



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:46 am GMT

PDB ID : 2HLF  
Title : Structure of the Escherichia coli ClC chloride channel Y445E mutant and Fab complex  
Authors : Accardi, A.; Lobet, S.; Williams, C.; Miller, C.; Dutzler, R.  
Deposited on : 2006-07-07  
Resolution : 3.30 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

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

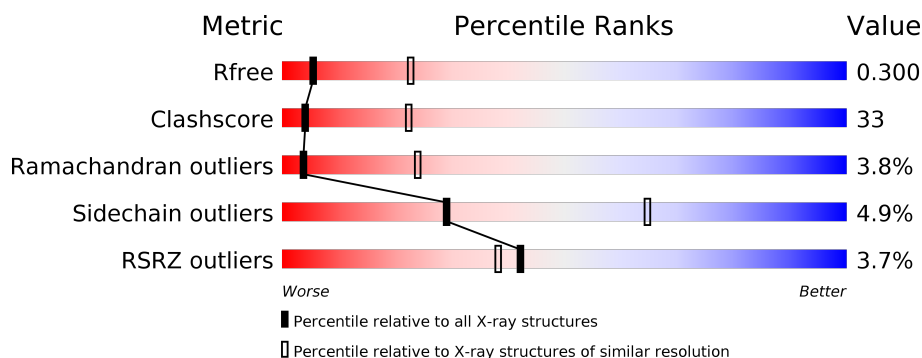
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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. 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	444	<div> <div>41%</div> <div>53%</div> <div>5%</div> </div>
1	B	444	<div> <div>38%</div> <div>53%</div> <div>8%</div> </div>
2	C	221	<div> <div>65%</div> <div>35%</div> </div>
2	E	221	<div> <div>60%</div> <div>38%</div> </div>
3	D	211	<div> <div>57%</div> <div>37%</div> </div>
3	F	211	<div> <div>59%</div> <div>36%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BR	A	1	-	-	X	X
4	BR	B	2	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13220 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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3331	2186	560	565	20			
1	B	441	Total	C	N	O	S	0	0	0
			3301	2170	553	558	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLU	TYR	ENGINEERED	UNP P37019
B	445	GLU	TYR	ENGINEERED	UNP P37019

- Molecule 2 is a protein called Fab Fragment, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called Fab Fragment, Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Br	0	0
			1	1		

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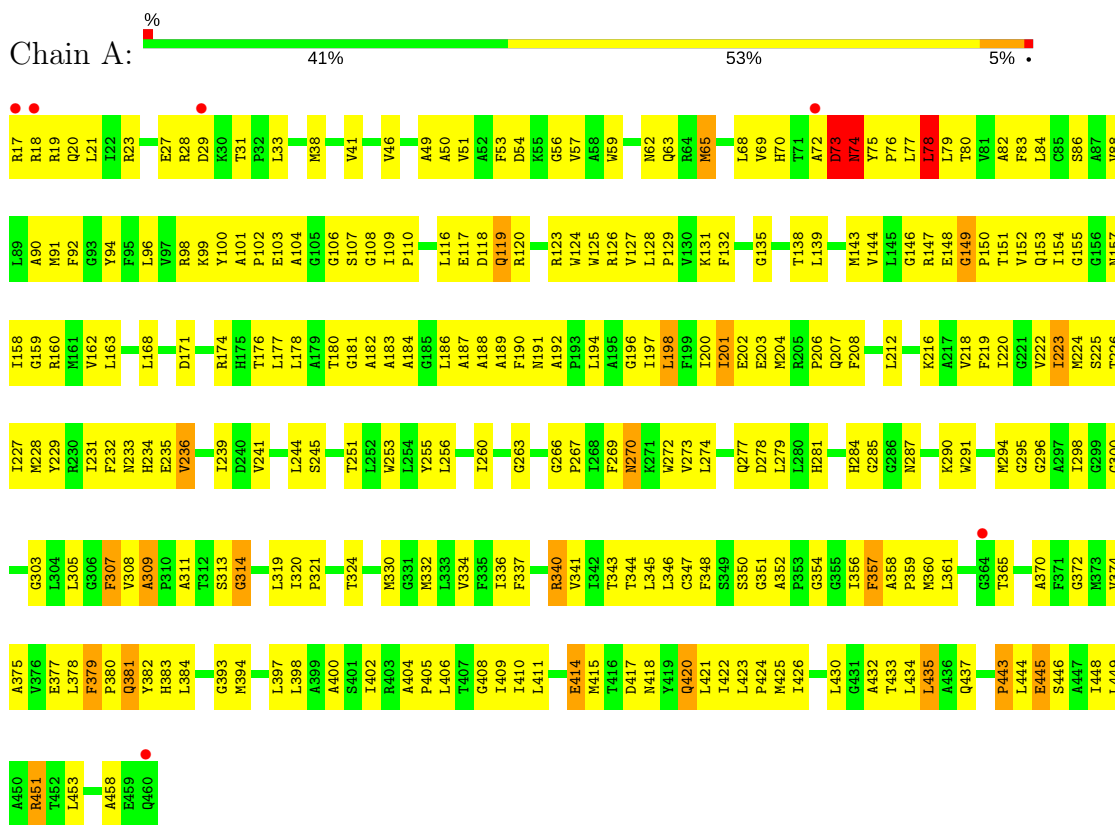
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Br	0	0
			1	1		

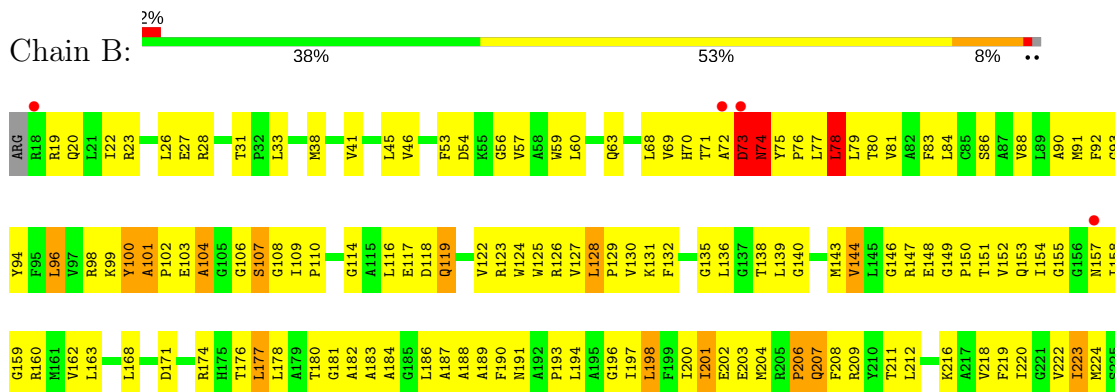
### 3 Residue-property plots

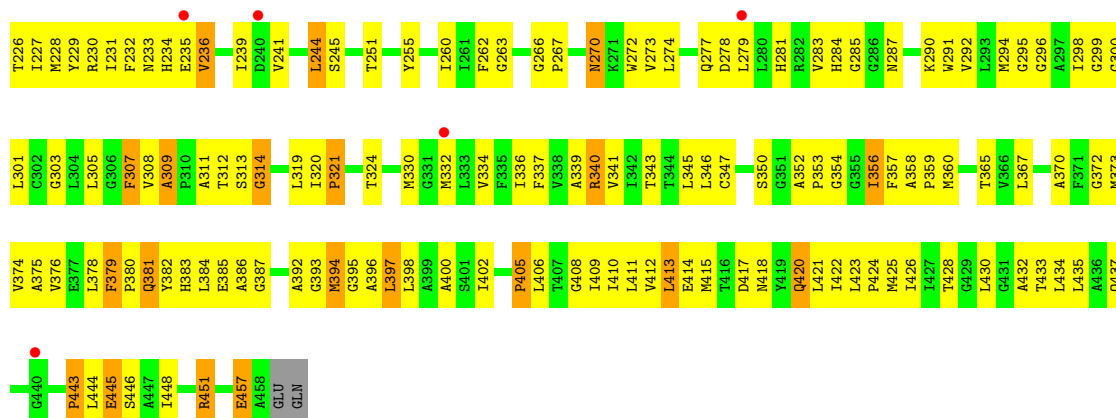
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: H(+)/Cl(-) exchange transporter clcA

