



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:55 AM UTC

PDB ID : 5YQ0 / pdb_00005yq0
Title : Crystal structure of secreted protein CofJ from ETEC.
Authors : Oki, H.; Kawahara, K.; Maruno, T.; Imai, T.; Muroga, Y.; Fukakusa, S.;
Iwashita, T.; Kobayashi, Y.; Matsuda, S.; Kodama, T.; Iida, T.; Yoshida, T.;
Ohkubo, T.; Nakamura, S.
Deposited on : 2017-11-04
Resolution : 1.76 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
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

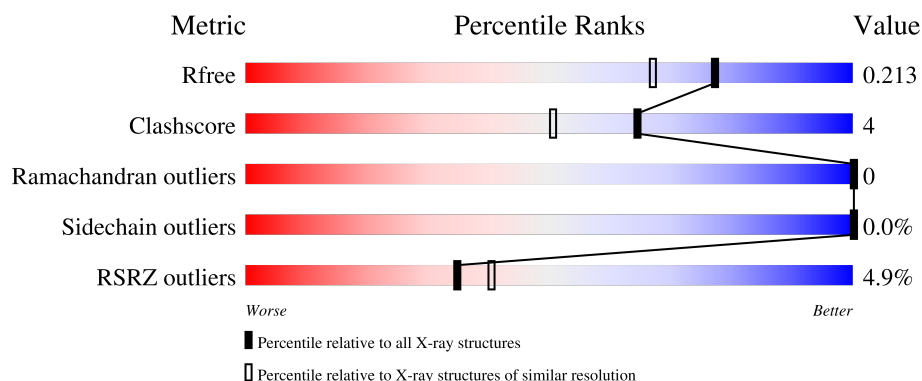
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	326	5% 86% 6% 8%
1	B	326	4% 85% 7% 8%
1	C	326	4% 89% 7% 7%
1	D	326	4% 85% 7% 8%
1	E	326	2% 87% 5% 8%

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Mol	Chain	Length	Quality of chain
1	F	326	5% 87% 6% 8%
1	G	326	9% 83% 9% 8%
1	H	326	3% 86% 6% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22745 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 CofJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2460	1559	419	474	8			
1	B	301	Total	C	N	O	S	0	0	0
			2460	1559	419	474	8			
1	C	304	Total	C	N	O	S	0	0	0
			2477	1568	422	479	8			
1	D	301	Total	C	N	O	S	0	0	0
			2460	1559	419	474	8			
1	E	301	Total	C	N	O	S	0	0	0
			2460	1559	419	474	8			
1	F	301	Total	C	N	O	S	0	0	0
			2460	1559	419	474	8			
1	G	301	Total	C	N	O	S	0	0	0
			2460	1559	419	474	8			
1	H	301	Total	C	N	O	S	0	0	0
			2460	1559	419	474	8			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Ca	0	0
			2	2		
2	E	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	409	Total	O	0	0
			409	409		

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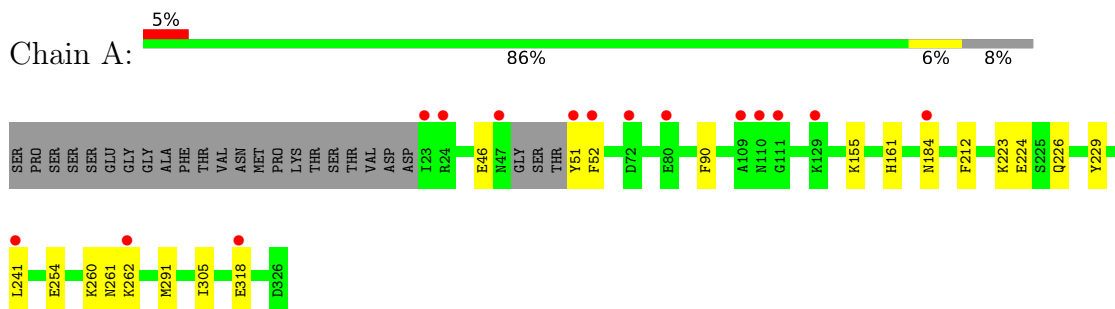
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	355	Total 355	O 355	0	0
3	C	403	Total 403	O 403	0	0
3	D	395	Total 395	O 395	0	0
3	E	395	Total 395	O 395	0	0
3	F	367	Total 367	O 367	0	0
3	G	316	Total 316	O 316	0	0
3	H	404	Total 404	O 404	0	0

