



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:00 AM UTC

PDB ID : 4POF / pdb_00004pof
Title : PfMCM N-terminal domain without DNA
Authors : Froelich, C.A.; Kang, S.; Epling, L.B.; Bell, S.P.; Enemark, E.J.
Deposited on : 2014-02-25
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

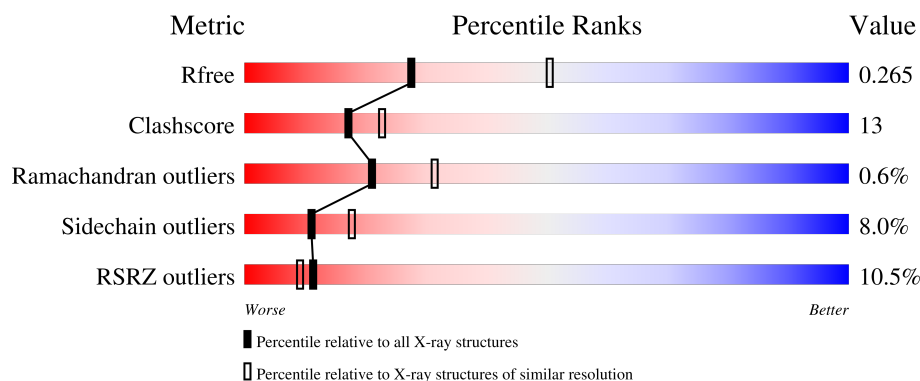
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	11% 70% 25% ..
1	B	257	12% 69% 26% 5% .
1	C	257	11% 70% 25% ..
1	D	257	8% 73% 22% ..
1	E	257	8% 71% 24% ..

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Mol	Chain	Length	Quality of chain
1	F	257	12% 71% 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12258 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
			2042	1294	350	389	9			
1	B	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	C	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	D	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	E	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			
1	F	255	Total	C	N	O	S	0	0	0
			2042	1294	350	389	9			

There are 12 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
B	0	SER	-	expression tag	UNP Q8U3I4
B	1	VAL	-	expression tag	UNP Q8U3I4
C	0	SER	-	expression tag	UNP Q8U3I4
C	1	VAL	-	expression tag	UNP Q8U3I4
D	0	SER	-	expression tag	UNP Q8U3I4
D	1	VAL	-	expression tag	UNP Q8U3I4
E	0	SER	-	expression tag	UNP Q8U3I4
E	1	VAL	-	expression tag	UNP Q8U3I4
F	0	SER	-	expression tag	UNP Q8U3I4
F	1	VAL	-	expression tag	UNP Q8U3I4

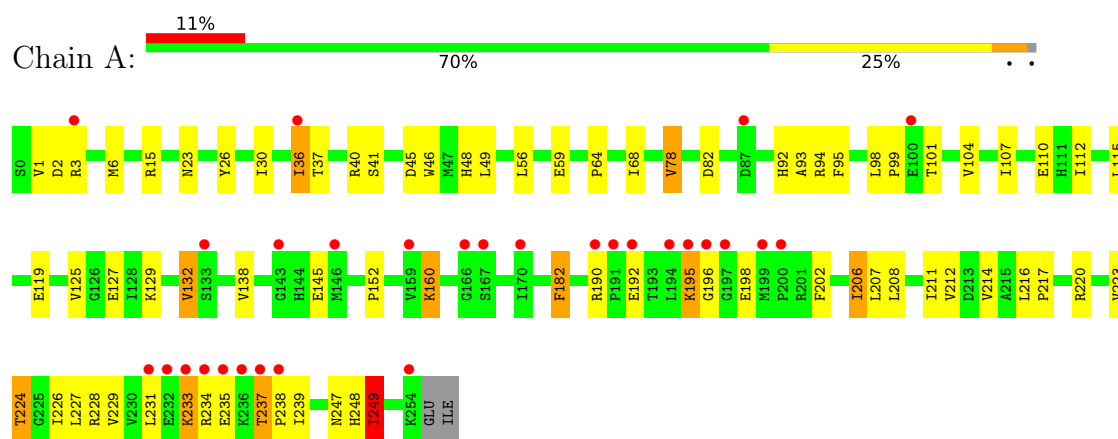
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

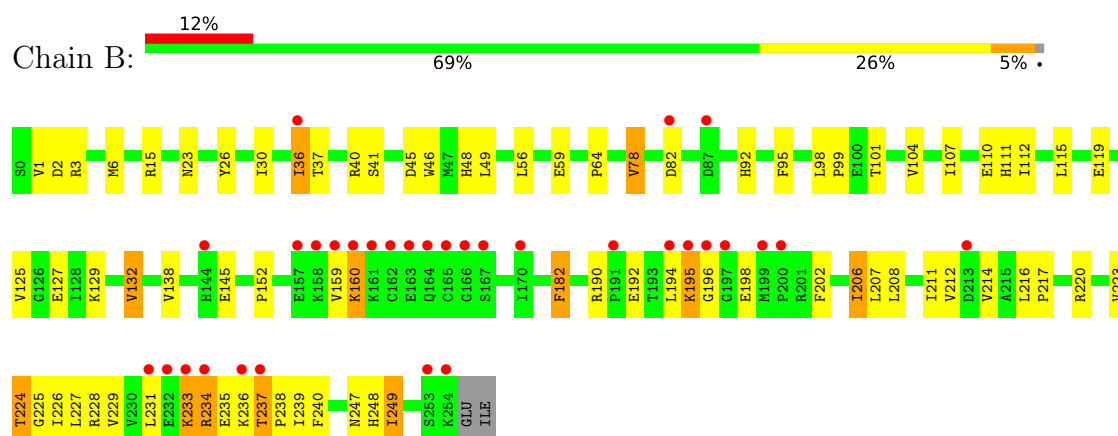
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

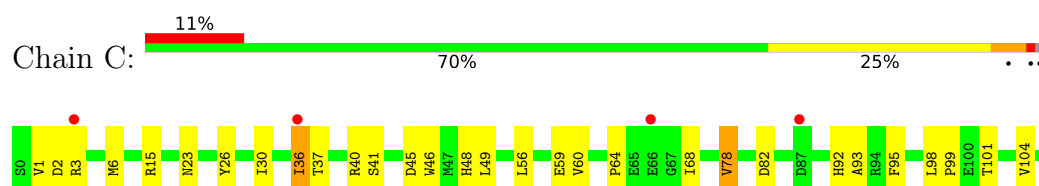
• Molecule 1: Cell division control protein 21

