



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:03 am GMT

PDB ID : 5AA5  
Title : Actinobacterial-type NiFe-hydrogenase from *Ralstonia eutropha* H16 at 2.85 Angstrom resolution  
Authors : Schaefer, C.; Bommer, M.; Hennig, S.; Jeoung, J.H.; Dobbek, H.; Lenz, O.  
Deposited on : 2015-07-23  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

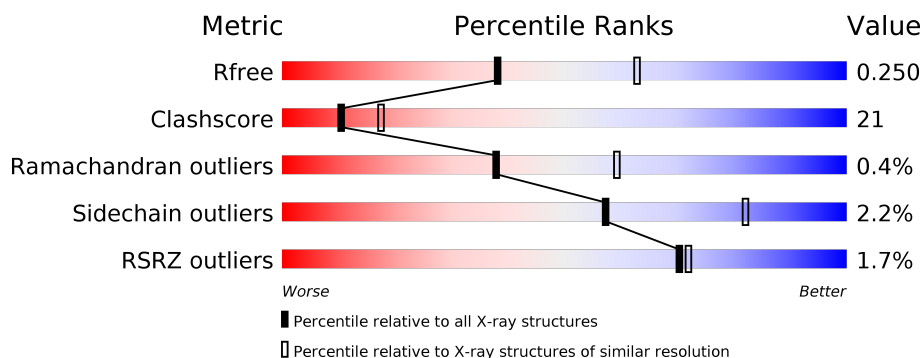
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	351	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>..</div> </div> </div>
1	B	351	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>33%</div> <div>..</div> </div> </div>
1	D	351	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>..</div> </div> </div>
1	F	351	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>33%</div> <div>..</div> </div> </div>
1	H	351	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>36%</div> <div>..</div> </div> </div>
1	M	351	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>32%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	C	579	
2	E	579	
2	G	579	
2	I	579	
2	K	579	
2	L	579	

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
3	SF4	B	501	-	-	-	X
3	SF4	M	702	-	-	X	-
4	MLA	A	505	-	-	-	X
5	NFU	C	701	-	-	X	-
5	NFU	E	701	-	-	X	-
5	NFU	I	701	-	-	X	-
5	NFU	L	701	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42867 atoms, of which 2 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.

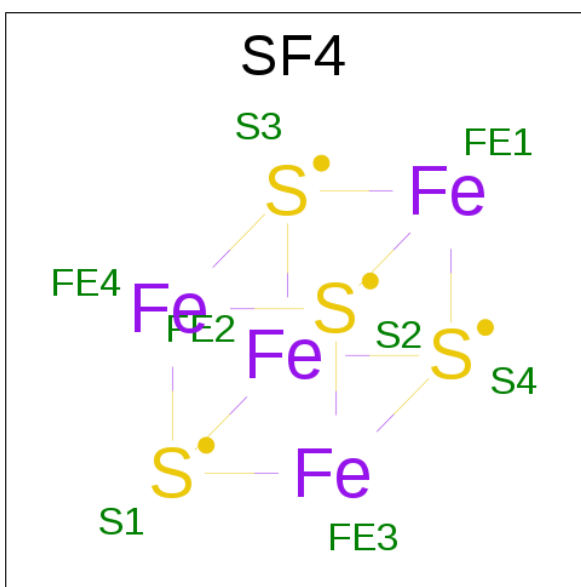
- Molecule 1 is a protein called NIFE-HYDROGENASE SMALL SUBUNIT, HOFK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			
1	B	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			
1	D	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			
1	F	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			
1	H	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			
1	M	345	Total	C	N	O	S	0	0	0
			2616	1676	447	473	20			

- Molecule 2 is a protein called NIFE-HYDROGENASE LARGE SUBUNIT, HOFG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	561	Total	C	N	O	S	0	0	0
			4495	2875	775	819	26			
2	E	559	Total	C	N	O	S	0	0	0
			4478	2863	772	817	26			
2	G	561	Total	C	N	O	S	0	0	0
			4495	2875	775	819	26			
2	I	560	Total	C	N	O	S	0	0	0
			4486	2869	773	818	26			
2	K	561	Total	C	N	O	S	0	0	0
			4495	2875	775	819	26			
2	L	560	Total	C	N	O	S	0	0	0
			4486	2869	773	818	26			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



