



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 07:02 pm BST

PDB ID : 6BKJ  
Title : Crystal Structure of Human Calpain-3 Protease Core in Complex with Leupeptin  
Authors : Ye, Q.; Campbell, R.L.; Davies, P.L.  
Deposited on : 2017-11-08  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

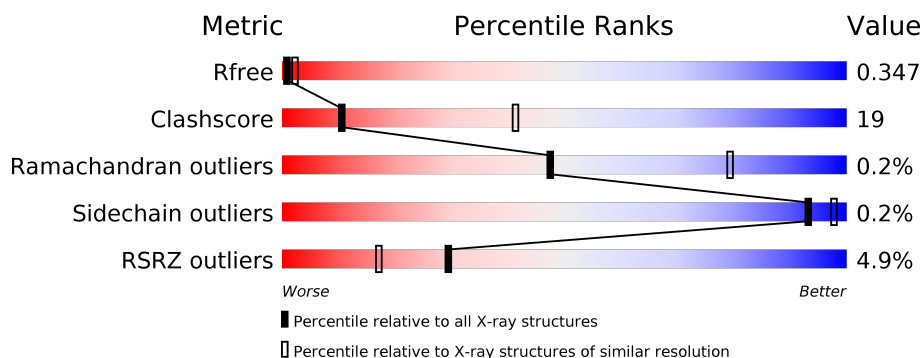
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	382	<div> <div>4%</div> <div>63%18%20%</div> </div>
1	B	382	<div> <div>5%</div> <div>60%20%20%</div> </div>
1	C	382	<div> <div>%</div> <div>59%20%20%</div> </div>
1	D	382	<div> <div>5%</div> <div>62%19%20%</div> </div>
2	F	4	<div> <div>25%</div> <div>75%25%</div> </div>
2	G	4	<div> <div>25%</div> <div>75%25%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	4	
2	I	4	

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
2	AR7	F	358	-	-	-	X
2	AR7	G	358	-	-	-	X
2	AR7	H	358	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10293 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 Calpain-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2534	1633	423	463	15			
1	B	307	Total	C	N	O	S	0	0	0
			2530	1630	422	463	15			
1	C	304	Total	C	N	O	S	0	0	0
			2510	1619	419	457	15			
1	D	307	Total	C	N	O	S	0	0	0
			2544	1641	423	465	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	LEU	-	expression tag	UNP P20807
A	421	GLU	-	expression tag	UNP P20807
A	422	HIS	-	expression tag	UNP P20807
A	423	HIS	-	expression tag	UNP P20807
A	424	HIS	-	expression tag	UNP P20807
A	425	HIS	-	expression tag	UNP P20807
A	426	HIS	-	expression tag	UNP P20807
A	427	HIS	-	expression tag	UNP P20807
B	420	LEU	-	expression tag	UNP P20807
B	421	GLU	-	expression tag	UNP P20807
B	422	HIS	-	expression tag	UNP P20807
B	423	HIS	-	expression tag	UNP P20807
B	424	HIS	-	expression tag	UNP P20807
B	425	HIS	-	expression tag	UNP P20807
B	426	HIS	-	expression tag	UNP P20807
B	427	HIS	-	expression tag	UNP P20807
C	420	LEU	-	expression tag	UNP P20807
C	421	GLU	-	expression tag	UNP P20807
C	422	HIS	-	expression tag	UNP P20807
C	423	HIS	-	expression tag	UNP P20807
C	424	HIS	-	expression tag	UNP P20807

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Chain	Residue	Modelled	Actual	Comment	Reference
C	425	HIS	-	expression tag	UNP P20807
C	426	HIS	-	expression tag	UNP P20807
C	427	HIS	-	expression tag	UNP P20807
D	420	LEU	-	expression tag	UNP P20807
D	421	GLU	-	expression tag	UNP P20807
D	422	HIS	-	expression tag	UNP P20807
D	423	HIS	-	expression tag	UNP P20807
D	424	HIS	-	expression tag	UNP P20807
D	425	HIS	-	expression tag	UNP P20807
D	426	HIS	-	expression tag	UNP P20807
D	427	HIS	-	expression tag	UNP P20807

- Molecule 2 is a protein called Leupeptin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	4	Total	C	N	O	0	0	0
			30	20	6	4			
2	G	4	Total	C	N	O	0	0	0
			30	20	6	4			
2	H	4	Total	C	N	O	0	0	0
			30	20	6	4			
2	I	4	Total	C	N	O	0	0	0
			30	20	6	4			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		

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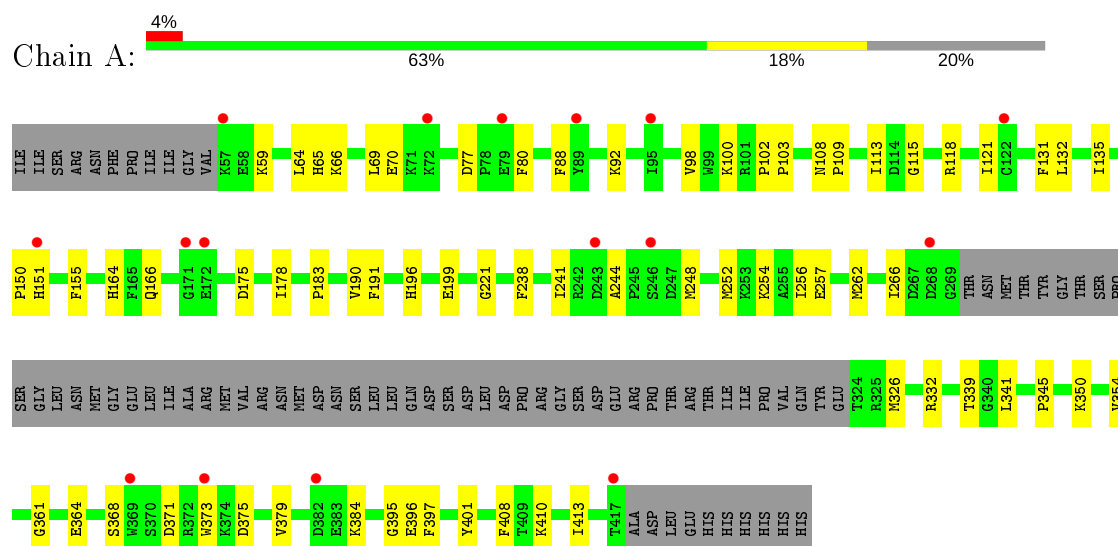
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	11	Total 11	O 11	0	0
4	C	9	Total 9	O 9	0	0
4	D	12	Total 12	O 12	0	0
4	H	1	Total 1	O 1	0	0