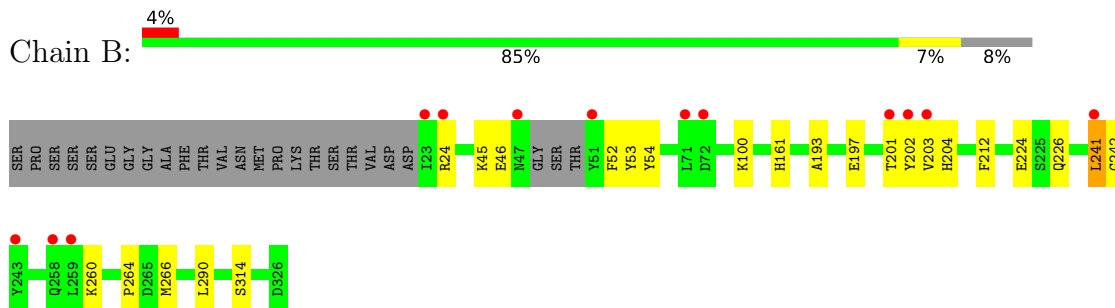
3 Residue-property plots [i](#)

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.

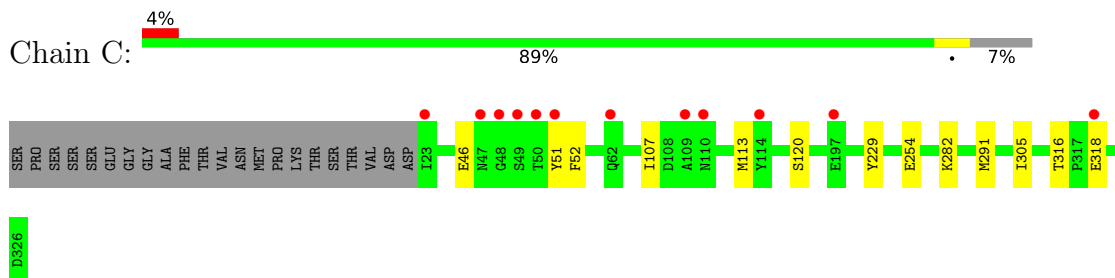
- Molecule 1: CofJ



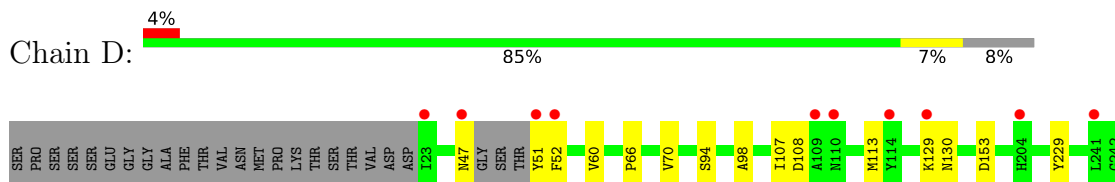
- Molecule 1: CofJ

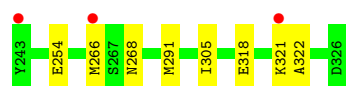


- Molecule 1: CofJ

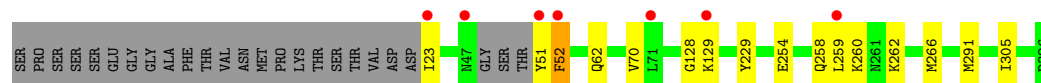
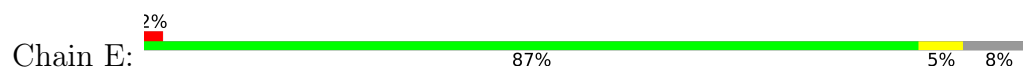