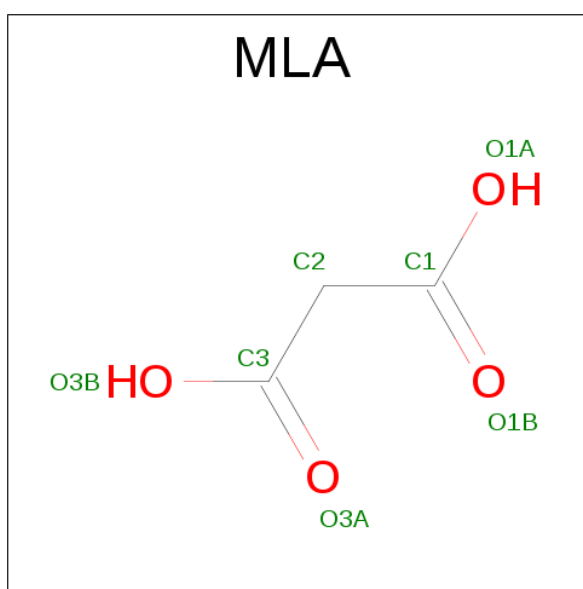
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		
3	H	1	Total	Fe	S	0	0
			8	4	4		
3	H	1	Total	Fe	S	0	0
			8	4	4		

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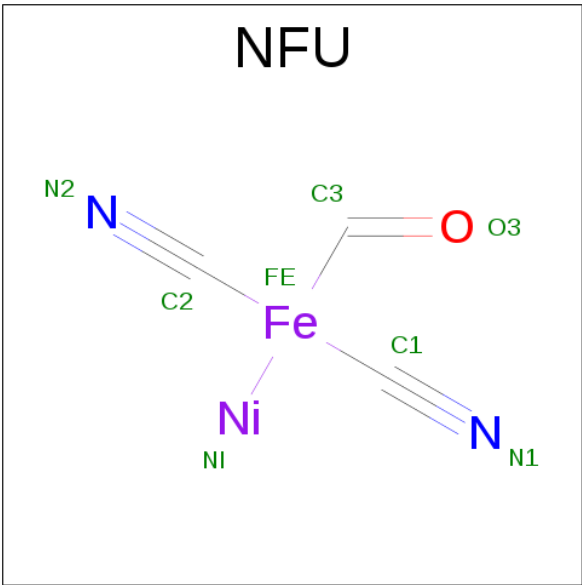
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is MALONIC ACID (three-letter code: MLA) (formula:  $C_3H_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			7	3	4			
4	A	1	Total	C	O		0	0
			7	3	4			
4	A	1	Total	C	H	O	0	0
			9	3	2	4		
4	D	1	Total	C	O		0	0
			7	3	4			
4	F	1	Total	C	O		0	0
			7	3	4			
4	M	1	Total	C	O		0	0
			7	3	4			

- Molecule 5 is FORMYL[BIS(HYDROCYANATO-1KAPPAC)]IRONNICKEL(Fe-Ni) (three-letter code: NFU) (formula:  $C_3HFeN_2NiO$ ).

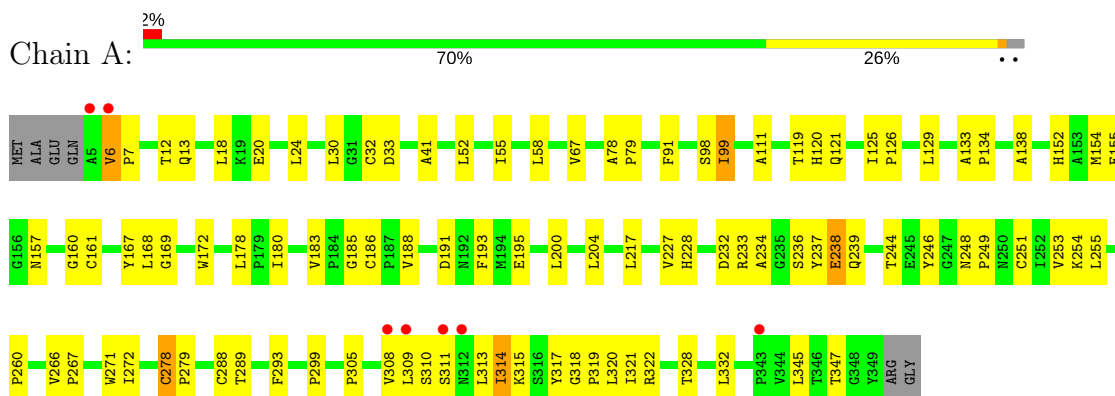


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
5	E	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
5	G	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
5	I	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
5	K	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		
5	L	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		

