



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2025 – 01:14 pm BST

PDB ID : 9RMM / pdb_00009rmm
Title : Crystal structure of outer membrane SilC
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Deposited on : 2025-06-18
Resolution : 3.20 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : **FAILED**
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

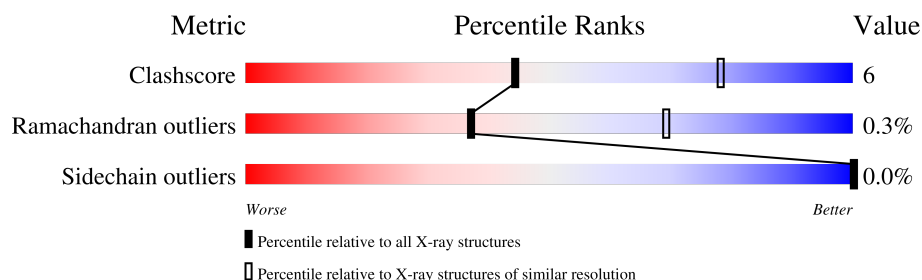
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	462	
1	B	462	
1	D	462	
1	E	462	
1	F	462	
2	C	463	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20536 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 Probable outer membrane lipoprotein SilC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	1	0
			3430	2150	601	674	5			
1	B	435	Total	C	N	O	S	0	0	0
			3410	2138	595	672	5			
1	D	437	Total	C	N	O	S	0	0	0
			3422	2146	597	674	5			
1	E	437	Total	C	N	O	S	0	0	0
			3422	2146	597	674	5			
1	F	438	Total	C	N	O	S	0	0	0
			3427	2149	598	675	5			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	LYS	-	expression tag	UNP Q9ZHD2
B	444	LYS	-	expression tag	UNP Q9ZHD2
D	444	LYS	-	expression tag	UNP Q9ZHD2
E	444	LYS	-	expression tag	UNP Q9ZHD2
F	444	LYS	-	expression tag	UNP Q9ZHD2

- Molecule 2 is a protein called Probable outer membrane lipoprotein SilC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	437	Total	C	N	O	S	0	0	0
			3425	2147	599	674	5			

There are 2 discrepancies between the modelled and reference sequences:

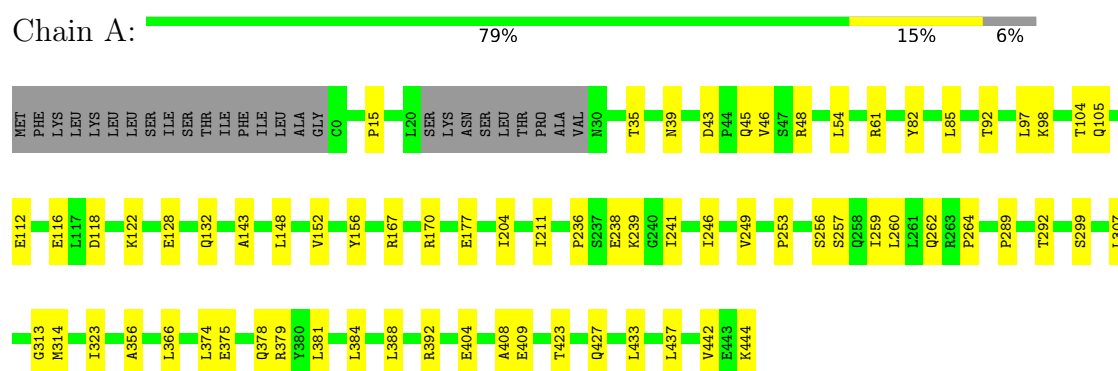
Chain	Residue	Modelled	Actual	Comment	Reference
C	444	LYS	-	expression tag	UNP Q9ZHD2
C	445	HIS	-	expression tag	UNP Q9ZHD2

