W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 02:16 PM JST

PDB ID	:	7CUX
Title	:	Crystal structure of human Schlafen 5 N'-terminal domain (SLFN5-N) involved in ssRNA cleaving and DNA binding
Authors	:	Yang, J.Y.; Luo, M.; Ou, J.Y.; Wang, Z.W.; Gao, S.
Deposited on	:	2020-08-25
Resolution	:	3.29 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.29 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		12
Ramachandran outliers		1.8%
Sidechain outliers		0.6%
RSRZ outliers		14.9%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
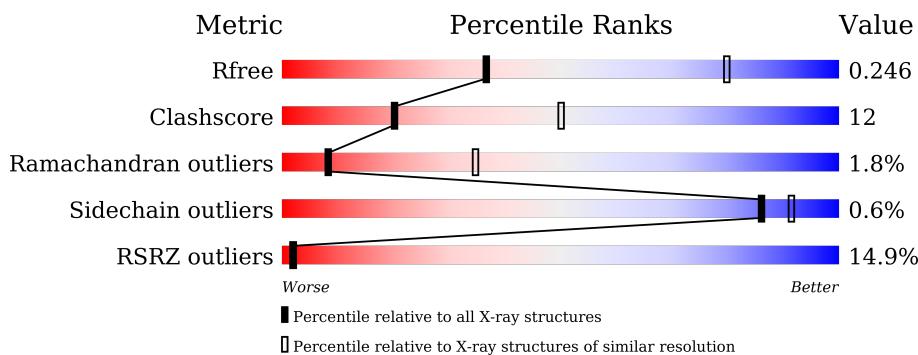
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	326	15% · 60% · 29% · 10%
1	B	326	10% · 63% · 27% · 10%
1	C	326	16% · 64% · 25% · 11%
1	D	326	13% · 67% · 23% · 10%
1	E	326	13% · 62% · 27% · 10%
1	F	326	14% · 63% · 27% · 9%
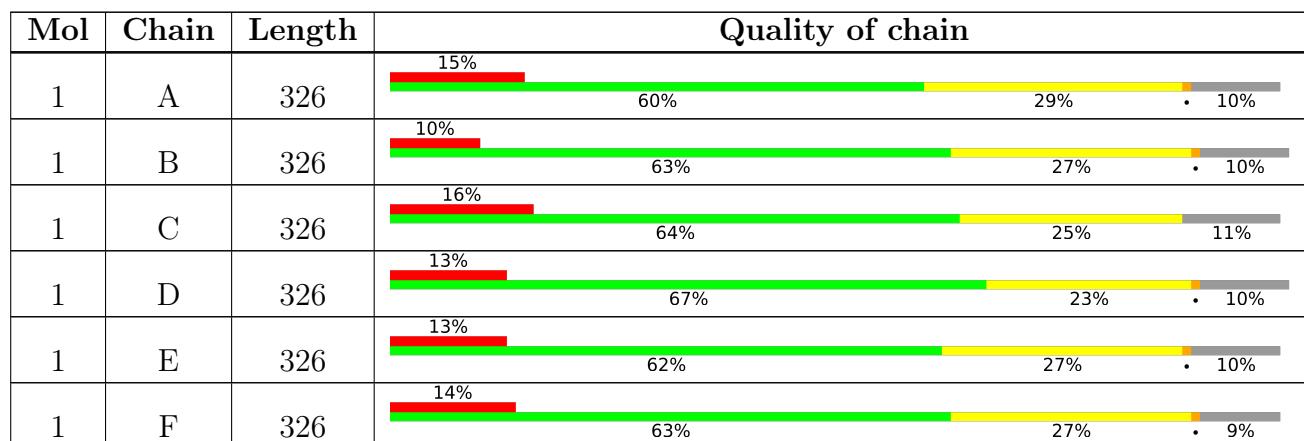
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14075 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 Schlafen family member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2330	1472	414	425	19			
1	B	295	Total	C	N	O	S	0	0	0
			2345	1479	419	428	19			
1	C	291	Total	C	N	O	S	0	0	0
			2327	1471	413	424	19			
1	D	295	Total	C	N	O	S	0	0	0
			2355	1489	419	428	19			
1	E	295	Total	C	N	O	S	0	0	0
			2351	1485	419	428	19			
1	F	296	Total	C	N	O	S	0	0	0
			2361	1491	420	431	19			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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: Schlafen family member 5

• Molecule 1: Schlafen family member 5

• Molecule 1: Schlafen family member 5

Chain C:

● Molecule 1: Schlafen family member 5

Chain D:

● Molecule 1: Schlafen family member 5

Chain E:

