



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:21 am BST

PDB ID : 1ZM9  
Title : Structure of eEF2-ETA in complex with PJ34  
Authors : Joergensen, R.; Merrill, A.R.; Yates, S.P.; Marquez, V.E.; Schwan, A.L.; Boesen, T.; Andersen, G.R.  
Deposited on : 2005-05-10  
Resolution : 2.80 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  
buster-report : 1.1.7 (2018)  
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

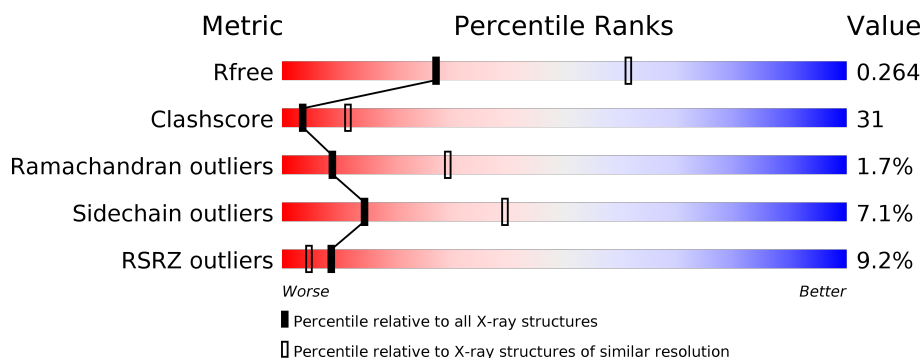
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	842	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>40%</div> <div>• •</div> </div> </div>
1	C	842	<div> <div>6%</div> <div> <div></div> <div>43%</div> <div>49%</div> <div>5%</div> <div>•</div> </div> </div>
1	E	842	<div> <div>26%</div> <div> <div></div> <div>48%</div> <div>46%</div> <div>• •</div> </div> </div>
2	B	207	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>38%</div> <div>6%</div> </div> </div>
2	D	207	<div> <div></div> <div> <div></div> <div>59%</div> <div>35%</div> <div>5%</div> </div> </div>
2	F	207	<div> <div></div> <div> <div></div> <div>60%</div> <div>34%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24042 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	C	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	E	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			

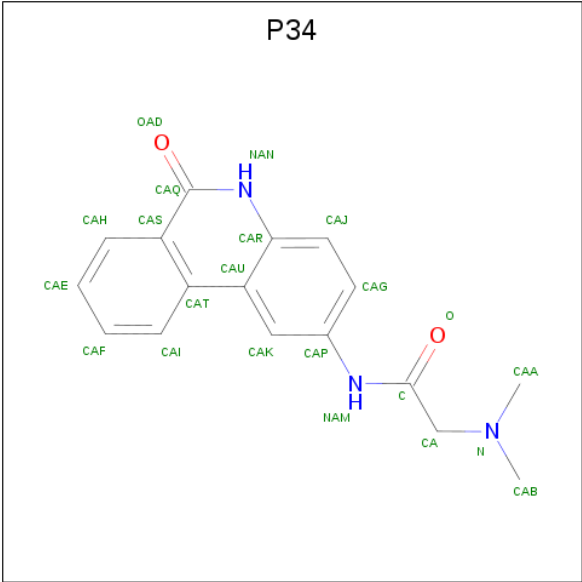
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324
C	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324
E	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324

- Molecule 2 is a protein called exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1587	1001	283	303			
2	D	207	Total	C	N	O	0	0	0
			1587	1001	283	303			
2	F	207	Total	C	N	O	0	0	0
			1587	1001	283	303			

- Molecule 3 is N 2 ,N 2 -DIMETHYL-N 1 -(6-OXO-5,6-DIHYDROPHENANTHRIDIN-2-Y L)GLYCINAMIDE (three-letter code: P34) (formula: C<sub>17</sub>H<sub>17</sub>N<sub>3</sub>O<sub>2</sub>).

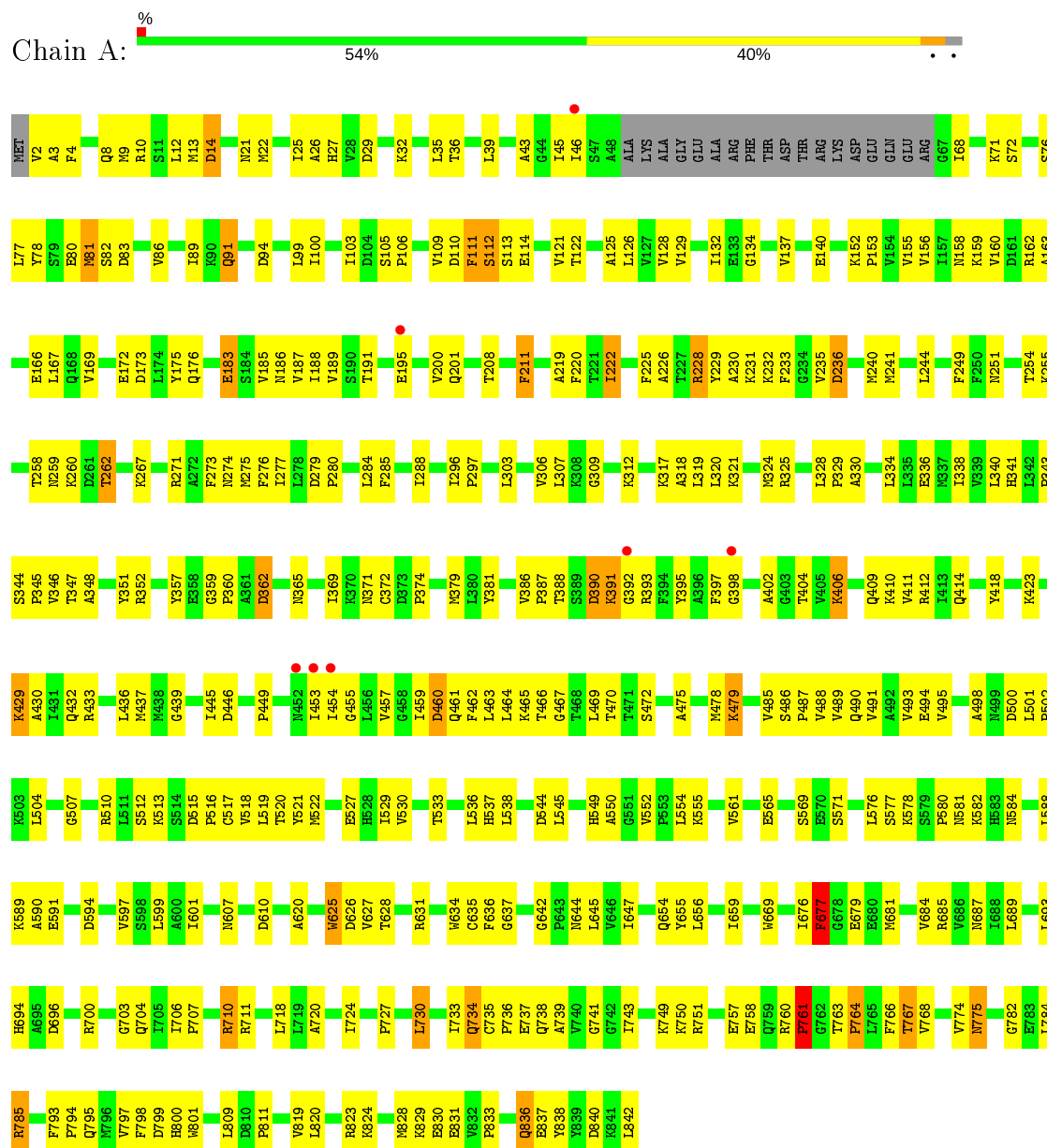


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			22	17	3	2		
3	D	1	Total	C	N	O	0	0
			22	17	3	2		
3	F	1	Total	C	N	O	0	0
			22	17	3	2		

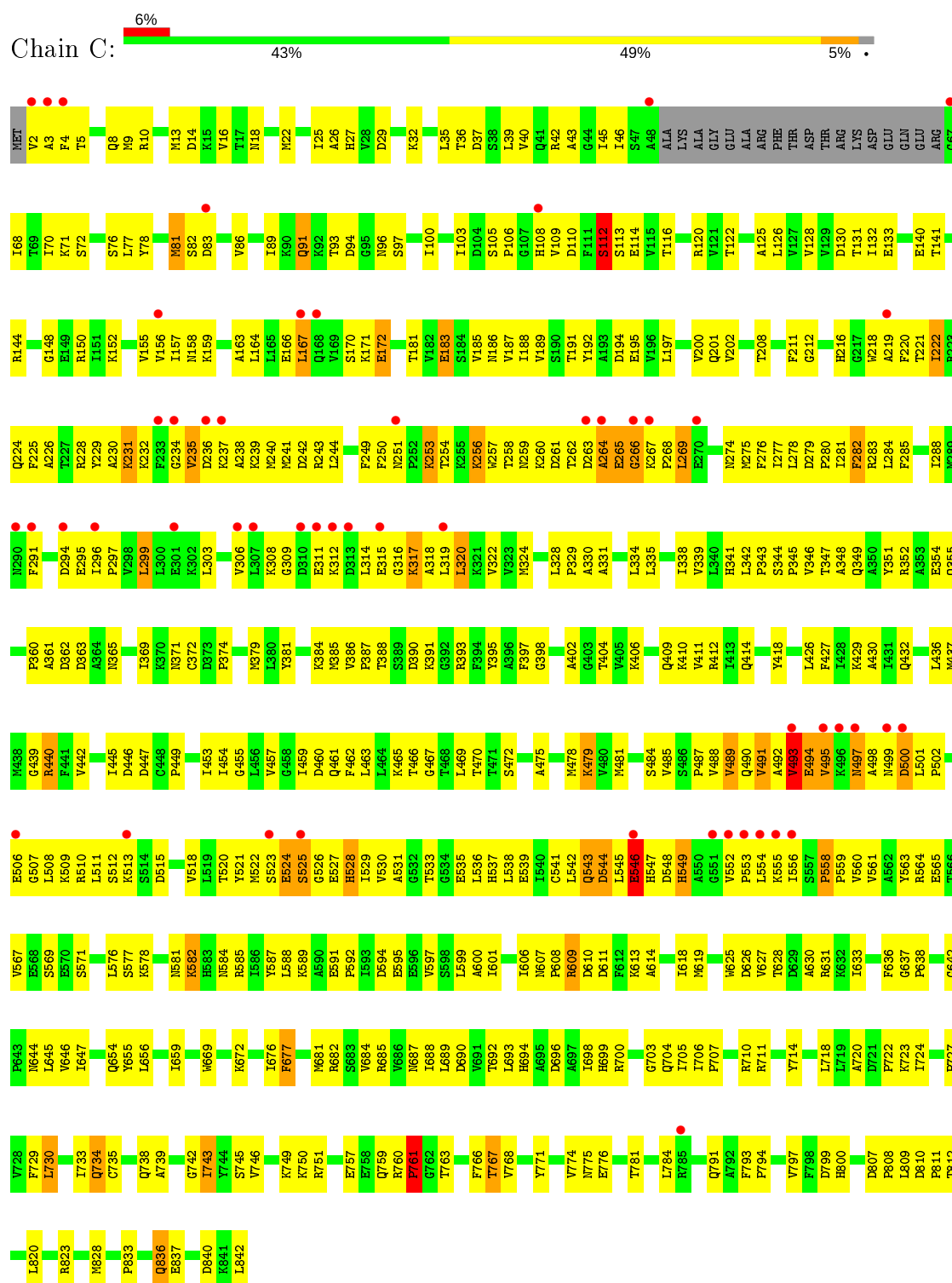
### 3 Residue-property plots

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.

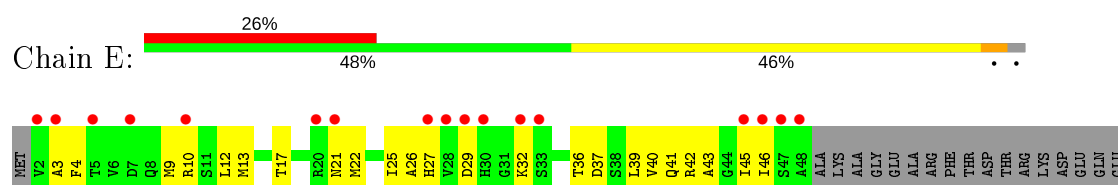
#### • Molecule 1: Elongation factor 2

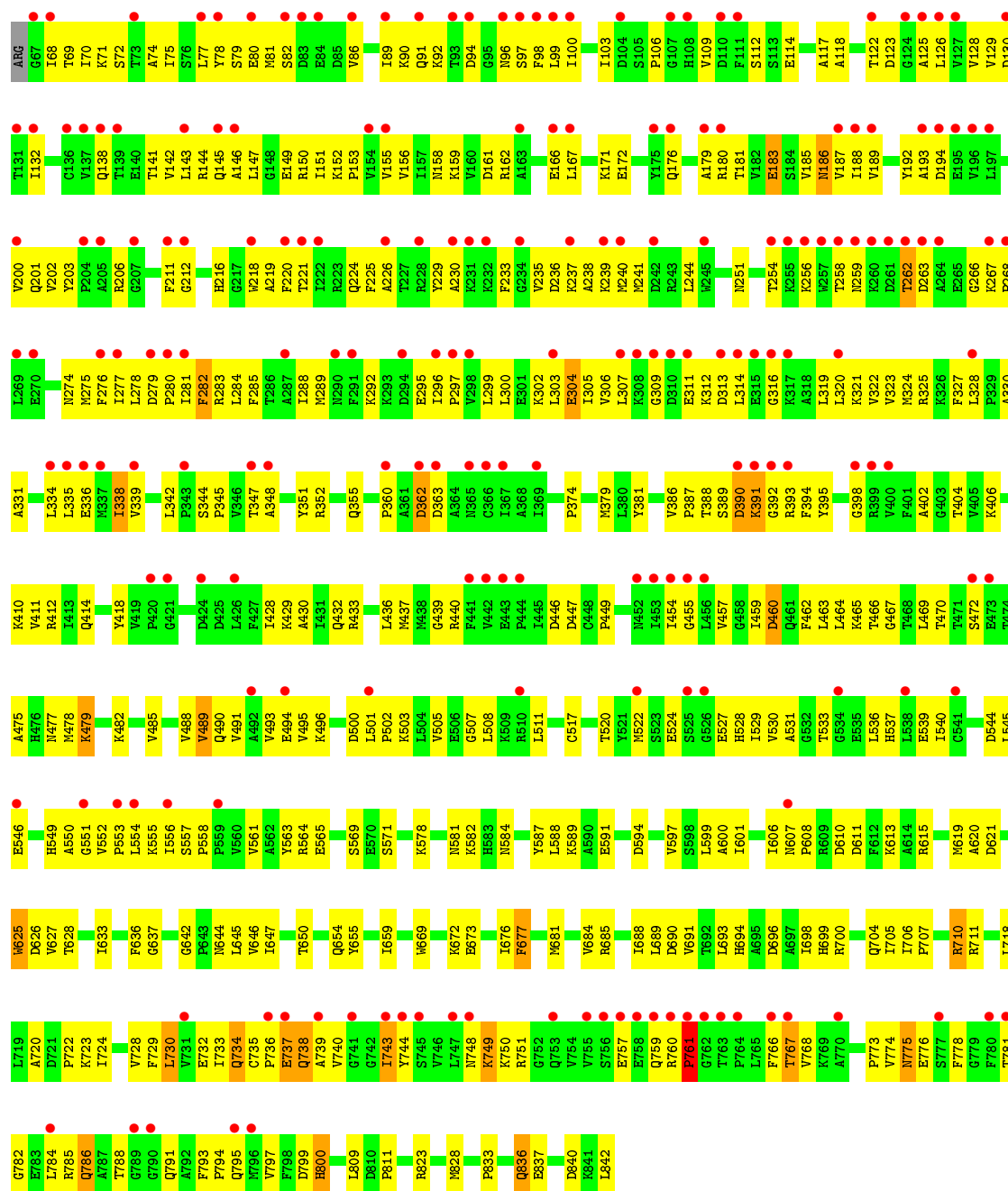


#### • Molecule 1: Elongation factor 2

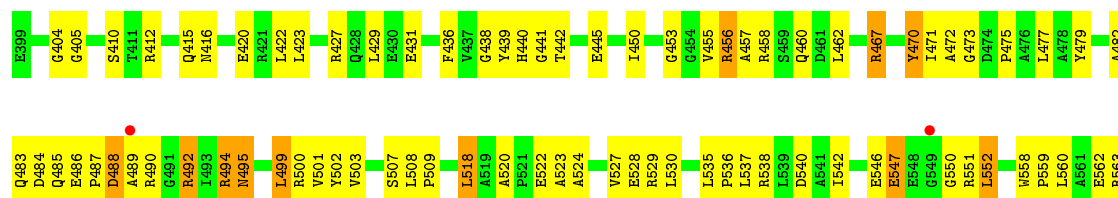


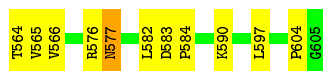
• Molecule 1: Elongation factor 2



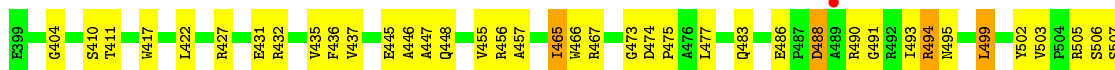


• Molecule 2: exotoxin A

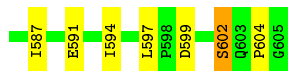




• Molecule 2: exotoxin A



• Molecule 2: exotoxin A





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	330.84Å 68.74Å 191.46Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 99.3 (29.70-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.254 , 0.274 0.249 , 0.264	Depositor DCC
$R_{free}$ test set	2056 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	24042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0789e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DDE, P34

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	0.48	0/6517	0.67	1/8823 (0.0%)
1	C	0.50	0/6517	0.71	1/8823 (0.0%)
1	E	0.44	0/6517	0.64	0/8823
2	B	0.52	0/1626	0.76	0/2216
2	D	0.54	0/1626	0.77	1/2216 (0.0%)
2	F	0.49	0/1626	0.75	1/2216 (0.0%)
All	All	0.48	0/24429	0.69	4/33117 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ASP	N-CA-C	-6.10	94.52	111.00
2	D	518	LEU	N-CA-C	5.83	126.73	111.00
2	F	518	LEU	N-CA-C	5.53	125.94	111.00
1	C	498	ALA	N-CA-C	5.23	125.12	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	6405	0	6472	339	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6405	0	6472	503	0
1	E	6405	0	6472	437	0
2	B	1587	0	1539	95	0
2	D	1587	0	1539	85	0
2	F	1587	0	1539	82	0
3	B	22	0	17	0	0
3	D	22	0	17	0	0
3	F	22	0	17	1	0
All	All	24042	0	24084	1514	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 31.