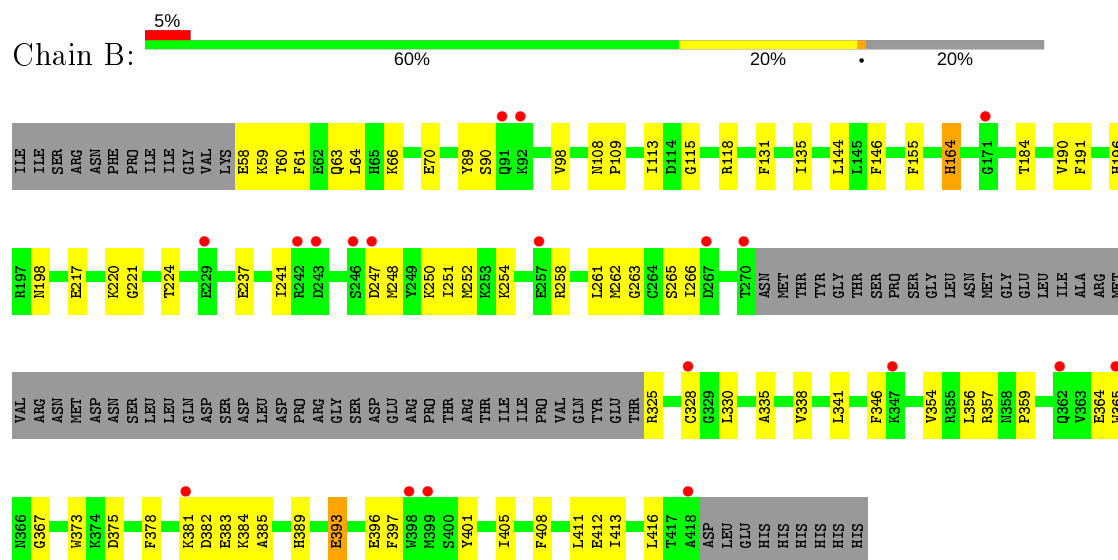
### 3 Residue-property plots [i](#)

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: Calpain-3



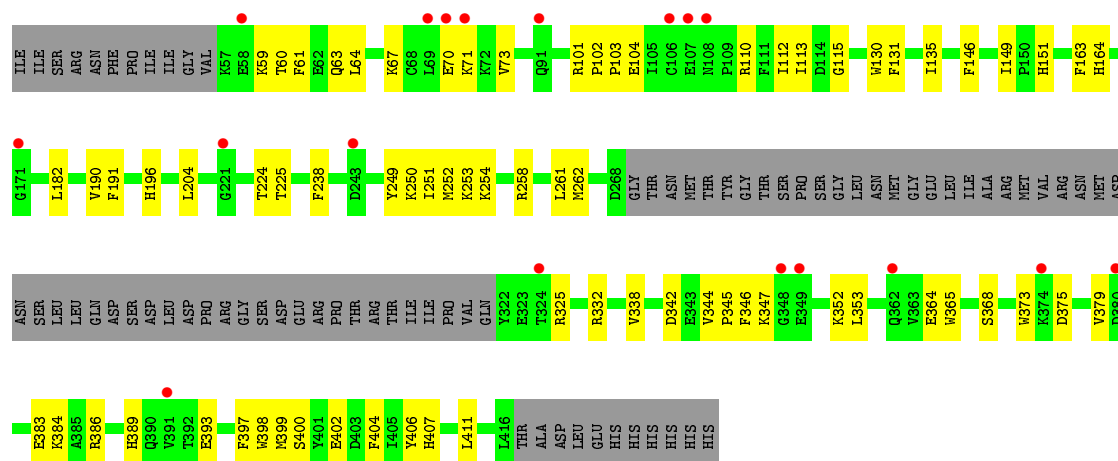
#### • Molecule 1: Calpain-3



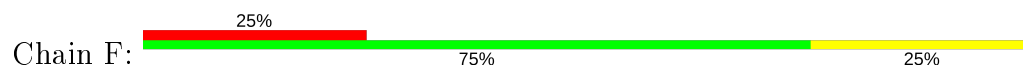
#### • Molecule 1: Calpain-3



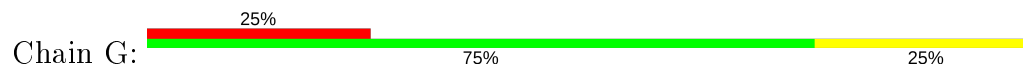
- Molecule 1: Calpain-3



- Molecule 2: Leupeptin



- Molecule 2: Leupeptin

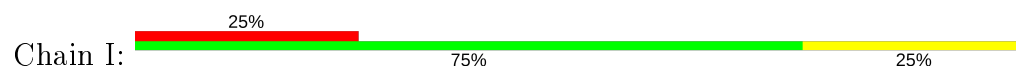


- Molecule 2: Leupeptin





● Molecule 2: Leupeptin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.93Å 106.69Å 234.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.99 – 3.20 17.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (17.99-3.20) 97.1 (17.99-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 3.21Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.277 , 0.353 0.279 , 0.347	Depositor DCC
$R_{free}$ test set	1139 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	118.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 105.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, ACE, AR7

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	0.55	0/2608	0.73	0/3527
1	B	0.56	0/2604	0.75	0/3523
1	C	0.55	0/2584	0.75	0/3496
1	D	0.55	0/2619	0.76	0/3542
2	F	0.50	0/16	1.08	0/21
2	G	0.89	0/16	1.27	0/21
2	H	0.64	0/16	0.71	0/21
2	I	0.73	0/16	1.20	0/21
All	All	0.56	0/10479	0.75	0/14172

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	2534	0	2419	92	0
1	B	2530	0	2411	86	0
1	C	2510	0	2395	110	0
1	D	2544	0	2424	87	0
2	F	30	0	37	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	30	0	37	2	0
2	H	30	0	37	1	0
2	I	30	0	38	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	14	0	0	0	0
4	B	11	0	0	0	0
4	C	9	0	0	0	0
4	D	12	0	0	0	0
4	H	1	0	0	0	0
All	All	10293	0	9798	371	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 19.

