU
1	F	23	ARG
1	F	33	LEU
1	F	42	LEU
1	F	44	ASN
1	F	46	LEU
1	F	49	VAL
1	F	60	ARG
1	F	80	LYS
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
1	F	169	LEU
1	F	171	LEU
1	F	179	ASN
1	F	183	LEU
1	F	223	ASN
1	F	224	GLN
1	F	250	ASN

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Mol	Chain	Res	Type
1	F	256	LEU
1	F	257	THR
1	F	260	ARG
1	F	268	ASN
1	F	294	VAL
1	F	306	GLU
1	F	311	GLU
1	F	333	GLU
1	F	351	ASN
1	G	33	LEU
1	G	39	VAL
1	G	44	ASN
1	G	61	ILE
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	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
1	G	331	ILE
1	H	2	MET
1	H	33	LEU
1	H	34	THR
1	H	44	ASN

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Mol	Chain	Res	Type
1	H	60	ARG
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	294	VAL
1	H	350	GLN
1	I	8	LEU
1	I	18	ASN
1	I	20	THR
1	I	32	LEU
1	I	46	LEU
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	141	ASN
1	I	143	GLN
1	I	144	THR
1	I	169	LEU
1	I	171	LEU
1	I	183	LEU
1	I	186	ASP
1	I	208	ARG

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Mol	Chain	Res	Type
1	I	222	ASP
1	I	236	GLU
1	I	247	GLN
1	I	250	ASN
1	I	256	LEU
1	I	257	THR
1	I	294	VAL
1	I	303	MET
1	I	351	ASN
1	J	12	LEU
1	J	46	LEU
1	J	82	THR
1	J	88	ASN
1	J	89	GLU
1	J	91	ASN
1	J	95	GLN
1	J	103	MET
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	206	ILE
1	J	224	GLN
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	32	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	94	LEU
1	K	117	LEU
1	K	125	ASN
1	K	151	THR
1	K	156	ILE
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	325	GLN
1	K	331	ILE
1	L	12	LEU
1	L	27	GLN
1	L	32	LEU
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	88	ASN
1	L	91	ASN
1	L	94	LEU
1	L	103	MET
1	L	114	GLU
1	L	117	LEU
1	L	141	ASN
1	L	158	MET
1	L	168	LYS
1	L	171	LEU
1	L	183	LEU
1	L	190	LEU
1	L	191	LYS
1	L	257	THR

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Mol	Chain	Res	Type
1	L	259	GLU
1	L	266	GLU
1	L	268	ASN
1	L	294	VAL
1	L	341	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (172) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	95	GLN
1	A	109	HIS
1	A	166	ASN
1	A	181	GLN
1	A	194	HIS
1	A	213	GLN
1	A	224	GLN
1	A	317	ASN
1	A	351	ASN
1	B	18	ASN
1	B	88	ASN
1	B	90	GLN
1	B	91	ASN
1	B	107	GLN
1	B	181	GLN
1	B	200	ASN
1	B	224	GLN
1	B	234	HIS
1	B	268	ASN
1	B	317	ASN
1	B	339	GLN
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

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Mol	Chain	Res	Type
1	C	317	ASN
1	C	325	GLN
1	D	18	ASN
1	D	27	GLN
1	D	30	GLN
1	D	107	GLN
1	D	109	HIS
1	D	125	ASN
1	D	141	ASN
1	D	172	ASN
1	D	181	GLN
1	D	204	HIS
1	D	213	GLN
1	D	223	ASN
1	D	250	ASN
1	D	258	HIS
1	D	286	GLN
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	181	GLN
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	351	ASN
1	F	27	GLN
1	F	30	GLN
1	F	44	ASN
1	F	88	ASN
1	F	91	ASN
1	F	109	HIS
1	F	125	ASN
1	F	141	ASN
1	F	172	ASN
1	F	181	GLN
1	F	200	ASN

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Mol	Chain	Res	Type
1	F	213	GLN
1	F	234	HIS
1	F	250	ASN
1	F	317	ASN
1	F	325	GLN
1	F	339	GLN
1	F	351	ASN
1	G	30	GLN
1	G	44	ASN
1	G	88	ASN
1	G	91	ASN
1	G	95	GLN
1	G	102	HIS
1	G	141	ASN
1	G	166	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	286	GLN
1	G	297	HIS
1	G	310	ASN
1	G	317	ASN
1	G	325	GLN
1	H	30	GLN
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	204	HIS
1	H	213	GLN
1	H	223	ASN
1	H	250	ASN
1	H	268	ASN
1	H	317	ASN
1	H	325	GLN