All (1514) 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:552:VAL:HG22	1:E:553:PRO:CD	1.53	1.37
1:E:552:VAL:CG2	1:E:553:PRO:HD3	1.65	1.27
1:C:546:GLU:HA	1:C:554:LEU:CD1	1.71	1.18
1:C:500:ASP:OD2	1:C:552:VAL:HG11	1.44	1.18
1:C:231:LYS:HE3	1:C:232:LYS:HG3	1.26	1.15
1:C:315:GLU:HA	1:C:319:LEU:HB2	1.26	1.09
1:C:253:LYS:HE3	1:C:253:LYS:HA	1.34	1.09
1:C:291:PHE:HE1	1:C:315:GLU:HB2	1.16	1.08
1:E:495:VAL:HG12	1:E:554:LEU:HD23	1.35	1.08
2:F:546:GLU:HG3	2:F:547:GLU:HG3	1.33	1.07
1:C:545:LEU:O	1:C:546:GLU:O	1.72	1.07
1:E:556:ILE:HG22	1:E:557:SER:H	1.21	1.06
1:C:256:LYS:CA	1:C:256:LYS:HE2	1.84	1.05
2:D:546:GLU:HG3	2:D:547:GLU:HG3	1.32	1.05
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.39	1.04
2:B:546:GLU:HG3	2:B:547:GLU:HG3	1.31	1.03
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.37	1.02
1:E:503:LYS:HB3	1:E:551:GLY:HA3	1.42	1.02
1:A:10:ARG:HD3	1:A:445:ILE:HD11	1.40	1.02
2:D:531:ILE:HD11	2:D:533:HIS:O	1.59	1.00
1:E:786:GLN:N	1:E:786:GLN:OE1	1.95	1.00
1:C:256:LYS:HA	1:C:256:LYS:CE	1.92	0.99
2:B:488:ASP:OD2	2:B:490:ARG:HG2	1.62	0.99
1:A:533:THR:H	1:A:537:HIS:CD2	1.81	0.99
2:B:477:LEU:HD13	2:B:551:ARG:NH1	1.78	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:HIS:HD2	1:A:696:ASP:H	1.12	0.98
1:C:256:LYS:HA	1:C:256:LYS:HE2	0.98	0.97
1:A:27:HIS:HD2	1:A:29:ASP:H	1.09	0.97
2:B:490:ARG:HD2	2:B:492:ARG:HD2	1.47	0.96
1:C:2:VAL:HG22	1:C:3:ALA:H	1.28	0.96
1:A:819:VAL:O	1:A:823:ARG:HG3	1.63	0.96
1:A:533:THR:H	1:A:537:HIS:HD2	1.00	0.95
1:E:27:HIS:HD2	1:E:29:ASP:H	1.12	0.95
2:D:527:VAL:O	2:D:531:ILE:HG23	1.66	0.94
1:A:737:GLU:HG3	1:A:766:PHE:CE2	2.03	0.94
1:E:694:HIS:HD2	1:E:696:ASP:H	1.11	0.94
1:E:546:GLU:HB2	1:E:554:LEU:HD12	1.46	0.94
1:A:429:LYS:HE3	1:A:430:ALA:H	1.31	0.94
1:C:546:GLU:HA	1:C:554:LEU:HD12	1.50	0.93
2:B:490:ARG:CD	2:B:492:ARG:HD2	1.97	0.93
1:C:291:PHE:CE1	1:C:315:GLU:HB2	2.03	0.92
1:E:404:THR:HG22	1:E:449:PRO:HA	1.51	0.92
1:E:495:VAL:CG1	1:E:554:LEU:HD23	1.99	0.92
1:C:42:ARG:HG3	1:C:331:ALA:CB	1.98	0.92
1:C:511:LEU:HA	1:C:549:HIS:CE1	2.05	0.91
1:C:288:ILE:HG23	1:C:319:LEU:CD2	2.00	0.91
1:C:166:GLU:C	1:C:167:LEU:HD12	1.90	0.91
1:C:265:GLU:HG3	1:C:266:GLY:H	1.32	0.91
1:C:523:SER:OG	1:C:527:GLU:HB2	1.69	0.91
1:A:578:LYS:HE3	1:A:840:ASP:OD1	1.69	0.90
1:A:404:THR:HG22	1:A:449:PRO:HA	1.52	0.90
1:A:45:ILE:HD12	1:A:76:SER:HB3	1.54	0.90
1:C:759:GLN:HB3	1:C:766:PHE:CE2	2.05	0.90
1:C:296:ILE:HD13	1:C:319:LEU:HD21	1.55	0.89
1:C:110:ASP:OD1	1:C:781:THR:HG21	1.72	0.88
1:C:2:VAL:HG22	1:C:3:ALA:N	1.84	0.88
1:C:234:GLY:O	1:C:235:VAL:HG23	1.72	0.88
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.54	0.88
1:C:536:LEU:HD12	1:C:537:HIS:N	1.88	0.88
1:C:404:THR:HG22	1:C:449:PRO:HA	1.53	0.88
1:C:4:PHE:HD1	1:C:8:GLN:OE1	1.57	0.88
1:C:694:HIS:HD2	1:C:696:ASP:H	1.19	0.87
2:D:520:ALA:HB3	2:D:522:GLU:OE2	1.75	0.87
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.55	0.87
1:E:91:GLN:HE22	1:E:344:SER:H	1.18	0.87
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:PRO:HB3	1:A:837:GLU:OE1	1.76	0.85
2:D:556:LEU:HD22	2:D:560:LEU:HD13	1.58	0.84
1:C:546:GLU:HA	1:C:554:LEU:HD11	1.58	0.84
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.59	0.84
1:C:288:ILE:HG23	1:C:319:LEU:CG	2.08	0.83
1:C:546:GLU:CA	1:C:554:LEU:CD1	2.55	0.83
1:A:500:ASP:HB2	1:A:552:VAL:HG11	1.59	0.83
1:C:27:HIS:HD2	1:C:29:ASP:H	1.22	0.83
1:C:157:ILE:CD1	1:C:181:THR:HG21	2.07	0.83
1:E:552:VAL:HG22	1:E:553:PRO:HD3	0.86	0.83
1:A:828:MET:CE	2:B:576:ARG:HE	1.91	0.83
1:E:524:GLU:HA	2:F:492:ARG:HH12	1.44	0.83
1:C:546:GLU:CA	1:C:554:LEU:HD12	2.07	0.83
1:E:500:ASP:OD2	1:E:552:VAL:HG21	1.77	0.82
1:A:828:MET:HE1	2:B:576:ARG:HE	1.44	0.82
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.60	0.82
1:A:533:THR:N	1:A:537:HIS:HD2	1.77	0.82
1:C:484:SER:HB3	1:C:797:VAL:CG2	2.10	0.82
2:D:527:VAL:HG13	2:D:542:ILE:HD12	1.62	0.81
1:E:495:VAL:HG12	1:E:554:LEU:CD2	2.09	0.81
2:D:477:LEU:HB2	2:D:551:ARG:HD2	1.63	0.81
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.60	0.81
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.62	0.81
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.61	0.81
1:C:2:VAL:CG2	1:C:3:ALA:H	1.94	0.81
1:E:27:HIS:CD2	1:E:29:ASP:H	1.98	0.81
1:A:27:HIS:CD2	1:A:29:ASP:H	1.96	0.80
1:C:638:PRO:HB3	1:C:672:LYS:HG2	1.61	0.80
1:E:694:HIS:O	1:E:700:ARG:HD3	1.82	0.80
1:C:243:ARG:NH1	1:C:257:TRP:CG	2.50	0.80
1:C:171:LYS:HG2	1:C:282:PHE:CD1	2.16	0.80
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.63	0.80
1:C:511:LEU:CA	1:C:549:HIS:CE1	2.64	0.80
1:C:836:GLN:HE21	1:C:836:GLN:H	1.28	0.80
2:F:503:VAL:HG12	2:F:564:THR:HG22	1.64	0.80
1:E:152:LYS:HD2	1:E:200:VAL:CG2	2.12	0.79
1:E:300:LEU:HG	1:E:305:ILE:HB	1.65	0.79
1:E:152:LYS:HD2	1:E:200:VAL:HG23	1.64	0.79
1:C:311:GLU:HA	1:C:314:LEU:HD13	1.64	0.79
2:B:427:ARG:O	2:B:431:GLU:HG3	1.83	0.79
1:C:157:ILE:HD11	1:C:181:THR:HG21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:503:LYS:HB3	1:E:551:GLY:CA	2.12	0.79
1:A:561:VAL:HG21	1:A:775:ASN:HA	1.63	0.78
1:A:737:GLU:HG3	1:A:766:PHE:HE2	1.45	0.78
1:C:229:TYR:CE2	1:C:276:PHE:HB3	2.19	0.78
2:F:488:ASP:CG	2:F:492:ARG:HB2	2.03	0.78
1:C:494:GLU:O	1:C:555:LYS:HB3	1.84	0.78
1:E:496:LYS:HB2	1:E:555:LYS:HZ3	1.48	0.78
2:F:513:ARG:HH11	2:F:513:ARG:HB2	1.49	0.78
1:E:237:LYS:HA	1:E:240:MET:HB3	1.64	0.78
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.65	0.78
1:E:496:LYS:HD3	1:E:555:LYS:HE2	1.66	0.78
1:A:230:ALA:O	1:A:235:VAL:HG22	1.83	0.77
1:E:552:VAL:HG22	1:E:553:PRO:HD2	1.60	0.77
1:E:147:LEU:CD1	1:E:192:TYR:HB2	2.14	0.77
1:E:412:ARG:HG2	1:E:412:ARG:HH11	1.50	0.77
1:E:552:VAL:CG2	1:E:553:PRO:CD	2.42	0.77
1:E:734:GLN:N	1:E:734:GLN:HE21	1.81	0.77
1:A:644:ASN:HD22	1:A:684:VAL:HB	1.49	0.77
1:C:265:GLU:HG3	1:C:266:GLY:N	1.99	0.77
1:C:311:GLU:HA	1:C:314:LEU:CD1	2.15	0.77
1:E:836:GLN:HE21	1:E:836:GLN:H	1.28	0.77
1:A:627:VAL:HG12	2:F:405:GLY:HA2	1.66	0.76
1:E:141:THR:HA	1:E:144:ARG:NH2	2.00	0.76
1:E:556:ILE:HG22	1:E:557:SER:N	2.00	0.76
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.68	0.76
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.68	0.76
1:C:836:GLN:NE2	1:C:836:GLN:H	1.84	0.76
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.15	0.76
1:C:288:ILE:HG23	1:C:319:LEU:HG	1.66	0.75
1:E:71:LYS:HE3	1:E:387:PRO:CD	2.16	0.75
1:E:155:VAL:HG23	1:E:202:VAL:HG11	1.69	0.75
1:E:736:PRO:HB2	1:E:738:GLN:CG	2.16	0.75
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.67	0.75
1:A:321:LYS:O	1:A:325:ARG:HG3	1.87	0.75
1:C:191:THR:O	1:C:763:THR:HG22	1.86	0.75
2:D:455:VAL:O	2:D:456:ARG:HG2	1.87	0.75
2:D:427:ARG:O	2:D:431:GLU:HG3	1.86	0.75
1:E:74:ALA:O	1:E:439:GLY:HA2	1.86	0.75
2:B:552:LEU:HD12	2:B:552:LEU:N	2.01	0.74
2:F:488:ASP:OD2	2:F:492:ARG:HB2	1.87	0.74
1:C:166:GLU:HB3	1:C:167:LEU:CD1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:ILE:O	1:E:342:LEU:HB2	1.87	0.74
2:B:467:ARG:HG3	2:B:558:TRP:CD1	2.22	0.74
1:A:544:ASP:O	1:A:549:HIS:HD2	1.71	0.74
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.68	0.74
1:E:500:ASP:O	1:E:503:LYS:HB2	1.87	0.74
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.70	0.74
1:C:391:LYS:HE3	1:C:393:ARG:HG3	1.70	0.73
1:C:584:ASN:ND2	1:C:694:HIS:H	1.86	0.73
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.70	0.73
1:E:786:GLN:OE1	1:E:786:GLN:CA	2.36	0.73
1:E:836:GLN:NE2	1:E:836:GLN:H	1.85	0.73
2:B:438:GLY:HA3	2:B:471:ILE:HD13	1.70	0.73
1:C:454:ILE:HG13	1:C:455:GLY:H	1.54	0.73
1:E:591:GLU:O	1:E:685:ARG:HB3	1.89	0.73
2:B:439:TYR:CE2	2:B:475:PRO:HD3	2.24	0.73
1:C:552:VAL:HB	1:C:553:PRO:CD	2.18	0.73
1:C:291:PHE:HE1	1:C:315:GLU:CB	1.97	0.72
1:A:251:ASN:HB3	1:A:254:THR:OG1	1.89	0.72
1:A:258:THR:HG22	1:A:259:ASN:N	2.03	0.72
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.71	0.72
1:C:533:THR:H	1:C:537:HIS:CD2	2.08	0.72
1:E:10:ARG:HG3	1:E:10:ARG:HH11	1.54	0.72
2:B:477:LEU:HD13	2:B:551:ARG:HH12	1.53	0.72
2:F:488:ASP:OD2	2:F:492:ARG:HD3	1.89	0.72
1:E:26:ALA:CB	1:E:128:VAL:HB	2.19	0.72
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.71	0.72
1:E:503:LYS:CB	1:E:551:GLY:HA3	2.17	0.72
1:C:320:LEU:HD12	1:C:324:MET:HG3	1.71	0.72
1:C:494:GLU:OE1	1:C:494:GLU:HA	1.87	0.72
1:C:509:LYS:HD2	1:C:509:LYS:N	2.05	0.72
1:C:533:THR:H	1:C:537:HIS:HD2	1.37	0.71
2:D:531:ILE:HD12	2:D:533:HIS:CE1	2.25	0.71
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.71	0.71
1:C:288:ILE:CG2	1:C:319:LEU:HG	2.20	0.71
1:C:158:ASN:ND2	1:C:159:LYS:HG2	2.06	0.71
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.73	0.71
1:C:584:ASN:HD21	1:C:694:HIS:H	1.38	0.71
1:A:694:HIS:CD2	1:A:696:ASP:H	2.03	0.71
1:C:251:ASN:OD1	1:C:269:LEU:HD11	1.91	0.71
1:E:482:LYS:HD3	1:E:797:VAL:HG11	1.71	0.71
1:E:508:LEU:HD22	1:E:520:THR:HB	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:HIS:HB2	2:B:471:ILE:HG22	1.71	0.71
1:E:185:VAL:O	1:E:189:VAL:HG23	1.91	0.70
1:A:836:GLN:HE21	1:A:836:GLN:H	1.37	0.70
2:B:552:LEU:HD12	2:B:552:LEU:H	1.56	0.70
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.06	0.70
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.72	0.70
1:C:509:LYS:O	1:C:513:LYS:HE3	1.91	0.70
1:E:331:ALA:O	1:E:335:LEU:HG	1.90	0.70
1:C:258:THR:HG22	1:C:260:LYS:H	1.56	0.70
1:E:226:ALA:O	1:E:230:ALA:HB2	1.92	0.70
1:E:459:ILE:HG21	1:E:463:LEU:HD12	1.74	0.70
1:C:757:GLU:HG3	1:C:768:VAL:HG22	1.73	0.70
1:C:546:GLU:HA	1:C:554:LEU:CG	2.22	0.70
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.74	0.70
1:C:545:LEU:O	1:C:546:GLU:C	2.24	0.70
1:E:236:ASP:OD1	1:E:238:ALA:HB3	1.92	0.70
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.72	0.70
1:E:496:LYS:HD3	1:E:555:LYS:CE	2.21	0.70
1:E:556:ILE:CG2	1:E:557:SER:H	2.04	0.70
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.72	0.70
1:E:454:ILE:HG13	1:E:455:GLY:H	1.55	0.70
1:A:820:LEU:HD11	1:A:830:GLU:HG2	1.74	0.69
1:A:391:LYS:HB3	1:A:393:ARG:HG2	1.74	0.69
1:A:410:LYS:HA	1:A:430:ALA:HA	1.74	0.69
1:C:571:SER:HB2	1:C:589:LYS:HG2	1.73	0.69
1:C:694:HIS:O	1:C:700:ARG:HD3	1.92	0.69
1:C:231:LYS:HE3	1:C:232:LYS:CG	2.14	0.69
1:C:251:ASN:HB2	1:C:254:THR:OG1	1.91	0.69
1:C:511:LEU:HD13	1:C:549:HIS:CD2	2.27	0.69
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.73	0.69
1:C:511:LEU:HD22	1:C:545:LEU:HD13	1.73	0.69
1:A:235:VAL:HG21	1:A:240:MET:HB2	1.73	0.69
1:A:429:LYS:HE3	1:A:430:ALA:N	2.07	0.69
1:C:45:ILE:HD11	1:C:78:TYR:CB	2.23	0.69
1:C:171:LYS:HG2	1:C:282:PHE:CE1	2.28	0.69
1:E:142:VAL:O	1:E:145:GLN:HB2	1.92	0.69
1:E:186:ASN:CG	1:E:201:GLN:HE21	1.96	0.69
1:A:828:MET:CE	2:B:576:ARG:NE	2.56	0.69
1:C:538:LEU:O	1:C:542:LEU:HG	1.93	0.69
1:E:203:TYR:HD2	1:E:206:ARG:HD2	1.56	0.69
1:A:669:TRP:HZ2	2:B:490:ARG:CD	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:LEU:HA	1:C:549:HIS:NE2	2.06	0.68
1:A:757:GLU:HG3	1:A:768:VAL:HG22	1.75	0.68
1:E:737:GLU:HG3	1:E:766:PHE:CE1	2.29	0.68
1:A:392:GLY:HA2	1:A:513:LYS:HE2	1.74	0.68
1:E:581:ASN:ND2	1:E:704:GLN:HG3	2.08	0.68
2:D:488:ASP:OD2	2:D:490:ARG:HG2	1.94	0.68
1:A:273:PHE:CD1	1:A:277:ILE:HD12	2.28	0.68
1:A:581:ASN:ND2	1:A:704:GLN:HG3	2.09	0.68
2:F:522:GLU:CD	2:F:522:GLU:H	1.97	0.68
1:C:694:HIS:CD2	1:C:696:ASP:H	2.09	0.68
1:A:591:GLU:O	1:A:685:ARG:HB3	1.94	0.68
1:A:824:LYS:HE3	1:A:830:GLU:OE2	1.94	0.68
1:C:225:PHE:CD2	1:C:277:ILE:HG13	2.29	0.67
1:E:546:GLU:CB	1:E:554:LEU:HD12	2.23	0.67
1:C:3:ALA:HA	1:C:46:ILE:O	1.94	0.67
1:E:785:ARG:NH2	1:E:786:GLN:HE22	1.93	0.67
1:C:497:ASN:N	1:C:497:ASN:HD22	1.91	0.67
2:D:552:LEU:HD12	2:D:552:LEU:N	2.10	0.67
1:E:334:LEU:O	1:E:338:ILE:HG12	1.95	0.67
1:A:571:SER:HB2	1:A:589:LYS:HG2	1.74	0.67
1:C:530:VAL:HG12	1:C:530:VAL:O	1.95	0.67
2:D:417:TRP:CZ2	2:D:568:PRO:HD2	2.29	0.67
1:A:694:HIS:O	1:A:700:ARG:HD3	1.95	0.67
1:C:315:GLU:CA	1:C:319:LEU:HB2	2.16	0.67
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.77	0.67
1:C:497:ASN:N	1:C:497:ASN:ND2	2.42	0.67
1:E:91:GLN:NE2	1:E:344:SER:H	1.91	0.67
1:E:694:HIS:CD2	1:E:696:ASP:H	2.02	0.67
1:A:258:THR:HG22	1:A:259:ASN:H	1.58	0.67
1:C:543:GLN:HG2	1:C:544:ASP:N	2.08	0.67
1:E:710:ARG:HH11	1:E:710:ARG:HG3	1.60	0.67
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.76	0.67
2:B:503:VAL:HG12	2:B:564:THR:HG22	1.77	0.67
1:C:354:GLU:OE2	1:C:361:ALA:HB1	1.95	0.67
1:C:591:GLU:O	1:C:685:ARG:HB3	1.94	0.67
1:C:488:VAL:HG23	1:C:489:VAL:HG22	1.77	0.67
1:E:591:GLU:CG	1:E:685:ARG:HG2	2.24	0.67
1:A:836:GLN:NE2	1:A:836:GLN:H	1.92	0.66
2:D:465:ILE:H	2:D:465:ILE:HD13	1.59	0.66
1:A:285:PHE:HE2	1:A:324:MET:SD	2.18	0.66
1:E:496:LYS:HD3	1:E:555:LYS:NZ	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:736:PRO:HB2	1:E:738:GLN:HG2	1.77	0.66
1:C:530:VAL:O	1:C:538:LEU:CD1	2.44	0.66
1:E:292:LYS:HD3	1:E:295:GLU:OE2	1.95	0.66
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.30	0.66
1:E:589:LYS:HE3	1:E:689:LEU:HD11	1.76	0.66
1:A:594:ASP:HB2	1:A:597:VAL:HG23	1.77	0.66
1:C:311:GLU:O	1:C:314:LEU:HD13	1.96	0.66
1:E:307:LEU:HD13	1:E:312:LYS:HA	1.77	0.66
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.30	0.66
1:C:253:LYS:CE	1:C:253:LYS:HA	2.21	0.66
1:C:243:ARG:NH1	1:C:257:TRP:CD1	2.64	0.66
1:C:578:LYS:HE3	1:C:840:ASP:OD1	1.95	0.66
1:A:27:HIS:HD2	1:A:29:ASP:N	1.89	0.66
1:A:429:LYS:HG3	1:A:430:ALA:H	1.59	0.66
1:C:132:ILE:HG23	1:C:133:GLU:N	2.11	0.66
1:C:72:SER:HA	1:C:439:GLY:O	1.96	0.66
1:C:759:GLN:HB3	1:C:766:PHE:CD2	2.31	0.66
1:E:495:VAL:CG1	1:E:554:LEU:CD2	2.71	0.65
1:A:25:ILE:HD12	1:A:125:ALA:HB1	1.77	0.65
1:C:454:ILE:HG13	1:C:455:GLY:N	2.12	0.65
1:C:226:ALA:O	1:C:230:ALA:HB2	1.96	0.65
1:C:493:VAL:HG21	1:C:545:LEU:HD21	1.77	0.65
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.76	0.65
1:A:734:GLN:HE21	1:A:734:GLN:N	1.95	0.65
1:C:231:LYS:HG2	1:C:232:LYS:N	2.10	0.65
1:E:75:ILE:HD13	1:E:439:GLY:CA	2.27	0.65
2:F:537:LEU:O	2:F:538:ARG:HD3	1.96	0.65
1:E:578:LYS:HE3	1:E:840:ASP:OD1	1.96	0.65
1:E:759:GLN:HB2	1:E:766:PHE:CE2	2.31	0.65
1:A:3:ALA:HA	1:A:46:ILE:O	1.96	0.65
2:B:479:TYR:CD2	2:B:582:LEU:HB2	2.31	0.65
1:C:492:ALA:HA	1:C:528:HIS:O	1.96	0.65
2:D:523:ALA:O	2:D:527:VAL:HG23	1.96	0.65
1:E:258:THR:HG22	1:E:259:ASN:H	1.61	0.65
1:C:183:GLU:O	1:C:187:VAL:HG23	1.97	0.65
2:F:548:GLU:HG2	2:F:548:GLU:O	1.96	0.65
1:A:258:THR:CG2	1:A:260:LYS:HG2	2.27	0.65
1:C:490:GLN:O	1:C:491:VAL:HG13	1.97	0.65
1:A:828:MET:HE1	2:B:576:ARG:NE	2.11	0.64
1:C:609:ARG:HH11	1:C:609:ARG:HG3	1.62	0.64
1:C:167:LEU:N	1:C:167:LEU:HD12	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.36	0.64
1:A:493:VAL:HG12	1:A:554:LEU:HD22	1.79	0.64
1:E:311:GLU:HB3	1:E:322:VAL:HG11	1.79	0.64
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.80	0.64
1:A:429:LYS:HG3	1:A:430:ALA:N	2.12	0.64
1:C:157:ILE:HD11	1:C:181:THR:CG2	2.26	0.64
1:C:27:HIS:CD2	1:C:29:ASP:H	2.10	0.64
1:E:89:ILE:C	1:E:91:GLN:H	2.01	0.64
2:F:467:ARG:HG3	2:F:558:TRP:CD1	2.31	0.64
1:C:384:LYS:HB2	1:C:465:LYS:HE3	1.78	0.64
1:C:507:GLY:HA2	1:C:510:ARG:HD2	1.79	0.64
1:C:541:CYS:O	1:C:545:LEU:HB2	1.98	0.64
2:F:556:LEU:HD22	2:F:560:LEU:CD1	2.26	0.64
1:C:484:SER:HB3	1:C:797:VAL:HG23	1.80	0.64
1:E:454:ILE:HG13	1:E:455:GLY:N	2.12	0.64
1:E:162:ARG:O	1:E:166:GLU:HB2	1.98	0.64
1:E:75:ILE:HD13	1:E:439:GLY:HA3	1.79	0.64
1:A:581:ASN:O	1:A:582:LYS:HB2	1.98	0.63
2:F:504:PRO:HD3	2:F:563:ARG:O	1.98	0.63
1:C:265:GLU:OE2	1:C:267:LYS:HE3	1.97	0.63
1:C:166:GLU:HB3	1:C:167:LEU:HD12	1.79	0.63
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.78	0.63
1:E:781:THR:O	1:E:785:ARG:HG3	1.97	0.63
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.80	0.63
1:E:528:HIS:O	1:E:529:ILE:HD13	1.99	0.63
1:C:529:ILE:N	1:C:529:ILE:HD12	2.14	0.63
1:C:192:TYR:HA	1:C:763:THR:HG21	1.79	0.63
1:C:609:ARG:NH1	1:C:609:ARG:HG3	2.13	0.63
1:C:581:ASN:ND2	1:C:704:GLN:HG3	2.14	0.63
1:A:454:ILE:HG13	1:A:455:GLY:H	1.64	0.63
1:C:148:GLY:HA2	1:C:760:ARG:NH2	2.13	0.63
1:E:528:HIS:C	1:E:529:ILE:HD13	2.18	0.63
2:B:537:LEU:O	2:B:538:ARG:HD3	1.98	0.63
2:B:495:ASN:N	2:B:495:ASN:HD22	1.96	0.63
1:E:710:ARG:NH1	1:E:710:ARG:HG3	2.14	0.62
1:A:288:ILE:HG23	1:A:319:LEU:HD23	1.80	0.62
1:A:459:ILE:HG21	1:A:463:LEU:HD12	1.81	0.62
1:A:654:GLN:HG2	1:A:655:TYR:CD2	2.34	0.62
1:C:35:LEU:HD22	1:C:334:LEU:HD11	1.82	0.62
1:E:153:PRO:HD2	1:E:200:VAL:HG22	1.81	0.62
1:A:581:ASN:HD21	1:A:704:GLN:HG3	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:LEU:C	1:C:501:LEU:HD23	2.19	0.62
1:E:500:ASP:CB	1:E:552:VAL:HG11	2.29	0.62
1:A:710:ARG:HG3	1:A:710:ARG:HH11	1.63	0.62
1:C:2:VAL:CG2	1:C:3:ALA:N	2.53	0.62
1:C:588:LEU:C	1:C:588:LEU:HD12	2.19	0.62
1:E:584:ASN:ND2	1:E:694:HIS:H	1.97	0.62
1:A:504:LEU:HD13	1:A:554:LEU:HD21	1.82	0.62
1:C:311:GLU:CA	1:C:314:LEU:HD13	2.29	0.62
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.81	0.62
2:B:410:SER:OG	2:B:412:ARG:HB3	1.99	0.62
2:F:493:ILE:HG22	2:F:493:ILE:O	2.00	0.62
2:F:552:LEU:HD12	2:F:552:LEU:N	2.15	0.62
1:A:735:CYS:SG	1:A:739:ALA:HB3	2.40	0.62
1:C:384:LYS:CB	1:C:465:LYS:HE3	2.30	0.62
1:E:321:LYS:O	1:E:325:ARG:HG3	1.99	0.62
1:A:809:LEU:O	1:A:811:PRO:HD3	2.00	0.62
1:A:406:LYS:HG3	1:A:409:GLN:HB2	1.82	0.61
1:A:647:ILE:HG13	1:A:685:ARG:HE	1.63	0.61
