



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:43 AM UTC

PDB ID : 4YWM / pdb_00004ywm
Title : Pyrococcus furiosus MCM N-terminal domain beta-turn triple mutant pentameric ring
Authors : Froelich, C.A.; Enemark, E.J.
Deposited on : 2015-03-20
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 Phenix2.0
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

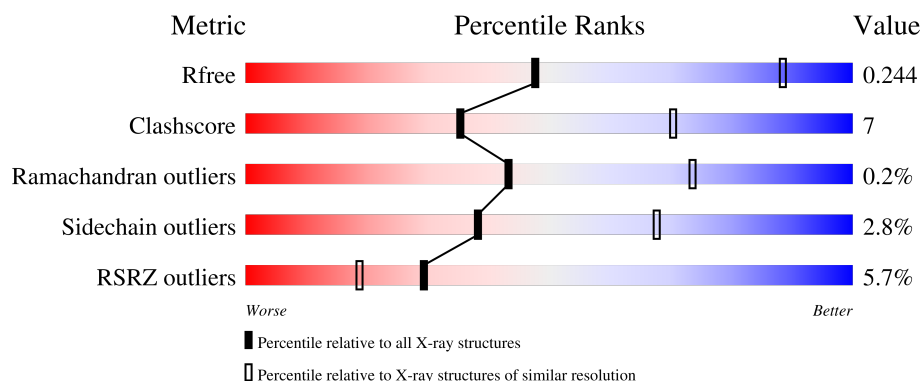
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



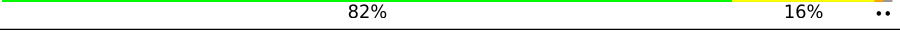
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	257	5% 79% 19% .
1	B	257	5% 79% 19% ..
1	C	257	3% 80% 18% ..
1	D	257	5% 76% 23% .
1	E	257	5% 81% 18% ..

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Mol	Chain	Length	Quality of chain
1	F	257	 4% 83% 15% ..
1	G	257	 7% 81% 17% ..
1	H	257	 4% 84% 14% ..
1	I	257	 11% 83% 15% ..
1	J	257	 7% 82% 16% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20305 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 Cell division control protein 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2028	1285	345	389	9			
1	B	255	Total	C	N	O	S	0	0	0
			2028	1285	345	389	9			
1	C	255	Total	C	N	O	S	0	0	0
			2028	1285	345	389	9			
1	D	255	Total	C	N	O	S	0	0	0
			2028	1285	345	389	9			
1	E	255	Total	C	N	O	S	0	0	0
			2028	1285	345	389	9			
1	F	254	Total	C	N	O	S	0	0	0
			2023	1282	344	388	9			
1	G	254	Total	C	N	O	S	0	0	0
			2023	1282	344	388	9			
1	H	254	Total	C	N	O	S	0	0	0
			2023	1282	344	388	9			
1	I	254	Total	C	N	O	S	0	0	0
			2023	1282	344	388	9			
1	J	254	Total	C	N	O	S	0	0	0
			2023	1282	344	388	9			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q8U3I4
A	1	VAL	-	expression tag	UNP Q8U3I4
A	233	ALA	LYS	engineered mutation	UNP Q8U3I4
A	234	ALA	ARG	engineered mutation	UNP Q8U3I4
A	236	ALA	LYS	engineered mutation	UNP Q8U3I4
B	0	SER	-	expression tag	UNP Q8U3I4
B	1	VAL	-	expression tag	UNP Q8U3I4
B	233	ALA	LYS	engineered mutation	UNP Q8U3I4
B	234	ALA	ARG	engineered mutation	UNP Q8U3I4

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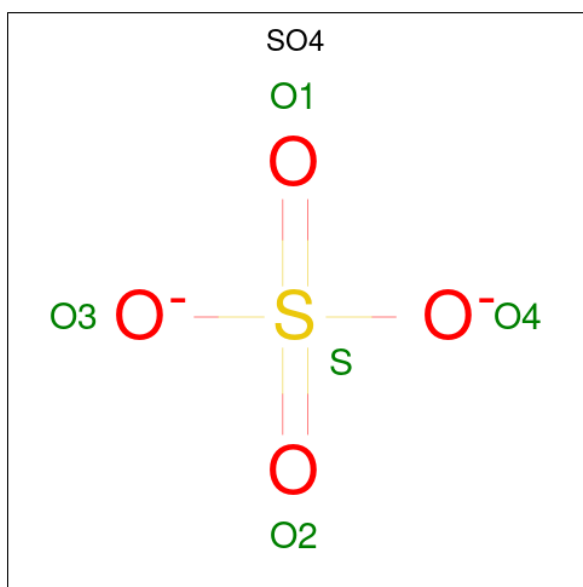
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Chain	Residue	Modelled	Actual	Comment	Reference
B	236	ALA	LYS	engineered mutation	UNP Q8U3I4
C	0	SER	-	expression tag	UNP Q8U3I4
C	1	VAL	-	expression tag	UNP Q8U3I4
C	233	ALA	LYS	engineered mutation	UNP Q8U3I4
C	234	ALA	ARG	engineered mutation	UNP Q8U3I4
C	236	ALA	LYS	engineered mutation	UNP Q8U3I4
D	0	SER	-	expression tag	UNP Q8U3I4
D	1	VAL	-	expression tag	UNP Q8U3I4
D	233	ALA	LYS	engineered mutation	UNP Q8U3I4
D	234	ALA	ARG	engineered mutation	UNP Q8U3I4
D	236	ALA	LYS	engineered mutation	UNP Q8U3I4
E	0	SER	-	expression tag	UNP Q8U3I4
E	1	VAL	-	expression tag	UNP Q8U3I4
E	233	ALA	LYS	engineered mutation	UNP Q8U3I4
E	234	ALA	ARG	engineered mutation	UNP Q8U3I4
E	236	ALA	LYS	engineered mutation	UNP Q8U3I4
F	0	SER	-	expression tag	UNP Q8U3I4
F	1	VAL	-	expression tag	UNP Q8U3I4
F	233	ALA	LYS	engineered mutation	UNP Q8U3I4
F	234	ALA	ARG	engineered mutation	UNP Q8U3I4
F	236	ALA	LYS	engineered mutation	UNP Q8U3I4
G	0	SER	-	expression tag	UNP Q8U3I4
G	1	VAL	-	expression tag	UNP Q8U3I4
G	233	ALA	LYS	engineered mutation	UNP Q8U3I4
G	234	ALA	ARG	engineered mutation	UNP Q8U3I4
G	236	ALA	LYS	engineered mutation	UNP Q8U3I4
H	0	SER	-	expression tag	UNP Q8U3I4
H	1	VAL	-	expression tag	UNP Q8U3I4
H	233	ALA	LYS	engineered mutation	UNP Q8U3I4
H	234	ALA	ARG	engineered mutation	UNP Q8U3I4
H	236	ALA	LYS	engineered mutation	UNP Q8U3I4
I	0	SER	-	expression tag	UNP Q8U3I4
I	1	VAL	-	expression tag	UNP Q8U3I4
I	233	ALA	LYS	engineered mutation	UNP Q8U3I4
I	234	ALA	ARG	engineered mutation	UNP Q8U3I4
I	236	ALA	LYS	engineered mutation	UNP Q8U3I4
J	0	SER	-	expression tag	UNP Q8U3I4
J	1	VAL	-	expression tag	UNP Q8U3I4
J	233	ALA	LYS	engineered mutation	UNP Q8U3I4
J	234	ALA	ARG	engineered mutation	UNP Q8U3I4
J	236	ALA	LYS	engineered mutation	UNP Q8U3I4