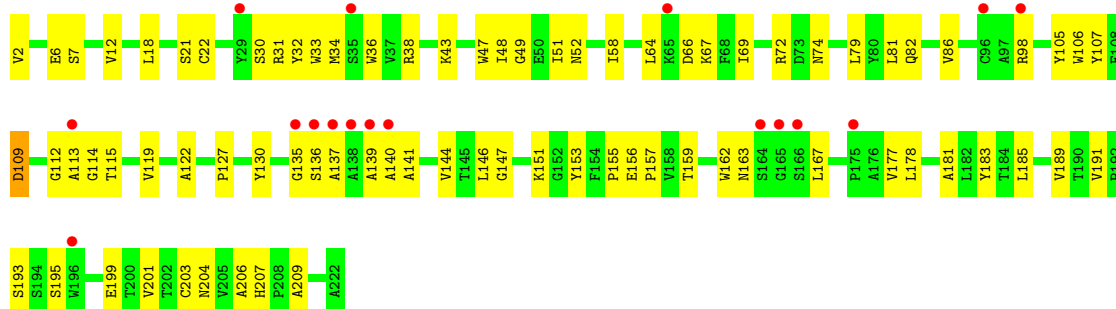


- Molecule 1: H(+)/Cl(-) exchange transporter clcA

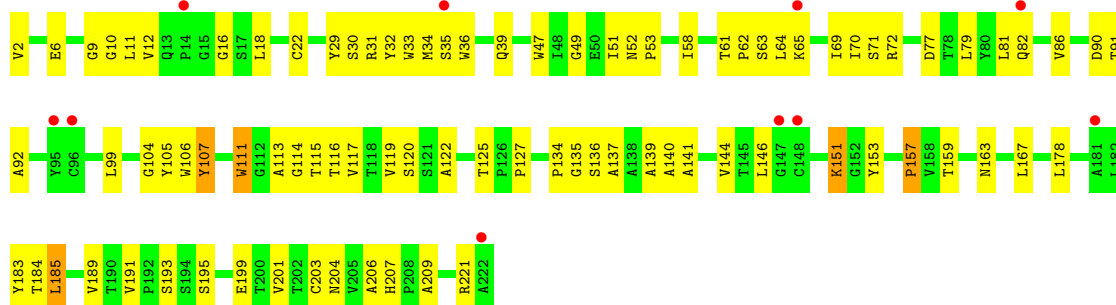




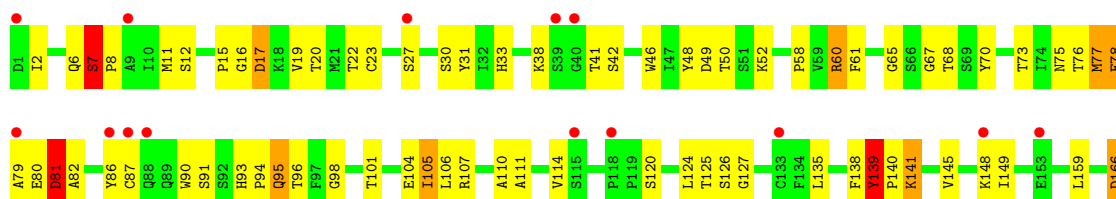
• Molecule 2: Fab Fragment, Heavy chain

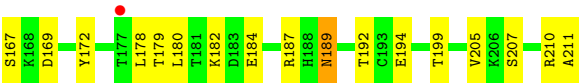


• Molecule 2: Fab Fragment, Heavy chain

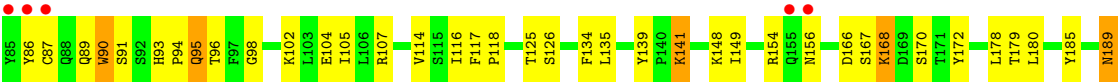


• Molecule 3: Fab Fragment, Light chain





● Molecule 3: Fab Fragment, Light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.84Å 97.59Å 171.54Å 90.00° 131.52° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 20.01 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-3.30) 97.9 (20.01-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.29Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.281 , 0.309 0.265 , 0.300	Depositor DCC
$R_{free}$ test set	2089 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	141.2	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 84.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.57	0/3402	0.75	1/4615 (0.0%)
1	B	0.62	0/3372	0.76	1/4577 (0.0%)
2	C	0.84	0/1721	0.80	0/2355
2	E	0.93	0/1721	0.86	0/2355
3	D	1.02	8/1660 (0.5%)	1.16	19/2257 (0.8%)
3	F	1.02	6/1660 (0.4%)	0.97	8/2257 (0.4%)
All	All	0.79	14/13536 (0.1%)	0.86	29/18416 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
3	F	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	78	GLU	CD-OE1	-13.10	1.11	1.25
3	D	141	LYS	CD-CE	-11.20	1.23	1.51
3	D	78	GLU	CD-OE2	-11.02	1.13	1.25
3	F	141	LYS	CD-CE	-9.70	1.26	1.51
3	D	68	THR	CB-CG2	-8.91	1.23	1.52
3	F	68	THR	CB-CG2	-8.61	1.24	1.52
3	D	77	MET	SD-CE	-7.51	1.35	1.77
3	D	141	LYS	CE-NZ	-6.60	1.32	1.49
3	F	90	TRP	CG-CD1	-6.36	1.27	1.36
3	F	141	LYS	CE-NZ	-6.36	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	81	ASP	CG-OD2	-6.22	1.11	1.25
3	F	35	TYR	CG-CD1	-5.67	1.31	1.39
3	D	81	ASP	CG-OD1	-5.47	1.12	1.25
3	F	102	LYS	CE-NZ	-5.07	1.36	1.49

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	78	GLU	OE1-CD-OE2	-15.80	104.34	123.30
3	D	139	TYR	CB-CG-CD2	14.71	129.82	121.00
3	F	60	ARG	NE-CZ-NH2	13.92	127.26	120.30
3	D	81	ASP	CB-CG-OD1	13.23	130.21	118.30
3	F	17	ASP	CB-CG-OD2	11.20	128.38	118.30
3	D	139	TYR	CB-CG-CD1	-9.73	115.16	121.00
3	D	139	TYR	C-N-CA	-9.65	81.48	122.00
3	D	139	TYR	C-N-CD	9.49	148.33	128.40
3	D	81	ASP	OD1-CG-OD2	-9.04	106.12	123.30
3	D	60	ARG	NE-CZ-NH2	-8.88	115.86	120.30
3	D	166	ASP	CB-CG-OD1	8.73	126.16	118.30
3	D	60	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	78	LEU	CA-CB-CG	7.21	131.88	115.30
3	D	17	ASP	CB-CG-OD2	7.16	124.75	118.30
1	B	78	LEU	CA-CB-CG	7.09	131.60	115.30
3	D	68	THR	OG1-CB-CG2	-6.64	94.72	110.00
3	F	68	THR	OG1-CB-CG2	-6.34	95.42	110.00
3	D	81	ASP	CB-CG-OD2	5.97	123.67	118.30
3	F	15	PRO	CA-N-CD	-5.93	103.19	111.50
3	D	78	GLU	CG-CD-OE2	5.80	129.90	118.30
3	F	60	ARG	NE-CZ-NH1	-5.59	117.51	120.30
3	D	138	PHE	O-C-N	5.58	131.64	122.70
3	D	77	MET	CG-SD-CE	5.41	108.86	100.20
3	D	138	PHE	C-N-CA	-5.38	108.25	121.70
3	D	166	ASP	OD1-CG-OD2	-5.37	113.10	123.30
3	F	166	ASP	CB-CG-OD1	5.32	123.09	118.30
3	F	7	SER	C-N-CD	5.28	139.49	128.40
3	D	7	SER	C-N-CD	5.06	139.03	128.40
3	F	166	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	139	TYR	Peptide
3	F	139	TYR	Sidechain

## 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	3331	0	3481	305	0
1	B	3301	0	3454	322	0
2	C	1672	0	1654	69	0
2	E	1672	0	1654	86	0
3	D	1621	0	1546	79	0
3	F	1621	0	1546	78	0
4	A	1	0	0	2	0
4	B	1	0	0	5	0
All	All	13220	0	13335	870	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 33.