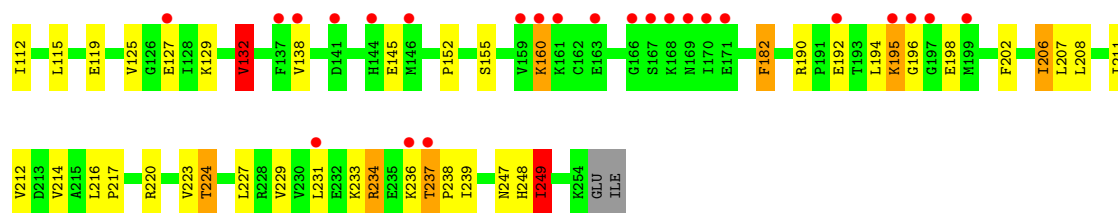


• Molecule 1: Cell division control protein 21

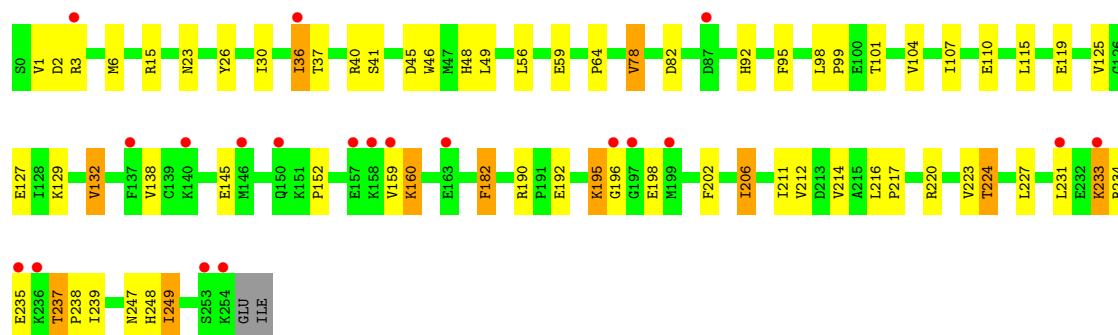
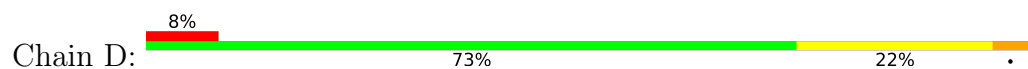


• Molecule 1: Cell division control protein 21

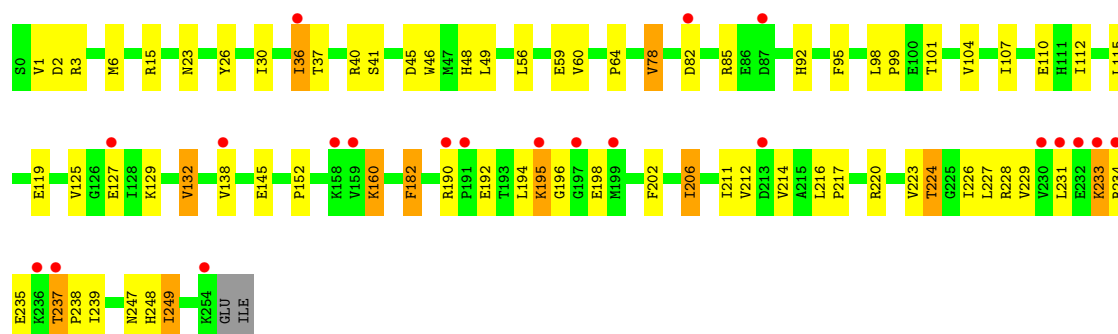




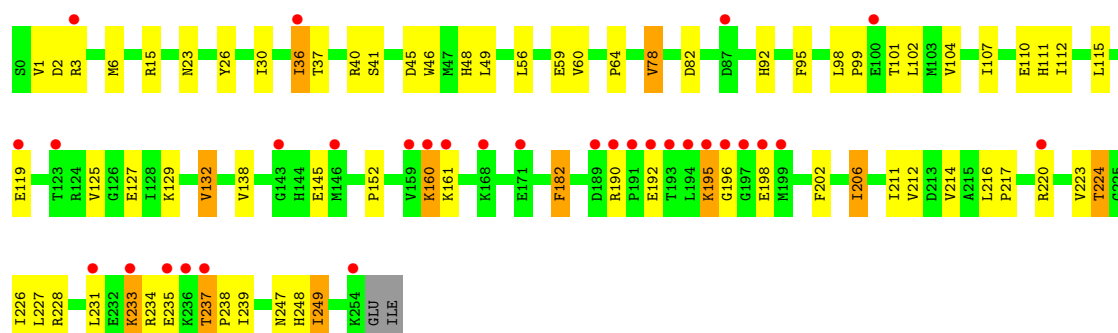
● Molecule 1: Cell division control protein 21



● Molecule 1: Cell division control protein 21



● Molecule 1: Cell division control protein 21



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.85Å 103.06Å 122.44Å 90.00° 119.85° 90.00°	Depositor
Resolution (Å)	47.33 – 2.65 47.33 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.33-2.65) 98.6 (47.33-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.259 , 0.270 0.253 , 0.265	Depositor DCC
R_{free} test set	3839 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	1.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for l,k,-h-l 0.022 for -h-l,k,h 0.000 for -h-l,-k,l 0.000 for h,-k,-h-l 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12258	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2446e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.71	0/2077	0.98	4/2805 (0.1%)
1	B	0.66	0/2077	0.96	4/2805 (0.1%)
1	C	0.66	0/2077	0.96	4/2805 (0.1%)
1	D	0.64	0/2077	0.94	3/2805 (0.1%)
1	E	0.62	0/2077	0.94	3/2805 (0.1%)
1	F	0.73	1/2077 (0.0%)	1.00	3/2805 (0.1%)
All	All	0.67	1/12462 (0.0%)	0.96	21/16830 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	111	HIS	CA-C	-5.04	1.45	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	VAL	CB-CA-C	-11.49	99.62	111.80
1	E	132	VAL	CB-CA-C	-11.30	99.82	111.80
1	A	132	VAL	CB-CA-C	-10.95	100.20	111.80
1	C	132	VAL	CB-CA-C	-10.59	100.57	111.80
1	D	132	VAL	CB-CA-C	-10.53	100.64	111.80
1	F	132	VAL	CB-CA-C	-10.46	100.71	111.80
1	D	196	GLY	N-CA-C	-7.02	105.53	115.43
1	B	196	GLY	N-CA-C	-6.99	105.57	115.43
1	C	196	GLY	N-CA-C	-6.92	105.67	115.43
1	A	196	GLY	N-CA-C	-6.82	105.82	115.43
1	E	196	GLY	N-CA-C	-6.75	105.91	115.43
1	F	196	GLY	N-CA-C	-6.66	106.05	115.43
1	C	195	LYS	N-CA-C	6.20	120.73	109.32
1	F	195	LYS	N-CA-C	6.13	120.60	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	LYS	N-CA-C	6.09	120.53	109.32
1	E	195	LYS	N-CA-C	6.06	120.47	109.32
1	A	195	LYS	N-CA-C	6.03	120.42	109.32
1	B	195	LYS	N-CA-C	6.00	120.36	109.32
1	B	225	GLY	N-CA-C	5.79	119.05	110.42
1	A	249	ILE	CB-CA-C	-5.29	102.23	110.69
1	C	249	ILE	CB-CA-C	-5.04	102.63	110.69

