



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:50 am GMT

PDB ID : 5JM6
Title : Structure of Chaetomium thermophilum mApel
Authors : Bertipaglia, C.; Jakobi, A.J.; Wilmanns, M.; Sachse, C.
Deposited on : 2016-04-28
Resolution : 2.76 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

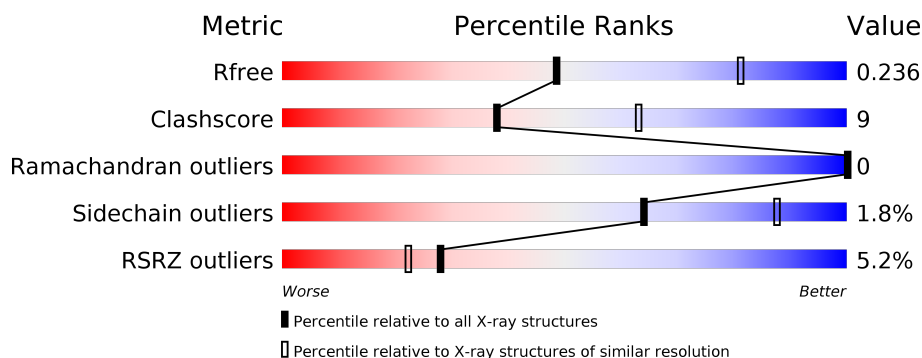
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	519	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	519	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>18%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	519	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	519	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>
1	E	519	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>18%</div> <div>•</div> <div>14%</div> </div> </div>
1	F	519	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20685 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 Aminopeptidase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3399	2177	581	625	16			
1	E	445	Total	C	N	O	S	0	0	0
			3399	2177	581	625	16			
1	F	445	Total	C	N	O	S	0	0	0
			3399	2177	581	625	16			
1	B	445	Total	C	N	O	S	0	0	0
			3399	2177	581	625	16			
1	C	445	Total	C	N	O	S	0	0	0
			3399	2177	581	625	16			
1	D	445	Total	C	N	O	S	0	0	0
			3399	2177	581	625	16			

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

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

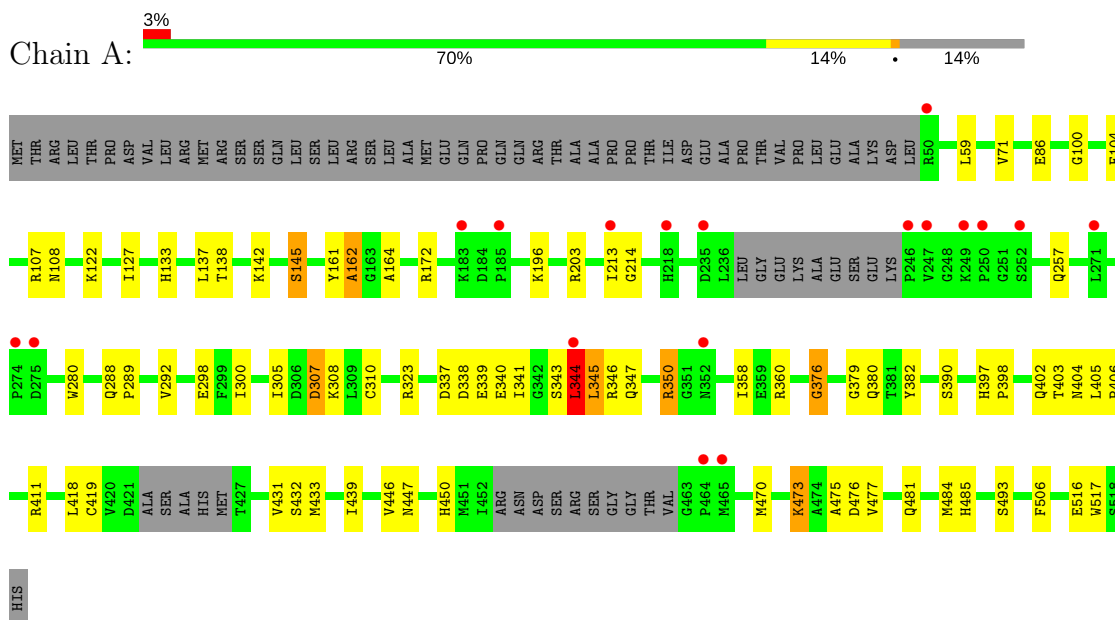
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	E	52	Total 52	O 52	0	0
3	F	51	Total 51	O 51	0	0
3	B	49	Total 49	O 49	0	0
3	C	41	Total 41	O 41	0	0
3	D	57	Total 57	O 57	0	0

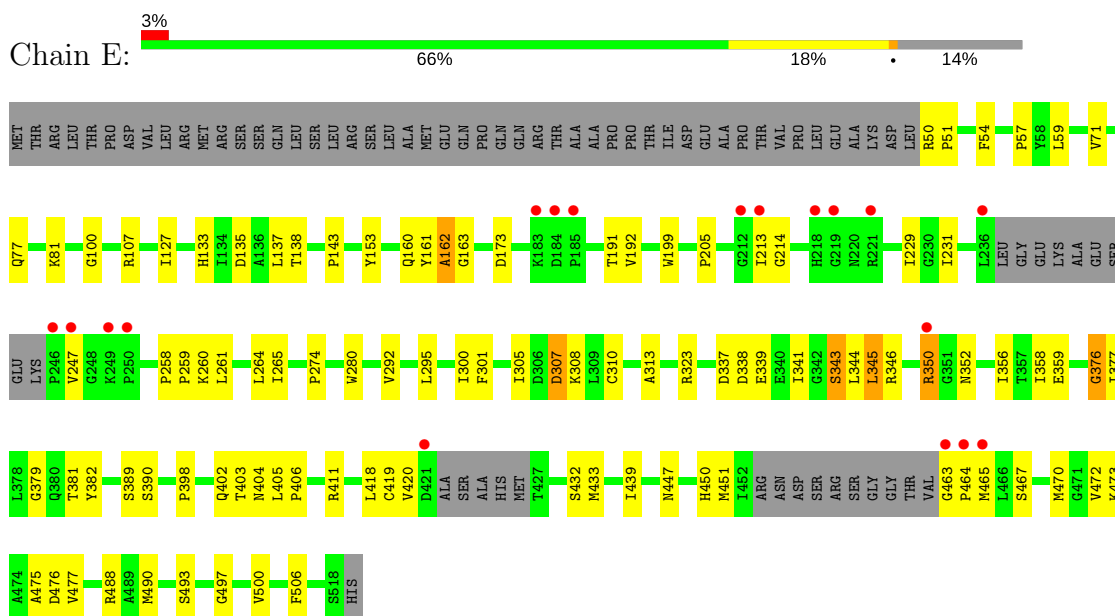
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Aminopeptidase-like protein



