



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:37 AM UTC

PDB ID : 7Q5N / pdb_00007q5n
Title : Crystal structure of Chaetomium thermophilum Ahp1-Urm1 complex
Authors : Ravichandran, K.E.; Wilk, P.; Grudnik, P.; Glatt, S.
Deposited on : 2021-11-04
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

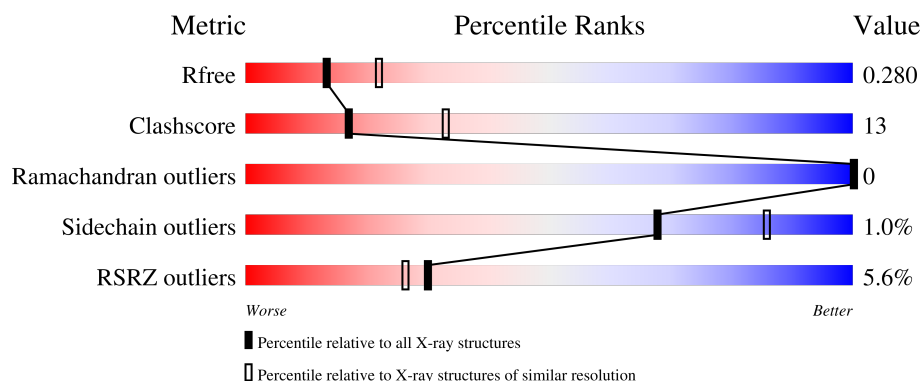
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	174	0% 89% 9% .
1	B	174	5% 86% 12% ..
1	C	174	6% 73% 24% .
1	D	174	8% 76% 22% .
1	E	174	6% 81% 16% .

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Mol	Chain	Length	Quality of chain
1	F	174	
2	G	111	
2	H	111	
2	I	111	
2	J	111	
2	K	111	
2	L	111	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CSS	A	60	-	-	X	-
1	CSS	B	60	-	-	X	-
1	CSS	D	60	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12664 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 Thioredoxin domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1256	795	212	245	4			
1	B	172	Total	C	N	O	S	0	0	0
			1268	804	214	246	4			
1	C	169	Total	C	N	O	S	0	0	0
			1247	790	210	243	4			
1	D	170	Total	C	N	O	S	0	0	0
			1251	792	211	244	4			
1	E	169	Total	C	N	O	S	0	0	0
			1247	790	210	243	4			
1	F	168	Total	C	N	O	S	0	0	0
			1239	785	209	242	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G0S1P8
A	0	ALA	-	expression tag	UNP G0S1P8
A	30	SER	CYS	engineered mutation	UNP G0S1P8
B	-1	GLY	-	expression tag	UNP G0S1P8
B	0	ALA	-	expression tag	UNP G0S1P8
B	30	SER	CYS	engineered mutation	UNP G0S1P8
C	-1	GLY	-	expression tag	UNP G0S1P8
C	0	ALA	-	expression tag	UNP G0S1P8
C	30	SER	CYS	engineered mutation	UNP G0S1P8
D	-1	GLY	-	expression tag	UNP G0S1P8
D	0	ALA	-	expression tag	UNP G0S1P8
D	30	SER	CYS	engineered mutation	UNP G0S1P8
E	-1	GLY	-	expression tag	UNP G0S1P8
E	0	ALA	-	expression tag	UNP G0S1P8
E	30	SER	CYS	engineered mutation	UNP G0S1P8
F	-1	GLY	-	expression tag	UNP G0S1P8
F	0	ALA	-	expression tag	UNP G0S1P8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	SER	CYS	engineered mutation	UNP G0S1P8

- Molecule 2 is a protein called Ubiquitin-related modifier 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	103	Total	C	N	O	S	0	0	0
			821	525	134	160	2			
2	H	104	Total	C	N	O	S	1	0	0
			829	531	135	161	2			
2	I	104	Total	C	N	O	S	0	0	0
			829	531	135	161	2			
2	J	103	Total	C	N	O	S	0	0	0
			821	525	134	160	2			
2	K	104	Total	C	N	O	S	0	0	0
			829	531	135	161	2			
2	L	104	Total	C	N	O	S	0	0	0
			829	531	135	161	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP G0SE11
G	2	ALA	-	expression tag	UNP G0SE11
G	55	SER	CYS	engineered mutation	UNP G0SE11
H	1	MET	-	initiating methionine	UNP G0SE11
H	2	ALA	-	expression tag	UNP G0SE11
H	55	SER	CYS	engineered mutation	UNP G0SE11
I	1	MET	-	initiating methionine	UNP G0SE11
I	2	ALA	-	expression tag	UNP G0SE11
I	55	SER	CYS	engineered mutation	UNP G0SE11
J	1	MET	-	initiating methionine	UNP G0SE11
J	2	ALA	-	expression tag	UNP G0SE11
J	55	SER	CYS	engineered mutation	UNP G0SE11
K	1	MET	-	initiating methionine	UNP G0SE11
K	2	ALA	-	expression tag	UNP G0SE11
K	55	SER	CYS	engineered mutation	UNP G0SE11
L	1	MET	-	initiating methionine	UNP G0SE11
L	2	ALA	-	expression tag	UNP G0SE11
L	55	SER	CYS	engineered mutation	UNP G0SE11

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	3	Total Zn 3 3	0	0
3	C	3	Total Zn 3 3	0	0
3	D	2	Total Zn 2 2	0	0
3	E	3	Total Zn 3 3	0	0
3	F	2	Total Zn 2 2	0	0
3	G	1	Total Zn 1 1	0	0
3	H	8	Total Zn 8 8	0	0
3	I	5	Total Zn 5 5	0	0
3	J	4	Total Zn 4 4	0	0
3	K	6	Total Zn 6 6	0	0
3	L	3	Total Zn 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	33	Total O 33 33	0	0
4	B	22	Total O 22 22	0	0
4	C	9	Total O 9 9	0	0
4	D	11	Total O 11 11	0	0
4	E	15	Total O 15 15	0	0
4	F	4	Total O 4 4	0	0
4	G	6	Total O 6 6	0	0
4	H	12	Total O 12 12	0	0

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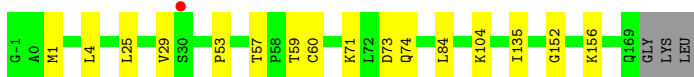
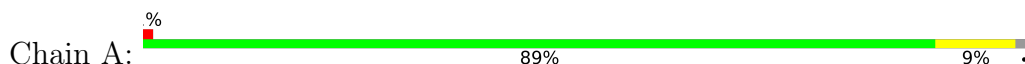
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	9	Total 9	O 9	0	0
4	J	6	Total 6	O 6	0	0
4	K	21	Total 21	O 21	0	0
4	L	9	Total 9	O 9	0	0

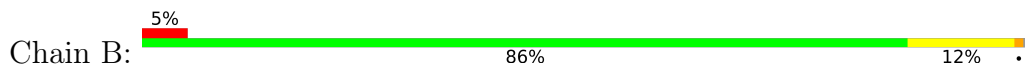
3 Residue-property plots [i](#)

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.