- Molecule 1: CofJ

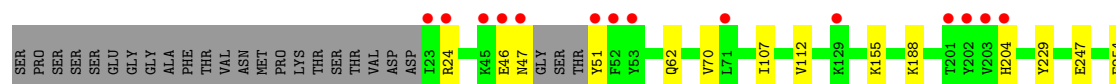
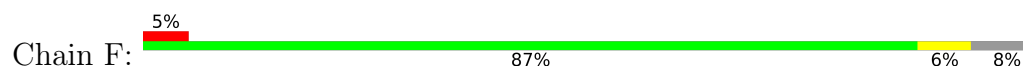




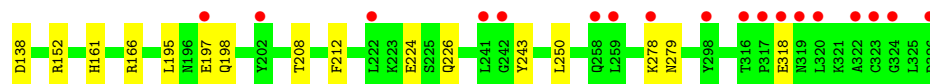
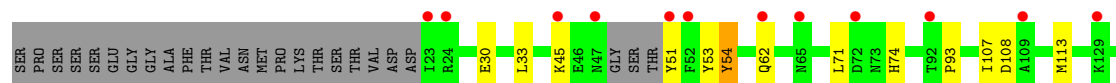
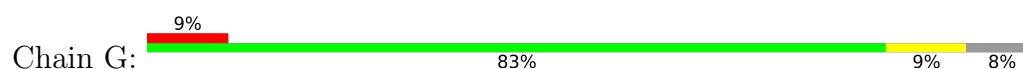
● Molecule 1: CofJ



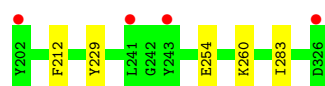
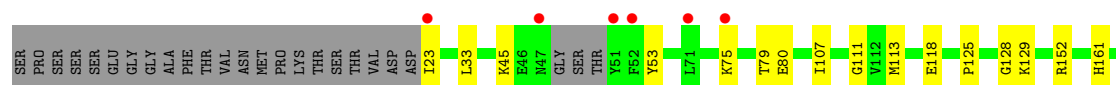
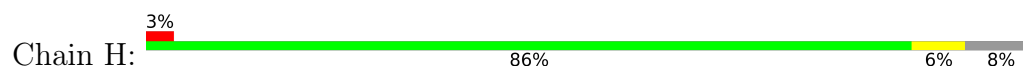
● Molecule 1: CofJ



● Molecule 1: CofJ



● Molecule 1: CofJ



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.21Å 147.54Å 149.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.23 – 1.76 49.23 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.23-1.76) 99.4 (49.23-1.76)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.180 , 0.211 0.182 , 0.213	Depositor DCC
R_{free} test set	30616 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -l,-k,-h 0.000 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22745	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.3009e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA

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	0.40	0/2523	0.61	0/3413
1	B	0.41	2/2523 (0.1%)	0.57	0/3413
1	C	0.37	1/2541 (0.0%)	0.59	0/3439
1	D	0.36	1/2523 (0.0%)	0.58	0/3413
1	E	0.34	1/2523 (0.0%)	0.54	0/3413
1	F	0.30	0/2523	0.56	1/3413 (0.0%)
1	G	0.45	2/2523 (0.1%)	0.63	2/3413 (0.1%)
1	H	0.36	0/2523	0.58	1/3413 (0.0%)
All	All	0.37	7/20202 (0.0%)	0.58	4/27330 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	71	LEU	C-N	8.99	1.46	1.33
1	D	52	PHE	C-O	-7.08	1.15	1.23
1	G	54	TYR	C-N	-6.87	1.24	1.33
1	E	52	PHE	C-O	-6.05	1.16	1.24
1	B	290	LEU	C-O	-5.60	1.17	1.24
1	B	52	PHE	C-O	-5.39	1.17	1.23
1	C	52	PHE	C-O	-5.39	1.16	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	71	LEU	CA-C-N	-6.96	110.58	122.56
1	G	71	LEU	C-N-CA	-6.96	110.58	122.56
1	H	129	LYS	N-CA-C	6.68	118.56	111.28
1	F	204	HIS	N-CA-C	5.59	118.30	111.82