3 Residue-property plots [i](#)

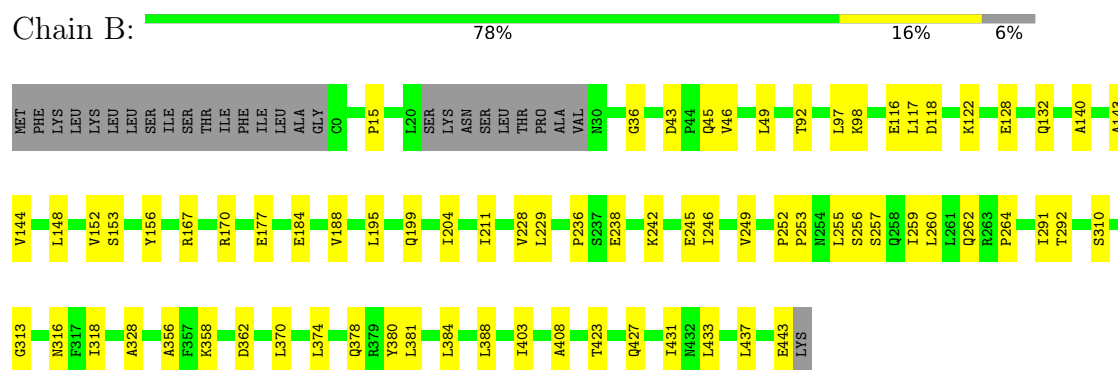
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

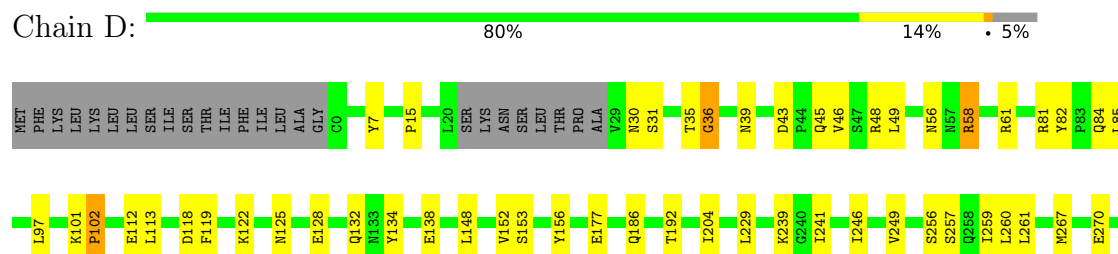
- Molecule 1: Probable outer membrane lipoprotein SilC

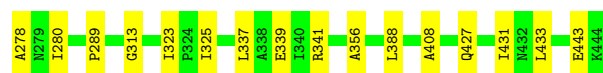


- Molecule 1: Probable outer membrane lipoprotein SilC



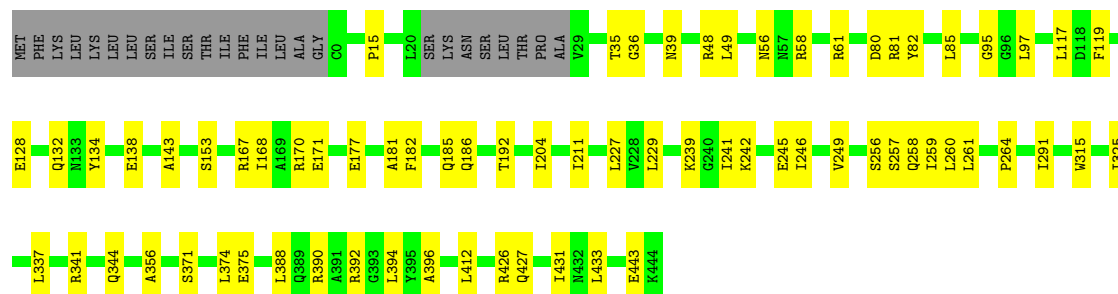
- Molecule 1: Probable outer membrane lipoprotein SilC





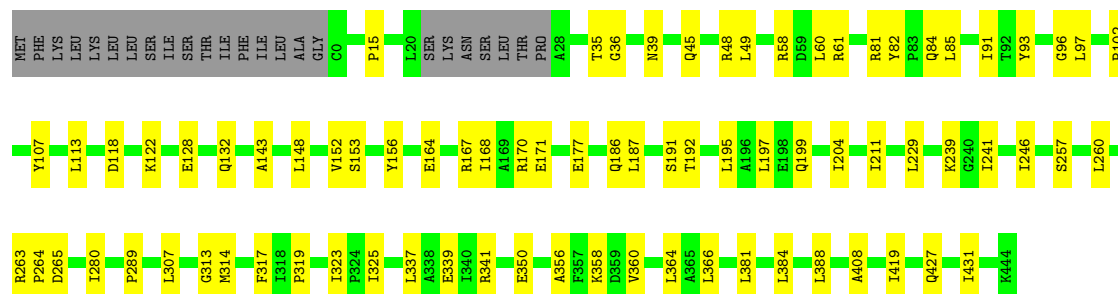
- Molecule 1: Probable outer membrane lipoprotein SilC