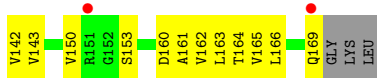
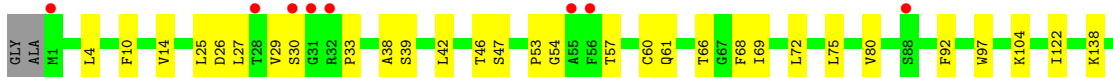
- Molecule 1: Thioredoxin domain-containing protein



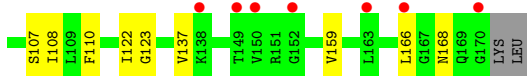
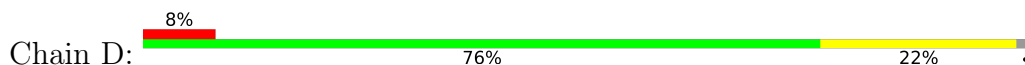
- Molecule 1: Thioredoxin domain-containing protein



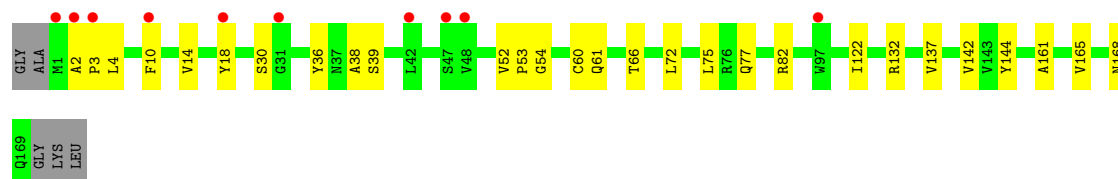
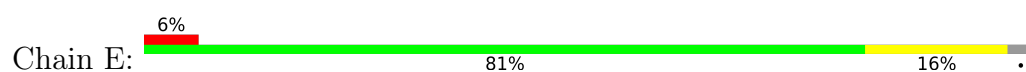
- Molecule 1: Thioredoxin domain-containing protein



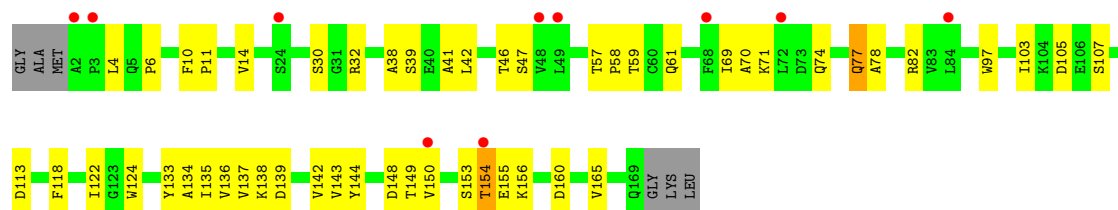
- Molecule 1: Thioredoxin domain-containing protein



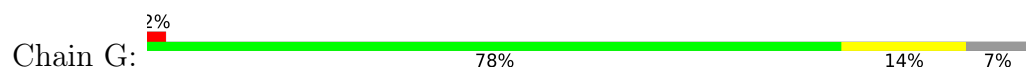
- Molecule 1: Thioredoxin domain-containing protein



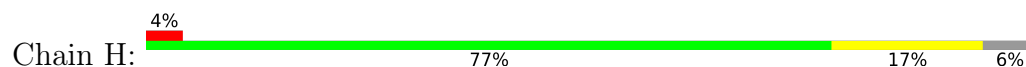
- Molecule 1: Thioredoxin domain-containing protein



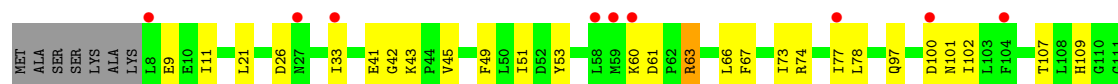
- Molecule 2: Ubiquitin-related modifier 1



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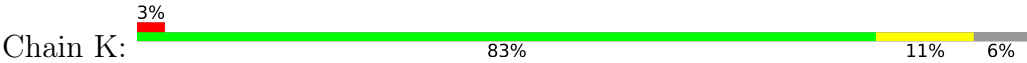


- Molecule 2: Ubiquitin-related modifier 1

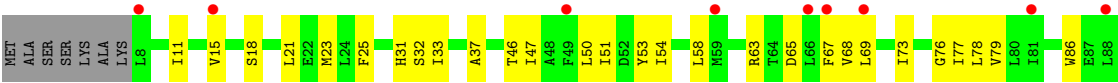




● Molecule 2: Ubiquitin-related modifier 1



● Molecule 2: Ubiquitin-related modifier 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	185.43Å 197.22Å 139.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 2.50 48.47 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.47-2.50) 99.3 (48.47-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.234 , 0.272 0.244 , 0.280	Depositor DCC
R_{free} test set	4366 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12664	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: ZN, CSS