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	2460	0	2333	25	0
1	B	2460	0	2333	20	0
1	C	2477	0	2349	8	0
1	D	2460	0	2333	24	0
1	E	2460	0	2333	14	0
1	F	2460	0	2333	14	0
1	G	2460	0	2333	34	0
1	H	2460	0	2333	17	0
2	C	2	0	0	0	0
2	E	1	0	0	0	0
2	H	1	0	0	0	0
3	A	409	0	0	2	0
3	B	355	0	0	5	0
3	C	403	0	0	1	0
3	D	395	0	0	1	0
3	E	395	0	0	2	0
3	F	367	0	0	2	0
3	G	316	0	0	4	0
3	H	404	0	0	2	0
All	All	22745	0	18680	149	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 4.

All (149) 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:G:45:LYS:NZ	1:G:51:TYR:HB2	1.73	1.04
1:G:278:LYS:HE2	3:G:636:HOH:O	1.57	1.04
1:E:129:LYS:HE2	1:E:129:LYS:N	1.72	1.00
1:D:321:LYS:HE2	3:D:733:HOH:O	1.65	0.97
1:G:318:GLU:OE1	1:G:318:GLU:N	1.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:CE2	1:A:241:LEU:CD1	2.50	0.94
1:E:128:GLY:C	1:E:129:LYS:HE2	1.93	0.94
1:A:52:PHE:CE2	1:A:241:LEU:HD12	2.03	0.94
1:G:45:LYS:NZ	1:G:51:TYR:CB	2.34	0.91
1:D:318:GLU:O	1:D:321:LYS:HG3	1.77	0.85
1:A:260:LYS:O	1:A:262:LYS:HD2	1.81	0.81
1:F:46:GLU:O	1:F:47:ASN:CG	2.25	0.79
1:G:318:GLU:H	1:G:318:GLU:CD	1.92	0.77
1:A:229:TYR:OH	1:A:254:GLU:HG3	1.84	0.77
1:F:24:ARG:HG2	1:G:30:GLU:OE2	1.86	0.74
1:A:318:GLU:N	1:A:318:GLU:OE1	2.20	0.74
1:G:45:LYS:HZ1	1:G:51:TYR:CB	1.99	0.72
1:G:138:ASP:OD1	1:H:118:GLU:HG3	1.89	0.72
1:G:45:LYS:HZ1	1:G:51:TYR:HB3	1.53	0.72
1:A:52:PHE:CE2	1:A:241:LEU:HD11	2.26	0.70
1:F:318:GLU:H	1:F:318:GLU:CD	1.97	0.69
1:E:129:LYS:HE2	1:E:129:LYS:CA	2.23	0.69
1:G:152:ARG:HD3	3:G:656:HOH:O	1.93	0.68
1:C:46:GLU:O	1:C:51:TYR:HA	1.95	0.66
1:A:52:PHE:HE2	1:A:241:LEU:CD1	2.08	0.66
1:A:52:PHE:HE2	1:A:241:LEU:HD12	1.56	0.66
1:G:45:LYS:HZ2	1:G:51:TYR:HB2	1.57	0.66
1:A:261:ASN:C	1:A:262:LYS:HG3	2.20	0.65
1:C:120:SER:HB3	1:D:66:PRO:HG2	1.78	0.64
1:D:229:TYR:OH	1:D:254:GLU:HG3	1.98	0.64
1:A:241:LEU:H	1:A:241:LEU:HD23	1.62	0.63
1:A:46:GLU:O	1:A:51:TYR:HA	1.98	0.63
1:H:229:TYR:OH	1:H:254:GLU:HG3	1.99	0.63