All (870) 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:A:381:GLN:N	1:A:381:GLN:HE21	1.41	1.17
1:A:381:GLN:NE2	1:A:381:GLN:H	1.44	1.14
1:B:381:GLN:N	1:B:381:GLN:HE21	1.46	1.11
1:B:381:GLN:NE2	1:B:381:GLN:H	1.49	1.10
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.33	1.08
2:E:9:GLY:H	2:E:115:THR:HG21	1.18	1.06
1:A:119:GLN:HA	1:A:119:GLN:HE21	1.20	1.06
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.39	1.04
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.41	1.03
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.40	0.99
1:B:119:GLN:HE21	1:B:119:GLN:HA	1.27	0.99
1:B:107:SER:HB3	4:B:2:BR:BR	2.19	0.98
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.27	0.94
3:D:95:GLN:H	3:D:95:GLN:CD	1.72	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.51	0.92
3:F:95:GLN:H	3:F:95:GLN:CD	1.68	0.92
1:B:148:GLU:HG2	1:B:357:PHE:HB3	1.52	0.91
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.06	0.90
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.54	0.88
1:B:68:LEU:HD22	1:B:78:LEU:CD2	2.04	0.87
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.38	0.87
3:F:13:ALA:HB3	3:F:77:MET:HE3	1.56	0.87
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.39	0.86
1:B:68:LEU:HD22	1:B:78:LEU:HD23	1.55	0.86
1:B:227:ILE:O	1:B:231:ILE:HG12	1.76	0.85
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.58	0.84
2:C:113:ALA:HA	3:D:42:SER:OG	1.78	0.84
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.57	0.84
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.60	0.84
3:D:6:GLN:HE22	3:D:86:TYR:HA	1.40	0.84
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.13	0.84
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.41	0.83
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.60	0.83
1:B:154:ILE:O	1:B:158:ILE:HG12	1.77	0.83
1:B:110:PRO:HD2	4:B:2:BR:BR	2.34	0.83
1:A:148:GLU:HG2	1:A:357:PHE:HB3	1.61	0.83
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.13	0.83
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.61	0.82
1:A:430:LEU:HD22	1:B:223:ILE:HD12	1.59	0.82
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.61	0.82
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.59	0.82
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.59	0.82
1:A:267:PRO:O	1:A:270:ASN:HB2	1.80	0.82
1:B:298:ILE:HG23	1:B:346:LEU:HD23	1.61	0.82
1:A:422:ILE:HA	1:A:425:MET:HE3	1.62	0.81
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.61	0.81
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.62	0.81
1:A:119:GLN:HA	1:A:119:GLN:NE2	1.95	0.81
3:D:95:GLN:N	3:D:95:GLN:CD	2.30	0.81
2:E:9:GLY:N	2:E:115:THR:HG21	1.96	0.80
1:B:374:VAL:HG12	1:B:378:LEU:HD11	1.63	0.80
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.61	0.80
1:B:119:GLN:NE2	1:B:119:GLN:HA	1.96	0.80
1:B:267:PRO:O	1:B:270:ASN:HB2	1.82	0.80
1:A:19:ARG:HB2	1:A:19:ARG:NH1	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:HG22	1:A:218:VAL:HA	1.64	0.79
1:B:398:LEU:O	1:B:402:ILE:HG22	1.81	0.79
1:B:279:LEU:O	1:B:279:LEU:HD23	1.81	0.79
2:E:221:ARG:HH12	3:F:118:PRO:HB2	1.46	0.79
1:A:227:ILE:O	1:A:231:ILE:HG12	1.83	0.78
1:A:298:ILE:HG23	1:A:346:LEU:HD23	1.64	0.78
1:A:287:ASN:ND2	1:A:290:LYS:HG3	1.98	0.78
1:B:422:ILE:HA	1:B:425:MET:HE2	1.66	0.78
3:F:13:ALA:HB3	3:F:77:MET:CE	2.14	0.77
1:A:197:ILE:HD13	1:A:219:PHE:CD1	2.19	0.77
1:A:74:ASN:C	1:A:74:ASN:HD22	1.87	0.77
1:B:197:ILE:HD13	1:B:219:PHE:CD1	2.20	0.77
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.18	0.77
1:B:187:ALA:O	1:B:189:ALA:N	2.17	0.77
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.65	0.77
1:B:421:LEU:O	1:B:424:PRO:HD2	1.85	0.76
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.66	0.76
1:B:86:SER:OG	1:B:303:GLY:HA3	1.86	0.76
3:F:107:ARG:CD	3:F:170:SER:HB2	2.15	0.76
3:F:95:GLN:N	3:F:95:GLN:CD	2.34	0.76
3:D:189:ASN:HD21	3:D:211:ALA:H	1.34	0.76
1:A:86:SER:OG	1:A:303:GLY:HA3	1.85	0.76
1:B:320:ILE:HG23	1:B:365:THR:HG21	1.69	0.75
1:A:398:LEU:O	1:A:402:ILE:HG22	1.86	0.75
1:B:110:PRO:HG3	1:B:445:GLU:HB3	1.68	0.75
1:A:68:LEU:HD22	1:A:78:LEU:CD2	2.16	0.75
3:F:38:LYS:O	3:F:41:THR:HG22	1.87	0.75
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.15	0.75
3:F:189:ASN:HD21	3:F:211:ALA:H	1.33	0.75
1:B:135:GLY:HA2	1:B:138:THR:OG1	1.86	0.74
1:A:154:ILE:O	1:A:158:ILE:HG12	1.87	0.74
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.67	0.74
1:B:104:ALA:HB2	1:B:127:VAL:HG13	1.70	0.74
1:B:109:ILE:HB	1:B:110:PRO:HD3	1.68	0.74
1:A:119:GLN:CA	1:A:119:GLN:HE21	2.00	0.74
2:C:38:ARG:HD3	2:C:48:ILE:HD11	1.70	0.74
2:E:134:PRO:O	2:E:221:ARG:HG3	1.87	0.74
1:A:409:ILE:HD11	1:A:426:ILE:HA	1.71	0.73
1:A:155:GLY:O	1:A:158:ILE:HB	1.88	0.73
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.23	0.73
1:B:346:LEU:O	1:B:350:SER:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:VAL:HG12	1:A:378:LEU:HD11	1.71	0.73
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.72	0.72
1:A:320:ILE:HG23	1:A:365:THR:HG21	1.71	0.72
1:B:336:ILE:O	1:B:340:ARG:HG3	1.90	0.71
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.73	0.71
1:A:135:GLY:HA2	1:A:138:THR:OG1	1.90	0.71
1:A:444:LEU:O	1:A:448:ILE:HG13	1.91	0.71
1:A:200:ILE:HA	1:A:204:MET:HB2	1.73	0.70
2:C:195:SER:O	2:C:199:GLU:HB3	1.92	0.70
3:D:106:LEU:HD23	3:D:107:ARG:N	2.06	0.70
1:A:116:LEU:HD23	1:A:178:LEU:HD23	1.72	0.69
1:A:409:ILE:CD1	1:A:426:ILE:HA	2.22	0.69
1:B:119:GLN:CA	1:B:119:GLN:HE21	2.03	0.69
3:F:38:LYS:NZ	3:F:80:GLU:O	2.24	0.69
1:B:150:PRO:O	1:B:154:ILE:HG13	1.92	0.69
1:A:208:PHE:HZ	1:B:28:ARG:HB2	1.57	0.69
1:A:346:LEU:O	1:A:350:SER:HB3	1.92	0.69
3:D:7:SER:HB2	3:D:22:THR:HB	1.74	0.69
3:F:107:ARG:HD2	3:F:170:SER:HB2	1.72	0.69
1:A:150:PRO:O	1:A:154:ILE:HG13	1.93	0.69
1:A:200:ILE:HG22	1:A:201:ILE:N	2.05	0.69
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.23	0.69
2:E:9:GLY:HA3	2:E:115:THR:HG22	1.73	0.68
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.29	0.68
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.28	0.68
1:A:28:ARG:HH22	1:B:203:GLU:CD	1.95	0.68
2:C:7:SER:HA	2:C:115:THR:HG21	1.75	0.68
1:A:337:PHE:O	1:A:341:VAL:HG23	1.92	0.68
1:A:68:LEU:HD22	1:A:78:LEU:HD23	1.75	0.68
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.76	0.68
1:A:406:LEU:HD13	1:B:219:PHE:CZ	2.28	0.67
1:A:202:GLU:O	1:A:202:GLU:HG2	1.94	0.67
1:A:279:LEU:O	1:A:279:LEU:HD23	1.94	0.67
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.77	0.67
3:D:125:THR:HG22	3:D:125:THR:O	1.93	0.67
3:D:6:GLN:NE2	3:D:87:CYS:H	1.92	0.67
1:B:155:GLY:O	1:B:158:ILE:HB	1.95	0.67
1:B:180:THR:HG22	1:B:218:VAL:HA	1.77	0.67
1:B:287:ASN:ND2	1:B:290:LYS:HG3	2.08	0.67
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.76	0.67
1:B:148:GLU:CG	1:B:357:PHE:HB3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLU:H	1:B:148:GLU:CD	1.98	0.66
3:D:30:SER:HA	3:D:70:TYR:OH	1.96	0.66
2:E:221:ARG:NH1	3:F:118:PRO:HB2	2.11	0.66
1:A:398:LEU:O	1:A:402:ILE:CG2	2.44	0.65
1:A:444:LEU:HD13	1:A:444:LEU:O	1.96	0.65
1:B:116:LEU:HD23	1:B:178:LEU:HD23	1.78	0.65
1:B:374:VAL:HG12	1:B:378:LEU:CD1	2.27	0.65
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.61	0.65
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.79	0.65
1:A:171:ASP:HB2	1:A:212:LEU:HD22	1.79	0.65
1:A:223:ILE:HD11	1:B:426:ILE:CG2	2.26	0.65
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.77	0.65
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.76	0.65
1:A:146:GLY:HA3	1:A:148:GLU:OE2	1.95	0.65
2:C:6:GLU:O	2:C:115:THR:HG23	1.96	0.65
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.79	0.65
1:A:171:ASP:CB	1:A:212:LEU:HD22	2.27	0.65
1:B:200:ILE:HG22	1:B:201:ILE:N	2.12	0.65
1:B:337:PHE:O	1:B:341:VAL:HG23	1.97	0.64
1:B:90:ALA:HB3	1:B:296:GLY:HA2	1.79	0.64
3:F:30:SER:HA	3:F:70:TYR:OH	1.97	0.64
1:B:270:ASN:ND2	1:B:444:LEU:HD23	2.11	0.64
1:B:74:ASN:HD22	1:B:74:ASN:C	2.00	0.64
2:C:163:ASN:ND2	2:C:167:LEU:HD22	2.12	0.64
1:B:444:LEU:O	1:B:448:ILE:HG13	1.97	0.64
3:D:95:GLN:N	3:D:95:GLN:OE1	2.31	0.64
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.33	0.64
3:F:78:GLU:O	3:F:81:ASP:HB2	1.97	0.64
1:B:200:ILE:HA	1:B:204:MET:HB2	1.79	0.64
1:B:421:LEU:C	1:B:424:PRO:HD2	2.17	0.64
1:A:381:GLN:HE21	1:A:381:GLN:H	0.70	0.64
1:B:144:VAL:HG12	1:B:144:VAL:O	1.98	0.64
3:D:31:TYR:HA	3:D:50:THR:OG1	1.98	0.64
2:E:163:ASN:ND2	2:E:167:LEU:HD22	2.13	0.64
2:E:195:SER:O	2:E:199:GLU:HB3	1.97	0.64
3:D:7:SER:CB	3:D:22:THR:HB	2.28	0.63
3:F:141:LYS:HB3	3:F:172:TYR:CD1	2.33	0.63
1:A:332:MET:O	1:A:336:ILE:HG13	1.99	0.63
1:B:413:LEU:O	1:B:415:MET:N	2.31	0.63
3:F:95:GLN:H	3:F:95:GLN:NE2	1.96	0.63
1:A:148:GLU:CG	1:A:357:PHE:HB3	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.80	0.63
2:E:185:LEU:O	2:E:185:LEU:HD12	1.99	0.63
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.79	0.63
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.34	0.63
1:A:223:ILE:HG22	1:A:224:MET:N	2.14	0.63
1:A:360:MET:HG2	1:A:397:LEU:HD12	1.81	0.63
1:B:191:ASN:HB2	1:B:229:TYR:CE2	2.34	0.63
2:E:185:LEU:C	2:E:185:LEU:HD12	2.19	0.63
1:A:19:ARG:HB2	1:A:19:ARG:HH11	1.61	0.63
1:A:28:ARG:HD2	1:B:207:GLN:HG2	1.79	0.63
1:A:410:ILE:HD11	1:B:194:LEU:HD13	1.79	0.63
1:B:202:GLU:HG2	1:B:202:GLU:O	1.99	0.63
1:A:241:VAL:HG12	1:A:241:VAL:O	1.98	0.62
1:A:443:PRO:HB2	1:A:446:SER:HB2	1.81	0.62
1:B:150:PRO:HD3	1:B:354:GLY:CA	2.20	0.62
3:F:125:THR:O	3:F:125:THR:HG22	1.98	0.62
1:A:144:VAL:HG12	1:A:144:VAL:O	1.99	0.62
1:A:92:PHE:O	1:A:96:LEU:HD23	1.99	0.62
3:F:6:GLN:NE2	3:F:87:CYS:H	1.97	0.62
3:F:31:TYR:HA	3:F:50:THR:OG1	1.99	0.62
1:A:160:ARG:HH12	1:A:174:ARG:HD2	1.64	0.62
1:B:234:HIS:CE1	3:D:52:LYS:NZ	2.67	0.62
2:E:18:LEU:HD11	2:E:117:VAL:HG22	1.82	0.62
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.34	0.62
1:A:203:GLU:CD	1:B:28:ARG:HH22	2.03	0.61
1:A:336:ILE:O	1:A:340:ARG:HG3	2.00	0.61
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.65	0.61
1:B:400:ALA:HB2	1:B:432:ALA:HB1	1.80	0.61