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

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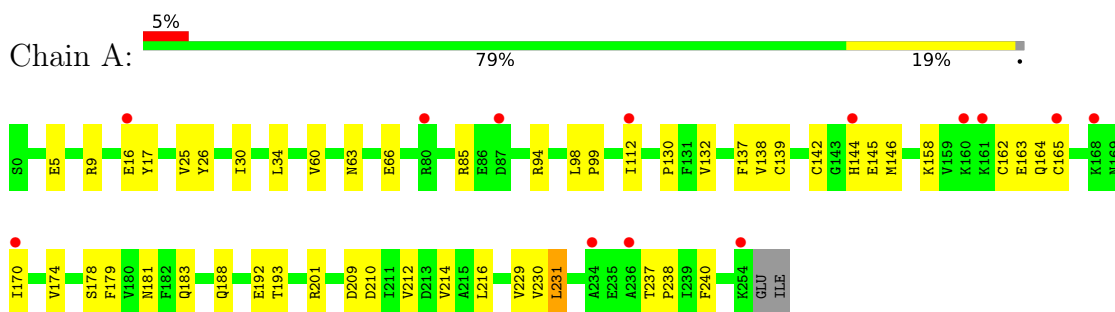
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		

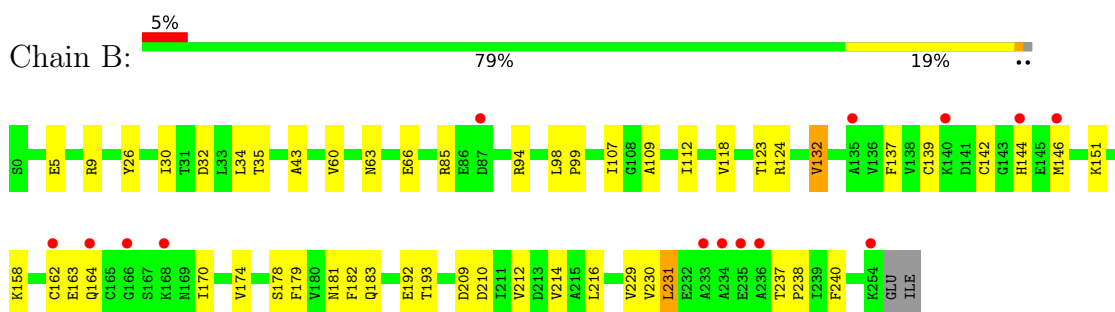
3 Residue-property plots [i](#)

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.

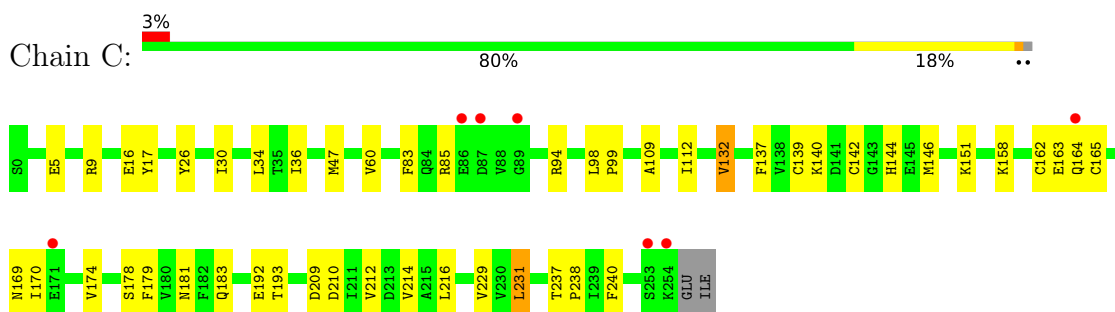
- Molecule 1: Cell division control protein 21



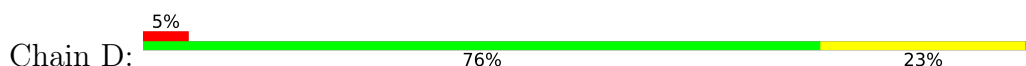
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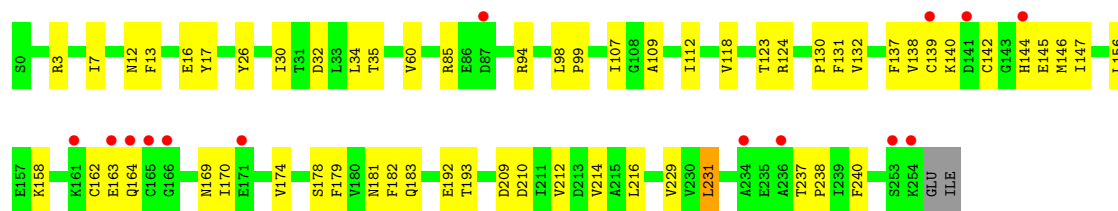


- Molecule 1: Cell division control protein 21

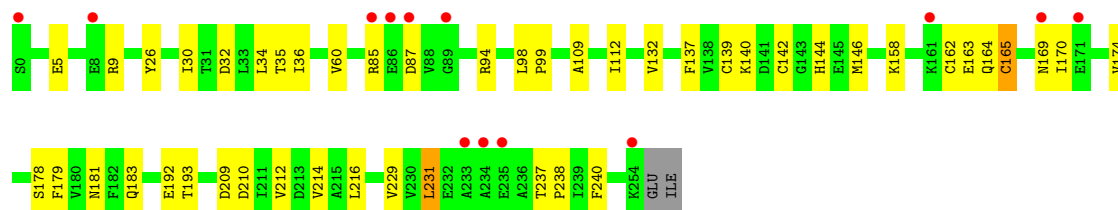
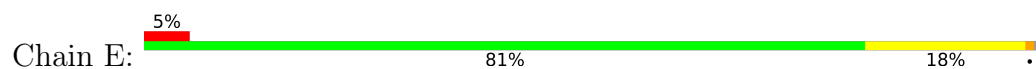


- Molecule 1: Cell division control protein 21

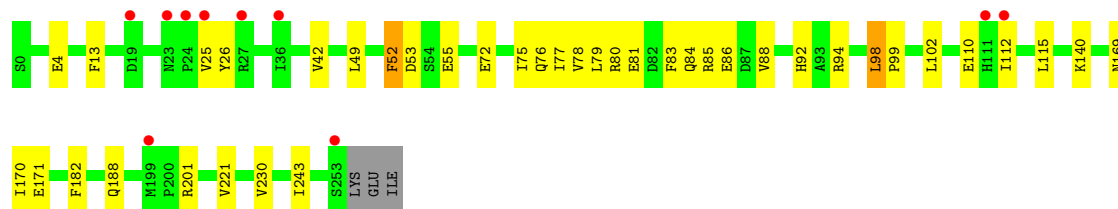
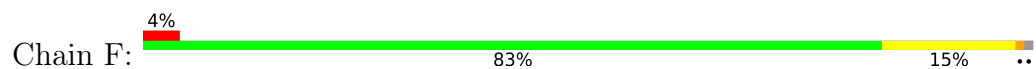