Chain E: 79% 15% 5%



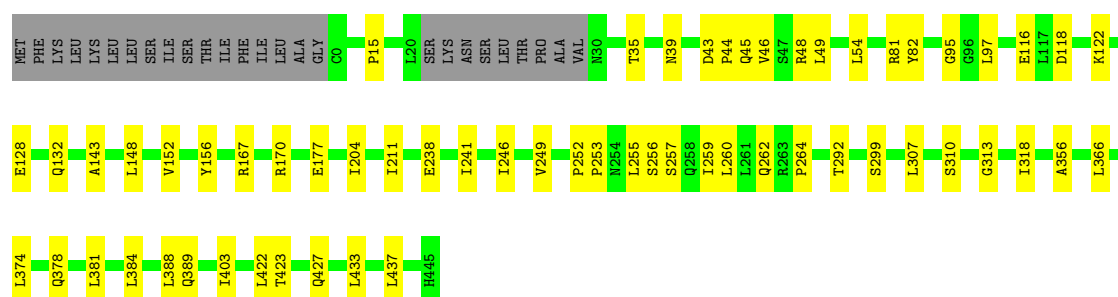
- Molecule 1: Probable outer membrane lipoprotein SilC

Chain F: 78% 17% 5%



- Molecule 2: Probable outer membrane lipoprotein SilC

Chain C: 81% 13% 6%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.06Å 326.79Å 88.10Å 90.00° 120.27° 90.00°	Depositor
Resolution (Å)	44.29 – 3.20	Depositor
% Data completeness (in resolution range)	99.4 (44.29-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.237 , 0.284	Depositor
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.456	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.387 for -h-l,k,h 0.387 for l,k,-h-l 0.339 for l,-k,h 0.340 for h,-k,-h-l 0.339 for -h-l,-k,l	Xtriage
Total number of atoms	20536	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.38% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/3486	0.68	0/4718
1	B	0.49	0/3466	0.68	0/4693
1	D	0.48	0/3478	0.71	0/4710
1	E	0.47	0/3478	0.69	0/4710
1	F	0.47	0/3483	0.70	0/4717
2	C	0.48	0/3482	0.67	0/4715
All	All	0.48	0/20873	0.69	0/28263

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	58	ARG	Sidechain

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	3430	0	3394	43	0
1	B	3410	0	3369	47	0
1	D	3422	0	3380	42	0
1	E	3422	0	3380	46	0
1	F	3427	0	3385	47	0
2	C	3425	0	3378	40	0
All	All	20536	0	20286	240	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 6.

