



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:33 PM UTC

PDB ID : 4UV2 / pdb_00004uv2
Title : Structure of the curli transport lipoprotein CsgG in a non-lipidated, pre-pore conformation
Authors : Goyal, P.; Krasteva, P.V.; Gerven, N.V.; Gubellini, F.; Broeck, I.V.D.; Troupiotis-Tsailaki, A.; Jonckheere, W.; Pehau-Arnaudet, G.; Pinkner, J.S.; Chapman, M.R.; Hultgren, S.J.; Howorka, S.; Fronzes, R.; Remaut, H.
Deposited on : 2014-08-04
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

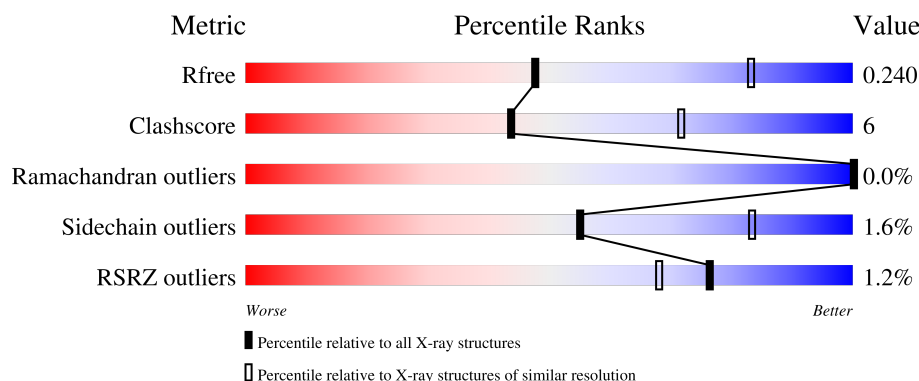
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	262	
1	B	262	
1	C	262	
1	D	262	

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Mol	Chain	Length	Quality of chain
1	E	262	 % 81% 11% 8%
1	F	262	 2% 76% 13% 11%
1	G	262	 % 75% 15% 10%
1	H	262	 % 69% 20% 10%
1	I	262	 % 80% 9% 10%
1	J	262	 2% 72% 15% 13%
1	K	262	 % 77% 12% 11%
1	L	262	 % 76% 12% 11%
1	M	262	 % 69% 13% 17%
1	N	262	 % 77% 12% 11%
1	O	262	 2% 71% 13% 17%
1	P	262	 2% 69% 13% 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28853 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 CURLI PRODUCTION TRANSPORT COMPONENT CSGG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	Se	95	0	0
			1817	1151	312	348	1	5			
1	B	236	Total	C	N	O	S	Se	75	0	0
			1835	1162	317	350	1	5			
1	C	234	Total	C	N	O	S	Se	41	0	0
			1817	1151	312	348	1	5			
1	D	235	Total	C	N	O	S	Se	68	0	0
			1828	1157	316	349	1	5			
1	E	241	Total	C	N	O	S	Se	91	0	0
			1879	1187	326	360	1	5			
1	F	234	Total	C	N	O	S	Se	115	0	0
			1821	1152	315	348	1	5			
1	G	235	Total	C	N	O	S	Se	121	0	0
			1830	1157	317	350	1	5			
1	H	236	Total	C	N	O	S	Se	72	0	0
			1835	1162	317	350	1	5			
1	I	235	Total	C	N	O	S	Se	117	0	0
			1828	1157	316	349	1	5			
1	J	228	Total	C	N	O	S	Se	110	0	0
			1785	1131	309	339	1	5			
1	K	234	Total	C	N	O	S	Se	119	0	0
			1821	1152	315	348	1	5			
1	L	234	Total	C	N	O	S	Se	119	0	0
			1821	1152	315	348	1	5			
1	M	217	Total	C	N	O	S	Se	80	0	0
			1705	1079	294	326	1	5			
1	N	233	Total	C	N	O	S	Se	162	0	0
			1814	1147	314	347	1	5			
1	O	218	Total	C	N	O	S	Se	92	0	0
			1714	1085	296	327	1	5			
1	P	216	Total	C	N	O	S	Se	99	0	0
			1703	1080	293	324	1	5			

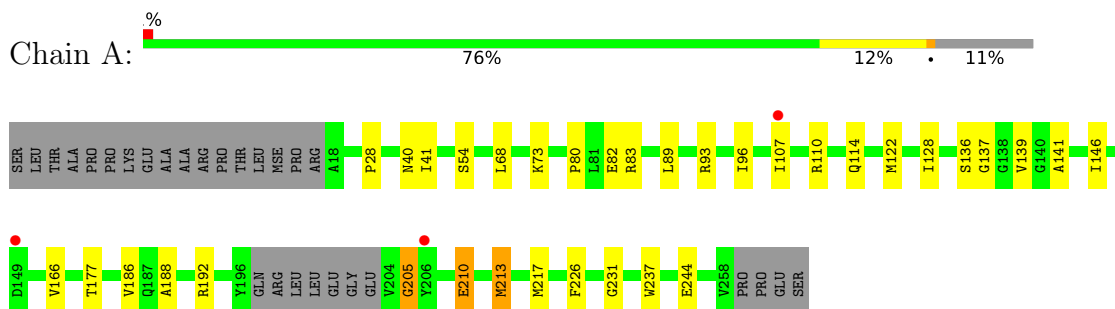
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P0AEA2
B	1	SER	-	expression tag	UNP P0AEA2
C	1	SER	-	expression tag	UNP P0AEA2
D	1	SER	-	expression tag	UNP P0AEA2
E	1	SER	-	expression tag	UNP P0AEA2
F	1	SER	-	expression tag	UNP P0AEA2
G	1	SER	-	expression tag	UNP P0AEA2
H	1	SER	-	expression tag	UNP P0AEA2
I	1	SER	-	expression tag	UNP P0AEA2
J	1	SER	-	expression tag	UNP P0AEA2
K	1	SER	-	expression tag	UNP P0AEA2
L	1	SER	-	expression tag	UNP P0AEA2
M	1	SER	-	expression tag	UNP P0AEA2
N	1	SER	-	expression tag	UNP P0AEA2
O	1	SER	-	expression tag	UNP P0AEA2
P	1	SER	-	expression tag	UNP P0AEA2

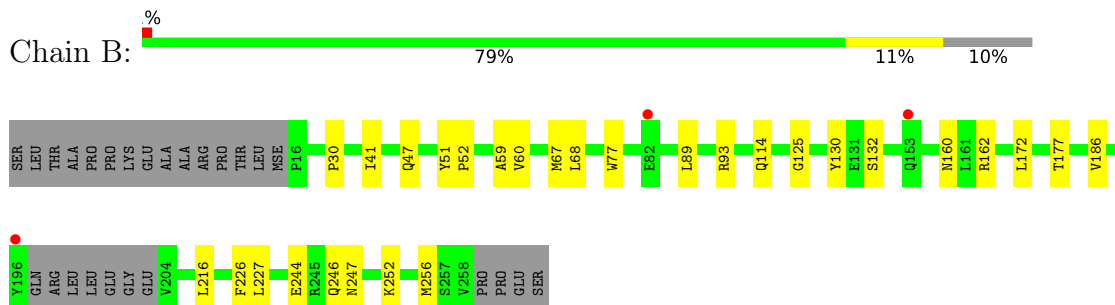
3 Residue-property plots

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.