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	0.38	0/1272	0.57	1/1730 (0.1%)
1	B	0.21	0/1284	0.36	0/1745
1	C	0.26	0/1263	0.41	0/1718
1	D	0.38	0/1267	0.60	2/1723 (0.1%)
1	E	0.57	0/1263	0.88	4/1718 (0.2%)
1	F	0.48	0/1255	0.82	5/1708 (0.3%)
2	G	0.33	0/838	0.50	0/1137
2	H	0.28	0/846	0.45	1/1148 (0.1%)
2	I	0.60	0/846	0.92	0/1148
2	J	0.62	3/838 (0.4%)	0.82	2/1137 (0.2%)
2	K	0.15	0/846	0.29	0/1148
2	L	0.20	0/846	0.40	0/1148
All	All	0.40	3/12664 (0.0%)	0.62	15/17208 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	110	GLY	C-N	-6.87	1.23	1.33
2	J	111	GLY	C-O	6.81	1.37	1.23
2	J	111	GLY	CA-C	-5.52	1.42	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	110	GLY	O-C-N	8.93	134.31	122.70
1	F	57	THR	CA-CB-OG1	-8.13	97.40	109.60
1	F	154	THR	N-CA-C	-6.81	102.26	113.50
1	F	58	PRO	N-CA-C	6.50	122.76	113.47
1	F	143	VAL	N-CA-C	-6.28	107.38	113.53
1	E	3	PRO	CA-C-N	-6.12	114.38	123.00
1	E	3	PRO	C-N-CA	-6.12	114.38	123.00
1	D	82	ARG	CA-C-O	-5.96	113.80	120.66
2	H	93	ALA	N-CA-C	-5.94	105.77	114.39
2	J	91	GLU	CB-CA-C	-5.85	109.84	116.63
1	A	84	LEU	CA-C-O	-5.83	114.02	120.38
1	F	30	SER	N-CA-C	5.31	118.58	110.20
1	E	77	GLN	N-CA-C	-5.21	106.92	113.28
1	E	2	ALA	CA-C-O	-5.00	116.63	120.48
1	D	82	ARG	N-CA-C	5.00	117.59	109.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	110	GLY	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1256	0	1250	14	0
1	B	1268	0	1269	22	0
1	C	1247	0	1242	38	0
1	D	1251	0	1245	40	0
1	E	1247	0	1242	18	0
1	F	1239	0	1230	45	0
2	G	821	0	809	14	0
2	H	829	0	820	15	0
2	I	829	0	820	31	0
2	J	821	0	809	42	0
2	K	829	0	820	8	0
2	L	829	0	820	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	H	8	0	0	0	0
3	I	5	0	0	0	0
3	J	4	0	0	1	0
3	K	6	0	0	0	0
3	L	3	0	0	0	0
4	A	33	0	0	1	0
4	B	22	0	0	5	0
4	C	9	0	0	3	0
4	D	11	0	0	3	0
4	E	15	0	0	4	0
4	F	4	0	0	0	0
4	G	6	0	0	0	0
4	H	12	0	0	2	0
4	I	9	0	0	5	0
4	J	6	0	0	0	0
4	K	21	0	0	2	0
4	L	9	0	0	6	0
All	All	12664	0	12376	317	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 13.