All (371) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:PHE:CZ	1:C:93:PHE:HB2	1.53	1.39
1:A:244:ALA:HB1	1:A:248:MET:CE	1.59	1.29
1:B:401:TYR:CE2	1:B:405:ILE:HD11	1.76	1.19
1:B:373:TRP:CZ3	1:B:375:ASP:HB2	1.79	1.16
1:C:88:PHE:CE1	1:C:93:PHE:HB2	1.80	1.16
1:D:59:LYS:HB3	1:D:64:LEU:HD11	1.31	1.06
1:B:59:LYS:HB3	1:B:64:LEU:HD11	1.36	1.05
1:A:244:ALA:HB1	1:A:248:MET:HE3	1.05	1.04
1:B:382:ASP:OD1	1:B:383:GLU:N	1.89	1.04
1:A:373:TRP:HE1	1:A:375:ASP:HB2	1.18	1.03
1:B:401:TYR:CZ	1:B:405:ILE:HD11	1.93	1.03
1:C:169:ARG:NH1	1:C:212:LEU:HD21	1.74	1.01
1:C:88:PHE:CZ	1:C:93:PHE:CB	2.44	1.00
1:D:365:TRP:CZ3	1:D:399:MET:HB2	1.96	1.00
1:C:61:PHE:CE1	1:C:162:ILE:HG12	1.98	0.98
1:C:61:PHE:HE1	1:C:162:ILE:HG12	1.26	0.98
1:C:93:PHE:HB3	1:C:94:PRO:HD2	1.43	0.97
1:A:131:PHE:CZ	1:A:135:ILE:HD11	1.98	0.97
1:A:121:ILE:CG2	1:A:132:LEU:HD22	1.95	0.96
1:B:265:SER:O	1:B:408:PHE:HD1	1.47	0.95
1:C:90:SER:HB3	1:C:93:PHE:HE2	1.28	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:PHE:CE1	1:C:190:VAL:HG11	2.02	0.93
1:D:250:LYS:NZ	1:D:254:LYS:HE3	1.83	0.93
1:A:183:PRO:HG2	1:A:191:PHE:CE2	2.02	0.93
1:C:97:PHE:HE1	1:C:190:VAL:HG11	1.33	0.93
1:D:59:LYS:HB3	1:D:64:LEU:CD1	1.99	0.92
1:A:368:SER:HA	1:A:373:TRP:CE3	2.05	0.92
1:B:384:LYS:HG2	1:B:389:HIS:HB3	1.53	0.90
1:D:365:TRP:HZ3	1:D:399:MET:HA	1.37	0.89
1:D:365:TRP:CZ3	1:D:399:MET:CB	2.55	0.89
1:A:244:ALA:CB	1:A:248:MET:HE3	2.00	0.89
1:B:263:GLY:O	1:B:412:GLU:HG2	1.73	0.88
1:B:59:LYS:HB3	1:B:64:LEU:CD1	2.04	0.88
1:C:93:PHE:HB3	1:C:94:PRO:CD	2.04	0.88
1:A:373:TRP:NE1	1:A:375:ASP:HB2	1.89	0.86
1:C:169:ARG:HH11	1:C:212:LEU:HD21	1.37	0.86
1:A:244:ALA:HB1	1:A:248:MET:HE1	1.58	0.85
1:D:102:PRO:HB2	1:D:103:PRO:HD3	1.58	0.84
1:C:95:ILE:HG22	1:C:95:ILE:O	1.78	0.83
1:C:191:PHE:CE2	1:C:216:TYR:HD2	1.95	0.83
1:A:244:ALA:CB	1:A:248:MET:CE	2.52	0.82
1:D:365:TRP:CZ3	1:D:368:SER:O	2.32	0.82
1:C:88:PHE:CD1	1:C:93:PHE:HD2	1.97	0.81
1:B:248:MET:HA	1:B:251:ILE:HD12	1.62	0.81
1:C:386:ARG:HH11	1:C:386:ARG:HG3	1.46	0.81
1:C:131:PHE:CE1	1:C:135:ILE:HD11	2.16	0.80
1:B:401:TYR:CE2	1:B:405:ILE:CD1	2.63	0.80
1:C:191:PHE:CE2	1:C:216:TYR:CD2	2.69	0.80
1:A:183:PRO:HG2	1:A:191:PHE:HE2	1.45	0.78
1:D:365:TRP:CH2	1:D:368:SER:O	2.36	0.77
1:C:90:SER:CB	1:C:93:PHE:HE2	1.97	0.77
1:A:326:MET:CE	1:A:332:ARG:HG3	2.15	0.77
1:C:358:ASN:HD22	1:C:363:VAL:HG13	1.48	0.77
1:A:121:ILE:HG22	1:A:132:LEU:HD22	1.66	0.77
1:D:250:LYS:HZ1	1:D:254:LYS:HE3	1.49	0.76
1:C:90:SER:HB3	1:C:93:PHE:CE2	2.18	0.74
2:I:356:LEU:O	2:I:356:LEU:HD12	1.86	0.74
1:C:212:LEU:HD12	1:C:212:LEU:O	1.87	0.74
1:A:65:HIS:NE2	1:A:69:LEU:HD11	2.02	0.74
1:C:266:ILE:HG13	1:C:332:ARG:HA	1.70	0.74
1:C:132:LEU:N	1:C:132:LEU:HD23	2.03	0.74
1:B:266:ILE:HG13	1:B:408:PHE:CD1	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:ARG:HD2	1:D:332:ARG:H	1.54	0.72
1:A:410:LYS:NZ	1:C:327:ALA:HB2	2.04	0.72
1:C:131:PHE:CZ	1:C:135:ILE:HD11	2.24	0.72
1:C:358:ASN:ND2	1:C:363:VAL:HG13	2.03	0.72
1:A:183:PRO:CG	1:A:191:PHE:HE2	2.03	0.72
1:D:365:TRP:CZ3	1:D:399:MET:HA	2.24	0.72
1:B:262:MET:CE	1:B:338:VAL:HG11	2.20	0.72
1:B:217:GLU:CG	1:B:220:LYS:HE2	2.20	0.71
1:C:253:LYS:O	1:C:257:GLU:HG3	1.89	0.71
1:B:381:LYS:O	1:B:384:LYS:HB3	1.89	0.71
1:A:150:PRO:HG2	1:A:164:HIS:CE1	2.25	0.71
1:D:406:TYR:HE1	1:D:407:HIS:CE1	2.08	0.71
1:B:373:TRP:CH2	1:B:375:ASP:HB2	2.26	0.71