1:B:220:ILE:O	1:B:224:MET:HG2	2.00	0.61
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.30	0.61
1:B:110:PRO:CD	4:B:2:BR:BR	3.03	0.61
2:C:185:LEU:HD12	2:C:185:LEU:C	2.21	0.61
1:B:223:ILE:HG22	1:B:224:MET:N	2.14	0.61
1:B:160:ARG:HH12	1:B:174:ARG:HD2	1.66	0.61
1:B:360:MET:HG2	1:B:397:LEU:HD12	1.82	0.61
2:C:30:SER:C	2:C:32:TYR:H	2.04	0.61
1:B:91:MET:HG3	1:B:296:GLY:HA3	1.83	0.61
2:E:39:GLN:O	2:E:92:ALA:HB1	2.01	0.61
1:A:379:PHE:HA	1:A:381:GLN:HE22	1.64	0.60
1:B:187:ALA:C	1:B:189:ALA:H	2.05	0.60
1:A:201:ILE:HG13	1:A:201:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:189:ASN:HD21	3:D:211:ALA:N	1.97	0.60
1:A:159:GLY:O	1:A:162:VAL:HG22	2.01	0.60
2:E:91:THR:OG1	2:E:119:VAL:HG23	2.00	0.60
1:A:190:PHE:HB3	1:A:415:MET:SD	2.42	0.60
2:E:30:SER:C	2:E:32:TYR:H	2.05	0.60
3:F:116:ILE:HD13	3:F:193:CYS:HB2	1.84	0.60
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.84	0.60
3:F:7:SER:HB3	3:F:8:PRO:CD	2.31	0.60
1:A:216:LYS:HZ1	1:B:433:THR:HG22	1.67	0.60
1:A:219:PHE:CZ	1:B:406:LEU:HD13	2.38	0.59
1:A:451:ARG:HB3	1:A:451:ARG:HH11	1.67	0.59
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.02	0.59
2:C:146:LEU:HD12	2:C:201:VAL:HG11	1.84	0.59
3:F:76:THR:HG22	3:F:76:THR:O	2.02	0.59
1:A:18:ARG:HB2	1:B:119:GLN:OE1	2.02	0.59
1:A:263:GLY:HA3	1:A:435:LEU:HB2	1.83	0.59
1:B:212:LEU:HD12	1:B:212:LEU:N	2.18	0.59
1:B:360:MET:CG	1:B:397:LEU:HD12	2.32	0.59
1:B:92:PHE:O	1:B:96:LEU:HD23	2.03	0.59
2:C:163:ASN:HD22	2:C:167:LEU:HD22	1.66	0.59
1:A:207:GLN:HG2	1:B:28:ARG:HD2	1.85	0.59
1:A:357:PHE:CE1	1:A:402:ILE:HD13	2.36	0.59
3:D:95:GLN:H	3:D:95:GLN:NE2	2.00	0.59
1:A:406:LEU:HD13	1:B:219:PHE:CE1	2.38	0.59
1:B:75:TYR:CE2	1:B:79:LEU:HD11	2.38	0.59
1:B:234:HIS:HE1	3:D:52:LYS:HZ3	1.51	0.59
1:A:448:ILE:HD13	4:A:1:BR:BR	2.58	0.59
1:B:311:ALA:O	1:B:336:ILE:HG23	2.03	0.59
1:B:383:HIS:HB3	2:E:33:TRP:CZ2	2.38	0.59
1:A:287:ASN:HD22	1:A:290:LYS:CG	2.08	0.59
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.85	0.59
2:E:63:SER:OG	2:E:64:LEU:N	2.36	0.59
1:A:244:LEU:HB2	1:A:418:ASN:OD1	2.03	0.58
1:A:313:SER:OG	1:A:314:GLY:N	2.30	0.58
3:F:2:ILE:HD12	3:F:27:SER:HB2	1.83	0.58
1:B:98:ARG:NE	1:B:98:ARG:HA	2.18	0.58
2:E:163:ASN:HD22	2:E:167:LEU:HD22	1.67	0.58
1:A:182:ALA:HB3	1:A:200:ILE:HD11	1.86	0.58
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.84	0.58
1:B:90:ALA:O	1:B:94:TYR:HD1	1.86	0.58
3:D:192:THR:HG22	3:D:207:SER:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PRO:HG2	4:B:2:BR:BR	2.58	0.58
1:B:357:PHE:CE1	1:B:402:ILE:HD13	2.38	0.58
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.14	0.58
1:A:219:PHE:CE1	1:B:406:LEU:HD13	2.39	0.58
1:A:241:VAL:HG12	1:A:244:LEU:HD21	1.84	0.58
3:D:2:ILE:HD12	3:D:27:SER:HB2	1.85	0.58
3:F:189:ASN:HD21	3:F:211:ALA:N	1.99	0.58
2:C:6:GLU:CG	2:C:114:GLY:HA2	2.33	0.58
3:D:78:GLU:O	3:D:81:ASP:HB2	2.03	0.58
3:F:82:ALA:HB2	3:F:105:ILE:HG12	1.86	0.58
1:A:104:ALA:HB2	1:A:127:VAL:HG13	1.86	0.58
1:A:405:PRO:HG2	1:A:406:LEU:H	1.68	0.58
1:B:144:VAL:HG21	1:B:343:THR:HB	1.84	0.58
2:C:86:VAL:HG12	2:C:119:VAL:CG1	2.33	0.58
3:F:20:THR:HG23	3:F:73:THR:OG1	2.03	0.58
1:A:143:MET:HE2	1:A:347:CYS:HB3	1.85	0.58
3:F:192:THR:HG22	3:F:207:SER:CB	2.34	0.58
1:A:28:ARG:NH2	1:B:203:GLU:OE1	2.37	0.57
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.85	0.57
1:A:421:LEU:O	1:A:425:MET:HG3	2.04	0.57
1:A:78:LEU:HD11	1:A:307:PHE:CE2	2.40	0.57
2:E:144:VAL:O	2:E:144:VAL:HG13	2.04	0.57
1:B:380:PRO:HD2	1:B:381:GLN:NE2	2.19	0.57
1:A:163:LEU:HD12	1:A:168:LEU:HB2	1.86	0.57
1:A:251:THR:HG22	1:A:255:TYR:HE1	1.70	0.57
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.69	0.57
1:A:91:MET:CG	1:A:296:GLY:HA3	2.35	0.57
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.40	0.57
1:A:360:MET:CG	1:A:397:LEU:HD12	2.35	0.57
1:B:320:ILE:HG23	1:B:365:THR:CG2	2.34	0.57
1:B:74:ASN:ND2	1:B:76:PRO:HD2	2.20	0.57
1:B:148:GLU:HG2	1:B:357:PHE:CB	2.28	0.56
1:B:408:GLY:O	1:B:411:LEU:N	2.37	0.56
1:B:171:ASP:HB2	1:B:212:LEU:HD22	1.87	0.56
1:B:234:HIS:CE1	3:D:52:LYS:HZ1	2.22	0.56
2:E:51:ILE:CD1	2:E:72:ARG:HG2	2.35	0.56
1:A:200:ILE:HG22	1:A:201:ILE:CG2	2.36	0.56
1:A:68:LEU:HD22	1:A:78:LEU:HD22	1.86	0.56
3:F:7:SER:CB	3:F:8:PRO:HD3	2.33	0.56
1:A:123:ARG:HA	1:A:125:TRP:CH2	2.41	0.56
3:D:60:ARG:NH2	3:D:81:ASP:OD1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:LEU:HA	1:B:308:VAL:HG22	1.88	0.56
3:D:106:LEU:HD23	3:D:107:ARG:H	1.69	0.56
1:A:98:ARG:HA	1:A:98:ARG:NE	2.21	0.56
1:B:235:GLU:O	1:B:236:VAL:HG23	2.05	0.56
3:D:17:ASP:H	3:D:76:THR:HA	1.71	0.56
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.40	0.56
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.87	0.56
1:A:186:LEU:O	1:A:186:LEU:HG	2.06	0.55
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.88	0.55
3:D:7:SER:HB3	3:D:8:PRO:CD	2.32	0.55
2:E:104:GLY:O	2:E:106:TRP:CD1	2.60	0.55
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.87	0.55
1:A:212:LEU:N	1:A:212:LEU:HD12	2.22	0.55
1:B:139:LEU:HD11	1:B:146:GLY:O	2.06	0.55
1:B:370:ALA:O	1:B:374:VAL:HG23	2.05	0.55
1:B:379:PHE:HA	1:B:381:GLN:HE22	1.70	0.55
3:D:110:ALA:C	3:D:199:THR:HG21	2.26	0.55
3:D:60:ARG:HD2	3:D:76:THR:O	2.06	0.55
1:A:370:ALA:O	1:A:374:VAL:HG23	2.06	0.55
1:B:68:LEU:HD22	1:B:78:LEU:HD22	1.84	0.55
1:A:186:LEU:HD23	1:A:196:GLY:HA2	1.88	0.55
1:B:451:ARG:HB3	1:B:451:ARG:HH11	1.71	0.55
1:A:341:VAL:O	1:A:345:LEU:HG	2.07	0.55
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.72	0.55
1:A:28:ARG:HB2	1:B:208:PHE:HZ	1.72	0.55
1:A:208:PHE:CZ	1:B:28:ARG:HB2	2.40	0.55
1:B:100:TYR:O	1:B:101:ALA:HB2	2.05	0.55
2:C:7:SER:HA	2:C:115:THR:CG2	2.36	0.55
1:B:182:ALA:HB3	1:B:200:ILE:HD11	1.89	0.55
2:C:6:GLU:HA	2:C:22:CYS:HA	1.89	0.55
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.42	0.55
3:D:75:ASN:O	3:D:76:THR:HB	2.07	0.55
1:B:405:PRO:HG2	1:B:406:LEU:H	1.70	0.55
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.89	0.55
3:F:7:SER:HB2	3:F:22:THR:HB	1.89	0.55
1:A:203:GLU:OE1	1:B:28:ARG:NH2	2.41	0.54
1:B:244:LEU:HB2	1:B:418:ASN:OD1	2.08	0.54
1:B:38:MET:O	1:B:41:VAL:HG12	2.07	0.54
2:C:2:VAL:O	2:C:2:VAL:HG23	2.07	0.54
1:A:33:LEU:O	1:A:33:LEU:HD23	2.07	0.54
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASP:CB	1:B:212:LEU:HD22	2.37	0.54
2:E:10:GLY:N	2:E:116:THR:O	2.38	0.54
1:B:251:THR:HG22	1:B:255:TYR:HE1	1.72	0.54
1:B:190:PHE:HB3	1:B:415:MET:SD	2.48	0.54
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.39	0.54
3:D:8:PRO:O	3:D:101:THR:HG23	2.07	0.54
2:E:6:GLU:CD	2:E:114:GLY:H	2.11	0.54
2:E:12:VAL:HG11	2:E:18:LEU:HB3	1.88	0.54
1:A:74:ASN:ND2	1:A:76:PRO:HD2	2.23	0.54
1:B:263:GLY:HA3	1:B:435:LEU:HB2	1.90	0.54
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.90	0.54
1:A:374:VAL:HG12	1:A:378:LEU:CD1	2.37	0.54
1:A:108:GLY:HA3	1:A:153:GLN:NE2	2.22	0.54
2:C:141:ALA:O	2:C:193:SER:HB2	2.08	0.54
1:B:398:LEU:O	1:B:402:ILE:CG2	2.55	0.53
3:D:38:LYS:O	3:D:41:THR:HG22	2.08	0.53
1:B:234:HIS:HE1	3:D:52:LYS:NZ	2.05	0.53
1:A:200:ILE:HG22	1:A:201:ILE:HG22	1.90	0.53
1:A:379:PHE:CA	1:A:381:GLN:HE22	2.21	0.53
3:D:189:ASN:HD22	3:D:210:ARG:HB2	1.72	0.53
3:D:7:SER:CB	3:D:8:PRO:HD3	2.35	0.53
3:D:79:ALA:C	3:D:81:ASP:H	2.11	0.53
1:A:197:ILE:CG1	1:A:222:VAL:HG21	2.38	0.53
1:A:207:GLN:HG2	1:B:28:ARG:CD	2.39	0.53
1:A:380:PRO:HD2	1:A:381:GLN:HE22	1.73	0.53
1:A:417:ASP:O	1:A:417:ASP:OD2	2.26	0.53
1:A:74:ASN:C	1:A:74:ASN:ND2	2.58	0.53
3:D:82:ALA:HB2	3:D:105:ILE:HG13	1.89	0.53
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.91	0.53
1:A:382:TYR:HB3	1:A:384:LEU:HD21	1.91	0.53
2:E:6:GLU:HA	2:E:22:CYS:HA	1.91	0.53
2:E:69:ILE:HB	2:E:82:GLN:HB2	1.90	0.53
1:B:197:ILE:CG1	1:B:222:VAL:HG21	2.39	0.53
1:B:78:LEU:HD11	1:B:307:PHE:CE2	2.44	0.53
1:A:147:ARG:O	1:A:150:PRO:HD2	2.08	0.53
1:B:98:ARG:HD2	1:B:291:TRP:CD2	2.44	0.53
2:E:11:LEU:HD11	2:E:120:SER:HB3	1.91	0.53
3:F:189:ASN:HD22	3:F:210:ARG:HB2	1.73	0.53
1:A:234:HIS:H	1:A:234:HIS:CD2	2.27	0.52
1:B:99:LYS:HG2	1:B:100:TYR:CE1	2.45	0.52
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7:SER:CB	3:F:22:THR:HB	2.39	0.52
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.91	0.52
1:A:31:THR:H	1:B:437:GLN:HE22	1.57	0.52
2:C:7:SER:CA	2:C:115:THR:HG21	2.38	0.52
3:D:141:LYS:HB3	3:D:172:TYR:CD1	2.44	0.52
3:D:192:THR:HG22	3:D:207:SER:HB2	1.92	0.52
1:A:109:ILE:HB	1:A:110:PRO:HD3	1.90	0.52
3:F:2:ILE:CD1	3:F:27:SER:HB2	2.39	0.52
2:C:12:VAL:HG11	2:C:18:LEU:HB3	1.91	0.52
1:A:151:THR:O	1:A:155:GLY:N	2.34	0.52
1:A:74:ASN:ND2	1:A:77:LEU:H	2.07	0.52
1:B:108:GLY:HA3	1:B:153:GLN:NE2	2.24	0.52
1:A:320:ILE:HG23	1:A:365:THR:CG2	2.40	0.52
1:B:147:ARG:N	1:B:148:GLU:OE2	2.42	0.52
1:B:393:GLY:O	1:B:395:GLY:N	2.43	0.52
1:A:408:GLY:O	1:A:411:LEU:N	2.40	0.52
1:B:106:GLY:O	1:B:131:LYS:NZ	2.42	0.52
1:B:381:GLN:CA	1:B:381:GLN:HE21	2.22	0.52
2:C:185:LEU:HD12	2:C:185:LEU:O	2.09	0.52
1:B:110:PRO:CG	4:B:2:BR:BR	3.13	0.52
1:B:91:MET:CG	1:B:296:GLY:HA3	2.40	0.52
1:A:433:THR:CG2	1:B:216:LYS:HE2	2.40	0.51
1:A:449:LEU:O	1:A:453:LEU:HB2	2.10	0.51
1:B:33:LEU:HD23	1:B:33:LEU:O	2.10	0.51
1:A:274:LEU:O	1:A:277:GLN:CB	2.58	0.51
1:A:187:ALA:C	1:A:189:ALA:H	2.13	0.51
1:B:332:MET:O	1:B:336:ILE:HG13	2.09	0.51
1:B:330:MET:HE2	1:B:334:VAL:HG23	1.91	0.51
1:B:409:ILE:HD11	1:B:426:ILE:HA	1.93	0.51
2:C:30:SER:O	2:C:32:TYR:N	2.44	0.51
3:F:15:PRO:CD	3:F:105:ILE:HG23	2.40	0.51
1:B:270:ASN:O	1:B:273:VAL:HG12	2.10	0.51
1:B:298:ILE:O	1:B:301:LEU:HB3	2.11	0.51
3:D:148:LYS:HB2	3:D:192:THR:OG1	2.11	0.51
2:E:18:LEU:HD11	2:E:117:VAL:CG2	2.40	0.51
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.45	0.51
3:F:75:ASN:O	3:F:76:THR:HB	2.10	0.51
1:B:53:PHE:O	1:B:57:VAL:HG23	2.11	0.51
1:B:77:LEU:O	1:B:80:THR:HB	2.11	0.51
2:E:141:ALA:O	2:E:193:SER:HB2	2.11	0.51
2:C:69:ILE:HB	2:C:82:GLN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:PHE:O	1:A:273:VAL:HG12	2.11	0.51
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.92	0.51
1:B:409:ILE:CD1	1:B:426:ILE:HA	2.40	0.51