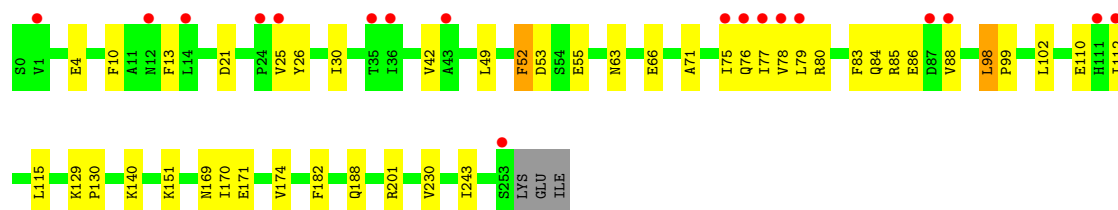
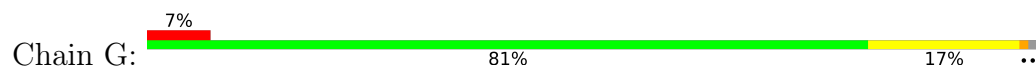
• Molecule 1: Cell division control protein 21



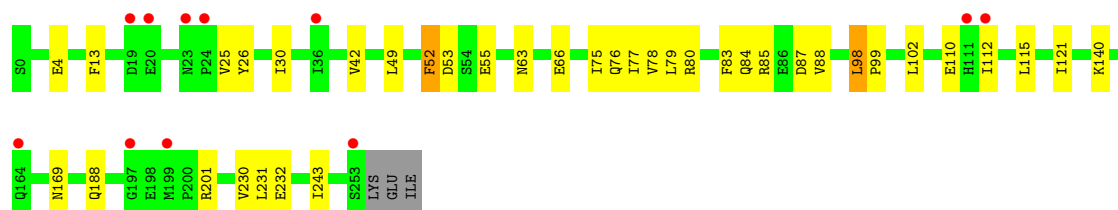
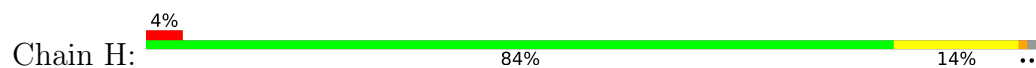
• Molecule 1: Cell division control protein 21



• Molecule 1: Cell division control protein 21

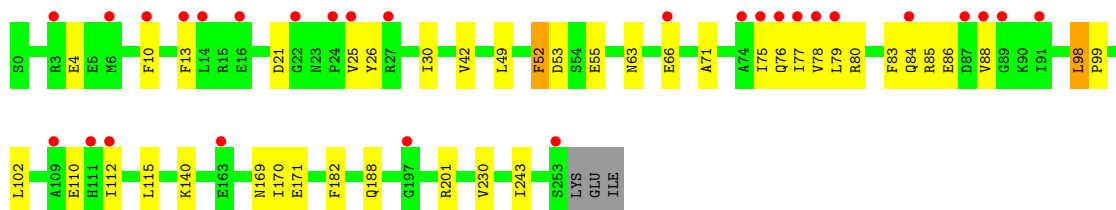


• Molecule 1: Cell division control protein 21



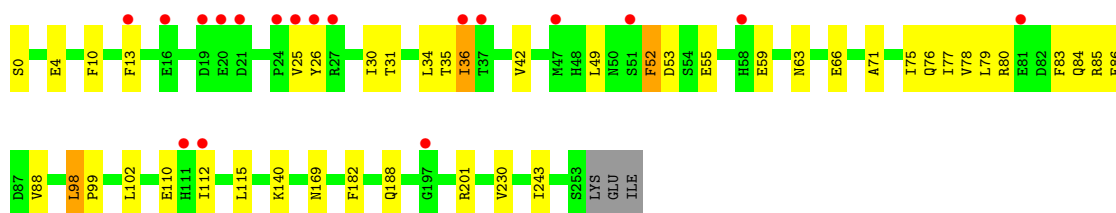
● Molecule 1: Cell division control protein 21

Chain I:  11% 83% 15% ..



● Molecule 1: Cell division control protein 21

Chain J:  7% 82% 16% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.71Å 210.71Å 209.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-3.20) 97.7 (50.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.237 , 0.270 (Not available) , 0.244	Depositor DCC
R_{free} test set	4328 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20305	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN

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	0.80	1/2063 (0.0%)	0.94	0/2790
1	B	0.90	2/2063 (0.1%)	1.00	2/2790 (0.1%)
1	C	0.91	0/2063	0.97	2/2790 (0.1%)
1	D	0.91	0/2063	0.99	1/2790 (0.0%)
1	E	0.85	0/2063	0.95	0/2790
1	F	0.78	0/2058	0.92	1/2783 (0.0%)
1	G	0.84	0/2058	0.97	1/2783 (0.0%)
1	H	0.76	0/2058	0.92	0/2783
1	I	0.86	0/2058	0.97	0/2783
1	J	0.72	0/2058	0.89	0/2783
All	All	0.83	3/20605 (0.0%)	0.95	7/27865 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	VAL	N-CA	-5.55	1.39	1.46
1	B	43	ALA	CA-C	-5.13	1.46	1.52
1	B	230	VAL	N-CA	-5.05	1.40	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	VAL	CB-CA-C	-6.07	105.76	112.68
1	B	132	VAL	CB-CA-C	-5.95	105.89	112.68
1	D	147	ILE	N-CA-C	5.79	116.92	108.58
1	C	151	LYS	N-CA-C	-5.64	101.63	110.14
1	G	151	LYS	N-CA-C	-5.18	103.16	110.31
1	F	221	VAL	N-CA-C	5.17	116.14	108.65
1	B	151	LYS	N-CA-C	-5.07	102.49	110.14