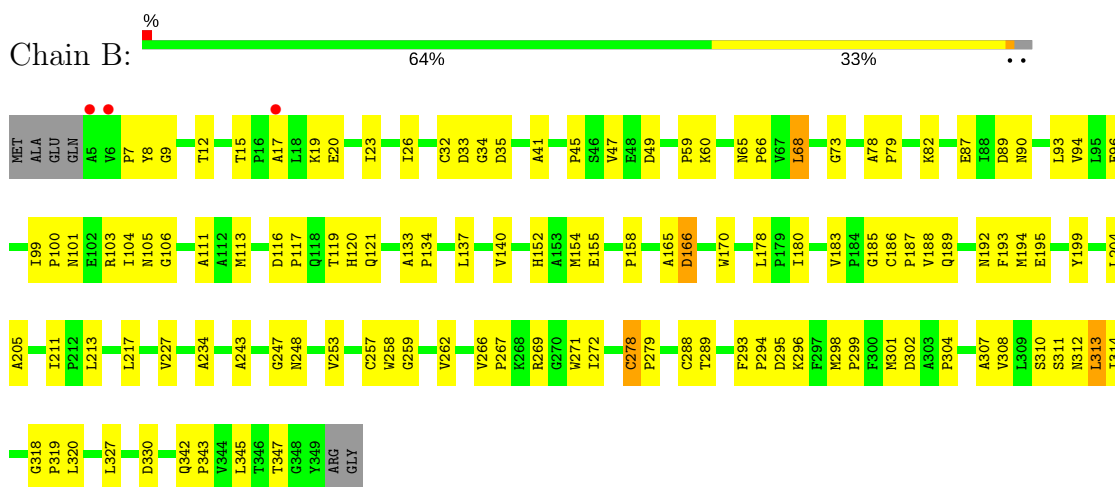
### 3 Residue-property plots

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.

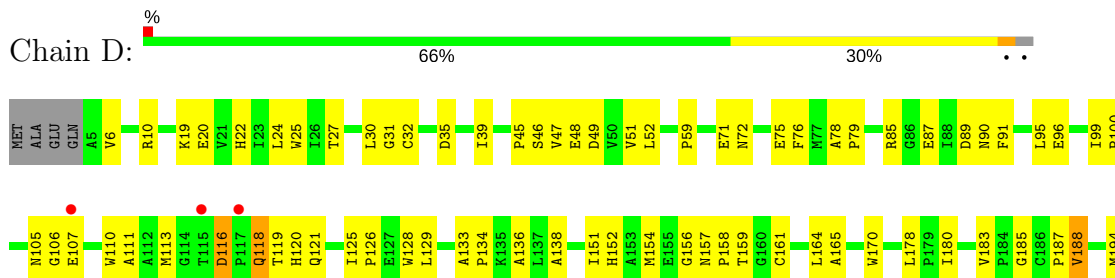
#### • Molecule 1: NIFE-HYDROGENASE SMALL SUBUNIT, HOFK



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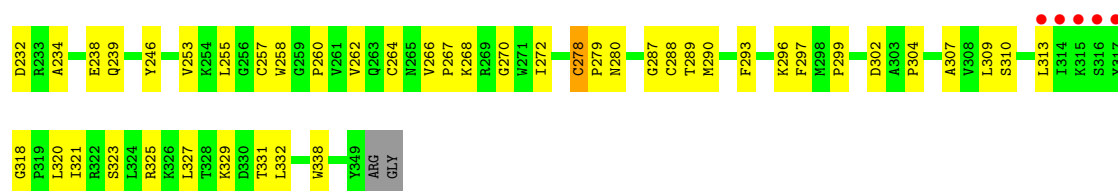