All (240) 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:F:239:LYS:NZ	1:F:241:ILE:O	2.04	0.91
1:A:98:LYS:HD3	1:B:310:SER:HB2	1.75	0.68
1:B:167:ARG:NH1	1:B:238:GLU:OE2	2.25	0.68
1:A:143:ALA:HB2	1:A:264:PRO:HB2	1.76	0.68
1:B:374:LEU:HD21	1:B:423:THR:HG22	1.76	0.67
1:A:442:VAL:HG12	1:A:444:LYS:H	1.59	0.66
2:C:48:ARG:HH21	2:C:49:LEU:HD21	1.61	0.65
1:A:128:GLU:OE2	1:A:132:GLN:NE2	2.29	0.65
1:A:167:ARG:NH1	1:A:238:GLU:OE2	2.31	0.64
2:C:143:ALA:HB2	2:C:264:PRO:HB2	1.78	0.64
1:D:261:LEU:O	1:D:267:MET:HE3	1.97	0.64
2:C:128:GLU:OE2	2:C:132:GLN:NE2	2.30	0.64
1:F:246:ILE:HD12	1:F:427:GLN:HB2	1.80	0.63
1:B:98:LYS:HD3	2:C:310:SER:HB2	1.80	0.62
1:E:371:SER:O	1:E:375:GLU:HG2	1.99	0.62
1:A:116:GLU:HG2	1:A:292:THR:HG22	1.82	0.62
2:C:246:ILE:HD12	2:C:427:GLN:HB2	1.80	0.62
1:E:97:LEU:HD12	1:F:313:GLY:HA3	1.80	0.62
1:E:246:ILE:HD12	1:E:427:GLN:HB2	1.82	0.61
1:A:313:GLY:HA3	2:C:97:LEU:HD12	1.83	0.61
1:B:36:GLY:HA3	1:B:443:GLU:C	2.26	0.61
2:C:15:PRO:O	2:C:257:SER:OG	2.17	0.60
1:A:177:GLU:HA	1:A:204:ILE:HD11	1.83	0.60
2:C:374:LEU:HD21	2:C:423:THR:HG22	1.83	0.59
1:B:143:ALA:HB2	1:B:264:PRO:HB2	1.85	0.58
1:B:15:PRO:O	1:B:257:SER:OG	2.20	0.57
1:F:45:GLN:HG2	1:F:156:TYR:CE1	2.38	0.57
1:A:249:VAL:HG21	1:A:433:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:LEU:O	1:F:152:VAL:HG23	2.05	0.57
1:D:260:LEU:HD22	1:D:356:ALA:HB1	1.85	0.57
1:A:246:ILE:HD12	1:A:427:GLN:HB2	1.87	0.57
1:E:49:LEU:HD22	1:E:229:LEU:HD11	1.86	0.57
1:A:15:PRO:O	1:A:257:SER:OG	2.17	0.57
1:D:85:LEU:O	1:E:325:ILE:HB	2.05	0.56
1:D:45:GLN:HG2	1:D:156:TYR:CE1	2.41	0.56
1:E:56:ASN:HA	1:E:61:ARG:HH21	1.71	0.56
2:C:249:VAL:HG21	2:C:433:LEU:HG	1.88	0.56
1:E:177:GLU:HA	1:E:204:ILE:HD11	1.89	0.55
1:E:227:LEU:HD22	1:F:358:LYS:HD2	1.88	0.55
1:B:246:ILE:HD12	1:B:427:GLN:HB2	1.88	0.54
1:E:143:ALA:HB2	1:E:264:PRO:HB2	1.88	0.54
1:A:388:LEU:HD13	1:A:408:ALA:HB3	1.89	0.54
1:A:43:ASP:HB3	1:A:46:VAL:HG12	1.88	0.54
1:A:92:THR:HG23	1:B:318:ILE:HG12	1.88	0.54
1:E:249:VAL:HG21	1:E:433:LEU:HD22	1.89	0.54
1:F:48:ARG:HH21	1:F:49:LEU:HD21	1.73	0.54
1:D:289:PRO:HG3	1:D:323:ILE:HG23	1.89	0.53
2:C:170:ARG:HA	2:C:211:ILE:HD11	1.90	0.53
1:F:143:ALA:HB2	1:F:264:PRO:HB2	1.91	0.53
1:D:30:ASN:OD1	1:D:31:SER:N	2.41	0.53
1:E:167:ARG:O	1:E:171:GLU:HG2	2.09	0.53
1:A:256:SER:O	1:A:259:ILE:HG22	2.08	0.52
2:C:256:SER:O	2:C:259:ILE:HG22	2.09	0.52
1:D:97:LEU:HD21	1:E:315:TRP:HB3	1.91	0.52
1:B:249:VAL:HG21	1:B:433:LEU:HG	1.91	0.52
1:B:252:PRO:HD2	1:B:255:LEU:HD13	1.91	0.52
1:B:184:GLU:O	1:B:188:VAL:HG23	2.10	0.52
1:A:85:LEU:HD12	1:A:112:GLU:O	2.10	0.51
1:B:128:GLU:OE2	1:B:132:GLN:NE2	2.42	0.51
1:D:134:TYR:OH	1:D:138:GLU:OE2	2.21	0.51
1:A:118:ASP:OD1	1:A:122:LYS:N	2.42	0.51
1:B:97:LEU:HD12	2:C:313:GLY:HA3	1.92	0.51