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	2028	0	2028	35	0
1	B	2028	0	2028	37	0
1	C	2028	0	2028	40	1
1	D	2028	0	2028	44	0
1	E	2028	0	2028	32	1
1	F	2023	0	2026	28	0
1	G	2023	0	2026	31	1
1	H	2023	0	2026	28	0
1	I	2023	0	2026	29	1
1	J	2023	0	2026	30	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
All	All	20305	0	20270	301	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (301) 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:B:112:ILE:HG12	1:C:174:VAL:HG11	1.46	0.95
1:C:240:PHE:CE1	1:D:132:VAL:HG23	2.09	0.87
1:H:98:LEU:HB3	1:H:99:PRO:HD2	1.59	0.84
1:I:98:LEU:HB3	1:I:99:PRO:HD2	1.60	0.84
1:J:98:LEU:HB3	1:J:99:PRO:HD2	1.60	0.84
1:A:174:VAL:HG11	1:E:112:ILE:HG12	1.57	0.83
1:D:142:CYS:SG	1:D:144:HIS:HB2	2.19	0.82
1:A:209:ASP:O	1:A:212:VAL:HG12	1.80	0.81
1:F:98:LEU:HB3	1:F:99:PRO:HD2	1.60	0.81
1:B:142:CYS:SG	1:B:144:HIS:HB2	2.22	0.80
1:G:98:LEU:HB3	1:G:99:PRO:HD2	1.63	0.79
1:B:209:ASP:O	1:B:212:VAL:HG12	1.84	0.77
1:C:209:ASP:O	1:C:212:VAL:HG12	1.84	0.77
1:D:209:ASP:O	1:D:212:VAL:HG12	1.85	0.77
1:B:112:ILE:HG12	1:C:174:VAL:CG1	2.16	0.76
1:C:240:PHE:CE1	1:D:132:VAL:CG2	2.68	0.76
1:E:209:ASP:O	1:E:212:VAL:HG12	1.88	0.74
1:A:174:VAL:CG1	1:E:112:ILE:HG12	2.16	0.74
1:C:112:ILE:HG12	1:D:174:VAL:CG1	2.18	0.74
1:A:142:CYS:SG	1:A:144:HIS:HB2	2.30	0.72
1:D:112:ILE:HG12	1:E:174:VAL:HG11	1.71	0.72
1:G:83:PHE:O	1:G:85:ARG:HG2	1.92	0.69
1:I:83:PHE:O	1:I:85:ARG:HG2	1.92	0.69
1:G:42:VAL:HG21	1:G:75:ILE:HD13	1.75	0.68
1:I:42:VAL:HG21	1:I:75:ILE:HD13	1.76	0.68
1:C:231:LEU:HD21	1:D:156:LEU:HD22	1.74	0.67
1:A:112:ILE:HG12	1:B:174:VAL:CG1	2.25	0.67
1:H:42:VAL:HG21	1:H:75:ILE:HD13	1.76	0.66
1:F:42:VAL:HG21	1:F:75:ILE:HD13	1.76	0.66
1:D:112:ILE:HG12	1:E:174:VAL:CG1	2.26	0.65
1:A:112:ILE:HG12	1:B:174:VAL:HG11	1.79	0.64
1:C:112:ILE:HG12	1:D:174:VAL:HG11	1.80	0.63
1:J:42:VAL:HG21	1:J:75:ILE:HD13	1.79	0.63
1:G:77:ILE:O	1:G:80:ARG:N	2.30	0.63
1:A:237:THR:OG1	1:A:238:PRO:HD2	1.99	0.63
1:H:77:ILE:O	1:H:80:ARG:N	2.33	0.61
1:B:237:THR:OG1	1:B:238:PRO:HD2	2.00	0.61
1:I:98:LEU:HD11	1:I:115:LEU:HD23	1.83	0.61
1:J:188:GLN:HB2	1:J:201:ARG:O	2.02	0.60
1:C:112:ILE:HG12	1:D:174:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:THR:OG1	1:E:238:PRO:HD2	2.02	0.59
1:D:237:THR:OG1	1:D:238:PRO:HD2	2.02	0.59
1:J:77:ILE:O	1:J:80:ARG:N	2.34	0.59
1:A:34:LEU:HG	1:A:85:ARG:NH1	2.18	0.58
1:A:132:VAL:HG23	1:E:240:PHE:CE1	2.38	0.58
1:A:240:PHE:CE1	1:B:132:VAL:CG2	2.86	0.58
1:H:83:PHE:O	1:H:85:ARG:HG2	2.04	0.58
1:I:77:ILE:O	1:I:80:ARG:N	2.37	0.58
1:H:98:LEU:HD11	1:H:115:LEU:HD23	1.86	0.57
1:A:240:PHE:CE1	1:B:132:VAL:HG23	2.39	0.57
1:G:98:LEU:HD11	1:G:115:LEU:HD23	1.87	0.57
1:C:26:TYR:O	1:C:30:ILE:HG13	2.04	0.57
1:G:140:LYS:HB2	1:G:169:ASN:ND2	2.20	0.56
1:F:77:ILE:O	1:F:80:ARG:N	2.37	0.56
1:H:52:PHE:HD1	1:H:53:ASP:HB2	1.70	0.56
1:B:34:LEU:HG	1:B:85:ARG:NH1	2.21	0.56
1:F:83:PHE:O	1:F:85:ARG:HG2	2.05	0.56
1:D:34:LEU:HG	1:D:85:ARG:NH1	2.21	0.56
1:J:83:PHE:O	1:J:85:ARG:HG2	2.06	0.55
1:C:231:LEU:HD21	1:D:156:LEU:CD2	2.37	0.55
1:H:52:PHE:CD1	1:H:53:ASP:HB2	2.41	0.55
1:C:142:CYS:SG	1:C:144:HIS:HB2	2.47	0.55
1:F:52:PHE:HD1	1:F:53:ASP:HB2	1.73	0.54
1:F:188:GLN:HB2	1:F:201:ARG:O	2.07	0.54
1:E:26:TYR:O	1:E:30:ILE:HG13	2.07	0.54
1:H:140:LYS:HB2	1:H:169:ASN:ND2	2.22	0.54
1:J:140:LYS:HB2	1:J:169:ASN:ND2	2.22	0.54
1:C:34:LEU:HG	1:C:85:ARG:NH1	2.23	0.54
1:B:26:TYR:O	1:B:30:ILE:HG13	2.07	0.54
1:B:137:PHE:CZ	1:B:158:LYS:HA	2.43	0.54
1:C:237:THR:OG1	1:C:238:PRO:HD2	2.08	0.54
1:F:52:PHE:CD1	1:F:53:ASP:HB2	2.43	0.54
1:H:188:GLN:HB2	1:H:201:ARG:O	2.08	0.54
1:I:80:ARG:HA	1:I:85:ARG:H	1.73	0.54
1:J:98:LEU:HD11	1:J:115:LEU:HD23	1.89	0.53
1:H:112:ILE:H	1:H:112:ILE:HD12	1.73	0.53
1:A:26:TYR:O	1:A:30:ILE:HG13	2.09	0.53
1:B:98:LEU:HB3	1:B:99:PRO:HD2	1.91	0.53
1:C:231:LEU:HD13	1:C:240:PHE:CZ	2.44	0.53
1:A:183:GLN:CB	1:A:212:VAL:HG23	2.39	0.53
1:D:183:GLN:CB	1:D:212:VAL:HG23	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:52:PHE:CD1	1:I:53:ASP:HB2	2.44	0.53
1:G:112:ILE:HD12	1:G:112:ILE:H	1.74	0.53
1:I:140:LYS:HB2	1:I:169:ASN:ND2	2.24	0.53
1:J:52:PHE:CD1	1:J:53:ASP:HB2	2.44	0.53
1:J:79:LEU:HD13	1:J:88:VAL:HG21	1.91	0.53
1:F:98:LEU:HD11	1:F:115:LEU:HD23	1.90	0.52
1:J:112:ILE:H	1:J:112:ILE:HD12	1.73	0.52
1:E:94:ARG:NH1	1:E:210:ASP:OD1	2.43	0.52
1:F:112:ILE:HD12	1:F:112:ILE:H	1.73	0.52
1:J:52:PHE:HD1	1:J:53:ASP:HB2	1.74	0.52
1:D:181:ASN:CB	1:D:212:VAL:HG11	2.39	0.52
1:F:98:LEU:HB3	1:F:99:PRO:CD	2.37	0.52
1:D:137:PHE:CZ	1:D:158:LYS:HA	2.45	0.51
1:G:52:PHE:CD1	1:G:52:PHE:C	2.88	0.51
1:G:52:PHE:CD1	1:G:53:ASP:HB2	2.46	0.51
1:J:80:ARG:HA	1:J:85:ARG:H	1.75	0.51
1:B:229:VAL:HG23	1:B:229:VAL:O	2.11	0.51
1:I:52:PHE:HD1	1:I:53:ASP:HB2	1.76	0.51
1:B:183:GLN:CB	1:B:212:VAL:HG23	2.41	0.51
1:D:26:TYR:O	1:D:30:ILE:HG13	2.11	0.51
1:A:181:ASN:CB	1:A:212:VAL:HG11	2.40	0.50
1:H:79:LEU:HD13	1:H:88:VAL:HG21	1.92	0.50
1:H:98:LEU:HB3	1:H:99:PRO:CD	2.36	0.50
1:I:112:ILE:HD12	1:I:112:ILE:H	1.76	0.50
1:B:94:ARG:NH1	1:B:210:ASP:OD1	2.44	0.50
1:D:183:GLN:HB2	1:D:212:VAL:HG23	1.94	0.50
1:C:183:GLN:CB	1:C:212:VAL:HG23	2.42	0.49
1:F:140:LYS:HB2	1:F:169:ASN:ND2	2.27	0.49
1:A:130:PRO:HG2	1:E:240:PHE:HB2	1.93	0.49
1:E:183:GLN:CB	1:E:212:VAL:HG23	2.42	0.49
1:I:76:GLN:OE1	1:I:76:GLN:HA	2.12	0.49
1:A:183:GLN:HB2	1:A:212:VAL:HG23	1.95	0.49
1:E:98:LEU:HB3	1:E:99:PRO:HD2	1.94	0.49
1:F:52:PHE:CD1	1:F:52:PHE:C	2.91	0.49
1:E:142:CYS:SG	1:E:144:HIS:HB2	2.53	0.49
1:F:79:LEU:HD13	1:F:88:VAL:HG21	1.94	0.49
1:A:231:LEU:HD13	1:A:240:PHE:CZ	2.47	0.49
1:C:183:GLN:HB2	1:C:212:VAL:HG23	1.95	0.49
1:D:32:ASP:O	1:D:35:THR:HG22	2.13	0.49
1:F:80:ARG:HA	1:F:85:ARG:H	1.77	0.49
1:I:26:TYR:O	1:I:30:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:52:PHE:CD1	1:J:52:PHE:C	2.90	0.49
1:B:181:ASN:CB	1:B:212:VAL:HG11	2.42	0.49
1:D:142:CYS:SG	1:D:144:HIS:CB	2.99	0.49
1:I:52:PHE:CD1	1:I:52:PHE:C	2.90	0.49
1:D:94:ARG:NH1	1:D:210:ASP:OD1	2.45	0.49
1:J:98:LEU:HB3	1:J:99:PRO:CD	2.37	0.48
1:E:34:LEU:HG	1:E:85:ARG:NH1	2.28	0.48
1:B:132:VAL:HG22	1:B:179:PHE:CE2	2.48	0.48
1:C:181:ASN:CB	1:C:212:VAL:HG11	2.44	0.48
1:H:52:PHE:CD1	1:H:52:PHE:C	2.91	0.48
1:A:137:PHE:CZ	1:A:158:LYS:HA	2.48	0.48
1:G:80:ARG:HA	1:G:85:ARG:H	1.79	0.48
1:D:139:CYS:HA	1:D:170:ILE:HG12	1.95	0.48
1:H:102:LEU:HD13	1:H:110:GLU:HG3	1.95	0.48
1:E:139:CYS:HA	1:E:170:ILE:HG12	1.95	0.48
1:H:80:ARG:HA	1:H:85:ARG:H	1.78	0.48
1:D:132:VAL:HG22	1:D:179:PHE:CE2	2.49	0.47
1:G:52:PHE:HD1	1:G:53:ASP:HB2	1.78	0.47
1:E:231:LEU:HD13	1:E:240:PHE:CZ	2.49	0.47
1:E:183:GLN:HB2	1:E:212:VAL:HG23	1.96	0.47
1:I:13:PHE:CE1	1:I:49:LEU:HA	2.50	0.47
1:I:98:LEU:HB3	1:I:99:PRO:CD	2.38	0.47
1:B:139:CYS:HA	1:B:170:ILE:HG12	1.97	0.47
1:D:16:GLU:O	1:D:17:TYR:C	2.58	0.47
1:D:98:LEU:HB3	1:D:99:PRO:HD2	1.96	0.47
1:J:0:SER:HB2	1:J:59:GLU:OE1	2.15	0.47