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	2042	0	2052	51	1
1	B	2042	0	2052	56	0
1	C	2042	0	2052	53	0
1	D	2042	0	2052	47	0
1	E	2042	0	2052	55	0
1	F	2042	0	2052	50	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
All	All	12258	0	12312	310	1

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 13.

All (310) 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:C:41:SER:HB3	1:C:92:HIS:HB2	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ILE:HB	1:B:249:ILE:HD11	1.49	0.95
1:F:41:SER:HB3	1:F:92:HIS:HB2	1.52	0.92
1:B:41:SER:HB3	1:B:92:HIS:HB2	1.52	0.91
1:D:160:LYS:H	1:D:160:LYS:HD3	1.36	0.91
1:D:41:SER:HB3	1:D:92:HIS:HB2	1.51	0.91
1:E:160:LYS:H	1:E:160:LYS:HD3	1.37	0.90
1:C:160:LYS:H	1:C:160:LYS:HD3	1.36	0.90
1:E:211:ILE:HB	1:E:249:ILE:HD11	1.55	0.89
1:D:211:ILE:HB	1:D:249:ILE:HD11	1.54	0.88
1:E:41:SER:HB3	1:E:92:HIS:HB2	1.56	0.87
1:F:160:LYS:HD3	1:F:160:LYS:H	1.37	0.87
1:A:160:LYS:HD3	1:A:160:LYS:H	1.38	0.87
1:F:211:ILE:HB	1:F:249:ILE:HD11	1.56	0.86
1:C:211:ILE:HB	1:C:249:ILE:HD11	1.55	0.86
1:B:160:LYS:H	1:B:160:LYS:HD3	1.39	0.86
1:A:211:ILE:HB	1:A:249:ILE:HD11	1.58	0.85
1:A:41:SER:HB3	1:A:92:HIS:HB2	1.61	0.82
1:C:30:ILE:HD13	1:C:78:VAL:HG21	1.63	0.79
1:F:30:ILE:HD13	1:F:78:VAL:HG21	1.66	0.78
1:B:30:ILE:HD13	1:B:78:VAL:HG21	1.67	0.77
1:D:30:ILE:HD13	1:D:78:VAL:HG21	1.66	0.75
1:E:30:ILE:HD13	1:E:78:VAL:HG21	1.68	0.75
1:F:30:ILE:HD13	1:F:78:VAL:CG2	2.19	0.73
1:C:30:ILE:HD13	1:C:78:VAL:CG2	2.19	0.73
1:C:95:PHE:H	1:C:247:ASN:HD21	1.38	0.72
1:F:95:PHE:H	1:F:247:ASN:HD21	1.37	0.71
1:D:30:ILE:HD13	1:D:78:VAL:CG2	2.21	0.70
1:D:95:PHE:H	1:D:247:ASN:HD21	1.39	0.70
1:E:95:PHE:H	1:E:247:ASN:HD21	1.38	0.69
1:B:95:PHE:H	1:B:247:ASN:HD21	1.38	0.69
1:E:30:ILE:HD13	1:E:78:VAL:CG2	2.24	0.68
1:A:95:PHE:H	1:A:247:ASN:HD21	1.40	0.68
1:D:231:LEU:HD12	1:D:231:LEU:H	1.60	0.67
1:F:226:ILE:HG22	1:F:228:ARG:HD3	1.77	0.67
1:B:30:ILE:HD13	1:B:78:VAL:CG2	2.24	0.67
1:B:138:VAL:HG22	1:B:145:GLU:HG2	1.77	0.66
1:F:231:LEU:H	1:F:231:LEU:HD12	1.61	0.66
1:E:138:VAL:HG22	1:E:145:GLU:HG2	1.78	0.66
1:A:30:ILE:HD13	1:A:78:VAL:HG21	1.76	0.65
1:D:138:VAL:HG22	1:D:145:GLU:HG2	1.78	0.65
1:C:138:VAL:HG22	1:C:145:GLU:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:LEU:HD12	1:E:231:LEU:H	1.62	0.65
1:C:36:ILE:CD1	1:C:37:THR:H	2.10	0.64
1:A:138:VAL:HG22	1:A:145:GLU:HG2	1.78	0.64
1:C:231:LEU:HD12	1:C:231:LEU:H	1.62	0.64
1:D:40:ARG:HH21	1:D:40:ARG:HG3	1.63	0.64
1:F:36:ILE:CD1	1:F:37:THR:H	2.10	0.64
1:B:36:ILE:CD1	1:B:37:THR:H	2.10	0.63
1:F:138:VAL:HG22	1:F:145:GLU:HG2	1.80	0.63
1:A:30:ILE:HD13	1:A:78:VAL:CG2	2.28	0.63
1:E:36:ILE:CD1	1:E:37:THR:H	2.12	0.63
1:E:40:ARG:HH21	1:E:40:ARG:HG3	1.64	0.63
1:A:36:ILE:CD1	1:A:37:THR:H	2.12	0.62
1:E:190:ARG:HG2	1:E:192:GLU:HG2	1.81	0.62
1:B:190:ARG:HG2	1:B:192:GLU:HG2	1.81	0.62
1:F:190:ARG:HG2	1:F:192:GLU:HG2	1.81	0.62
1:C:190:ARG:HG2	1:C:192:GLU:HG2	1.82	0.62
1:B:49:LEU:HD11	1:B:56:LEU:HD23	1.82	0.62
1:A:195:LYS:HA	1:A:198:GLU:CB	2.30	0.61
1:D:36:ILE:CD1	1:D:37:THR:H	2.13	0.61
1:B:45:ASP:HB3	1:B:48:HIS:CD2	2.36	0.61
1:D:195:LYS:HA	1:D:198:GLU:CB	2.30	0.61
1:F:64:PRO:HB3	1:F:115:LEU:HB2	1.83	0.61
1:A:40:ARG:HH21	1:A:40:ARG:HG3	1.66	0.61
1:E:160:LYS:H	1:E:160:LYS:CD	2.11	0.61
1:C:195:LYS:HA	1:C:198:GLU:CB	2.31	0.61
1:D:160:LYS:H	1:D:160:LYS:CD	2.10	0.61
1:C:45:ASP:HB3	1:C:48:HIS:CD2	2.36	0.60
1:A:190:ARG:HG2	1:A:192:GLU:HG2	1.83	0.60
1:A:231:LEU:H	1:A:231:LEU:HD12	1.65	0.60
1:D:190:ARG:HG2	1:D:192:GLU:HG2	1.82	0.60
1:E:195:LYS:HA	1:E:198:GLU:CB	2.30	0.60
1:F:49:LEU:HD11	1:F:56:LEU:HD23	1.84	0.60
1:C:160:LYS:H	1:C:160:LYS:CD	2.10	0.60
1:A:226:ILE:HG22	1:A:228:ARG:HD3	1.84	0.60
1:A:45:ASP:HB3	1:A:48:HIS:CD2	2.37	0.60
1:B:95:PHE:H	1:B:247:ASN:ND2	1.99	0.59
1:F:195:LYS:HA	1:F:198:GLU:CB	2.32	0.59
1:B:195:LYS:HA	1:B:198:GLU:CB	2.33	0.59
1:B:231:LEU:HD12	1:B:231:LEU:H	1.67	0.59
1:C:49:LEU:HD11	1:C:56:LEU:HD23	1.83	0.59
1:C:40:ARG:HH21	1:C:40:ARG:HG3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ILE:HG22	1:B:228:ARG:HD3	1.85	0.59
1:F:40:ARG:HH21	1:F:40:ARG:HG3	1.67	0.59
1:F:41:SER:CB	1:F:92:HIS:HB2	2.31	0.58
1:D:95:PHE:H	1:D:247:ASN:ND2	2.01	0.58
1:E:45:ASP:HB3	1:E:48:HIS:CD2	2.38	0.58
1:F:95:PHE:H	1:F:247:ASN:ND2	2.02	0.58
1:E:95:PHE:H	1:E:247:ASN:ND2	2.01	0.58
1:C:41:SER:CB	1:C:92:HIS:HB2	2.30	0.58
1:D:49:LEU:HD11	1:D:56:LEU:HD23	1.85	0.58
1:D:64:PRO:HB3	1:D:115:LEU:HB2	1.86	0.57
1:A:49:LEU:HD11	1:A:56:LEU:HD23	1.87	0.57
1:C:26:TYR:OH	1:C:48:HIS:HD2	1.87	0.57
1:D:45:ASP:HB3	1:D:48:HIS:CD2	2.40	0.57
1:E:49:LEU:HD11	1:E:56:LEU:HD23	1.85	0.57