1:C:191:PHE:HD2	1:C:216:TYR:HE2	1.38	0.71
1:A:65:HIS:NE2	1:A:69:LEU:CD1	2.54	0.70
1:D:384:LYS:HG3	1:D:389:HIS:HB3	1.72	0.70
1:A:113:ILE:HG13	1:A:199:GLU:HG3	1.73	0.70
1:A:65:HIS:CD2	1:A:69:LEU:HD12	2.26	0.70
1:D:250:LYS:HZ2	1:D:254:LYS:HE3	1.53	0.70
1:A:121:ILE:CG2	1:A:132:LEU:CD2	2.68	0.70
1:C:358:ASN:ND2	1:C:363:VAL:CG1	2.56	0.69
1:D:251:ILE:HA	1:D:254:LYS:HZ3	1.58	0.69
1:D:406:TYR:CE1	1:D:407:HIS:CE1	2.81	0.69
1:C:61:PHE:O	1:C:65:HIS:N	2.23	0.69
1:D:59:LYS:CB	1:D:64:LEU:HD11	2.18	0.68
1:A:183:PRO:CB	1:A:191:PHE:HE2	2.06	0.68
1:D:252:MET:HE2	1:D:411:LEU:HD22	1.75	0.68
2:F:356:LEU:C	2:F:356:LEU:HD12	2.13	0.68
1:C:210:ALA:HB2	1:C:219:LEU:HD11	1.76	0.68
1:D:113:ILE:HD12	1:D:196:HIS:ND1	2.08	0.68
1:C:98:VAL:HG23	1:C:184:THR:OG1	1.95	0.67
1:C:88:PHE:CD1	1:C:93:PHE:CD2	2.82	0.67
1:C:191:PHE:HD2	1:C:216:TYR:CE2	2.12	0.67
1:A:326:MET:HE1	1:A:332:ARG:HG3	1.76	0.67
1:C:191:PHE:CD2	1:C:216:TYR:CE2	2.83	0.67
1:B:265:SER:O	1:B:408:PHE:CD1	2.39	0.66
1:D:262:MET:HE2	1:D:411:LEU:HD11	1.78	0.66
1:D:262:MET:HG3	1:D:338:VAL:HB	1.76	0.66
1:D:101:ARG:HB2	1:D:104:GLU:HG3	1.77	0.66
1:D:61:PHE:CE2	1:D:164:HIS:CE1	2.84	0.66
1:C:266:ILE:HG22	1:C:408:PHE:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:THR:O	1:C:64:LEU:N	2.24	0.65
1:A:410:LYS:HZ1	1:C:327:ALA:HB2	1.60	0.65
1:A:379:VAL:HB	1:A:384:LYS:HE3	1.79	0.65
1:C:146:PHE:HD1	1:C:151:HIS:CD2	2.15	0.65
1:A:326:MET:HE2	1:A:332:ARG:HG3	1.79	0.65
1:A:131:PHE:CE2	1:A:135:ILE:HD11	2.31	0.64
1:B:266:ILE:HG13	1:B:408:PHE:CE1	2.33	0.64
1:D:102:PRO:CB	1:D:103:PRO:HD3	2.27	0.64
1:A:410:LYS:NZ	1:C:327:ALA:CB	2.60	0.64
1:C:88:PHE:CE1	1:C:93:PHE:CB	2.72	0.64
1:D:252:MET:CE	1:D:411:LEU:HD22	2.28	0.64
1:D:146:PHE:HD1	1:D:151:HIS:CD2	2.16	0.64
1:D:251:ILE:HA	1:D:254:LYS:NZ	2.12	0.64
1:B:328:CYS:HB2	1:B:365:TRP:CZ3	2.33	0.63
1:A:98:VAL:CG1	1:A:100:LYS:HE2	2.28	0.63
1:A:183:PRO:CG	1:A:191:PHE:CE2	2.78	0.63
1:D:393:GLU:OE1	1:D:393:GLU:HA	1.99	0.62
1:A:256:ILE:CD1	1:A:262:MET:CE	2.77	0.62
1:B:217:GLU:HG3	1:B:220:LYS:HE2	1.80	0.62
1:B:373:TRP:CZ3	1:B:375:ASP:CB	2.70	0.62
1:D:365:TRP:CZ3	1:D:399:MET:CA	2.83	0.61
1:B:217:GLU:HG2	1:B:220:LYS:HE2	1.80	0.61
1:C:169:ARG:NH1	1:C:212:LEU:CD2	2.59	0.61
1:C:191:PHE:HE2	1:C:216:TYR:CD2	2.16	0.61
1:A:244:ALA:CB	1:A:248:MET:HE1	2.26	0.61
1:C:191:PHE:CD2	1:C:216:TYR:CD2	2.89	0.61
1:B:261:LEU:HD12	1:B:261:LEU:N	2.16	0.61
2:F:356:LEU:O	2:F:356:LEU:HD12	2.01	0.61
1:D:130:TRP:HA	1:D:224:THR:HG22	1.83	0.60
1:C:196:HIS:CE1	1:C:198:ASN:HB2	2.36	0.60
1:C:266:ILE:CG2	1:C:408:PHE:HA	2.31	0.60
1:C:169:ARG:HH11	1:C:212:LEU:CD2	2.12	0.60
1:B:265:SER:C	1:B:408:PHE:HD1	2.04	0.60
1:A:121:ILE:HG23	1:A:132:LEU:HD22	1.82	0.59
1:A:368:SER:HA	1:A:373:TRP:CZ3	2.37	0.59
1:A:364:GLU:HB2	1:A:397:PHE:CD2	2.37	0.59
1:B:338:VAL:HA	1:B:356:LEU:HD23	1.83	0.59
1:A:98:VAL:HG11	1:A:100:LYS:HE2	1.84	0.59
1:D:365:TRP:HZ3	1:D:399:MET:CA	2.11	0.59
1:C:97:PHE:HE1	1:C:190:VAL:CG1	2.10	0.59
1:C:60:THR:HG23	1:C:63:GLN:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LYS:HE3	1:C:378:PHE:CD2	2.37	0.59
1:D:252:MET:HE1	1:D:404:PHE:CE2	2.38	0.58
1:A:410:LYS:HZ1	1:C:327:ALA:CB	2.17	0.58
1:B:263:GLY:C	1:B:412:GLU:HG2	2.24	0.58
1:D:102:PRO:HB2	1:D:103:PRO:CD	2.32	0.58
1:A:183:PRO:HB2	1:A:191:PHE:HE2	1.68	0.58
1:A:256:ILE:HD11	1:A:262:MET:CE	2.34	0.57
1:D:383:GLU:HA	1:D:386:ARG:HG2	1.87	0.57