1:G:138:ASP:OD2	1:G:138:ASP:O	2.18	0.62
1:B:24:ARG:NH2	3:B:403:HOH:O	2.32	0.62
1:D:321:LYS:HD2	1:D:322:ALA:N	2.15	0.62
1:F:46:GLU:O	1:F:47:ASN:ND2	2.32	0.62
1:H:260:LYS:NZ	3:H:504:HOH:O	2.34	0.61
1:D:318:GLU:HG3	1:D:321:LYS:HE3	1.82	0.61
1:H:107:ILE:HD11	1:H:113:MET:HE3	1.83	0.60
1:B:241:LEU:H	1:B:241:LEU:HD23	1.66	0.60
1:E:129:LYS:N	1:E:129:LYS:CE	2.57	0.59
1:G:107:ILE:HD11	1:G:113:MET:HE2	1.83	0.58
1:G:45:LYS:HZ3	1:G:51:TYR:HB2	1.65	0.58
1:D:129:LYS:O	1:D:130:ASN:HB2	2.04	0.58
1:G:45:LYS:NZ	1:G:51:TYR:HB3	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:LYS:NZ	3:C:501:HOH:O	2.38	0.57
1:H:125:PRO:HA	1:H:128:GLY:O	2.04	0.57
1:H:79:THR:C	1:H:80:GLU:HG2	2.30	0.56
1:A:261:ASN:O	1:A:262:LYS:HG3	2.05	0.56
1:E:260:LYS:NZ	3:E:506:HOH:O	2.38	0.56
1:G:197:GLU:HG3	1:G:198:GLN:N	2.20	0.56
1:C:120:SER:HB3	1:D:66:PRO:CG	2.35	0.56
1:A:90:PHE:CE1	1:A:155:LYS:HG3	2.40	0.56
1:E:229:TYR:OH	1:E:254:GLU:HG3	2.06	0.56
1:G:318:GLU:N	1:G:318:GLU:CD	2.56	0.55
1:B:45:LYS:HB2	1:B:53:TYR:CE2	2.41	0.54
1:G:278:LYS:HG3	3:G:540:HOH:O	2.07	0.54
1:A:318:GLU:H	1:A:318:GLU:CD	2.16	0.53
1:A:52:PHE:CD2	1:A:241:LEU:HD11	2.44	0.52
1:A:241:LEU:O	1:A:241:LEU:HG	2.08	0.52
1:B:224:GLU:HG3	1:B:226:GLN:H	1.74	0.52
1:F:318:GLU:CD	1:F:318:GLU:N	2.67	0.52
1:G:224:GLU:HG3	1:G:226:GLN:H	1.73	0.52
1:B:201:THR:HG21	1:B:242:GLY:O	2.08	0.52
1:B:24:ARG:NH1	1:D:94:SER:OG	2.42	0.52
1:D:51:TYR:C	1:D:51:TYR:CD1	2.88	0.52
1:H:107:ILE:HD13	1:H:113:MET:HA	1.92	0.51
1:G:93:PRO:HB2	1:G:107:ILE:HD13	1.93	0.51
1:B:202:TYR:O	1:B:204:HIS:ND1	2.43	0.51
1:B:264:PRO:HB2	1:B:266:MET:HE3	1.91	0.51
1:C:229:TYR:OH	1:C:254:GLU:HG3	2.11	0.51
1:E:51:TYR:CE2	1:E:52:PHE:CZ	2.99	0.50
1:A:241:LEU:HD23	1:A:241:LEU:N	2.25	0.50
1:G:54:TYR:OH	1:G:243:TYR:OH	2.25	0.49
1:H:107:ILE:CG2	1:H:111:GLY:HA2	2.42	0.49
1:A:46:GLU:O	1:A:51:TYR:CA	2.60	0.49
1:G:51:TYR:HD1	1:G:53:TYR:HE1	1.61	0.49
1:D:60:VAL:O	1:D:70:VAL:HG22	2.13	0.48