1:A:64:PRO:HB3	1:A:115:LEU:HB2	1.86	0.57
1:E:64:PRO:HB3	1:E:115:LEU:HB2	1.87	0.56
1:F:160:LYS:H	1:F:160:LYS:CD	2.11	0.56
1:B:64:PRO:HB3	1:B:115:LEU:HB2	1.87	0.56
1:C:95:PHE:H	1:C:247:ASN:ND2	2.03	0.56
1:B:95:PHE:O	1:B:224:THR:HG21	2.05	0.56
1:E:95:PHE:O	1:E:224:THR:HG21	2.05	0.56
1:B:160:LYS:H	1:B:160:LYS:CD	2.13	0.56
1:A:26:TYR:OH	1:A:48:HIS:HD2	1.88	0.56
1:D:41:SER:CB	1:D:92:HIS:HB2	2.29	0.56
1:A:95:PHE:H	1:A:247:ASN:ND2	2.04	0.56
1:C:64:PRO:HB3	1:C:115:LEU:HB2	1.88	0.55
1:B:40:ARG:HH21	1:B:40:ARG:HG3	1.71	0.55
1:B:41:SER:CB	1:B:92:HIS:HB2	2.31	0.55
1:E:15:ARG:HH21	1:E:82:ASP:CG	2.15	0.55
1:F:214:VAL:HG11	1:F:249:ILE:HD13	1.88	0.55
1:D:26:TYR:OH	1:D:48:HIS:HD2	1.91	0.54
1:E:182:PHE:C	1:E:182:PHE:CD2	2.86	0.54
1:F:226:ILE:CG2	1:F:228:ARG:HD3	2.37	0.54
1:B:15:ARG:HH21	1:B:82:ASP:CG	2.16	0.54
1:F:36:ILE:HD12	1:F:37:THR:H	1.72	0.54
1:A:98:LEU:HB3	1:A:99:PRO:HD2	1.89	0.53
1:B:182:PHE:C	1:B:182:PHE:CD2	2.85	0.53
1:E:224:THR:HG22	1:E:248:HIS:HB3	1.90	0.53
1:B:224:THR:HG22	1:B:248:HIS:HB3	1.90	0.53
1:B:98:LEU:HB3	1:B:99:PRO:HD2	1.91	0.53
1:E:41:SER:CB	1:E:92:HIS:HB2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:LEU:HB3	1:D:99:PRO:HD2	1.89	0.53
1:E:36:ILE:HD12	1:E:37:THR:H	1.73	0.53
1:E:98:LEU:HB3	1:E:99:PRO:HD2	1.91	0.53
1:B:240:PHE:CE2	1:C:132:VAL:HG22	2.44	0.53
1:C:182:PHE:C	1:C:182:PHE:CD2	2.86	0.53
1:A:160:LYS:H	1:A:160:LYS:CD	2.13	0.52
1:C:15:ARG:HH21	1:C:82:ASP:CG	2.17	0.52
1:F:3:ARG:HG2	1:F:3:ARG:HH21	1.74	0.52
1:F:26:TYR:OH	1:F:48:HIS:HD2	1.92	0.52
1:A:182:PHE:CD2	1:A:182:PHE:C	2.86	0.52
1:D:214:VAL:HG11	1:D:249:ILE:HD13	1.90	0.52
1:F:152:PRO:HB2	1:F:206:ILE:HD12	1.92	0.52
1:A:224:THR:HG22	1:A:248:HIS:HB3	1.92	0.52
1:A:237:THR:HG22	1:A:238:PRO:HD2	1.92	0.52
1:A:15:ARG:HH21	1:A:82:ASP:CG	2.17	0.51
1:B:237:THR:HG22	1:B:238:PRO:HD2	1.90	0.51
1:C:237:THR:HG22	1:C:238:PRO:HD2	1.92	0.51
1:D:3:ARG:HH21	1:D:3:ARG:HG2	1.76	0.51
1:D:15:ARG:HH21	1:D:82:ASP:CG	2.18	0.51
1:D:36:ILE:HD12	1:D:37:THR:H	1.74	0.51
1:B:214:VAL:HG11	1:B:249:ILE:HD13	1.91	0.51
1:C:98:LEU:HB3	1:C:99:PRO:HD2	1.92	0.51
1:B:3:ARG:HG2	1:B:3:ARG:HH21	1.76	0.51
1:C:30:ILE:CD1	1:C:78:VAL:HG21	2.35	0.51
1:D:30:ILE:CD1	1:D:78:VAL:HG21	2.40	0.51
1:D:182:PHE:C	1:D:182:PHE:CD2	2.89	0.51
1:E:226:ILE:HG22	1:E:228:ARG:HD3	1.92	0.51
1:C:95:PHE:O	1:C:224:THR:HG21	2.11	0.51
1:D:2:ASP:O	1:D:6:MET:HB2	2.11	0.51
1:F:30:ILE:CD1	1:F:78:VAL:HG21	2.38	0.51
1:F:195:LYS:HA	1:F:198:GLU:HB2	1.93	0.51
1:A:3:ARG:HG2	1:A:3:ARG:HH21	1.76	0.50
1:A:36:ILE:HD12	1:A:37:THR:H	1.75	0.50
1:E:3:ARG:HG2	1:E:3:ARG:HH21	1.76	0.50
1:E:195:LYS:HA	1:E:198:GLU:HB2	1.93	0.50
1:F:104:VAL:HA	1:F:107:ILE:CD1	2.41	0.50
1:F:125:VAL:HG22	1:F:217:PRO:HD3	1.93	0.50
1:F:182:PHE:C	1:F:182:PHE:CD2	2.90	0.50
1:A:195:LYS:HA	1:A:198:GLU:HB2	1.93	0.50
1:D:195:LYS:HA	1:D:198:GLU:HB2	1.92	0.50
1:E:214:VAL:HG11	1:E:249:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:VAL:HG11	1:C:249:ILE:HD13	1.93	0.50
1:D:224:THR:HG22	1:D:248:HIS:HB3	1.93	0.50
1:A:1:VAL:HG23	1:A:59:GLU:HG3	1.93	0.50
1:C:3:ARG:HG2	1:C:3:ARG:HH21	1.76	0.50
1:C:104:VAL:HA	1:C:107:ILE:CD1	2.42	0.50
1:F:15:ARG:HH21	1:F:82:ASP:CG	2.19	0.50
1:F:202:PHE:C	1:F:202:PHE:CD2	2.90	0.50
1:A:104:VAL:HA	1:A:107:ILE:CD1	2.41	0.49
1:C:195:LYS:HA	1:C:198:GLU:HB2	1.93	0.49
1:D:152:PRO:HB2	1:D:206:ILE:HD12	1.94	0.49
1:D:237:THR:HG22	1:D:238:PRO:HD2	1.94	0.49
1:A:127:GLU:HG3	1:A:129:LYS:HE3	1.93	0.49
1:B:26:TYR:OH	1:B:48:HIS:HD2	1.94	0.49
1:C:224:THR:HG22	1:C:248:HIS:HB3	1.94	0.49
1:A:95:PHE:O	1:A:224:THR:HG21	2.11	0.49
1:B:36:ILE:HD12	1:B:37:THR:H	1.75	0.49
1:F:46:TRP:CE3	1:F:99:PRO:HD3	2.47	0.49
1:A:152:PRO:HB2	1:A:206:ILE:HD12	1.95	0.49
1:E:237:THR:HG22	1:E:238:PRO:HD2	1.95	0.49
1:D:95:PHE:O	1:D:224:THR:HG21	2.12	0.49
1:F:2:ASP:O	1:F:6:MET:HB2	2.12	0.49
1:E:127:GLU:HG3	1:E:129:LYS:HE3	1.95	0.49
1:C:36:ILE:HD12	1:C:37:THR:H	1.74	0.49
1:F:45:ASP:HB3	1:F:48:HIS:CD2	2.48	0.49
1:A:237:THR:HG22	1:A:239:ILE:HD13	1.94	0.49
1:C:2:ASP:O	1:C:6:MET:HB2	2.12	0.49
1:B:127:GLU:HG3	1:B:129:LYS:HE3	1.95	0.49
1:A:41:SER:CB	1:A:92:HIS:HB2	2.38	0.48
1:C:202:PHE:C	1:C:202:PHE:CD2	2.91	0.48
1:E:2:ASP:O	1:E:6:MET:HB2	2.13	0.48
1:B:195:LYS:HA	1:B:198:GLU:HB2	1.95	0.48
1:F:95:PHE:O	1:F:224:THR:HG21	2.13	0.48
1:F:127:GLU:HG3	1:F:129:LYS:HE3	1.95	0.48
1:B:2:ASP:O	1:B:6:MET:HB2	2.14	0.48
1:D:1:VAL:HG23	1:D:59:GLU:HG3	1.95	0.48
1:E:26:TYR:OH	1:E:48:HIS:HD2	1.95	0.48
1:B:36:ILE:HD13	1:B:37:THR:H	1.79	0.48
1:F:1:VAL:HG23	1:F:59:GLU:HG3	1.95	0.48
1:F:237:THR:HG22	1:F:239:ILE:HD13	1.96	0.48