• Molecule 1: Aminopeptidase-like protein

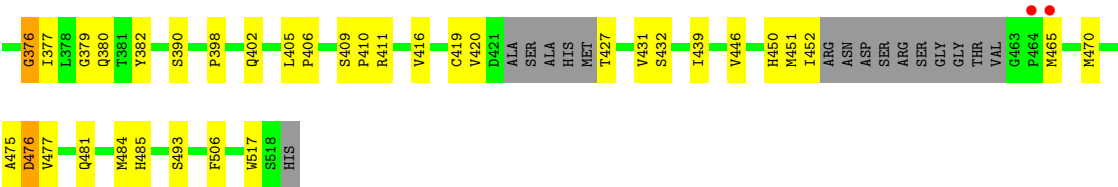


[illegible]

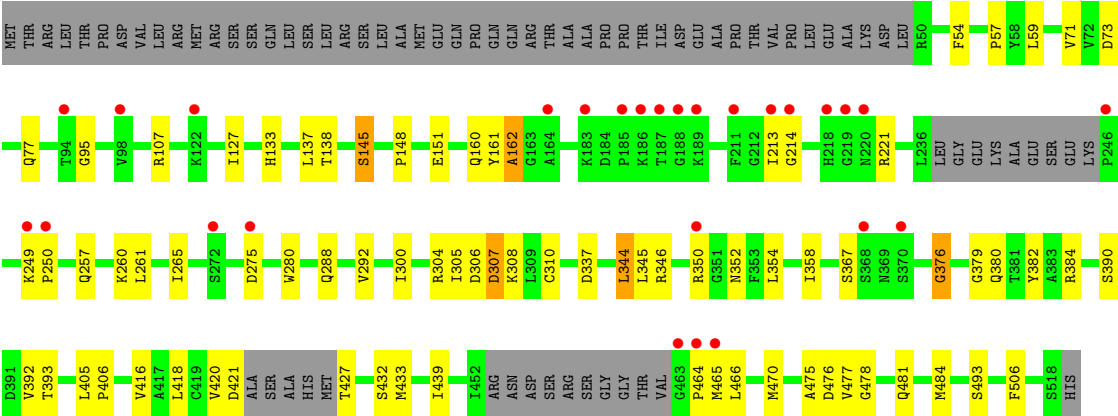
Chain B:

Item	Category
G444	66%
H450	66%
M451	66%
L452	66%
ARG	66%
ASN	66%
ASP	66%
SER	66%
ARG	66%
SER	66%
GLY	66%
GLY	66%
THR	66%
VAL	66%
G463	66%
P464	66%
M465	66%
L466	66%
S467	66%
K473	66%
V477	66%
Q481	66%
L482	66%
S483	66%
M484	66%
H485	66%
S486	66%
L487	66%
M490	66%
S493	66%
K501	66%
F506	66%
S518	66%
HIS	66%
L344	18%
L346	18%
R346	18%
R350	18%
G351	18%
N352	18%
L356	18%
S357	18%
L358	18%
E363	18%
G376	18%
L377	18%
L378	18%
G379	18%
Q380	18%
T381	18%
V382	18%
A383	18%
R384	18%
S390	18%
D391	18%
V392	18%
A395	18%
F400	18%
T401	18%
Q402	18%
T403	18%
M404	18%
L405	18%
P406	18%
R411	18%
V416	18%
A417	18%
L418	18%
C419	18%
V420	18%
D421	18%
ALA	18%
SER	18%
ALA	18%
HIS	18%
MET	18%
T427	18%
T428	18%
D429	18%
M433	18%
L439	18%
S443	18%
G214	14%
G217	14%
H218	14%
G219	14%
N220	14%
R221	14%
L236	14%
LEU	14%
GLY	14%
GLU	14%
LYS	14%
ALA	14%
GLU	14%
GLU	14%
LYS	14%
P246	14%
R249	14%
K250	14%
A251	14%
Q257	14%
L261	14%
L265	14%
L266	14%
L269	14%
G270	14%
Q271	14%
S272	14%
D273	14%
P274	14%
D275	14%
W280	14%
V292	14%
T300	14%
L305	14%
D306	14%
R307	14%
K308	14%
L309	14%
C310	14%
A324	14%
P325	14%
D337	14%
D338	14%
I341	14%
G342	14%
G212	14%
T213	14%

Chain C:



● Molecule 1: Aminopeptidase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	121.02Å 143.89Å 201.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 2.76 53.75 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.07-2.76) 98.6 (53.75-2.76)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.77Å)	Xtriage
Refinement program	PHENIX (dev_2313: ???)	Depositor
R, R_{free}	0.208 , 0.242 0.204 , 0.236	Depositor DCC
R_{free} test set	4506 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20685	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.28	0/3481	0.60	3/4728 (0.1%)
1	B	0.28	0/3481	0.56	2/4728 (0.0%)
1	C	0.28	0/3481	0.55	0/4728
1	D	0.29	0/3481	0.57	1/4728 (0.0%)
1	E	0.29	0/3481	0.58	1/4728 (0.0%)
1	F	0.27	0/3481	0.57	3/4728 (0.1%)
All	All	0.28	0/20886	0.57	10/28368 (0.0%)

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
1	A	0	3
1	B	0	2
1	C	0	2
1	D	0	3
1	E	0	2
1	F	0	3
All	All	0	15

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	LEU	CA-CB-CG	9.96	138.20	115.30
1	F	345	LEU	CA-CB-CG	8.20	134.16	115.30
1	A	345	LEU	CA-CB-CG	7.16	131.76	115.30
1	D	344	LEU	CA-CB-CG	6.89	131.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	344	LEU	CA-CB-CG	6.63	130.54	115.30
1	F	137	LEU	CA-CB-CG	5.74	128.50	115.30
1	E	350	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	345	LEU	CB-CG-CD1	-5.38	101.86	111.00
1	B	307	ASP	N-CA-C	5.06	124.66	111.00
1	B	306	ASP	C-N-CA	5.04	134.29	121.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	ALA	Peptide
1	A	344	LEU	Peptide
1	A	376	GLY	Peptide
1	B	376	GLY	Peptide
1	B	95	GLY	Peptide
1	C	376	GLY	Peptide
1	C	95	GLY	Peptide
1	D	162	ALA	Peptide
1	D	376	GLY	Peptide
1	D	95	GLY	Peptide
1	E	162	ALA	Peptide
1	E	376	GLY	Peptide
1	F	344	LEU	Peptide
1	F	376	GLY	Peptide
1	F	95	GLY	Peptide