All (317) 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:E:53:PRO:HB2	4:E:302:HOH:O	1.33	1.21
2:L:54:ILE:HA	2:L:58:LEU:HD23	1.32	1.11
2:L:25:PHE:HB3	4:L:302:HOH:O	1.55	1.06
1:A:57:THR:OG1	1:A:60:CSS:SD	2.08	1.04
2:I:9:GLU:HB2	4:I:402:HOH:O	1.55	1.04
2:L:25:PHE:CB	4:L:302:HOH:O	2.03	1.03
1:E:60:CSS:SD	4:E:302:HOH:O	2.20	0.98
1:B:57:THR:OG1	1:B:60:CSS:SD	2.11	0.98
1:A:60:CSS:SD	4:A:317:HOH:O	2.22	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:THR:OG1	1:D:60:CSS:SD	2.26	0.93
1:F:14:VAL:HG23	1:F:38:ALA:HB3	1.52	0.88
1:D:60:CSS:SD	4:D:408:HOH:O	2.31	0.86
1:C:42:LEU:HD22	1:C:47:SER:OG	1.76	0.85
2:K:109:HIS:CE1	4:K:403:HOH:O	2.28	0.85
1:C:10:PHE:HE1	1:C:14:VAL:HG11	1.42	0.84
1:D:60:CSS:SD	4:D:410:HOH:O	2.36	0.83
2:L:31:HIS:ND1	4:L:301:HOH:O	2.11	0.83
1:E:14:VAL:HG23	1:E:38:ALA:HB3	1.62	0.81
1:D:4:LEU:HD22	1:D:122:ILE:CD1	2.11	0.81
2:J:24:LEU:HD11	2:J:59:MET:SD	2.21	0.81
1:C:61:GLN:O	1:C:66:THR:HG23	1.81	0.81
1:B:61:GLN:HE21	1:B:97:TRP:HE1	1.29	0.79
1:C:60:CSS:SD	4:C:305:HOH:O	2.41	0.78
1:D:4:LEU:HD22	1:D:122:ILE:HD13	1.65	0.77
1:C:75:LEU:HD22	1:C:80:VAL:HG21	1.69	0.75
1:F:153:SER:HA	2:L:23:MET:HE1	1.67	0.75
1:C:14:VAL:HG12	1:C:39:SER:OG	1.87	0.74
2:L:25:PHE:HB2	4:L:302:HOH:O	1.78	0.74
1:C:61:GLN:OE1	1:C:97:TRP:NE1	2.21	0.74
1:D:4:LEU:CD2	1:D:122:ILE:HD13	2.17	0.74
2:H:14:THR:OG1	2:H:101:ASN:OD1	2.05	0.73
1:E:4:LEU:HD11	1:E:142:VAL:HG21	1.69	0.73
2:I:97:GLN:HB2	2:I:100:ASP:OD2	1.89	0.73
2:K:59:MET:HE1	2:K:64:THR:HA	1.70	0.72
2:J:11:ILE:HG23	2:J:37:ALA:HB2	1.72	0.71
2:I:63:ARG:NH1	2:I:66:LEU:HD11	2.05	0.71
2:G:88:LEU:HD21	2:J:108:LEU:CD1	2.21	0.69
1:B:61:GLN:HE22	1:B:101:ASN:HD21	1.41	0.68
1:F:136:VAL:HG12	1:F:144:TYR:HB3	1.75	0.67
2:I:63:ARG:HH11	2:I:66:LEU:HD11	1.60	0.66
2:J:24:LEU:HD22	2:J:25:PHE:CE2	2.31	0.65
1:C:163:LEU:HA	1:C:166:LEU:HD12	1.79	0.65
1:D:42:LEU:HB3	1:D:137:VAL:HG21	1.76	0.65
1:F:41:ALA:O	1:F:82:ARG:NH1	2.29	0.65
1:D:14:VAL:HG23	1:D:38:ALA:HB3	1.79	0.65
1:B:60:CSS:SD	4:B:316:HOH:O	2.55	0.64
1:A:53:PRO:HD2	1:A:60:CSS:SG	2.36	0.64
1:B:61:GLN:NE2	1:B:97:TRP:HE1	1.94	0.64
1:C:46:THR:HG22	1:C:138:LYS:HD2	1.78	0.64
1:E:144:TYR:CD2	1:E:165:VAL:HG21	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:VAL:HG22	1:D:39:SER:OG	1.98	0.64
2:J:11:ILE:C	2:J:11:ILE:HD12	2.23	0.64
2:I:43:LYS:NZ	4:I:401:HOH:O	2.32	0.63
2:L:31:HIS:NE2	4:L:302:HOH:O	2.28	0.63
1:F:42:LEU:HD22	1:F:47:SER:OG	1.98	0.63
1:F:105:ASP:OD1	1:F:107:SER:OG	2.12	0.63
2:J:87:GLU:OE2	3:J:201:ZN:ZN	1.46	0.63
2:L:15:VAL:HG12	2:L:102:ILE:HD11	1.79	0.63
1:D:122:ILE:HG22	1:D:123:GLY:N	2.12	0.62
2:I:51:ILE:HD13	2:I:73:ILE:HB	1.82	0.62
1:B:60:CSS:SD	4:B:313:HOH:O	2.56	0.61
1:C:14:VAL:HG13	1:C:38:ALA:HB3	1.82	0.61
2:I:9:GLU:CB	4:I:402:HOH:O	2.30	0.61
2:L:32:SER:C	2:L:33:ILE:HD12	2.25	0.61
2:G:88:LEU:HD21	2:J:108:LEU:HD11	1.83	0.60
1:F:155:GLU:OE2	1:F:156:LYS:NZ	2.30	0.60
2:J:47:ILE:HD11	2:J:94:TYR:HD2	1.66	0.60
1:D:69:ILE:HD13	1:D:103:ILE:HD11	1.84	0.60
1:F:148:ASP:HB3	1:F:153:SER:HB3	1.84	0.59
2:I:26:ASP:HB2	2:I:60:LYS:CD	2.33	0.59
2:I:9:GLU:C	4:I:402:HOH:O	2.46	0.59
1:D:69:ILE:HA	1:D:72:LEU:HD21	1.84	0.59
2:I:63:ARG:NH1	2:I:66:LEU:CD1	2.66	0.59
2:J:103:LEU:HD11	2:J:105:VAL:HG22	1.83	0.58
2:G:11:ILE:HD11	2:G:97:GLN:C	2.28	0.58
1:A:57:THR:CB	1:A:60:CSS:HD	2.12	0.58
1:A:73:ASP:OD1	1:A:74:GLN:N	2.36	0.58
2:G:13:ILE:HD13	2:G:35:LEU:HD11	1.86	0.58
2:J:32:SER:C	2:J:33:ILE:HD12	2.29	0.58
1:C:160:ASP:HA	1:C:163:LEU:HD12	1.86	0.57
2:G:59:MET:HE1	2:G:64:THR:HA	1.86	0.57
1:C:162:VAL:HG12	1:C:166:LEU:HD11	1.86	0.57
2:J:11:ILE:CD1	2:J:13:ILE:HG23	2.35	0.57
2:H:8:LEU:N	4:H:301:HOH:O	2.38	0.57
1:F:46:THR:HG23	1:F:138:LYS:HD3	1.86	0.56
2:I:26:ASP:HB2	2:I:60:LYS:HD2	1.86	0.56
1:F:14:VAL:CG2	1:F:38:ALA:HB3	2.32	0.56
2:J:35:LEU:HD11	2:J:50:LEU:HD23	1.86	0.56
2:L:50:LEU:HD21	2:L:102:ILE:CD1	2.35	0.56
1:F:153:SER:HA	2:L:23:MET:CE	2.35	0.56
2:I:33:ILE:HG12	2:I:53:TYR:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:CD2	1:C:80:VAL:HG21	2.36	0.56
1:C:46:THR:CG2	1:C:138:LYS:HD2	2.36	0.55
2:G:29:ARG:NH2	2:J:101:ASN:OD1	2.39	0.55
1:B:49:LEU:HD11	1:B:86:ILE:HD13	1.87	0.55
1:B:57:THR:CB	1:B:60:CSS:HD	2.15	0.55
1:D:122:ILE:HG22	1:D:123:GLY:H	1.71	0.55
1:F:155:GLU:HG3	1:F:156:LYS:N	2.20	0.55
1:D:58:PRO:O	1:D:62:GLU:N	2.38	0.55
2:L:11:ILE:HD11	2:L:37:ALA:HA	1.90	0.54
2:L:96:ILE:H	2:L:96:ILE:HD12	1.73	0.54
1:C:33:PRO:CG	1:C:92:PHE:HE1	2.21	0.54
2:J:103:LEU:HD12	2:J:104:PHE:N	2.22	0.54
1:F:4:LEU:HD21	1:F:142:VAL:HG11	1.90	0.54
2:J:21:LEU:HD22	2:J:106:SER:HB2	1.88	0.54
1:F:71:LYS:NZ	1:F:74:GLN:HG3	2.23	0.54
1:B:32:ARG:HB3	4:B:301:HOH:O	2.08	0.53
2:J:18:SER:O	2:J:21:LEU:HD23	2.08	0.53
2:I:109:HIS:CE1	4:I:404:HOH:O	2.61	0.53
1:C:68:PHE:O	1:C:72:LEU:HD22	2.09	0.53
1:C:150:VAL:HG23	1:C:153:SER:HB2	1.89	0.53
2:J:74:ARG:NH2	2:J:77:ILE:HD11	2.23	0.53
2:J:74:ARG:NH2	2:J:106:SER:OG	2.41	0.52
2:J:51:ILE:HD11	2:J:104:PHE:CE1	2.44	0.52
1:F:134:ALA:C	1:F:135:ILE:HD12	2.33	0.52
1:C:69:ILE:HA	1:C:72:LEU:CD2	2.40	0.52
1:D:122:ILE:CG2	1:D:123:GLY:N	2.73	0.52
2:L:96:ILE:HD12	2:L:96:ILE:N	2.25	0.52
1:D:4:LEU:HD23	1:D:4:LEU:H	1.74	0.51
1:E:161:ALA:O	1:E:165:VAL:HG23	2.09	0.51
2:L:65:ASP:OD1	2:L:65:ASP:N	2.43	0.51
2:H:33:ILE:HD13	2:H:53:TYR:HE2	1.74	0.51