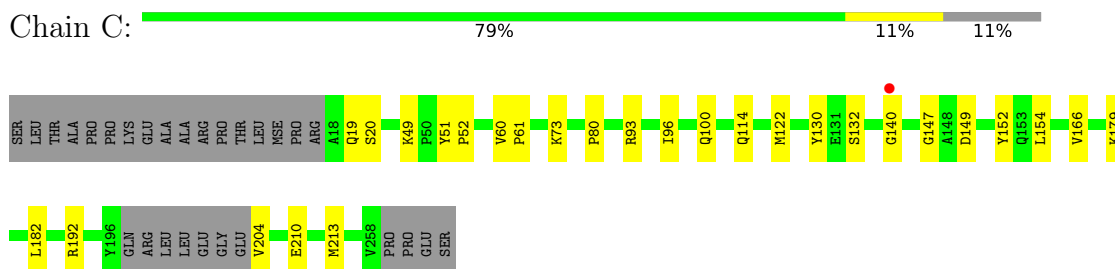
• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



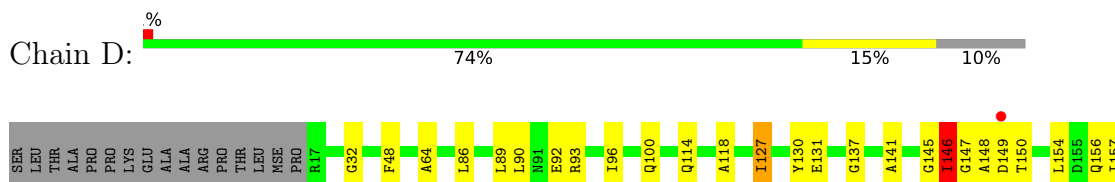
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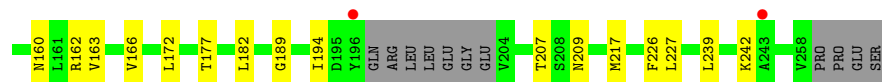


• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG

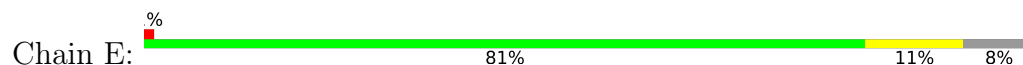


• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG

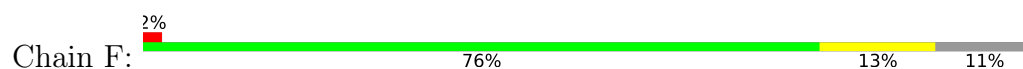




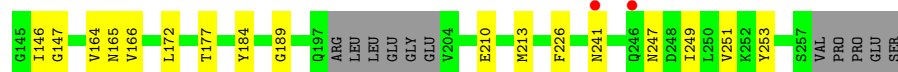
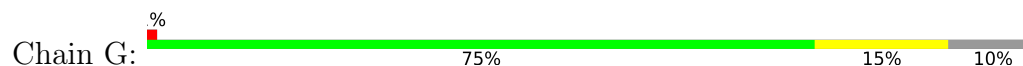
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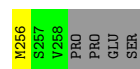
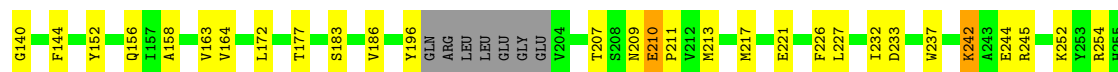
• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



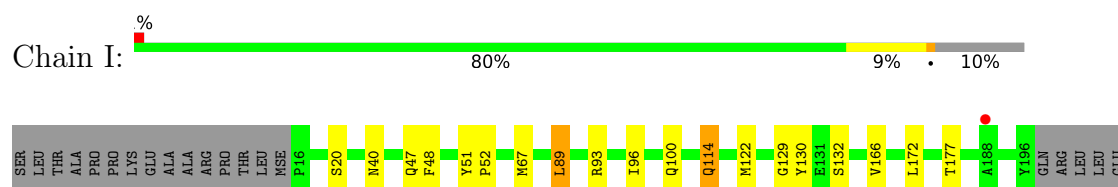
• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



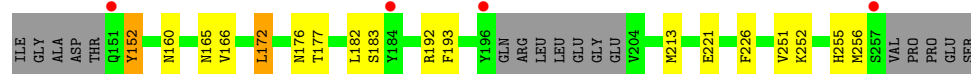
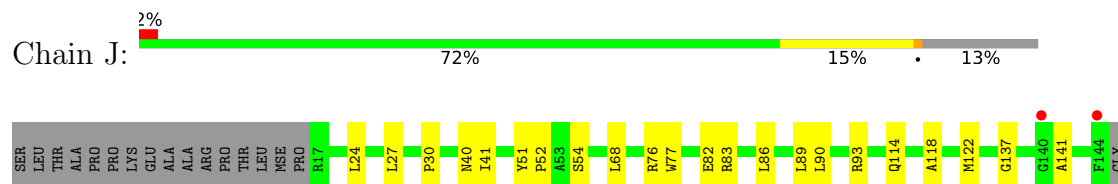
• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



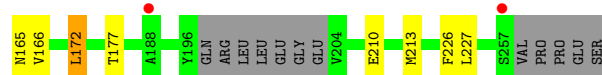
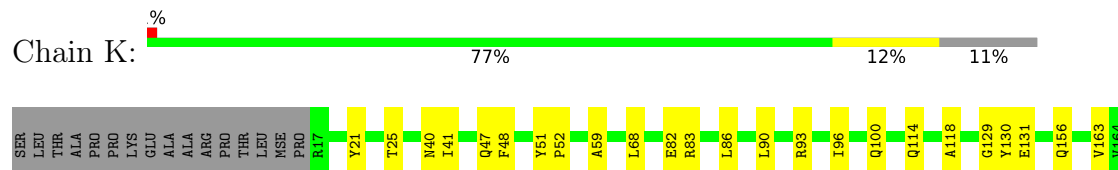
• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



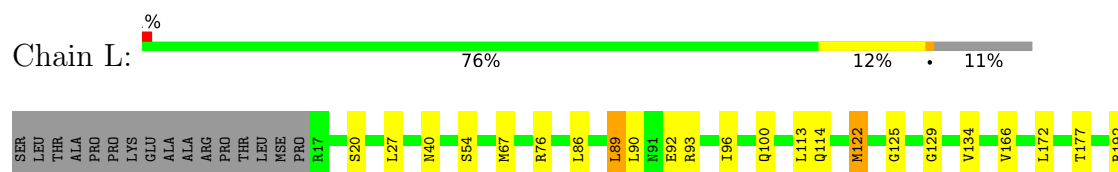
• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



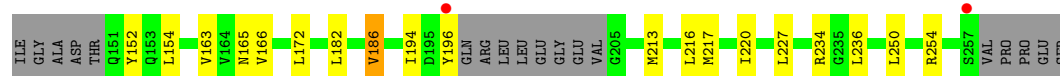
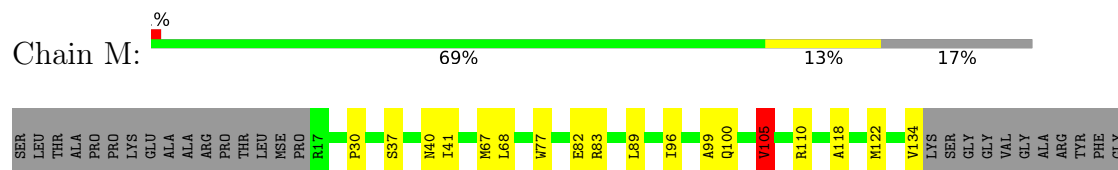
• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