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	3399	0	3406	58	1
1	B	3399	0	3406	75	0
1	C	3399	0	3406	68	2
1	D	3399	0	3406	51	0
1	E	3399	0	3406	80	0
1	F	3399	0	3406	49	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	29	0	0	3	0
3	B	49	0	0	9	0
3	C	41	0	0	3	0
3	D	57	0	0	8	0
3	E	52	0	0	5	0
3	F	51	0	0	2	1
All	All	20685	0	20436	357	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (357) 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:350:ARG:NH2	1:E:465:MET:HB2	1.76	0.99
1:E:339:GLU:OE2	1:E:343:SER:OG	1.93	0.86
1:E:339:GLU:OE1	1:E:463:GLY:N	2.08	0.85
1:B:344:LEU:HD11	1:B:350:ARG:HG2	1.60	0.83
1:C:304:ARG:NH2	3:C:701:HOH:O	2.11	0.83
1:E:350:ARG:HH22	1:E:465:MET:HB2	1.42	0.82
1:E:343:SER:O	1:E:350:ARG:HB2	1.80	0.80
1:B:346:ARG:NH2	3:B:706:HOH:O	2.16	0.78
1:C:161:TYR:CE2	1:C:341:ILE:HD11	2.20	0.77
1:B:344:LEU:CD1	1:B:350:ARG:HG2	2.15	0.76
1:F:107:ARG:HD3	1:F:346:ARG:HG2	1.67	0.76
1:A:100:GLY:O	1:A:323:ARG:NH1	2.19	0.76
1:B:418:LEU:HD23	1:B:433:MET:HG2	1.67	0.75
1:E:107:ARG:HD3	1:E:346:ARG:HG2	1.69	0.75
1:E:345:LEU:CD1	1:E:346:ARG:H	2.00	0.75
1:A:203:ARG:NH1	3:A:703:HOH:O	2.20	0.75
1:E:344:LEU:HD12	1:E:350:ARG:HB3	1.69	0.74
1:B:78:LYS:NZ	3:B:703:HOH:O	2.12	0.74
1:E:205:PRO:O	3:E:701:HOH:O	2.03	0.74
1:A:137:LEU:HG	1:A:162:ALA:HB3	1.70	0.74
1:D:418:LEU:HD23	1:D:433:MET:HG2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:LEU:HD23	1:D:465:MET:SD	2.28	0.73
1:B:404:ASN:OD1	3:B:701:HOH:O	2.05	0.73
1:A:137:LEU:HG	1:A:162:ALA:CB	2.18	0.73
1:A:107:ARG:HD3	1:A:346:ARG:HG2	1.70	0.72
1:A:418:LEU:HD23	1:A:433:MET:HG2	1.70	0.72
1:A:419:CYS:SG	1:A:450:HIS:ND1	2.63	0.72
1:B:107:ARG:HD3	1:B:346:ARG:HG2	1.72	0.72
1:E:137:LEU:HD22	1:E:162:ALA:HB1	1.72	0.71
1:F:348:GLY:O	3:F:701:HOH:O	2.08	0.71
1:F:170:TRP:O	3:F:702:HOH:O	2.08	0.71
1:A:127:ILE:HD13	1:A:358:ILE:HD13	1.72	0.71
1:C:107:ARG:HD3	1:C:346:ARG:HG2	1.73	0.70
1:B:307:ASP:OD1	1:B:310:CYS:HB2	1.91	0.70
1:E:231:ILE:O	3:E:702:HOH:O	2.09	0.69
1:E:490:MET:HE1	1:C:205:PRO:HB3	1.74	0.69
1:B:195:VAL:HG22	1:B:269:LEU:HD21	1.75	0.69
1:A:142:LYS:HD3	1:C:451:MET:HE1	1.75	0.69
1:A:404:ASN:OD1	3:A:701:HOH:O	2.11	0.68
1:B:109:GLY:O	3:B:702:HOH:O	2.10	0.68
1:D:337:ASP:O	3:D:703:HOH:O	2.11	0.68
1:E:173:ASP:OD1	3:E:703:HOH:O	2.12	0.68
1:C:344:LEU:HD12	1:C:344:LEU:C	2.14	0.67
1:D:151:GLU:OE2	3:D:702:HOH:O	2.11	0.67
1:C:145:SER:OG	1:C:257:GLN:NE2	2.28	0.67
1:E:345:LEU:HD12	1:E:346:ARG:H	1.59	0.67
1:B:51:PRO:O	3:B:704:HOH:O	2.13	0.66
1:E:50:ARG:HG3	1:E:51:PRO:HD3	1.77	0.66
1:B:405:LEU:HD12	1:B:406:PRO:HD2	1.78	0.66
1:A:516:GLU:OE2	3:A:702:HOH:O	2.13	0.65
1:D:107:ARG:HD3	1:D:346:ARG:HG2	1.78	0.65
1:A:59:LEU:HD11	1:A:292:VAL:HG13	1.77	0.65
1:E:464:PRO:HB2	1:E:465:MET:HE2	1.78	0.65
1:F:59:LEU:HD11	1:F:292:VAL:HG13	1.79	0.65
1:E:127:ILE:HD13	1:E:358:ILE:HD13	1.79	0.64
1:E:418:LEU:HD23	1:E:433:MET:HG2	1.79	0.64
1:C:304:ARG:NH1	3:C:705:HOH:O	2.29	0.64
1:E:160:GLN:OE1	1:E:163:GLY:N	2.27	0.63
1:E:59:LEU:HD11	1:E:292:VAL:HG13	1.80	0.63
1:E:345:LEU:HD12	1:E:346:ARG:N	2.14	0.63
1:A:439:ILE:HD13	1:A:506:PHE:HA	1.80	0.63
1:B:429:ASP:OD1	1:B:473:LYS:NZ	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:419:CYS:SG	1:F:450:HIS:ND1	2.68	0.62
1:A:344:LEU:HB3	1:A:350:ARG:HG3	1.79	0.62
1:A:137:LEU:HD11	1:A:340:GLU:OE1	1.99	0.62
1:A:133:HIS:O	1:A:307:ASP:HB3	1.99	0.62
1:C:59:LEU:HD11	1:C:292:VAL:HG13	1.81	0.62
1:D:59:LEU:HD11	1:D:292:VAL:HG13	1.82	0.62
1:F:379:GLY:HA2	1:F:382:TYR:HB2	1.81	0.61
1:D:464:PRO:HB3	1:D:476:ASP:OD1	2.01	0.61
1:C:161:TYR:HE2	1:C:341:ILE:HD11	1.65	0.61
1:B:50:ARG:HA	1:B:53:HIS:ND1	2.16	0.61
1:B:352:ASN:OD1	1:B:356:ILE:HB	2.00	0.60
1:E:143:PRO:HG2	1:D:420:VAL:HG21	1.82	0.60
1:D:432:SER:HB3	1:D:475:ALA:HB2	1.84	0.60
1:F:127:ILE:HD13	1:F:358:ILE:HD13	1.84	0.60
1:B:363:GLU:OE2	3:B:705:HOH:O	2.16	0.60
1:E:344:LEU:HD23	1:D:465:MET:CE	2.31	0.60
1:E:419:CYS:SG	1:E:450:HIS:ND1	2.69	0.60
1:B:195:VAL:HG11	1:B:265:ILE:HD12	1.84	0.60
1:B:344:LEU:O	1:B:345:LEU:HG	2.01	0.60
1:D:384:ARG:NH1	3:D:713:HOH:O	2.34	0.60