2:C:167:LEU:HD21	2:C:191:VAL:HG11	1.93	0.51
1:B:284:HIS:HA	1:B:290:LYS:CB	2.40	0.51
2:E:9:GLY:H	2:E:115:THR:CG2	2.07	0.51
3:F:95:GLN:OE1	3:F:95:GLN:N	2.44	0.51
1:A:381:GLN:CA	1:A:381:GLN:HE21	2.17	0.50
1:B:241:VAL:HG12	1:B:244:LEU:HD21	1.93	0.50
1:B:27:GLU:OE1	1:B:27:GLU:HA	2.11	0.50
1:A:38:MET:HG3	1:A:168:LEU:CD1	2.36	0.50
1:B:312:THR:HG22	1:B:339:ALA:HB3	1.94	0.50
2:C:32:TYR:CD2	2:C:98:ARG:HG3	2.46	0.50
1:B:187:ALA:C	1:B:189:ALA:N	2.64	0.50
1:B:287:ASN:HD22	1:B:290:LYS:CG	2.18	0.50
2:E:125:THR:O	2:E:153:TYR:HA	2.12	0.50
3:F:27:SER:O	3:F:68:THR:HG22	2.11	0.50
1:A:294:MET:HG2	1:A:294:MET:O	2.12	0.50
2:C:64:LEU:HB2	2:C:67:LYS:HB2	1.93	0.50
2:E:207:HIS:CE1	2:E:209:ALA:HB3	2.46	0.50
3:F:154:ARG:HE	3:F:156:ASN:HB2	1.77	0.50
1:A:144:VAL:HG21	1:A:343:THR:HB	1.93	0.50
2:C:159:THR:OG1	2:C:206:ALA:HB3	2.12	0.50
2:E:221:ARG:HH11	3:F:118:PRO:HD2	1.77	0.50
1:A:99:LYS:HG2	1:A:100:TYR:CE1	2.46	0.50
1:A:90:ALA:O	1:A:94:TYR:HD1	1.94	0.50
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.93	0.50
1:A:284:HIS:HA	1:A:290:LYS:CB	2.41	0.50
1:A:33:LEU:C	1:A:33:LEU:HD23	2.32	0.50
1:B:405:PRO:O	1:B:408:GLY:N	2.45	0.50
3:D:20:THR:HG23	3:D:73:THR:OG1	2.11	0.50
1:B:117:GLU:O	1:B:118:ASP:HB2	2.12	0.50
1:B:128:LEU:HB2	1:B:129:PRO:HD3	1.92	0.50
1:B:224:MET:O	1:B:228:MET:HG2	2.12	0.50
1:B:78:LEU:HD21	1:B:307:PHE:CE1	2.47	0.50
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.47	0.50
3:F:168:LYS:HD3	3:F:168:LYS:N	2.27	0.50
1:A:281:HIS:O	1:A:285:GLY:HA2	2.12	0.49
1:B:99:LYS:CG	1:B:100:TYR:CE1	2.95	0.49
1:B:235:GLU:O	1:B:236:VAL:CG2	2.59	0.49
2:E:9:GLY:HA3	2:E:115:THR:CG2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ILE:HG13	1:A:222:VAL:HG21	1.94	0.49
1:A:28:ARG:CD	1:B:207:GLN:HG2	2.42	0.49
1:B:229:TYR:CE1	1:B:233:ASN:ND2	2.80	0.49
1:B:284:HIS:HA	1:B:290:LYS:HB2	1.93	0.49
3:D:58:PRO:HG2	3:D:61:PHE:HD1	1.78	0.49
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.30	0.49
1:A:426:ILE:CG2	1:B:223:ILE:HD11	2.42	0.49
1:A:444:LEU:HD13	1:A:444:LEU:C	2.32	0.49
1:B:153:GLN:O	1:B:155:GLY:N	2.45	0.49
2:C:86:VAL:HG12	2:C:119:VAL:HG11	1.94	0.49
1:A:110:PRO:HG3	1:A:445:GLU:HB3	1.95	0.49
1:B:270:ASN:HD21	1:B:444:LEU:HB2	1.78	0.49
2:C:189:VAL:O	2:C:189:VAL:HG13	2.12	0.49
1:A:171:ASP:HB3	1:A:212:LEU:HD22	1.94	0.49
1:A:272:TRP:CD1	1:A:272:TRP:N	2.78	0.49
1:A:372:GLY:O	1:A:375:ALA:HB3	2.12	0.49
1:B:86:SER:HB3	1:B:299:GLY:O	2.12	0.49
2:E:146:LEU:HD12	2:E:201:VAL:HG11	1.93	0.49
2:E:30:SER:O	2:E:32:TYR:N	2.46	0.49
1:B:190:PHE:CD1	1:B:411:LEU:HD11	2.48	0.49
1:A:226:THR:HG21	1:B:423:LEU:HD11	1.95	0.49
2:E:159:THR:OG1	2:E:206:ALA:HB3	2.12	0.49
1:A:200:ILE:CG2	1:A:201:ILE:N	2.74	0.49
1:A:27:GLU:OE1	1:A:27:GLU:HA	2.13	0.49
1:B:94:TYR:CE1	1:B:295:GLY:HA3	2.48	0.49
1:B:92:PHE:CD1	1:B:92:PHE:C	2.86	0.49
2:E:135:GLY:C	2:E:137:ALA:H	2.16	0.49
2:E:2:VAL:O	2:E:2:VAL:HG23	2.13	0.49
1:A:239:ILE:HG22	1:A:241:VAL:HG23	1.95	0.48
1:B:357:PHE:CE1	1:B:402:ILE:CD1	2.96	0.48
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.42	0.48
1:A:84:LEU:O	1:A:88:VAL:HG23	2.13	0.48
2:C:135:GLY:C	2:C:137:ALA:H	2.16	0.48
1:A:19:ARG:HB2	1:A:19:ARG:CZ	2.43	0.48
1:A:314:GLY:O	1:A:340:ARG:NH2	2.46	0.48
1:B:96:LEU:O	1:B:130:VAL:HG13	2.13	0.48
1:B:270:ASN:O	1:B:273:VAL:CG1	2.62	0.48
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.48	0.48
1:A:46:VAL:HG11	1:A:184:ALA:CB	2.43	0.48
1:A:311:ALA:O	1:A:336:ILE:HG23	2.13	0.48
1:A:148:GLU:OE1	1:A:357:PHE:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LEU:O	1:B:277:GLN:CB	2.61	0.48
1:A:98:ARG:HD2	1:A:291:TRP:CD2	2.48	0.48
1:B:176:THR:HG22	1:B:177:LEU:HD23	1.96	0.48
1:B:143:MET:HE3	1:B:347:CYS:SG	2.54	0.48
2:C:113:ALA:HA	3:D:42:SER:HG	1.75	0.48
3:D:93:HIS:CG	3:D:94:PRO:HA	2.48	0.48
1:A:69:VAL:HA	1:A:72:ALA:HB2	1.95	0.48
3:D:111:ALA:HA	3:D:199:THR:OG1	2.13	0.48
1:A:187:ALA:O	1:A:189:ALA:N	2.47	0.48
1:A:356:ILE:HG12	1:A:356:ILE:O	2.13	0.48
2:E:151:LYS:HB2	2:E:184:THR:OG1	2.14	0.48
1:A:330:MET:HE2	1:A:334:VAL:HG23	1.95	0.48
1:A:356:ILE:HG23	1:A:360:MET:CE	2.38	0.48
3:F:93:HIS:CG	3:F:94:PRO:HA	2.49	0.48
1:B:153:GLN:O	1:B:154:ILE:C	2.52	0.48
1:B:266:GLY:N	1:B:267:PRO:CD	2.77	0.48
1:B:422:ILE:HD12	1:B:425:MET:CE	2.43	0.48
2:E:167:LEU:HD21	2:E:191:VAL:HG11	1.96	0.48
1:A:19:ARG:CB	1:A:19:ARG:CZ	2.92	0.47
1:A:267:PRO:O	1:A:270:ASN:N	2.46	0.47
1:A:270:ASN:HD21	1:A:444:LEU:HB2	1.79	0.47
1:B:186:LEU:HG	1:B:186:LEU:O	2.13	0.47
1:B:94:TYR:CD1	1:B:295:GLY:HA3	2.49	0.47
1:B:412:VAL:O	1:B:413:LEU:C	2.52	0.47
2:C:86:VAL:CG1	2:C:119:VAL:CG2	2.92	0.47
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.96	0.47
3:F:48:TYR:O	3:F:49:ASP:C	2.48	0.47
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.17	0.47
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.96	0.47
1:A:235:GLU:O	1:A:236:VAL:HG23	2.14	0.47
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.49	0.47
1:A:148:GLU:O	1:A:149:GLY:C	2.52	0.47
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.96	0.47
1:B:86:SER:HB2	1:B:300:GLY:HA2	1.97	0.47
2:E:86:VAL:HG12	2:E:119:VAL:CG1	2.44	0.47
1:A:86:SER:HB2	1:A:300:GLY:HA2	1.96	0.47
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.49	0.47
1:B:159:GLY:O	1:B:162:VAL:HG22	2.14	0.47
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.95	0.47
3:F:12:SER:HA	3:F:104:GLU:O	2.14	0.47
3:F:192:THR:HG22	3:F:207:SER:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:ND2	1:A:444:LEU:HD23	2.30	0.47
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.49	0.47
1:B:356:ILE:O	1:B:356:ILE:HG12	2.15	0.47
1:B:392:ALA:O	1:B:428:THR:HG21	2.14	0.47
2:E:105:TYR:N	2:E:105:TYR:CD1	2.82	0.47
1:A:192:ALA:HB1	1:A:414:GLU:OE2	2.14	0.47
1:A:430:LEU:HD22	1:B:223:ILE:CD1	2.38	0.47
1:B:382:TYR:HB3	1:B:384:LEU:HD21	1.96	0.47
1:A:245:SER:O	1:A:420:GLN:NE2	2.48	0.47
1:B:123:ARG:HA	1:B:125:TRP:CH2	2.50	0.47
1:B:59:TRP:O	1:B:63:GLN:HG2	2.15	0.47
2:E:9:GLY:N	2:E:115:THR:CG2	2.75	0.47
1:A:231:ILE:HB	1:A:232:PHE:CD1	2.50	0.47
1:A:380:PRO:HD2	1:A:381:GLN:NE2	2.29	0.47
1:A:357:PHE:CE1	1:A:402:ILE:CD1	2.98	0.47
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.97	0.47
1:B:422:ILE:HD12	1:B:425:MET:HE3	1.95	0.47
2:C:6:GLU:HA	2:C:21:SER:O	2.13	0.47
1:B:71:THR:O	1:B:78:LEU:HB2	2.15	0.47
2:E:52:ASN:HB2	2:E:53:PRO:HD2	1.96	0.47
3:F:22:THR:CG2	3:F:23:CYS:N	2.78	0.47
3:D:15:PRO:HA	3:D:77:MET:O	2.14	0.47
2:E:185:LEU:C	2:E:185:LEU:CD1	2.83	0.47
1:B:38:MET:CG	1:B:168:LEU:HD11	2.39	0.46
3:F:89:GLN:NE2	3:F:95:GLN:HA	2.29	0.46
1:A:20:GLN:O	1:A:23:ARG:HB3	2.15	0.46
1:A:418:ASN:HB3	1:A:420:GLN:OE1	2.15	0.46
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.97	0.46
1:B:54:ASP:OD1	1:B:147:ARG:NH2	2.48	0.46
2:C:112:GLY:O	3:D:42:SER:OG	2.32	0.46
3:D:149:ILE:HD11	3:D:178:LEU:HD21	1.97	0.46
3:F:107:ARG:CG	3:F:170:SER:HB2	2.45	0.46
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.49	0.46
1:B:211:THR:HG22	1:B:212:LEU:N	2.31	0.46
2:E:30:SER:C	2:E:32:TYR:N	2.68	0.46
1:A:147:ARG:N	1:A:148:GLU:OE2	2.48	0.46
1:A:73:ASP:N	1:A:73:ASP:OD1	2.36	0.46
1:A:78:LEU:HD13	1:A:79:LEU:N	2.30	0.46
1:B:119:GLN:CA	1:B:119:GLN:NE2	2.68	0.46
1:B:294:MET:HG2	1:B:294:MET:O	2.14	0.46
3:D:141:LYS:HD3	3:D:172:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:17:ASP:N	3:D:76:THR:HA	2.30	0.46
2:E:16:GLY:O	2:E:86:VAL:HG23	2.15	0.46
2:E:52:ASN:HB2	2:E:53:PRO:CD	2.44	0.46
1:A:38:MET:CG	1:A:168:LEU:HD11	2.37	0.46
1:A:46:VAL:HG11	1:A:184:ALA:HB3	1.97	0.46
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.51	0.46
3:D:6:GLN:HE21	3:D:98:GLY:HA3	1.79	0.46
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.97	0.46
1:A:100:TYR:O	1:A:101:ALA:HB2	2.16	0.46
1:A:190:PHE:O	1:A:191:ASN:C	2.53	0.46
1:A:148:GLU:CD	1:A:357:PHE:HB3	2.36	0.46
2:C:147:GLY:HA2	2:C:162:TRP:CH2	2.51	0.46
1:B:151:THR:O	1:B:155:GLY:N	2.44	0.46
1:B:313:SER:O	1:B:340:ARG:NH2	2.44	0.46
1:B:393:GLY:O	1:B:394:MET:C	2.54	0.46
2:C:6:GLU:CD	2:C:114:GLY:HA2	2.36	0.46
2:E:35:SER:HB3	2:E:99:LEU:HD21	1.98	0.46
3:F:189:ASN:ND2	3:F:210:ARG:HB2	2.31	0.46
1:A:155:GLY:HA3	1:A:181:GLY:O	2.15	0.46
1:A:49:ALA:O	1:A:51:VAL:N	2.49	0.46
3:D:166:ASP:OD1	3:D:167:SER:N	2.49	0.46
3:F:15:PRO:HD3	3:F:105:ILE:HG23	1.97	0.46
1:A:202:GLU:OE1	1:A:404:ALA:HB1	2.15	0.46
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.39	0.46
1:B:176:THR:O	1:B:180:THR:HG23	2.15	0.46
3:D:12:SER:HA	3:D:104:GLU:O	2.16	0.46
3:D:189:ASN:ND2	3:D:210:ARG:HB2	2.31	0.46
1:A:117:GLU:O	1:A:118:ASP:HB2	2.15	0.46
1:A:59:TRP:O	1:A:62:ASN:HB3	2.16	0.46
1:A:94:TYR:CD1	1:A:295:GLY:HA3	2.51	0.46
1:B:68:LEU:HD13	1:B:307:PHE:CD1	2.51	0.46
1:B:33:LEU:HD23	1:B:33:LEU:C	2.36	0.46
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.51	0.46
2:E:61:THR:O	2:E:63:SER:N	2.49	0.46
1:A:266:GLY:N	1:A:267:PRO:CD	2.78	0.45
1:A:148:GLU:HG2	1:A:357:PHE:CB	2.39	0.45
1:A:433:THR:HG22	1:B:216:LYS:HZ1	1.81	0.45
1:B:408:GLY:O	1:B:409:ILE:C	2.54	0.45
2:E:29:TYR:HB2	2:E:77:ASP:OD2	2.16	0.45
1:A:160:ARG:HH12	1:A:174:ARG:CD	2.28	0.45
1:B:101:ALA:N	1:B:102:PRO:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:ILE:HG23	2:C:51:ILE:O	2.16	0.45
2:E:106:TRP:CD1	2:E:106:TRP:N	2.83	0.45
3:F:1:ASP:HB3	3:F:94:PRO:HD2	1.98	0.45
1:A:77:LEU:O	1:A:80:THR:HB	2.16	0.45
1:B:239:ILE:HG22	1:B:241:VAL:HG23	1.98	0.45
1:B:308:VAL:O	1:B:309:ALA:HB2	2.16	0.45
2:C:86:VAL:HG11	2:C:119:VAL:HG22	1.99	0.45
1:A:148:GLU:H	1:A:148:GLU:CD	2.18	0.45
1:A:148:GLU:OE1	1:A:357:PHE:HB3	2.16	0.45
1:A:423:LEU:HD11	1:B:226:THR:HG21	1.97	0.45
1:A:433:THR:HG22	1:B:216:LYS:HE2	1.98	0.45
2:E:111:TRP:N	2:E:111:TRP:CD1	2.84	0.45
1:A:139:LEU:HD11	1:A:146:GLY:O	2.17	0.45
1:A:151:THR:O	1:A:152:VAL:C	2.54	0.45
1:A:187:ALA:C	1:A:189:ALA:N	2.69	0.45
1:B:267:PRO:O	1:B:270:ASN:N	2.49	0.45
2:E:189:VAL:HG13	2:E:189:VAL:O	2.16	0.45
2:E:86:VAL:HG13	2:E:90:ASP:HB2	1.99	0.45
2:E:91:THR:O	2:E:92:ALA:HB2	2.17	0.45
2:E:39:GLN:C	2:E:92:ALA:HB1	2.37	0.45