• Molecule 1: Schlafen family member 5

Chain F:
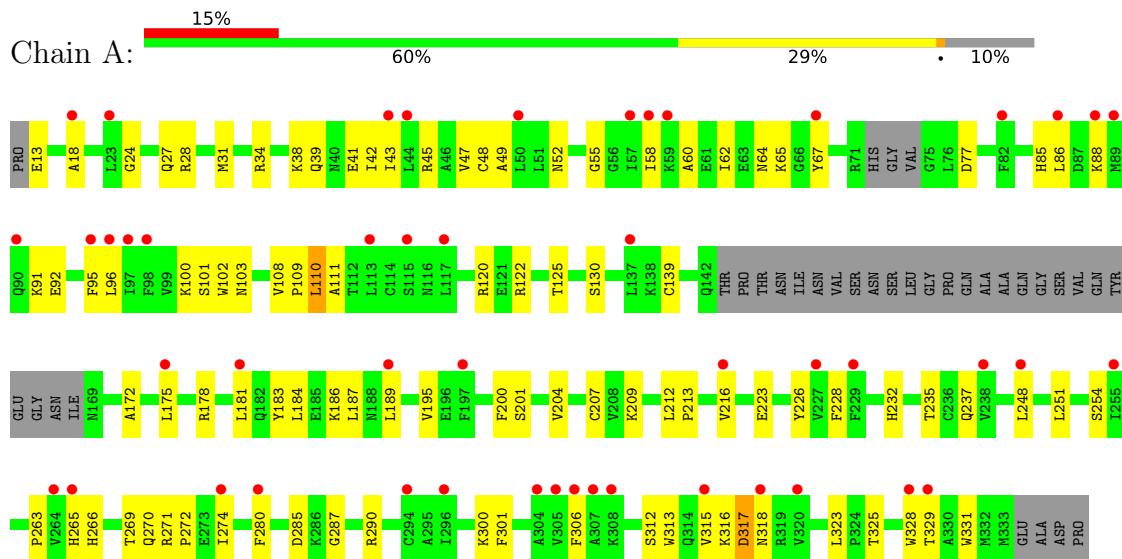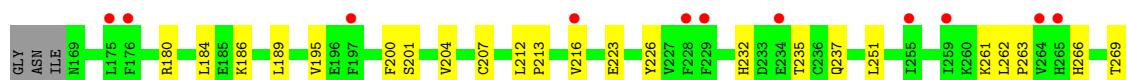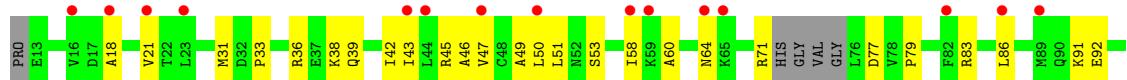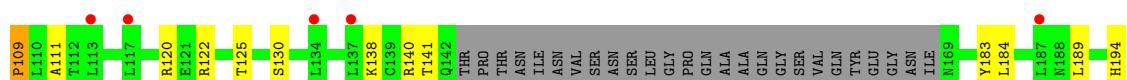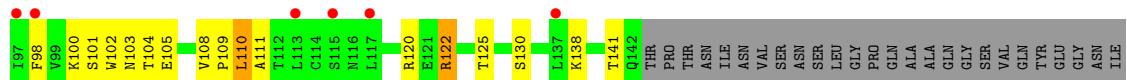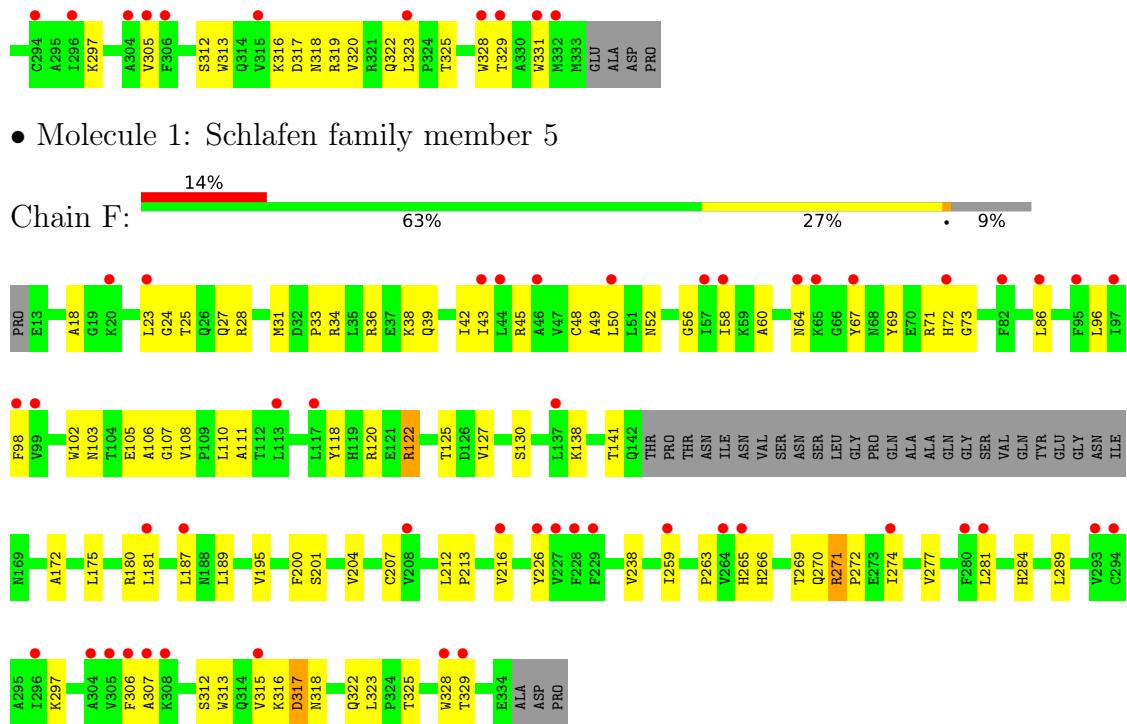
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	211.86Å 156.44Å 131.46Å 90.00° 110.38° 90.00°	Depositor
Resolution (Å)	41.08 – 3.29 123.23 – 3.29	Depositor EDS
% Data completeness (in resolution range)	71.9 (41.08-3.29) 72.2 (123.23-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575, REFMAC 7.0.077	Depositor
R, R_{free}	0.201 , 0.247 0.204 , 0.246	Depositor DCC
R_{free} test set	2175 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	128.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 145.8	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.031 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.044 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14075	wwPDB-VP
Average B, all atoms (Å^2)	164.0	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 46.73 % 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 1.0974e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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	0.26	0/2375	0.50	0/3201
1	B	0.26	0/2392	0.51	0/3224
1	C	0.26	0/2372	0.49	0/3196
1	D	0.26	0/2402	0.50	0/3240
1	E	0.26	0/2398	0.51	0/3232
1	F	0.26	0/2408	0.50	0/3246
All	All	0.26	0/14347	0.50	0/19339

There are no bond length outliers.

There are no bond angle outliers.

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	2330	0	2322	66	0
1	B	2345	0	2320	56	0
1	C	2327	0	2321	62	0
1	D	2355	0	2355	51	0
1	E	2351	0	2340	64	0
1	F	2361	0	2350	62	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	14075	0	14008	351	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 12.