1:E:488:ARG:O	1:C:203:ARG:NH2	2.35	0.59
1:E:352:ASN:OD1	1:E:356:ILE:HB	2.02	0.59
1:A:379:GLY:HA2	1:A:382:TYR:HB2	1.84	0.59
1:B:145:SER:OG	1:B:257:GLN:NE2	2.35	0.59
1:E:379:GLY:HA2	1:E:382:TYR:HB2	1.84	0.59
1:E:465:MET:HG3	1:F:344:LEU:HD13	1.85	0.59
1:B:344:LEU:CD1	1:B:350:ARG:CG	2.80	0.59
1:E:345:LEU:CD1	1:E:346:ARG:N	2.66	0.59
1:C:233:ASN:HB3	1:C:236:LEU:HD12	1.85	0.59
1:F:133:HIS:O	1:F:307:ASP:HB3	2.02	0.59
1:B:59:LEU:HD11	1:B:292:VAL:HG13	1.83	0.59
1:E:337:ASP:OD1	1:E:338:ASP:N	2.35	0.58
1:B:307:ASP:OD2	1:B:391:ASP:HA	2.03	0.58
1:E:100:GLY:O	1:E:323:ARG:NH1	2.36	0.58
1:F:439:ILE:HD13	1:F:506:PHE:HA	1.85	0.57
1:A:405:LEU:HD12	1:A:406:PRO:HD2	1.85	0.57
1:B:439:ILE:HD13	1:B:506:PHE:HA	1.87	0.57
1:C:307:ASP:OD1	1:C:310:CYS:HB2	2.04	0.57
1:F:73:ASP:O	1:F:77:GLN:HG2	2.04	0.57
1:B:344:LEU:HD12	1:B:350:ARG:CB	2.34	0.57
1:C:419:CYS:SG	1:C:450:HIS:ND1	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:HD12	1:C:344:LEU:O	2.04	0.57
1:E:350:ARG:HH22	1:E:465:MET:CB	2.17	0.57
1:D:73:ASP:O	1:D:77:GLN:HG2	2.04	0.57
1:B:137:LEU:HD22	1:B:162:ALA:O	2.03	0.57
1:E:213:ILE:HG22	1:E:214:GLY:H	1.70	0.56
1:E:345:LEU:HD13	1:E:346:ARG:H	1.69	0.56
1:C:439:ILE:HD13	1:C:506:PHE:HA	1.88	0.56
1:F:405:LEU:HD12	1:F:406:PRO:HD2	1.87	0.56
1:D:137:LEU:HD22	1:D:162:ALA:HB1	1.88	0.56
1:B:127:ILE:HD13	1:B:358:ILE:HD13	1.88	0.56
1:D:307:ASP:OD1	1:D:310:CYS:HB2	2.06	0.56
1:E:313:ALA:HA	1:E:500:VAL:HG12	1.88	0.56
1:D:439:ILE:HD13	1:D:506:PHE:HA	1.88	0.56
1:C:300:ILE:HG13	1:C:493:SER:HA	1.86	0.55
1:F:464:PRO:HB3	1:F:476:ASP:OD2	2.06	0.55
1:E:161:TYR:CE2	1:E:341:ILE:HD11	2.42	0.55
1:C:379:GLY:HA2	1:C:382:TYR:HB2	1.87	0.55
1:D:107:ARG:NH1	1:D:352:ASN:OD1	2.25	0.55
1:C:343:SER:O	1:C:348:GLY:HA3	2.07	0.55
1:B:444:GLY:O	1:B:501:LYS:NZ	2.34	0.55
1:E:405:LEU:HD12	1:E:406:PRO:HD2	1.88	0.55
1:E:133:HIS:O	1:E:307:ASP:HB3	2.07	0.54
1:E:377:ILE:O	1:E:381:THR:HG23	2.07	0.54
1:A:345:LEU:HD23	1:C:465:MET:HG2	1.90	0.54
1:D:376:GLY:O	1:D:380:GLN:NE2	2.39	0.54
1:D:145:SER:OG	1:D:257:GLN:OE1	2.26	0.54
1:D:304:ARG:NH1	3:D:715:HOH:O	2.40	0.54
1:D:344:LEU:HD23	1:D:350:ARG:CB	2.38	0.54
1:B:191:THR:HG22	1:B:192:VAL:H	1.72	0.53
1:C:337:ASP:OD2	1:C:338:ASP:N	2.40	0.53
1:C:137:LEU:HD23	1:C:162:ALA:HB3	1.90	0.53
1:E:451:MET:SD	1:F:142:LYS:HD3	2.48	0.53
1:E:432:SER:HB3	1:E:475:ALA:HB2	1.90	0.53
1:A:145:SER:OG	1:A:257:GLN:OE1	2.27	0.53
1:A:305:ILE:O	1:A:307:ASP:N	2.41	0.53
1:D:344:LEU:HD23	1:D:350:ARG:HB3	1.90	0.53
1:C:127:ILE:HD13	1:C:358:ILE:HD13	1.91	0.53
1:E:137:LEU:HD22	1:E:162:ALA:CB	2.38	0.53
1:E:138:THR:O	1:E:161:TYR:HB3	2.08	0.53
1:F:50:ARG:HD2	1:F:501:LYS:NZ	2.24	0.53
1:A:432:SER:HB3	1:A:475:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:VAL:O	1:C:451:MET:HG3	2.09	0.53
1:C:405:LEU:HD12	1:C:406:PRO:HD2	1.91	0.53
1:E:439:ILE:HD13	1:E:506:PHE:HA	1.91	0.52
1:B:307:ASP:OD2	1:B:392:VAL:N	2.39	0.52
1:D:427:THR:HB	1:D:476:ASP:OD2	2.09	0.52
1:D:54:PHE:HA	1:D:57:PRO:HG2	1.91	0.52
1:E:305:ILE:O	1:E:307:ASP:N	2.42	0.52
1:D:305:ILE:O	1:D:307:ASP:N	2.42	0.52
1:D:379:GLY:HA2	1:D:382:TYR:HB2	1.92	0.52
1:E:490:MET:CE	1:C:205:PRO:HB3	2.39	0.52
1:D:288:GLN:OE1	3:D:704:HOH:O	2.19	0.52
1:E:191:THR:HG22	1:E:192:VAL:H	1.75	0.52
1:A:142:LYS:HD3	1:C:451:MET:CE	2.40	0.52
1:D:275:ASP:OD1	3:D:701:HOH:O	2.19	0.52
1:A:300:ILE:HG13	1:A:493:SER:HA	1.92	0.52
1:B:384:ARG:NH1	3:B:714:HOH:O	2.43	0.52
1:B:54:PHE:HA	1:B:57:PRO:HG2	1.91	0.52
1:A:431:VAL:HG13	1:A:517:TRP:CH2	2.45	0.51
1:C:161:TYR:CZ	1:C:341:ILE:HD11	2.45	0.51
1:F:86:GLU:HB2	1:F:104:PHE:CZ	2.45	0.51
1:B:305:ILE:O	1:B:307:ASP:N	2.43	0.51
1:B:307:ASP:OD2	1:B:391:ASP:OD1	2.28	0.51
1:B:416:VAL:HG11	1:B:477:VAL:HG13	1.93	0.51
1:C:305:ILE:O	1:C:307:ASP:N	2.44	0.51
1:C:137:LEU:HD22	1:C:164:ALA:HA	1.92	0.51
1:A:358:ILE:HD12	1:A:470:MET:CE	2.42	0.50
1:C:71:VAL:HG21	1:C:308:LYS:HE3	1.92	0.50
1:E:420:VAL:HG21	1:F:143:PRO:HG2	1.93	0.50
1:C:73:ASP:O	1:C:77:GLN:HG2	2.12	0.50
1:E:54:PHE:HA	1:E:57:PRO:HG2	1.93	0.50
1:E:398:PRO:HG3	1:C:153:TYR:CD1	2.47	0.50