1:C:127:GLU:HG3	1:C:129:LYS:HE3	1.95	0.48
1:C:1:VAL:HG23	1:C:59:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG11	1:A:249:ILE:HD13	1.96	0.47
1:A:104:VAL:HA	1:A:107:ILE:HD11	1.96	0.47
1:D:125:VAL:HG22	1:D:217:PRO:HD3	1.97	0.47
1:E:1:VAL:HG23	1:E:59:GLU:HG3	1.97	0.47
1:E:237:THR:HG22	1:E:239:ILE:HD13	1.96	0.47
1:F:237:THR:HG22	1:F:238:PRO:HD2	1.96	0.47
1:C:125:VAL:HG22	1:C:217:PRO:HD3	1.96	0.47
1:D:202:PHE:C	1:D:202:PHE:CD2	2.92	0.47
1:E:152:PRO:HB2	1:E:206:ILE:HD12	1.96	0.47
1:D:127:GLU:HG3	1:D:129:LYS:HE3	1.95	0.47
1:E:190:ARG:HD2	1:E:220:ARG:CZ	2.45	0.46
1:E:202:PHE:C	1:E:202:PHE:CD2	2.93	0.46
1:D:237:THR:HG22	1:D:239:ILE:HD13	1.97	0.46
1:F:224:THR:HG22	1:F:248:HIS:HB3	1.97	0.46
1:A:195:LYS:HA	1:A:198:GLU:HB3	1.98	0.46
1:F:104:VAL:HA	1:F:107:ILE:HD11	1.98	0.46
1:A:30:ILE:CD1	1:A:78:VAL:HG21	2.46	0.46
1:A:226:ILE:CG2	1:A:228:ARG:HD3	2.44	0.46
1:B:1:VAL:HG23	1:B:59:GLU:HG3	1.97	0.46
1:A:2:ASP:O	1:A:6:MET:HB2	2.15	0.46
1:D:160:LYS:HD3	1:D:160:LYS:N	2.18	0.46
1:E:30:ILE:CD1	1:E:78:VAL:HG21	2.42	0.46
1:E:112:ILE:HG12	1:E:229:VAL:HG13	1.97	0.46
1:B:202:PHE:C	1:B:202:PHE:CD2	2.94	0.45
1:C:36:ILE:HD13	1:C:37:THR:H	1.81	0.45
1:A:112:ILE:HG12	1:A:229:VAL:HG13	1.98	0.45
1:C:237:THR:HG22	1:C:239:ILE:HD13	1.98	0.45
1:F:98:LEU:HB3	1:F:99:PRO:HD2	1.99	0.45
1:A:202:PHE:C	1:A:202:PHE:CD2	2.94	0.45
1:D:224:THR:HG22	1:D:248:HIS:N	2.32	0.45
1:A:190:ARG:HD2	1:A:220:ARG:CZ	2.47	0.45
1:B:226:ILE:CG2	1:B:228:ARG:HD3	2.46	0.45
1:A:94:ARG:HG2	1:A:94:ARG:HH11	1.81	0.45
1:B:190:ARG:HD2	1:B:220:ARG:CZ	2.47	0.45
1:C:104:VAL:HA	1:C:107:ILE:HD11	1.98	0.45
1:A:125:VAL:HG22	1:A:217:PRO:HD3	2.00	0.44
1:D:190:ARG:HD2	1:D:220:ARG:CZ	2.46	0.44
1:E:104:VAL:HA	1:E:107:ILE:CD1	2.47	0.44
1:A:46:TRP:CE3	1:A:99:PRO:HD3	2.52	0.44
1:B:125:VAL:HG22	1:B:217:PRO:HD3	1.99	0.44
1:E:224:THR:HG22	1:E:248:HIS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LYS:O	1:D:235:GLU:HG2	2.18	0.44
1:B:30:ILE:CD1	1:B:78:VAL:HG21	2.43	0.43
1:C:194:LEU:HB3	1:C:195:LYS:H	1.47	0.43
1:D:104:VAL:HA	1:D:107:ILE:CD1	2.48	0.43
1:B:104:VAL:HA	1:B:107:ILE:CD1	2.48	0.43
1:F:224:THR:HG22	1:F:248:HIS:N	2.33	0.43
1:B:224:THR:HG22	1:B:248:HIS:N	2.33	0.43
1:B:237:THR:C	1:B:239:ILE:H	2.26	0.43
1:B:195:LYS:HA	1:B:198:GLU:HB3	2.01	0.43
1:C:46:TRP:CE3	1:C:99:PRO:HD3	2.54	0.43
1:C:224:THR:HG22	1:C:248:HIS:N	2.33	0.43
1:B:237:THR:HG22	1:B:239:ILE:HD13	1.99	0.43
1:E:125:VAL:HG22	1:E:217:PRO:HD3	1.99	0.43
1:A:224:THR:HG22	1:A:248:HIS:N	2.34	0.43
1:D:46:TRP:CE3	1:D:99:PRO:HD3	2.53	0.43
1:E:112:ILE:HG12	1:E:229:VAL:CG1	2.49	0.43
1:E:195:LYS:HA	1:E:198:GLU:HB3	1.99	0.43
1:A:207:LEU:O	1:A:208:LEU:HD23	2.19	0.42
1:F:195:LYS:HA	1:F:198:GLU:HB3	2.01	0.42
1:B:152:PRO:HB2	1:B:206:ILE:HD12	2.02	0.42
1:A:233:LYS:O	1:A:235:GLU:HG2	2.19	0.42
1:B:194:LEU:HB3	1:B:195:LYS:H	1.49	0.42
1:E:46:TRP:CE3	1:E:99:PRO:HD3	2.54	0.42
1:F:233:LYS:O	1:F:235:GLU:HG2	2.20	0.42
1:B:233:LYS:O	1:B:235:GLU:HG2	2.20	0.42
1:E:194:LEU:HB3	1:E:195:LYS:H	1.47	0.42
1:B:236:LYS:O	1:C:155:SER:HB2	2.20	0.42
1:C:112:ILE:HG12	1:C:229:VAL:HG13	2.02	0.42
1:F:190:ARG:HD2	1:F:220:ARG:CZ	2.50	0.42
1:C:190:ARG:HD2	1:C:220:ARG:CZ	2.49	0.41
1:A:68:ILE:HG23	1:A:93:ALA:HB3	2.02	0.41
1:B:112:ILE:HG12	1:B:229:VAL:HG13	2.02	0.41
1:B:224:THR:CG2	1:B:248:HIS:HB3	2.50	0.41
1:C:207:LEU:O	1:C:208:LEU:HD23	2.20	0.41
1:D:195:LYS:HA	1:D:198:GLU:HB3	1.98	0.41
1:E:104:VAL:HA	1:E:107:ILE:HD11	2.03	0.41
1:E:233:LYS:O	1:E:235:GLU:HG2	2.20	0.41
1:F:125:VAL:CG2	1:F:217:PRO:HD3	2.50	0.41
1:E:160:LYS:HD3	1:E:160:LYS:N	2.19	0.41
1:C:234:ARG:H	1:C:234:ARG:HD2	1.85	0.41
1:C:234:ARG:HG2	1:C:236:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:LYS:HD3	1:F:160:LYS:N	2.19	0.41
1:C:125:VAL:CG2	1:C:217:PRO:HD3	2.51	0.41
1:E:237:THR:HG22	1:E:239:ILE:CD1	2.51	0.41
1:C:195:LYS:HA	1:C:198:GLU:HB3	2.00	0.41
1:D:36:ILE:HD13	1:D:37:THR:H	1.85	0.41
1:E:237:THR:C	1:E:239:ILE:H	2.28	0.41
1:F:102:LEU:HD12	1:F:102:LEU:C	2.45	0.41
1:A:36:ILE:HD13	1:A:37:THR:H	1.83	0.41
1:C:152:PRO:HB2	1:C:206:ILE:HD12	2.02	0.41
1:B:46:TRP:CE3	1:B:99:PRO:HD3	2.56	0.40
1:E:224:THR:CG2	1:E:248:HIS:HB3	2.50	0.40
1:F:36:ILE:HD13	1:F:37:THR:H	1.83	0.40
1:B:104:VAL:HA	1:B:107:ILE:HD11	2.03	0.40
1:E:36:ILE:HD13	1:E:37:THR:H	1.85	0.40
1:E:226:ILE:CG2	1:E:228:ARG:HD3	2.51	0.40
1:B:207:LEU:O	1:B:208:LEU:HD23	2.22	0.40
1:D:224:THR:CG2	1:D:248:HIS:HB3	2.51	0.40
1:E:85:ARG:HA	1:E:85:ARG:HD3	1.97	0.40
1:B:111:HIS:O	1:B:112:ILE:C	2.64	0.40
1:B:234:ARG:HG2	1:B:236:LYS:H	1.85	0.40
1:C:68:ILE:HG23	1:C:93:ALA:HB3	2.04	0.40
1:D:237:THR:C	1:D:239:ILE:H	2.29	0.40