1:H:45:LYS:HE2	1:H:53:TYR:OH	2.12	0.48
1:H:107:ILE:HD11	1:H:113:MET:CE	2.44	0.48
1:G:197:GLU:CG	1:G:198:GLN:N	2.76	0.48
1:A:184:ASN:ND2	3:A:401:HOH:O	2.24	0.48
1:E:258:GLN:O	1:E:262:LYS:HE2	2.14	0.47
1:F:229:TYR:OH	1:F:254:GLU:HG3	2.14	0.47
1:D:318:GLU:O	1:D:321:LYS:CG	2.55	0.47
1:A:161:HIS:HB3	1:A:212:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:NH1	1:D:153:ASP:OD2	2.43	0.47
1:C:291:MET:HG2	1:C:305:ILE:HB	1.97	0.47
1:D:107:ILE:HD11	1:D:113:MET:HE3	1.96	0.47
1:F:155:LYS:NZ	3:F:410:HOH:O	2.47	0.47
1:A:291:MET:HG2	1:A:305:ILE:HB	1.96	0.47
1:B:193:ALA:O	1:B:197:GLU:HG3	2.15	0.46
1:A:260:LYS:O	1:A:262:LYS:CD	2.60	0.46
1:B:314:SER:HB2	1:D:98:ALA:HB3	1.96	0.46
1:D:291:MET:HG2	1:D:305:ILE:HB	1.95	0.46
1:H:161:HIS:HB3	1:H:212:PHE:CZ	2.50	0.46
1:B:202:TYR:O	1:B:204:HIS:CE1	2.69	0.46
1:D:266:MET:SD	1:D:268:ASN:O	2.73	0.46
1:D:318:GLU:C	1:D:321:LYS:HG3	2.40	0.46
1:D:318:GLU:O	1:D:321:LYS:HE3	2.16	0.46
1:F:51:TYR:N	1:F:51:TYR:CD1	2.84	0.46
1:D:51:TYR:C	1:D:51:TYR:HD1	2.23	0.46
1:E:259:LEU:HA	1:E:262:LYS:HE2	1.98	0.46
1:G:161:HIS:HB3	1:G:212:PHE:CZ	2.52	0.45
1:H:33:LEU:HB2	1:H:152:ARG:NE	2.32	0.45
1:B:241:LEU:HD23	1:B:241:LEU:N	2.29	0.45
1:H:152:ARG:NH2	1:H:283:ILE:O	2.49	0.45
1:E:23:ILE:N	3:E:513:HOH:O	2.50	0.45
1:G:45:LYS:HZ2	1:G:51:TYR:CB	2.20	0.44
1:C:316:THR:OG1	1:C:318:GLU:HG2	2.18	0.44
1:B:161:HIS:HB3	1:B:212:PHE:CZ	2.52	0.44
1:G:51:TYR:CE1	1:G:62:GLN:O	2.70	0.44
1:G:195:LEU:HD13	1:G:250:LEU:HD11	1.98	0.44
1:F:291:MET:HG2	1:F:305:ILE:HB	2.00	0.44
1:D:47:ASN:HA	1:D:51:TYR:N	2.33	0.44
1:F:188:LYS:NZ	3:F:404:HOH:O	2.31	0.44
1:B:224:GLU:OE2	1:B:226:GLN:HG2	2.18	0.44
1:D:129:LYS:O	1:D:130:ASN:CB	2.64	0.43
1:E:266:MET:HE2	1:E:266:MET:HB3	1.94	0.43
1:E:51:TYR:CE2	1:E:52:PHE:CE2	3.06	0.43
1:G:107:ILE:HG22	1:G:108:ASP:O	2.18	0.43
1:B:100:LYS:HD2	3:B:734:HOH:O	2.18	0.43
1:D:47:ASN:HA	1:D:51:TYR:CB	2.49	0.43
1:F:107:ILE:HA	1:F:112:VAL:O	2.19	0.43