All (351) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ILE:HD12	1:F:274:ILE:O	1.63	0.99
1:F:284:HIS:HA	1:F:289:LEU:HA	1.65	0.78
1:A:184:LEU:HD23	1:E:235:THR:HG21	1.68	0.75
1:E:28:ARG:HD3	1:E:76:LEU:HD11	1.67	0.74
1:C:184:LEU:HD23	1:D:235:THR:HG21	1.68	0.74
1:B:106:ALA:O	1:B:108:VAL:N	2.23	0.72
1:C:106:ALA:O	1:C:108:VAL:N	2.22	0.71
1:A:175:LEU:HD11	1:A:187:LEU:HD13	1.72	0.70
1:E:47:VAL:HG21	1:E:86:LEU:HD11	1.74	0.69
1:D:102:TRP:CD2	1:D:111:ALA:HB2	2.27	0.69
1:A:108:VAL:HG11	1:A:130:SER:HB3	1.75	0.69
1:F:270:GLN:O	1:F:272:PRO:HD3	1.93	0.69
1:A:316:LYS:O	1:A:318:ASN:N	2.25	0.69
1:A:189:LEU:HD21	1:A:195:VAL:HG11	1.76	0.67
1:F:28:ARG:HG2	1:F:31:MET:HE2	1.76	0.67
1:A:28:ARG:HG2	1:A:31:MET:HE2	1.75	0.67
1:D:120:ARG:HH11	1:D:125:THR:HG23	1.60	0.67
1:C:120:ARG:HH11	1:C:125:THR:HG23	1.60	0.67
1:E:189:LEU:HD21	1:E:195:VAL:HG11	1.77	0.67
1:C:316:LYS:O	1:C:318:ASN:N	2.28	0.67
1:F:106:ALA:O	1:F:108:VAL:N	2.29	0.66
1:F:316:LYS:O	1:F:318:ASN:N	2.29	0.66
1:C:47:VAL:O	1:C:51:LEU:HB2	1.95	0.66
1:B:270:GLN:O	1:B:272:PRO:HD3	1.97	0.65
1:B:312:SER:HB3	1:B:323:LEU:HD11	1.79	0.65
1:F:266:HIS:CE1	1:F:272:PRO:HD2	2.32	0.65
1:D:28:ARG:HD3	1:D:76:LEU:HD11	1.79	0.65
1:F:312:SER:HB3	1:F:323:LEU:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:GLY:HA3	1:D:83:ARG:HH21	1.62	0.64
1:A:120:ARG:HH11	1:A:125:THR:HG23	1.61	0.64
1:A:312:SER:HB3	1:A:323:LEU:HD11	1.79	0.64
1:F:25:THR:HG23	1:F:73:GLY:HA3	1.80	0.63
1:C:189:LEU:HD21	1:C:195:VAL:HG11	1.80	0.63
1:B:266:HIS:CE1	1:B:272:PRO:HD2	2.34	0.63
1:E:62:ILE:HD11	1:E:95:PHE:HB2	1.81	0.63
1:E:178:ARG:HE	1:F:180:ARG:HH22	1.46	0.62
1:E:312:SER:HB3	1:E:323:LEU:HD11	1.81	0.62
1:F:189:LEU:HD21	1:F:195:VAL:HG11	1.82	0.62
1:C:122:ARG:NH1	1:E:122:ARG:HH12	1.97	0.62
1:E:120:ARG:HB2	1:E:125:THR:HG22	1.83	0.61
1:A:325:THR:O	1:A:329:THR:HG22	2.00	0.61
1:F:181:LEU:HD23	1:F:238:VAL:HG21	1.83	0.61
1:F:269:THR:OG1	1:F:270:GLN:OE1	2.19	0.61
1:D:259:ILE:HA	1:D:262:LEU:HD23	1.83	0.61
1:E:120:ARG:HH11	1:E:125:THR:HG23	1.65	0.61
1:B:140:ARG:NH1	1:B:303:CYS:O	2.34	0.60
1:C:270:GLN:OE1	1:C:270:GLN:N	2.32	0.60
1:D:189:LEU:HD21	1:D:195:VAL:HG11	1.83	0.60
1:E:262:LEU:HD11	1:E:274:ILE:HD13	1.82	0.60
1:B:270:GLN:OE1	1:B:270:GLN:N	2.33	0.59
1:E:138:LYS:O	1:E:141:THR:HG22	2.03	0.59
1:B:58:ILE:O	1:B:96:LEU:HA	2.03	0.59
1:D:69:TYR:O	1:D:70:GLU:HG2	2.03	0.59
1:D:102:TRP:HZ2	1:D:108:VAL:HG13	1.67	0.58
1:D:312:SER:HB3	1:D:323:LEU:HD11	1.84	0.58
1:A:58:ILE:O	1:A:96:LEU:HA	2.03	0.58
1:A:269:THR:HG1	1:A:270:GLN:H	1.49	0.58
1:A:13:GLU:N	1:A:55:GLY:O	2.35	0.58
1:C:140:ARG:NH1	1:C:303:CYS:O	2.35	0.58
1:A:178:ARG:NH1	1:A:181:LEU:HD23	2.19	0.58
1:F:58:ILE:O	1:F:96:LEU:HA	2.04	0.58
1:B:325:THR:O	1:B:329:THR:HG22	2.04	0.58
1:E:103:ASN:O	1:E:104:THR:HG22	2.04	0.58
1:F:323:LEU:HD13	1:F:328:TRP:HB2	1.86	0.58
1:F:24:GLY:HA2	1:F:72:HIS:HA	1.85	0.58
1:B:189:LEU:HD21	1:B:195:VAL:HG11	1.86	0.57
1:F:86:LEU:HA	1:F:98:PHE:O	2.05	0.57
1:F:325:THR:O	1:F:329:THR:HG22	2.04	0.57
1:B:62:ILE:HD11	1:B:95:PHE:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ARG:HB2	1:D:125:THR:HG22	1.86	0.57
1:D:138:LYS:O	1:D:141:THR:HG22	2.05	0.57
1:D:325:THR:O	1:D:329:THR:HG22	2.05	0.57
1:C:33:PRO:O	1:C:36:ARG:HG2	2.05	0.56
1:F:108:VAL:HG21	1:F:130:SER:HB3	1.86	0.56
1:E:319:ARG:HH12	1:E:320:VAL:HG12	1.69	0.56
1:C:58:ILE:O	1:C:96:LEU:HA	2.04	0.56
1:F:27:GLN:HE21	1:F:67:TYR:HB3	1.70	0.56
1:D:140:ARG:NH1	1:D:303:CYS:O	2.39	0.56
1:C:18:ALA:HB3	1:C:60:ALA:HB2	1.87	0.56
1:C:138:LYS:O	1:C:141:THR:HG22	2.05	0.56
1:D:18:ALA:HB3	1:D:60:ALA:HB2	1.88	0.56
1:E:58:ILE:O	1:E:96:LEU:HA	2.05	0.56
1:F:284:HIS:ND1	1:F:289:LEU:HB3	2.21	0.55
1:A:39:GLN:O	1:A:43:ILE:HG12	2.06	0.55
1:E:75:GLY:O	1:E:76:LEU:HB2	2.06	0.55
1:A:48:CYS:O	1:A:52:ASN:ND2	2.39	0.55
1:C:102:TRP:CE3	1:C:111:ALA:HB2	2.42	0.55
1:A:27:GLN:HE21	1:A:67:TYR:HB3	1.71	0.55
1:E:325:THR:O	1:E:329:THR:HG22	2.06	0.54