1:B:43:ASP:HB3	1:B:46:VAL:HG12	1.91	0.51
1:D:337:LEU:HD22	1:D:341:ARG:NH2	2.26	0.51
2:C:389:GLN:OE1	1:E:239:LYS:NZ	2.19	0.51
2:C:45:GLN:HG2	2:C:156:TYR:CE1	2.46	0.51
2:C:241:ILE:HD11	1:E:388:LEU:HD13	1.92	0.50
1:E:134:TYR:OH	1:E:138:GLU:OE2	2.26	0.50
1:F:337:LEU:HD22	1:F:341:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:ASP:HB3	2:C:46:VAL:HG12	1.94	0.50
1:D:325:ILE:HG21	1:F:85:LEU:HD23	1.93	0.50
2:C:148:LEU:O	2:C:152:VAL:HG23	2.11	0.50
1:A:148:LEU:O	1:A:152:VAL:HG23	2.12	0.49
1:D:15:PRO:O	1:D:257:SER:OG	2.22	0.49
1:D:43:ASP:HB3	1:D:46:VAL:HG12	1.93	0.49
2:C:252:PRO:HD2	2:C:255:LEU:HD13	1.94	0.49
1:F:170:ARG:HA	1:F:211:ILE:HD11	1.93	0.49
1:F:260:LEU:HD22	1:F:356:ALA:HB1	1.93	0.49
1:F:167:ARG:O	1:F:171:GLU:HG2	2.13	0.49
1:F:35:THR:HB	1:F:39:ASN:OD1	2.13	0.49
1:B:374:LEU:CD2	1:B:423:THR:HG22	2.40	0.49
1:F:107:TYR:HB3	1:F:307:LEU:HD22	1.93	0.48
1:E:128:GLU:OE2	1:E:132:GLN:NE2	2.35	0.48
1:E:242:LYS:HD2	1:E:245:GLU:OE2	2.13	0.48
1:D:177:GLU:HA	1:D:204:ILE:HD11	1.96	0.48
1:F:49:LEU:HD22	1:F:229:LEU:HD11	1.95	0.48
1:A:374:LEU:HD21	1:A:423:THR:HG22	1.95	0.48
1:B:256:SER:O	1:B:259:ILE:HG22	2.13	0.48
2:C:388:LEU:HD23	1:E:241:ILE:HD11	1.96	0.48
1:F:186:GLN:HB3	1:F:192:THR:HG23	1.96	0.48
1:B:260:LEU:HD22	1:B:356:ALA:HB1	1.96	0.48
1:E:181:ALA:O	1:E:185:GLN:HG2	2.13	0.48
1:A:97:LEU:HD12	1:B:313:GLY:HA3	1.96	0.48
1:A:98:LYS:CD	1:B:310:SER:HB2	2.44	0.48
1:E:58:ARG:NH1	1:F:350:GLU:OE1	2.46	0.48
2:C:378:GLN:O	2:C:381:LEU:HB3	2.14	0.48
1:D:148:LEU:O	1:D:152:VAL:HG23	2.13	0.48
1:E:374:LEU:HD23	1:E:426:ARG:HH11	1.79	0.48
2:C:177:GLU:HA	2:C:204:ILE:HD11	1.96	0.47
1:D:289:PRO:HB3	1:D:323:ILE:HG12	1.95	0.47
1:A:45:GLN:HE21	1:A:236:PRO:HG3	1.78	0.47
1:A:314:MET:HG3	2:C:95:GLY:O	2.14	0.47
1:D:85:LEU:HD12	1:D:112:GLU:O	2.14	0.47
1:B:259:ILE:HG12	1:B:437:LEU:HD22	1.97	0.47
2:C:118:ASP:OD1	2:C:122:LYS:N	2.44	0.47
1:A:239:LYS:NZ	1:A:241:ILE:O	2.33	0.47
1:E:15:PRO:O	1:E:257:SER:OG	2.29	0.47
1:D:246:ILE:HD12	1:D:427:GLN:HB2	1.97	0.47
1:F:289:PRO:HB3	1:F:323:ILE:HG13	1.96	0.47
1:B:177:GLU:HA	1:B:204:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:NH2	1:A:409:GLU:OE2	2.41	0.46
1:A:437:LEU:HD23	1:A:437:LEU:HA	1.63	0.46
1:B:45:GLN:HG2	1:B:156:TYR:CE1	2.50	0.46
1:E:35:THR:HB	1:E:39:ASN:OD1	2.16	0.46
1:F:96:GLY:H	1:F:102:PRO:HD2	1.81	0.46
1:B:45:GLN:HE21	1:B:236:PRO:HG3	1.81	0.46
1:B:117:LEU:HB2	1:B:291:ILE:O	2.16	0.46
1:D:388:LEU:HD13	1:D:408:ALA:HB3	1.97	0.46
1:F:91:ILE:CG2	1:F:93:TYR:HE1	2.29	0.46
2:C:35:THR:HB	2:C:39:ASN:OD1	2.16	0.46
1:D:7:TYR:OH	1:D:270:GLU:OE2	2.30	0.45
2:C:437:LEU:HA	2:C:437:LEU:HD23	1.67	0.45
1:F:15:PRO:O	1:F:257:SER:OG	2.29	0.45
1:F:388:LEU:HD13	1:F:408:ALA:HB3	1.97	0.45
1:A:378:GLN:O	1:A:381:LEU:HB3	2.16	0.45