1:E:62:GLN:HG3	1:E:70:VAL:HA	2.00	0.42
1:F:62:GLN:HG3	1:F:70:VAL:HA	2.01	0.42
1:G:166:ARG:HD3	1:G:208:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:NH1	3:B:420:HOH:O	2.52	0.42
1:G:33:LEU:HB2	1:G:152:ARG:HG3	2.02	0.42
1:D:107:ILE:HG22	1:D:108:ASP:O	2.20	0.42
1:F:247:GLU:HB3	1:F:304:TYR:CE2	2.55	0.42
1:B:260:LYS:NZ	3:B:405:HOH:O	2.42	0.41
1:G:62:GLN:H	1:G:62:GLN:HG2	1.69	0.41
1:G:278:LYS:HG2	1:G:279:ASN:N	2.35	0.41
1:H:107:ILE:HD13	1:H:113:MET:CA	2.51	0.41
1:A:223:LYS:NZ	3:A:427:HOH:O	2.51	0.41
1:B:203:VAL:HA	3:B:641:HOH:O	2.20	0.41
1:A:52:PHE:CD2	1:A:241:LEU:CD1	3.02	0.41
1:B:46:GLU:HG3	1:B:54:TYR:HE2	1.85	0.41
1:C:107:ILE:HD13	1:C:113:MET:HA	2.03	0.41
1:G:51:TYR:CD2	1:G:51:TYR:N	2.89	0.41
1:H:107:ILE:HG23	1:H:111:GLY:C	2.46	0.41
1:A:224:GLU:HG3	1:A:226:GLN:H	1.85	0.41
1:H:23:ILE:N	3:H:520:HOH:O	2.54	0.40
1:E:291:MET:HG2	1:E:305:ILE:HB	2.02	0.40
1:G:74:HIS:HE1	3:G:662:HOH:O	2.04	0.40
1:H:75:LYS:HB2	1:H:75:LYS:HE3	1.92	0.40
1:F:46:GLU:O	1:F:47:ASN:CB	2.69	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	297/326 (91%)	291 (98%)	6 (2%)	0	100	100
1	B	297/326 (91%)	291 (98%)	6 (2%)	0	100	100
1	C	302/326 (93%)	295 (98%)	7 (2%)	0	100	100
1	D	297/326 (91%)	290 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	297/326 (91%)	292 (98%)	5 (2%)	0	100	100
1	F	297/326 (91%)	290 (98%)	7 (2%)	0	100	100
1	G	297/326 (91%)	291 (98%)	6 (2%)	0	100	100
1	H	297/326 (91%)	291 (98%)	6 (2%)	0	100	100
All	All	2381/2608 (91%)	2331 (98%)	50 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	266/287 (93%)	266 (100%)	0	100	100
1	B	266/287 (93%)	265 (100%)	1 (0%)	84	80
1	C	268/287 (93%)	268 (100%)	0	100	100
1	D	266/287 (93%)	266 (100%)	0	100	100
1	E	266/287 (93%)	266 (100%)	0	100	100
1	F	266/287 (93%)	266 (100%)	0	100	100
1	G	266/287 (93%)	266 (100%)	0	100	100
1	H	266/287 (93%)	266 (100%)	0	100	100
All	All	2130/2296 (93%)	2129 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	LEU