1:F:201:ARG:HH11	1:F:201:ARG:HG3	1.79	0.47
1:F:230:VAL:HG21	1:F:243:ILE:HG12	1.96	0.47
1:D:107:ILE:HD11	1:D:118:VAL:HG21	1.97	0.47
1:F:102:LEU:HD13	1:F:110:GLU:HG3	1.96	0.47
1:E:137:PHE:CZ	1:E:158:LYS:HA	2.50	0.47
1:C:162:CYS:HA	1:C:170:ILE:HD11	1.97	0.46
1:A:112:ILE:HG12	1:B:174:VAL:HG12	1.95	0.46
1:A:132:VAL:HG22	1:A:179:PHE:CE2	2.50	0.46
1:A:162:CYS:HA	1:A:170:ILE:HD11	1.97	0.46
1:B:183:GLN:HB2	1:B:212:VAL:HG23	1.97	0.46
1:D:109:ALA:O	1:D:112:ILE:HG22	2.15	0.46
1:G:13:PHE:CE1	1:G:49:LEU:HA	2.50	0.46
1:G:102:LEU:HD13	1:G:110:GLU:HG3	1.98	0.46
1:D:231:LEU:HD13	1:D:240:PHE:CZ	2.51	0.46
1:I:201:ARG:HG3	1:I:201:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:ARG:HG3	1:H:201:ARG:HH11	1.81	0.46
1:I:25:VAL:HG13	1:I:26:TYR:CD2	2.50	0.46
1:E:181:ASN:CB	1:E:212:VAL:HG11	2.46	0.46
1:G:230:VAL:HG21	1:G:243:ILE:HG12	1.98	0.46
1:A:229:VAL:HG22	1:B:174:VAL:HG11	1.97	0.46
1:B:109:ALA:O	1:B:112:ILE:HG22	2.16	0.46
1:E:132:VAL:HG22	1:E:179:PHE:CE2	2.51	0.46
1:I:79:LEU:HD13	1:I:88:VAL:HG21	1.96	0.46
1:H:13:PHE:CE1	1:H:49:LEU:HA	2.51	0.46
1:H:77:ILE:HG22	1:H:78:VAL:N	2.31	0.46
1:A:98:LEU:HB3	1:A:99:PRO:HD2	1.97	0.45
1:C:231:LEU:HD13	1:C:240:PHE:CE1	2.51	0.45
1:H:201:ARG:HG3	1:H:201:ARG:NH1	2.31	0.45
1:J:25:VAL:HG13	1:J:26:TYR:CD2	2.51	0.45
1:F:13:PHE:CE1	1:F:49:LEU:HA	2.52	0.45
1:J:230:VAL:HG21	1:J:243:ILE:HG12	1.97	0.45
1:G:188:GLN:HB2	1:G:201:ARG:O	2.17	0.45
1:I:102:LEU:HD13	1:I:110:GLU:HG3	1.99	0.45
1:B:162:CYS:HA	1:B:170:ILE:HD11	1.98	0.45
1:F:77:ILE:HG22	1:F:78:VAL:N	2.31	0.45
1:J:102:LEU:HD13	1:J:110:GLU:HG3	1.97	0.45
1:C:94:ARG:NH1	1:C:210:ASP:OD1	2.50	0.45
1:G:201:ARG:HG3	1:G:201:ARG:HH11	1.82	0.45
1:I:188:GLN:HB2	1:I:201:ARG:O	2.17	0.45
1:C:139:CYS:HA	1:C:170:ILE:HG12	1.99	0.44
1:B:112:ILE:HG23	1:B:112:ILE:O	2.17	0.44
1:C:36:ILE:HD11	1:G:182:PHE:CG	2.53	0.44
1:E:146:MET:HE3	1:E:163:GLU:HB3	1.99	0.44
1:C:98:LEU:HB3	1:C:99:PRO:HD2	1.97	0.44
1:G:25:VAL:HG13	1:G:26:TYR:CD2	2.52	0.44
1:G:79:LEU:HD13	1:G:88:VAL:HG21	1.97	0.44
1:A:139:CYS:HA	1:A:170:ILE:HG12	1.99	0.44
1:F:76:GLN:HA	1:F:76:GLN:OE1	2.17	0.44
1:C:240:PHE:CE1	1:D:132:VAL:HG21	2.48	0.44
1:D:229:VAL:O	1:D:229:VAL:HG23	2.18	0.44
1:C:83:PHE:HA	1:G:174:VAL:HG21	1.99	0.44
1:I:77:ILE:HG22	1:I:78:VAL:N	2.32	0.44
1:J:13:PHE:CE1	1:J:49:LEU:HA	2.53	0.44
1:J:201:ARG:HG3	1:J:201:ARG:HH11	1.83	0.43
1:F:170:ILE:HG22	1:F:171:GLU:N	2.33	0.43
1:C:240:PHE:HE1	1:D:132:VAL:HG23	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:ASN:O	1:D:13:PHE:C	2.61	0.43
1:E:36:ILE:HD11	1:I:182:PHE:CG	2.53	0.43
1:G:98:LEU:HB3	1:G:99:PRO:CD	2.40	0.43
1:C:132:VAL:HG22	1:C:179:PHE:CE2	2.53	0.43
1:G:76:GLN:OE1	1:G:76:GLN:HA	2.17	0.43
1:G:201:ARG:HG3	1:G:201:ARG:NH1	2.33	0.43
1:A:94:ARG:NH1	1:A:210:ASP:OD1	2.51	0.43
1:D:123:THR:HG22	1:D:124:ARG:HG3	2.00	0.43
1:D:162:CYS:HA	1:D:170:ILE:HD11	1.99	0.43
1:B:142:CYS:SG	1:B:144:HIS:CB	3.01	0.43
1:I:230:VAL:HG21	1:I:243:ILE:HG12	2.00	0.43
1:C:109:ALA:O	1:C:112:ILE:HG22	2.18	0.43
1:F:182:PHE:CD1	1:F:182:PHE:C	2.96	0.43
1:H:25:VAL:HG13	1:H:26:TYR:CD2	2.52	0.43
1:J:26:TYR:O	1:J:30:ILE:HG13	2.19	0.43
1:F:201:ARG:HG3	1:F:201:ARG:NH1	2.32	0.43
1:G:182:PHE:CD1	1:G:182:PHE:C	2.96	0.43
1:J:76:GLN:OE1	1:J:76:GLN:HA	2.19	0.43
1:A:5:GLU:O	1:A:9:ARG:HG2	2.18	0.43
1:C:5:GLU:O	1:C:9:ARG:HG2	2.19	0.43
1:D:181:ASN:HB3	1:D:212:VAL:HG11	2.00	0.43
1:C:146:MET:HE3	1:C:163:GLU:HB3	2.01	0.42
1:D:138:VAL:HG22	1:D:145:GLU:HG2	2.01	0.42
1:E:162:CYS:HA	1:E:170:ILE:HD11	2.01	0.42
1:J:77:ILE:HG22	1:J:78:VAL:N	2.33	0.42
1:E:5:GLU:O	1:E:9:ARG:HG2	2.18	0.42
1:I:63:ASN:HB3	1:I:66:GLU:OE2	2.19	0.42
1:A:63:ASN:HB3	1:A:66:GLU:OE2	2.19	0.42
1:A:181:ASN:HB3	1:A:212:VAL:HG11	2.00	0.42
1:C:240:PHE:HE1	1:D:132:VAL:CG2	2.26	0.42
1:H:230:VAL:HG21	1:H:243:ILE:HG12	2.00	0.42
1:A:146:MET:HE3	1:A:163:GLU:HB3	2.00	0.42
1:B:5:GLU:O	1:B:9:ARG:HG2	2.19	0.42
1:B:146:MET:HE3	1:B:163:GLU:HB3	2.00	0.42
1:H:102:LEU:CD1	1:H:110:GLU:HG3	2.49	0.42
1:I:201:ARG:HG3	1:I:201:ARG:NH1	2.34	0.42
1:J:10:PHE:CE2	1:J:71:ALA:HB2	2.54	0.42
1:B:32:ASP:O	1:B:35:THR:HG22	2.19	0.42
1:C:137:PHE:CZ	1:C:158:LYS:HA	2.55	0.42
1:G:80:ARG:HG3	1:G:86:GLU:CD	2.44	0.42
1:H:63:ASN:HB3	1:H:66:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:TYR:O	1:G:30:ILE:HG13	2.19	0.42
1:G:170:ILE:HG22	1:G:171:GLU:N	2.35	0.42
1:H:231:LEU:HD12	1:H:232:GLU:H	1.85	0.42
1:I:10:PHE:CE2	1:I:71:ALA:HB2	2.54	0.42
1:B:123:THR:HG22	1:B:124:ARG:HG3	2.02	0.42
1:C:238:PRO:HG2	1:D:131:PHE:CE1	2.55	0.42
1:E:229:VAL:O	1:E:229:VAL:HG23	2.19	0.42
1:G:10:PHE:CE2	1:G:71:ALA:HB2	2.54	0.42
1:A:229:VAL:O	1:A:229:VAL:HG23	2.19	0.42
1:D:182:PHE:CD1	1:D:182:PHE:C	2.98	0.42
1:H:76:GLN:HA	1:H:76:GLN:OE1	2.20	0.42
1:C:240:PHE:CD1	1:D:132:VAL:HG23	2.52	0.42
1:D:3:ARG:O	1:D:7:ILE:HG13	2.20	0.42
1:J:201:ARG:HG3	1:J:201:ARG:NH1	2.34	0.41
1:A:16:GLU:O	1:A:17:TYR:C	2.61	0.41
1:B:229:VAL:O	1:B:229:VAL:CG2	2.68	0.41
1:C:240:PHE:HB2	1:D:130:PRO:HG2	2.01	0.41
1:E:142:CYS:SG	1:E:165:CYS:HB3	2.60	0.41
1:F:25:VAL:HG13	1:F:26:TYR:CD2	2.54	0.41
1:G:63:ASN:HB3	1:G:66:GLU:OE2	2.19	0.41
1:J:31:THR:HA	1:J:34:LEU:HD12	2.01	0.41
1:B:231:LEU:HD13	1:B:240:PHE:CZ	2.54	0.41
1:C:112:ILE:HD13	1:C:229:VAL:HG13	2.03	0.41
1:C:140:LYS:HB2	1:C:169:ASN:ND2	2.35	0.41
1:G:77:ILE:HG22	1:G:78:VAL:N	2.35	0.41
1:I:170:ILE:HG22	1:I:171:GLU:N	2.36	0.41
1:B:85:ARG:HG3	1:B:85:ARG:HH11	1.85	0.41
1:B:107:ILE:HD11	1:B:118:VAL:HG21	2.02	0.41
1:C:47:MET:HE1	1:H:121:ILE:HD11	2.02	0.41
1:E:109:ALA:O	1:E:112:ILE:HG22	2.20	0.41
1:E:112:ILE:HD13	1:E:229:VAL:HG13	2.02	0.41
1:A:188:GLN:HB2	1:A:201:ARG:O	2.21	0.41
1:A:240:PHE:CE1	1:B:132:VAL:HG21	2.55	0.41
1:C:16:GLU:O	1:C:17:TYR:C	2.59	0.41
1:D:140:LYS:HB2	1:D:169:ASN:ND2	2.35	0.41
1:E:140:LYS:HB2	1:E:169:ASN:ND2	2.35	0.41
1:H:87:ASP:OD1	1:H:87:ASP:N	2.54	0.41
1:J:63:ASN:HB3	1:J:66:GLU:OE2	2.21	0.41
1:J:35:THR:HG22	1:J:36:ILE:N	2.36	0.41
1:J:80:ARG:HG3	1:J:86:GLU:CD	2.46	0.41
1:F:92:HIS:CD2	1:F:94:ARG:HH12	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:LYS:HB2	1:G:130:PRO:HD2	2.03	0.41
1:H:26:TYR:O	1:H:30:ILE:HG13	2.20	0.41
1:J:182:PHE:C	1:J:182:PHE:CD1	2.99	0.41
1:D:146:MET:HE3	1:D:163:GLU:HB3	2.02	0.40
1:B:182:PHE:CD1	1:B:182:PHE:C	2.98	0.40
1:A:132:VAL:CG2	1:E:240:PHE:CE1	3.02	0.40
1:A:138:VAL:HG22	1:A:145:GLU:HG2	2.03	0.40
1:B:63:ASN:HB3	1:B:66:GLU:OE2	2.22	0.40
1:E:87:ASP:OD1	1:E:87:ASP:N	2.54	0.40
1:F:72:GLU:OE1	1:F:92:HIS:HA	2.21	0.40
1:F:80:ARG:HH11	1:F:81:GLU:HG2	1.87	0.40
1:I:80:ARG:HG3	1:I:86:GLU:CD	2.46	0.40
1:I:182:PHE:CD1	1:I:182:PHE:C	2.99	0.40
1:E:32:ASP:O	1:E:35:THR:HG22	2.21	0.40
1:F:80:ARG:HG3	1:F:86:GLU:CD	2.46	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:HIS:ND1	1:I:21:ASP:O[4_545]	2.04	0.16
1:J:34:LEU:O	1:J:34:LEU:O[4_645]	2.17	0.03
1:E:144:HIS:ND1	1:G:21:ASP:O[4_655]	2.19	0.01