3:F:141:LYS:HB3	3:F:172:TYR:CE1	2.51	0.45
3:F:37:GLN:O	3:F:83:ALA:HB1	2.17	0.45
1:A:82:ALA:HB1	1:A:303:GLY:O	2.17	0.45
1:B:451:ARG:CB	1:B:451:ARG:HH11	2.30	0.45
2:C:72:ARG:HD3	2:C:74:ASN:OD1	2.17	0.45
3:F:179:THR:O	3:F:180:LEU:HD23	2.17	0.45
1:A:284:HIS:HA	1:A:290:LYS:HB2	1.99	0.45
1:A:308:VAL:O	1:A:309:ALA:HB2	2.17	0.45
1:B:314:GLY:O	1:B:340:ARG:NH2	2.50	0.45
2:E:33:TRP:CZ2	2:E:52:ASN:HB3	2.52	0.45
1:B:183:ALA:O	1:B:184:ALA:C	2.54	0.45
1:B:74:ASN:ND2	1:B:74:ASN:C	2.70	0.45
1:A:124:TRP:O	1:A:126:ARG:N	2.50	0.45
1:A:78:LEU:HD13	1:A:79:LEU:HD23	1.97	0.45
1:B:272:TRP:CD1	1:B:272:TRP:N	2.81	0.45
1:A:278:ASP:O	1:A:281:HIS:N	2.41	0.44
1:A:78:LEU:HD21	1:A:307:PHE:CE1	2.52	0.44
1:B:231:ILE:HB	1:B:232:PHE:CD1	2.52	0.44
3:F:107:ARG:HG2	3:F:170:SER:HB2	1.98	0.44
1:A:176:THR:HG22	1:A:177:LEU:HD23	1.98	0.44
1:A:358:ALA:HA	1:A:361:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:GLN:HE22	1:B:31:THR:H	1.65	0.44
2:C:30:SER:C	2:C:32:TYR:N	2.69	0.44
1:A:294:MET:O	1:A:298:ILE:HG13	2.17	0.44
1:B:69:VAL:HA	1:B:72:ALA:HB2	1.99	0.44
1:B:91:MET:O	1:B:93:GLY:N	2.50	0.44
1:A:106:GLY:O	1:A:131:LYS:NZ	2.50	0.44
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.99	0.44
1:A:29:ASP:OD2	1:A:216:LYS:NZ	2.50	0.44
2:C:144:VAL:HG13	2:C:144:VAL:O	2.17	0.44
2:C:51:ILE:CD1	2:C:72:ARG:HG2	2.47	0.44
2:C:86:VAL:CG1	2:C:119:VAL:HG22	2.47	0.44
1:A:73:ASP:O	1:A:75:TYR:N	2.50	0.44
1:B:74:ASN:HD22	1:B:76:PRO:HD2	1.82	0.44
2:E:51:ILE:O	2:E:51:ILE:HG23	2.17	0.44
3:D:90:TRP:CD2	3:D:95:GLN:HB3	2.52	0.44
1:A:358:ALA:HB3	1:A:359:PRO:CD	2.38	0.44
3:D:210:ARG:HH11	3:D:210:ARG:HG2	1.82	0.44
1:A:120:ARG:HB3	1:A:120:ARG:HE	1.56	0.44
1:B:20:GLN:O	1:B:23:ARG:HB3	2.18	0.44
1:B:420:GLN:HB2	1:B:420:GLN:HE21	1.52	0.44
1:B:22:ILE:O	1:B:26:LEU:HD12	2.17	0.44
1:B:73:ASP:O	1:B:75:TYR:N	2.51	0.44
3:D:141:LYS:HB3	3:D:172:TYR:CG	2.53	0.44
1:A:99:LYS:CG	1:A:100:TYR:CE1	3.01	0.43
1:A:53:PHE:O	1:A:57:VAL:HG23	2.18	0.43
1:B:100:TYR:N	1:B:100:TYR:CD1	2.86	0.43
1:B:148:GLU:O	1:B:152:VAL:HG23	2.17	0.43
1:B:267:PRO:O	1:B:270:ASN:CB	2.61	0.43
2:C:106:TRP:N	2:C:106:TRP:CD1	2.86	0.43
1:A:229:TYR:CE1	1:A:233:ASN:ND2	2.86	0.43
1:A:21:LEU:HD11	1:B:117:GLU:OE2	2.18	0.43
2:C:105:TYR:CD1	2:C:105:TYR:N	2.85	0.43
3:D:145:VAL:HA	3:D:194:GLU:O	2.18	0.43
3:F:149:ILE:HD11	3:F:178:LEU:HD21	2.00	0.43
1:A:183:ALA:O	1:A:184:ALA:C	2.55	0.43
1:A:94:TYR:CE1	1:A:295:GLY:HA3	2.53	0.43
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.54	0.43
1:A:451:ARG:HH11	1:A:451:ARG:CB	2.31	0.43
1:B:75:TYR:HB3	1:B:76:PRO:CD	2.38	0.43
2:C:139:ALA:O	2:C:141:ALA:N	2.52	0.43
2:C:156:GLU:HG2	2:C:183:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:TRP:H	2:E:106:TRP:HD1	1.66	0.43
1:A:109:ILE:N	1:A:110:PRO:CD	2.81	0.43
1:A:198:LEU:HD12	1:A:406:LEU:HG	2.01	0.43
1:A:393:GLY:O	1:A:394:MET:C	2.57	0.43
1:B:153:GLN:C	1:B:155:GLY:N	2.69	0.43
1:B:417:ASP:O	1:B:417:ASP:OD2	2.36	0.43
2:C:105:TYR:HD2	3:D:91:SER:HA	1.84	0.43
1:A:128:LEU:HB2	1:A:129:PRO:HD3	2.01	0.43
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.35	0.43
2:C:33:TRP:CZ2	2:C:52:ASN:HB3	2.53	0.43
3:D:127:GLY:O	3:D:182:LYS:N	2.45	0.43
1:A:406:LEU:HD13	1:B:219:PHE:HZ	1.80	0.43
1:B:381:GLN:H	1:B:381:GLN:HE21	0.67	0.43
2:E:221:ARG:NH1	3:F:118:PRO:HD2	2.33	0.43
1:B:420:GLN:H	1:B:420:GLN:HG3	1.38	0.43
3:F:185:TYR:HA	3:F:191:TYR:OH	2.19	0.43
1:B:91:MET:C	1:B:93:GLY:N	2.72	0.43
2:C:106:TRP:H	2:C:106:TRP:HD1	1.67	0.43
3:D:90:TRP:CE3	3:D:95:GLN:HG3	2.53	0.43
1:A:38:MET:O	1:A:41:VAL:HG12	2.19	0.43
1:B:393:GLY:O	1:B:396:ALA:N	2.35	0.43
2:E:29:TYR:CD2	2:E:77:ASP:HA	2.54	0.43
1:A:422:ILE:CG2	1:A:423:LEU:N	2.82	0.42
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.54	0.42
1:B:222:VAL:O	1:B:223:ILE:C	2.55	0.42
1:B:374:VAL:O	1:B:378:LEU:HG	2.19	0.42
3:D:184:GLU:O	3:D:187:ARG:HG2	2.19	0.42
1:B:270:ASN:HA	1:B:273:VAL:HG12	1.99	0.42
1:B:98:ARG:CD	1:B:291:TRP:CE3	2.94	0.42
1:B:313:SER:OG	1:B:314:GLY:N	2.52	0.42
1:B:38:MET:HG3	1:B:168:LEU:CD1	2.39	0.42
1:B:45:LEU:O	1:B:46:VAL:C	2.55	0.42
2:C:98:ARG:HD3	2:C:109:ASP:OD2	2.20	0.42
3:F:7:SER:CB	3:F:8:PRO:CD	2.95	0.42
1:B:284:HIS:CB	1:B:290:LYS:HB2	2.49	0.42
1:B:444:LEU:O	1:B:444:LEU:HD13	2.20	0.42
1:A:91:MET:O	1:A:92:PHE:C	2.57	0.42
1:B:127:VAL:O	1:B:128:LEU:C	2.57	0.42
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.54	0.42
1:B:114:GLY:O	1:B:117:GLU:N	2.51	0.42
1:B:409:ILE:HD13	1:B:426:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:18:LEU:H	2:E:18:LEU:HD23	1.84	0.42
1:A:180:THR:HG22	1:A:218:VAL:CA	2.44	0.42
1:A:54:ASP:OD1	1:A:147:ARG:NH2	2.48	0.42
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.35	0.42
1:B:212:LEU:CD1	1:B:212:LEU:N	2.83	0.42
1:B:223:ILE:CG2	1:B:224:MET:N	2.81	0.42
1:B:78:LEU:HD13	1:B:79:LEU:N	2.35	0.42
2:C:22:CYS:HB3	2:C:79:LEU:HB3	2.02	0.42
1:A:216:LYS:HE2	1:B:433:THR:CG2	2.50	0.42
1:A:253:TRP:O	1:A:256:LEU:HB3	2.20	0.42
1:A:270:ASN:HA	1:A:273:VAL:CG1	2.49	0.42
1:B:151:THR:O	1:B:152:VAL:C	2.57	0.42
1:B:385:GLU:O	1:B:386:ALA:C	2.58	0.42
1:A:381:GLN:HB3	3:D:93:HIS:HB2	2.01	0.42
2:E:104:GLY:O	2:E:106:TRP:HD1	2.02	0.42
2:E:71:SER:O	2:E:79:LEU:HD12	2.20	0.42
1:B:155:GLY:HA3	1:B:181:GLY:O	2.19	0.42
1:B:372:GLY:O	1:B:375:ALA:N	2.53	0.42
3:F:2:ILE:O	3:F:96:THR:HG21	2.20	0.42
1:A:147:ARG:O	1:A:148:GLU:C	2.58	0.42
1:B:124:TRP:O	1:B:126:ARG:N	2.53	0.42
1:B:198:LEU:HD12	1:B:406:LEU:HG	2.01	0.42
1:B:84:LEU:O	1:B:88:VAL:HG23	2.19	0.42
2:C:12:VAL:HG11	2:C:18:LEU:HD13	2.01	0.42
2:E:113:ALA:HA	3:F:42:SER:OG	2.18	0.42
1:A:281:HIS:O	1:A:285:GLY:N	2.53	0.41
1:A:62:ASN:O	1:A:65:MET:N	2.53	0.41
1:B:241:VAL:O	1:B:241:VAL:HG12	2.20	0.41
1:B:341:VAL:O	1:B:345:LEU:HG	2.20	0.41
1:B:379:PHE:CA	1:B:381:GLN:HE22	2.31	0.41
2:E:12:VAL:O	2:E:119:VAL:HA	2.20	0.41
1:A:124:TRP:C	1:A:126:ARG:N	2.73	0.41
1:A:320:ILE:HB	1:A:321:PRO:CD	2.45	0.41
1:B:278:ASP:O	1:B:281:HIS:N	2.40	0.41
2:C:122:ALA:HB1	2:C:181:ALA:HB1	2.01	0.41
3:D:22:THR:CG2	3:D:23:CYS:N	2.83	0.41
3:D:2:ILE:O	3:D:96:THR:HG21	2.20	0.41
2:E:139:ALA:O	2:E:141:ALA:N	2.53	0.41
2:E:127:PRO:CA	2:E:153:TYR:HB3	2.50	0.41
1:A:28:ARG:HB2	1:B:208:PHE:CZ	2.54	0.41
1:A:68:LEU:HD13	1:A:307:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HH22	1:B:102:PRO:HB3	1.85	0.41
1:B:60:LEU:HD12	1:B:136:LEU:O	2.19	0.41
2:C:64:LEU:H	2:C:64:LEU:HG	1.52	0.41
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.85	0.41
1:A:101:ALA:N	1:A:102:PRO:HD3	2.36	0.41
1:A:224:MET:O	1:A:228:MET:HG2	2.20	0.41
1:A:56:GLY:O	1:A:57:VAL:C	2.59	0.41
1:A:83:PHE:C	1:A:83:PHE:CD1	2.93	0.41
2:E:105:TYR:HD2	3:F:91:SER:HA	1.85	0.41
1:B:109:ILE:N	1:B:110:PRO:CD	2.83	0.41
1:B:197:ILE:HD11	1:B:219:PHE:HA	2.02	0.41
1:B:83:PHE:CD1	1:B:83:PHE:C	2.93	0.41
2:C:177:VAL:HG21	3:D:159:LEU:HD13	2.01	0.41
1:A:270:ASN:O	1:A:273:VAL:CG1	2.69	0.41
1:B:143:MET:HE2	1:B:347:CYS:HB3	2.02	0.41
1:B:274:LEU:O	1:B:277:GLN:HB2	2.20	0.41
1:B:91:MET:HG2	1:B:292:VAL:O	2.20	0.41
1:A:216:LYS:NZ	1:B:433:THR:HG22	2.33	0.41
3:D:11:MET:CE	3:D:19:VAL:HG13	2.50	0.41
2:E:69:ILE:HG22	2:E:69:ILE:O	2.19	0.41
1:A:448:ILE:HG21	4:A:1:BR:BR	2.75	0.41
1:A:225:SER:O	1:A:226:THR:C	2.58	0.41
1:A:409:ILE:HD13	1:A:426:ILE:HA	2.00	0.41
1:B:101:ALA:HB3	1:B:130:VAL:HG11	2.03	0.41
1:B:122:VAL:HG11	1:B:160:ARG:HB2	2.03	0.41
1:B:193:PRO:O	1:B:194:LEU:C	2.59	0.41
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.36	0.41
3:D:124:LEU:O	3:D:182:LYS:HD2	2.21	0.41
1:A:284:HIS:CB	1:A:290:LYS:HB2	2.51	0.41
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.54	0.41
1:A:194:LEU:HD13	1:B:410:ILE:HD11	2.03	0.41
1:A:437:GLN:NE2	1:B:31:THR:H	2.18	0.41
1:B:56:GLY:O	1:B:57:VAL:C	2.58	0.41
2:C:33:TRP:CH2	2:C:52:ASN:HB3	2.56	0.41
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.19	0.41
3:F:13:ALA:CB	3:F:77:MET:HE3	2.40	0.41
1:A:17:ARG:O	1:A:20:GLN:HB3	2.20	0.41
1:A:62:ASN:O	1:A:63:GLN:C	2.58	0.41
1:B:148:GLU:O	1:B:149:GLY:C	2.59	0.41
1:B:380:PRO:CD	1:B:381:GLN:NE2	2.84	0.41
1:B:92:PHE:CD1	1:B:92:PHE:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:38:LYS:HB2	3:D:41:THR:CG2	2.51	0.41
2:E:86:VAL:HG12	2:E:119:VAL:HG13	2.01	0.41
1:A:153:GLN:O	1:A:154:ILE:C	2.59	0.41
1:A:372:GLY:O	1:A:375:ALA:N	2.54	0.41
1:A:377:GLU:HG3	1:A:378:LEU:N	2.35	0.41
1:A:422:ILE:HA	1:A:422:ILE:HD12	1.86	0.41
1:B:307:PHE:CD2	1:B:307:PHE:O	2.74	0.41
2:C:18:LEU:HD23	2:C:18:LEU:H	1.85	0.41
2:C:36:TRP:HE1	2:C:79:LEU:HG	1.85	0.41
2:E:70:ILE:HG12	2:E:81:LEU:HD13	2.03	0.41
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.95	0.41
1:B:19:ARG:HA	1:B:19:ARG:HD2	1.92	0.40
1:B:381:GLN:N	1:B:381:GLN:NE2	2.31	0.40
3:F:114:VAL:HA	3:F:134:PHE:O	2.20	0.40
3:F:210:ARG:HG2	3:F:210:ARG:HH11	1.85	0.40
3:F:38:LYS:HB2	3:F:41:THR:CG2	2.51	0.40
1:A:216:LYS:HD3	1:B:434:LEU:CD2	2.50	0.40
1:B:320:ILE:O	1:B:321:PRO:C	2.60	0.40
2:C:43:LYS:NZ	2:C:43:LYS:HB3	2.36	0.40
2:E:178:LEU:HB2	2:E:183:TYR:CE2	2.56	0.40
1:A:235:GLU:O	1:A:236:VAL:CG2	2.69	0.40
1:A:241:VAL:CG1	1:A:241:VAL:O	2.67	0.40
1:B:281:HIS:O	1:B:285:GLY:N	2.53	0.40
1:B:148:GLU:CD	1:B:357:PHE:HB3	2.42	0.40
1:B:91:MET:O	1:B:92:PHE:C	2.59	0.40
3:D:12:SER:HB3	3:D:106:LEU:HB2	2.03	0.40
1:A:267:PRO:O	1:A:270:ASN:CB	2.61	0.40
1:A:348:PHE:O	1:A:351:GLY:N	2.46	0.40
2:C:130:TYR:HB3	3:D:120:SER:OG	2.21	0.40
3:D:179:THR:O	3:D:180:LEU:HD23	2.21	0.40
1:A:124:TRP:C	1:A:126:ARG:H	2.23	0.40
1:A:232:PHE:N	1:A:232:PHE:CD1	2.89	0.40
1:A:344:THR:O	1:A:345:LEU:C	2.59	0.40
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.37	0.40
2:E:144:VAL:O	2:E:144:VAL:CG1	2.69	0.40
2:E:51:ILE:HG13	2:E:58:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/444 (100%)	345 (78%)	80 (18%)	17 (4%)	4	24
1	B	439/444 (99%)	323 (74%)	89 (20%)	27 (6%)	2	13
2	C	219/221 (99%)	198 (90%)	16 (7%)	5 (2%)	7	36
2	E	219/221 (99%)	195 (89%)	17 (8%)	7 (3%)	5	29
3	D	209/211 (99%)	186 (89%)	15 (7%)	8 (4%)	4	24
3	F	209/211 (99%)	189 (90%)	18 (9%)	2 (1%)	18	53
All	All	1737/1752 (99%)	1436 (83%)	235 (14%)	66 (4%)	4	24