All (1) 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:A:192:GLU:O	1:F:161:LYS:NZ[2_545]	1.98	0.22

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%)	237 (94%)	15 (6%)	1 (0%)	30	42
1	B	253/257 (98%)	236 (93%)	15 (6%)	2 (1%)	16	24
1	C	253/257 (98%)	235 (93%)	17 (7%)	1 (0%)	30	42
1	D	253/257 (98%)	235 (93%)	16 (6%)	2 (1%)	16	24
1	E	253/257 (98%)	237 (94%)	15 (6%)	1 (0%)	30	42
1	F	253/257 (98%)	233 (92%)	18 (7%)	2 (1%)	16	24
All	All	1518/1542 (98%)	1413 (93%)	96 (6%)	9 (1%)	21	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	LYS
1	B	233	LYS
1	C	233	LYS
1	D	233	LYS
1	E	233	LYS
1	F	233	LYS
1	F	112	ILE
1	B	159	VAL
1	D	159	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	230/233 (99%)	212 (92%)	18 (8%)	11	18
1	B	230/233 (99%)	212 (92%)	18 (8%)	11	18
1	C	230/233 (99%)	211 (92%)	19 (8%)	10	16
1	D	230/233 (99%)	212 (92%)	18 (8%)	11	18
1	E	230/233 (99%)	211 (92%)	19 (8%)	10	16
1	F	230/233 (99%)	211 (92%)	19 (8%)	10	16
All	All	1380/1398 (99%)	1269 (92%)	111 (8%)	11	18