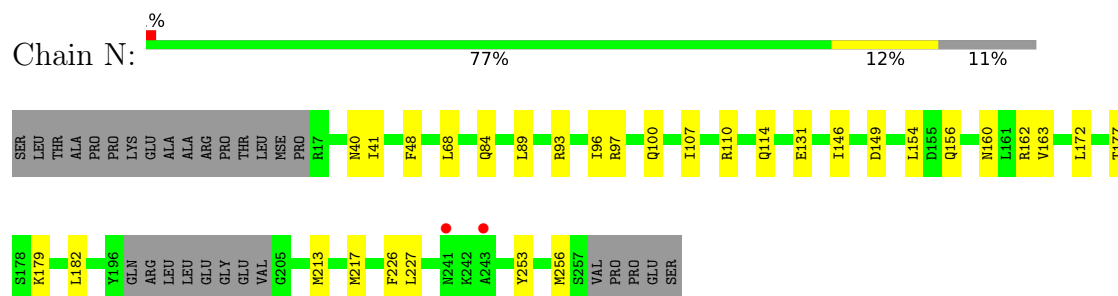
• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



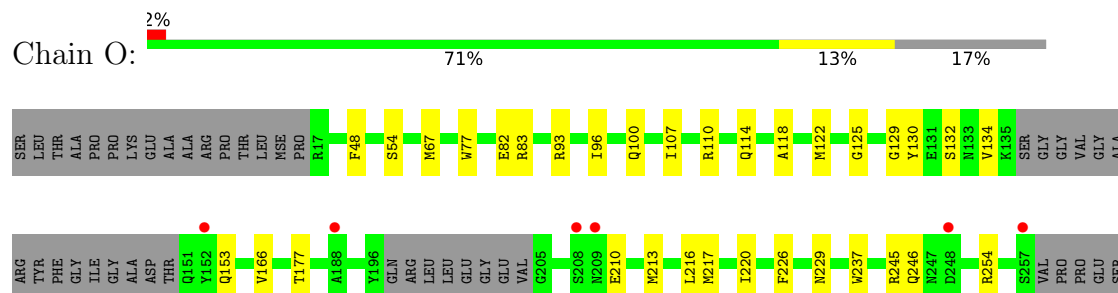
• Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



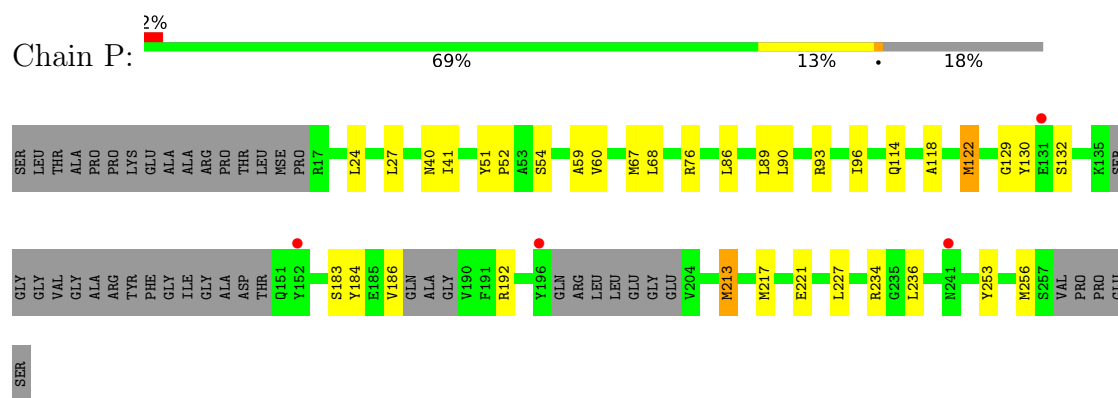
- Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



- Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



- Molecule 1: CURLI PRODUCTION TRANSPORT COMPONENT CSGG



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	101.33Å 103.60Å 141.74Å 111.33° 90.55° 118.21°	Depositor
Resolution (Å)	29.77 – 2.80 29.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.77-2.80) 98.9 (29.77-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.188 , 0.234 0.195 , 0.240	Depositor DCC
R_{free} test set	5624 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,-h-k,h+k+l 0.000 for -h-k,h,k+l 0.002 for h,-h-k,-l 0.019 for -h-k,k,-k-l 0.004 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28853	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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

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	0.64	0/1842	0.93	3/2491 (0.1%)
1	B	0.66	0/1861	0.92	2/2516 (0.1%)
1	C	0.62	0/1842	0.95	2/2491 (0.1%)
1	D	0.66	1/1853 (0.1%)	0.97	3/2505 (0.1%)
1	E	0.61	0/1905	0.89	0/2575
1	F	0.59	0/1846	0.93	2/2495 (0.1%)
1	G	0.66	0/1855	0.98	1/2507 (0.0%)
1	H	0.66	0/1861	0.94	2/2516 (0.1%)
1	I	0.59	0/1854	0.92	2/2506 (0.1%)
1	J	0.61	0/1809	0.93	2/2443 (0.1%)
1	K	0.61	0/1846	0.94	2/2495 (0.1%)
1	L	0.59	0/1846	0.93	2/2495 (0.1%)
1	M	0.63	1/1727 (0.1%)	0.94	4/2334 (0.2%)
1	N	0.61	0/1839	0.93	2/2485 (0.1%)
1	O	0.63	0/1736	0.93	1/2345 (0.0%)
1	P	0.65	0/1724	0.95	1/2328 (0.0%)
All	All	0.63	2/29246 (0.0%)	0.94	31/39527 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	105	VAL	CA-CB	5.08	1.59	1.54
1	D	127	ILE	CA-CB	-5.05	1.48	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ASN	N-CA-C	6.80	119.60	110.35
1	F	40	ASN	N-CA-C	6.53	119.23	110.35
1	A	186	VAL	N-CA-C	-6.44	106.68	111.90
1	J	40	ASN	N-CA-C	6.31	118.94	110.35
1	P	40	ASN	N-CA-C	6.27	118.88	110.35
1	L	40	ASN	N-CA-C	6.12	118.68	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	125	GLY	N-CA-C	6.11	120.70	110.56
1	H	210	GLU	N-CA-C	5.86	117.08	109.64
1	B	125	GLY	N-CA-C	5.83	120.24	110.56
1	C	49	LYS	CA-C-N	5.68	126.14	120.52
1	C	49	LYS	C-N-CA	5.68	126.14	120.52
1	M	186	VAL	N-CA-C	-5.64	107.33	111.90
1	A	205	GLY	N-CA-C	5.57	121.67	110.97
1	G	40	ASN	N-CA-C	5.53	117.86	110.35
1	I	47	GLN	N-CA-C	5.53	117.97	109.07
1	H	40	ASN	N-CA-C	5.52	117.86	110.35
1	N	40	ASN	N-CA-C	5.47	117.80	110.35
1	I	40	ASN	N-CA-C	5.40	117.70	110.35
1	K	47	GLN	N-CA-C	5.38	118.24	109.59
1	F	149	ASP	N-CA-C	-5.28	106.86	113.72
1	M	40	ASN	N-CA-C	5.27	117.52	110.35
1	J	152	TYR	N-CA-C	5.25	117.25	109.69
1	K	40	ASN	N-CA-C	5.24	117.47	110.35
1	M	37	SER	CA-C-N	-5.22	116.33	123.12
1	M	37	SER	C-N-CA	-5.22	116.33	123.12
1	B	47	GLN	N-CA-C	5.18	117.94	109.59
1	D	146	ILE	CA-C-N	5.09	126.28	120.53
1	D	146	ILE	C-N-CA	5.09	126.28	120.53
1	L	125	GLY	N-CA-C	5.08	118.99	110.56
1	N	149	ASP	N-CA-C	-5.05	107.50	113.97
1	D	32	GLY	N-CA-C	-5.03	103.13	110.87