1:C:241:ILE:HD12	1:C:408:PHE:C	2.25	0.57
1:B:98:VAL:HG13	1:B:184:THR:OG1	2.04	0.57
1:C:170:TYR:CG	1:C:170:TYR:O	2.58	0.57
1:B:413:ILE:HD12	1:B:413:ILE:N	2.19	0.56
1:D:262:MET:CG	1:D:338:VAL:HB	2.35	0.56
1:A:256:ILE:HG13	1:A:341:LEU:HD12	1.87	0.56
1:B:190:VAL:HG23	1:B:191:PHE:CD2	2.41	0.56
1:B:328:CYS:SG	1:B:365:TRP:HZ3	2.28	0.56
1:D:190:VAL:HG23	1:D:191:PHE:CD2	2.40	0.56
1:A:132:LEU:HD23	1:A:135:ILE:HD12	1.88	0.56
1:A:183:PRO:HB2	1:A:191:PHE:CE2	2.40	0.56
1:A:262:MET:HG2	1:A:413:ILE:HG12	1.87	0.56
1:D:261:LEU:N	1:D:261:LEU:HD12	2.21	0.56
1:B:58:GLU:HG2	1:B:59:LYS:HG2	1.89	0.55
1:C:386:ARG:NH1	1:C:386:ARG:HG3	2.16	0.55
1:C:81:PRO:HB2	1:C:82:PRO:HD2	1.88	0.55
1:A:256:ILE:HG12	1:A:262:MET:CE	2.36	0.55
1:C:212:LEU:HD12	1:C:212:LEU:C	2.26	0.55
1:B:393:GLU:HG2	1:B:393:GLU:O	2.06	0.55
1:C:196:HIS:HE1	1:C:198:ASN:HB2	1.71	0.55
1:A:65:HIS:CD2	1:A:69:LEU:CD1	2.89	0.55
1:C:347:LYS:HE3	1:C:378:PHE:CE2	2.41	0.55
1:D:365:TRP:CE3	1:D:399:MET:CB	2.90	0.55
1:D:365:TRP:HB2	1:D:397:PHE:CE2	2.42	0.55
1:D:252:MET:HE2	1:D:411:LEU:CD2	2.36	0.54
1:B:382:ASP:O	1:B:383:GLU:C	2.45	0.54
1:C:169:ARG:HD2	1:C:212:LEU:HD21	1.88	0.54
1:C:97:PHE:CD1	1:C:190:VAL:HG11	2.41	0.54
1:B:335:ALA:HB2	2:G:357:LEU:HD23	1.89	0.54
1:B:373:TRP:CE3	1:B:375:ASP:HB2	2.40	0.54
1:A:364:GLU:CB	1:A:397:PHE:CD2	2.91	0.54
1:C:232:THR:HB	1:C:416:LEU:HD21	1.90	0.53
1:C:60:THR:O	1:C:63:GLN:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ASN:O	1:C:139:THR:HG21	2.09	0.53
1:D:384:LYS:CG	1:D:389:HIS:HB3	2.37	0.53
1:B:247:ASP:HB2	1:B:250:LYS:HD2	1.89	0.53
1:B:224:THR:HB	1:B:412:GLU:OE1	2.07	0.53
1:C:239:PHE:CD2	1:C:411:LEU:HD23	2.43	0.53
1:D:225:THR:HG21	1:D:238:PHE:CZ	2.44	0.53
1:B:108:ASN:OD1	1:B:108:ASN:O	2.27	0.53
1:B:196:HIS:CE1	1:B:198:ASN:HB2	2.43	0.53
1:B:262:MET:HE1	1:B:338:VAL:HG11	1.91	0.53
1:A:121:ILE:HG23	1:A:132:LEU:CD2	2.39	0.52
1:B:131:PHE:CZ	1:B:135:ILE:HD11	2.44	0.52
1:A:118:ARG:NH1	1:A:396:GLU:OE2	2.42	0.52
1:B:254:LYS:HG3	1:B:258:ARG:NH1	2.24	0.52
1:C:257:GLU:O	1:D:110:ARG:NH2	2.42	0.52
1:B:325:ARG:HH11	1:B:325:ARG:HG3	1.74	0.52
1:B:381:LYS:O	1:B:385:ALA:N	2.38	0.52
1:B:59:LYS:CB	1:B:64:LEU:HD11	2.24	0.52
1:D:131:PHE:CZ	1:D:135:ILE:HD11	2.45	0.52
1:C:116:ALA:O	1:C:117:ASN:OD1	2.27	0.52
1:C:146:PHE:CD1	1:C:151:HIS:CD2	2.98	0.52
1:B:237:GLU:HG3	1:B:237:GLU:O	2.10	0.51
1:C:60:THR:C	1:C:64:LEU:HD12	2.31	0.51
1:D:365:TRP:HB3	1:D:397:PHE:CD2	2.46	0.51
1:C:163:PHE:CD2	1:C:204:LEU:HD13	2.46	0.51
1:A:254:LYS:HZ3	1:A:257:GLU:HG3	1.75	0.51
1:C:213:HIS:N	1:C:213:HIS:CD2	2.79	0.51
1:C:95:ILE:CG2	1:C:95:ILE:O	2.52	0.51
1:C:80:PHE:HB3	1:C:211:LYS:HZ2	1.76	0.51
1:A:77:ASP:OD2	1:A:80:PHE:HB3	2.11	0.50
1:D:365:TRP:CE3	1:D:399:MET:HB3	2.47	0.50
1:A:65:HIS:CD2	1:A:65:HIS:C	2.85	0.50
2:I:356:LEU:C	2:I:356:LEU:HD12	2.31	0.50
1:B:113:ILE:HD13	1:B:196:HIS:CE1	2.47	0.50
1:B:118:ARG:HD2	1:B:357:ARG:HD3	1.94	0.50
1:B:89:TYR:CD1	1:B:90:SER:N	2.80	0.50
1:D:254:LYS:O	1:D:258:ARG:HG3	2.12	0.50
1:C:262:MET:HG2	1:C:413:ILE:HG12	1.94	0.50
1:C:131:PHE:HE1	1:C:231:PHE:HZ	1.60	0.50
1:D:182:LEU:HD21	1:D:204:LEU:HD23	1.94	0.50
1:C:131:PHE:C	1:C:131:PHE:CD1	2.85	0.49
1:B:328:CYS:SG	1:B:365:TRP:CZ3	3.05	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:PHE:CD1	1:D:151:HIS:CD2	2.98	0.49
1:B:346:PHE:HE1	1:B:378:PHE:HB2	1.77	0.49
1:D:346:PHE:CD2	1:D:347:LYS:HG3	2.48	0.49