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Mol	Chain	Res	Type
1	I	18	ASN
1	I	30	GLN
1	I	88	ASN
1	I	91	ASN
1	I	102	HIS
1	I	141	ASN
1	I	172	ASN
1	I	181	GLN
1	I	234	HIS
1	I	250	ASN
1	I	268	ASN
1	I	317	ASN
1	I	325	GLN
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
1	J	181	GLN
1	J	250	ASN
1	J	325	GLN
1	K	30	GLN
1	K	44	ASN
1	K	88	ASN
1	K	95	GLN
1	K	107	GLN
1	K	143	GLN
1	K	172	ASN
1	K	181	GLN
1	K	200	ASN
1	K	234	HIS
1	K	250	ASN
1	K	268	ASN
1	K	277	ASN
1	K	317	ASN
1	K	325	GLN
1	L	27	GLN
1	L	30	GLN
1	L	44	ASN
1	L	88	ASN

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Mol	Chain	Res	Type
1	L	90	GLN
1	L	91	ASN
1	L	107	GLN
1	L	109	HIS
1	L	125	ASN
1	L	141	ASN
1	L	172	ASN
1	L	181	GLN
1	L	213	GLN
1	L	224	GLN
1	L	286	GLN
1	L	317	ASN
1	L	325	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](#)

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	403	-	2,2,2	0.75	0	1,1,1	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMT	B	402	-	2,2,2	0.72	0	1,1,1	0.23	0
4	ACY	J	403	-	3,3,3	0.83	0	3,3,3	0.73	0
3	FMT	L	404	-	2,2,2	0.77	0	1,1,1	0.28	0
3	FMT	D	404	-	2,2,2	0.75	0	1,1,1	0.21	0
3	FMT	A	404	-	2,2,2	0.65	0	1,1,1	0.25	0
3	FMT	L	405	-	2,2,2	0.83	0	1,1,1	0.25	0

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 [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	A	351/351 (100%)	0.11	12 (3%)	48	52	15, 27, 50, 63	0
1	B	351/351 (100%)	0.12	24 (6%)	23	26	15, 28, 52, 90	0
1	C	346/351 (98%)	0.34	25 (7%)	21	25	19, 31, 62, 88	0
1	D	341/351 (97%)	0.38	27 (7%)	18	20	18, 32, 60, 71	0
1	E	349/351 (99%)	0.37	19 (5%)	31	35	22, 33, 61, 86	0
1	F	344/351 (98%)	0.33	22 (6%)	25	28	20, 31, 58, 75	0
1	G	343/351 (97%)	0.62	36 (10%)	11	13	24, 41, 70, 85	0
1	H	347/351 (98%)	0.59	31 (8%)	15	17	22, 38, 69, 94	0
1	I	348/351 (99%)	0.75	48 (13%)	6	7	24, 43, 74, 113	0
1	J	341/351 (97%)	0.74	38 (11%)	10	11	26, 41, 63, 80	0
1	K	344/351 (98%)	0.64	30 (8%)	16	17	25, 42, 69, 84	0
1	L	348/351 (99%)	0.37	28 (8%)	18	20	17, 31, 58, 81	0
All	All	4153/4212 (98%)	0.45	340 (8%)	17	19	15, 35, 65, 113	0