1:C:427:THR:HB	1:C:476:ASP:OD1	2.12	0.49
1:D:416:VAL:HG11	1:D:477:VAL:HG12	1.94	0.49
1:A:137:LEU:HD23	1:A:164:ALA:HA	1.93	0.49
1:D:300:ILE:HG13	1:D:493:SER:HA	1.93	0.49
1:F:300:ILE:HG13	1:F:493:SER:HA	1.92	0.49
1:B:376:GLY:N	1:B:378:LEU:O	2.37	0.49
1:F:213:ILE:HG22	1:F:214:GLY:H	1.77	0.49
1:D:127:ILE:HD13	1:D:358:ILE:HD13	1.94	0.49
1:A:86:GLU:HB2	1:A:104:PHE:CZ	2.48	0.49
1:A:307:ASP:OD1	1:A:310:CYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:VAL:O	1:A:446:VAL:HG23	2.13	0.48
1:E:300:ILE:HG13	1:E:493:SER:HA	1.96	0.48
1:F:432:SER:HB3	1:F:475:ALA:HB2	1.96	0.48
1:D:393:THR:HG23	1:D:478:GLY:HA3	1.94	0.48
1:B:376:GLY:HA3	1:C:360:ARG:HD3	1.95	0.48
1:E:153:TYR:CD1	1:C:398:PRO:HG3	2.49	0.48
1:B:300:ILE:HG13	1:B:493:SER:HA	1.96	0.48
1:D:344:LEU:HG	1:D:350:ARG:HD2	1.95	0.48
1:C:137:LEU:HD11	1:C:485:HIS:CG	2.49	0.48
1:C:54:PHE:HA	1:C:57:PRO:HG2	1.94	0.48
1:D:390:SER:HA	1:D:477:VAL:O	2.13	0.48
1:F:305:ILE:O	1:F:307:ASP:N	2.47	0.48
1:B:71:VAL:HG21	1:B:308:LYS:HE3	1.96	0.48
1:B:52:GLU:OE2	1:B:52:GLU:N	2.41	0.48
1:D:421:ASP:O	3:D:706:HOH:O	2.20	0.48
1:B:344:LEU:HD12	1:B:350:ARG:CG	2.44	0.47
1:C:342:GLY:O	1:C:343:SER:HB2	2.14	0.47
1:A:213:ILE:HG22	1:A:214:GLY:H	1.80	0.47
1:C:138:THR:O	1:C:161:TYR:HB3	2.14	0.47
1:E:359:GLU:OE2	3:E:704:HOH:O	2.20	0.47
1:A:339:GLU:HA	1:A:343:SER:OG	2.14	0.47
1:F:307:ASP:OD1	1:F:310:CYS:HB2	2.14	0.47
1:A:71:VAL:HG21	1:A:308:LYS:HE3	1.96	0.47
1:B:379:GLY:HA2	1:B:382:TYR:HB2	1.97	0.47
1:A:344:LEU:CB	1:A:350:ARG:HG3	2.45	0.47
1:B:137:LEU:HD11	1:B:485:HIS:CG	2.50	0.47
1:A:133:HIS:NE2	1:A:307:ASP:HB2	2.30	0.47
1:D:416:VAL:CG1	1:D:477:VAL:HG12	2.45	0.47
1:F:195:VAL:HG21	1:F:265:ILE:HG23	1.97	0.47
1:B:405:LEU:HD21	1:C:142:LYS:HE2	1.97	0.47
1:F:376:GLY:O	1:F:380:GLN:HG3	2.15	0.47
1:D:405:LEU:HD12	1:D:406:PRO:HD2	1.97	0.47
1:B:261:LEU:O	1:B:265:ILE:HG12	2.15	0.46
1:D:133:HIS:O	1:D:307:ASP:HB3	2.14	0.46
1:E:350:ARG:HH21	1:E:465:MET:HB2	1.68	0.46
1:E:350:ARG:HA	1:E:350:ARG:HD3	1.42	0.46
1:A:481:GLN:NE2	1:A:484:MET:HA	2.30	0.46
1:B:419:CYS:SG	1:B:450:HIS:ND1	2.78	0.46
1:D:137:LEU:HD22	1:D:162:ALA:CB	2.45	0.46
1:E:260:LYS:O	1:E:260:LYS:HG3	2.14	0.46
1:B:191:THR:HG22	1:B:192:VAL:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:MET:C	1:E:467:SER:N	2.69	0.46
1:F:445:CYS:SG	1:F:501:LYS:HD3	2.56	0.46
1:E:358:ILE:HD12	1:E:470:MET:HE1	1.98	0.46
1:F:341:ILE:HG22	1:F:341:ILE:O	2.16	0.46
1:B:464:PRO:O	1:B:467:SER:OG	2.21	0.46
1:D:260:LYS:O	1:D:260:LYS:HG3	2.14	0.46
1:D:71:VAL:HG21	1:D:308:LYS:HE3	1.97	0.46
1:E:376:GLY:HA3	1:F:360:ARG:HD3	1.98	0.46
1:F:66:PRO:CG	1:F:196:LYS:HD2	2.46	0.46
1:B:395:ALA:O	3:B:707:HOH:O	2.21	0.45
1:F:140:ARG:HH11	1:F:281:GLU:HG2	1.82	0.45
1:B:187:THR:HB	1:B:189:LYS:HG2	1.98	0.45
1:C:341:ILE:HD12	1:C:341:ILE:H	1.81	0.45
1:D:261:LEU:O	1:D:265:ILE:HG12	2.16	0.45
1:D:481:GLN:NE2	1:D:484:MET:HA	2.32	0.45
1:B:196:LYS:HB2	1:B:196:LYS:HE3	1.65	0.45
1:C:213:ILE:HG22	1:C:214:GLY:H	1.80	0.45
1:E:344:LEU:CD1	1:E:350:ARG:HB3	2.42	0.45
1:F:337:ASP:OD1	1:F:338:ASP:N	2.50	0.45
1:A:402:GLN:HG2	1:A:403:THR:HG23	1.99	0.45
1:E:301:PHE:CE1	1:C:203:ARG:HD3	2.51	0.45
1:F:54:PHE:HA	1:F:57:PRO:HG2	1.98	0.45
1:F:261:LEU:O	1:F:265:ILE:HG12	2.17	0.45
1:A:360:ARG:HD3	1:C:376:GLY:HA3	1.99	0.45
1:D:213:ILE:HG22	1:D:214:GLY:H	1.82	0.44
1:C:431:VAL:HG13	1:C:517:TRP:CH2	2.52	0.44
1:E:465:MET:SD	1:F:345:LEU:HB3	2.57	0.44
1:E:497:GLY:O	1:E:500:VAL:HG22	2.18	0.44
1:A:138:THR:O	1:A:161:TYR:HB3	2.17	0.44
1:C:432:SER:HB3	1:C:475:ALA:HB2	2.00	0.44
1:E:472:VAL:HG12	1:E:473:LYS:O	2.17	0.44
1:F:187:THR:HB	1:F:189:LYS:HG2	1.98	0.44
1:D:148:PRO:O	3:D:705:HOH:O	2.20	0.44
1:F:354:LEU:HD23	1:F:466:LEU:HD22	1.98	0.44
1:B:481:GLN:NE2	1:B:484:MET:HA	2.33	0.44
1:C:133:HIS:O	1:C:307:ASP:HB3	2.18	0.44
1:D:358:ILE:HD12	1:D:470:MET:HE1	2.00	0.44
1:E:389:SER:OG	1:E:464:PRO:HA	2.17	0.44
1:A:133:HIS:CE1	1:A:307:ASP:HB2	2.53	0.44
1:A:337:ASP:OD1	1:A:338:ASP:N	2.51	0.44
1:E:199:TRP:HH2	1:E:264:LEU:HD11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:VAL:HG21	1:E:308:LYS:HE3	2.00	0.43