1:C:39:GLN:O	1:C:43:ILE:HG12	2.06	0.54
1:D:58:ILE:O	1:D:96:LEU:HA	2.07	0.54
1:E:270:GLN:OE1	1:E:270:GLN:N	2.35	0.54
1:A:323:LEU:HD13	1:A:328:TRP:HB2	1.90	0.54
1:C:120:ARG:HB2	1:C:125:THR:HG22	1.90	0.54
1:A:110:LEU:HD12	1:A:331:TRP:CD2	2.42	0.53
1:B:102:TRP:CE3	1:B:111:ALA:HB2	2.43	0.53
1:F:18:ALA:HB3	1:F:60:ALA:HB2	1.90	0.53
1:C:316:LYS:C	1:C:318:ASN:H	2.12	0.53
1:A:85:HIS:CE1	1:A:103:ASN:HD22	2.27	0.53
1:D:39:GLN:O	1:D:43:ILE:HG13	2.08	0.53
1:E:28:ARG:HG2	1:E:31:MET:HE1	1.91	0.53
1:F:274:ILE:HD12	1:F:274:ILE:C	2.29	0.53
1:A:34:ARG:O	1:A:38:LYS:HG3	2.09	0.52
1:B:220:ALA:HB1	1:B:301:PHE:HB2	1.91	0.52
1:C:86:LEU:HA	1:C:98:PHE:O	2.09	0.52
1:D:108:VAL:HG21	1:D:130:SER:HB3	1.91	0.52
1:C:318:ASN:OD1	1:C:319:ARG:N	2.42	0.52
1:B:39:GLN:O	1:B:43:ILE:HG12	2.08	0.52
1:B:284:HIS:ND1	1:B:289:LEU:HA	2.25	0.52
1:A:88:LYS:HD2	1:A:95:PHE:HZ	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:THR:OG1	1:B:270:GLN:OE1	2.25	0.52
1:E:102:TRP:CE3	1:E:111:ALA:HB2	2.44	0.52
1:B:106:ALA:C	1:B:108:VAL:H	2.12	0.52
1:D:49:ALA:HB1	1:D:315:VAL:HG13	1.91	0.52
1:E:39:GLN:O	1:E:43:ILE:HG12	2.09	0.52
1:E:323:LEU:HD13	1:E:328:TRP:HB2	1.90	0.52
1:F:48:CYS:O	1:F:52:ASN:ND2	2.43	0.52
1:B:140:ARG:NH1	1:B:301:PHE:O	2.41	0.51
1:A:24:GLY:O	1:A:28:ARG:N	2.38	0.51
1:A:316:LYS:C	1:A:318:ASN:H	2.13	0.51
1:B:263:PRO:HB2	1:B:306:PHE:HB2	1.93	0.51
1:E:284:HIS:ND1	1:E:289:LEU:HA	2.25	0.51
1:B:78:VAL:HG11	1:B:83:ARG:HD3	1.93	0.51
1:E:18:ALA:HB3	1:E:60:ALA:HB2	1.93	0.51
1:B:86:LEU:HA	1:B:98:PHE:O	2.11	0.50
1:B:316:LYS:O	1:B:318:ASN:N	2.44	0.50
1:D:50:LEU:HD22	1:D:56:GLY:HA3	1.93	0.50
1:C:269:THR:OG1	1:C:270:GLN:OE1	2.28	0.50
1:E:269:THR:OG1	1:E:270:GLN:OE1	2.28	0.50
1:B:220:ALA:HB3	1:B:305:VAL:HG11	1.94	0.50
1:C:49:ALA:HB2	1:C:320:VAL:HG23	1.93	0.50
1:C:106:ALA:C	1:C:108:VAL:H	2.12	0.50
1:A:316:LYS:NZ	1:A:317:ASP:OD2	2.40	0.50
1:B:50:LEU:HD22	1:B:56:GLY:HA3	1.93	0.50
1:B:48:CYS:O	1:B:52:ASN:ND2	2.44	0.50
1:E:72:HIS:HE1	1:E:76:LEU:HD13	1.77	0.50
1:D:86:LEU:HA	1:D:98:PHE:O	2.11	0.50
1:C:21:VAL:HG23	1:C:39:GLN:HB3	1.94	0.49
1:A:263:PRO:HB2	1:A:306:PHE:HB2	1.94	0.49
1:D:68:ASN:H	1:D:71:ARG:NH1	2.11	0.49
1:D:194:HIS:O	1:D:226:TYR:N	2.33	0.49
1:A:38:LYS:O	1:A:42:ILE:HG12	2.13	0.49
1:B:212:LEU:O	1:B:216:VAL:HG12	2.12	0.49
1:C:140:ARG:NH1	1:C:301:PHE:O	2.45	0.49
1:F:39:GLN:O	1:F:43:ILE:HG12	2.11	0.49
1:F:103:ASN:OD1	1:F:105:GLU:HG2	2.12	0.49
1:B:209:LYS:HE3	1:B:254:SER:HB3	1.93	0.49
1:F:274:ILE:O	1:F:274:ILE:CD1	2.50	0.49
1:C:122:ARG:NH2	1:E:122:ARG:HH22	2.11	0.49
1:F:181:LEU:HD13	1:F:281:LEU:HB3	1.94	0.49
1:D:34:ARG:O	1:D:38:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LEU:HD13	1:B:328:TRP:HB2	1.96	0.48
1:D:262:LEU:HD12	1:D:306:PHE:O	2.13	0.48
1:E:103:ASN:HD21	1:E:105:GLU:HB2	1.78	0.48
1:C:212:LEU:O	1:C:216:VAL:HG12	2.14	0.48
1:B:183:TYR:HB3	1:B:285:ASP:HB2	1.95	0.48
1:D:45:ARG:HG2	1:D:313:TRP:CE2	2.49	0.48
1:D:284:HIS:ND1	1:D:289:LEU:HA	2.28	0.48
1:B:31:MET:HE3	1:B:36:ARG:HA	1.96	0.48
1:C:223:GLU:HA	1:C:300:LYS:HD2	1.96	0.48
1:D:40:ASN:ND2	1:D:77:ASP:HB2	2.29	0.48
1:D:28:ARG:HG2	1:D:31:MET:HE1	1.96	0.47
1:A:266:HIS:CD2	1:A:271:ARG:HB3	2.49	0.47
1:E:24:GLY:HA2	1:E:72:HIS:HA	1.96	0.47
1:E:259:ILE:O	1:E:262:LEU:HG	2.14	0.47
1:F:138:LYS:O	1:F:141:THR:HG22	2.13	0.47
1:B:183:TYR:CB	1:B:285:ASP:HB2	2.45	0.47
1:C:49:ALA:HB1	1:C:315:VAL:HG13	1.96	0.47
1:E:200:PHE:CE1	1:E:204:VAL:HG23	2.49	0.47
1:E:232:HIS:HB3	1:E:235:THR:HG22	1.96	0.47
1:F:277:VAL:HG13	1:F:297:LYS:HB3	1.97	0.47
1:C:31:MET:O	1:C:36:ARG:NH2	2.35	0.47
1:F:120:ARG:HA	1:F:125:THR:HA	1.95	0.47
1:B:122:ARG:HD3	1:C:122:ARG:HH12	1.80	0.47
1:F:64:ASN:OD1	1:F:64:ASN:N	2.48	0.47
1:C:38:LYS:O	1:C:42:ILE:HG12	2.14	0.47
1:C:232:HIS:HB3	1:C:235:THR:HG22	1.97	0.47
1:D:269:THR:HG1	1:D:270:GLN:H	1.61	0.46
1:A:212:LEU:O	1:A:216:VAL:HG12	2.14	0.46
1:B:232:HIS:HB3	1:B:235:THR:HG22	1.97	0.46