1:E:48:ARG:HH21	1:E:49:LEU:HD21	1.82	0.45
1:A:45:GLN:HG2	1:A:156:TYR:CE1	2.52	0.45
1:B:92:THR:HG23	2:C:318:ILE:HG12	1.99	0.45
1:E:49:LEU:HB3	1:E:229:LEU:HD21	1.99	0.45
1:E:81:ARG:C	1:E:82:TYR:HD1	2.25	0.45
1:B:242:LYS:HD2	1:B:245:GLU:OE2	2.17	0.45
1:D:101:LYS:N	1:D:102:PRO:HD3	2.31	0.45
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.71	0.45
1:D:36:GLY:HA3	1:D:443:GLU:C	2.42	0.45
1:D:249:VAL:HG21	1:D:433:LEU:HG	2.00	0.44
1:E:186:GLN:HB3	1:E:192:THR:HG23	1.98	0.44
1:F:84:GLN:O	1:F:113:LEU:HA	2.17	0.44
1:F:128:GLU:OE2	1:F:132:GLN:NE2	2.40	0.44
1:A:170:ARG:HA	1:A:211:ILE:HD11	1.99	0.44
2:C:260:LEU:HD22	2:C:356:ALA:HB1	1.99	0.44
1:D:239:LYS:HE3	1:D:241:ILE:O	2.17	0.44
1:E:182:PHE:HZ	1:E:396:ALA:HB2	1.81	0.44
1:F:177:GLU:HA	1:F:204:ILE:HD11	1.98	0.44
1:F:381:LEU:HD22	1:F:419:ILE:HD12	2.00	0.44
1:A:35:THR:HB	1:A:39:ASN:OD1	2.18	0.44
1:E:260:LEU:HD22	1:E:356:ALA:HB1	1.98	0.44
1:E:337:LEU:HD22	1:E:341:ARG:NH2	2.32	0.44
1:D:81:ARG:C	1:D:82:TYR:HD1	2.25	0.44
1:E:85:LEU:O	1:F:325:ILE:HB	2.16	0.44
1:B:380:TYR:CZ	1:B:384:LEU:HD11	2.53	0.44
2:C:44:PRO:HG3	1:E:392:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ARG:HA	1:E:211:ILE:HD11	1.99	0.44
1:F:164:GLU:O	1:F:168:ILE:HG23	2.18	0.44
1:B:140:ALA:O	1:B:144:VAL:HG23	2.18	0.44
1:D:84:GLN:O	1:D:113:LEU:HA	2.17	0.44
2:C:374:LEU:HD13	2:C:422:LEU:HB3	2.00	0.43
1:D:35:THR:HB	1:D:39:ASN:OD1	2.18	0.43
1:A:104:THR:HG22	1:A:105:GLN:N	2.33	0.43
1:D:125:ASN:O	1:D:278:ALA:HB1	2.18	0.43
1:D:153:SER:OG	1:D:431:ILE:HD13	2.18	0.43
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.81	0.43
1:B:153:SER:OG	1:B:431:ILE:HD13	2.18	0.43
2:C:81:ARG:C	2:C:82:TYR:HD1	2.26	0.43
1:D:56:ASN:HA	1:D:61:ARG:HH21	1.83	0.43
1:E:256:SER:O	1:E:259:ILE:HG22	2.18	0.43
1:B:152:VAL:HG22	1:B:228:VAL:HG12	2.01	0.43
2:C:116:GLU:HG2	2:C:292:THR:HG22	2.00	0.43
1:D:134:TYR:CZ	1:D:138:GLU:OE2	2.72	0.43
1:E:36:GLY:HA3	1:E:443:GLU:C	2.44	0.43
1:A:375:GLU:O	1:A:379:ARG:HG2	2.18	0.43
1:E:153:SER:OG	1:E:431:ILE:HD13	2.18	0.43
1:B:378:GLN:O	1:B:381:LEU:HB3	2.19	0.43
1:F:187:LEU:CD2	1:F:197:LEU:HD22	2.48	0.43
1:E:95:GLY:O	1:F:314:MET:HG3	2.18	0.43
1:F:81:ARG:C	1:F:82:TYR:HD1	2.26	0.43
1:F:153:SER:OG	1:F:431:ILE:HD13	2.19	0.43
1:A:260:LEU:HD22	1:A:356:ALA:HB1	2.00	0.43
1:B:195:LEU:O	1:B:199:GLN:HG3	2.19	0.43
1:F:58:ARG:NH1	1:F:61:ARG:CZ	2.82	0.43
1:F:360:VAL:O	1:F:364:LEU:HG	2.19	0.43
1:E:168:ILE:HA	1:E:171:GLU:CG	2.49	0.43
1:A:82:TYR:HB2	1:B:328:ALA:HB2	1.99	0.42
1:B:370:LEU:HD23	1:B:370:LEU:HA	1.74	0.42
1:D:119:PHE:HD1	1:D:119:PHE:O	2.01	0.42
1:F:280:ILE:HD11	1:F:339:GLU:HA	1.99	0.42
1:F:366:LEU:HA	1:F:366:LEU:HD23	1.75	0.42
1:B:118:ASP:OD1	1:B:122:LYS:N	2.48	0.42
1:B:259:ILE:O	1:B:262:GLN:HG3	2.19	0.42
1:D:128:GLU:OE2	1:D:132:GLN:NE2	2.45	0.42