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	79	GLU	6.3
1	E	272	SER	6.1
1	D	309	PRO	6.0
1	I	273	LEU	5.9
1	D	118	THR	5.4
1	K	306	GLU	4.9
1	E	118	THR	4.9
1	I	276	PRO	4.9
1	I	275	THR	4.7
1	I	20	THR	4.6
1	L	307	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	272	SER	4.4
1	G	275	THR	4.4
1	I	193	THR	4.3
1	D	269	ALA	4.3
1	J	195	SER	4.3
1	C	78	ASN	4.2
1	H	269	ALA	4.2
1	E	309	PRO	4.1
1	H	351	ASN	4.1
1	E	220	GLY	4.1
1	C	276	PRO	4.1
1	L	309	PRO	4.0
1	L	267	TYR	4.0
1	K	351	ASN	4.0
1	B	20	THR	3.9
1	G	75	THR	3.9
1	J	194	HIS	3.9
1	I	256	LEU	3.9
1	G	79	GLU	3.9
1	D	307	ASP	3.8
1	A	351	ASN	3.8
1	J	78	ASN	3.8
1	H	84	LEU	3.8
1	J	193	THR	3.8
1	I	274	ASP	3.8
1	G	309	PRO	3.8
1	L	305	PRO	3.8
1	I	194	HIS	3.8
1	A	17	TRP	3.7
1	J	278	ALA	3.7
1	K	191	LYS	3.7
1	C	277	ASN	3.7
1	E	275	THR	3.7
1	K	331	ILE	3.7
1	J	115	MET	3.7
1	D	304	ALA	3.7
1	I	17	TRP	3.6
1	H	118	THR	3.6
1	G	78	ASN	3.6
1	H	270	GLU	3.6
1	B	29	PHE	3.5
1	G	76	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	269	ALA	3.5
1	I	19	PRO	3.5
1	F	118	THR	3.5
1	G	15	GLY	3.5
1	K	192	ASP	3.5
1	E	277	ASN	3.4
1	G	120	THR	3.4
1	H	79	GLU	3.4
1	E	270	GLU	3.3
1	H	267	TYR	3.3
1	A	65	ASN	3.3
1	I	191	LYS	3.3
1	I	195	SER	3.3
1	J	279	CYS	3.3
1	L	271	ARG	3.3
1	F	78	ASN	3.3
1	L	270	GLU	3.3
1	B	28	SER	3.2
1	H	76	PRO	3.2
1	J	269	ALA	3.2
1	F	277	ASN	3.2
1	I	192	ASP	3.2
1	H	268	ASN	3.2
1	G	117	LEU	3.2
1	J	117	LEU	3.2
1	D	74	ARG	3.2
1	I	271	ARG	3.2
1	K	81	ILE	3.2
1	J	116	ASP	3.2
1	A	219	SER	3.2
1	H	309	PRO	3.1
1	A	18	ASN	3.1
1	K	276	PRO	3.1
1	G	192	ASP	3.1
1	J	16	LEU	3.1
1	F	220	GLY	3.1
1	J	350	GLN	3.1
1	D	305	PRO	3.1
1	H	78	ASN	3.1
1	I	116	ASP	3.1
1	L	274	ASP	3.1
1	I	117	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	276	PRO	3.0
1	F	114	GLU	3.0
1	L	116	ASP	3.0
1	H	117	LEU	3.0
1	I	201	VAL	3.0
1	J	158	MET	3.0
1	J	190	LEU	3.0
1	J	149	GLY	3.0
1	K	277	ASN	3.0
1	K	118	THR	3.0
1	J	306	GLU	3.0
1	B	14	PHE	3.0
1	D	117	LEU	3.0
1	F	44	ASN	3.0
1	B	309	PRO	3.0
1	C	76	PRO	3.0
1	L	289	ASP	3.0
1	I	18	ASN	3.0
1	I	114	GLU	3.0
1	I	200	ASN	3.0
1	D	116	ASP	3.0
1	F	278	ALA	2.9
1	C	116	ASP	2.9
1	L	117	LEU	2.9
1	I	115	MET	2.9
1	F	306	GLU	2.9
1	J	114	GLU	2.9
1	G	77	ASP	2.8
1	K	116	ASP	2.8
1	B	67	GLU	2.8
1	C	223	ASN	2.8
1	D	113	SER	2.8
1	I	78	ASN	2.8
1	I	219	SER	2.8
1	I	150	PRO	2.8
1	K	268	ASN	2.8
1	I	29	PHE	2.8
1	I	270	GLU	2.8