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	1817	0	1823	23	0
1	B	1835	0	1844	18	0
1	C	1817	0	1823	18	0
1	D	1828	0	1836	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1879	0	1886	19	0
1	F	1821	0	1827	24	0
1	G	1830	0	1835	29	0
1	H	1835	0	1844	39	0
1	I	1828	0	1835	19	0
1	J	1785	0	1793	23	0
1	K	1821	0	1827	22	0
1	L	1821	0	1827	23	0
1	M	1705	0	1712	27	0
1	N	1814	0	1818	23	0
1	O	1714	0	1725	24	0
1	P	1703	0	1717	22	0
All	All	28853	0	28972	329	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 (329) 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:H:28:PRO:HB3	1:H:244:GLU:HG2	1.49	0.95
1:A:122:MSE:HE2	1:A:166:VAL:HG22	1.52	0.90
1:C:122:MSE:HE1	1:D:89:LEU:HA	1.53	0.90
1:O:67:MSE:HE2	1:O:220:ILE:HD12	1.52	0.88
1:M:67:MSE:HE2	1:M:220:ILE:HD12	1.60	0.84
1:N:131:GLU:HG2	1:N:156:GLN:HG2	1.60	0.81
1:F:122:MSE:HE1	1:G:89:LEU:HA	1.63	0.80
1:G:105:VAL:HG12	1:M:110:ARG:NH2	1.96	0.80
1:O:67:MSE:HE1	1:O:216:LEU:HG	1.63	0.80
1:I:67:MSE:HE2	1:I:220:ILE:HD12	1.67	0.75
1:D:207:THR:HG22	1:D:209:ASN:H	1.51	0.73
1:C:192:ARG:HH21	1:C:204:VAL:HG11	1.51	0.73
1:G:41:ILE:HD11	1:G:68:LEU:HD22	1.71	0.72
1:B:41:ILE:HD11	1:B:68:LEU:HD22	1.74	0.69
1:D:146:ILE:HG21	1:D:150:THR:HG21	1.75	0.69
1:G:128:ILE:HG13	1:H:213:MSE:HE1	1.76	0.68
1:F:107:ILE:HD13	1:N:107:ILE:HD13	1.76	0.67
1:K:129:GLY:HA3	1:L:213:MSE:HE1	1.76	0.67
1:J:251:VAL:O	1:J:255:HIS:ND1	2.25	0.67
1:H:207:THR:HG22	1:H:209:ASN:H	1.60	0.67
1:I:230:ASP:OD2	1:I:234:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HG	1:H:122:MSE:HE1	1.77	0.66
1:M:122:MSE:HE1	1:N:89:LEU:HA	1.76	0.66
1:I:67:MSE:HE1	1:I:217:MSE:HA	1.79	0.65
1:O:129:GLY:HA3	1:P:213:MSE:HE1	1.79	0.64
1:G:144:PHE:HB3	1:G:146:ILE:CD1	2.27	0.64
1:H:242:LYS:O	1:H:245:ARG:HG3	1.98	0.64
1:J:122:MSE:HE2	1:J:166:VAL:HG22	1.81	0.62
1:C:93:ARG:NH2	1:C:114:GLN:O	2.33	0.62
1:G:122:MSE:HE1	1:H:89:LEU:HG	1.82	0.62
1:M:67:MSE:HE1	1:M:216:LEU:HG	1.81	0.61
1:D:163:VAL:HG23	1:D:227:LEU:HD11	1.84	0.60
1:A:122:MSE:HE1	1:B:89:LEU:HA	1.82	0.60
1:G:144:PHE:HB3	1:G:146:ILE:HD12	1.83	0.60
1:K:41:ILE:HD11	1:K:68:LEU:HD22	1.82	0.60
1:H:207:THR:HG22	1:H:209:ASN:N	2.17	0.60
1:L:122:MSE:HE2	1:L:166:VAL:HG22	1.85	0.59
1:F:30:PRO:HA	1:F:239:LEU:HA	1.85	0.59
1:G:210:GLU:O	1:G:213:MSE:HB3	2.03	0.59
1:O:229:ASN:ND2	1:O:254:ARG:HG3	2.18	0.58
1:M:82:GLU:O	1:M:83:ARG:HD3	2.02	0.58
1:D:177:THR:HG22	1:D:226:PHE:CD2	2.37	0.58
1:D:207:THR:HG22	1:D:209:ASN:N	2.16	0.58
1:M:67:MSE:HE3	1:M:217:MSE:HA	1.85	0.58
1:B:93:ARG:NH2	1:B:114:GLN:O	2.37	0.57
1:K:82:GLU:O	1:K:83:ARG:HD3	2.04	0.57
1:F:130:TYR:OH	1:F:132:SER:HB2	2.04	0.56
1:P:41:ILE:HD11	1:P:68:LEU:HD22	1.87	0.56
1:D:146:ILE:HG22	1:D:147:GLY:H	1.70	0.56
1:F:234:ARG:HB2	1:F:236:LEU:HD13	1.87	0.56
1:L:192:ARG:HD3	1:L:206:TYR:CZ	2.41	0.56
1:H:131:GLU:HG2	1:H:156:GLN:HB3	1.87	0.56
1:P:93:ARG:NH2	1:P:114:GLN:O	2.39	0.56
1:O:67:MSE:HE3	1:O:217:MSE:HA	1.87	0.56
1:I:67:MSE:CE	1:I:217:MSE:HA	2.35	0.56
1:D:146:ILE:HG22	1:D:147:GLY:N	2.21	0.55
1:D:166:VAL:HA	1:E:89:LEU:HD21	1.89	0.55
1:A:82:GLU:O	1:A:83:ARG:HD3	2.07	0.55
1:I:122:MSE:HE2	1:I:166:VAL:HG22	1.89	0.55
1:N:154:LEU:HD12	1:N:182:LEU:HD21	1.87	0.55
1:O:107:ILE:HD12	1:O:110:ARG:HE	1.72	0.54
1:P:86:LEU:O	1:P:90:LEU:HG	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:93:ARG:NH2	1:K:114:GLN:O	2.40	0.54
1:O:93:ARG:NH2	1:O:114:GLN:O	2.41	0.54
1:B:252:LYS:HE2	1:B:256:MSE:CE	2.38	0.54
1:E:93:ARG:NH2	1:E:114:GLN:O	2.41	0.54
1:H:177:THR:HG22	1:H:226:PHE:CD2	2.42	0.53
1:L:210:GLU:O	1:L:213:MSE:HB3	2.09	0.53
1:M:67:MSE:CE	1:M:220:ILE:HD12	2.36	0.53
1:M:118:ALA:HB1	1:N:96:ILE:HG12	1.89	0.53
1:B:59:ALA:HB1	1:B:130:TYR:CE2	2.44	0.53
1:D:177:THR:HG22	1:D:226:PHE:CE2	2.44	0.53
1:F:122:MSE:HE3	1:F:166:VAL:HG22	1.89	0.53
1:I:177:THR:HG22	1:I:226:PHE:CD2	2.44	0.53
1:A:107:ILE:O	1:A:110:ARG:HG2	2.08	0.53
1:E:195:ASP:O	1:E:197:GLN:N	2.42	0.53
1:A:93:ARG:NH2	1:A:114:GLN:O	2.42	0.52
1:B:160:ASN:OD1	1:B:162:ARG:NH1	2.40	0.52
1:C:122:MSE:CE	1:C:166:VAL:HG22	2.39	0.52
1:L:93:ARG:NH2	1:L:114:GLN:O	2.43	0.52
1:N:93:ARG:NH2	1:N:114:GLN:O	2.43	0.52
1:E:73:LYS:HG3	1:E:80:PRO:HG2	1.91	0.52
1:G:166:VAL:HA	1:H:89:LEU:HD21	1.90	0.52
1:K:177:THR:HG22	1:K:226:PHE:CE2	2.44	0.52
1:G:130:TYR:OH	1:G:132:SER:HB2	2.10	0.52
1:D:141:ALA:O	1:D:145:GLY:N	2.42	0.52
1:G:93:ARG:NH2	1:G:114:GLN:O	2.42	0.52
1:K:21:TYR:CZ	1:K:25:THR:HG21	2.44	0.52
1:N:107:ILE:HD12	1:N:110:ARG:HE	1.74	0.52
1:I:96:ILE:O	1:I:100:GLN:HG2	2.10	0.52
1:G:177:THR:HG22	1:G:226:PHE:CD2	2.45	0.52
1:J:165:ASN:HB2	1:J:172:LEU:CD1	2.40	0.52
1:M:41:ILE:HD11	1:M:68:LEU:HD22	1.92	0.52
1:B:244:GLU:HG2	1:B:247:ASN:HB2	1.91	0.51
1:J:24:LEU:HD22	1:J:221:GLU:HG2	1.91	0.51
1:F:77:TRP:HZ3	1:F:237:TRP:CD1	2.28	0.51
1:G:63:SER:OG	1:G:67:MSE:HE3	2.10	0.51
1:I:93:ARG:NH2	1:I:114:GLN:O	2.43	0.51
1:P:27:LEU:O	1:P:76:ARG:NH2	2.43	0.51
1:F:93:ARG:NH2	1:F:114:GLN:O	2.44	0.51
1:P:24:LEU:HD22	1:P:221:GLU:HG2	1.92	0.51
1:F:41:ILE:HD11	1:F:68:LEU:HD22	1.92	0.51
1:G:146:ILE:HG22	1:G:147:GLY:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:96:ILE:HG12	1:P:118:ALA:HB1	1.92	0.51
1:C:154:LEU:HD12	1:C:182:LEU:HD21	1.93	0.51
1:M:163:VAL:HG23	1:M:227:LEU:HD11	1.94	0.50
1:O:130:TYR:OH	1:O:132:SER:HB2	2.11	0.50
1:J:137:GLY:HA2	1:J:141:ALA:HB2	1.93	0.50
1:N:41:ILE:HD11	1:N:68:LEU:HD22	1.93	0.50
1:O:177:THR:HG22	1:O:226:PHE:CD2	2.46	0.50
1:M:250:LEU:O	1:M:254:ARG:HB2	2.11	0.50
1:J:82:GLU:O	1:J:83:ARG:HD3	2.12	0.50
1:K:165:ASN:HB2	1:K:172:LEU:HD13	1.94	0.50
1:O:82:GLU:O	1:O:83:ARG:HD3	2.12	0.50
1:B:30:PRO:HB3	1:B:77:TRP:CZ3	2.47	0.50
1:E:128:ILE:HG13	1:F:213:MSE:HE1	1.93	0.50
1:E:130:TYR:OH	1:E:132:SER:HB2	2.12	0.49
1:C:122:MSE:HE2	1:C:166:VAL:HG22	1.93	0.49
1:F:231:GLY:HA2	1:F:236:LEU:HD22	1.93	0.49
1:H:28:PRO:CB	1:H:244:GLU:HG2	2.32	0.49
1:L:177:THR:HG22	1:L:226:PHE:CD2	2.47	0.49
1:A:28:PRO:HB3	1:A:244:GLU:HG2	1.94	0.49
1:A:122:MSE:HE1	1:B:89:LEU:HD13	1.95	0.49
1:O:210:GLU:O	1:O:213:MSE:HB3	2.13	0.49
1:G:105:VAL:HG12	1:M:110:ARG:HH22	1.72	0.49
1:J:252:LYS:HG2	1:J:256:MSE:HE3	1.94	0.49
1:H:30:PRO:HB3	1:H:77:TRP:CZ3	2.48	0.49
1:J:177:THR:HG22	1:J:226:PHE:CD2	2.48	0.49
1:H:130:TYR:OH	1:H:132:SER:HB2	2.13	0.48
1:M:96:ILE:O	1:M:100:GLN:HG2	2.13	0.48
1:E:166:VAL:HA	1:F:89:LEU:HD21	1.95	0.48
1:I:129:GLY:HA3	1:J:213:MSE:HE1	1.94	0.48
1:D:137:GLY:CA	1:D:148:ALA:HA	2.43	0.48
1:D:160:ASN:OD1	1:D:162:ARG:NH1	2.46	0.48
1:A:137:GLY:HA2	1:A:141:ALA:HB2	1.96	0.48
1:K:118:ALA:HB1	1:L:96:ILE:HG12	1.96	0.48
1:L:129:GLY:HA3	1:M:213:MSE:HE1	1.96	0.48
1:O:118:ALA:HB1	1:P:96:ILE:HG12	1.94	0.48
1:H:152:TYR:HB2	1:H:183:SER:O	2.14	0.48
1:J:93:ARG:NH2	1:J:114:GLN:O	2.47	0.48
1:C:122:MSE:HE2	1:D:92:GLU:HG3	1.96	0.47
1:D:130:TYR:HD1	1:D:157:ILE:HG12	1.79	0.47
1:M:30:PRO:HB3	1:M:77:TRP:CZ3	2.49	0.47
1:O:134:VAL:HA	1:O:153:GLN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:89:LEU:O	1:J:93:ARG:HG3	2.14	0.47
1:M:154:LEU:HD12	1:M:182:LEU:HD21	1.96	0.47
1:D:154:LEU:HD12	1:D:182:LEU:HD21	1.95	0.47
1:G:96:ILE:O	1:G:100:GLN:HG2	2.14	0.47
1:H:163:VAL:HG23	1:H:227:LEU:HD11	1.97	0.47
1:L:177:THR:HG22	1:L:226:PHE:CE2	2.49	0.47
1:M:234:ARG:HB2	1:M:236:LEU:HD13	1.96	0.47
1:C:192:ARG:NH2	1:C:204:VAL:HG11	2.25	0.47
1:E:160:ASN:OD1	1:E:162:ARG:NH1	2.47	0.47
1:A:188:ALA:O	1:H:196:TYR:OH	2.22	0.47
1:E:118:ALA:HB1	1:F:96:ILE:HG12	1.96	0.47
1:F:130:TYR:CZ	1:F:132:SER:HB2	2.49	0.47
1:K:131:GLU:HG2	1:K:156:GLN:HB3	1.97	0.47
1:J:27:LEU:O	1:J:76:ARG:NH2	2.48	0.47
1:K:48:PHE:HB2	1:L:54:SER:HB3	1.97	0.47
1:H:131:GLU:CG	1:H:156:GLN:HB3	2.45	0.47
1:M:99:ALA:O	1:M:105:VAL:HG23	2.15	0.47
1:N:48:PHE:HB2	1:O:54:SER:HB3	1.96	0.47
1:A:177:THR:HG22	1:A:226:PHE:CD2	2.50	0.46
1:C:147:GLY:C	1:C:149:ASP:H	2.23	0.46
1:G:146:ILE:HD11	1:G:184:TYR:OH	2.15	0.46
1:J:118:ALA:HB1	1:K:96:ILE:HG12	1.97	0.46
1:N:84:GLN:H	1:N:84:GLN:CD	2.22	0.46
1:O:77:TRP:HZ3	1:O:237:TRP:CD1	2.32	0.46