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	36	ILE
1	A	78	VAL
1	A	101	THR
1	A	110	GLU
1	A	119	GLU
1	A	132	VAL
1	A	160	LYS
1	A	182	PHE
1	A	206	ILE
1	A	212	VAL
1	A	216	LEU
1	A	223	VAL
1	A	224	THR
1	A	227	LEU
1	A	234	ARG
1	A	237	THR
1	A	249	ILE
1	B	23	ASN
1	B	36	ILE
1	B	78	VAL
1	B	101	THR
1	B	110	GLU
1	B	119	GLU
1	B	132	VAL
1	B	160	LYS
1	B	182	PHE
1	B	206	ILE
1	B	212	VAL
1	B	216	LEU
1	B	223	VAL
1	B	224	THR
1	B	227	LEU
1	B	234	ARG
1	B	237	THR
1	B	249	ILE
1	C	23	ASN
1	C	36	ILE
1	C	60	VAL
1	C	78	VAL
1	C	101	THR
1	C	110	GLU

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Mol	Chain	Res	Type
1	C	119	GLU
1	C	132	VAL
1	C	160	LYS
1	C	182	PHE
1	C	206	ILE
1	C	212	VAL
1	C	216	LEU
1	C	223	VAL
1	C	224	THR
1	C	227	LEU
1	C	234	ARG
1	C	237	THR
1	C	249	ILE
1	D	23	ASN
1	D	36	ILE
1	D	78	VAL
1	D	101	THR
1	D	110	GLU
1	D	119	GLU
1	D	132	VAL
1	D	160	LYS
1	D	182	PHE
1	D	206	ILE
1	D	212	VAL
1	D	216	LEU
1	D	223	VAL
1	D	224	THR
1	D	227	LEU
1	D	234	ARG
1	D	237	THR
1	D	249	ILE
1	E	23	ASN
1	E	36	ILE
1	E	60	VAL
1	E	78	VAL
1	E	101	THR
1	E	110	GLU
1	E	119	GLU
1	E	132	VAL
1	E	160	LYS
1	E	182	PHE
1	E	206	ILE

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Mol	Chain	Res	Type
1	E	212	VAL
1	E	216	LEU
1	E	223	VAL
1	E	224	THR
1	E	227	LEU
1	E	234	ARG
1	E	237	THR
1	E	249	ILE
1	F	23	ASN
1	F	36	ILE
1	F	60	VAL
1	F	78	VAL
1	F	101	THR
1	F	110	GLU
1	F	119	GLU
1	F	132	VAL
1	F	160	LYS
1	F	182	PHE
1	F	206	ILE
1	F	212	VAL
1	F	216	LEU
1	F	223	VAL
1	F	224	THR
1	F	227	LEU
1	F	234	ARG
1	F	237	THR
1	F	249	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	48	HIS
1	A	63	ASN
1	A	117	GLN
1	A	164	GLN
1	A	169	ASN
1	A	188	GLN
1	A	247	ASN
1	B	12	ASN
1	B	48	HIS
1	B	63	ASN