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	107	SER
1	A	307	PHE
1	A	309	ALA
1	B	188	ALA
1	B	309	ALA
1	B	414	GLU
2	C	140	ALA
3	D	7	SER
3	D	139	TYR
3	D	140	PRO
3	D	169	ASP
2	E	140	ALA
3	F	7	SER
1	A	236	VAL
1	A	314	GLY
1	A	414	GLU
1	B	74	ASN
1	B	107	SER
1	B	132	PHE

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Mol	Chain	Res	Type
1	B	223	ILE
1	B	236	VAL
1	B	307	PHE
1	B	314	GLY
1	B	387	GLY
1	B	394	MET
3	D	67	GLY
2	E	122	ALA
1	A	132	PHE
1	B	73	ASP
1	B	104	ALA
1	B	413	LEU
3	D	80	GLU
3	D	126	SER
1	A	73	ASP
1	A	188	ALA
1	A	201	ILE
1	A	443	PRO
1	A	458	ALA
1	B	245	SER
1	B	443	PRO
2	C	31	ARG
2	C	136	SER
2	E	31	ARG
3	F	126	SER
1	A	223	ILE
1	B	96	LEU
1	B	206	PRO
2	C	109	ASP
2	E	65	LYS
2	E	136	SER
1	A	50	ALA
1	B	101	ALA
1	B	128	LEU
1	B	376	VAL
1	B	140	GLY
1	B	144	VAL
1	B	283	VAL
2	E	62	PRO
1	A	149	GLY
1	B	201	ILE
3	D	105	ILE