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.14	0.61
1:A:222:ILE:HG22	1:A:241:MET:HB2	1.81	0.61
1:C:311:GLU:OE2	1:C:322:VAL:HG11	2.01	0.61
2:D:455:VAL:O	2:D:456:ARG:CG	2.48	0.61
1:A:2:VAL:HG22	1:A:3:ALA:N	2.15	0.61
2:B:477:LEU:HD13	2:B:551:ARG:HH11	1.65	0.61
1:C:103:ILE:HD12	1:C:122:THR:HG22	1.81	0.61
1:E:508:LEU:HD22	1:E:520:THR:CG2	2.31	0.61
1:E:607:ASN:HB3	1:E:610:ASP:OD2	1.99	0.61
2:D:457:ALA:HB2	2:D:558:TRP:CD2	2.35	0.61
1:E:81:MET:O	1:E:96:ASN:HB3	2.00	0.61
1:E:410:LYS:HA	1:E:430:ALA:HA	1.82	0.61
1:E:126:LEU:HD11	1:E:156:VAL:HG21	1.83	0.61
1:C:584:ASN:HD22	1:C:693:LEU:HA	1.66	0.61
1:C:749:LYS:O	1:C:750:LYS:HD2	2.00	0.61
1:E:495:VAL:HA	1:E:554:LEU:HA	1.81	0.61
1:A:162:ARG:O	1:A:166:GLU:HB2	2.00	0.61
1:A:669:TRP:CZ2	2:B:490:ARG:HD2	2.36	0.61
1:C:296:ILE:CD1	1:C:319:LEU:HD21	2.29	0.61
1:C:563:TYR:O	1:C:564:ARG:HD2	2.01	0.60
1:C:591:GLU:CG	1:C:685:ARG:HG2	2.30	0.60
1:C:810:ASP:OD1	1:C:812:THR:HG22	2.01	0.60
1:A:584:ASN:ND2	1:A:694:HIS:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:GLU:CG	1:A:766:PHE:CE2	2.82	0.60
2:D:417:TRP:CH2	2:D:568:PRO:HD2	2.35	0.60
1:C:703:GLY:HA2	2:D:493:ILE:HD13	1.84	0.60
1:A:158:ASN:ND2	1:A:159:LYS:HG2	2.16	0.60
1:C:192:TYR:HA	1:C:763:THR:CG2	2.31	0.60
1:C:506:GLU:O	1:C:510:ARG:HG3	2.01	0.60
1:E:285:PHE:CE2	1:E:320:LEU:HD11	2.36	0.60
2:F:537:LEU:O	2:F:538:ARG:CD	2.49	0.60
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.82	0.60
1:C:410:LYS:HE2	1:C:430:ALA:HB2	1.83	0.60
1:E:126:LEU:HD11	1:E:156:VAL:CG2	2.31	0.60
1:A:550:ALA:O	1:A:552:VAL:HG23	2.01	0.60
2:F:420:GLU:H	2:F:420:GLU:CD	2.05	0.60
1:C:491:VAL:O	1:C:529:ILE:HA	2.02	0.60
1:C:734:GLN:HE21	1:C:734:GLN:N	1.98	0.60
1:E:694:HIS:HD2	1:E:696:ASP:N	1.93	0.59
1:A:183:GLU:O	1:A:187:VAL:HG23	2.03	0.59
1:A:229:TYR:CE2	1:A:276:PHE:HB3	2.36	0.59
1:E:167:LEU:H	1:E:167:LEU:HD12	1.66	0.59
1:C:258:THR:HG22	1:C:259:ASN:N	2.18	0.59
1:C:784:LEU:CD2	1:C:794:PRO:HG3	2.32	0.59
1:E:412:ARG:HH12	1:E:428:ILE:HD11	1.67	0.59
1:A:381:TYR:O	1:A:398:GLY:HA3	2.02	0.59
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.85	0.59
1:E:258:THR:HG22	1:E:259:ASN:N	2.18	0.59
1:E:749:LYS:O	1:E:750:LYS:HD2	2.02	0.59
1:C:251:ASN:H	1:C:251:ASN:HD22	1.50	0.59
2:F:556:LEU:HD22	2:F:560:LEU:HD13	1.84	0.59
1:E:493:VAL:HG12	1:E:494:GLU:N	2.17	0.59
2:B:455:VAL:C	2:B:456:ARG:HD2	2.23	0.59
1:C:535:GLU:O	1:C:539:GLU:HG3	2.03	0.59
1:E:500:ASP:HA	1:E:503:LYS:HD2	1.83	0.59
1:A:454:ILE:HG13	1:A:455:GLY:N	2.17	0.59
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.84	0.59
2:B:530:LEU:HD23	2:B:604:PRO:HD3	1.85	0.59
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.83	0.59
1:C:258:THR:HG22	1:C:259:ASN:H	1.68	0.59
1:C:569:SER:O	1:C:720:ALA:HB1	2.02	0.59
1:A:737:GLU:HG3	1:A:766:PHE:CD2	2.37	0.59
2:B:457:ALA:O	2:B:458:ARG:HG3	2.03	0.59
1:C:581:ASN:O	1:C:582:LYS:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:HD2	1:A:517:CYS:SG	2.43	0.58
1:E:584:ASN:HD21	1:E:694:HIS:H	1.49	0.58
1:E:591:GLU:HG2	1:E:685:ARG:HG2	1.84	0.58
1:A:240:MET:O	1:A:244:LEU:HG	2.03	0.58
1:E:147:LEU:HD12	1:E:192:TYR:HB2	1.86	0.58
1:E:153:PRO:HD2	1:E:200:VAL:CG2	2.33	0.58
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.68	0.58
1:A:466:THR:HG22	1:A:467:GLY:N	2.19	0.58
1:E:91:GLN:HE22	1:E:344:SER:N	1.95	0.58
2:F:487:PRO:HA	2:F:492:ARG:O	2.02	0.58
1:A:459:ILE:HD11	1:A:469:LEU:HD21	1.84	0.58
1:A:591:GLU:CG	1:A:685:ARG:HG2	2.34	0.58
1:C:221:THR:OG1	1:C:224:GLN:HG3	2.02	0.58
1:C:384:LYS:HB2	1:C:465:LYS:NZ	2.18	0.58
1:C:412:ARG:HH11	1:C:412:ARG:HG2	1.68	0.58
1:C:611:ASP:OD2	1:C:613:LYS:HB2	2.04	0.58
1:E:581:ASN:O	1:E:582:LYS:HB2	2.02	0.58
1:E:588:LEU:HD12	1:E:588:LEU:C	2.23	0.58
1:C:45:ILE:HD11	1:C:78:TYR:N	2.19	0.58
1:C:511:LEU:CD1	1:C:549:HIS:NE2	2.67	0.58
1:C:45:ILE:HG12	1:C:76:SER:O	2.04	0.58
1:C:384:LYS:HB2	1:C:465:LYS:CE	2.34	0.58
1:E:158:ASN:HD22	1:E:159:LYS:HG3	1.67	0.58
1:E:225:PHE:CG	1:E:277:ILE:HD12	2.39	0.58
1:A:591:GLU:HG2	1:A:685:ARG:HG2	1.86	0.58
1:C:410:LYS:HA	1:C:430:ALA:HA	1.84	0.58
1:C:544:ASP:O	1:C:549:HIS:N	2.37	0.58
1:C:609:ARG:HH11	1:C:609:ARG:CG	2.17	0.58
2:D:508:LEU:N	2:D:509:PRO:CD	2.67	0.58
1:E:152:LYS:CD	1:E:200:VAL:HG23	2.33	0.58
1:E:69:THR:OG1	1:E:389:SER:HB3	2.04	0.58
1:C:132:ILE:HG23	1:C:133:GLU:H	1.68	0.58
1:E:412:ARG:HG2	1:E:412:ARG:NH1	2.13	0.58
2:D:546:GLU:HG3	2:D:547:GLU:CG	2.22	0.57
1:E:203:TYR:CD2	1:E:206:ARG:HD2	2.37	0.57
2:F:417:TRP:CE2	2:F:568:PRO:HB2	2.39	0.57
1:A:411:VAL:HG12	1:A:412:ARG:N	2.18	0.57
1:C:543:GLN:CG	1:C:544:ASP:N	2.67	0.57
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.85	0.57
1:A:169:VAL:HG22	1:A:173:ASP:HB2	1.86	0.57
1:C:236:ASP:OD2	1:C:239:LYS:HE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:ASN:HB3	1:C:610:ASP:CG	2.24	0.57
1:A:737:GLU:CG	1:A:766:PHE:HE2	2.14	0.57
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.40	0.57
1:A:828:MET:HE2	2:B:576:ARG:HE	1.69	0.57
1:C:594:ASP:HB2	1:C:597:VAL:HG23	1.85	0.57
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.68	0.57
1:C:654:GLN:HG2	1:C:655:TYR:CD2	2.39	0.57
2:D:546:GLU:CG	2:D:547:GLU:HG3	2.21	0.57
1:E:508:LEU:HD22	1:E:520:THR:CB	2.35	0.57
2:F:445:GLU:OE1	2:F:494:ARG:NH2	2.37	0.57
1:A:669:TRP:CZ2	2:B:490:ARG:CD	2.87	0.57
1:C:91:GLN:O	1:C:93:THR:HG23	2.04	0.57
1:E:581:ASN:HD21	1:E:704:GLN:HG3	1.69	0.57
1:A:175:TYR:HD2	1:A:176:GLN:HE21	1.53	0.57
1:A:561:VAL:HG21	1:A:775:ASN:CA	2.32	0.57
1:A:72:SER:HA	1:A:439:GLY:O	2.05	0.57
1:C:263:ASP:O	1:C:265:GLU:N	2.35	0.57
1:C:426:LEU:O	1:C:427:PHE:CD1	2.58	0.57
1:E:569:SER:O	1:E:720:ALA:HB1	2.05	0.57
1:A:584:ASN:HD21	1:A:694:HIS:H	1.52	0.57
2:D:465:ILE:HG12	2:D:466:TRP:CD1	2.39	0.57
2:D:529:ARG:NH1	2:D:604:PRO:HG2	2.19	0.57
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.35	0.57
1:E:303:LEU:O	1:E:304:GLU:HB2	2.05	0.57
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.86	0.57
1:C:167:LEU:N	1:C:167:LEU:CD1	2.68	0.56
1:C:200:VAL:O	1:C:200:VAL:HG13	2.05	0.56
1:E:225:PHE:CD2	1:E:277:ILE:HD12	2.40	0.56
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.70	0.56
1:A:140:GLU:HG3	1:A:188:ILE:CD1	2.35	0.56
1:A:321:LYS:HZ2	1:A:325:ARG:HD3	1.70	0.56
1:A:35:LEU:HD22	1:A:334:LEU:HD11	1.86	0.56
1:A:429:LYS:CE	1:A:430:ALA:H	2.12	0.56
2:B:457:ALA:HB2	2:B:558:TRP:CD2	2.40	0.56
1:C:25:ILE:HD12	1:C:125:ALA:HB1	1.87	0.56
1:E:307:LEU:HB2	1:E:312:LYS:HE2	1.87	0.56
1:A:32:LYS:NZ	1:A:105:SER:HB2	2.21	0.56
2:D:445:GLU:OE1	2:D:494:ARG:NH2	2.38	0.56
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.87	0.56
2:F:570:ALA:HB3	2:F:591:GLU:OE1	2.05	0.56
1:A:710:ARG:NH1	1:A:710:ARG:HG3	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:PRO:O	1:C:349:GLN:HG3	2.05	0.56
2:F:582:LEU:HD21	2:F:587:ILE:HD11	1.88	0.56
1:A:348:ALA:HA	1:A:351:TYR:CE2	2.41	0.56
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.87	0.56
1:E:279:ASP:O	1:E:283:ARG:HG2	2.06	0.56
1:A:631:ARG:NH2	2:F:406:ASP:OD2	2.38	0.56
1:C:116:THR:HB	1:C:481:MET:HE3	1.88	0.56
1:C:126:LEU:HD11	1:C:156:VAL:CG2	2.36	0.56
1:C:344:SER:C	1:C:346:VAL:H	2.09	0.56
1:C:571:SER:HB2	1:C:589:LYS:CG	2.35	0.56
1:E:43:ALA:HB1	1:E:78:TYR:O	2.06	0.56
2:F:473:GLY:HA3	2:F:597:LEU:HD11	1.87	0.56
1:C:529:ILE:HG22	1:C:530:VAL:N	2.20	0.56
1:C:750:LYS:O	1:C:751:ARG:HB2	2.05	0.56
1:E:132:ILE:N	1:E:132:ILE:HD12	2.20	0.56
1:A:565:GLU:CD	1:A:676:ILE:HB	2.26	0.56
1:C:348:ALA:O	1:C:352:ARG:HB2	2.05	0.56
1:C:494:GLU:OE1	1:C:494:GLU:CA	2.53	0.56
1:C:4:PHE:CD1	1:C:8:GLN:OE1	2.48	0.56
2:D:576:ARG:HH11	2:D:576:ARG:HG3	1.70	0.56
1:C:222:ILE:HG22	1:C:241:MET:HB2	1.88	0.56
2:B:546:GLU:HG3	2:B:547:GLU:CG	2.22	0.56
2:B:563:ARG:HG3	2:B:563:ARG:HH11	1.71	0.56
1:C:234:GLY:O	1:C:235:VAL:CG2	2.50	0.56
1:C:381:TYR:O	1:C:398:GLY:HA3	2.05	0.56
1:C:499:ASN:O	1:C:502:PRO:HD2	2.05	0.56
1:C:647:ILE:HG13	1:C:685:ARG:HE	1.70	0.56
2:B:455:VAL:O	2:B:456:ARG:HD2	2.06	0.55
1:C:412:ARG:NH1	1:C:412:ARG:HG2	2.21	0.55
1:C:511:LEU:HD13	1:C:549:HIS:NE2	2.21	0.55
1:E:183:GLU:OE1	1:E:186:ASN:ND2	2.39	0.55
1:E:200:VAL:O	1:E:200:VAL:HG22	2.06	0.55
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.88	0.55
1:C:208:THR:HG22	1:C:341:HIS:CG	2.41	0.55
1:C:545:LEU:HA	1:C:549:HIS:HB2	1.88	0.55
1:E:493:VAL:CG1	1:E:494:GLU:N	2.69	0.55
1:C:637:GLY:O	1:C:642:GLY:HA3	2.06	0.55
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.88	0.55
1:A:758:GLU:O	1:A:766:PHE:HD1	1.89	0.55
1:C:253:LYS:HE3	1:C:253:LYS:CA	2.22	0.55
1:C:546:GLU:HA	1:C:554:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:VAL:HG13	1:C:688:ILE:CD1	2.36	0.55
1:A:730:LEU:HB2	1:A:799:ASP:HB2	1.89	0.55
1:A:45:ILE:HB	1:A:76:SER:HB2	1.87	0.55
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.88	0.55
2:B:471:ILE:HG21	2:B:501:VAL:HG21	1.88	0.55
1:C:132:ILE:HG23	1:C:133:GLU:HG3	1.87	0.55
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.36	0.55
1:C:735:CYS:SG	1:C:739:ALA:HB3	2.47	0.55
1:E:809:LEU:O	1:E:811:PRO:HD3	2.06	0.55
1:A:258:THR:HG21	1:A:260:LYS:HG2	1.88	0.55
1:A:277:ILE:O	1:A:280:PRO:HD2	2.07	0.55
1:A:191:THR:O	1:A:763:THR:HG22	2.07	0.55
1:C:239:LYS:O	1:C:243:ARG:HG3	2.07	0.55
1:C:291:PHE:CE1	1:C:315:GLU:OE1	2.60	0.55
1:C:522:MET:HA	1:C:527:GLU:O	2.06	0.55
1:E:307:LEU:HD12	1:E:312:LYS:HD3	1.89	0.55
1:A:348:ALA:O	1:A:352:ARG:HB2	2.07	0.55
1:A:109:VAL:CG1	1:A:793:PHE:HE1	2.20	0.55
2:D:520:ALA:HB1	2:D:521:PRO:CD	2.36	0.55
1:E:348:ALA:O	1:E:352:ARG:HB2	2.07	0.55
2:F:530:LEU:HA	2:F:604:PRO:HG3	1.88	0.55
1:C:311:GLU:OE2	1:C:322:VAL:CG1	2.54	0.55
2:D:432:ARG:HA	2:D:432:ARG:CZ	2.37	0.55
1:E:432:GLN:HB2	1:E:457:VAL:O	2.07	0.55
1:C:511:LEU:N	1:C:549:HIS:CE1	2.75	0.55
1:C:552:VAL:HB	1:C:553:PRO:HD3	1.88	0.55
1:E:391:LYS:HG3	1:E:392:GLY:H	1.72	0.55
1:E:749:LYS:HG3	1:E:749:LYS:O	2.06	0.55
1:C:508:LEU:HD23	1:C:545:LEU:HD11	1.89	0.55
1:C:591:GLU:HG2	1:C:685:ARG:HG2	1.88	0.55
1:E:10:ARG:HG3	1:E:10:ARG:NH1	2.15	0.55
1:E:494:GLU:HA	1:E:494:GLU:OE1	2.07	0.55
1:A:365:ASN:O	1:A:369:ILE:HG12	2.07	0.54
1:E:240:MET:O	1:E:244:LEU:HG	2.06	0.54
1:A:321:LYS:NZ	1:A:325:ARG:HD3	2.22	0.54
1:C:189:VAL:CG1	1:C:200:VAL:HG12	2.36	0.54
1:C:411:VAL:HG12	1:C:412:ARG:N	2.22	0.54
1:C:581:ASN:HD21	1:C:704:GLN:HG3	1.71	0.54
1:C:109:VAL:HG13	1:C:793:PHE:HE1	1.72	0.54
2:D:465:ILE:H	2:D:465:ILE:CD1	2.21	0.54
2:D:570:ALA:HB3	2:D:591:GLU:OE1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ALA:HA	1:E:151:ILE:HD12	1.89	0.54
1:E:284:LEU:HD13	1:E:324:MET:HE3	1.89	0.54
1:C:251:ASN:H	1:C:251:ASN:ND2	2.06	0.54
1:E:706:ILE:HB	1:E:707:PRO:HD3	1.90	0.54
1:E:522:MET:HB2	2:F:490:ARG:HH12	1.71	0.54
1:A:391:LYS:HG3	1:A:392:GLY:H	1.72	0.54
2:D:574:ASP:OD1	2:D:575:PRO:HD2	2.07	0.54
1:E:740:VAL:HG21	1:E:766:PHE:CD1	2.43	0.54
1:A:155:VAL:HG12	1:A:156:VAL:N	2.22	0.54
1:A:501:LEU:C	1:A:501:LEU:HD23	2.28	0.54
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.43	0.54
1:C:285:PHE:HE2	1:C:324:MET:SD	2.31	0.54
2:D:518:LEU:HD11	2:D:542:ILE:HD13	1.89	0.54
2:D:527:VAL:CG1	2:D:542:ILE:HD12	2.37	0.54
1:E:145:GLN:NE2	1:E:793:PHE:CZ	2.76	0.54
1:A:459:ILE:CD1	1:A:469:LEU:HD21	2.38	0.54
1:C:565:GLU:OE1	1:C:676:ILE:HG12	2.07	0.54
1:E:39:LEU:CD1	1:E:334:LEU:HD12	2.37	0.54
1:E:545:LEU:O	1:E:550:ALA:HB3	2.08	0.54
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.48	0.54
1:E:740:VAL:HG21	1:E:766:PHE:HD1	1.72	0.54
1:C:226:ALA:CB	1:C:241:MET:HB3	2.38	0.54
2:F:440:HIS:HB2	2:F:471:ILE:HG22	1.88	0.54
1:E:26:ALA:O	1:E:32:LYS:HD2	2.07	0.54
1:A:100:ILE:HD13	1:A:338:ILE:HG21	1.90	0.54
1:A:588:LEU:HD12	1:A:588:LEU:C	2.28	0.54
1:A:799:ASP:OD1	1:A:800:HIS:HD2	1.91	0.54
1:C:459:ILE:HG21	1:C:463:LEU:HD12	1.89	0.54
1:E:114:GLU:O	1:E:117:ALA:HB3	2.08	0.54
1:E:39:LEU:HD11	1:E:334:LEU:CD1	2.38	0.54
1:E:556:ILE:HD12	1:E:556:ILE:N	2.23	0.54
1:C:530:VAL:O	1:C:538:LEU:HD11	2.08	0.53
1:C:784:LEU:HD23	1:C:794:PRO:CG	2.35	0.53
1:E:284:LEU:HD11	1:E:303:LEU:CD1	2.37	0.53
1:E:524:GLU:HG3	1:E:669:TRP:CZ3	2.43	0.53
1:E:571:SER:HB2	1:E:589:LYS:HG2	1.89	0.53
1:A:103:ILE:HD11	1:A:453:ILE:HG12	1.89	0.53
1:A:25:ILE:CD1	1:A:125:ALA:HB1	2.38	0.53
1:A:155:VAL:CG1	1:A:156:VAL:N	2.72	0.53
1:A:220:PHE:HB3	1:A:328:LEU:HD13	1.89	0.53
1:C:200:VAL:O	1:C:200:VAL:CG1	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:LEU:HD11	1:E:334:LEU:HD12	1.89	0.53
2:B:546:GLU:CG	2:B:547:GLU:HG3	2.22	0.53
1:C:158:ASN:HD22	1:C:159:LYS:HG2	1.72	0.53
1:E:186:ASN:HB2	1:E:201:GLN:HG2	1.90	0.53
1:E:72:SER:HA	1:E:439:GLY:O	2.08	0.53
1:A:569:SER:O	1:A:720:ALA:HB1	2.08	0.53
1:C:43:ALA:HB1	1:C:78:TYR:O	2.07	0.53
1:E:411:VAL:HG12	1:E:412:ARG:N	2.22	0.53
1:E:607:ASN:HB3	1:E:610:ASP:CG	2.29	0.53
1:E:693:LEU:HB3	1:E:700:ARG:HD2	1.91	0.53
1:A:200:VAL:O	1:A:200:VAL:HG13	2.08	0.53
1:A:644:ASN:ND2	1:A:684:VAL:HB	2.20	0.53
1:A:584:ASN:HD22	1:A:693:LEU:HA	1.73	0.53
1:A:175:TYR:HD2	1:A:176:GLN:NE2	2.07	0.53
1:C:263:ASP:OD1	1:C:264:ALA:N	2.42	0.53
1:C:148:GLY:HA2	1:C:760:ARG:HH22	1.70	0.53
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.91	0.53
1:C:16:VAL:HG12	1:C:346:VAL:HG23	1.90	0.53
1:C:220:PHE:HB3	1:C:328:LEU:HD13	1.91	0.53
1:C:42:ARG:HG3	1:C:331:ALA:HB3	1.88	0.53
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.73	0.53
1:C:644:ASN:ND2	1:C:684:VAL:H	2.06	0.53
1:E:563:TYR:O	1:E:564:ARG:HD2	2.08	0.53
1:A:507:GLY:HA2	1:A:510:ARG:HB2	1.89	0.53
1:A:647:ILE:HB	1:A:687:ASN:ND2	2.24	0.53
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.89	0.53
1:A:306:VAL:O	1:A:306:VAL:HG23	2.09	0.53
2:B:490:ARG:HD2	2:B:492:ARG:CD	2.29	0.53
1:C:157:ILE:HD12	1:C:181:THR:HG21	1.89	0.53
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.91	0.53
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.44	0.53
2:F:429:LEU:O	2:F:434:TYR:HB2	2.09	0.53
1:A:111:PHE:HB3	1:A:114:GLU:HG2	1.89	0.52
1:A:71:LYS:HB3	1:A:386:VAL:HG23	1.90	0.52
1:A:43:ALA:HB1	1:A:78:TYR:O	2.10	0.52
2:B:462:LEU:O	2:B:467:ARG:NH2	2.42	0.52
2:B:484:ASP:OD2	2:B:494:ARG:HG2	2.09	0.52
2:B:440:HIS:O	2:B:499:LEU:HB2	2.09	0.52
1:E:611:ASP:OD2	1:E:613:LYS:HB2	2.08	0.52
2:F:457:ALA:HB2	2:F:558:TRP:CD2	2.45	0.52
2:F:462:LEU:O	2:F:467:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ALA:O	1:A:235:VAL:CG2	2.57	0.52
1:A:750:LYS:O	1:A:751:ARG:HB2	2.09	0.52
2:D:584:PRO:HA	2:D:587:ILE:HD13	1.91	0.52
2:D:589:ASP:O	2:D:592:GLN:N	2.41	0.52
1:A:820:LEU:CD1	1:A:830:GLU:HG2	2.38	0.52
1:A:828:MET:HE2	2:B:576:ARG:NE	2.22	0.52
1:C:265:GLU:OE2	1:C:267:LYS:HG3	2.08	0.52
1:E:167:LEU:N	1:E:167:LEU:HD12	2.24	0.52
1:E:561:VAL:HG21	1:E:775:ASN:CB	2.39	0.52
1:A:493:VAL:CG1	1:A:554:LEU:HD22	2.38	0.52
1:A:4:PHE:HA	1:A:8:GLN:OE1	2.10	0.52
2:B:467:ARG:HG3	2:B:558:TRP:HD1	1.71	0.52
1:C:390:ASP:O	1:C:391:LYS:HB2	2.10	0.52
1:E:3:ALA:HA	1:E:46:ILE:O	2.09	0.52
1:E:707:PRO:O	1:E:711:ARG:HG3	2.10	0.52
2:B:535:LEU:HB3	2:B:536:PRO:HA	1.92	0.52
1:C:315:GLU:O	1:C:318:ALA:HB3	2.09	0.52
1:C:722:PRO:O	1:C:723:LYS:HD2	2.09	0.52
1:E:176:GLN:O	1:E:180:ARG:HG3	2.09	0.52
1:E:338:ILE:HA	1:E:342:LEU:HG	1.90	0.52
1:E:71:LYS:HB3	1:E:386:VAL:CG2	2.39	0.52
1:E:491:VAL:O	1:E:529:ILE:HG23	2.10	0.52
1:C:126:LEU:HD11	1:C:156:VAL:HG21	1.91	0.52
1:C:231:LYS:CG	1:C:232:LYS:N	2.72	0.52
1:C:539:GLU:HA	1:C:542:LEU:HD12	1.92	0.52
1:C:565:GLU:CD	1:C:676:ILE:HB	2.30	0.52
1:E:828:MET:CE	2:F:576:ARG:HE	2.23	0.52
1:E:82:SER:O	1:E:86:VAL:HG23	2.09	0.52
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.92	0.52
1:A:12:LEU:HG	1:A:99:LEU:HB2	1.91	0.52
1:C:710:ARG:NH1	1:C:714:TYR:CE2	2.78	0.52
1:E:9:MET:O	1:E:12:LEU:HB3	2.10	0.52
1:E:482:LYS:HB3	1:E:797:VAL:HG21	1.92	0.52
2:B:490:ARG:NE	2:B:492:ARG:HD2	2.24	0.52
1:C:525:SER:OG	1:C:527:GLU:HG2	2.10	0.52
1:E:186:ASN:OD1	1:E:186:ASN:C	2.48	0.52
1:A:707:PRO:O	1:A:711:ARG:HG3	2.10	0.52
1:E:80:GLU:HA	1:E:96:ASN:O	2.10	0.52
2:F:518:LEU:HD22	2:F:518:LEU:N	2.24	0.52
1:A:208:THR:HG22	1:A:341:HIS:CG	2.44	0.52
1:A:344:SER:C	1:A:346:VAL:H	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:SER:OG	1:C:527:GLU:CG	2.58	0.52
1:E:626:ASP:C	1:E:628:THR:N	2.63	0.52
1:E:654:GLN:HG2	1:E:655:TYR:CD2	2.44	0.52
1:C:284:LEU:O	1:C:288:ILE:HB	2.10	0.51
2:D:531:ILE:CD1	2:D:533:HIS:O	2.45	0.51
1:E:103:ILE:HD12	1:E:103:ILE:N	2.24	0.51
1:A:411:VAL:HG13	1:A:470:THR:O	2.11	0.51
1:E:284:LEU:HD23	1:E:299:LEU:CD2	2.40	0.51
2:F:520:ALA:HB1	2:F:522:GLU:OE2	2.10	0.51
1:C:542:LEU:O	1:C:545:LEU:HB3	2.10	0.51
1:E:39:LEU:HB3	1:E:77:LEU:HD21	1.91	0.51
1:A:186:ASN:CB	1:A:201:GLN:HG2	2.41	0.51
1:A:429:LYS:CG	1:A:430:ALA:H	2.24	0.51
1:C:116:THR:C	1:C:481:MET:HE3	2.31	0.51
1:C:627:VAL:HG21	1:C:631:ARG:NH2	2.24	0.51
1:C:638:PRO:HB3	1:C:672:LYS:CG	2.37	0.51
1:E:179:ALA:O	1:E:183:GLU:HB2	2.10	0.51
1:E:478:MET:O	1:E:479:LYS:C	2.49	0.51
1:A:647:ILE:HG13	1:A:685:ARG:NE	2.25	0.51
1:E:739:ALA:HB2	1:E:791:GLN:OE1	2.09	0.51
1:A:749:LYS:O	1:A:750:LYS:HD2	2.10	0.51
1:C:220:PHE:HA	1:C:224:GLN:OE1	2.10	0.51
1:C:478:MET:O	1:C:479:LYS:C	2.49	0.51
1:C:521:TYR:O	1:C:529:ILE:HD12	2.11	0.51
1:C:546:GLU:N	1:C:554:LEU:HD12	2.26	0.51
1:C:669:TRP:C	1:C:669:TRP:CD1	2.83	0.51
1:A:284:LEU:HD11	1:A:303:LEU:CD1	2.41	0.51
2:B:450:ILE:HG23	2:B:455:VAL:HG23	1.91	0.51