2:J:65:ASP:OD1	2:J:69:LEU:CD2	2.58	0.51
2:L:11:ILE:HD11	2:L:37:ALA:CA	2.41	0.51
2:L:18:SER:O	2:L:21:LEU:HD12	2.10	0.51
2:H:64:THR:HG22	2:H:68:VAL:HG12	1.93	0.51
2:L:46:THR:C	2:L:96:ILE:HD11	2.35	0.51
2:G:13:ILE:CD1	2:G:35:LEU:HD11	2.41	0.51
2:J:21:LEU:CD2	2:J:106:SER:HB2	2.41	0.51
2:L:11:ILE:HD11	2:L:37:ALA:HB2	1.93	0.51
2:L:15:VAL:HG12	2:L:102:ILE:CD1	2.40	0.51
2:L:50:LEU:HD21	2:L:102:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:PHE:CE2	1:D:58:PRO:HD3	2.47	0.50
2:H:29:ARG:NH1	2:K:83:ASP:O	2.44	0.50
2:H:65:ASP:N	2:H:65:ASP:OD1	2.43	0.50
2:J:17:PHE:HZ	2:J:54:ILE:HD13	1.77	0.50
1:C:160:ASP:O	1:C:164:THR:HG23	2.11	0.50
2:G:88:LEU:HD21	2:J:108:LEU:HD13	1.91	0.50
2:I:78:LEU:CD1	2:I:107:THR:HG23	2.42	0.50
2:J:50:LEU:HD13	2:J:54:ILE:HG13	1.93	0.50
2:L:31:HIS:CE1	4:L:302:HOH:O	2.64	0.50
1:F:69:ILE:HD11	1:F:103:ILE:HD11	1.93	0.50
1:E:53:PRO:HD2	1:E:60:CSS:SG	2.53	0.49
1:C:122:ILE:HG22	1:C:122:ILE:O	2.12	0.49
1:C:150:VAL:HG23	1:C:153:SER:CB	2.42	0.49
1:D:122:ILE:CG2	1:D:123:GLY:H	2.25	0.49
1:D:67:GLY:C	1:D:159:VAL:HG21	2.37	0.49
2:J:17:PHE:CE2	2:J:25:PHE:CE2	3.00	0.49
2:H:33:ILE:HD13	2:H:53:TYR:CE2	2.47	0.49
1:D:60:CSS:O	1:D:65:VAL:HG12	2.13	0.49
1:D:89:ASN:ND2	4:D:402:HOH:O	2.46	0.49
2:L:86:TRP:CE3	2:L:91:GLU:O	2.66	0.48
1:B:144:TYR:HB2	1:B:165:VAL:HG21	1.94	0.48
1:A:29:VAL:HG23	1:A:29:VAL:O	2.13	0.48
2:G:13:ILE:HD13	2:G:35:LEU:CD1	2.42	0.48
1:D:10:PHE:HE2	1:D:14:VAL:HG21	1.79	0.48
2:K:64:THR:HG22	2:K:68:VAL:HG12	1.96	0.48
2:L:58:LEU:N	2:L:58:LEU:HD22	2.28	0.48
2:J:11:ILE:HD12	2:J:11:ILE:O	2.12	0.48
1:B:32:ARG:N	4:B:301:HOH:O	2.40	0.47
2:L:11:ILE:HD12	2:L:11:ILE:N	2.29	0.47
2:L:54:ILE:CA	2:L:58:LEU:HD23	2.24	0.47
2:I:41:GLU:HB3	2:I:43:LYS:HE3	1.96	0.47
1:D:47:SER:HB2	1:D:137:VAL:HG22	1.96	0.47
1:A:71:LYS:HG2	1:A:74:GLN:CD	2.39	0.47
1:F:10:PHE:HE2	1:F:14:VAL:HG21	1.79	0.47
2:I:73:ILE:HD12	2:I:74:ARG:H	1.79	0.47
2:K:30:ARG:HG2	4:K:419:HOH:O	2.13	0.47
2:J:55:SER:HA	2:J:59:MET:HG3	1.95	0.47
2:J:96:ILE:HD12	2:J:96:ILE:O	2.14	0.47
1:D:32:ARG:NH2	2:L:92:GLU:OE2	2.48	0.47
1:E:122:ILE:HG22	1:E:122:ILE:O	2.15	0.47
1:C:46:THR:HG22	1:C:138:LYS:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:ILE:O	1:F:70:ALA:HB3	2.15	0.46
2:J:24:LEU:HD22	2:J:25:PHE:CZ	2.50	0.46
1:F:32:ARG:HH11	2:H:91:GLU:CD	2.24	0.46
2:H:66:LEU:O	2:H:74:ARG:NH1	2.48	0.46
2:L:11:ILE:HD11	2:L:37:ALA:CB	2.45	0.46
2:L:51:ILE:HD13	2:L:73:ILE:HB	1.96	0.46
2:K:43:LYS:HA	2:K:43:LYS:HD3	1.77	0.46
1:B:36:TYR:CE1	1:B:84:LEU:HD21	2.51	0.46
1:F:154:THR:O	1:F:154:THR:HG22	2.16	0.46
2:I:73:ILE:HD11	2:I:77:ILE:HD12	1.96	0.46
2:L:47:ILE:N	2:L:96:ILE:HD11	2.31	0.46
1:B:61:GLN:NE2	1:B:97:TRP:NE1	2.62	0.46
1:B:73:ASP:OD1	1:B:73:ASP:N	2.48	0.45
1:E:132:ARG:NH1	4:E:301:HOH:O	2.46	0.45
1:F:148:ASP:HA	1:F:156:LYS:HE2	1.98	0.45
2:I:42:GLY:C	2:I:43:LYS:HE2	2.41	0.45
2:K:21:LEU:CD2	2:K:106:SER:HB2	2.46	0.45
1:C:33:PRO:CG	1:C:92:PHE:CE1	2.99	0.45
1:E:72:LEU:HA	1:E:75:LEU:HD12	1.98	0.45
2:I:33:ILE:HD11	2:I:53:TYR:OH	2.16	0.45
1:F:42:LEU:HB3	1:F:137:VAL:HG21	1.98	0.45
1:E:54:GLY:N	4:E:302:HOH:O	2.50	0.45
2:I:78:LEU:N	2:I:78:LEU:HD12	2.31	0.45
1:F:160:ASP:HB2	2:L:63:ARG:HD3	1.98	0.45
2:J:24:LEU:HD23	2:J:24:LEU:C	2.42	0.45
1:E:38:ALA:O	1:E:39:SER:C	2.58	0.45
1:F:61:GLN:HG2	1:F:97:TRP:HE1	1.82	0.45
1:B:111:LEU:HD12	1:B:111:LEU:N	2.32	0.45
1:D:32:ARG:HH21	2:L:92:GLU:CD	2.25	0.45
1:E:10:PHE:HD2	1:E:137:VAL:HG21	1.81	0.45
1:F:149:THR:HG23	1:F:149:THR:O	2.17	0.45
2:I:63:ARG:HB2	2:I:66:LEU:HD12	1.98	0.45
1:F:113:ASP:C	1:F:113:ASP:OD1	2.60	0.44
2:I:102:ILE:N	2:I:102:ILE:HD12	2.31	0.44
2:L:53:TYR:CD2	2:L:58:LEU:HD21	2.52	0.44
1:E:18:TYR:CD1	1:E:36:TYR:HB2	2.53	0.44
2:H:59:MET:HE1	2:H:64:THR:HA	1.99	0.44
2:I:78:LEU:HD11	2:I:107:THR:HG23	1.99	0.44
1:E:168:ASN:N	1:E:168:ASN:HD22	2.16	0.44
1:D:10:PHE:CE2	1:D:14:VAL:HG21	2.52	0.44
1:D:27:LEU:HD23	1:D:99:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:LEU:CD2	1:F:47:SER:CB	2.96	0.44
1:F:11:PRO:HB2	1:F:14:VAL:CG1	2.48	0.44
2:I:101:ASN:C	2:I:102:ILE:HD12	2.43	0.44
1:B:32:ARG:CB	4:B:301:HOH:O	2.65	0.44
1:D:25:LEU:HD21	1:D:104:LYS:HB3	2.00	0.44
1:B:69:ILE:HA	1:B:72:LEU:CD2	2.48	0.44
1:C:69:ILE:HA	1:C:72:LEU:HD21	1.99	0.44
1:D:26:ASP:OD1	1:D:28:THR:OG1	2.35	0.44
1:F:122:ILE:HG22	1:F:122:ILE:O	2.18	0.44
1:C:54:GLY:O	1:C:57:THR:OG1	2.36	0.43
1:F:14:VAL:HG22	1:F:39:SER:OG	2.18	0.43
2:I:26:ASP:HB2	2:I:60:LYS:HD3	1.99	0.43
2:J:10:GLU:OE2	2:J:36:PRO:HA	2.19	0.43
2:J:23:MET:HG3	2:J:27:ASN:OD1	2.18	0.43
1:D:103:ILE:HD13	1:D:103:ILE:N	2.33	0.43
2:H:13:ILE:HD11	2:H:35:LEU:HD11	1.99	0.43
2:H:81:ILE:HG23	2:H:102:ILE:CD1	2.48	0.43
2:H:109:HIS:CE1	4:H:305:HOH:O	2.71	0.43
2:I:21:LEU:HD11	2:I:77:ILE:HG23	2.00	0.43
2:J:24:LEU:HD21	2:J:59:MET:HA	2.00	0.43
1:A:25:LEU:CD1	1:A:104:LYS:HB3	2.48	0.43
1:E:14:VAL:CG2	1:E:38:ALA:HB3	2.42	0.43
1:F:59:THR:HG23	2:L:110:GLY:HA3	2.00	0.43
2:L:76:GLY:O	2:L:107:THR:HG22	2.19	0.43
1:E:61:GLN:O	1:E:66:THR:OG1	2.37	0.43
2:J:55:SER:HA	2:J:59:MET:CG	2.49	0.43
2:L:11:ILE:CD1	2:L:37:ALA:HA	2.49	0.43
1:B:18:TYR:CB	1:B:111:LEU:HG	2.49	0.43
2:I:43:LYS:HE2	2:I:43:LYS:N	2.33	0.43
2:J:33:ILE:HD12	2:J:33:ILE:N	2.34	0.43
2:L:79:VAL:HG12	2:L:86:TRP:HB3	2.00	0.43
2:J:59:MET:CE	2:J:64:THR:HA	2.49	0.43