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	253/257 (98%)	234 (92%)	17 (7%)	2 (1%)	16	50
1	B	253/257 (98%)	235 (93%)	17 (7%)	1 (0%)	30	62
1	C	253/257 (98%)	235 (93%)	17 (7%)	1 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	253/257 (98%)	235 (93%)	17 (7%)	1 (0%)	30	62
1	E	253/257 (98%)	235 (93%)	17 (7%)	1 (0%)	30	62
1	F	252/257 (98%)	237 (94%)	15 (6%)	0	100	100
1	G	252/257 (98%)	236 (94%)	16 (6%)	0	100	100
1	H	252/257 (98%)	235 (93%)	17 (7%)	0	100	100
1	I	252/257 (98%)	232 (92%)	20 (8%)	0	100	100
1	J	252/257 (98%)	235 (93%)	17 (7%)	0	100	100
All	All	2525/2570 (98%)	2349 (93%)	170 (7%)	6 (0%)	43	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	192	GLU
1	A	192	GLU
1	C	192	GLU
1	D	192	GLU
1	E	192	GLU
1	A	25	VAL

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	227/230 (99%)	219 (96%)	8 (4%)	32	64
1	B	227/230 (99%)	220 (97%)	7 (3%)	35	66
1	C	227/230 (99%)	219 (96%)	8 (4%)	32	64
1	D	227/230 (99%)	220 (97%)	7 (3%)	35	66
1	E	227/230 (99%)	219 (96%)	8 (4%)	32	64
1	F	227/230 (99%)	222 (98%)	5 (2%)	45	71
1	G	227/230 (99%)	222 (98%)	5 (2%)	45	71
1	H	227/230 (99%)	222 (98%)	5 (2%)	45	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	227/230 (99%)	222 (98%)	5 (2%)	45	71
1	J	227/230 (99%)	221 (97%)	6 (3%)	40	69
All	All	2270/2300 (99%)	2206 (97%)	64 (3%)	38	68