1:C:521:TYR:CD1	1:C:529:ILE:HD13	2.46	0.51
1:C:589:LYS:HE3	1:C:689:LEU:HD11	1.92	0.51
1:E:171:LYS:NZ	1:E:283:ARG:NH2	2.58	0.51
1:A:91:GLN:HE22	1:A:343:PRO:HA	1.76	0.51
1:C:256:LYS:HD3	1:C:257:TRP:H	1.75	0.51
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.93	0.51
1:E:254:THR:O	1:E:256:LYS:HG3	2.11	0.51
2:F:513:ARG:CB	2:F:513:ARG:HH11	2.21	0.51
2:B:453:GLY:O	2:B:456:ARG:HD3	2.11	0.51
1:C:262:THR:OG1	1:C:263:ASP:N	2.44	0.51
1:C:365:ASN:O	1:C:369:ILE:HG12	2.11	0.51
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.41	0.51
1:E:597:VAL:O	1:E:601:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LEU:O	1:C:319:LEU:HD13	2.11	0.50
1:E:12:LEU:HG	1:E:99:LEU:HB2	1.93	0.50
1:E:536:LEU:O	1:E:539:GLU:N	2.44	0.50
1:E:620:ALA:HA	1:E:625:TRP:O	2.10	0.50
1:C:156:VAL:HG21	1:C:334:LEU:HD22	1.94	0.50
2:D:551:ARG:HG3	2:D:551:ARG:HH11	1.76	0.50
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.75	0.50
2:F:524:ALA:O	2:F:528:GLU:HG3	2.11	0.50
1:A:229:TYR:CZ	1:A:276:PHE:HB3	2.46	0.50
2:B:436:PHE:HB2	2:B:502:TYR:CE2	2.46	0.50
1:C:42:ARG:HG3	1:C:331:ALA:HB1	1.88	0.50
1:C:543:GLN:HA	1:C:546:GLU:HG3	1.92	0.50
1:E:488:VAL:HG23	1:E:489:VAL:CG2	2.42	0.50
1:A:172:GLU:OE2	1:A:271:ARG:NH2	2.45	0.50
1:A:200:VAL:CG1	1:A:200:VAL:O	2.59	0.50
1:A:627:VAL:O	1:A:631:ARG:HG3	2.12	0.50
2:B:429:LEU:HD21	2:B:565:VAL:HG11	1.93	0.50
1:C:644:ASN:HD22	1:C:684:VAL:H	1.58	0.50
1:C:739:ALA:HB2	1:C:791:GLN:OE1	2.11	0.50
1:C:823:ARG:NH1	1:C:828:MET:HB2	2.27	0.50
1:E:36:THR:O	1:E:40:VAL:HG23	2.11	0.50
1:E:496:LYS:HG3	1:E:496:LYS:O	2.11	0.50
2:F:546:GLU:CG	2:F:547:GLU:HG3	2.24	0.50
1:A:404:THR:HG22	1:A:449:PRO:CA	2.35	0.50
1:C:315:GLU:HA	1:C:319:LEU:CB	2.19	0.50
1:C:404:THR:HG22	1:C:449:PRO:CA	2.36	0.50
1:C:524:GLU:C	1:C:526:GLY:H	2.15	0.50
1:C:823:ARG:NH2	1:C:833:PRO:HD3	2.26	0.50
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.93	0.50
1:A:565:GLU:O	1:A:681:MET:HA	2.11	0.50
2:B:495:ASN:N	2:B:495:ASN:ND2	2.60	0.50
1:C:235:VAL:CG1	1:C:236:ASP:N	2.75	0.50
1:C:70:ILE:N	1:C:440:ARG:O	2.39	0.50
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.93	0.50
1:E:728:VAL:HB	1:E:800:HIS:CD2	2.47	0.50
1:A:103:ILE:HD12	1:A:122:THR:HG22	1.93	0.50
1:C:100:ILE:HD13	1:C:338:ILE:HG21	1.93	0.50
1:C:840:ASP:OD1	1:C:842:LEU:HD13	2.10	0.50
1:E:404:THR:HG22	1:E:449:PRO:CA	2.35	0.50
1:E:786:GLN:N	1:E:786:GLN:CD	2.65	0.50
1:A:186:ASN:CG	1:A:201:GLN:HG2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PHE:CE2	1:A:277:ILE:HG23	2.47	0.50
1:C:523:SER:O	1:C:526:GLY:N	2.42	0.50
2:D:455:VAL:HG12	2:D:456:ARG:N	2.27	0.50
1:E:237:LYS:HA	1:E:240:MET:CB	2.36	0.50
1:E:436:LEU:HD23	1:E:454:ILE:CD1	2.42	0.50
1:E:545:LEU:O	1:E:550:ALA:CB	2.60	0.50
1:E:644:ASN:HD22	1:E:684:VAL:HB	1.77	0.50
2:B:488:ASP:OD1	2:B:489:ALA:N	2.45	0.49
1:C:809:LEU:O	1:C:811:PRO:HD3	2.11	0.49
1:E:565:GLU:O	1:E:681:MET:HA	2.12	0.49
1:A:478:MET:O	1:A:479:LYS:C	2.50	0.49
1:A:669:TRP:HZ2	2:B:490:ARG:HD2	1.73	0.49
1:C:693:LEU:HB3	1:C:700:ARG:HD2	1.94	0.49
2:D:465:ILE:N	2:D:465:ILE:HD13	2.26	0.49
1:A:824:LYS:CE	1:A:830:GLU:OE2	2.58	0.49
1:C:294:ASP:OD1	1:C:295:GLU:N	2.45	0.49
1:E:466:THR:HG22	1:E:467:GLY:N	2.27	0.49
2:F:470:TYR:CE2	2:F:555:ILE:HG12	2.47	0.49
2:F:522:GLU:N	2:F:522:GLU:OE1	2.44	0.49
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.94	0.49
1:A:3:ALA:HA	1:A:46:ILE:HG22	1.94	0.49
1:A:485:VAL:HG22	1:A:485:VAL:O	2.12	0.49
1:A:491:VAL:HG13	1:A:538:LEU:HD21	1.95	0.49
1:C:231:LYS:CE	1:C:232:LYS:HG3	2.19	0.49
1:C:265:GLU:CG	1:C:266:GLY:H	2.14	0.49
1:C:291:PHE:CZ	1:C:316:GLY:CA	2.95	0.49
1:C:45:ILE:HB	1:C:76:SER:HB2	1.95	0.49
1:E:633:ILE:HG12	1:E:647:ILE:CD1	2.42	0.49
1:C:552:VAL:HB	1:C:553:PRO:HD2	1.92	0.49
1:C:614:ALA:O	1:C:618:ILE:HG12	2.11	0.49
2:D:436:PHE:HB2	2:D:502:TYR:CE2	2.47	0.49
1:E:325:ARG:HH11	1:E:325:ARG:HG2	1.77	0.49
1:A:186:ASN:HB3	1:A:201:GLN:HG2	1.94	0.49
1:A:501:LEU:HB3	1:A:502:PRO:HD3	1.94	0.49
2:B:552:LEU:CD1	2:B:552:LEU:N	2.72	0.49
2:B:500:ARG:O	2:B:566:VAL:HG13	2.12	0.49
2:D:507:SER:C	2:D:509:PRO:HD2	2.33	0.49
1:E:503:LYS:CG	1:E:551:GLY:HA3	2.42	0.49
1:E:650:THR:CG2	1:E:688:ILE:HG22	2.42	0.49
1:E:584:ASN:HD22	1:E:693:LEU:HA	1.78	0.49
1:A:21:ASN:ND2	1:A:345:PRO:HG3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:SER:HB2	1:A:589:LYS:CG	2.40	0.49
1:A:703:GLY:HA3	2:B:485:GLN:O	2.13	0.49
1:C:152:LYS:HD2	1:C:200:VAL:HG22	1.94	0.49
1:C:546:GLU:CA	1:C:554:LEU:HD11	2.35	0.49
1:E:734:GLN:H	1:E:734:GLN:HE21	1.59	0.49
1:E:734:GLN:N	1:E:734:GLN:NE2	2.55	0.49
1:E:784:LEU:HD23	1:E:794:PRO:CG	2.38	0.49
1:A:110:ASP:C	1:A:112:SER:H	2.16	0.49
1:A:22:MET:HA	1:A:122:THR:HB	1.95	0.49
1:A:258:THR:CG2	1:A:259:ASN:N	2.73	0.49
1:C:523:SER:HG	1:C:527:GLU:HB2	1.73	0.49
1:C:647:ILE:HG13	1:C:685:ARG:NE	2.28	0.49
1:C:698:ILE:HG23	1:C:699:DDE:N	2.28	0.49
1:E:491:VAL:O	1:E:529:ILE:CG2	2.61	0.49
1:A:222:ILE:HD13	1:A:222:ILE:N	2.27	0.49
1:C:240:MET:O	1:C:244:LEU:HG	2.13	0.49
1:C:509:LYS:O	1:C:513:LYS:HG3	2.13	0.49
1:C:543:GLN:HG2	1:C:544:ASP:OD1	2.13	0.49
1:C:743:ILE:HD13	1:C:784:LEU:HD11	1.93	0.49
1:E:289:MET:HE1	1:E:316:GLY:HA2	1.95	0.49
1:A:433:ARG:HB2	1:A:457:VAL:HB	1.95	0.49
1:A:549:HIS:H	1:A:549:HIS:CD2	2.29	0.49
1:C:120:ARG:NH1	1:C:479:LYS:HG3	2.27	0.49
1:C:277:ILE:HG22	1:C:278:LEU:N	2.27	0.49
1:C:410:LYS:HG3	1:C:429:LYS:O	2.12	0.49
1:E:501:LEU:HD23	1:E:501:LEU:C	2.33	0.49
2:F:505:ARG:HH11	2:F:505:ARG:HG3	1.78	0.49
1:C:384:LYS:HB2	1:C:465:LYS:HZ2	1.78	0.48
2:D:447:ALA:HA	2:D:499:LEU:HD21	1.95	0.48
1:E:229:TYR:CE2	1:E:276:PHE:HB3	2.47	0.48
1:E:626:ASP:O	1:E:628:THR:N	2.46	0.48
1:C:212:GLY:HA2	1:C:218:TRP:CZ3	2.48	0.48
1:C:216:HIS:CE1	1:C:317:LYS:NZ	2.82	0.48
1:C:311:GLU:C	1:C:314:LEU:HD13	2.34	0.48
1:C:32:LYS:NZ	1:C:105:SER:HB2	2.27	0.48
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.93	0.48
2:D:477:LEU:HD13	2:D:551:ARG:NH1	2.28	0.48
1:E:307:LEU:HB2	1:E:312:LYS:CE	2.42	0.48
1:E:546:GLU:OE2	1:E:554:LEU:N	2.34	0.48
1:A:10:ARG:NH1	1:A:14:ASP:OD2	2.46	0.48
1:A:9:MET:O	1:A:13:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LEU:HD13	1:A:312:LYS:HA	1.96	0.48
1:C:236:ASP:OD1	1:C:238:ALA:HB3	2.13	0.48
1:C:268:PRO:O	1:C:269:LEU:HD23	2.13	0.48
1:C:116:THR:HB	1:C:481:MET:CE	2.43	0.48
1:C:647:ILE:HB	1:C:687:ASN:ND2	2.27	0.48
2:D:511:PHE:CE1	2:D:560:LEU:HD11	2.49	0.48
2:D:457:ALA:HB2	2:D:558:TRP:CE3	2.49	0.48
1:E:278:LEU:O	1:E:282:PHE:HB2	2.13	0.48
2:F:479:TYR:CD2	2:F:582:LEU:HD13	2.48	0.48
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.94	0.48
1:A:388:THR:HG21	1:A:395:TYR:CG	2.48	0.48
1:C:283:ARG:HB3	1:C:299:LEU:HD21	1.96	0.48
1:C:746:VAL:HA	1:C:749:LYS:HG2	1.96	0.48
1:E:527:GLU:HB3	1:E:529:ILE:HD11	1.95	0.48
2:F:530:LEU:HD21	2:F:602:SER:O	2.13	0.48
1:A:486:SER:O	1:A:488:VAL:HG13	2.13	0.48
1:C:459:ILE:CD1	1:C:469:LEU:HD21	2.44	0.48
1:E:22:MET:HA	1:E:122:THR:HB	1.94	0.48
1:A:262:THR:HG22	1:A:267:LYS:O	2.13	0.48
1:C:385:MET:H	1:C:465:LYS:HD2	1.78	0.48
1:E:711:ARG:HD2	2:F:577:ASN:HD21	1.79	0.48
2:F:420:GLU:N	2:F:420:GLU:CD	2.67	0.48
1:A:520:THR:HA	1:A:529:ILE:O	2.13	0.48
1:A:819:VAL:O	1:A:823:ARG:CG	2.50	0.48
1:C:284:LEU:HD11	1:C:303:LEU:CD1	2.44	0.48
1:E:144:ARG:HG2	1:E:192:TYR:CD2	2.49	0.48
1:E:386:VAL:HG11	1:E:437:MET:CE	2.43	0.48
1:E:536:LEU:HD11	1:E:540:ILE:HD11	1.96	0.48
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.49	0.48
1:A:597:VAL:O	1:A:601:ILE:HG13	2.14	0.48
2:B:441:GLY:O	2:B:442:THR:HB	2.13	0.48
1:E:25:ILE:HG12	1:E:125:ALA:HB1	1.95	0.48
1:A:285:PHE:CE2	1:A:320:LEU:HD11	2.48	0.48
1:A:797:VAL:HG22	1:A:798:PHE:N	2.29	0.48
1:C:436:LEU:HD23	1:C:454:ILE:CD1	2.44	0.48
1:E:141:THR:HA	1:E:144:ARG:CZ	2.44	0.48
1:E:17:THR:HB	1:E:92:LYS:O	2.13	0.48
1:E:381:TYR:O	1:E:398:GLY:HA3	2.14	0.48
1:E:411:VAL:HG13	1:E:470:THR:O	2.14	0.48
1:E:500:ASP:CG	1:E:552:VAL:HG11	2.34	0.48
1:E:546:GLU:HG3	1:E:554:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:784:LEU:CD2	1:E:794:PRO:HG3	2.37	0.48
1:A:232:LYS:O	1:A:232:LYS:HD2	2.14	0.48
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.49	0.48
1:A:763:THR:HB	1:A:764:PRO:HD2	1.96	0.48
1:C:155:VAL:HG12	1:C:156:VAL:N	2.27	0.48
1:C:410:LYS:HG3	1:C:429:LYS:C	2.35	0.48
1:C:520:THR:HG22	1:C:530:VAL:HG22	1.96	0.48
2:B:477:LEU:CD1	2:B:551:ARG:NH1	2.65	0.47
1:C:711:ARG:HD2	2:D:577:ASN:HD21	1.79	0.47
1:E:183:GLU:O	1:E:187:VAL:HG23	2.14	0.47
1:E:508:LEU:CD2	1:E:520:THR:CG2	2.92	0.47
1:E:782:GLY:HA2	1:E:785:ARG:HE	1.79	0.47
1:A:158:ASN:HD22	1:A:159:LYS:HG2	1.78	0.47
1:A:336:GLU:HG2	1:A:340:LEU:HD12	1.96	0.47
1:A:411:VAL:CG1	1:A:412:ARG:N	2.77	0.47
1:A:423:LYS:HG2	1:A:423:LYS:O	2.14	0.47
1:C:261:ASP:O	1:C:269:LEU:N	2.46	0.47
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.94	0.47
1:C:70:ILE:O	1:C:440:ARG:HG3	2.14	0.47
1:E:132:ILE:HD13	1:E:162:ARG:HD3	1.95	0.47
2:F:484:ASP:OD2	2:F:494:ARG:N	2.44	0.47
1:A:429:LYS:CG	1:A:430:ALA:N	2.78	0.47
1:A:634:TRP:O	1:A:635:CYS:HB3	2.14	0.47
1:E:729:PHE:CE2	1:E:774:VAL:HG22	2.49	0.47
1:E:729:PHE:CZ	1:E:774:VAL:HG22	2.49	0.47
2:B:438:GLY:HA3	2:B:471:ILE:CD1	2.41	0.47
2:D:523:ALA:O	2:D:524:ALA:C	2.53	0.47
1:E:77:LEU:CB	1:E:100:ILE:HB	2.44	0.47
1:E:335:LEU:O	1:E:339:VAL:HG23	2.14	0.47
1:E:69:THR:O	1:E:389:SER:N	2.47	0.47
1:E:500:ASP:OD2	1:E:552:VAL:HG11	2.15	0.47
1:E:836:GLN:HE21	1:E:836:GLN:N	2.06	0.47
1:A:106:PRO:HG3	1:A:114:GLU:HG3	1.96	0.47
1:A:235:VAL:CG2	1:A:240:MET:HB2	2.43	0.47
2:B:445:GLU:OE1	2:B:494:ARG:NH2	2.38	0.47
1:C:224:GLN:O	1:C:228:ARG:HG3	2.14	0.47
1:C:25:ILE:CD1	1:C:125:ALA:HB1	2.44	0.47
1:C:565:GLU:O	1:C:681:MET:HA	2.14	0.47
1:C:275:MET:HE1	1:C:276:PHE:CZ	2.49	0.47
1:C:411:VAL:HG11	1:C:469:LEU:HB3	1.96	0.47
2:D:527:VAL:HG22	2:D:542:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:659:ILE:HD13	1:E:693:LEU:HD21	1.96	0.47
1:E:823:ARG:NH1	1:E:828:MET:HB2	2.29	0.47
1:A:219:ALA:HB3	1:A:330:ALA:HA	1.97	0.47
1:C:587:TYR:CD2	1:C:690:ASP:HB3	2.49	0.47
2:D:531:ILE:HG13	2:D:533:HIS:H	1.78	0.47
1:E:221:THR:OG1	1:E:224:GLN:HG3	2.15	0.47
1:A:162:ARG:HG3	1:A:166:GLU:OE2	2.14	0.47
1:A:676:ILE:O	1:A:677:PHE:HB3	2.15	0.47
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.95	0.47
1:C:110:ASP:OD1	1:C:781:THR:CG2	2.55	0.47
1:C:636:PHE:CD1	1:C:645:LEU:HD21	2.50	0.47
1:E:150:ARG:CZ	1:E:355:GLN:OE1	2.62	0.47
2:F:440:HIS:O	2:F:499:LEU:HB2	2.14	0.47
1:A:175:TYR:CD2	1:A:176:GLN:NE2	2.83	0.47
1:A:461:GLN:NE2	1:A:462:PHE:CE2	2.83	0.47
1:C:291:PHE:CZ	1:C:316:GLY:HA2	2.49	0.47
1:C:636:PHE:CE1	1:C:645:LEU:HD21	2.50	0.47
2:D:542:ILE:HG23	2:D:542:ILE:O	2.13	0.47
1:E:546:GLU:HG3	1:E:554:LEU:N	2.30	0.47
1:A:129:VAL:HG13	1:A:134:GLY:O	2.14	0.47
2:B:508:LEU:N	2:B:509:PRO:CD	2.78	0.47
1:C:155:VAL:CG1	1:C:156:VAL:N	2.77	0.47
1:C:262:THR:HA	1:C:267:LYS:O	2.14	0.47
1:C:244:LEU:HD22	1:C:277:ILE:CD1	2.45	0.47
1:C:454:ILE:CG1	1:C:455:GLY:H	2.26	0.47
1:C:459:ILE:HD11	1:C:469:LEU:HD21	1.96	0.47
1:A:676:ILE:HG22	1:A:677:PHE:CD2	2.50	0.47
2:B:420:GLU:CD	2:B:420:GLU:H	2.19	0.47
2:B:524:ALA:O	2:B:528:GLU:HG3	2.15	0.47
1:C:279:ASP:HB3	1:C:280:PRO:CD	2.43	0.47
1:C:306:VAL:HG23	1:C:306:VAL:O	2.14	0.47
1:C:371:ASN:O	1:C:372:CYS:C	2.53	0.47
1:C:490:GLN:O	1:C:491:VAL:CG1	2.62	0.47
1:C:729:PHE:O	1:C:771:TYR:HA	2.15	0.47
1:C:836:GLN:N	1:C:836:GLN:HE21	2.06	0.47
1:C:82:SER:O	1:C:86:VAL:HG23	2.15	0.47
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.14	0.47
1:E:646:VAL:HG13	1:E:688:ILE:CD1	2.45	0.47
1:A:258:THR:HG22	1:A:260:LYS:HG2	1.95	0.46
1:A:386:VAL:HG11	1:A:437:MET:CE	2.45	0.46
2:B:423:LEU:HD11	2:B:590:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:563:ARG:HG3	2:B:563:ARG:NH1	2.30	0.46
1:C:130:ASP:OD2	1:C:132:ILE:HG22	2.15	0.46
2:D:520:ALA:HB3	2:D:522:GLU:CD	2.33	0.46
1:C:45:ILE:HG12	1:C:76:SER:C	2.36	0.46
1:E:4:PHE:CE2	1:E:45:ILE:HD12	2.50	0.46
2:F:488:ASP:OD2	2:F:492:ARG:CD	2.61	0.46
1:A:823:ARG:NH1	1:A:831:GLU:O	2.48	0.46
1:C:211:PHE:CD2	1:C:211:PHE:N	2.84	0.46
1:C:222:ILE:HD13	1:C:222:ILE:N	2.30	0.46
1:C:348:ALA:HA	1:C:351:TYR:CE2	2.51	0.46
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.97	0.46
1:C:700:ARG:HB2	1:C:700:ARG:HE	1.42	0.46
1:E:581:ASN:ND2	1:E:699:DDE:O	2.49	0.46
1:A:296:ILE:N	1:A:297:PRO:HD2	2.30	0.46
1:A:512:SER:HA	1:A:518:VAL:CG1	2.46	0.46
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.97	0.46
1:C:338:ILE:O	1:C:342:LEU:HB2	2.16	0.46
1:E:736:PRO:O	1:E:738:GLN:N	2.48	0.46
1:E:750:LYS:O	1:E:751:ARG:HB2	2.15	0.46
2:F:505:ARG:NH1	2:F:505:ARG:HG3	2.31	0.46
2:B:507:SER:C	2:B:509:PRO:HD2	2.35	0.46
1:C:3:ALA:HA	1:C:46:ILE:HG22	1.98	0.46
2:D:575:PRO:HG2	2:D:576:ARG:N	2.31	0.46
1:E:149:GLU:O	1:E:150:ARG:HB2	2.15	0.46
1:E:296:ILE:O	1:E:300:LEU:HB2	2.15	0.46
1:A:249:PHE:CD2	1:A:249:PHE:N	2.83	0.46
2:B:415:GLN:O	2:B:416:ASN:HB2	2.16	0.46
1:C:317:LYS:HD2	1:C:317:LYS:HA	1.53	0.46
1:E:143:LEU:O	1:E:147:LEU:HG	2.15	0.46
1:E:237:LYS:O	1:E:241:MET:HG2	2.14	0.46
1:E:493:VAL:CG1	1:E:494:GLU:H	2.29	0.46
1:E:646:VAL:HG13	1:E:688:ILE:HD13	1.97	0.46
1:E:743:ILE:HD13	1:E:784:LEU:HD11	1.96	0.46
2:F:510:GLY:O	2:F:512:TYR:CD1	2.69	0.46
1:A:186:ASN:OD1	1:A:201:GLN:HG2	2.15	0.46
1:A:414:GLN:HB3	1:A:418:TYR:CD2	2.49	0.46
1:E:181:THR:O	1:E:185:VAL:HG23	2.16	0.46
1:E:150:ARG:NH1	1:E:351:TYR:O	2.49	0.46
1:E:500:ASP:OD1	1:E:503:LYS:HD2	2.16	0.46
1:E:552:VAL:CB	1:E:553:PRO:CD	2.93	0.46
1:E:607:ASN:HA	1:E:608:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:VAL:CG2	1:A:3:ALA:N	2.79	0.46
1:A:824:LYS:HE3	1:A:830:GLU:CD	2.35	0.46
1:C:335:LEU:O	1:C:339:VAL:HG23	2.16	0.46
1:C:45:ILE:HD11	1:C:78:TYR:HB3	1.95	0.46
1:C:497:ASN:H	1:C:497:ASN:HD22	1.60	0.46
1:C:552:VAL:CB	1:C:553:PRO:CD	2.84	0.46
1:C:707:PRO:O	1:C:711:ARG:HG3	2.16	0.46
2:D:505:ARG:C	2:D:507:SER:H	2.19	0.46
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.31	0.46
1:E:735:CYS:SG	1:E:736:PRO:HD2	2.56	0.46
1:E:74:ALA:O	1:E:439:GLY:CA	2.59	0.46
1:A:77:LEU:HB2	1:A:100:ILE:HB	1.96	0.46
1:A:694:HIS:HD2	1:A:696:ASP:N	1.95	0.46
1:A:700:ARG:HB2	1:A:700:ARG:HE	1.42	0.46
1:E:454:ILE:CG1	1:E:455:GLY:N	2.79	0.46
1:E:536:LEU:O	1:E:539:GLU:HB3	2.15	0.46
1:E:70:ILE:HG22	1:E:388:THR:HG22	1.97	0.46
1:E:732:GLU:N	1:E:795:GLN:O	2.45	0.46
1:A:186:ASN:HB3	1:A:201:GLN:HE21	1.81	0.46
1:C:314:LEU:HD21	1:C:322:VAL:HG21	1.97	0.46
1:C:490:GLN:HB2	1:C:529:ILE:CG2	2.46	0.46
2:D:495:ASN:OD1	2:D:495:ASN:N	2.48	0.46
2:D:576:ARG:NH1	2:D:576:ARG:HG3	2.29	0.46
2:D:588:PRO:O	2:D:591:GLU:N	2.46	0.46
1:E:262:THR:HG21	1:E:266:GLY:HA2	1.97	0.46
1:A:220:PHE:C	1:A:220:PHE:CD1	2.90	0.45
1:C:685:ARG:HE	1:C:687:ASN:HD21	1.64	0.45
1:E:32:LYS:NZ	1:E:106:PRO:O	2.49	0.45
1:E:202:VAL:O	1:E:202:VAL:HG23	2.16	0.45
2:F:422:LEU:HD13	2:F:594:ILE:HD11	1.97	0.45
2:B:404:GLY:HA2	1:C:626:ASP:CG	2.36	0.45
1:C:344:SER:C	1:C:346:VAL:N	2.70	0.45
1:C:685:ARG:NE	1:C:687:ASN:HD21	2.13	0.45
1:C:585:ARG:HD2	1:C:692:THR:OG1	2.16	0.45
1:E:221:THR:HG21	1:E:336:GLU:OE1	2.15	0.45
1:E:433:ARG:HB3	1:E:457:VAL:HB	1.98	0.45
1:E:606:ILE:HD12	1:E:619:MET:CG	2.46	0.45
1:E:75:ILE:HD13	1:E:439:GLY:HA2	1.98	0.45
1:A:727:PRO:HB3	1:A:801:TRP:CZ3	2.51	0.45
2:B:460:GLN:HB3	2:B:467:ARG:HD3	1.97	0.45
2:B:546:GLU:HG2	2:B:550:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:HH11	2:B:577:ASN:HD21	1.63	0.45
2:D:552:LEU:CD1	2:D:552:LEU:N	2.78	0.45
1:E:89:ILE:C	1:E:91:GLN:N	2.68	0.45
2:B:583:ASP:HA	2:B:584:PRO:HD2	1.85	0.45
1:C:186:ASN:OD1	1:C:202:VAL:N	2.48	0.45
1:E:109:VAL:O	1:E:109:VAL:HG12	2.16	0.45
2:B:457:ALA:HB2	2:B:558:TRP:CE3	2.51	0.45
1:C:411:VAL:CG1	1:C:412:ARG:N	2.80	0.45
1:C:454:ILE:CG1	1:C:455:GLY:N	2.79	0.45
2:D:518:LEU:H	2:D:518:LEU:HD22	1.81	0.45
2:D:518:LEU:N	2:D:518:LEU:HD22	2.31	0.45
1:E:823:ARG:HG2	1:E:823:ARG:NH1	2.30	0.45
1:E:840:ASP:OD1	1:E:842:LEU:HD13	2.15	0.45
1:A:591:GLU:HG2	1:A:685:ARG:CG	2.46	0.45
1:C:705:ILE:HD12	1:C:705:ILE:N	2.31	0.45
1:E:414:GLN:HB3	1:E:418:TYR:CD2	2.51	0.45
2:F:457:ALA:HB2	2:F:558:TRP:CE3	2.52	0.45
1:A:167:LEU:N	1:A:167:LEU:HD12	2.32	0.45
1:C:249:PHE:N	1:C:249:PHE:CD2	2.85	0.45
1:C:253:LYS:HG3	1:C:253:LYS:O	2.17	0.45
1:C:374:PRO:O	1:C:404:THR:HG23	2.17	0.45
1:C:485:VAL:O	1:C:485:VAL:HG22	2.15	0.45
1:C:546:GLU:HB2	1:C:547:HIS:H	1.36	0.45
1:C:656:LEU:O	1:C:659:ILE:HG12	2.16	0.45
1:E:591:GLU:HG2	1:E:685:ARG:CG	2.45	0.45
1:E:89:ILE:HG22	1:E:91:GLN:HB3	1.99	0.45
1:A:620:ALA:HA	1:A:625:TRP:O	2.17	0.45
1:A:627:VAL:HG11	2:F:406:ASP:OD1	2.16	0.45
2:B:551:ARG:NH1	2:B:551:ARG:HG3	2.31	0.45
1:C:116:THR:CB	1:C:481:MET:HE3	2.47	0.45
1:C:256:LYS:CD	1:C:257:TRP:H	2.29	0.45
1:C:294:ASP:OD1	1:C:295:GLU:HG3	2.17	0.45
1:C:296:ILE:N	1:C:297:PRO:HD2	2.32	0.45
1:C:588:LEU:O	1:C:588:LEU:HD12	2.17	0.45
1:E:274:ASN:O	1:E:279:ASP:HB2	2.16	0.45
1:E:505:VAL:HG12	1:E:505:VAL:O	2.17	0.45
1:E:507:GLY:CA	1:E:549:HIS:HB3	2.46	0.45
2:F:470:TYR:CD2	2:F:555:ILE:HG12	2.52	0.45
1:A:258:THR:HG22	1:A:260:LYS:H	1.82	0.45
1:A:550:ALA:C	1:A:552:VAL:N	2.71	0.45
1:A:581:ASN:O	1:A:582:LYS:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ASN:HB3	1:A:610:ASP:OD2	2.17	0.45
1:C:152:LYS:CD	1:C:200:VAL:HG22	2.45	0.45
1:E:109:VAL:HG23	1:E:138:GLN:CD	2.38	0.45
1:E:314:LEU:CD1	1:E:322:VAL:HG21	2.47	0.45