2:J:60:LYS:HE2	2:J:60:LYS:HA	2.01	0.43
1:F:71:LYS:HZ3	1:F:74:GLN:HG3	1.82	0.42
1:F:77:GLN:HE21	1:F:77:GLN:HB3	1.52	0.42
2:G:45:VAL:HG13	2:G:96:ILE:HB	1.99	0.42
2:G:95:GLU:O	2:G:97:GLN:OE1	2.37	0.42
1:A:4:LEU:HD23	1:A:135:ILE:HD13	2.01	0.42
1:C:60:CSS:SD	4:C:306:HOH:O	2.61	0.42
1:D:69:ILE:O	1:D:72:LEU:CD2	2.67	0.42
1:E:52:VAL:HB	1:E:60:CSS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:35:LEU:HB3	2:J:36:PRO:HD2	2.01	0.42
2:J:103:LEU:HD11	2:J:105:VAL:CG2	2.49	0.42
1:F:42:LEU:CD2	1:F:47:SER:HB2	2.49	0.42
2:L:50:LEU:CD2	2:L:102:ILE:CD1	2.98	0.42
1:B:169:GLN:HE21	1:B:169:GLN:HB2	1.72	0.42
1:F:138:LYS:NZ	1:F:139:ASP:OD2	2.50	0.42
2:H:91:GLU:H	2:H:91:GLU:HG2	1.52	0.42
2:L:50:LEU:O	2:L:53:TYR:N	2.52	0.42
2:L:69:LEU:HD13	2:L:69:LEU:C	2.44	0.42
2:L:73:ILE:HD11	2:L:77:ILE:HG21	2.02	0.42
1:D:78:ALA:HB1	1:D:166:LEU:HD12	2.02	0.42
1:C:4:LEU:HD22	1:C:142:VAL:HG21	2.01	0.42
1:C:161:ALA:O	1:C:165:VAL:HG12	2.19	0.42
1:F:103:ILE:N	1:F:103:ILE:HD13	2.34	0.42
1:F:135:ILE:HD12	1:F:135:ILE:N	2.35	0.42
2:J:59:MET:O	2:J:60:LYS:HE2	2.20	0.42
1:A:59:THR:HG21	1:A:152:GLY:HA2	2.02	0.42
1:F:150:VAL:HG13	1:F:153:SER:HB2	2.02	0.42
1:D:78:ALA:HB1	1:D:166:LEU:CD1	2.50	0.41
1:F:118:PHE:CD1	1:F:118:PHE:C	2.98	0.41
1:A:29:VAL:O	1:A:29:VAL:CG2	2.69	0.41
1:D:48:VAL:HB	1:D:83:VAL:HG22	2.01	0.41
1:F:6:PRO:HA	1:F:142:VAL:HG23	2.01	0.41
1:F:124:TRP:HE3	1:F:133:TYR:CG	2.38	0.41
1:C:53:PRO:HB2	4:C:306:HOH:O	2.18	0.41
1:C:143:VAL:HG11	1:C:169:GLN:HE21	1.85	0.41
1:F:148:ASP:O	1:F:149:THR:HG22	2.20	0.41
1:F:155:GLU:HG3	1:F:156:LYS:HG3	2.01	0.41
2:I:11:ILE:HD11	2:I:97:GLN:C	2.45	0.41
2:I:67:PHE:O	2:I:73:ILE:HD12	2.20	0.41
2:L:67:PHE:HD2	2:L:68:VAL:HG13	1.85	0.41
1:B:29:VAL:CG2	1:C:26:ASP:OD2	2.68	0.41
1:C:10:PHE:CE1	1:C:14:VAL:HG11	2.35	0.41
1:F:47:SER:HB3	1:F:82:ARG:HG2	2.02	0.41
2:H:81:ILE:HG23	2:H:102:ILE:HD13	2.02	0.41
2:J:36:PRO:HG2	2:J:38:LYS:O	2.21	0.41
2:K:11:ILE:HD11	2:K:97:GLN:C	2.45	0.41
1:A:1:MET:HE3	1:A:1:MET:HB3	1.94	0.41
1:B:109:LEU:HB3	1:B:111:LEU:HD11	2.02	0.41
1:D:108:ILE:HG22	1:D:110:PHE:CE1	2.56	0.41
2:L:50:LEU:C	2:L:50:LEU:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:50:LEU:O	2:G:54:ILE:HG13	2.21	0.41
1:A:25:LEU:HD11	1:A:104:LYS:HB3	2.02	0.41
1:C:27:LEU:CD1	1:D:27:LEU:HD11	2.51	0.41
1:A:156:LYS:HA	1:A:156:LYS:HD2	1.83	0.41
1:C:25:LEU:CD1	1:C:104:LYS:HB3	2.50	0.41
1:C:33:PRO:HG2	1:C:92:PHE:HE1	1.85	0.41
1:C:143:VAL:HG11	1:C:169:GLN:NE2	2.35	0.41
1:D:107:SER:O	1:D:108:ILE:HD12	2.20	0.41
2:G:52:ASP:OD1	2:G:56:LYS:NZ	2.51	0.41
2:I:63:ARG:HD2	2:I:66:LEU:HD11	2.03	0.41
1:C:42:LEU:CD2	1:C:47:SER:OG	2.57	0.41
2:I:45:VAL:CG2	2:I:49:PHE:HD2	2.34	0.40
2:L:50:LEU:HD11	2:L:54:ILE:HD11	2.03	0.40
2:J:61:ASP:OD1	2:J:61:ASP:C	2.64	0.40
1:B:10:PHE:CD2	1:B:42:LEU:HD23	2.56	0.40
1:D:72:LEU:N	1:D:72:LEU:HD22	2.36	0.40
2:L:78:LEU:HB2	2:L:105:VAL:HG13	2.03	0.40
1:D:29:VAL:O	1:D:29:VAL:HG23	2.21	0.40
1:F:77:GLN:O	1:F:78:ALA:HB3	2.21	0.40
1:D:168:ASN:OD1	1:D:168:ASN:N	2.55	0.40
2:G:59:MET:HE1	2:G:64:THR:HG22	2.02	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	168/174 (97%)	160 (95%)	8 (5%)	0	100	100
1	B	169/174 (97%)	161 (95%)	8 (5%)	0	100	100
1	C	166/174 (95%)	160 (96%)	6 (4%)	0	100	100
1	D	167/174 (96%)	158 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	166/174 (95%)	160 (96%)	6 (4%)	0	100	100
1	F	165/174 (95%)	155 (94%)	10 (6%)	0	100	100
2	G	101/111 (91%)	96 (95%)	5 (5%)	0	100	100
2	H	102/111 (92%)	98 (96%)	4 (4%)	0	100	100
2	I	102/111 (92%)	96 (94%)	6 (6%)	0	100	100
2	J	101/111 (91%)	92 (91%)	9 (9%)	0	100	100
2	K	102/111 (92%)	98 (96%)	4 (4%)	0	100	100
2	L	102/111 (92%)	95 (93%)	7 (7%)	0	100	100
All	All	1611/1710 (94%)	1529 (95%)	82 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	132/134 (98%)	132 (100%)	0	100	100
1	B	134/134 (100%)	133 (99%)	1 (1%)	76	89
1	C	132/134 (98%)	130 (98%)	2 (2%)	57	80
1	D	132/134 (98%)	132 (100%)	0	100	100
1	E	132/134 (98%)	130 (98%)	2 (2%)	57	80
1	F	131/134 (98%)	129 (98%)	2 (2%)	57	80
2	G	92/98 (94%)	91 (99%)	1 (1%)	65	84
2	H	93/98 (95%)	93 (100%)	0	100	100
2	I	93/98 (95%)	91 (98%)	2 (2%)	45	73
2	J	92/98 (94%)	91 (99%)	1 (1%)	65	84
2	K	93/98 (95%)	92 (99%)	1 (1%)	65	84
2	L	93/98 (95%)	92 (99%)	1 (1%)	65	84
All	All	1349/1392 (97%)	1336 (99%)	13 (1%)	68	86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	169	GLN
1	C	29	VAL
1	C	30	SER
1	E	30	SER
1	E	82	ARG
1	F	77	GLN
1	F	165	VAL
2	G	34	SER
2	I	61	ASP
2	I	63	ARG
2	J	14	THR
2	K	55	SER
2	L	102	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	B	61	GLN
1	B	126	ASN
1	B	169	GLN
1	C	169	GLN
1	D	126	ASN
1	E	74	GLN
1	E	77	GLN
1	E	168	ASN
1	F	77	GLN
2	G	27	ASN
2	G	71	ASN
2	G	82	ASN
2	G	97	GLN
2	H	72	HIS
2	H	97	GLN
2	I	31	HIS
2	I	97	GLN
2	J	97	GLN
2	K	71	ASN
2	L	71	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	CSS	A	60	1	4,6,7	1.21	0	2,6,8	0.56	0
1	CSS	C	60	1	4,6,7	0.98	0	2,6,8	0.59	0
1	CSS	E	60	1	4,6,7	0.76	0	2,6,8	0.86	0
1	CSS	B	60	1	4,6,7	1.04	0	2,6,8	0.17	0
1	CSS	F	60	1	4,6,7	1.07	0	2,6,8	0.19	0
1	CSS	D	60	1	4,6,7	0.97	0	2,6,8	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSS	A	60	1	-	0/1/5/7	-
1	CSS	C	60	1	-	0/1/5/7	-
1	CSS	E	60	1	-	0/1/5/7	-
1	CSS	B	60	1	-	0/1/5/7	-
1	CSS	F	60	1	-	0/1/5/7	-
1	CSS	D	60	1	-	0/1/5/7	-