1:B:337:ASP:OD1	1:B:338:ASP:N	2.51	0.43
1:B:402:GLN:HG3	1:B:402:GLN:H	1.46	0.43
1:C:107:ARG:NH1	1:C:352:ASN:OD1	2.29	0.43
1:C:161:TYR:OH	1:C:341:ILE:HD11	2.19	0.43
1:D:345:LEU:HD12	1:D:346:ARG:H	1.84	0.43
1:E:307:ASP:OD1	1:E:310:CYS:HB2	2.18	0.43
1:B:86:GLU:HB2	1:B:104:PHE:CZ	2.54	0.43
1:A:345:LEU:HD13	1:C:427:THR:HA	2.01	0.43
1:C:446:VAL:O	3:C:702:HOH:O	2.22	0.43
1:A:345:LEU:CD1	1:C:427:THR:HA	2.49	0.43
1:B:213:ILE:HG22	1:B:214:GLY:H	1.84	0.43
1:B:249:LYS:HB3	1:B:249:LYS:HE3	1.91	0.43
1:B:416:VAL:CG1	1:B:477:VAL:HG13	2.49	0.42
1:C:345:LEU:HA	1:C:345:LEU:HD12	1.87	0.42
1:C:376:GLY:O	1:C:380:GLN:HG3	2.19	0.42
1:A:473:LYS:HA	1:A:473:LYS:HD2	1.55	0.42
1:B:484:MET:O	1:B:485:HIS:HB2	2.19	0.42
1:B:73:ASP:O	1:B:77:GLN:HG2	2.19	0.42
1:E:258:PRO:HA	1:E:259:PRO:HD3	1.94	0.42
1:E:402:GLN:HG2	1:E:403:THR:HG23	2.01	0.42
1:A:346:ARG:HD3	1:A:347:GLN:HE21	1.84	0.42
1:C:484:MET:O	1:C:485:HIS:HB2	2.18	0.42
1:E:135:ASP:OD2	1:E:161:TYR:OH	2.29	0.42
1:F:484:MET:O	1:F:485:HIS:HB2	2.19	0.42
1:B:162:ALA:HB2	1:B:341:ILE:HD11	2.00	0.42
1:C:390:SER:HA	1:C:477:VAL:O	2.20	0.42
1:E:404:ASN:OD1	3:E:705:HOH:O	2.22	0.42
1:B:90:ARG:NH1	3:B:716:HOH:O	2.50	0.42
1:A:298:GLU:O	1:A:493:SER:N	2.42	0.42
1:E:390:SER:HA	1:E:477:VAL:O	2.19	0.42
1:E:418:LEU:HD13	1:E:447:ASN:HB3	2.02	0.42
1:A:341:ILE:O	1:A:341:ILE:HG22	2.20	0.42
1:B:138:THR:O	1:B:161:TYR:HB3	2.19	0.42
1:C:196:LYS:HE3	1:C:196:LYS:HB2	1.81	0.42
1:B:103:TYR:HB2	1:B:115:PHE:CZ	2.55	0.42
1:B:344:LEU:HD12	1:B:350:ARG:HG2	1.97	0.42
1:C:452:ILE:H	1:C:452:ILE:HG13	1.71	0.42
1:D:160:GLN:HG3	1:D:221:ARG:NH1	2.34	0.42
1:F:71:VAL:HG21	1:F:308:LYS:HE3	2.02	0.42
1:A:376:GLY:O	1:A:380:GLN:NE2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:HB3	1:B:93:TRP:CE2	2.55	0.42
1:B:169:TRP:CD2	1:B:487:ILE:HD12	2.55	0.41
1:B:482:LEU:HB2	1:B:490:MET:HG3	2.02	0.41
1:D:138:THR:O	1:D:161:TYR:HB3	2.20	0.41
1:C:481:GLN:NE2	1:C:484:MET:HA	2.34	0.41
1:F:140:ARG:NH1	1:F:281:GLU:HG2	2.35	0.41
1:A:122:LYS:HE3	1:A:122:LYS:HB2	1.92	0.41
1:A:484:MET:O	1:A:485:HIS:HB2	2.20	0.41
1:C:409:SER:HA	1:C:410:PRO:HD3	1.88	0.41
1:E:261:LEU:O	1:E:265:ILE:HG12	2.20	0.41
1:F:191:THR:OG1	1:F:192:VAL:N	2.53	0.41
1:F:298:GLU:O	1:F:493:SER:N	2.48	0.41
1:B:377:ILE:HA	1:B:377:ILE:HD12	1.91	0.41
1:C:377:ILE:HA	1:C:377:ILE:HD12	1.92	0.41
1:A:196:LYS:HB2	1:A:196:LYS:HE3	1.78	0.41
1:A:137:LEU:CD1	1:A:340:GLU:OE1	2.68	0.41
1:B:390:SER:HA	1:B:477:VAL:O	2.20	0.41
1:C:257:GLN:HE21	1:C:280:TRP:HZ2	1.68	0.41
1:F:409:SER:HA	1:F:410:PRO:HD3	1.90	0.41
1:B:257:GLN:HE21	1:B:280:TRP:HZ2	1.68	0.41
1:B:376:GLY:O	1:B:380:GLN:HG3	2.20	0.41
1:D:354:LEU:HD23	1:D:466:LEU:HD22	2.03	0.41
1:A:418:LEU:HD13	1:A:447:ASN:HB3	2.02	0.41
1:C:358:ILE:HD12	1:C:470:MET:HE1	2.03	0.41
1:F:497:GLY:O	1:F:500:VAL:HG12	2.21	0.41
1:A:137:LEU:HG	1:A:162:ALA:HB1	2.01	0.41
1:B:266:LEU:HB3	1:B:271:LEU:O	2.21	0.41
1:E:247:VAL:HG12	1:E:274:PRO:CG	2.51	0.41
1:F:133:HIS:NE2	1:F:307:ASP:HB2	2.35	0.41
1:A:108:ASN:HB3	1:A:347:GLN:HG2	2.03	0.40
1:B:443:SER:O	1:B:501:LYS:HE2	2.21	0.40
1:D:249:LYS:HA	1:D:250:PRO:HD2	1.88	0.40
1:E:77:GLN:HG3	1:E:81:LYS:HE3	2.03	0.40
1:B:81:LYS:HD2	1:B:81:LYS:HA	1.81	0.40
1:F:108:ASN:HB3	1:F:347:GLN:HG2	2.04	0.40
1:F:428:THR:HG22	1:F:433:MET:HG3	2.04	0.40
1:A:288:GLN:HA	1:A:289:PRO:HD3	1.99	0.40
1:A:390:SER:HA	1:A:477:VAL:O	2.21	0.40
1:B:98:VAL:HG12	1:B:99:PRO:O	2.21	0.40
1:E:295:LEU:HD11	1:C:229:ILE:HD12	2.04	0.40
1:C:416:VAL:HG11	1:C:477:VAL:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:472:VAL:HG12	1:F:473:LYS:O	2.22	0.40
1:A:397:HIS:HA	1:A:398:PRO:HD3	1.96	0.40
1:C:261:LEU:O	1:C:265:ILE:HG12	2.22	0.40
1:D:306:ASP:HA	1:D:392:VAL:HG21	2.03	0.40
1:E:229:ILE:HD12	1:C:295:LEU:HD11	2.02	0.40
1:F:300:ILE:HB	1:F:491:THR:HG22	2.04	0.40
1:F:481:GLN:NE2	1:F:484:MET:HA	2.37	0.40
1:F:491:THR:HG23	1:F:492:GLY:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:ARG:NH2	1:C:323:ARG:O[4_555]	2.01	0.19
1:F:323:ARG:O	1:C:323:ARG:NH2[4_555]	2.12	0.08
1:A:172:ARG:NH2	3:F:702:HOH:O[2_555]	2.18	0.02