1:E:235:THR:HG23	1:E:237:GLN:H	1.80	0.46
1:E:262:LEU:HD13	1:E:305:VAL:HG13	1.97	0.46
1:E:33:PRO:HB3	1:E:36:ARG:HH21	1.79	0.46
1:E:108:VAL:HG21	1:E:130:SER:HB3	1.97	0.46
1:D:44:LEU:HD21	1:D:77:ASP:O	2.16	0.46
1:D:65:LYS:HE2	1:D:93:ASN:HB3	1.96	0.46
1:E:28:ARG:CD	1:E:76:LEU:HD11	2.42	0.46
1:E:187:LEU:HD11	1:E:238:VAL:HG23	1.97	0.46
1:B:252:ARG:CZ	1:B:278:LEU:HD23	2.46	0.46
1:B:265:HIS:CG	1:B:329:THR:HG21	2.51	0.46
1:F:34:ARG:O	1:F:38:LYS:HG3	2.16	0.46
1:F:266:HIS:CD2	1:F:271:ARG:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:HIS:CG	1:D:329:THR:HG21	2.51	0.46
1:E:31:MET:HE3	1:E:36:ARG:HA	1.98	0.46
1:B:64:ASN:OD1	1:B:64:ASN:N	2.49	0.45
1:D:195:VAL:HA	1:D:226:TYR:O	2.16	0.45
1:A:232:HIS:HB3	1:A:235:THR:HG22	1.99	0.45
1:B:85:HIS:CE1	1:B:103:ASN:HD22	2.34	0.45
1:D:40:ASN:HD21	1:D:77:ASP:HB2	1.81	0.45
1:D:321:ARG:HA	1:D:321:ARG:HD2	1.62	0.45
1:A:120:ARG:HB2	1:A:125:THR:HG22	1.99	0.45
1:A:122:ARG:NH1	1:F:122:ARG:HE	2.14	0.45
1:C:64:ASN:OD1	1:C:64:ASN:N	2.49	0.45
1:C:226:TYR:CE2	1:C:297:LYS:HD2	2.51	0.45
1:C:45:ARG:HG2	1:C:313:TRP:CE2	2.52	0.45
1:C:261:LYS:HB3	1:C:261:LYS:HE2	1.79	0.45
1:D:245:LYS:HE3	1:D:245:LYS:HB3	1.77	0.45
1:E:45:ARG:HG2	1:E:313:TRP:CE2	2.52	0.45
1:C:235:THR:HG23	1:C:237:GLN:HG3	1.98	0.45
1:F:38:LYS:O	1:F:42:ILE:HG12	2.17	0.45
1:C:79:PRO:O	1:C:83:ARG:HG3	2.17	0.45
1:C:213:PRO:HB3	1:C:262:LEU:HD21	1.98	0.45
1:F:106:ALA:O	1:F:108:VAL:HG12	2.17	0.44
1:F:263:PRO:HB2	1:F:306:PHE:HB2	1.99	0.44
1:B:109:PRO:O	1:B:110:LEU:HD23	2.18	0.44
1:B:269:THR:HG1	1:B:270:GLN:H	1.64	0.44
1:C:108:VAL:HG21	1:C:130:SER:HB3	1.98	0.44
1:D:140:ARG:NH1	1:D:301:PHE:O	2.48	0.44
1:F:200:PHE:CE1	1:F:204:VAL:HG13	2.53	0.44
1:B:18:ALA:HB3	1:B:60:ALA:HB2	2.00	0.44
1:E:212:LEU:O	1:E:216:VAL:HG12	2.17	0.44
1:E:265:HIS:CG	1:E:329:THR:HG21	2.52	0.44
1:E:27:GLN:HE21	1:E:67:TYR:HB3	1.82	0.44
1:A:64:ASN:OD1	1:A:64:ASN:N	2.49	0.44
1:B:138:LYS:O	1:B:141:THR:HG22	2.18	0.44
1:E:201:SER:OG	1:E:207:CYS:HB2	2.18	0.44
1:D:201:SER:OG	1:D:207:CYS:HB2	2.17	0.44
1:F:212:LEU:O	1:F:216:VAL:HG12	2.17	0.44
1:B:108:VAL:HG21	1:B:130:SER:HB3	2.00	0.44
1:B:235:THR:HG23	1:B:237:GLN:H	1.82	0.44
1:D:266:HIS:CE1	1:D:272:PRO:HD2	2.53	0.44
1:E:64:ASN:OD1	1:E:64:ASN:N	2.46	0.44
1:F:270:GLN:O	1:F:270:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HG22	1:A:301:PHE:CD1	2.52	0.43
1:C:50:LEU:HD12	1:C:315:VAL:HG11	2.00	0.43
1:E:100:LYS:HG2	1:E:101:SER:N	2.33	0.43
1:A:49:ALA:HB1	1:A:315:VAL:HG13	2.00	0.43
1:B:120:ARG:HA	1:B:125:THR:HA	2.01	0.43
1:E:269:THR:HG1	1:E:270:GLN:H	1.66	0.43
1:A:18:ALA:HB3	1:A:60:ALA:HB2	2.00	0.43
1:F:175:LEU:HD21	1:F:187:LEU:HD13	2.00	0.43
1:A:62:ILE:HG13	1:A:65:LYS:HG2	1.99	0.43
1:E:226:TYR:CE2	1:E:297:LYS:HD2	2.53	0.43
1:F:212:LEU:N	1:F:213:PRO:HD2	2.33	0.43
1:A:201:SER:OG	1:A:207:CYS:HB2	2.18	0.43
1:C:212:LEU:N	1:C:213:PRO:HD2	2.34	0.43
1:E:110:LEU:HD23	1:E:331:TRP:CG	2.53	0.43
1:E:316:LYS:O	1:E:318:ASN:N	2.52	0.43
1:C:195:VAL:HA	1:C:226:TYR:O	2.19	0.43
1:D:235:THR:HG23	1:D:237:GLN:H	1.83	0.43
1:F:106:ALA:C	1:F:108:VAL:H	2.19	0.43
1:A:212:LEU:N	1:A:213:PRO:HD2	2.34	0.43
1:C:100:LYS:HG2	1:C:101:SER:N	2.34	0.43
1:A:172:ALA:HA	1:A:189:LEU:HD22	2.01	0.43
1:A:195:VAL:HA	1:A:226:TYR:O	2.18	0.43
1:A:209:LYS:HE3	1:A:254:SER:HB3	2.01	0.43
1:B:265:HIS:CD2	1:B:329:THR:HG21	2.54	0.43
1:A:91:LYS:HG3	1:A:92:GLU:CD	2.40	0.42
1:C:33:PRO:HA	1:C:36:ARG:NE	2.34	0.42
1:D:232:HIS:HB3	1:D:235:THR:HG22	2.00	0.42
1:D:259:ILE:HA	1:D:262:LEU:CD2	2.48	0.42
1:F:313:TRP:HA	1:F:322:GLN:HA	2.01	0.42
1:B:313:TRP:HA	1:B:322:GLN:HA	2.01	0.42
1:E:109:PRO:O	1:E:110:LEU:HG	2.19	0.42
1:E:319:ARG:HD2	1:E:319:ARG:HA	1.87	0.42
1:A:200:PHE:CE1	1:A:204:VAL:HG13	2.54	0.42
1:F:33:PRO:O	1:F:36:ARG:HB3	2.19	0.42
1:F:274:ILE:C	1:F:274:ILE:CD1	2.88	0.42
1:A:183:TYR:CB	1:A:285:ASP:HB2	2.50	0.42
1:B:28:ARG:HG2	1:B:31:MET:HE1	2.00	0.42