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.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	60	CSS	4	0
1	C	60	CSS	2	0
1	E	60	CSS	3	0
1	B	60	CSS	4	0
1	D	60	CSS	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 41 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	170/174 (97%)	0.23	1 (0%) 85 83	58, 73, 100, 143	0
1	B	171/174 (98%)	0.29	9 (5%) 32 28	59, 80, 112, 150	0
1	C	168/174 (96%)	0.58	10 (5%) 27 24	75, 99, 133, 163	1 (0%)
1	D	169/174 (97%)	0.81	14 (8%) 17 15	87, 131, 165, 190	0
1	E	168/174 (96%)	0.59	10 (5%) 27 24	81, 106, 152, 182	0
1	F	167/174 (95%)	0.86	10 (5%) 27 24	86, 128, 177, 204	0
2	G	103/111 (92%)	0.64	2 (1%) 66 62	77, 121, 162, 178	0
2	H	104/111 (93%)	0.52	4 (3%) 44 39	69, 89, 139, 179	1 (0%)
2	I	104/111 (93%)	0.80	9 (8%) 16 14	90, 114, 161, 185	1 (0%)
2	J	103/111 (92%)	0.98	9 (8%) 16 14	80, 134, 181, 201	0
2	K	104/111 (93%)	0.44	3 (2%) 53 49	68, 89, 122, 166	0
2	L	104/111 (93%)	0.87	10 (9%) 13 11	101, 137, 170, 205	0
All	All	1635/1710 (95%)	0.62	91 (5%) 30 26	58, 105, 162, 205	3 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	LEU	6.6
2	J	66	LEU	5.1
2	L	90	GLY	4.8
2	K	8	LEU	4.6
1	B	170	GLY	4.5
2	I	8	LEU	4.5
1	F	2	ALA	3.9
2	K	111	GLY	3.9
1	D	170	GLY	3.8
2	L	15	VAL	3.7
1	E	47	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	J	111	GLY	3.3
2	I	59	MET	3.3
1	C	88	SER	3.3
1	A	30	SER	3.2
1	E	1	MET	3.2
2	J	110	GLY	3.2
2	L	8	LEU	3.1
1	B	3	PRO	3.1
1	D	2	ALA	3.1
2	L	88	LEU	3.0
1	C	56	PHE	3.0
1	E	10	PHE	3.0
1	D	149	THR	3.0
1	F	24	SER	2.9
1	B	30	SER	2.9
1	D	166	LEU	2.9
1	E	2	ALA	2.9
2	I	60	LYS	2.8
1	C	55	ALA	2.8
1	D	4	LEU	2.8
1	C	1	MET	2.8
1	B	2	ALA	2.8
1	D	163	LEU	2.8
2	H	88	LEU	2.7
2	H	90	GLY	2.6
2	H	8	LEU	2.6
1	C	151	ARG	2.6
2	I	27	ASN	2.6
1	D	30	SER	2.6
1	C	31	GLY	2.5
1	F	3	PRO	2.5
1	F	150	VAL	2.5
2	J	26	ASP	2.5
1	F	49	LEU	2.5
2	L	67	PHE	2.5
2	G	93	ALA	2.4
1	E	3	PRO	2.4
2	I	100	ASP	2.4
2	G	111	GLY	2.4
1	F	72	LEU	2.4
1	E	97	TRP	2.4
1	C	30	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	28	THR	2.3
2	I	58	LEU	2.3
2	K	69	LEU	2.3
2	J	109	HIS	2.3
1	C	32	ARG	2.3
2	L	69	LEU	2.3
1	F	68	PHE	2.3
2	L	49	PHE	2.3
1	B	169	GLN	2.2
2	I	104	PHE	2.2
1	E	18	TYR	2.2
2	I	33	ILE	2.2
1	E	48	VAL	2.2
1	B	1	MET	2.2
1	E	31	GLY	2.2
1	F	48	VAL	2.2
2	I	77	ILE	2.2
1	D	138	LYS	2.2
1	D	93	VAL	2.1
2	L	59	MET	2.1
1	D	152	GLY	2.1
2	L	81	ILE	2.1
2	J	62	PRO	2.1
1	C	169	GLN	2.1
1	D	22	THR	2.1
1	B	32	ARG	2.1
2	H	91	GLU	2.1
1	B	141	LYS	2.1
1	D	150	VAL	2.1
1	F	84	LEU	2.1
2	J	51	ILE	2.1
1	D	16	PHE	2.0
2	J	78	LEU	2.0
1	D	31	GLY	2.0
2	J	86	TRP	2.0
1	E	42	LEU	2.0
2	L	66	LEU	2.0
1	F	154	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSS	F	60	7/8	0.83	0.17	103,106,119,120	0
1	CSS	E	60	7/8	0.92	0.11	75,85,94,100	0
1	CSS	C	60	7/8	0.93	0.11	68,84,89,89	0
1	CSS	B	60	7/8	0.95	0.15	56,60,80,100	0
1	CSS	A	60	7/8	0.97	0.10	56,76,81,84	0
1	CSS	D	60	7/8	0.97	0.11	96,97,103,104	0