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	437/519 (84%)	429 (98%)	8 (2%)	0	100	100
1	B	437/519 (84%)	430 (98%)	7 (2%)	0	100	100
1	C	437/519 (84%)	428 (98%)	9 (2%)	0	100	100
1	D	437/519 (84%)	429 (98%)	8 (2%)	0	100	100
1	E	437/519 (84%)	423 (97%)	14 (3%)	0	100	100
1	F	437/519 (84%)	427 (98%)	10 (2%)	0	100	100
All	All	2622/3114 (84%)	2566 (98%)	56 (2%)	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	367/430 (85%)	359 (98%)	8 (2%)	57	85
1	B	367/430 (85%)	360 (98%)	7 (2%)	62	87
1	C	367/430 (85%)	355 (97%)	12 (3%)	43	74
1	D	367/430 (85%)	363 (99%)	4 (1%)	78	92
1	E	367/430 (85%)	361 (98%)	6 (2%)	68	89
1	F	367/430 (85%)	365 (100%)	2 (0%)	91	96
All	All	2202/2580 (85%)	2163 (98%)	39 (2%)	64	87

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	SER
1	A	280	TRP
1	A	307	ASP
1	A	344	LEU
1	A	350	ARG
1	A	411	ARG
1	A	473	LYS
1	A	476	ASP
1	E	280	TRP
1	E	307	ASP
1	E	343	SER
1	E	345	LEU
1	E	411	ARG
1	E	476	ASP
1	F	280	TRP
1	F	307	ASP
1	B	187	THR
1	B	249	LYS
1	B	280	TRP
1	B	307	ASP
1	B	350	ARG
1	B	402	GLN