1:N:177:THR:HG22	1:N:226:PHE:CD2	2.50	0.46
1:E:130:TYR:CZ	1:E:132:SER:HB2	2.50	0.46
1:F:24:LEU:HD11	1:F:75:SER:HB3	1.98	0.46
1:M:182:LEU:HD12	1:M:194:ILE:HD11	1.97	0.46
1:O:245:ARG:HG2	1:O:254:ARG:HH12	1.80	0.46
1:G:213:MSE:HE2	1:G:213:MSE:HB2	1.67	0.46
1:K:210:GLU:O	1:K:213:MSE:HB3	2.16	0.46
1:I:67:MSE:CE	1:I:220:ILE:HD12	2.41	0.46
1:I:130:TYR:OH	1:I:132:SER:HB2	2.16	0.46
1:O:96:ILE:O	1:O:100:GLN:HG2	2.16	0.46
1:A:54:SER:HB3	1:H:48:PHE:HB2	1.98	0.46
1:B:67:MSE:HE1	1:B:216:LEU:HD23	1.98	0.46
1:K:177:THR:HG22	1:K:226:PHE:CD2	2.50	0.46
1:L:86:LEU:O	1:L:90:LEU:HG	2.15	0.46
1:P:234:ARG:HB2	1:P:236:LEU:HD13	1.97	0.46
1:H:177:THR:HG22	1:H:226:PHE:CE2	2.51	0.46
1:O:67:MSE:CE	1:O:216:LEU:HG	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:TYR:CG	1:B:52:PRO:HA	2.51	0.46
1:G:34:ILE:HD12	1:G:77:TRP:O	2.16	0.46
1:K:83:ARG:NE	1:L:92:GLU:OE2	2.39	0.46
1:N:156:GLN:HA	1:N:179:LYS:O	2.15	0.45
1:H:122:MSE:HE3	1:H:164:VAL:HB	1.98	0.45
1:B:227:LEU:HD12	1:B:227:LEU:HA	1.73	0.45
1:N:131:GLU:HG2	1:N:156:GLN:CG	2.40	0.45
1:J:41:ILE:HD11	1:J:68:LEU:HD22	1.99	0.45
1:M:182:LEU:HB2	1:M:194:ILE:HG13	1.99	0.45
1:A:96:ILE:HG12	1:H:118:ALA:HB1	1.98	0.45
1:F:33:LYS:NZ	1:F:76:ARG:HA	2.32	0.45
1:F:122:MSE:HE1	1:G:89:LEU:HD23	1.98	0.45
1:F:227:LEU:HD12	1:F:227:LEU:HA	1.76	0.45
1:J:165:ASN:HB2	1:J:172:LEU:HD11	1.98	0.45
1:A:177:THR:HG22	1:A:226:PHE:CE2	2.52	0.45
1:O:122:MSE:HE2	1:P:89:LEU:HG	1.98	0.45
1:A:41:ILE:HD11	1:A:68:LEU:HD22	1.99	0.44
1:K:86:LEU:O	1:K:90:LEU:HG	2.16	0.44
1:D:64:ALA:HB2	1:D:127:ILE:HD11	1.99	0.44
1:K:165:ASN:HB2	1:K:172:LEU:CD1	2.47	0.44
1:C:210:GLU:O	1:C:213:MSE:HB3	2.17	0.44
1:E:201:GLU:OE1	1:E:201:GLU:N	2.51	0.44
1:M:182:LEU:HG	1:M:196:TYR:HE1	1.83	0.44
1:A:213:MSE:HE3	1:A:217:MSE:CE	2.47	0.44
1:N:177:THR:HG22	1:N:226:PHE:CE2	2.52	0.44
1:C:130:TYR:OH	1:C:132:SER:HB2	2.18	0.44
1:H:24:LEU:HD22	1:H:221:GLU:HG2	1.99	0.44
1:J:152:TYR:N	1:J:152:TYR:CD1	2.86	0.44
1:K:96:ILE:O	1:K:100:GLN:HG2	2.18	0.44
1:L:247:ASN:OD1	1:L:249:ILE:N	2.47	0.44
1:I:89:LEU:HG	1:P:122:MSE:HE1	2.00	0.44
1:J:160:ASN:HB2	1:J:176:ASN:OD1	2.17	0.44
1:A:73:LYS:HG3	1:A:80:PRO:HG2	1.99	0.44
1:G:146:ILE:HG22	1:G:147:GLY:H	1.82	0.44
1:L:122:MSE:HE1	1:M:89:LEU:HG	1.99	0.44
1:E:195:ASP:O	1:E:198:ARG:N	2.43	0.44
1:F:33:LYS:HZ3	1:F:76:ARG:HA	1.83	0.44
1:F:154:LEU:HD11	1:G:189:GLY:HA3	2.00	0.44
1:H:140:GLY:O	1:H:144:PHE:HB2	2.18	0.44
1:G:128:ILE:HG13	1:H:213:MSE:CE	2.46	0.43
1:D:93:ARG:NH2	1:D:114:GLN:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:ALA:HB1	1:H:130:TYR:CE2	2.52	0.43
1:B:30:PRO:HB3	1:B:77:TRP:CE3	2.53	0.43
1:H:130:TYR:CZ	1:H:132:SER:HB2	2.52	0.43
1:H:233:ASP:CG	1:H:254:ARG:HH12	2.26	0.43
1:J:183:SER:HA	1:J:192:ARG:O	2.18	0.43
1:N:163:VAL:HG23	1:N:227:LEU:HD11	1.99	0.43
1:P:253:TYR:HA	1:P:256:MSE:HG3	1.99	0.43
1:O:130:TYR:CZ	1:O:132:SER:HB2	2.53	0.43
1:C:140:GLY:HA3	1:C:152:TYR:CZ	2.54	0.43
1:E:186:VAL:HG11	1:E:192:ARG:HG3	2.01	0.43
1:I:213:MSE:HE1	1:P:129:GLY:HA3	2.00	0.43
1:K:59:ALA:HB1	1:K:130:TYR:CE2	2.53	0.43
1:N:160:ASN:OD1	1:N:162:ARG:NH1	2.51	0.43
1:L:96:ILE:O	1:L:100:GLN:HG2	2.19	0.43
1:P:51:TYR:CG	1:P:52:PRO:HA	2.53	0.43
1:P:59:ALA:HB1	1:P:130:TYR:CE2	2.54	0.43
1:H:67:MSE:SE	1:H:217:MSE:HG3	2.68	0.43
1:N:93:ARG:NH1	1:N:97:ARG:HH22	2.17	0.43
1:B:177:THR:HG22	1:B:226:PHE:CD2	2.54	0.43
1:G:165:ASN:HB2	1:G:172:LEU:HG	2.00	0.43
1:K:51:TYR:CG	1:K:52:PRO:HA	2.54	0.43
1:M:166:VAL:HA	1:N:89:LEU:HD21	2.01	0.43
1:I:51:TYR:CG	1:I:52:PRO:HA	2.54	0.43
1:L:20:SER:HG	1:L:218:SER:HG	1.62	0.43
1:B:177:THR:HG22	1:B:226:PHE:CE2	2.54	0.42
1:C:73:LYS:HG3	1:C:80:PRO:HG2	2.01	0.42
1:F:122:MSE:CE	1:F:166:VAL:HG22	2.48	0.42
1:H:73:LYS:HG3	1:H:80:PRO:HG2	2.00	0.42
1:I:20:SER:HB3	1:I:221:GLU:OE1	2.19	0.42
1:J:30:PRO:HB3	1:J:77:TRP:CZ3	2.54	0.42
1:A:141:ALA:HA	1:A:146:ILE:HG13	2.00	0.42
1:D:118:ALA:HB1	1:E:96:ILE:HG12	2.01	0.42
1:G:249:ILE:O	1:G:253:TYR:HD1	2.02	0.42
1:L:67:MSE:HE2	1:L:217:MSE:SE	2.70	0.42
1:P:130:TYR:OH	1:P:132:SER:HB2	2.19	0.42
1:D:242:LYS:HE3	1:D:242:LYS:HB2	1.82	0.42
1:A:231:GLY:HA3	1:A:237:TRP:CE2	2.54	0.42
1:D:96:ILE:O	1:D:100:GLN:HG2	2.20	0.42
1:E:163:VAL:HG23	1:E:227:LEU:HD11	2.01	0.42
1:K:163:VAL:HG23	1:K:227:LEU:HD11	2.00	0.42
1:K:166:VAL:HA	1:L:89:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLN:HG2	1:C:20:SER:N	2.35	0.42
1:D:147:GLY:C	1:D:149:ASP:H	2.28	0.42
1:O:107:ILE:HD11	1:O:110:ARG:HH21	1.85	0.42
1:L:27:LEU:O	1:L:76:ARG:NH2	2.53	0.42
1:H:122:MSE:HE2	1:H:122:MSE:HB3	1.88	0.42
1:J:182:LEU:O	1:J:193:PHE:HA	2.19	0.42
1:K:213:MSE:HE2	1:K:213:MSE:HB2	1.65	0.42
1:D:137:GLY:HA2	1:D:148:ALA:HA	2.02	0.42
1:H:30:PRO:HB3	1:H:77:TRP:CH2	2.54	0.42
1:N:96:ILE:O	1:N:100:GLN:HG2	2.20	0.42
1:A:192:ARG:HA	1:A:205:GLY:O	2.19	0.41
1:C:154:LEU:HD11	1:D:189:GLY:HA3	2.02	0.41
1:L:227:LEU:HD12	1:L:227:LEU:HA	1.75	0.41
1:C:96:ILE:O	1:C:100:GLN:HG2	2.20	0.41
1:D:48:PHE:HB2	1:E:54:SER:HB3	2.01	0.41
1:H:210:GLU:HA	1:H:211:PRO:HD3	1.92	0.41
1:N:213:MSE:HA	1:N:213:MSE:HE3	2.01	0.41
1:P:183:SER:HA	1:P:192:ARG:O	2.19	0.41
1:A:210:GLU:HG3	1:H:131:GLU:HB3	2.01	0.41
1:G:247:ASN:O	1:G:251:VAL:HG13	2.21	0.41
1:M:152:TYR:CD1	1:M:152:TYR:N	2.88	0.41
1:F:51:TYR:CG	1:F:52:PRO:HA	2.56	0.41
1:L:113:LEU:HD23	1:L:113:LEU:HA	1.88	0.41
1:O:177:THR:HG22	1:O:226:PHE:CE2	2.55	0.41
1:A:213:MSE:HE1	1:H:158:ALA:CB	2.50	0.41
1:B:130:TYR:OH	1:B:132:SER:HB2	2.21	0.41
1:H:51:TYR:CG	1:H:52:PRO:HA	2.56	0.41
1:I:177:THR:HG22	1:I:226:PHE:CE2	2.56	0.41
1:N:227:LEU:HD12	1:N:227:LEU:HA	1.76	0.41
1:G:118:ALA:HB1	1:H:96:ILE:HG12	2.02	0.41
1:O:166:VAL:HA	1:P:89:LEU:HD21	2.03	0.41
1:P:227:LEU:HD12	1:P:227:LEU:HA	1.94	0.41
1:D:86:LEU:O	1:D:90:LEU:HG	2.20	0.41
1:D:131:GLU:HG2	1:D:156:GLN:HB3	2.03	0.41
1:E:48:PHE:HB2	1:F:54:SER:HB3	2.03	0.41
1:G:122:MSE:HE3	1:G:164:VAL:HB	2.03	0.41
1:G:137:GLY:HA2	1:G:141:ALA:HB2	2.02	0.41
1:H:86:LEU:O	1:H:90:LEU:HG	2.21	0.41
1:M:165:ASN:HB2	1:M:172:LEU:HG	2.02	0.41
1:N:154:LEU:HD12	1:N:182:LEU:CD2	2.50	0.41
1:F:59:ALA:HB1	1:F:130:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:67:MSE:HE2	1:P:217:MSE:HE3	2.03	0.41
1:P:184:TYR:CE1	1:P:192:ARG:HB2	2.55	0.41
1:M:227:LEU:HD12	1:M:227:LEU:HA	1.83	0.40
1:A:122:MSE:CE	1:B:89:LEU:HD13	2.51	0.40
1:C:51:TYR:CG	1:C:52:PRO:HA	2.56	0.40
1:E:194:ILE:HG12	1:E:204:VAL:HG22	2.03	0.40
1:H:232:ILE:HA	1:H:237:TRP:O	2.21	0.40
1:H:252:LYS:HE2	1:H:256:MSE:CE	2.51	0.40
1:I:213:MSE:HE2	1:I:213:MSE:HB2	1.91	0.40
1:J:51:TYR:CG	1:J:52:PRO:HA	2.57	0.40
1:L:231:GLY:HA3	1:L:237:TRP:NE1	2.36	0.40
1:B:244:GLU:CG	1:B:247:ASN:HB2	2.51	0.40
1:C:60:VAL:HG12	1:C:61:PRO:O	2.20	0.40
1:E:77:TRP:HZ3	1:E:237:TRP:CD1	2.39	0.40
1:I:48:PHE:HB2	1:J:54:SER:HB3	2.03	0.40
1:J:86:LEU:O	1:J:90:LEU:HG	2.21	0.40
1:M:213:MSE:HE2	1:M:213:MSE:HB2	1.83	0.40
1:N:253:TYR:HA	1:N:256:MSE:HE3	2.03	0.40
1:D:207:THR:CG2	1:D:209:ASN:H	2.30	0.40
1:L:89:LEU:O	1:L:93:ARG:HG3	2.22	0.40
1:O:48:PHE:HB2	1:P:54:SER:HB3	2.04	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	230/262 (88%)	228 (99%)	2 (1%)	0	100	100
1	B	232/262 (88%)	229 (99%)	3 (1%)	0	100	100
1	C	230/262 (88%)	228 (99%)	2 (1%)	0	100	100
1	D	231/262 (88%)	227 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	239/262 (91%)	234 (98%)	4 (2%)	1 (0%)	30	60
1	F	230/262 (88%)	226 (98%)	4 (2%)	0	100	100
1	G	231/262 (88%)	227 (98%)	4 (2%)	0	100	100
1	H	232/262 (88%)	229 (99%)	3 (1%)	0	100	100
1	I	231/262 (88%)	228 (99%)	3 (1%)	0	100	100
1	J	222/262 (85%)	218 (98%)	4 (2%)	0	100	100
1	K	230/262 (88%)	224 (97%)	6 (3%)	0	100	100
1	L	230/262 (88%)	225 (98%)	5 (2%)	0	100	100
1	M	211/262 (80%)	207 (98%)	4 (2%)	0	100	100
1	N	229/262 (87%)	224 (98%)	5 (2%)	0	100	100
1	O	212/262 (81%)	208 (98%)	4 (2%)	0	100	100
1	P	208/262 (79%)	207 (100%)	1 (0%)	0	100	100
All	All	3628/4192 (86%)	3569 (98%)	58 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	196	TYR