1:E:119:PHE:HD1	1:E:119:PHE:O	2.02	0.42
1:D:280:ILE:HD11	1:D:339:GLU:HA	2.02	0.42
2:C:54:LEU:HA	2:C:54:LEU:HD23	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:LEU:O	1:F:199:GLN:HG3	2.19	0.42
1:F:263:ARG:HB3	1:F:265:ASP:OD1	2.19	0.42
1:B:49:LEU:HD22	1:B:229:LEU:HD11	2.01	0.42
1:B:148:LEU:O	1:B:152:VAL:HG23	2.20	0.42
1:B:437:LEU:HD23	1:B:437:LEU:HA	1.60	0.42
2:C:381:LEU:O	2:C:384:LEU:N	2.51	0.42
1:F:118:ASP:OD1	1:F:122:LYS:N	2.50	0.42
2:C:246:ILE:CD1	2:C:427:GLN:HB2	2.50	0.42
1:D:313:GLY:HA3	1:F:97:LEU:HD12	2.01	0.42
1:A:45:GLN:NE2	1:A:48:ARG:NH2	2.68	0.42
1:A:381:LEU:O	1:A:384:LEU:N	2.53	0.42
1:E:36:GLY:HA3	1:E:443:GLU:O	2.20	0.42
2:C:167:ARG:NH1	2:C:238:GLU:OE2	2.53	0.42
2:C:366:LEU:HD23	2:C:366:LEU:HA	1.70	0.41
1:D:186:GLN:HB3	1:D:192:THR:HG23	2.01	0.41
1:D:325:ILE:HB	1:F:85:LEU:O	2.21	0.41
1:E:80:ASP:N	1:E:80:ASP:OD1	2.51	0.41
2:C:259:ILE:O	2:C:262:GLN:HG3	2.19	0.41
1:B:403:ILE:HD13	1:B:403:ILE:HG21	1.82	0.41
1:B:117:LEU:HD22	1:B:291:ILE:HB	2.02	0.41
1:E:388:LEU:HD12	1:E:412:LEU:HD22	2.02	0.41
1:A:299:SER:OG	1:A:307:LEU:O	2.39	0.41
1:E:390:ARG:O	1:E:394:LEU:HD13	2.21	0.41
1:B:316:ASN:OD1	1:B:318:ILE:HG13	2.21	0.41
1:F:186:GLN:HB3	1:F:191:SER:HB2	2.02	0.41
1:B:358:LYS:NZ	1:B:362:ASP:OD2	2.53	0.41
1:B:388:LEU:HD13	1:B:408:ALA:HB3	2.02	0.41
2:C:299:SER:OG	2:C:307:LEU:O	2.39	0.41
1:D:118:ASP:OD1	1:D:122:LYS:N	2.53	0.41
1:D:261:LEU:HD23	1:D:261:LEU:HA	1.77	0.41
1:F:317:PHE:CD1	1:F:319:PRO:HD3	2.56	0.41
1:F:246:ILE:CD1	1:F:427:GLN:HB2	2.49	0.41
1:A:404:GLU:OE1	2:C:403:ILE:HB	2.21	0.40
1:D:49:LEU:HD22	1:D:229:LEU:HD11	2.02	0.40
1:D:256:SER:O	1:D:259:ILE:HG22	2.21	0.40
1:E:117:LEU:HB2	1:E:291:ILE:O	2.21	0.40
1:E:261:LEU:HA	1:E:261:LEU:HD23	1.73	0.40
1:A:45:GLN:NE2	1:A:48:ARG:HH21	2.20	0.40
1:A:259:ILE:O	1:A:262:GLN:HG3	2.21	0.40
1:A:289:PRO:HB3	1:A:323:ILE:HG13	2.03	0.40
1:D:58:ARG:NH1	1:D:61:ARG:NH1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:LEU:HD12	1:F:60:LEU:HA	1.85	0.40
1:F:384:LEU:HA	1:F:384:LEU:HD23	1.93	0.40
1:B:170:ARG:HA	1:B:211:ILE:HD11	2.02	0.40
1:E:341:ARG:O	1:E:344:GLN:HB2	2.22	0.40
1:B:116:GLU:HG2	1:B:292:THR:HG22	2.02	0.40
2:C:374:LEU:CD2	2:C:423:THR:HG22	2.50	0.40
1:D:45:GLN:OE1	1:D:48:ARG:NH2	2.54	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	433/462 (94%)	416 (96%)	16 (4%)	1 (0%)	44	75
1	B	431/462 (93%)	416 (96%)	14 (3%)	1 (0%)	44	75
1	D	433/462 (94%)	416 (96%)	15 (4%)	2 (0%)	25	60
1	E	433/462 (94%)	419 (97%)	13 (3%)	1 (0%)	44	75
1	F	434/462 (94%)	411 (95%)	22 (5%)	1 (0%)	44	75
2	C	433/463 (94%)	416 (96%)	16 (4%)	1 (0%)	44	75
All	All	2597/2773 (94%)	2494 (96%)	96 (4%)	7 (0%)	37	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	36	GLY
1	B	253	PRO
1	E	258	GLN
1	A	253	PRO
1	D	102	PRO