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.52	0.45
1:E:379:MET:SD	1:E:470:THR:HG22	2.57	0.45
2:F:552:LEU:H	2:F:552:LEU:HD12	1.80	0.45
1:A:324:MET:HA	1:A:324:MET:HE2	1.99	0.45
1:C:186:ASN:HB3	1:C:201:GLN:HE21	1.82	0.45
1:C:262:THR:CA	1:C:269:LEU:HG	2.47	0.45
1:C:288:ILE:HD13	1:C:319:LEU:HG	1.98	0.45
1:C:495:VAL:CG1	1:C:554:LEU:HD23	2.46	0.45
1:C:807:ASP:OD2	1:C:808:PRO:HD2	2.17	0.45
2:D:546:GLU:OE1	2:D:551:ARG:NH1	2.50	0.45
2:F:406:ASP:O	2:F:416:ASN:ND2	2.42	0.45
2:F:498:LEU:O	2:F:569:SER:HB3	2.17	0.45
1:A:760:ARG:O	1:A:761:PRO:C	2.56	0.44
1:A:840:ASP:OD1	1:A:842:LEU:HD13	2.17	0.44
2:D:455:VAL:C	2:D:456:ARG:HG2	2.37	0.44
2:D:437:VAL:HG11	2:D:511:PHE:CE2	2.51	0.44
1:E:495:VAL:HG12	1:E:553:PRO:O	2.16	0.44
1:E:736:PRO:O	1:E:737:GLU:C	2.55	0.44
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.80	0.44
1:C:216:HIS:NE2	1:C:317:LYS:NZ	2.65	0.44
1:C:522:MET:SD	1:C:528:HIS:HA	2.57	0.44
1:C:626:ASP:C	1:C:628:THR:N	2.70	0.44
1:C:647:ILE:HB	1:C:687:ASN:HD22	1.83	0.44
2:D:535:LEU:HB3	2:D:536:PRO:HA	1.99	0.44
1:E:218:TRP:HA	1:E:328:LEU:O	2.17	0.44
1:E:305:ILE:HG21	1:E:323:VAL:HG13	1.99	0.44
2:B:558:TRP:O	2:B:562:GLU:HG3	2.17	0.44
1:C:186:ASN:HB3	1:C:201:GLN:HG2	1.99	0.44
1:E:167:LEU:H	1:E:167:LEU:CD1	2.29	0.44
1:E:672:LYS:HG3	1:E:673:GLU:HG3	2.00	0.44
1:A:211:PHE:O	1:A:219:ALA:HA	2.17	0.44
2:B:523:ALA:O	2:B:524:ALA:C	2.54	0.44
1:C:391:LYS:HE3	1:C:393:ARG:CG	2.45	0.44
1:C:42:ARG:HG3	1:C:331:ALA:HB2	1.93	0.44
1:C:567:VAL:HG23	1:C:592:PRO:HG3	1.99	0.44
1:C:646:VAL:HG13	1:C:688:ILE:HD13	1.97	0.44
2:D:522:GLU:OE1	2:D:522:GLU:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:LYS:NZ	1:E:283:ARG:HH21	2.15	0.44
1:E:565:GLU:CD	1:E:676:ILE:HB	2.38	0.44
2:F:433:GLY:O	2:F:505:ARG:HB2	2.16	0.44
1:A:226:ALA:CB	1:A:241:MET:HB3	2.47	0.44
1:A:739:ALA:C	1:A:741:GLY:N	2.70	0.44
1:A:82:SER:O	1:A:86:VAL:HG23	2.17	0.44
1:C:411:VAL:HG13	1:C:470:THR:O	2.17	0.44
2:D:538:ARG:HA	2:D:538:ARG:HD2	1.63	0.44
1:E:594:ASP:HB2	1:E:597:VAL:HG23	1.99	0.44
1:E:647:ILE:HG13	1:E:685:ARG:HE	1.82	0.44
1:A:189:VAL:CG1	1:A:200:VAL:HG12	2.48	0.44
2:B:410:SER:OG	2:B:412:ARG:CB	2.64	0.44
1:C:250:PHE:HB3	1:C:275:MET:HE1	1.99	0.44
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.99	0.44
1:A:155:VAL:HG21	1:A:185:VAL:HG11	2.00	0.44
1:C:110:ASP:C	1:C:112:SER:H	2.20	0.44
1:C:397:PHE:HD1	1:C:437:MET:HG3	1.83	0.44
1:E:496:LYS:HB2	1:E:555:LYS:NZ	2.27	0.44
2:F:479:TYR:CG	2:F:582:LEU:HB2	2.52	0.44
1:A:411:VAL:HG11	1:A:469:LEU:HB3	1.99	0.44
1:C:106:PRO:HG3	1:C:114:GLU:HG3	1.99	0.44
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.74	0.44
1:C:727:PRO:HG2	1:C:774:VAL:HB	2.00	0.44
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.99	0.44
2:D:551:ARG:HG3	2:D:551:ARG:NH1	2.33	0.44
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.53	0.44
1:E:533:THR:H	1:E:537:HIS:CD2	2.35	0.44
1:E:736:PRO:HB3	1:E:738:GLN:CD	2.38	0.44
2:B:495:ASN:H	2:B:495:ASN:ND2	2.16	0.44
2:D:508:LEU:HD23	2:D:508:LEU:HA	1.74	0.44
2:D:518:LEU:HD21	2:D:544:GLY:HA3	2.00	0.44
1:E:736:PRO:CB	1:E:738:GLN:CD	2.87	0.44
1:A:13:MET:SD	1:A:436:LEU:HD21	2.58	0.43
1:A:659:ILE:HD13	1:A:693:LEU:HD21	1.99	0.43
1:A:733:ILE:O	1:A:767:THR:HA	2.18	0.43
2:B:523:ALA:O	2:B:527:VAL:HG23	2.18	0.43
1:C:600:ALA:HB1	1:C:606:ILE:HG12	1.98	0.43
1:E:303:LEU:O	1:E:304:GLU:CB	2.66	0.43
1:E:37:ASP:O	1:E:41:GLN:HG3	2.18	0.43
1:E:387:PRO:HG3	1:E:394:PHE:CE1	2.52	0.43
1:E:89:ILE:O	1:E:91:GLN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PHE:CD2	1:A:211:PHE:N	2.86	0.43
1:A:436:LEU:HD23	1:A:454:ILE:CD1	2.49	0.43
1:A:45:ILE:HD12	1:A:76:SER:CB	2.38	0.43
1:C:414:GLN:HB3	1:C:418:TYR:CD2	2.52	0.43
1:C:395:TYR:CE1	1:C:457:VAL:HG13	2.53	0.43
1:C:546:GLU:N	1:C:554:LEU:CD1	2.80	0.43
1:C:5:THR:OG1	1:C:8:GLN:HG3	2.18	0.43
2:D:528:GLU:HA	2:D:531:ILE:HG12	2.00	0.43
2:D:575:PRO:HG2	2:D:576:ARG:H	1.82	0.43
2:F:427:ARG:CG	2:F:428:GLN:N	2.80	0.43
2:F:521:PRO:O	2:F:524:ALA:HB3	2.18	0.43
1:A:132:ILE:HD12	1:A:162:ARG:NE	2.33	0.43
1:A:494:GLU:HB3	1:A:555:LYS:HB3	1.99	0.43
1:A:495:VAL:HG13	1:A:504:LEU:HD22	2.00	0.43
2:B:470:TYR:N	2:B:470:TYR:CD1	2.86	0.43
1:C:141:THR:O	1:C:144:ARG:HB2	2.19	0.43
1:E:40:VAL:C	1:E:42:ARG:H	2.21	0.43
1:A:823:ARG:NH1	1:A:829:LYS:O	2.51	0.43
2:D:552:LEU:HD12	2:D:552:LEU:H	1.83	0.43
1:E:360:PRO:HB2	1:E:363:ASP:HB2	2.00	0.43
1:E:411:VAL:CG1	1:E:412:ARG:N	2.81	0.43
1:E:495:VAL:HA	1:E:554:LEU:HD23	2.00	0.43
1:E:735:CYS:HA	1:E:736:PRO:HD3	1.82	0.43
2:F:546:GLU:CG	2:F:547:GLU:N	2.81	0.43
1:A:172:GLU:CD	1:A:271:ARG:HH21	2.22	0.43
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.99	0.43
1:C:291:PHE:HZ	1:C:316:GLY:CA	2.31	0.43
1:E:388:THR:HG21	1:E:395:TYR:CD1	2.54	0.43
2:F:538:ARG:HD2	2:F:538:ARG:HA	1.60	0.43
2:F:546:GLU:OE1	2:F:551:ARG:N	2.46	0.43
1:A:647:ILE:HB	1:A:687:ASN:HD22	1.83	0.43
1:C:132:ILE:CG2	1:C:133:GLU:N	2.79	0.43
1:E:508:LEU:HD21	1:E:530:VAL:CG2	2.48	0.43
1:E:700:ARG:O	1:E:705:ILE:HD13	2.17	0.43
2:F:427:ARG:O	2:F:431:GLU:HG3	2.19	0.43
1:A:693:LEU:HB3	1:A:700:ARG:HD2	2.01	0.43
1:A:711:ARG:NH1	1:A:838:TYR:HA	2.33	0.43
1:C:186:ASN:CB	1:C:201:GLN:HG2	2.49	0.43
1:C:360:PRO:HB2	1:C:363:ASP:HB2	2.00	0.43
1:C:607:ASN:HB3	1:C:610:ASP:OD2	2.18	0.43
1:E:13:MET:SD	1:E:436:LEU:HD21	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:454:ILE:CG1	1:E:455:GLY:H	2.26	0.43
1:E:740:VAL:O	1:E:740:VAL:HG12	2.18	0.43
1:E:79:SER:O	1:E:98:PHE:N	2.52	0.43
1:A:273:PHE:HD1	1:A:277:ILE:HD12	1.81	0.43
1:E:220:PHE:HB3	1:E:328:LEU:HD13	2.00	0.43
1:E:251:ASN:HB3	1:E:254:THR:OG1	2.18	0.43
1:E:429:LYS:HG3	1:E:462:PHE:CE1	2.54	0.43
1:E:669:TRP:CZ2	2:F:492:ARG:HG2	2.53	0.43
1:E:690:ASP:OD1	1:E:691:VAL:N	2.50	0.43
1:A:488:VAL:HG23	1:A:489:VAL:HG23	2.00	0.43
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.89	0.43
1:A:727:PRO:HG2	1:A:774:VAL:HB	2.00	0.43
1:C:9:MET:O	1:C:13:MET:HG3	2.19	0.43
1:C:194:ASP:HB2	1:C:197:LEU:HG	2.01	0.43
1:E:129:VAL:HG12	1:E:130:ASP:N	2.33	0.43
1:E:711:ARG:HD2	2:F:577:ASN:ND2	2.33	0.43
1:A:466:THR:CG2	1:A:467:GLY:N	2.82	0.43
1:C:10:ARG:CZ	1:C:449:PRO:HD3	2.48	0.43
1:C:595:GLU:OE2	1:C:682:ARG:NH1	2.51	0.43
1:C:606:ILE:HD12	1:C:619:MET:CG	2.49	0.43
1:E:118:ALA:O	1:E:122:THR:HG23	2.19	0.43
1:E:189:VAL:O	1:E:193:ALA:CB	2.67	0.43
1:E:600:ALA:HB1	1:E:606:ILE:HG12	1.99	0.43
1:A:129:VAL:HG13	1:A:134:GLY:C	2.39	0.42
1:A:26:ALA:CB	1:A:128:VAL:HB	2.48	0.42
1:C:216:HIS:CE1	1:C:317:LYS:HZ1	2.37	0.42
1:C:22:MET:HA	1:C:122:THR:HB	2.00	0.42
1:C:277:ILE:O	1:C:281:ILE:HD12	2.18	0.42
1:A:103:ILE:HD13	1:A:121:VAL:HG23	2.00	0.42
1:C:521:TYR:CE2	1:C:529:ILE:HB	2.54	0.42
1:C:91:GLN:HE22	1:C:343:PRO:HA	1.84	0.42
1:E:490:GLN:O	1:E:491:VAL:HG13	2.19	0.42
2:B:552:LEU:CD1	2:B:552:LEU:H	2.26	0.42
1:C:386:VAL:HA	1:C:387:PRO:HD3	1.72	0.42
2:D:435:VAL:HB	2:D:505:ARG:HH11	1.84	0.42
1:E:522:MET:HB2	2:F:490:ARG:NH1	2.34	0.42
1:E:705:ILE:N	1:E:705:ILE:HD12	2.35	0.42
1:E:722:PRO:O	1:E:723:LYS:HD2	2.19	0.42
2:F:510:GLY:O	2:F:512:TYR:CE1	2.72	0.42
1:A:580:PRO:HD2	1:A:704:GLN:OE1	2.19	0.42
1:C:536:LEU:CD1	1:C:537:HIS:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:474:ASP:O	2:D:475:PRO:C	2.57	0.42
2:D:518:LEU:HD21	2:D:544:GLY:CA	2.49	0.42
1:E:211:PHE:N	1:E:211:PHE:CD2	2.87	0.42
1:E:418:TYR:HB3	1:E:477:ASN:HD21	1.84	0.42
1:E:778:PHE:N	1:E:778:PHE:CD2	2.87	0.42
2:F:464:ALA:O	2:F:467:ARG:HB3	2.19	0.42
2:F:498:LEU:HD23	2:F:498:LEU:HA	1.74	0.42
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.55	0.42
2:B:439:TYR:O	2:B:471:ILE:HB	2.20	0.42
2:B:577:ASN:HD22	2:B:577:ASN:C	2.23	0.42
1:C:742:GLY:O	1:C:745:SER:HB3	2.20	0.42
2:D:503:VAL:HG12	2:D:564:THR:HG22	2.01	0.42
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.55	0.42
1:E:43:ALA:O	1:E:77:LEU:HA	2.19	0.42
1:E:406:LYS:HB3	1:E:447:ASP:HB3	2.01	0.42
1:E:636:PHE:CE1	1:E:645:LEU:HD21	2.54	0.42
1:E:68:ILE:HG23	1:E:390:ASP:HB2	2.01	0.42
1:A:167:LEU:H	1:A:167:LEU:HD12	1.83	0.42
1:A:357:TYR:CE2	1:A:359:GLY:HA3	2.55	0.42
1:A:518:VAL:HG22	1:A:519:LEU:N	2.35	0.42
1:A:676:ILE:HG22	1:A:677:PHE:HD2	1.85	0.42
1:C:108:HIS:HD2	1:C:110:ASP:H	1.66	0.42
1:C:131:THR:HG21	1:C:163:ALA:HB2	2.01	0.42
1:C:150:ARG:HG3	1:C:355:GLN:OE1	2.19	0.42
2:D:455:VAL:O	2:D:456:ARG:CD	2.68	0.42
2:D:531:ILE:HG13	2:D:532:GLY:N	2.33	0.42
2:D:561:ALA:HA	2:D:564:THR:HG23	2.01	0.42
1:E:235:VAL:HG11	1:E:239:LYS:HD3	2.02	0.42
1:E:296:ILE:N	1:E:297:PRO:HD2	2.35	0.42
1:A:126:LEU:HD11	1:A:156:VAL:CG2	2.50	0.42
1:A:360:PRO:C	1:A:362:ASP:H	2.22	0.42
1:A:397:PHE:HD1	1:A:437:MET:HG3	1.84	0.42
1:A:495:VAL:HA	1:A:554:LEU:HD23	2.01	0.42
1:A:644:ASN:ND2	1:A:684:VAL:H	2.17	0.42
1:A:565:GLU:HG2	1:A:676:ILE:HD12	2.02	0.42
1:C:360:PRO:C	1:C:362:ASP:H	2.22	0.42
1:C:495:VAL:HG12	1:C:554:LEU:HD23	2.01	0.42
1:C:487:PRO:HB3	1:C:531:ALA:HB1	2.02	0.42
1:C:626:ASP:O	1:C:628:THR:N	2.53	0.42
1:C:659:ILE:HD13	1:C:693:LEU:HD21	2.02	0.42
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:VAL:O	1:E:306:VAL:HG23	2.19	0.42
1:E:500:ASP:CB	1:E:552:VAL:CG1	2.98	0.42
2:F:479:TYR:CE2	2:F:582:LEU:HD13	2.54	0.42
1:A:106:PRO:CG	1:A:114:GLU:HG3	2.48	0.42
1:A:392:GLY:CA	1:A:513:LYS:HE2	2.43	0.42
1:C:547:HIS:CD2	1:C:548:ASP:OD1	2.72	0.42
1:C:799:ASP:OD1	1:C:800:HIS:HD2	2.03	0.42
2:D:467:ARG:HG3	2:D:558:TRP:CD1	2.54	0.42
1:E:412:ARG:HH12	1:E:428:ILE:CD1	2.32	0.42
1:E:500:ASP:HB3	1:E:552:VAL:CG1	2.50	0.42
1:E:773:PRO:HB2	1:E:776:GLU:HB2	2.01	0.42
2:F:437:VAL:HG11	2:F:511:PHE:CE2	2.54	0.42
1:A:406:LYS:O	1:A:409:GLN:HB3	2.19	0.42
1:A:647:ILE:CG1	1:A:685:ARG:HE	2.31	0.42
1:C:172:GLU:HA	1:C:274:ASN:HD21	1.84	0.42
1:C:288:ILE:HG21	1:C:319:LEU:HG	2.01	0.42
1:C:576:LEU:HD12	1:C:577:SER:N	2.34	0.42
1:E:485:VAL:HG22	1:E:485:VAL:O	2.20	0.42
1:E:500:ASP:OD1	1:E:503:LYS:CD	2.68	0.42
1:E:626:ASP:O	1:E:627:VAL:C	2.57	0.42
2:F:472:ALA:HB2	3:F:702:P34:HAE	2.02	0.42
1:A:782:GLY:O	1:A:785:ARG:HB3	2.20	0.42
1:C:211:PHE:O	1:C:219:ALA:HA	2.19	0.42
1:C:258:THR:HG22	1:C:260:LYS:N	2.29	0.42
1:C:529:ILE:HG22	1:C:530:VAL:H	1.83	0.42
1:C:536:LEU:HD12	1:C:537:HIS:H	1.75	0.42
2:D:446:ALA:O	2:D:447:ALA:C	2.56	0.42
1:E:144:ARG:HG2	1:E:192:TYR:CG	2.55	0.42
1:E:25:ILE:HG23	1:E:142:VAL:HG11	2.02	0.42
1:E:171:LYS:HZ1	1:E:283:ARG:NH2	2.18	0.42
1:A:153:PRO:HD2	1:A:200:VAL:HG13	2.01	0.41
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.55	0.41
1:E:736:PRO:CB	1:E:738:GLN:HG2	2.49	0.41
1:A:231:LYS:C	1:A:233:PHE:H	2.23	0.41
1:A:654:GLN:HG2	1:A:655:TYR:CG	2.55	0.41
2:B:522:GLU:N	2:B:522:GLU:OE1	2.41	0.41
1:C:521:TYR:O	1:C:529:ILE:CD1	2.67	0.41
1:E:123:ASP:O	1:E:151:ILE:HG23	2.20	0.41
1:E:25:ILE:HG23	1:E:142:VAL:CG1	2.49	0.41
1:A:89:ILE:HG22	1:A:91:GLN:HG2	2.02	0.41
2:B:507:SER:C	2:B:509:PRO:CD	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ILE:O	1:C:280:PRO:HD2	2.20	0.41
1:C:406:LYS:O	1:C:409:GLN:HB3	2.20	0.41
1:C:751:ARG:NH2	1:C:776:GLU:HG3	2.35	0.41
1:E:307:LEU:HB2	1:E:312:LYS:CD	2.50	0.41
1:A:32:LYS:HZ1	1:A:105:SER:HB2	1.82	0.41
1:A:371:ASN:O	1:A:372:CYS:C	2.58	0.41
1:C:466:THR:HG22	1:C:467:GLY:N	2.35	0.41
1:C:523:SER:O	1:C:524:GLU:C	2.58	0.41
1:E:188:ILE:HG23	1:E:192:TYR:CD2	2.56	0.41
1:E:759:GLN:HB2	1:E:766:PHE:HE2	1.81	0.41
1:E:760:ARG:O	1:E:761:PRO:C	2.59	0.41
1:A:160:VAL:O	1:A:163:ALA:HB3	2.21	0.41
1:A:521:TYR:CZ	1:A:529:ILE:HD12	2.55	0.41
1:A:737:GLU:CG	1:A:766:PHE:CD2	3.03	0.41
1:C:37:ASP:O	1:C:40:VAL:N	2.53	0.41
1:C:388:THR:HG21	1:C:395:TYR:CD1	2.55	0.41
1:C:760:ARG:O	1:C:761:PRO:C	2.59	0.41
1:E:46:ILE:H	1:E:46:ILE:HD12	1.85	0.41
1:E:736:PRO:CB	1:E:738:GLN:CG	2.95	0.41
2:F:495:ASN:OD1	2:F:495:ASN:N	2.54	0.41
1:A:112:SER:HB3	1:A:794:PRO:O	2.19	0.41
1:A:137:VAL:O	1:A:140:GLU:HB3	2.20	0.41
1:A:374:PRO:O	1:A:404:THR:HG23	2.21	0.41
2:B:520:ALA:HB1	2:B:522:GLU:OE1	2.21	0.41
1:C:132:ILE:CG2	1:C:133:GLU:H	2.33	0.41
1:C:493:VAL:HG21	1:C:545:LEU:CD2	2.46	0.41
1:C:558:PRO:HA	1:C:559:PRO:HD3	1.79	0.41
1:C:581:ASN:O	1:C:582:LYS:CB	2.68	0.41
1:C:613:LYS:HD3	1:C:631:ARG:NH1	2.35	0.41
1:E:126:LEU:HD11	1:E:156:VAL:HG23	2.02	0.41
1:E:267:LYS:HA	1:E:268:PRO:HD3	1.85	0.41
1:E:360:PRO:C	1:E:362:ASP:H	2.24	0.41
1:E:374:PRO:O	1:E:404:THR:HG23	2.21	0.41
1:E:386:VAL:HA	1:E:387:PRO:HD3	1.81	0.41
1:A:254:THR:O	1:A:255:LYS:HB2	2.20	0.41
1:A:2:VAL:HG22	1:A:3:ALA:H	1.84	0.41
1:A:485:VAL:O	1:A:487:PRO:HD3	2.21	0.41
1:A:656:LEU:O	1:A:659:ILE:HG12	2.21	0.41
1:A:80:GLU:C	1:A:81:MET:HG2	2.40	0.41
2:B:450:ILE:HG23	2:B:455:VAL:CG2	2.51	0.41
1:C:237:LYS:HA	1:C:240:MET:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ILE:HA	1:C:462:PHE:HD2	1.84	0.41
1:C:563:TYR:O	1:C:564:ARG:CD	2.67	0.41
2:F:467:ARG:HG3	2:F:558:TRP:HD1	1.84	0.41
1:E:828:MET:HE3	2:F:576:ARG:HE	1.84	0.41
1:A:550:ALA:O	1:A:552:VAL:N	2.54	0.41
1:A:636:PHE:CD1	1:A:645:LEU:HD21	2.56	0.41
1:C:18:ASN:HB3	1:C:97:SER:O	2.21	0.41
1:C:459:ILE:O	1:C:462:PHE:N	2.46	0.41
1:C:560:VAL:HG12	1:C:561:VAL:N	2.35	0.41
1:C:601:ILE:HG12	1:C:606:ILE:HB	2.03	0.41
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.56	0.41
1:A:258:THR:CG2	1:A:259:ASN:H	2.29	0.41
1:A:317:LYS:O	1:A:318:ALA:C	2.59	0.41
1:A:391:LYS:O	1:A:513:LYS:HE2	2.20	0.41
1:A:735:CYS:HA	1:A:736:PRO:HD3	1.88	0.41
1:A:578:LYS:HG2	1:A:840:ASP:OD2	2.20	0.41
2:B:482:ALA:O	2:B:483:GLN:HB3	2.20	0.41
1:C:308:LYS:HB2	1:C:311:GLU:OE1	2.20	0.41
1:C:436:LEU:O	1:C:442:VAL:HA	2.21	0.41
1:C:4:PHE:HD2	1:C:45:ILE:HG23	1.85	0.41
1:C:630:ALA:O	1:C:633:ILE:HG13	2.21	0.41
1:C:698:ILE:CG2	1:C:699:DDE:N	2.83	0.41
1:C:823:ARG:HH11	1:C:828:MET:HB2	1.86	0.41
1:E:488:VAL:HG23	1:E:489:VAL:HG22	2.03	0.41
1:E:615:ARG:HG2	1:E:619:MET:HE1	2.03	0.41
1:E:710:ARG:CG	1:E:710:ARG:HH11	2.30	0.41
1:E:759:GLN:HB2	1:E:766:PHE:CD2	2.56	0.41
1:E:733:ILE:O	1:E:767:THR:HA	2.21	0.41
1:A:637:GLY:O	1:A:642:GLY:HA3	2.21	0.41
2:B:490:ARG:CG	2:B:492:ARG:HD2	2.51	0.41
2:B:499:LEU:HB3	2:B:566:VAL:HG11	2.03	0.41
1:C:70:ILE:HG12	1:C:440:ARG:O	2.21	0.41
1:C:807:ASP:OD2	1:C:808:PRO:N	2.54	0.41
2:D:531:ILE:CG1	2:D:532:GLY:N	2.84	0.41
2:F:531:ILE:HG22	2:F:533:HIS:H	1.85	0.41
1:A:228:ARG:HG2	1:A:229:TYR:N	2.36	0.41
1:A:589:LYS:HE3	1:A:689:LEU:HD11	2.03	0.41
2:B:471:ILE:HD12	2:B:472:ALA:N	2.36	0.41
1:C:388:THR:HG21	1:C:395:TYR:CG	2.56	0.41
1:C:506:GLU:HG3	1:C:510:ARG:HE	1.86	0.41
1:C:530:VAL:O	1:C:538:LEU:HD13	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:MET:O	1:C:96:ASN:HB3	2.21	0.41
1:E:276:PHE:C	1:E:277:ILE:HD13	2.41	0.41
1:E:511:LEU:HA	1:E:549:HIS:CE1	2.56	0.41
1:E:737:GLU:HG3	1:E:766:PHE:CZ	2.56	0.41
1:A:488:VAL:HG23	1:A:489:VAL:CG2	2.51	0.40
2:B:529:ARG:NH1	2:B:604:PRO:HG3	2.36	0.40
1:C:637:GLY:O	1:C:642:GLY:CA	2.69	0.40
1:E:730:LEU:C	1:E:730:LEU:CD2	2.90	0.40
1:E:744:TYR:O	1:E:748:ASN:ND2	2.53	0.40
2:F:486:GLU:HB2	2:F:487:PRO:HD2	2.03	0.40
1:A:169:VAL:CG2	1:A:173:ASP:HB2	2.51	0.40
1:A:677:PHE:N	1:A:677:PHE:CD2	2.89	0.40
1:C:156:VAL:HG21	1:C:334:LEU:CD2	2.51	0.40
1:C:228:ARG:C	1:C:230:ALA:H	2.25	0.40
1:C:251:ASN:HB2	1:C:254:THR:HG1	1.84	0.40
1:C:71:LYS:HB3	1:C:386:VAL:HG23	2.03	0.40
1:C:484:SER:CB	1:C:797:VAL:HG23	2.48	0.40
1:C:807:ASP:OD2	1:C:808:PRO:CD	2.69	0.40
1:A:522:MET:HA	1:A:527:GLU:O	2.21	0.40
1:A:590:ALA:HA	1:A:685:ARG:O	2.21	0.40
2:B:486:GLU:HB3	2:B:487:PRO:HD2	2.03	0.40
2:B:542:ILE:HG23	2:B:542:ILE:O	2.22	0.40
1:C:226:ALA:HB2	1:C:241:MET:HB3	2.03	0.40
1:C:291:PHE:CE1	1:C:316:GLY:N	2.89	0.40
1:E:241:MET:HA	1:E:244:LEU:HD12	2.03	0.40
1:E:4:PHE:CD2	1:E:45:ILE:HD12	2.56	0.40
1:E:637:GLY:O	1:E:642:GLY:HA3	2.21	0.40
1:E:587:TYR:CD2	1:E:690:ASP:HB3	2.57	0.40
1:A:228:ARG:C	1:A:230:ALA:H	2.24	0.40
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.92	0.40
1:A:515:ASP:OD1	1:A:516:PRO:HD2	2.21	0.40
1:C:386:VAL:HG11	1:C:437:MET:CE	2.51	0.40
1:C:591:GLU:HG2	1:C:685:ARG:CG	2.49	0.40
2:D:527:VAL:HG22	2:D:542:ILE:HD12	2.03	0.40
1:E:739:ALA:HB1	1:E:788:THR:HB	2.03	0.40
1:E:786:GLN:H	1:E:786:GLN:CD	2.23	0.40
2:F:571:ILE:CD1	2:F:587:ILE:HD12	2.51	0.40
1:A:390:ASP:O	1:A:391:LYS:CB	2.67	0.40
1:A:395:TYR:CE1	1:A:457:VAL:HG13	2.56	0.40
1:A:490:GLN:HA	1:A:530:VAL:O	2.21	0.40
1:A:576:LEU:HD12	1:A:577:SER:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ASP:C	1:A:628:THR:N	2.72	0.40
1:C:581:ASN:ND2	1:C:699:DDE:O	2.55	0.40
1:C:733:ILE:O	1:C:767:THR:HA	2.21	0.40
2:D:447:ALA:O	2:D:448:GLN:C	2.60	0.40
2:D:555:ILE:O	2:D:555:ILE:HG22	2.21	0.40
1:E:188:ILE:HG23	1:E:192:TYR:CE2	2.57	0.40
1:E:158:ASN:HA	1:E:212:GLY:O	2.21	0.40
1:E:289:MET:CE	1:E:316:GLY:C	2.90	0.40
1:E:325:ARG:NH1	1:E:325:ARG:HG2	2.36	0.40
1:E:823:ARG:NH2	1:E:833:PRO:HD3	2.35	0.40
1:E:92:LYS:HE3	1:E:92:LYS:HB2	1.72	0.40
1:E:78:TYR:CE1	1:E:97:SER:HB3	2.51	0.40
2:F:560:LEU:O	2:F:563:ARG:HB2	2.21	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	818/842 (97%)	729 (89%)	76 (9%)	13 (2%)	9	31
1	C	818/842 (97%)	726 (89%)	75 (9%)	17 (2%)	7	23
1	E	818/842 (97%)	714 (87%)	87 (11%)	17 (2%)	7	23
2	B	205/207 (99%)	183 (89%)	21 (10%)	1 (0%)	29	61
2	D	205/207 (99%)	177 (86%)	24 (12%)	4 (2%)	7	24
2	F	205/207 (99%)	180 (88%)	24 (12%)	1 (0%)	29	61
All	All	3069/3147 (98%)	2709 (88%)	307 (10%)	53 (2%)	9	29