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	ZN	F	301	1/1	0.38	0.20	168,168,168,168	1
3	ZN	B	203	1/1	0.56	0.18	204,204,204,204	0
3	ZN	J	203	1/1	0.68	0.12	165,165,165,165	0
3	ZN	H	208	1/1	0.75	0.18	160,160,160,160	0
3	ZN	B	202	1/1	0.76	0.10	165,165,165,165	0
3	ZN	D	302	1/1	0.77	0.07	202,202,202,202	0
3	ZN	C	201	1/1	0.77	0.08	189,189,189,189	0
3	ZN	J	202	1/1	0.78	0.09	206,206,206,206	0
3	ZN	C	203	1/1	0.79	0.18	155,155,155,155	1
3	ZN	E	202	1/1	0.79	0.10	180,180,180,180	0
3	ZN	J	204	1/1	0.81	0.13	151,151,151,151	1
3	ZN	D	301	1/1	0.83	0.12	155,155,155,155	1
3	ZN	B	201	1/1	0.85	0.27	64,64,64,64	1
3	ZN	K	306	1/1	0.85	0.15	179,179,179,179	0
3	ZN	K	302	1/1	0.86	0.15	153,153,153,153	0
3	ZN	E	203	1/1	0.86	0.18	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	L	201	1/1	0.87	0.06	208,208,208,208	0
3	ZN	H	203	1/1	0.88	0.09	162,162,162,162	0
3	ZN	I	301	1/1	0.88	0.08	144,144,144,144	1
3	ZN	C	202	1/1	0.90	0.07	165,165,165,165	0
3	ZN	I	304	1/1	0.90	0.08	146,146,146,146	0
3	ZN	A	201	1/1	0.91	0.10	163,163,163,163	0
3	ZN	H	205	1/1	0.91	0.11	136,136,136,136	0
3	ZN	H	207	1/1	0.91	0.08	98,98,98,98	0
3	ZN	H	201	1/1	0.91	0.12	92,92,92,92	0
3	ZN	I	303	1/1	0.92	0.12	134,134,134,134	0
3	ZN	E	201	1/1	0.92	0.04	186,186,186,186	0
3	ZN	L	202	1/1	0.92	0.09	164,164,164,164	0
3	ZN	F	302	1/1	0.93	0.06	171,171,171,171	0
3	ZN	H	206	1/1	0.94	0.14	118,118,118,118	0
3	ZN	K	303	1/1	0.94	0.12	142,142,142,142	0
3	ZN	K	304	1/1	0.94	0.13	130,130,130,130	0
3	ZN	I	302	1/1	0.95	0.16	156,156,156,156	0
3	ZN	H	202	1/1	0.95	0.05	89,89,89,89	1
3	ZN	K	301	1/1	0.95	0.07	163,163,163,163	0
3	ZN	L	203	1/1	0.96	0.06	115,115,115,115	0
3	ZN	I	305	1/1	0.97	0.07	113,113,113,113	0
3	ZN	K	305	1/1	0.97	0.07	135,135,135,135	0
3	ZN	H	204	1/1	0.98	0.09	93,93,93,93	0
3	ZN	G	201	1/1	0.98	0.05	117,117,117,117	0
3	ZN	J	201	1/1	0.98	0.05	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.