1	K	1	GLU	2.8
1	L	311	GLU	2.8
1	H	20	THR	2.8
1	H	75	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	276	PRO	2.8
1	B	66	SER	2.7
1	C	269	ALA	2.7
1	B	26	ARG	2.7
1	D	308	ARG	2.7
1	J	113	SER	2.7
1	A	14	PHE	2.7
1	J	112	LEU	2.7
1	B	21	TYR	2.7
1	I	202	ILE	2.7
1	J	161	CYS	2.7
1	J	77	ASP	2.7
1	D	219	SER	2.7
1	J	219	SER	2.7
1	C	279	CYS	2.7
1	E	77	ASP	2.7
1	B	30	GLN	2.6
1	C	271	ARG	2.6
1	D	267	TYR	2.6
1	I	21	TYR	2.6
1	C	27	GLN	2.6
1	D	350	GLN	2.6
1	J	326	GLY	2.6
1	I	311	GLU	2.6
1	K	223	ASN	2.6
1	F	309	PRO	2.6
1	G	349	LEU	2.6
1	L	84	LEU	2.6
1	J	29	PHE	2.5
1	D	311	GLU	2.5
1	J	204	HIS	2.5
1	B	271	ARG	2.5
1	L	276	PRO	2.5
1	F	14	PHE	2.5
1	H	14	PHE	2.5
1	H	223	ASN	2.5
1	I	23	ARG	2.5
1	K	305	PRO	2.5
1	D	29	PHE	2.5
1	A	267	TYR	2.5
1	E	116	ASP	2.5
1	F	116	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	67	GLU	2.5
1	B	219	SER	2.5
1	E	219	SER	2.5
1	K	121	THR	2.5
1	C	309	PRO	2.5
1	I	197	PRO	2.5
1	H	199	ARG	2.5
1	I	14	PHE	2.5
1	B	351	ASN	2.5
1	C	77	ASP	2.4
1	H	116	ASP	2.4
1	L	222	ASP	2.4
1	I	279	CYS	2.4
1	L	265	SER	2.4
1	G	194	HIS	2.4
1	D	220	GLY	2.4
1	K	279	CYS	2.4
1	G	24	SER	2.4
1	C	120	THR	2.4
1	E	264	ALA	2.4
1	F	268	ASN	2.4
1	H	306	GLU	2.4
1	A	77	ASP	2.4
1	K	307	ASP	2.4
1	I	196	SER	2.4
1	I	26	ARG	2.4
1	L	121	THR	2.4
1	B	114	GLU	2.4
1	G	90	GLN	2.4
1	J	203	ASP	2.4
1	G	206	ILE	2.4
1	E	80	LYS	2.4
1	H	219	SER	2.4
1	C	20	THR	2.4
1	B	19	PRO	2.4
1	G	276	PRO	2.4
1	G	267	TYR	2.3
1	K	311	GLU	2.3
1	F	350	GLN	2.3
1	K	350	GLN	2.3
1	J	277	ASN	2.3
1	L	46	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	290	GLY	2.3
1	J	206	ILE	2.3
1	H	17	TRP	2.3
1	B	78	ASN	2.3
1	A	256	LEU	2.3
1	J	196	SER	2.3
1	J	280	ILE	2.3
1	C	270	GLU	2.3
1	D	310	ASN	2.3
1	D	77	ASP	2.3
1	F	17	TRP	2.3
1	F	267	TYR	2.3
1	H	16	LEU	2.3
1	I	40	TYR	2.3
1	L	21	TYR	2.3
1	K	2	MET	2.3
1	A	350	GLN	2.3
1	L	278	ALA	2.3
1	I	158	MET	2.3
1	L	266	GLU	2.2
1	H	90	GLN	2.2
1	I	113	SER	2.2
1	J	198	SER	2.2
1	K	265	SER	2.2
1	E	120	THR	2.2
1	G	19	PRO	2.2
1	G	257	THR	2.2
1	K	20	THR	2.2
1	B	23	ARG	2.2
1	B	166	ASN	2.2
1	I	65	ASN	2.2
1	C	117	LEU	2.2
1	A	271	ARG	2.2
1	C	110	ARG	2.2
1	D	26	ARG	2.2
1	G	199	ARG	2.2
1	B	18	ASN	2.2
1	F	81	ILE	2.2
1	G	118	THR	2.2
1	H	80	LYS	2.2
1	K	78	ASN	2.2
1	L	303	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	1	GLU	2.2
1	I	161	CYS	2.2
1	K	90	GLN	2.2
1	E	267	TYR	2.2
1	J	66	SER	2.2