1:D:212:LEU:N	1:D:213:PRO:HD2	2.34	0.42
1:F:23:LEU:HB3	1:F:72:HIS:CG	2.55	0.42
1:B:212:LEU:N	1:B:213:PRO:HD2	2.35	0.42
1:D:91:LYS:HG3	1:D:92:GLU:CD	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:TYR:CE2	1:B:297:LYS:HD2	2.55	0.42
1:C:53:SER:OG	1:C:315:VAL:HG22	2.18	0.42
1:C:91:LYS:HD2	1:C:91:LYS:HA	1.85	0.42
1:C:313:TRP:HA	1:C:322:GLN:HA	2.01	0.42
1:E:212:LEU:N	1:E:213:PRO:HD2	2.34	0.42
1:B:110:LEU:HD22	1:B:331:TRP:CD1	2.55	0.42
1:C:201:SER:OG	1:C:207:CYS:HB2	2.20	0.42
1:C:263:PRO:HB2	1:C:306:PHE:HB2	2.01	0.42
1:E:57:ILE:HD12	1:E:98:PHE:CD2	2.54	0.42
1:F:226:TYR:CE2	1:F:297:LYS:HD2	2.55	0.42
1:A:45:ARG:HG2	1:A:313:TRP:CE2	2.54	0.42
1:D:183:TYR:CB	1:D:285:ASP:HB2	2.50	0.42
1:D:266:HIS:NE2	1:D:272:PRO:O	2.51	0.42
1:A:235:THR:HG23	1:A:237:GLN:H	1.84	0.42
1:B:45:ARG:HG2	1:B:313:TRP:CE2	2.55	0.42
1:B:115:SER:O	1:B:117:LEU:HD22	2.20	0.42
1:C:266:HIS:CD2	1:C:271:ARG:HB3	2.55	0.42
1:C:266:HIS:NE2	1:C:272:PRO:O	2.52	0.41
1:E:44:LEU:HD21	1:E:77:ASP:O	2.20	0.41
1:A:175:LEU:HD22	1:A:228:PHE:CE1	2.56	0.41
1:C:200:PHE:CE1	1:C:204:VAL:HG23	2.55	0.41
1:E:82:PHE:CE1	1:E:111:ALA:HB1	2.55	0.41
1:F:49:ALA:HB1	1:F:315:VAL:HG13	2.03	0.41
1:F:118:TYR:CE2	1:F:127:VAL:HB	2.55	0.41
1:A:248:LEU:HD22	1:A:280:PHE:CG	2.55	0.41
1:B:201:SER:OG	1:B:207:CYS:HB2	2.21	0.41
1:F:45:ARG:HG2	1:F:313:TRP:CE2	2.55	0.41
1:F:49:ALA:HA	1:F:313:TRP:O	2.20	0.41
1:F:213:PRO:HB2	1:F:307:ALA:HB1	2.02	0.41
1:A:175:LEU:HA	1:A:178:ARG:HG3	2.02	0.41
1:A:265:HIS:CD2	1:A:329:THR:HG21	2.55	0.41
1:C:91:LYS:HG3	1:C:92:GLU:CD	2.40	0.41
1:E:313:TRP:CE3	1:E:322:GLN:HB3	2.55	0.41
1:F:201:SER:OG	1:F:207:CYS:HB2	2.21	0.41
1:A:235:THR:HG21	1:E:184:LEU:HD13	2.02	0.41
1:B:122:ARG:HD3	1:C:122:ARG:NH1	2.36	0.41
1:B:200:PHE:CE1	1:B:204:VAL:HG13	2.55	0.41
1:B:270:GLN:O	1:B:270:GLN:HG2	2.21	0.41
1:C:43:ILE:HG12	1:C:43:ILE:H	1.74	0.41
1:C:71:ARG:HD2	1:C:71:ARG:HA	1.74	0.41
1:F:50:LEU:HD22	1:F:56:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASN:OD1	1:A:110:LEU:HG	2.21	0.41
1:A:102:TRP:CE3	1:A:111:ALA:HB2	2.55	0.41
1:A:251:LEU:HD23	1:A:251:LEU:O	2.21	0.41
1:D:183:TYR:HB3	1:D:285:ASP:HB2	2.02	0.41
1:E:195:VAL:HA	1:E:226:TYR:O	2.21	0.41
1:F:259:ILE:HG22	1:F:274:ILE:HG12	2.02	0.41
1:C:235:THR:HG21	1:D:184:LEU:HD13	2.02	0.41
1:D:108:VAL:HA	1:D:109:PRO:HD3	1.86	0.41
1:A:100:LYS:HG2	1:A:101:SER:N	2.36	0.41
1:B:33:PRO:HB3	1:B:36:ARG:NH2	2.35	0.41
1:A:235:THR:HG23	1:A:237:GLN:HG3	2.03	0.41
1:C:46:ALA:O	1:C:50:LEU:HD13	2.20	0.41
1:D:212:LEU:O	1:D:216:VAL:HG12	2.20	0.41
1:E:251:LEU:HD23	1:E:251:LEU:O	2.21	0.41
1:F:69:TYR:C	1:F:71:ARG:H	2.23	0.41
1:F:172:ALA:HA	1:F:189:LEU:HD22	2.02	0.41
1:A:49:ALA:HA	1:A:313:TRP:O	2.22	0.41
1:A:52:ASN:OD1	1:A:111:ALA:N	2.40	0.41
1:A:223:GLU:HA	1:A:300:LYS:HD2	2.02	0.41
1:E:44:LEU:HA	1:E:47:VAL:HG12	2.03	0.41
1:F:265:HIS:CG	1:F:329:THR:HG21	2.56	0.41
1:A:24:GLY:HA3	1:A:27:GLN:CD	2.41	0.40
1:A:109:PRO:O	1:A:110:LEU:HB3	2.22	0.40
1:A:266:HIS:CE1	1:A:272:PRO:HD2	2.55	0.40
1:C:316:LYS:C	1:C:318:ASN:N	2.74	0.40
1:E:183:TYR:CB	1:E:285:ASP:HB2	2.51	0.40
1:A:24:GLY:HA3	1:A:27:GLN:NE2	2.36	0.40
1:A:47:VAL:HG11	1:A:86:LEU:HD11	2.03	0.40
1:C:180:ARG:HG3	1:C:284:HIS:CD2	2.56	0.40
1:C:251:LEU:O	1:C:251:LEU:HD23	2.21	0.40
1:E:89:MET:HB3	1:E:96:LEU:HB2	2.03	0.40
1:A:91:LYS:HD2	1:A:91:LYS:HA	1.91	0.40
1:A:331:TRP:O	1:A:331:TRP:HD1	2.05	0.40
1:E:38:LYS:O	1:E:42:ILE:HG12	2.22	0.40
1:F:102:TRP:CE3	1:F:111:ALA:HB2	2.56	0.40
1:F:195:VAL:HA	1:F:226:TYR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	286/326 (88%)	265 (93%)	17 (6%)	4 (1%)	11	38
1	B	291/326 (89%)	271 (93%)	13 (4%)	7 (2%)	6	28
1	C	285/326 (87%)	265 (93%)	16 (6%)	4 (1%)	11	38
1	D	291/326 (89%)	269 (92%)	18 (6%)	4 (1%)	11	38
1	E	291/326 (89%)	263 (90%)	21 (7%)	7 (2%)	6	28
1	F	292/326 (90%)	270 (92%)	17 (6%)	5 (2%)	9	35
All	All	1736/1956 (89%)	1603 (92%)	102 (6%)	31 (2%)	8	35