1:B:196:HIS:HE1	1:B:198:ASN:HB2	1.77	0.48
1:B:241:ILE:HG21	1:B:405:ILE:O	2.14	0.48
1:C:131:PHE:HE2	1:C:206:GLU:HA	1.78	0.48
1:C:81:PRO:CB	1:C:82:PRO:HD2	2.42	0.48
1:D:261:LEU:N	1:D:261:LEU:CD1	2.77	0.48
1:D:344:VAL:CG2	1:D:345:PRO:HD2	2.44	0.48
1:C:115:GLY:HA3	1:D:115:GLY:HA3	1.96	0.48
1:C:88:PHE:CE1	1:C:93:PHE:HD2	2.30	0.48
1:D:346:PHE:CE2	1:D:347:LYS:HG3	2.48	0.48
1:D:163:PHE:CD2	1:D:204:LEU:HD13	2.49	0.48
1:C:169:ARG:HD2	1:C:212:LEU:CD2	2.43	0.48
1:D:146:PHE:CD1	1:D:151:HIS:NE2	2.82	0.48
1:C:146:PHE:CD1	1:C:151:HIS:NE2	2.81	0.48
1:C:190:VAL:HG23	1:C:191:PHE:CD1	2.48	0.47
1:A:221:GLY:HA3	2:F:356:LEU:HD13	1.94	0.47
1:B:60:THR:OG1	1:B:63:GLN:HG3	2.15	0.47
1:B:252:MET:HG2	1:B:411:LEU:HD21	1.96	0.47
1:B:382:ASP:O	1:B:385:ALA:N	2.47	0.47
1:A:256:ILE:HD11	1:A:262:MET:HE1	1.96	0.47
1:B:364:GLU:HB3	1:B:397:PHE:CD2	2.50	0.47
1:B:412:GLU:O	1:B:412:GLU:HG3	2.14	0.47
1:A:256:ILE:HG12	1:A:262:MET:HE1	1.95	0.47
1:C:88:PHE:CE1	1:C:93:PHE:CD2	3.03	0.47
1:A:252:MET:HB3	1:A:341:LEU:HD11	1.97	0.47
1:B:330:LEU:HG	1:B:365:TRP:HE3	1.80	0.47
1:D:364:GLU:HB3	1:D:397:PHE:CD1	2.49	0.47
1:D:113:ILE:CD1	1:D:196:HIS:ND1	2.77	0.46
1:C:61:PHE:HD1	1:C:177:VAL:HG13	1.80	0.46
1:D:250:LYS:O	1:D:254:LYS:HG3	2.15	0.46
1:C:130:TRP:HB2	1:C:224:THR:HA	1.97	0.46
1:D:262:MET:HG3	1:D:338:VAL:CB	2.45	0.46
1:B:109:PRO:HG2	1:B:155:PHE:HB3	1.97	0.46
1:B:118:ARG:NH2	1:B:396:GLU:OE1	2.43	0.46
1:C:131:PHE:CE1	1:C:231:PHE:HZ	2.34	0.46
2:H:357:LEU:HA	2:H:357:LEU:HD23	1.75	0.46
1:A:131:PHE:CD2	1:A:132:LEU:HG	2.51	0.46
1:A:88:PHE:CE1	1:A:92:LYS:HG2	2.50	0.46
1:C:113:ILE:O	1:C:114:ASP:OD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:TYR:CE2	1:D:352:LYS:HB3	2.52	0.46
1:D:60:THR:OG1	1:D:63:GLN:HG3	2.16	0.46
1:A:221:GLY:CA	2:F:356:LEU:HD13	2.45	0.46
1:A:150:PRO:CG	1:A:164:HIS:CE1	2.96	0.45
1:C:239:PHE:HE2	1:C:413:ILE:HG13	1.81	0.45
1:A:66:LYS:O	1:A:70:GLU:HG2	2.15	0.45
2:F:356:LEU:C	2:F:356:LEU:CD1	2.85	0.45
1:A:364:GLU:OE1	1:A:371:ASP:OD2	2.34	0.45
1:A:77:ASP:OD2	1:A:80:PHE:N	2.49	0.45
1:A:131:PHE:HD2	1:A:132:LEU:HG	1.82	0.45
1:C:128:ASP:OD1	1:C:128:ASP:N	2.49	0.45
1:C:203:ALA:O	1:C:206:GLU:HG2	2.16	0.45
1:A:151:HIS:HB2	1:B:146:PHE:CD2	2.52	0.45
1:A:361:GLY:HA2	1:A:395:GLY:HA3	1.99	0.45
1:C:234:GLY:HA3	1:C:415:ASN:O	2.17	0.45
1:A:190:VAL:HG23	1:A:191:PHE:CD2	2.52	0.44
1:B:262:MET:HE3	1:B:338:VAL:HG21	1.99	0.44
1:D:112:ILE:HD13	1:D:151:HIS:CE1	2.52	0.44
1:B:61:PHE:CZ	1:B:164:HIS:CD2	3.05	0.44
1:C:60:THR:CG2	1:C:63:GLN:HB2	2.47	0.44
1:A:248:MET:HB3	1:A:401:TYR:OH	2.18	0.44
1:B:60:THR:OG1	1:B:63:GLN:CG	2.65	0.44
1:C:66:LYS:O	1:C:70:GLU:HG3	2.17	0.44
1:D:146:PHE:HD1	1:D:151:HIS:NE2	2.16	0.44
1:A:238:PHE:HB2	1:A:410:LYS:HE2	1.98	0.44
1:B:144:LEU:HD11	1:B:416:LEU:HD11	1.98	0.44
1:D:60:THR:OG1	1:D:63:GLN:CG	2.65	0.44
1:A:108:ASN:HA	1:A:109:PRO:HD2	1.82	0.44
1:C:169:ARG:CZ	1:C:212:LEU:HD21	2.43	0.43
1:D:400:SER:OG	1:D:402:GLU:HG2	2.17	0.43
1:A:150:PRO:CB	1:A:164:HIS:CE1	3.01	0.43
1:A:178:ILE:O	1:A:178:ILE:HG13	2.18	0.43
1:B:109:PRO:HG2	1:B:155:PHE:CB	2.47	0.43
1:B:217:GLU:HG3	1:B:220:LYS:CE	2.48	0.43
1:B:262:MET:HE2	1:B:338:VAL:HG11	1.97	0.43
1:A:256:ILE:CG1	1:A:262:MET:HE1	2.49	0.43
1:A:266:ILE:HG22	1:A:332:ARG:HG2	2.00	0.43
1:A:241:ILE:HG13	1:A:408:PHE:O	2.19	0.43
1:A:118:ARG:NH1	1:A:339:THR:HB	2.33	0.43
1:B:262:MET:HE2	1:B:338:VAL:CG1	2.49	0.43