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Mol	Chain	Res	Type
1	B	117	GLN
1	B	164	GLN
1	B	169	ASN
1	B	188	GLN
1	B	247	ASN
1	C	48	HIS
1	C	63	ASN
1	C	117	GLN
1	C	164	GLN
1	C	169	ASN
1	C	188	GLN
1	C	247	ASN
1	D	12	ASN
1	D	48	HIS
1	D	63	ASN
1	D	117	GLN
1	D	164	GLN
1	D	169	ASN
1	D	188	GLN
1	D	247	ASN
1	E	12	ASN
1	E	48	HIS
1	E	63	ASN
1	E	117	GLN
1	E	164	GLN
1	E	169	ASN
1	E	188	GLN
1	E	247	ASN
1	F	12	ASN
1	F	48	HIS
1	F	63	ASN
1	F	117	GLN
1	F	164	GLN
1	F	169	ASN
1	F	188	GLN
1	F	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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%)	0.72	29 (11%) 10 8	35, 65, 144, 162	0
1	B	255/257 (99%)	0.71	32 (12%) 8 6	39, 68, 135, 169	0
1	C	255/257 (99%)	0.69	28 (10%) 10 8	37, 69, 153, 170	0
1	D	255/257 (99%)	0.62	20 (7%) 19 15	40, 69, 159, 184	0
1	E	255/257 (99%)	0.56	21 (8%) 17 14	44, 73, 158, 182	0
1	F	255/257 (99%)	0.70	31 (12%) 8 7	35, 65, 142, 161	0
All	All	1530/1542 (99%)	0.67	161 (10%) 11 9	35, 68, 150, 184	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	194	LEU	5.3
1	F	196	GLY	5.2
1	F	193	THR	5.1
1	D	197	GLY	4.7
1	F	195	LYS	4.6
1	B	161	LYS	4.2
1	F	231	LEU	4.1
1	B	159	VAL	4.0
1	F	190	ARG	4.0
1	D	254	LYS	3.9
1	B	231	LEU	3.9
1	A	231	LEU	3.9
1	B	166	GLY	3.8
1	A	254	LYS	3.8
1	E	87	ASP	3.8
1	A	194	LEU	3.8
1	F	159	VAL	3.7
1	C	141	ASP	3.7
1	B	160	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	197	GLY	3.7
1	D	159	VAL	3.7
1	A	197	GLY	3.6
1	E	233	LYS	3.6
1	F	192	GLU	3.6
1	C	231	LEU	3.6
1	B	199	MET	3.5
1	C	146	MET	3.5
1	A	237	THR	3.5
1	B	170	ILE	3.5
1	B	87	ASP	3.5
1	B	157	GLU	3.5
1	C	159	VAL	3.4
1	A	195	LYS	3.4
1	E	199	MET	3.4
1	D	140	LYS	3.4
1	F	254	LYS	3.4
1	E	231	LEU	3.3
1	D	236	LYS	3.3
1	F	36	ILE	3.3
1	D	231	LEU	3.3
1	D	233	LYS	3.3
1	A	196	GLY	3.3
1	D	36	ILE	3.3
1	F	236	LYS	3.2
1	A	36	ILE	3.2
1	B	164	GLN	3.2
1	C	144	HIS	3.2
1	A	233	LYS	3.1
1	C	170	ILE	3.1
1	B	158	LYS	3.1
1	A	199	MET	3.1
1	A	192	GLU	3.1
1	B	195	LYS	3.1
1	E	195	LYS	3.0
1	C	3	ARG	2.9
1	F	237	THR	2.9
1	B	236	LYS	2.9
1	A	159	VAL	2.9
1	E	191	PRO	2.9
1	A	236	LYS	2.8
1	E	237	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	150	GLN	2.8
1	C	160	LYS	2.8
1	A	143	GLY	2.8
1	B	197	GLY	2.8
1	A	87	ASP	2.8
1	F	3	ARG	2.8
1	F	143	GLY	2.8
1	B	163	GLU	2.8
1	C	192	GLU	2.8
1	A	191	PRO	2.7
1	C	36	ILE	2.7
1	C	197	GLY	2.7
1	F	197	GLY	2.7
1	C	138	VAL	2.7
1	B	191	PRO	2.7
1	B	233	LYS	2.7
1	A	190	ARG	2.7
1	B	82	ASP	2.7
1	F	87	ASP	2.7
1	D	158	LYS	2.7
1	F	199	MET	2.6
1	C	166	GLY	2.6
1	C	171	GLU	2.6
1	C	161	LYS	2.6
1	E	254	LYS	2.6
1	B	237	THR	2.6
1	A	166	GLY	2.6
1	B	196	GLY	2.6
1	F	146	MET	2.6
1	F	233	LYS	2.6
1	B	165	CYS	2.6
1	F	100	GLU	2.6
1	E	82	ASP	2.6
1	F	220	ARG	2.6
1	B	254	LYS	2.6
1	E	159	VAL	2.6
1	C	87	ASP	2.5
1	B	36	ILE	2.5
1	E	236	LYS	2.5
1	A	146	MET	2.5
1	D	196	GLY	2.5
1	C	199	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	234	ARG	2.5
1	D	3	ARG	2.5
1	C	66	GLU	2.5
1	B	213	ASP	2.4
1	E	232	GLU	2.4
1	D	146	MET	2.4
1	C	168	LYS	2.4
1	A	100	GLU	2.4
1	D	199	MET	2.4
1	C	236	LYS	2.4
1	C	127	GLU	2.4
1	D	235	GLU	2.4
1	C	237	THR	2.3
1	F	119	GLU	2.3
1	F	198	GLU	2.3
1	C	167	SER	2.3
1	A	232	GLU	2.3
1	F	189	ASP	2.3
1	D	137	PHE	2.3
1	F	160	LYS	2.3
1	D	157	GLU	2.3
1	F	235	GLU	2.3
1	A	167	SER	2.3
1	B	194	LEU	2.3
1	A	170	ILE	2.2
1	C	195	LYS	2.2
1	B	232	GLU	2.2
1	C	163	GLU	2.2
1	A	133	SER	2.2
1	E	230	VAL	2.2
1	B	162	CYS	2.2
1	A	235	GLU	2.2
1	B	234	ARG	2.2
1	B	167	SER	2.2
1	E	138	VAL	2.2
1	E	158	LYS	2.2
1	F	161	LYS	2.2
1	D	87	ASP	2.2
1	F	123	THR	2.1
1	E	213	ASP	2.1
1	F	171	GLU	2.1
1	E	190	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	137	PHE	2.1
1	D	253	SER	2.1
1	F	191	PRO	2.1
1	C	169	ASN	2.1
1	B	253	SER	2.1
1	D	163	GLU	2.1
1	E	127	GLU	2.1
1	A	238	PRO	2.1
1	B	200	PRO	2.1
1	E	36	ILE	2.1
1	B	144	HIS	2.0
1	A	3	ARG	2.0
1	E	234	ARG	2.0
1	F	168	LYS	2.0
1	A	200	PRO	2.0
1	C	196	GLY	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($\text{\AA}^2$)	Q<0.9
2	ZN	C	301	1/1	0.91	0.11	141,141,141,141	0
2	ZN	B	301	1/1	0.92	0.09	116,116,116,116	0
2	ZN	E	301	1/1	0.96	0.05	163,163,163,163	0
2	ZN	F	301	1/1	0.96	0.06	141,141,141,141	0
2	ZN	A	301	1/1	0.97	0.06	141,141,141,141	0
2	ZN	D	301	1/1	0.97	0.06	165,165,165,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.