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	164	GLN
1	A	165	CYS
1	A	178	SER
1	A	193	THR
1	A	214	VAL
1	A	216	LEU
1	A	231	LEU
1	B	60	VAL
1	B	164	GLN
1	B	178	SER
1	B	193	THR
1	B	214	VAL
1	B	216	LEU
1	B	231	LEU
1	C	60	VAL
1	C	164	GLN
1	C	165	CYS
1	C	178	SER
1	C	193	THR
1	C	214	VAL
1	C	216	LEU
1	C	231	LEU
1	D	60	VAL
1	D	164	GLN
1	D	178	SER
1	D	193	THR
1	D	214	VAL
1	D	216	LEU
1	D	231	LEU
1	E	60	VAL
1	E	164	GLN
1	E	165	CYS
1	E	178	SER

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Mol	Chain	Res	Type
1	E	193	THR
1	E	214	VAL
1	E	216	LEU
1	E	231	LEU
1	F	4	GLU
1	F	52	PHE
1	F	55	GLU
1	F	84	GLN
1	F	98	LEU
1	G	4	GLU
1	G	52	PHE
1	G	55	GLU
1	G	84	GLN
1	G	98	LEU
1	H	4	GLU
1	H	52	PHE
1	H	55	GLU
1	H	84	GLN
1	H	98	LEU
1	I	4	GLU
1	I	52	PHE
1	I	55	GLU
1	I	84	GLN
1	I	98	LEU
1	J	4	GLU
1	J	36	ILE
1	J	52	PHE
1	J	55	GLU
1	J	84	GLN
1	J	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	117	GLN
1	A	169	ASN
1	A	175	ASN
1	B	50	ASN
1	B	58	HIS
1	B	117	GLN
1	B	169	ASN

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Mol	Chain	Res	Type
1	B	175	ASN
1	C	50	ASN
1	C	58	HIS
1	C	117	GLN
1	C	175	ASN
1	C	188	GLN
1	D	117	GLN
1	D	169	ASN
1	E	50	ASN
1	E	58	HIS
1	E	117	GLN
1	E	169	ASN
1	E	175	ASN
1	F	58	HIS
1	F	92	HIS
1	G	92	HIS
1	H	58	HIS
1	H	92	HIS
1	I	58	HIS
1	I	92	HIS
1	I	169	ASN
1	J	58	HIS
1	J	92	HIS
1	J	188	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 ⓘ

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	SO4	F	302	-	4,4,4	0.38	0	6,6,6	0.63	0
3	SO4	I	302	-	4,4,4	0.31	0	6,6,6	0.47	0
3	SO4	D	302	-	4,4,4	0.37	0	6,6,6	0.26	0
3	SO4	H	302	-	4,4,4	0.39	0	6,6,6	0.46	0
3	SO4	J	302	-	4,4,4	0.41	0	6,6,6	0.70	0
3	SO4	E	302	-	4,4,4	0.34	0	6,6,6	0.48	0
3	SO4	B	302	-	4,4,4	0.46	0	6,6,6	0.63	0
3	SO4	G	302	-	4,4,4	0.24	0	6,6,6	0.43	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.

No monomer is involved in short contacts.