1	G	74	ARG	2.2
1	L	263	LYS	2.2
1	K	44	ASN	2.2
1	F	276	PRO	2.2
1	L	275	THR	2.2
1	G	119	ASP	2.2
1	H	77	ASP	2.2
1	E	269	ALA	2.2
1	I	204	HIS	2.2
1	F	16	LEU	2.2
1	B	22	SER	2.2
1	B	110	ARG	2.2
1	B	1	GLU	2.1
1	B	79	GLU	2.1
1	C	14	PHE	2.1
1	D	14	PHE	2.1
1	K	29	PHE	2.1
1	G	350	GLN	2.1
1	H	15	GLY	2.1
1	G	278	ALA	2.1
1	C	336	ARG	2.1
1	G	84	LEU	2.1
1	I	112	LEU	2.1
1	I	147	LEU	2.1
1	G	113	SER	2.1
1	C	21	TYR	2.1
1	G	277	ASN	2.1
1	K	166	ASN	2.1
1	K	267	TYR	2.1
1	J	67	GLU	2.1
1	J	119	ASP	2.1
1	A	309	PRO	2.1
1	J	17	TRP	2.1
1	I	325	GLN	2.1
1	F	23	ARG	2.1
1	H	308	ARG	2.1
1	B	16	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	351	ASN	2.1
1	G	212	GLU	2.1
1	J	166	ASN	2.1
1	C	267	TYR	2.1
1	D	20	THR	2.1
1	F	76	PRO	2.1
1	J	118	THR	2.1
1	K	14	PHE	2.1
1	C	219	SER	2.1
1	G	28	SER	2.1
1	H	221	SER	2.1
1	I	262	SER	2.1
1	L	113	SER	2.1
1	L	114	GLU	2.1
1	C	166	ASN	2.1
1	D	120	THR	2.1
1	E	20	THR	2.1
1	G	193	THR	2.1
1	K	209	HIS	2.1
1	H	83	VAL	2.1
1	C	266	GLU	2.0
1	E	306	GLU	2.0
1	I	154	SER	2.1
1	L	304	ALA	2.1
1	L	77	ASP	2.0
1	D	121	THR	2.0
1	G	191	LYS	2.0
1	D	24	SER	2.0
1	E	24	SER	2.0
1	G	17	TRP	2.0
1	E	307	ASP	2.0
1	G	116	ASP	2.0
1	I	203	ASP	2.0
1	D	23	ARG	2.0
1	G	60	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
2	MG	D	402	1/1	0.76	0.14	44,44,44,44	0
4	ACY	J	403	4/4	0.76	0.21	57,57,57,57	0
2	MG	L	402	1/1	0.79	0.23	60,60,60,60	0
2	MG	I	402	1/1	0.83	0.12	64,64,64,64	0
3	FMT	L	405	3/3	0.85	0.19	35,35,35,35	0
2	MG	L	403	1/1	0.86	0.13	49,49,49,49	0
2	MG	E	401	1/1	0.86	0.08	47,47,47,47	0
2	MG	H	401	1/1	0.86	0.14	63,63,63,63	0
3	FMT	B	402	3/3	0.88	0.13	44,44,44,44	0
2	MG	L	401	1/1	0.90	0.08	34,34,34,34	0
2	MG	A	402	1/1	0.90	0.07	31,31,31,31	0
2	MG	J	401	1/1	0.90	0.09	46,46,46,46	0
3	FMT	A	403	3/3	0.91	0.11	39,39,39,39	0
2	MG	D	403	1/1	0.91	0.08	54,54,54,54	0
2	MG	C	401	1/1	0.92	0.06	39,39,39,39	0
2	MG	C	402	1/1	0.92	0.13	59,59,59,59	0
3	FMT	A	404	3/3	0.92	0.10	34,34,34,35	0
2	MG	I	401	1/1	0.94	0.05	34,34,34,34	0
2	MG	F	402	1/1	0.94	0.08	46,46,46,46	0
2	MG	D	401	1/1	0.94	0.06	34,34,34,34	0
2	MG	J	402	1/1	0.94	0.11	39,39,39,39	0
2	MG	A	401	1/1	0.95	0.07	27,27,27,27	0
3	FMT	D	404	3/3	0.97	0.06	21,21,21,21	0
2	MG	B	401	1/1	0.97	0.04	35,35,35,35	0
2	MG	F	401	1/1	0.97	0.13	30,30,30,30	0
3	FMT	L	404	3/3	0.98	0.04	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.