All (53) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	112	SER
1	A	498	ALA
1	A	761	PRO
2	B	518	LEU
1	C	235	VAL
1	C	264	ALA
1	C	546	GLU
1	C	761	PRO
1	E	112	SER
1	E	761	PRO
1	A	309	GLY
1	A	677	PHE
1	C	112	SER
1	C	309	GLY
1	E	90	LYS
1	E	233	PHE
1	E	304	GLU
1	E	479	LYS
1	A	390	ASP
1	A	479	LYS
1	C	266	GLY
1	C	479	LYS
1	C	525	SER
1	C	677	PHE
2	D	491	GLY
2	D	506	SER
1	E	390	ASP
1	E	558	PRO
1	E	621	ASP
1	A	111	PHE
1	A	446	ASP
1	A	460	ASP
1	C	265	GLU
1	E	446	ASP
1	E	677	PHE
1	C	446	ASP
1	E	302	LYS
1	E	737	GLU
2	F	404	GLY
1	C	329	PRO
2	D	604	PRO
1	E	460	ASP
1	C	493	VAL

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Mol	Chain	Res	Type
1	C	558	PRO
1	C	743	ILE
1	E	743	ILE
1	A	329	PRO
1	C	491	VAL
1	E	309	GLY
1	E	338	ILE
2	D	404	GLY
1	A	743	ILE
1	A	764	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	699/714 (98%)	659 (94%)	40 (6%)	20	50
1	C	699/714 (98%)	638 (91%)	61 (9%)	10	30
1	E	699/714 (98%)	663 (95%)	36 (5%)	23	55
2	B	161/162 (99%)	145 (90%)	16 (10%)	8	23
2	D	161/162 (99%)	146 (91%)	15 (9%)	9	26
2	F	161/162 (99%)	146 (91%)	15 (9%)	9	26
All	All	2580/2628 (98%)	2397 (93%)	183 (7%)	14	39