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	GLY
1	A	317	ASP
1	B	77	ASP
1	B	107	GLY
1	B	110	LEU
1	B	287	GLY
1	B	317	ASP
1	C	107	GLY
1	C	110	LEU
1	C	317	ASP
1	E	69	TYR
1	E	76	LEU
1	E	110	LEU
1	F	107	GLY
1	F	110	LEU
1	F	317	ASP
1	A	77	ASP
1	D	77	ASP
1	D	318	ASN
1	E	55	GLY

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Mol	Chain	Res	Type
1	E	77	ASP
1	B	271	ARG
1	C	77	ASP
1	D	122	ARG
1	E	122	ARG
1	E	317	ASP
1	F	271	ARG
1	B	122	ARG
1	F	122	ARG
1	A	110	LEU
1	D	109	PRO

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	257/285 (90%)	253 (98%)	4 (2%)	62	79
1	B	257/285 (90%)	255 (99%)	2 (1%)	81	89
1	C	258/285 (90%)	257 (100%)	1 (0%)	91	95
1	D	260/285 (91%)	259 (100%)	1 (0%)	91	95
1	E	258/285 (90%)	257 (100%)	1 (0%)	91	95
1	F	260/285 (91%)	259 (100%)	1 (0%)	91	95
All	All	1550/1710 (91%)	1540 (99%)	10 (1%)	86	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	139	CYS
1	A	186	LYS
1	A	290	ARG
1	B	186	LYS
1	B	332	MET
1	C	186	LYS