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Mol	Chain	Res	Type
1	B	411	ARG
1	C	111	SER
1	C	145	SER
1	C	161	TYR
1	C	184	ASP
1	C	260	LYS
1	C	280	TRP
1	C	307	ASP
1	C	343	SER
1	C	344	LEU
1	C	402	GLN
1	C	411	ARG
1	C	476	ASP
1	D	145	SER
1	D	280	TRP
1	D	307	ASP
1	D	367	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	E	65	ASN
1	E	369	ASN
1	F	53	HIS
1	B	125	ASN
1	B	257	GLN
1	C	257	GLN
1	C	369	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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	445/519 (85%)	0.25	18 (4%)	39	33	26, 39, 66, 82	0
1	B	445/519 (85%)	0.30	30 (6%)	19	14	26, 40, 68, 80	0
1	C	445/519 (85%)	0.31	25 (5%)	25	20	26, 39, 69, 81	0
1	D	445/519 (85%)	0.32	27 (6%)	22	17	29, 40, 67, 84	0
1	E	445/519 (85%)	0.17	18 (4%)	39	33	28, 40, 67, 84	0
1	F	445/519 (85%)	0.17	21 (4%)	32	26	26, 40, 68, 83	0
All	All	2670/3114 (85%)	0.25	139 (5%)	28	22	26, 40, 68, 84	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	HIS	8.6
1	C	185	PRO	6.0
1	D	187	THR	5.6
1	C	186	LYS	5.5
1	A	250	PRO	5.4
1	D	250	PRO	5.4
1	D	186	LYS	5.4
1	E	218	HIS	5.3
1	F	186	LYS	5.3
1	C	219	GLY	5.2
1	D	185	PRO	5.2
1	E	185	PRO	5.2
1	B	185	PRO	5.1
1	E	250	PRO	5.1
1	A	246	PRO	5.0
1	D	465	MET	4.9
1	F	218	HIS	4.8
1	F	185	PRO	4.8
1	D	188	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	185	PRO	4.6
1	F	272	SER	4.6
1	C	250	PRO	4.6
1	A	218	HIS	4.6
1	C	187	THR	4.5
1	D	219	GLY	4.3
1	A	465	MET	4.3
1	C	248	GLY	4.3
1	F	187	THR	4.2
1	B	218	HIS	4.1
1	F	465	MET	3.9
1	E	247	VAL	3.9
1	C	465	MET	3.9
1	B	187	THR	3.8
1	B	167	GLU	3.8
1	F	271	LEU	3.7
1	B	188	GLY	3.7
1	B	463	GLY	3.7
1	C	212	GLY	3.6
1	D	246	PRO	3.6
1	C	249	LYS	3.6
1	B	186	LYS	3.5
1	B	250	PRO	3.5
1	B	94	THR	3.5
1	C	271	LEU	3.5
1	E	465	MET	3.5
1	F	219	GLY	3.4
1	B	213	ILE	3.3
1	B	465	MET	3.3
1	B	220	ASN	3.3
1	E	212	GLY	3.2
1	F	250	PRO	3.2
1	B	219	GLY	3.2
1	E	184	ASP	3.1
1	D	218	HIS	3.1
1	C	184	ASP	3.1
1	A	344	LEU	3.1
1	B	164	ALA	3.1
1	C	183	LYS	3.1
1	C	270	GLY	3.1
1	C	191	THR	3.1
1	F	270	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	214	GLY	3.0
1	B	464	PRO	3.0
1	C	350	ARG	3.0
1	B	212	GLY	3.0
1	A	271	LEU	3.0
1	C	464	PRO	2.9
1	C	188	GLY	2.9
1	F	246	PRO	2.9
1	D	122	LYS	2.9
1	A	464	PRO	2.9
1	D	189	LYS	2.8
1	D	249	LYS	2.8
1	D	350	ARG	2.8
1	E	213	ILE	2.8
1	D	94	THR	2.8
1	E	219	GLY	2.7
1	A	247	VAL	2.7
1	D	213	ILE	2.7
1	D	370	SER	2.7
1	D	220	ASN	2.6
1	F	184	ASP	2.6
1	E	350	ARG	2.6
1	D	272	SER	2.6
1	C	164	ALA	2.6
1	F	236	LEU	2.6
1	D	464	PRO	2.6
1	D	463	GLY	2.6
1	A	274	PRO	2.5
1	B	275	ASP	2.5
1	B	217	GLY	2.5
1	C	247	VAL	2.5
1	B	273	ASP	2.5
1	F	247	VAL	2.5
1	E	246	PRO	2.5
1	E	464	PRO	2.5
1	B	249	LYS	2.5
1	D	183	LYS	2.5
1	E	183	LYS	2.4
1	F	265	ILE	2.4
1	C	246	PRO	2.4
1	B	221	ARG	2.3
1	C	275	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	272	SER	2.3
1	D	164	ALA	2.3
1	A	249	LYS	2.3
1	B	324	ALA	2.3
1	C	161	TYR	2.3
1	B	189	LYS	2.3
1	C	189	LYS	2.3
1	A	213	ILE	2.3
1	F	463	GLY	2.3
1	B	342	GLY	2.3
1	C	220	ASN	2.3
1	E	249	LYS	2.2
1	D	98	VAL	2.2
1	D	368	SER	2.2
1	A	275	ASP	2.2
1	B	350	ARG	2.2
1	E	421	ASP	2.2
1	E	221	ARG	2.2
1	B	184	ASP	2.2
1	A	50	ARG	2.2
1	D	275	ASP	2.2
1	A	183	LYS	2.2
1	B	400	PHE	2.1
1	B	325	PRO	2.1
1	F	276	SER	2.1
1	A	352	ASN	2.1
1	F	464	PRO	2.1
1	F	213	ILE	2.1
1	A	235	ASP	2.1
1	A	252	SER	2.0
1	E	463	GLY	2.0
1	D	211	PHE	2.0
1	F	194	LEU	2.0
1	F	188	GLY	2.0
1	D	214	GLY	2.0
1	E	236	LEU	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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	C	601	1/1	0.79	0.21	0.48	96,96,96,96	0
2	ZN	D	601	1/1	0.79	0.20	0.08	96,96,96,96	0
2	ZN	F	601	1/1	0.72	0.20	0.05	96,96,96,96	0
2	ZN	B	601	1/1	0.87	0.19	-0.01	96,96,96,96	0
2	ZN	E	601	1/1	0.73	0.18	-0.10	96,96,96,96	0
2	ZN	A	601	1/1	0.59	0.21	-0.23	111,111,111,111	0
2	ZN	E	602	1/1	0.97	0.06	-2.21	73,73,73,73	0
2	ZN	B	602	1/1	0.95	0.08	-2.26	68,68,68,68	0
2	ZN	D	602	1/1	0.89	0.07	-2.45	68,68,68,68	0
2	ZN	A	602	1/1	0.96	0.07	-2.94	71,71,71,71	0
2	ZN	F	602	1/1	0.97	0.06	-2.98	74,74,74,74	0
2	ZN	C	602	1/1	0.94	0.07	-4.94	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.