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	199/217 (92%)	194 (98%)	5 (2%)	42	76
1	B	201/217 (93%)	197 (98%)	4 (2%)	48	80
1	C	199/217 (92%)	198 (100%)	1 (0%)	81	93
1	D	200/217 (92%)	195 (98%)	5 (2%)	42	76
1	E	205/217 (94%)	202 (98%)	3 (2%)	57	84
1	F	199/217 (92%)	194 (98%)	5 (2%)	42	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	200/217 (92%)	198 (99%)	2 (1%)	68	88
1	H	201/217 (93%)	195 (97%)	6 (3%)	36	72
1	I	200/217 (92%)	197 (98%)	3 (2%)	57	84
1	J	196/217 (90%)	195 (100%)	1 (0%)	81	93
1	K	199/217 (92%)	198 (100%)	1 (0%)	81	93
1	L	199/217 (92%)	195 (98%)	4 (2%)	48	80
1	M	189/217 (87%)	186 (98%)	3 (2%)	55	83
1	N	198/217 (91%)	195 (98%)	3 (2%)	57	84
1	O	190/217 (88%)	189 (100%)	1 (0%)	81	93
1	P	190/217 (88%)	186 (98%)	4 (2%)	47	79
All	All	3165/3472 (91%)	3114 (98%)	51 (2%)	55	83