1:C:146:PHE:HE1	1:C:151:HIS:CE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:LYS:O	1:D:71:LYS:HG2	2.18	0.43
1:A:379:VAL:HB	1:A:384:LYS:CE	2.47	0.43
1:A:98:VAL:HG12	1:A:100:LYS:HE2	1.97	0.43
1:A:113:ILE:HD12	1:A:196:HIS:ND1	2.34	0.43
1:C:131:PHE:CE1	1:C:135:ILE:CD1	2.96	0.43
1:A:345:PRO:HD3	1:A:350:LYS:NZ	2.33	0.43
1:B:265:SER:C	1:B:408:PHE:CD1	2.89	0.43
1:C:60:THR:H	1:C:63:GLN:HB3	1.84	0.43
1:C:98:VAL:HG21	1:C:100:LYS:HZ1	1.83	0.43
1:D:146:PHE:CE1	1:D:151:HIS:CE1	3.07	0.43
1:A:166:GLN:HG2	1:A:175:ASP:OD1	2.19	0.42
1:B:241:ILE:HG23	1:B:405:ILE:HG23	2.01	0.42
1:D:345:PRO:HG2	1:D:379:VAL:HG13	2.01	0.42
1:A:77:ASP:OD2	1:A:80:PHE:CB	2.67	0.42
1:A:256:ILE:CD1	1:A:262:MET:HE1	2.48	0.42
1:B:221:GLY:HA2	2:G:357:LEU:O	2.19	0.42
1:C:151:HIS:HB3	1:D:146:PHE:CD2	2.55	0.42
1:D:365:TRP:CB	1:D:397:PHE:CE2	3.02	0.42
1:B:261:LEU:CD1	1:B:261:LEU:N	2.83	0.42
1:D:373:TRP:CH2	1:D:375:ASP:HB2	2.54	0.42
1:A:59:LYS:HB2	1:A:64:LEU:HD21	2.02	0.42
1:C:146:PHE:HD1	1:C:151:HIS:NE2	2.14	0.42
1:D:61:PHE:CD2	1:D:164:HIS:CE1	3.08	0.42
1:D:253:LYS:NZ	1:D:342:ASP:HA	2.34	0.42
1:A:166:GLN:CD	1:A:175:ASP:OD1	2.58	0.42
1:B:346:PHE:CE1	1:B:378:PHE:HB2	2.53	0.42
1:C:268:ASP:HA	1:C:332:ARG:HD3	2.02	0.42
1:B:252:MET:HB3	1:B:341:LEU:HD11	2.02	0.41
1:A:341:LEU:HD23	1:A:354:VAL:HG22	2.02	0.41
1:D:59:LYS:HA	1:D:63:GLN:OE1	2.20	0.41
1:C:112:ILE:HD13	1:C:151:HIS:CE1	2.55	0.41
1:A:103:PRO:HD3	1:A:155:PHE:HE2	1.85	0.41
1:B:341:LEU:HD23	1:B:354:VAL:HG22	2.03	0.41
1:B:262:MET:HG2	1:B:413:ILE:HG13	2.03	0.41
1:D:146:PHE:HE1	1:D:151:HIS:CE1	2.38	0.41
1:C:146:PHE:CE1	1:C:151:HIS:CE1	3.08	0.41
1:D:149:ILE:O	1:D:151:HIS:HD2	2.04	0.41
1:A:256:ILE:CG1	1:A:262:MET:CE	2.97	0.41
1:B:383:GLU:HA	1:B:383:GLU:OE1	2.19	0.41
1:B:66:LYS:O	1:B:70:GLU:HG2	2.20	0.41
1:C:266:ILE:HD11	1:C:331:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:LYS:HD3	1:C:412:GLU:CD	2.41	0.41
1:D:406:TYR:CD1	1:D:407:HIS:CE1	3.08	0.41
1:A:115:GLY:HA3	1:B:115:GLY:HA3	2.01	0.41
1:C:191:PHE:CD2	1:C:216:TYR:HE2	2.23	0.41
1:D:365:TRP:CE3	1:D:399:MET:HB2	2.51	0.41
1:D:406:TYR:CD1	1:D:407:HIS:ND1	2.89	0.41
1:D:353:LEU:HB3	1:D:398:TRP:CE3	2.56	0.41
1:D:67:LYS:O	1:D:70:GLU:HG2	2.21	0.41
1:A:65:HIS:NE2	1:A:69:LEU:HD12	2.29	0.41
1:B:373:TRP:CH2	1:B:375:ASP:CB	3.01	0.41
1:C:151:HIS:ND1	1:D:146:PHE:CZ	2.85	0.41
1:D:384:LYS:HG3	1:D:389:HIS:ND1	2.36	0.41
1:B:248:MET:HB3	1:B:401:TYR:OH	2.21	0.41
1:A:102:PRO:HB2	1:A:155:PHE:CE2	2.55	0.40
1:B:375:ASP:OD1	1:B:378:PHE:CE2	2.74	0.40
1:A:256:ILE:HG12	1:A:262:MET:HE2	2.02	0.40
1:C:61:PHE:N	1:C:64:LEU:HD12	2.36	0.40
1:D:71:LYS:HB2	1:D:73:VAL:HG22	2.03	0.40
1:D:365:TRP:CH2	1:D:399:MET:HB2	2.51	0.40
1:B:365:TRP:NE1	1:B:367:GLY:CA	2.84	0.40
1:B:59:LYS:HA	1:B:63:GLN:OE1	2.22	0.40
1:C:97:PHE:CE1	1:C:190:VAL:HG21	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	303/382 (79%)	292 (96%)	11 (4%)	0	100	100
1	B	303/382 (79%)	291 (96%)	10 (3%)	2 (1%)	22	61
1	C	300/382 (78%)	286 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	303/382 (79%)	291 (96%)	12 (4%)	0	100	100
2	F	2/4 (50%)	2 (100%)	0	0	100	100
2	G	2/4 (50%)	2 (100%)	0	0	100	100
2	H	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
2	I	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
All	All	1217/1544 (79%)	1166 (96%)	49 (4%)	2 (0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	393	GLU
1	B	359	PRO