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	36	THR
1	A	68	ILE
1	A	81	MET
1	A	83	ASP
1	A	91	GLN
1	A	94	ASP
1	A	113	SER

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Mol	Chain	Res	Type
1	A	152	LYS
1	A	183	GLU
1	A	195	GLU
1	A	211	PHE
1	A	222	ILE
1	A	228	ARG
1	A	236	ASP
1	A	262	THR
1	A	275	MET
1	A	347	THR
1	A	362	ASP
1	A	391	LYS
1	A	406	LYS
1	A	429	LYS
1	A	432	GLN
1	A	460	ASP
1	A	536	LEU
1	A	599	LEU
1	A	625	TRP
1	A	677	PHE
1	A	710	ARG
1	A	718	LEU
1	A	724	ILE
1	A	730	LEU
1	A	734	GLN
1	A	738	GLN
1	A	761	PRO
1	A	767	THR
1	A	775	ASN
1	A	785	ARG
1	A	795	GLN
1	A	836	GLN
2	B	422	LEU
2	B	456	ARG
2	B	467	ARG
2	B	470	TYR
2	B	488	ASP
2	B	492	ARG
2	B	494	ARG
2	B	495	ASN
2	B	499	LEU
2	B	518	LEU

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Mol	Chain	Res	Type
2	B	540	ASP
2	B	547	GLU
2	B	552	LEU
2	B	559	PRO
2	B	560	LEU
2	B	577	ASN
1	C	14	ASP
1	C	36	THR
1	C	68	ILE
1	C	81	MET
1	C	83	ASP
1	C	91	GLN
1	C	94	ASP
1	C	112	SER
1	C	113	SER
1	C	164	LEU
1	C	167	LEU
1	C	170	SER
1	C	172	GLU
1	C	183	GLU
1	C	195	GLU
1	C	222	ILE
1	C	231	LYS
1	C	242	ASP
1	C	253	LYS
1	C	256	LYS
1	C	269	LEU
1	C	282	PHE
1	C	299	LEU
1	C	312	LYS
1	C	317	LYS
1	C	320	LEU
1	C	347	THR
1	C	432	GLN
1	C	440	ARG
1	C	460	ASP
1	C	461	GLN
1	C	489	VAL
1	C	493	VAL
1	C	494	GLU
1	C	495	VAL
1	C	497	ASN

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Mol	Chain	Res	Type
1	C	500	ASP
1	C	512	SER
1	C	524	GLU
1	C	528	HIS
1	C	543	GLN
1	C	544	ASP
1	C	546	GLU
1	C	549	HIS
1	C	556	ILE
1	C	582	LYS
1	C	599	LEU
1	C	609	ARG
1	C	625	TRP
1	C	677	PHE
1	C	718	LEU
1	C	724	ILE
1	C	730	LEU
1	C	734	GLN
1	C	738	GLN
1	C	761	PRO
1	C	767	THR
1	C	775	ASN
1	C	820	LEU
1	C	836	GLN
1	C	837	GLU
2	D	410	SER
2	D	411	THR
2	D	422	LEU
2	D	465	ILE
2	D	483	GLN
2	D	486	GLU
2	D	488	ASP
2	D	494	ARG
2	D	499	LEU
2	D	538	ARG
2	D	540	ASP
2	D	547	GLU
2	D	551	ARG
2	D	560	LEU
2	D	577	ASN
1	E	94	ASP
1	E	161	ASP

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Mol	Chain	Res	Type
1	E	183	GLU
1	E	186	ASN
1	E	194	ASP
1	E	216	HIS
1	E	262	THR
1	E	263	ASP
1	E	275	MET
1	E	282	PHE
1	E	313	ASP
1	E	347	THR
1	E	362	ASP
1	E	391	LYS
1	E	440	ARG
1	E	460	ASP
1	E	489	VAL
1	E	544	ASP
1	E	599	LEU
1	E	625	TRP
1	E	677	PHE
1	E	698	ILE
1	E	710	ARG
1	E	718	LEU
1	E	724	ILE
1	E	730	LEU
1	E	734	GLN
1	E	738	GLN
1	E	749	LYS
1	E	761	PRO
1	E	767	THR
1	E	775	ASN
1	E	786	GLN
1	E	800	HIS
1	E	836	GLN
1	E	837	GLU
2	F	411	THR
2	F	422	LEU
2	F	437	VAL
2	F	494	ARG
2	F	498	LEU
2	F	513	ARG
2	F	522	GLU
2	F	538	ARG

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Mol	Chain	Res	Type
2	F	540	ASP
2	F	547	GLU
2	F	548	GLU
2	F	560	LEU
2	F	577	ASN
2	F	599	ASP
2	F	602	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	91	GLN
1	A	108	HIS
1	A	138	GLN
1	A	176	GLN
1	A	201	GLN
1	A	274	ASN
1	A	371	ASN
1	A	414	GLN
1	A	528	HIS
1	A	537	HIS
1	A	549	HIS
1	A	581	ASN
1	A	583	HIS
1	A	584	ASN
1	A	644	ASN
1	A	687	ASN
1	A	694	HIS
1	A	734	GLN
1	A	738	GLN
1	A	748	ASN
1	A	753	GLN
1	A	800	HIS
1	A	836	GLN
2	B	428	GLN
2	B	448	GLN
2	B	495	ASN
2	B	577	ASN
1	C	27	HIS
1	C	91	GLN
1	C	138	GLN

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Mol	Chain	Res	Type
1	C	201	GLN
1	C	251	ASN
1	C	371	ASN
1	C	414	GLN
1	C	490	GLN
1	C	497	ASN
1	C	537	HIS
1	C	581	ASN
1	C	583	HIS
1	C	584	ASN
1	C	644	ASN
1	C	687	ASN
1	C	694	HIS
1	C	734	GLN
1	C	738	GLN
1	C	753	GLN
1	C	800	HIS
1	C	836	GLN
2	D	428	GLN
2	D	448	GLN
2	D	577	ASN
1	E	27	HIS
1	E	91	GLN
1	E	138	GLN
1	E	201	GLN
1	E	371	ASN
1	E	414	GLN
1	E	537	HIS
1	E	549	HIS
1	E	581	ASN
1	E	583	HIS
1	E	584	ASN
1	E	644	ASN
1	E	687	ASN
1	E	694	HIS
1	E	734	GLN
1	E	748	ASN
1	E	753	GLN
1	E	800	HIS
1	E	836	GLN
2	F	428	GLN
2	F	448	GLN

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Mol	Chain	Res	Type
2	F	460	GLN
2	F	577	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	DDE	C	699	1	5,10,21	0.70	0	3,12,30	1.42	1 (33%)
1	DDE	A	699	1	5,10,21	0.79	0	3,12,30	1.38	1 (33%)
1	DDE	E	699	1	5,10,21	0.65	0	3,12,30	1.40	1 (33%)

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	DDE	C	699	1	-	0/5/6/23	0/1/1/1
1	DDE	A	699	1	-	0/5/6/23	0/1/1/1
1	DDE	E	699	1	-	0/5/6/23	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	DDE	CD2-NE2-CE1	2.06	109.00	105.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	DDE	CD2-NE2-CE1	2.03	108.95	105.78
1	E	699	DDE	CD2-NE2-CE1	2.03	108.94	105.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	699	DDE	3	0
1	E	699	DDE	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands 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	$\# Z  > 2$
3	P34	F	702	-	23,24,24	2.30	11 (47%)	30,34,34	2.90	9 (30%)
3	P34	D	701	-	23,24,24	2.15	9 (39%)	30,34,34	2.64	10 (33%)
3	P34	B	700	-	23,24,24	2.37	11 (47%)	30,34,34	2.79	10 (33%)

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
3	P34	F	702	-	-	3/8/8/8	0/3/3/3
3	P34	D	701	-	-	2/8/8/8	0/3/3/3
3	P34	B	700	-	-	4/8/8/8	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	P34	CAQ-NAN	5.19	1.42	1.33
3	D	701	P34	CAQ-NAN	4.89	1.41	1.33
3	F	702	P34	CAQ-NAN	4.39	1.40	1.33
3	B	700	P34	CAR-NAN	4.04	1.42	1.35
3	B	700	P34	CAG-CAP	3.98	1.46	1.39
3	D	701	P34	CAR-NAN	3.76	1.41	1.35
3	F	702	P34	CAR-NAN	3.72	1.41	1.35
3	F	702	P34	CAJ-CAG	3.66	1.44	1.36
3	F	702	P34	CAG-CAP	3.44	1.45	1.39
3	B	700	P34	CAJ-CAG	3.43	1.43	1.36
3	D	701	P34	CAP-NAM	-3.18	1.35	1.41
3	D	701	P34	CAG-CAP	3.11	1.44	1.39
3	F	702	P34	CAP-NAM	-3.05	1.35	1.41
3	B	700	P34	CA-C	3.04	1.57	1.52
3	F	702	P34	CA-C	2.98	1.57	1.52
3	F	702	P34	CAK-CAP	2.84	1.43	1.37
3	D	701	P34	CAE-CAH	2.77	1.43	1.36
3	B	700	P34	CAE-CAH	2.75	1.43	1.36
3	D	701	P34	CAF-CAI	2.68	1.42	1.36
3	B	700	P34	CAP-NAM	-2.67	1.36	1.41
3	F	702	P34	CAF-CAI	2.61	1.42	1.36
3	F	702	P34	CAE-CAH	2.52	1.42	1.36
3	D	701	P34	CA-C	2.49	1.56	1.52
3	D	701	P34	CAJ-CAG	2.49	1.41	1.36
3	B	700	P34	CAF-CAI	2.40	1.42	1.36
3	B	700	P34	CAK-CAP	2.39	1.42	1.37
3	D	701	P34	CAK-CAP	2.38	1.42	1.37
3	B	700	P34	CAU-CAR	2.37	1.46	1.41
3	F	702	P34	CAU-CAR	2.27	1.45	1.41
3	B	700	P34	CAK-CAU	2.17	1.45	1.41
3	F	702	P34	CAH-CAS	2.03	1.45	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	702	P34	CAU-CAR-NAN	-8.42	119.03	123.60
3	B	700	P34	CAU-CAR-NAN	-8.18	119.16	123.60
3	D	701	P34	CAU-CAR-NAN	-6.66	119.98	123.60
3	F	702	P34	CAS-CAQ-NAN	-6.45	119.91	124.40
3	D	701	P34	CAS-CAQ-NAN	-6.38	119.96	124.40
3	F	702	P34	CAP-NAM-C	6.16	138.28	127.50
3	B	700	P34	CAP-NAM-C	5.98	137.95	127.50
3	B	700	P34	CAS-CAQ-NAN	-5.81	120.35	124.40
3	D	701	P34	CAP-NAM-C	5.61	137.30	127.50
3	F	702	P34	CA-C-NAM	5.22	123.94	114.12
3	D	701	P34	CA-C-NAM	4.80	123.15	114.12
3	B	700	P34	CA-C-NAM	4.54	122.65	114.12
3	F	702	P34	O-C-NAM	-4.41	115.58	123.63
3	B	700	P34	O-C-NAM	-4.16	116.04	123.63
3	F	702	P34	CAQ-NAN-CAR	4.13	122.50	116.83
3	D	701	P34	O-C-NAM	-3.93	116.47	123.63
3	B	700	P34	CAK-CAP-NAM	-3.73	110.69	123.13
3	F	702	P34	CAK-CAP-NAM	-3.66	110.95	123.13
3	B	700	P34	CAQ-NAN-CAR	3.49	121.62	116.83
3	D	701	P34	CAK-CAP-NAM	-3.46	111.59	123.13
3	D	701	P34	CAQ-NAN-CAR	3.16	121.17	116.83
3	B	700	P34	CAG-CAP-NAM	2.99	130.45	120.40
3	F	702	P34	CAG-CAP-NAM	2.80	129.81	120.40
3	D	701	P34	CAG-CAJ-CAR	-2.79	117.32	120.84
3	D	701	P34	CAG-CAP-NAM	2.77	129.73	120.40
3	B	700	P34	CAG-CAJ-CAR	-2.68	117.46	120.84
3	F	702	P34	CAG-CAJ-CAR	-2.26	117.99	120.84
3	D	701	P34	CAJ-CAR-CAU	2.14	123.00	120.05
3	B	700	P34	CAB-N-CA	2.01	113.69	110.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