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	255/257 (99%)	0.13	13 (5%)	33	21	34, 63, 127, 163	0
1	B	255/257 (99%)	0.04	14 (5%)	30	19	22, 48, 123, 186	0
1	C	255/257 (99%)	0.02	7 (2%)	56	36	29, 55, 106, 152	0
1	D	255/257 (99%)	0.06	14 (5%)	30	19	24, 47, 120, 168	0
1	E	255/257 (99%)	0.13	13 (5%)	33	21	31, 58, 108, 182	0
1	F	254/257 (98%)	0.43	10 (3%)	43	27	37, 74, 133, 210	0
1	G	254/257 (98%)	0.39	18 (7%)	22	14	26, 65, 117, 174	0
1	H	254/257 (98%)	0.36	11 (4%)	40	24	34, 72, 132, 216	0
1	I	254/257 (98%)	0.61	28 (11%)	10	7	26, 69, 118, 154	0
1	J	254/257 (98%)	0.54	18 (7%)	22	14	44, 85, 146, 216	0
All	All	2545/2570 (99%)	0.27	146 (5%)	29	19	22, 63, 127, 216	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	112	ILE	5.6
1	F	112	ILE	5.2
1	H	112	ILE	4.8
1	I	24	PRO	4.7
1	B	144	HIS	4.5
1	D	144	HIS	4.3
1	G	112	ILE	4.3
1	I	14	LEU	4.2
1	I	112	ILE	4.1
1	G	88	VAL	4.0
1	G	24	PRO	3.9
1	J	36	ILE	3.9
1	E	87	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	J	24	PRO	3.6
1	I	16	GLU	3.6
1	D	141	ASP	3.6
1	H	19	ASP	3.5
1	B	146	MET	3.5
1	I	76	GLN	3.5
1	I	89	GLY	3.5
1	I	197	GLY	3.5
1	H	36	ILE	3.4
1	C	253	SER	3.4
1	F	24	PRO	3.4
1	I	78	VAL	3.3
1	B	236	ALA	3.3
1	I	6	MET	3.3
1	H	23	ASN	3.3
1	E	89	GLY	3.3
1	G	14	LEU	3.0
1	H	24	PRO	3.0
1	J	19	ASP	3.0
1	B	254	LYS	3.0
1	C	254	LYS	3.0
1	D	171	GLU	3.0
1	G	87	ASP	3.0
1	I	75	ILE	3.0
1	C	87	ASP	3.0
1	F	111	HIS	3.0
1	I	88	VAL	3.0
1	B	87	ASP	3.0
1	I	79	LEU	2.9
1	F	19	ASP	2.9
1	F	253	SER	2.9
1	A	160	LYS	2.9
1	I	77	ILE	2.9
1	H	20	GLU	2.9
1	I	25	VAL	2.9
1	D	254	LYS	2.9
1	I	87	ASP	2.8
1	H	111	HIS	2.8
1	D	234	ALA	2.8
1	J	37	THR	2.7
1	D	166	GLY	2.7
1	J	25	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	254	LYS	2.7
1	A	87	ASP	2.7
1	I	111	HIS	2.7
1	F	23	ASN	2.7
1	G	76	GLN	2.7
1	A	234	ALA	2.7
1	I	13	PHE	2.6
1	G	77	ILE	2.6
1	B	164	GLN	2.6
1	J	20	GLU	2.6
1	G	79	LEU	2.6
1	I	109	ALA	2.6
1	A	168	LYS	2.6
1	D	163	GLU	2.6
1	E	171	GLU	2.6
1	I	74	ALA	2.6
1	I	27	ARG	2.6
1	I	10	PHE	2.6
1	E	234	ALA	2.6
1	J	58	HIS	2.5
1	E	0	SER	2.5
1	A	254	LYS	2.5
1	B	233	ALA	2.5
1	E	86	GLU	2.5
1	A	112	ILE	2.5
1	I	84	GLN	2.5
1	G	253	SER	2.5
1	B	135	ALA	2.4
1	D	139	CYS	2.4
1	C	86	GLU	2.4
1	G	111	HIS	2.4
1	D	165	CYS	2.4
1	J	21	ASP	2.4
1	B	234	ALA	2.4
1	D	87	ASP	2.4
1	I	3	ARG	2.4
1	J	47	MET	2.3
1	H	164	GLN	2.3
1	B	162	CYS	2.3
1	G	75	ILE	2.3
1	E	235	GLU	2.3
1	A	236	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	233	ALA	2.3
1	A	16	GLU	2.3
1	D	236	ALA	2.3
1	A	144	HIS	2.3
1	J	51	SER	2.3
1	C	171	GLU	2.3
1	G	25	VAL	2.3
1	C	89	GLY	2.3
1	H	197	GLY	2.3
1	F	199	MET	2.3
1	G	36	ILE	2.2
1	I	91	ILE	2.2
1	J	197	GLY	2.2
1	A	80	ARG	2.2
1	J	27	ARG	2.2
1	D	164	GLN	2.2
1	B	140	LYS	2.2
1	D	161	LYS	2.2
1	E	85	ARG	2.2
1	A	165	CYS	2.2
1	I	66	GLU	2.2
1	J	16	GLU	2.2
1	J	111	HIS	2.2
1	F	36	ILE	2.2
1	J	26	TYR	2.2
1	H	199	MET	2.2
1	A	161	LYS	2.2
1	G	43	ALA	2.2
1	A	170	ILE	2.1
1	H	253	SER	2.1
1	G	35	THR	2.1
1	J	13	PHE	2.1
1	F	25	VAL	2.1
1	E	161	LYS	2.1
1	I	163	GLU	2.1
1	I	253	SER	2.1
1	G	12	ASN	2.1
1	G	1	VAL	2.1
1	B	166	GLY	2.1
1	I	22	GLY	2.1
1	E	8	GLU	2.1
1	D	253	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	78	VAL	2.1
1	E	169	ASN	2.1
1	B	235	GLU	2.1
1	F	27	ARG	2.0
1	C	164	GLN	2.0
1	B	168	LYS	2.0
1	J	81	GLU	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](#)

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
3	SO4	B	302	5/5	0.74	0.17	106,106,106,106	0
3	SO4	D	302	5/5	0.76	0.19	115,115,115,115	0
3	SO4	E	302	5/5	0.80	0.12	104,104,104,104	0
3	SO4	J	302	5/5	0.90	0.14	79,79,79,79	0
3	SO4	F	302	5/5	0.91	0.10	83,83,83,83	0
3	SO4	H	302	5/5	0.91	0.15	79,79,79,79	0
2	ZN	B	301	1/1	0.91	0.10	183,183,183,183	0
2	ZN	D	301	1/1	0.92	0.10	143,143,143,143	0
2	ZN	A	301	1/1	0.93	0.08	167,167,167,167	0
2	ZN	G	301	1/1	0.97	0.04	103,103,103,103	0
3	SO4	I	302	5/5	0.97	0.07	59,59,59,59	0
3	SO4	G	302	5/5	0.97	0.06	63,63,63,63	0
2	ZN	E	301	1/1	0.98	0.04	67,67,67,67	0
2	ZN	I	301	1/1	0.98	0.03	103,103,103,103	0
2	ZN	C	301	1/1	0.99	0.03	70,70,70,70	0
2	ZN	H	301	1/1	0.99	0.03	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	F	301	1/1	0.99	0.03	73,73,73,73	0
2	ZN	J	301	1/1	0.99	0.03	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.