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Mol	Chain	Res	Type
2	C	253	PRO
1	D	36	GLY

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	367/389 (94%)	365 (100%)	2 (0%)	86	93
1	B	365/389 (94%)	365 (100%)	0	100	100
1	D	366/389 (94%)	366 (100%)	0	100	100
1	E	366/389 (94%)	366 (100%)	0	100	100
1	F	366/389 (94%)	366 (100%)	0	100	100
2	C	366/390 (94%)	366 (100%)	0	100	100
All	All	2196/2335 (94%)	2194 (100%)	2 (0%)	100	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61[A]	ARG
1	A	61[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	416	GLN
1	A	429	ASN
1	B	199	GLN
1	B	262	GLN
1	B	416	GLN
1	B	427	GLN
1	B	429	ASN
2	C	203	GLN

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Mol	Chain	Res	Type
2	C	262	GLN
2	C	348	ASN
2	C	373	GLN
2	C	416	GLN
1	D	56	ASN
1	D	86	ASN
1	D	145	HIS
1	D	327	ASN
1	D	348	ASN
1	D	416	GLN
1	E	220	GLN
1	E	327	ASN
1	E	377	GLN
1	E	416	GLN
1	E	427	GLN
1	F	86	ASN
1	F	145	HIS
1	F	327	ASN
1	F	416	GLN
1	F	429	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.