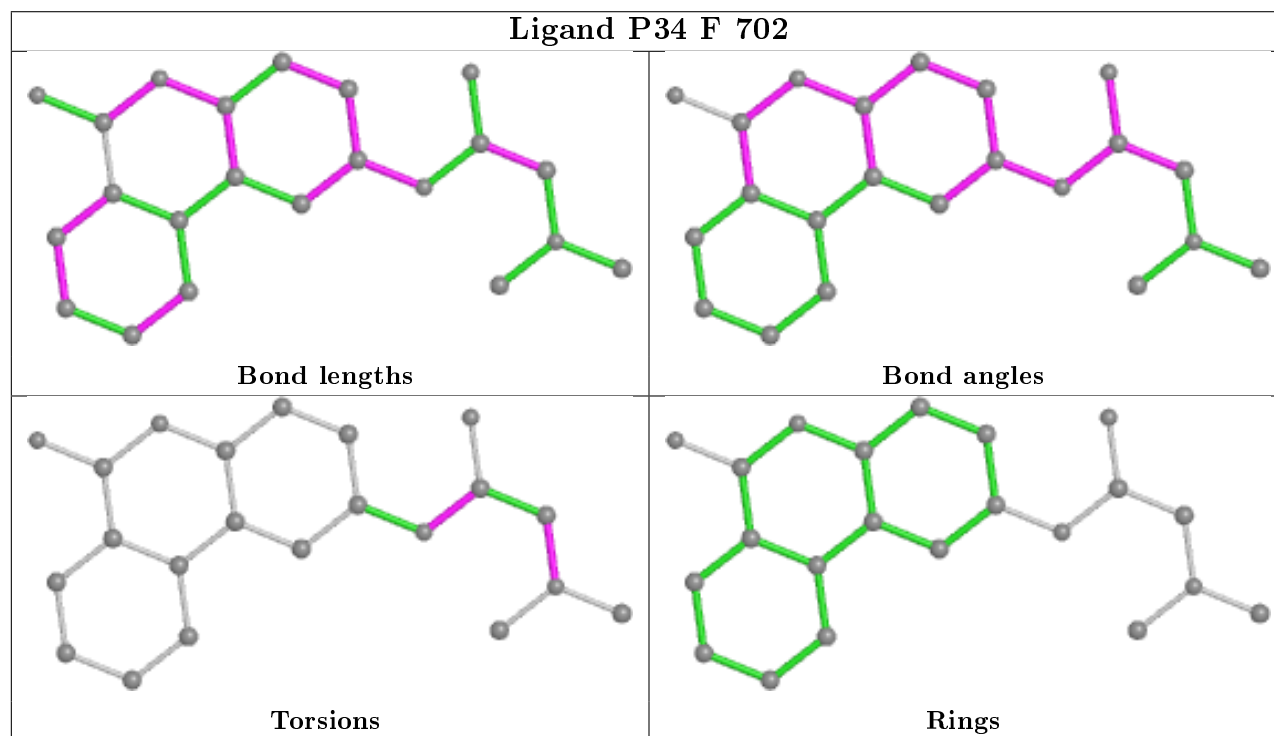
Mol	Chain	Res	Type	Atoms
3	F	702	P34	C-CA-N-CAB
3	F	702	P34	CA-C-NAM-CAP
3	D	701	P34	CA-C-NAM-CAP
3	B	700	P34	C-CA-N-CAA
3	B	700	P34	C-CA-N-CAB
3	B	700	P34	CA-C-NAM-CAP
3	F	702	P34	O-C-NAM-CAP
3	D	701	P34	O-C-NAM-CAP
3	B	700	P34	O-C-NAM-CAP

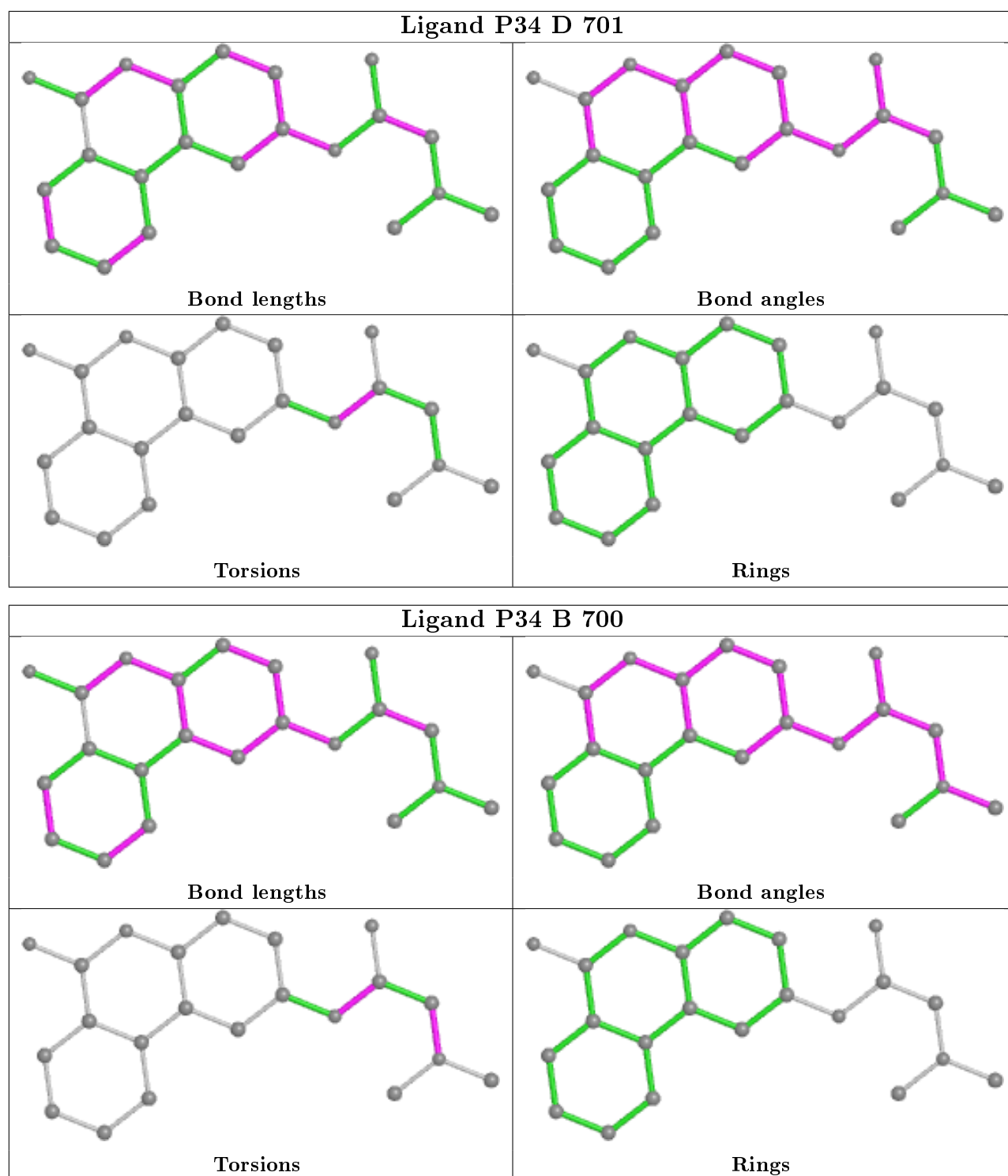
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	702	P34	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	822/842 (97%)	0.00	7 (0%) 84 80	16, 52, 85, 106	0
1	C	822/842 (97%)	0.36	52 (6%) 20 12	19, 66, 124, 136	0
1	E	822/842 (97%)	1.24	220 (26%) 0 0	20, 105, 128, 148	0
2	B	207/207 (100%)	-0.36	2 (0%) 82 77	9, 32, 61, 79	0
2	D	207/207 (100%)	-0.22	1 (0%) 91 88	11, 33, 64, 79	0
2	F	207/207 (100%)	-0.22	1 (0%) 91 88	18, 38, 70, 84	0
All	All	3087/3147 (98%)	0.37	283 (9%) 9 5	9, 58, 122, 148	0

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	551	GLY	7.5
1	E	314	LEU	6.8
1	E	48	ALA	6.2
1	E	240	MET	6.1
1	E	759	GLN	6.1
1	E	257	TRP	6.0
1	E	280	PRO	6.0
1	E	197	LEU	5.9
1	E	231	LYS	5.9
1	E	167	LEU	5.9
1	E	761	PRO	5.8
1	E	146	ALA	5.7
1	E	362	ASP	5.7
1	C	499	ASN	5.7
1	C	552	VAL	5.5
1	E	308	LYS	5.5
1	E	80	GLU	5.3
1	E	179	ALA	5.3
1	E	110	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	163	ALA	5.1
1	E	315	GLU	5.1
1	E	47	SER	5.1
1	E	200	VAL	5.0
1	E	546	GLU	4.9
1	E	143	LEU	4.9
1	E	269	LEU	4.9
1	E	790	GLY	4.9
1	E	193	ALA	4.9
1	C	291	PHE	4.9
1	E	441	PHE	4.8
1	E	93	THR	4.8
1	E	256	LYS	4.8
1	E	777	SER	4.7
1	E	781	THR	4.7
1	E	108	HIS	4.6
1	E	194	ASP	4.6
1	E	762	GLY	4.6
1	E	67	GLY	4.6
1	E	335	LEU	4.5
1	E	317	LYS	4.5
1	E	264	ALA	4.5
1	C	554	LEU	4.5
1	C	168	GLN	4.4
1	E	189	VAL	4.4
1	E	262	THR	4.4
1	E	99	LEU	4.4
1	E	196	VAL	4.4
1	C	307	LEU	4.4
1	E	155	VAL	4.3
1	E	737	GLU	4.3
1	E	232	LYS	4.3
1	E	758	GLU	4.3
1	C	553	PRO	4.3
1	E	763	THR	4.2
1	E	290	ASN	4.2
1	E	46	ILE	4.2
1	E	195	GLU	4.2
1	E	230	ALA	4.2
1	E	554	LEU	4.2
1	C	251	ASN	4.2
1	C	495	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	255	LYS	4.2
1	E	444	PRO	4.1
1	E	86	VAL	4.1
1	C	497	ASN	4.1
1	E	757	GLU	4.1
1	E	307	LEU	4.1
1	E	258	THR	4.0
1	E	261	ASP	4.0
1	E	254	THR	3.9
1	E	166	GLU	3.9
1	E	310	ASP	3.9
1	E	755	VAL	3.9
1	E	398	GLY	3.9
1	E	132	ILE	3.8
1	E	760	ARG	3.8
1	E	316	GLY	3.8
1	E	176	GLN	3.8
1	E	311	GLU	3.8
1	E	784	LEU	3.7
1	E	263	ASP	3.7
1	C	167	LEU	3.7
1	E	21	ASN	3.7
1	E	347	THR	3.7
1	E	276	PHE	3.7
1	E	239	LYS	3.6
1	E	472	SER	3.6
1	E	492	ALA	3.6
1	E	136	CYS	3.6
1	E	551	GLY	3.6
1	E	455	GLY	3.6
1	E	242	ASP	3.5
1	E	259	ASN	3.5
1	E	175	TYR	3.5
1	E	84	GLU	3.5
1	E	367	ILE	3.5
1	E	89	ILE	3.5
1	E	138	GLN	3.5
1	E	245	TRP	3.4
1	E	78	TYR	3.4
1	E	541	CYS	3.4
1	E	294	ASP	3.4
1	E	127	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	301	GLU	3.3
1	E	228	ARG	3.3
1	E	731	VAL	3.3
1	E	392	GLY	3.3
1	E	770	ALA	3.3
1	E	212	GLY	3.3
1	E	764	PRO	3.2
1	E	220	PHE	3.2
1	E	343	PRO	3.2
1	E	328	LEU	3.2
1	E	96	ASN	3.2
1	E	348	ALA	3.2
1	C	311	GLU	3.2
1	A	392	GLY	3.1
1	E	27	HIS	3.1
1	E	221	THR	3.1
1	E	270	GLU	3.1
1	E	766	PHE	3.1
1	E	180	ARG	3.1
1	A	398	GLY	3.1
1	E	739	ALA	3.1
1	E	795	GLN	3.1
1	C	506	GLU	3.0
1	E	7	ASP	3.0
1	E	421	GLY	3.0
1	C	513	LYS	3.0
1	A	195	GLU	3.0
1	E	780	PHE	3.0
1	E	753	GLN	3.0
1	C	313	ASP	3.0
1	C	315	GLU	3.0
1	E	83	ASP	3.0
1	E	94	ASP	3.0
1	C	270	GLU	3.0
1	E	2	VAL	3.0
1	E	339	VAL	3.0
1	E	137	VAL	2.9
1	E	296	ILE	2.9
1	E	745	SER	2.9
1	C	2	VAL	2.9
1	E	453	ILE	2.9
1	E	391	LYS	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	29	ASP	2.8
1	E	107	GLY	2.8
1	E	211	PHE	2.8
1	E	789	GLY	2.8
1	E	452	ASN	2.8
1	A	46	ILE	2.8
1	E	443	GLU	2.8
1	A	454	ILE	2.8
1	E	97	SER	2.8
1	E	501	LEU	2.8
1	A	453	ILE	2.7
1	E	104	ASP	2.7
1	C	556	ILE	2.7
1	E	126	LEU	2.7
1	E	20	ARG	2.7
1	E	442	VAL	2.7
1	C	233	PHE	2.7
1	E	424	ASP	2.7
1	C	555	LYS	2.7
1	E	309	GLY	2.7
1	E	10	ARG	2.7
1	E	313	ASP	2.6
1	C	496	LYS	2.6
1	E	205	ALA	2.6
2	F	459	SER	2.6
1	C	234	GLY	2.6
1	E	399	ARG	2.6
1	E	122	THR	2.6
1	E	744	TYR	2.6
1	E	204	PRO	2.6
1	E	334	LEU	2.6
1	E	525	SER	2.6
1	E	337	MET	2.6
1	C	67	GLY	2.5
1	E	125	ALA	2.5
1	E	559	PRO	2.5
1	E	494	GLU	2.5
1	E	320	LEU	2.5
1	C	108	HIS	2.5
1	E	28	VAL	2.5
1	C	500	ASP	2.5
1	E	277	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	3	ALA	2.5
1	E	454	ILE	2.5
1	E	5	THR	2.5
1	E	360	PRO	2.5
2	B	489	ALA	2.5
1	E	222	ILE	2.5
1	E	747	LEU	2.5
1	C	525	SER	2.4
1	E	279	ASP	2.4
1	E	68	ILE	2.4
1	E	336	GLU	2.4
1	E	33	SER	2.4
1	E	98	PHE	2.4
1	C	523	SER	2.4
1	C	785	ARG	2.4
1	E	154	VAL	2.4
1	E	297	PRO	2.4
1	E	390	ASP	2.4
1	E	187	VAL	2.4
1	E	226	ALA	2.4
1	E	281	ILE	2.4
1	C	493	VAL	2.4
1	C	4	PHE	2.4
1	E	124	GLY	2.4
1	A	452	ASN	2.4
1	E	207	GLY	2.3
1	E	145	GLN	2.3
1	E	393	ARG	2.3
1	C	306	VAL	2.3
1	C	294	ASP	2.3
1	C	219	ALA	2.3
1	E	218	TRP	2.3
1	E	30	HIS	2.3
1	E	743	ILE	2.3
1	E	234	GLY	2.3
1	E	526	GLY	2.3
1	E	366	CYS	2.3
1	E	287	ALA	2.3
1	C	266	GLY	2.3
1	E	400	VAL	2.3
1	E	553	PRO	2.3
1	E	188	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	456	LEU	2.3
1	E	73	THR	2.3
1	E	303	LEU	2.3
1	E	45	ILE	2.3
1	E	510	ARG	2.3
1	E	756	SER	2.2
1	C	264	ALA	2.2
1	C	296	ILE	2.2
1	E	534	GLY	2.2
1	E	607	ASN	2.2
1	C	83	ASP	2.2
1	E	426	LEU	2.2
1	E	82	SER	2.2
1	E	556	ILE	2.2
1	E	32	LYS	2.2
2	D	489	ALA	2.2
1	E	267	LYS	2.2
1	C	48	ALA	2.2
1	E	139	THR	2.2
1	E	420	PRO	2.2
1	C	156	VAL	2.2
1	E	91	GLN	2.2
1	C	263	ASP	2.2
1	E	111	PHE	2.2
1	E	369	ILE	2.2
1	E	298	VAL	2.1
1	E	363	ASP	2.1
1	C	290	ASN	2.1
1	C	312	LYS	2.1
1	C	310	ASP	2.1
1	E	130	ASP	2.1
1	E	100	ILE	2.1
1	E	260	LYS	2.1
1	E	365	ASN	2.1
1	E	748	ASN	2.1
1	E	131	THR	2.1
1	E	3	ALA	2.1
1	C	237	LYS	2.1
1	C	267	LYS	2.1
1	E	473	GLU	2.1
1	E	77	LEU	2.1
2	B	549	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	291	PHE	2.1
1	E	538	LEU	2.0
1	C	319	LEU	2.0
1	C	236	ASP	2.0
1	C	546	GLU	2.0
1	E	741	GLY	2.0
1	E	767	THR	2.0
1	E	237	LYS	2.0
1	E	522	MET	2.0
1	E	796	MET	2.0
1	E	268	PRO	2.0
1	E	736	PRO	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
1	DDE	C	699	10/21	0.94	0.12	49,55,57,58	0
1	DDE	E	699	10/21	0.94	0.15	42,46,47,48	0
1	DDE	A	699	10/21	0.95	0.10	42,44,47,48	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

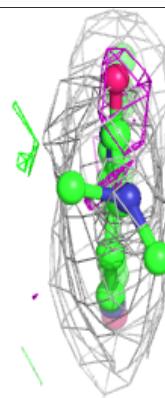
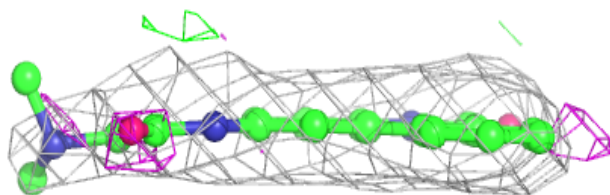
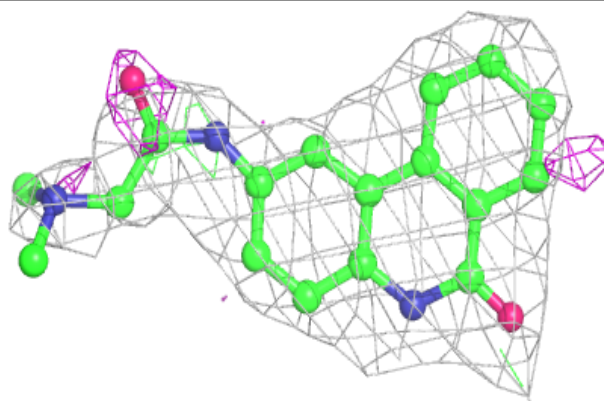
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	P34	D	701	22/22	0.89	0.25	18,24,54,55	0
3	P34	F	702	22/22	0.90	0.25	12,17,57,58	0
3	P34	B	700	22/22	0.92	0.18	8,13,34,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around P34 D 701:**

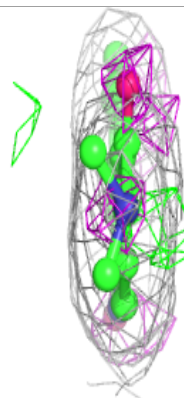
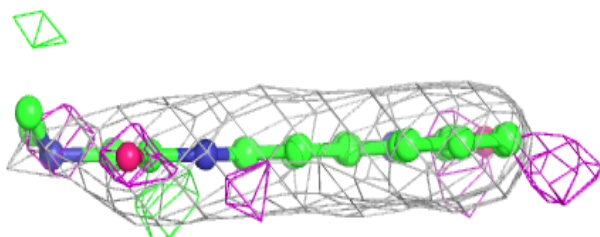
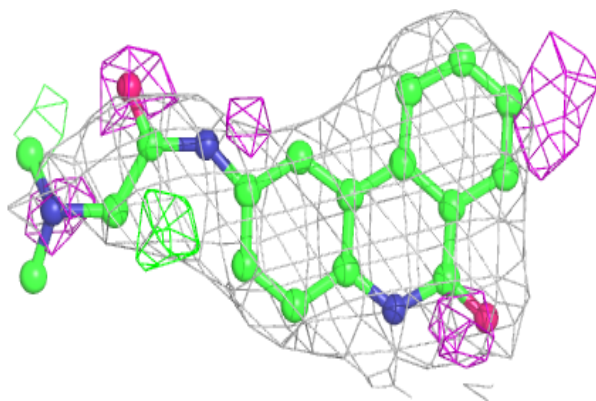
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



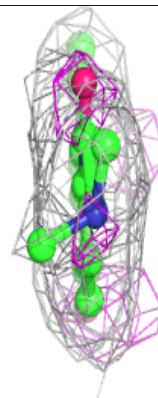
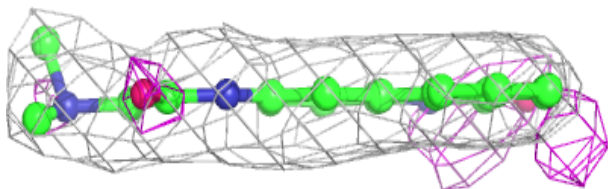
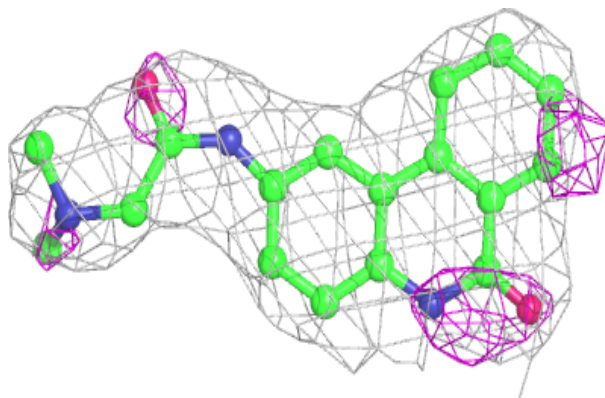


**Electron density around P34 F 702:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around P34 B 700:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.