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Mol	Chain	Res	Type
1	D	321	ARG
1	E	186	LYS
1	F	317	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	52	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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	292/326 (89%)	0.73	48 (16%)	1	2	83, 168, 243, 281	0
1	B	295/326 (90%)	0.71	34 (11%)	4	4	66, 139, 241, 274	0
1	C	291/326 (89%)	0.79	51 (17%)	1	1	81, 174, 257, 291	0
1	D	295/326 (90%)	0.72	42 (14%)	2	2	86, 166, 243, 268	0
1	E	295/326 (90%)	0.69	41 (13%)	2	2	80, 161, 232, 260	0
1	F	296/326 (90%)	0.80	46 (15%)	2	2	80, 158, 222, 284	0
All	All	1764/1956 (90%)	0.74	262 (14%)	2	2	66, 162, 242, 291	0

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	95	PHE	4.7
1	D	23	LEU	4.6
1	B	117	LEU	4.5
1	D	304	ALA	4.5
1	C	82	PHE	4.5
1	A	82	PHE	4.5
1	F	265	HIS	4.4
1	C	265	HIS	4.4
1	E	23	LEU	4.4
1	C	304	ALA	4.4
1	B	82	PHE	4.3
1	E	265	HIS	4.3
1	F	86	LEU	4.3
1	C	65	LYS	4.3
1	E	113	LEU	4.2
1	E	306	PHE	4.2
1	C	95	PHE	4.2
1	F	304	ALA	4.1
1	C	296	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	89	MET	4.0
1	A	98	PHE	4.0
1	B	216	VAL	4.0
1	B	23	LEU	4.0
1	A	274	ILE	3.9
1	B	64	ASN	3.9
1	F	65	LYS	3.9
1	A	88	LYS	3.8
1	B	95	PHE	3.8
1	D	265	HIS	3.8
1	D	306	PHE	3.7
1	A	229	PHE	3.7
1	A	306	PHE	3.7
1	C	113	LEU	3.7
1	F	329	THR	3.7
1	D	86	LEU	3.7
1	C	86	LEU	3.6
1	E	117	LEU	3.6
1	A	308	LYS	3.6
1	C	229	PHE	3.6
1	C	306	PHE	3.5
1	F	306	PHE	3.5
1	E	67	TYR	3.5
1	D	316	LYS	3.5
1	A	58	ILE	3.5
1	F	137	LEU	3.5
1	E	65	LYS	3.4
1	D	325	THR	3.4
1	C	328	TRP	3.4
1	A	44	LEU	3.4
1	A	280	PHE	3.4
1	B	89	MET	3.4
1	F	57	ILE	3.4
1	E	58	ILE	3.4
1	F	113	LEU	3.4
1	E	304	ALA	3.3
1	F	82	PHE	3.3
1	C	331	TRP	3.3
1	D	331	TRP	3.3
1	E	43	ILE	3.2
1	E	331	TRP	3.2
1	A	265	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	259	ILE	3.2
1	B	98	PHE	3.2
1	A	328	TRP	3.2
1	D	82	PHE	3.1
1	B	44	LEU	3.1
1	D	113	LEU	3.1
1	A	113	LEU	3.1
1	B	58	ILE	3.1
1	F	229	PHE	3.1
1	A	304	ALA	3.1
1	A	137	LEU	3.1
1	E	264	VAL	3.0
1	A	67	TYR	3.0
1	F	67	TYR	3.0
1	C	264	VAL	3.0
1	B	96	LEU	3.0
1	F	50	LEU	3.0
1	A	329	THR	3.0
1	C	117	LEU	3.0
1	D	229	PHE	3.0
1	F	20	LYS	3.0
1	A	307	ALA	3.0
1	C	274	ILE	3.0
1	A	59	LYS	2.9
1	E	229	PHE	2.9
1	A	86	LEU	2.9
1	C	310	PRO	2.9
1	B	115	SER	2.9
1	C	89	MET	2.9
1	D	72	HIS	2.9
1	E	95	PHE	2.9
1	B	22	THR	2.9
1	D	328	TRP	2.9
1	C	44	LEU	2.9
1	D	281	LEU	2.8
1	B	43	ILE	2.8
1	F	259	ILE	2.8
1	F	98	PHE	2.8
1	D	329	THR	2.8
1	A	95	PHE	2.8
1	C	332	MET	2.8
1	C	320	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	197	PHE	2.8
1	A	18	ALA	2.8
1	C	96	LEU	2.8
1	D	294	CYS	2.8
1	A	97	ILE	2.8
1	C	47	VAL	2.8
1	A	57	ILE	2.8
1	F	296	ILE	2.8
1	F	72	HIS	2.8
1	F	294	CYS	2.8
1	E	44	LEU	2.8
1	B	97	ILE	2.8
1	F	58	ILE	2.8
1	A	23	LEU	2.8
1	A	227	VAL	2.7
1	F	315	VAL	2.7
1	B	137	LEU	2.7
1	E	50	LEU	2.7
1	E	137	LEU	2.7
1	A	216	VAL	2.7
1	D	98	PHE	2.7
1	C	21	VAL	2.7
1	B	113	LEU	2.7
1	D	197	PHE	2.7
1	B	307	ALA	2.7
1	F	117	LEU	2.7
1	B	296	ILE	2.7
1	D	259	ILE	2.7
1	D	274	ILE	2.6
1	C	278	LEU	2.6
1	C	228	PHE	2.6
1	D	208	VAL	2.6
1	F	64	ASN	2.6
1	A	320	VAL	2.6
1	F	227	VAL	2.6
1	C	98	PHE	2.6
1	A	305	VAL	2.6
1	D	97	ILE	2.6
1	E	187	LEU	2.6
1	B	215	CYS	2.6
1	D	200	PHE	2.6
1	F	95	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	307	ALA	2.5
1	F	216	VAL	2.5
1	D	293	VAL	2.5
1	D	228	PHE	2.5
1	A	294	CYS	2.5
1	C	118	TYR	2.5
1	E	46	ALA	2.5
1	D	44	LEU	2.5
1	D	117	LEU	2.5
1	A	296	ILE	2.5
1	D	308	LYS	2.5
1	A	90	GLN	2.5
1	B	306	PHE	2.5
1	D	296	ILE	2.5
1	C	305	VAL	2.4
1	D	134	LEU	2.4
1	C	176	PHE	2.4
1	F	43	ILE	2.4
1	D	96	LEU	2.4
1	F	46	ALA	2.4
1	B	67	TYR	2.4
1	C	280	PHE	2.4
1	C	315	VAL	2.4
1	E	332	MET	2.4
1	D	137	LEU	2.4
1	F	208	VAL	2.4
1	A	115	SER	2.4
1	C	23	LEU	2.4
1	C	134	LEU	2.4
1	E	98	PHE	2.4
1	E	255	ILE	2.4
1	F	23	LEU	2.4
1	F	307	ALA	2.4
1	A	318	ASN	2.4
1	A	96	LEU	2.4
1	B	329	THR	2.4
1	C	325	THR	2.4
1	C	259	ILE	2.3
1	E	96	LEU	2.3
1	B	197	PHE	2.3
1	C	18	ALA	2.3
1	E	296	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	187	LEU	2.3
1	C	175	LEU	2.3
1	F	97	ILE	2.3
1	F	228	PHE	2.3
1	C	216	VAL	2.3
1	B	90	GLN	2.3
1	A	117	LEU	2.3
1	C	64	ASN	2.3
1	C	58	ILE	2.3
1	C	255	ILE	2.3
1	A	43	ILE	2.2
1	C	197	PHE	2.2
1	E	208	VAL	2.2
1	D	332	MET	2.2
1	F	274	ILE	2.2
1	D	216	VAL	2.2
1	D	227	VAL	2.2
1	D	187	LEU	2.2
1	B	86	LEU	2.2
1	E	323	LEU	2.2
1	D	323	LEU	2.2
1	D	90	GLN	2.2
1	A	248	LEU	2.2
1	D	307	ALA	2.2
1	F	181	LEU	2.2
1	E	213	PRO	2.2
1	C	234	GLU	2.2
1	F	99	VAL	2.2
1	E	329	THR	2.2
1	A	181	LEU	2.1
1	B	274	ILE	2.1
1	E	97	ILE	2.1
1	C	59	LYS	2.1
1	E	328	TRP	2.1
1	F	281	LEU	2.1
1	D	65	LYS	2.1
1	E	215	CYS	2.1
1	F	308	LYS	2.1
1	C	16	VAL	2.1
1	E	315	VAL	2.1
1	F	328	TRP	2.1
1	B	259	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	50	LEU	2.1
1	C	97	ILE	2.1
1	E	274	ILE	2.1
1	B	229	PHE	2.1
1	E	115	SER	2.1
1	B	212	LEU	2.1
1	A	238	VAL	2.1
1	E	305	VAL	2.1
1	F	264	VAL	2.1
1	C	333	MET	2.1
1	F	44	LEU	2.1
1	E	228	PHE	2.1
1	E	216	VAL	2.1
1	E	238	VAL	2.1
1	D	280	PHE	2.1
1	F	305	VAL	2.1
1	E	90	GLN	2.1
1	A	315	VAL	2.1
1	B	305	VAL	2.1
1	A	175	LEU	2.1
1	C	50	LEU	2.1
1	A	189	LEU	2.0
1	A	255	ILE	2.0
1	E	294	CYS	2.0
1	F	226	TYR	2.0
1	C	43	ILE	2.0
1	F	280	PHE	2.0
1	B	208	VAL	2.0
1	B	304	ALA	2.0
1	F	293	VAL	2.0
1	C	137	LEU	2.0
1	A	264	VAL	2.0
1	B	21	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	401	1/1	0.93	0.31	172,172,172,172	0
2	ZN	C	401	1/1	0.97	0.29	177,177,177,177	0
2	ZN	E	401	1/1	0.98	0.29	156,156,156,156	0
2	ZN	D	401	1/1	0.99	0.28	164,164,164,164	0
2	ZN	B	401	1/1	0.99	0.32	123,123,123,123	0
2	ZN	F	401	1/1	1.00	0.28	171,171,171,171	0

6.5　Other polymers ⓘ

There are no such residues in this entry.