### 5.3.2 Protein sidechains [i](#)

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	271/339 (80%)	271 (100%)	0	100	100
1	B	270/339 (80%)	269 (100%)	1 (0%)	91	95
1	C	268/339 (79%)	267 (100%)	1 (0%)	91	95
1	D	272/339 (80%)	272 (100%)	0	100	100
2	F	2/2 (100%)	2 (100%)	0	100	100
2	G	2/2 (100%)	2 (100%)	0	100	100
2	H	2/2 (100%)	2 (100%)	0	100	100
2	I	2/2 (100%)	2 (100%)	0	100	100
All	All	1089/1364 (80%)	1087 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	164	HIS

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Mol	Chain	Res	Type
1	C	334	HIS

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

Mol	Chain	Res	Type
1	C	213	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
2	AR7	H	358	2	10,10,11	1.54	2 (20%)	9,11,13	1.45	1 (11%)
2	AR7	G	358	1,2	10,10,11	1.62	2 (20%)	9,11,13	1.46	2 (22%)
2	AR7	F	358	1,2	10,10,11	1.61	3 (30%)	9,11,13	1.40	1 (11%)
2	AR7	I	358	1,2	10,10,11	1.55	3 (30%)	9,11,13	1.44	2 (22%)

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
2	AR7	H	358	2	-	0/9/9/11	-
2	AR7	G	358	1,2	-	2/9/9/11	-
2	AR7	F	358	1,2	-	2/9/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AR7	I	358	1,2	-	4/9/9/11	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	358	AR7	CZ-NE	-3.54	1.26	1.33
2	G	358	AR7	CZ-NE	-3.41	1.26	1.33
2	H	358	AR7	CZ-NE	-3.23	1.27	1.33
2	I	358	AR7	CZ-NE	-3.06	1.27	1.33
2	F	358	AR7	O-C	2.27	1.52	1.42
2	G	358	AR7	O-C	2.23	1.51	1.42
2	H	358	AR7	O-C	2.21	1.51	1.42
2	I	358	AR7	CZ-NH2	-2.20	1.25	1.34
2	I	358	AR7	O-C	2.11	1.51	1.42
2	F	358	AR7	CZ-NH2	-2.02	1.26	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	358	AR7	CB-CA-C	-3.60	107.32	112.25
2	F	358	AR7	O-C-CA	3.03	123.50	111.52
2	I	358	AR7	CG-CD-NE	-2.77	104.28	112.21
2	G	358	AR7	O-C-CA	2.76	122.44	111.52
2	I	358	AR7	O-C-CA	2.30	120.60	111.52
2	G	358	AR7	CG-CD-NE	-2.01	106.45	112.21

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	358	AR7	O-C-CA-N
2	F	358	AR7	O-C-CA-N
2	I	358	AR7	O-C-CA-N
2	I	358	AR7	N-CA-CB-CG
2	I	358	AR7	C-CA-CB-CG
2	I	358	AR7	NE-CD-CG-CB
2	F	358	AR7	NE-CD-CG-CB
2	G	358	AR7	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	307/382 (80%)	0.19	16 (5%) 27 15	75, 131, 181, 198	0
1	B	307/382 (80%)	0.29	19 (6%) 20 11	78, 131, 186, 212	0
1	C	304/382 (79%)	0.12	5 (1%) 72 59	79, 127, 163, 205	0
1	D	307/382 (80%)	0.37	18 (5%) 22 13	76, 130, 180, 204	0
2	F	2/4 (50%)	0.95	1 (50%) 0 0	127, 127, 127, 149	0
2	G	2/4 (50%)	1.32	1 (50%) 0 0	122, 122, 122, 126	0
2	H	2/4 (50%)	0.64	0 100 100	137, 137, 137, 157	0
2	I	2/4 (50%)	1.83	1 (50%) 0 0	135, 135, 135, 166	0
All	All	1233/1544 (79%)	0.25	61 (4%) 29 17	75, 130, 180, 212	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	324	THR	5.9
1	D	70	GLU	5.2
1	D	243	ASP	4.2
1	B	243	ASP	4.2
1	A	243	ASP	4.1
1	D	91	GLN	4.0
1	D	374	LYS	3.9
1	B	242	ARG	3.8
1	B	418	ALA	3.7
1	D	380	ASP	3.6
1	A	268	ASP	3.6
2	I	356	LEU	3.4
1	C	170	TYR	3.3
1	D	71	LYS	3.3
1	D	171	GLY	3.2
1	B	362	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	221	GLY	3.1
1	C	172	GLU	3.1
1	B	247	ASP	3.1
1	B	328	CYS	3.0
1	B	267	ASP	3.0
1	B	171	GLY	2.9
1	A	246	SER	2.9
1	B	246	SER	2.8
1	B	347	LYS	2.8
1	A	172	GLU	2.8
1	D	391	VAL	2.8
1	B	398	TRP	2.8
1	D	108	ASN	2.7
1	B	270	THR	2.7
1	A	72	LYS	2.6
2	G	356	LEU	2.6
1	D	107	GLU	2.6
1	A	89	TYR	2.6
1	D	58	GLU	2.5
1	A	95	ILE	2.5
1	B	399	MET	2.4
1	B	381	LYS	2.4
1	A	171	GLY	2.4
1	C	418	ALA	2.4
1	A	369	TRP	2.4
1	A	57	LYS	2.4
1	B	365	TRP	2.3
1	D	362	GLN	2.3
1	D	69	LEU	2.3
1	A	417	THR	2.3
1	D	349	GLU	2.3
1	A	151	HIS	2.3
1	C	417	THR	2.2
1	B	92	LYS	2.2
1	D	348	GLY	2.2
1	B	257	GLU	2.2
2	F	356	LEU	2.2
1	A	382	ASP	2.2
1	A	122	CYS	2.1
1	A	79	GLU	2.1
1	B	229	GLU	2.1
1	B	91	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	235	VAL	2.0
1	D	106	CYS	2.0
1	A	373	TRP	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	AR7	H	358	11/12	0.60	0.61	130,145,161,165	0
2	AR7	G	358	11/12	0.73	0.45	108,139,196,199	0
2	AR7	F	358	11/12	0.74	0.57	128,143,167,172	0
2	AR7	I	358	11/12	0.74	0.29	121,129,146,153	0

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CA	C	501	1/1	0.88	0.09	65,65,65,65	0
3	CA	D	502	1/1	0.91	0.09	109,109,109,109	0
3	CA	B	502	1/1	0.91	0.05	123,123,123,123	0
3	CA	C	502	1/1	0.92	0.07	94,94,94,94	0
3	CA	D	501	1/1	0.93	0.17	84,84,84,84	0
3	CA	A	501	1/1	0.94	0.09	73,73,73,73	0
3	CA	B	501	1/1	0.97	0.08	82,82,82,82	0
3	CA	A	502	1/1	0.98	0.06	100,100,100,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.