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Mol	Chain	Res	Type
1	A	206	PRO
1	B	405	PRO
2	C	157	PRO
2	E	157	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/335 (100%)	316 (94%)	19 (6%)	24	60
1	B	332/335 (99%)	306 (92%)	26 (8%)	15	46
2	C	181/181 (100%)	176 (97%)	5 (3%)	49	76
2	E	181/181 (100%)	174 (96%)	7 (4%)	37	70
3	D	185/185 (100%)	181 (98%)	4 (2%)	57	80
3	F	185/185 (100%)	177 (96%)	8 (4%)	33	68
All	All	1399/1402 (100%)	1330 (95%)	69 (5%)	29	65

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	MET
1	A	70	HIS
1	A	73	ASP
1	A	74	ASN
1	A	78	LEU
1	A	103	GLU
1	A	119	GLN
1	A	198	LEU
1	A	270	ASN
1	A	319	LEU
1	A	324	THR
1	A	340	ARG
1	A	357	PHE
1	A	379	PHE

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Mol	Chain	Res	Type
1	A	381	GLN
1	A	420	GLN
1	A	435	LEU
1	A	445	GLU
1	A	451	ARG
1	B	70	HIS
1	B	73	ASP
1	B	74	ASN
1	B	78	LEU
1	B	100	TYR
1	B	103	GLU
1	B	119	GLN
1	B	177	LEU
1	B	198	LEU
1	B	206	PRO
1	B	207	GLN
1	B	244	LEU
1	B	270	ASN
1	B	319	LEU
1	B	321	PRO
1	B	324	THR
1	B	340	ARG
1	B	356	ILE
1	B	373	MET
1	B	379	PHE
1	B	381	GLN
1	B	397	LEU
1	B	420	GLN
1	B	445	GLU
1	B	451	ARG
1	B	457	GLU
2	C	66	ASP
2	C	151	LYS
2	C	155	PRO
2	C	203	CYS
2	C	204	ASN
3	D	46	TRP
3	D	81	ASP
3	D	95	GLN
3	D	189	ASN
2	E	107	TYR
2	E	111	TRP

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Mol	Chain	Res	Type
2	E	151	LYS
2	E	157	PRO
2	E	185	LEU
2	E	203	CYS
2	E	204	ASN
3	F	15	PRO
3	F	17	ASP
3	F	60	ARG
3	F	69	SER
3	F	95	GLN
3	F	167	SER
3	F	168	LYS
3	F	189	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	74	ASN
1	A	119	GLN
1	A	153	GLN
1	A	157	ASN
1	A	207	GLN
1	A	234	HIS
1	A	270	ASN
1	A	277	GLN
1	A	287	ASN
1	A	327	ASN
1	A	381	GLN
1	A	437	GLN
1	B	62	ASN
1	B	74	ASN
1	B	153	GLN
1	B	157	ASN
1	B	207	GLN
1	B	234	HIS
1	B	270	ASN
1	B	277	GLN
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	383	HIS

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Mol	Chain	Res	Type
1	B	437	GLN
2	C	172	HIS
3	D	6	GLN
3	D	36	GLN
3	D	136	ASN
3	D	137	ASN
3	D	189	ASN
2	E	39	GLN
2	E	172	HIS
3	F	6	GLN
3	F	36	GLN
3	F	37	GLN
3	F	89	GLN
3	F	136	ASN
3	F	137	ASN
3	F	189	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	444/444 (100%)	-0.28	6 (1%) 75 73	65, 122, 172, 202	0
1	B	441/444 (99%)	-0.21	9 (2%) 65 63	62, 128, 180, 208	0
2	C	221/221 (100%)	0.12	17 (7%) 14 13	64, 119, 179, 208	0
2	E	221/221 (100%)	0.13	10 (4%) 34 32	65, 119, 176, 203	0
3	D	211/211 (100%)	0.34	15 (7%) 17 17	71, 146, 190, 208	0
3	F	211/211 (100%)	0.07	7 (3%) 47 44	57, 115, 171, 208	0
All	All	1749/1752 (99%)	-0.04	64 (3%) 42 38	57, 125, 180, 208	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	35	SER	8.3
3	D	87	CYS	4.8
3	D	133	CYS	4.1
2	E	148	CYS	3.8
1	B	235	GLU	3.7
2	C	139	ALA	3.6
2	C	166	SER	3.5
2	E	96	CYS	3.5
3	D	115	SER	3.5
1	B	73	ASP	3.4
2	C	136	SER	3.3
2	C	165	GLY	3.2
3	F	87	CYS	3.2
3	D	1	ASP	3.2
2	C	137	ALA	3.1
2	C	65	LYS	3.1
3	D	86	TYR	3.1
2	E	95	TYR	3.0
1	B	18	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	113	ALA	3.0
3	D	39	SER	2.9
2	C	96	CYS	2.9
2	C	135	GLY	2.9
1	A	72	ALA	2.9
3	D	27	SER	2.9
2	E	147	GLY	2.8
2	C	138	ALA	2.8
1	A	364	GLY	2.8
1	A	29	ASP	2.8
2	C	140	ALA	2.7
2	C	196	TRP	2.7
3	D	148	LYS	2.7
1	A	17	ARG	2.7
3	D	88	GLN	2.6
3	D	153	GLU	2.5
1	A	460	GLN	2.5
3	F	33	HIS	2.4
2	E	181	ALA	2.4
2	C	35	SER	2.4
2	E	14	PRO	2.4
1	B	440	GLY	2.4
2	E	82	GLN	2.4
2	E	65	LYS	2.3
1	A	18	ARG	2.3
3	D	40	GLY	2.3
3	F	155	GLN	2.3
3	F	86	TYR	2.3
1	B	279	LEU	2.3
3	F	85	TYR	2.3
3	F	34	TRP	2.2
2	C	175	PRO	2.2
1	B	157	ASN	2.2
2	C	29	TYR	2.2
3	D	177	THR	2.2
2	C	164	SER	2.2
1	B	240	ASP	2.2
1	B	332	MET	2.1
3	D	9	ALA	2.1
1	B	72	ALA	2.1
2	C	98	ARG	2.1
2	E	222	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	156	ASN	2.0
3	D	79	ALA	2.0
3	D	118	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	BR	A	1	1/1	0.83	0.92	12.85	76,76,76,76	0
4	BR	B	2	1/1	0.90	0.43	3.80	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.