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

Mol	Chain	Res	Type
1	A	74	HIS
1	A	183	ASN
1	A	196	ASN
1	B	116	ASN
1	B	240	ASN
1	B	279	ASN
1	C	116	ASN
1	D	65	ASN
1	D	184	ASN
1	D	228	ASN
1	F	42	GLN
1	F	47	ASN
1	F	62	GLN
1	F	130	ASN
1	F	184	ASN
1	F	240	ASN
1	G	116	ASN
1	H	228	ASN
1	H	240	ASN

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	301/326 (92%)	0.15	15 (4%) 34 39	14, 23, 39, 77	0
1	B	301/326 (92%)	0.17	13 (4%) 40 46	15, 23, 45, 82	0
1	C	304/326 (93%)	-0.01	12 (3%) 43 49	12, 21, 41, 70	0
1	D	301/326 (92%)	0.01	13 (4%) 40 46	14, 21, 37, 75	0
1	E	301/326 (92%)	-0.02	7 (2%) 61 67	13, 22, 39, 69	0
1	F	301/326 (92%)	0.21	17 (5%) 30 34	13, 24, 46, 88	0
1	G	301/326 (92%)	0.59	30 (9%) 12 14	18, 27, 48, 79	0
1	H	301/326 (92%)	0.03	10 (3%) 49 55	13, 21, 39, 76	0
All	All	2411/2608 (92%)	0.14	117 (4%) 35 40	12, 23, 43, 88	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	51	TYR	7.1
1	A	51	TYR	6.9
1	H	51	TYR	6.3
1	D	51	TYR	6.2
1	G	51	TYR	6.0
1	F	259	LEU	5.7
1	B	202	TYR	5.7
1	F	51	TYR	5.4
1	B	51	TYR	5.1
1	A	23	ILE	4.5
1	D	204	HIS	4.4
1	C	23	ILE	4.4
1	B	259	LEU	4.4
1	B	24	ARG	4.4
1	C	51	TYR	4.3
1	A	241	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	50	THR	4.2
1	H	75	LYS	4.2
1	B	23	ILE	4.1
1	D	129	LYS	4.0
1	D	23	ILE	3.9
1	F	47	ASN	3.8
1	A	262	LYS	3.8
1	G	241	LEU	3.8
1	B	241	LEU	3.7
1	G	52	PHE	3.7
1	A	109	ALA	3.6
1	A	52	PHE	3.5
1	F	52	PHE	3.5
1	E	129	LYS	3.5
1	G	259	LEU	3.5
1	F	202	TYR	3.5
1	H	202	TYR	3.5
1	B	47	ASN	3.4
1	D	47	ASN	3.4
1	A	72	ASP	3.4
1	G	72	ASP	3.4
1	H	23	ILE	3.4
1	G	326	ASP	3.4
1	G	197	GLU	3.2
1	G	320	LEU	3.2
1	G	129	LYS	3.2
1	G	322	ALA	3.2
1	E	47	ASN	3.2
1	H	71	LEU	3.2
1	G	323	CYS	3.2
1	B	203	VAL	3.1
1	H	241	LEU	3.1
1	G	317	PRO	3.0
1	F	45	LYS	3.0
1	G	23	ILE	3.0
1	F	53	TYR	3.0
1	B	201	THR	3.0
1	C	109	ALA	2.9
1	F	23	ILE	2.9
1	G	242	GLY	2.9
1	D	266	MET	2.9
1	G	324	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	48	GLY	2.8
1	G	47	ASN	2.8
1	G	92	THR	2.8
1	H	47	ASN	2.8
1	H	326	ASP	2.8
1	F	71	LEU	2.7
1	C	318	GLU	2.7
1	F	318	GLU	2.7
1	D	321	LYS	2.7
1	B	243	TYR	2.7
1	D	110	ASN	2.7
1	F	46	GLU	2.6
1	B	71	LEU	2.6
1	A	47	ASN	2.6
1	D	241	LEU	2.6
1	G	318	GLU	2.6
1	E	23	ILE	2.6
1	A	111	GLY	2.6
1	D	114	TYR	2.6
1	H	52	PHE	2.5
1	D	243	TYR	2.5
1	C	47	ASN	2.5
1	G	258	GLN	2.5
1	A	129	LYS	2.5
1	F	204	HIS	2.5
1	E	259	LEU	2.4
1	E	71	LEU	2.4
1	G	109	ALA	2.4
1	A	110	ASN	2.4
1	A	184	ASN	2.4
1	G	24	ARG	2.4
1	C	110	ASN	2.4
1	G	222	LEU	2.4
1	E	52	PHE	2.4
1	C	62	GLN	2.3
1	D	52	PHE	2.3
1	G	319	ASN	2.3
1	A	318	GLU	2.3
1	A	24	ARG	2.3
1	C	49	SER	2.3
1	C	114	TYR	2.3
1	D	109	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	258	GLN	2.2
1	G	202	TYR	2.2
1	B	258	GLN	2.2
1	F	24	ARG	2.2
1	G	45	LYS	2.2
1	A	80	GLU	2.1
1	G	65	ASN	2.1
1	C	197	GLU	2.1
1	G	298	TYR	2.1
1	H	243	TYR	2.1
1	G	62	GLN	2.1
1	F	201	THR	2.1
1	G	316	THR	2.1
1	B	72	ASP	2.0
1	F	203	VAL	2.0
1	F	129	LYS	2.0
1	G	278	LYS	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	CA	H	401	1/1	0.90	0.09	26,26,26,26	1
2	CA	C	401	1/1	0.93	0.08	23,23,23,23	1
2	CA	C	402	1/1	0.95	0.07	28,28,28,28	1
2	CA	E	401	1/1	0.98	0.04	20,20,20,20	1

6.5 Other polymers [i](#)

There are no such residues in this entry.