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ILE
1	A	136	SER
1	A	139	VAL
1	A	210	GLU
1	A	213	MSE
1	B	60	VAL
1	B	172	LEU
1	B	186	VAL
1	B	246	GLN
1	C	179	LYS
1	D	146	ILE
1	D	172	LEU
1	D	194	ILE
1	D	217	MSE
1	D	239	LEU
1	E	60	VAL
1	E	172	LEU
1	E	196	TYR
1	F	134	VAL
1	F	172	LEU
1	F	217	MSE
1	F	238	ASP
1	F	239	LEU

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Mol	Chain	Res	Type
1	G	19	GLN
1	G	241	ASN
1	H	60	VAL
1	H	107	ILE
1	H	134	VAL
1	H	172	LEU
1	H	186	VAL
1	H	242	LYS
1	I	89	LEU
1	I	114	GLN
1	I	172	LEU
1	J	172	LEU
1	K	172	LEU
1	L	89	LEU
1	L	122	MSE
1	L	134	VAL
1	L	172	LEU
1	M	105	VAL
1	M	134	VAL
1	M	186	VAL
1	N	146	ILE
1	N	172	LEU
1	N	217	MSE
1	O	246	GLN
1	P	60	VAL
1	P	122	MSE
1	P	186	VAL
1	P	213	MSE

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	19	GLN
1	A	246	GLN
1	B	19	GLN
1	B	120	ASN
1	B	209	ASN
1	C	120	ASN
1	D	19	GLN
1	D	47	GLN
1	D	120	ASN
1	D	153	GLN

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Mol	Chain	Res	Type
1	E	19	GLN
1	E	120	ASN
1	E	247	ASN
1	F	120	ASN
1	G	109	ASN
1	G	153	GLN
1	I	102	ASN
1	J	40	ASN
1	J	87	GLN
1	J	120	ASN
1	K	26	HIS
1	K	120	ASN
1	K	187	GLN
1	K	209	ASN
1	M	19	GLN
1	N	62	GLN
1	N	120	ASN
1	P	156	GLN
1	P	246	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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 ⓘ

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	229/262 (87%)	-0.23	3 (1%) 75 66	25, 46, 97, 128	26 (11%)
1	B	231/262 (88%)	-0.28	3 (1%) 75 66	17, 46, 87, 101	22 (9%)
1	C	229/262 (87%)	-0.39	1 (0%) 88 84	23, 48, 78, 103	15 (6%)
1	D	230/262 (87%)	-0.22	3 (1%) 75 66	21, 47, 90, 138	22 (9%)
1	E	236/262 (90%)	-0.25	2 (0%) 82 75	26, 49, 83, 104	30 (12%)
1	F	229/262 (87%)	-0.14	4 (1%) 69 60	20, 48, 97, 132	36 (15%)
1	G	230/262 (87%)	-0.13	3 (1%) 75 66	24, 46, 91, 123	36 (15%)
1	H	231/262 (88%)	-0.18	0 100 100	17, 46, 75, 95	29 (12%)
1	I	230/262 (87%)	-0.31	2 (0%) 81 74	22, 47, 81, 106	44 (19%)
1	J	223/262 (85%)	-0.13	6 (2%) 56 46	27, 48, 87, 118	33 (14%)
1	K	229/262 (87%)	-0.21	2 (0%) 81 74	25, 48, 92, 113	36 (15%)
1	L	229/262 (87%)	-0.10	2 (0%) 81 74	25, 54, 92, 116	35 (15%)
1	M	212/262 (80%)	-0.24	2 (0%) 81 74	24, 48, 79, 101	29 (13%)
1	N	228/262 (87%)	-0.09	2 (0%) 81 74	24, 50, 91, 123	53 (23%)
1	O	213/262 (81%)	-0.14	6 (2%) 55 45	21, 47, 88, 105	30 (14%)
1	P	211/262 (80%)	-0.10	4 (1%) 66 57	27, 50, 91, 112	29 (13%)
All	All	3620/4192 (86%)	-0.20	45 (1%) 76 68	17, 48, 89, 138	505 (13%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	ASP	3.9
1	F	196	TYR	3.9
1	O	188	ALA	3.4
1	G	241	ASN	3.4
1	J	151	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	257	SER	3.1
1	I	188	ALA	3.0
1	G	143	TYR	2.9
1	M	257	SER	2.8
1	N	241	ASN	2.8
1	A	149	ASP	2.7
1	J	144	PHE	2.7
1	P	196	TYR	2.7
1	P	131	GLU	2.6
1	A	206	TYR	2.6
1	C	140	GLY	2.6
1	O	208	SER	2.6
1	P	241	ASN	2.5
1	F	149	ASP	2.5
1	D	243	ALA	2.5
1	M	196	TYR	2.5
1	I	241	ASN	2.5
1	O	248	ASP	2.4
1	K	257	SER	2.4
1	K	188	ALA	2.4
1	A	107	ILE	2.4
1	N	243	ALA	2.3
1	L	257	SER	2.3
1	J	196	TYR	2.3
1	O	209	ASN	2.2
1	F	195	ASP	2.2
1	E	241	ASN	2.2
1	O	152	TYR	2.2
1	G	246	GLN	2.2
1	L	196	TYR	2.1
1	P	152	TYR	2.1
1	O	257	SER	2.1
1	F	150	THR	2.1
1	J	140	GLY	2.1
1	E	197	GLN	2.1
1	B	82	GLU	2.1
1	B	153	GLN	2.0
1	B	196	TYR	2.0
1	D	196	TYR	2.0
1	J	184	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.