#### • Molecule 1: NIFE-HYDROGENASE SMALL SUBUNIT, HOFK

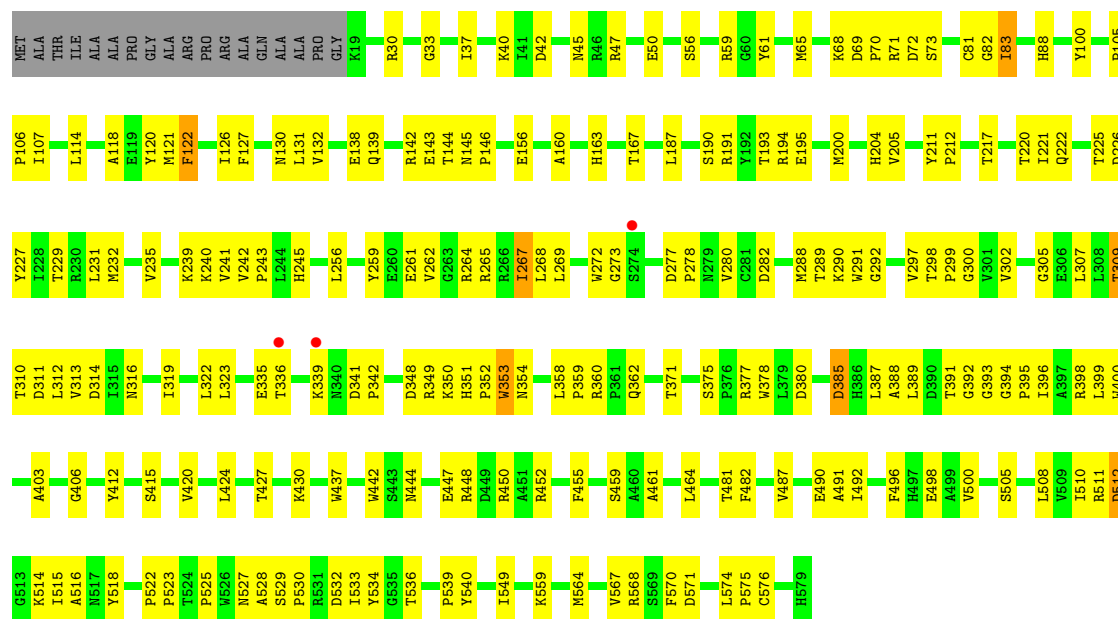




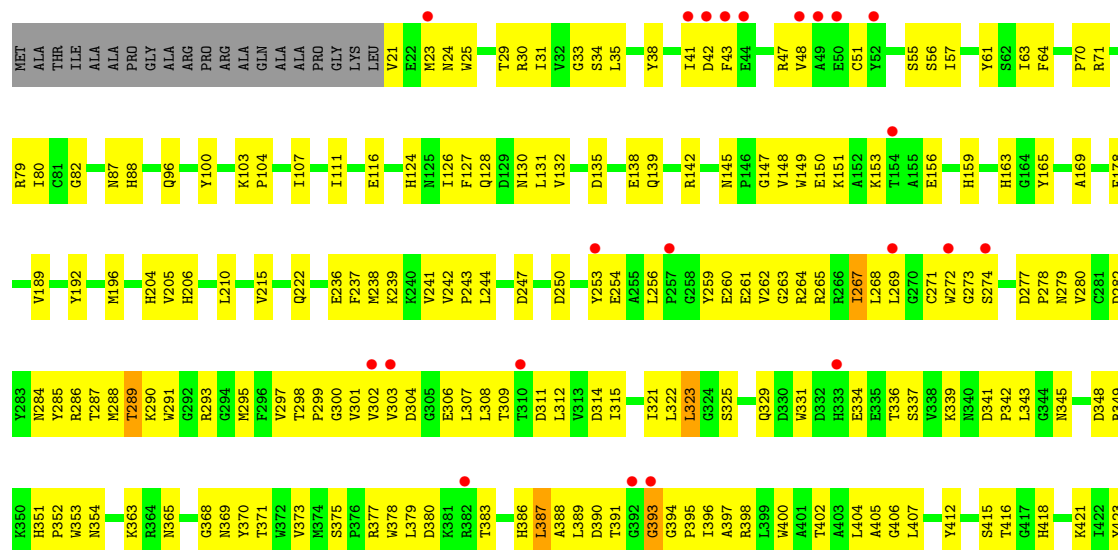


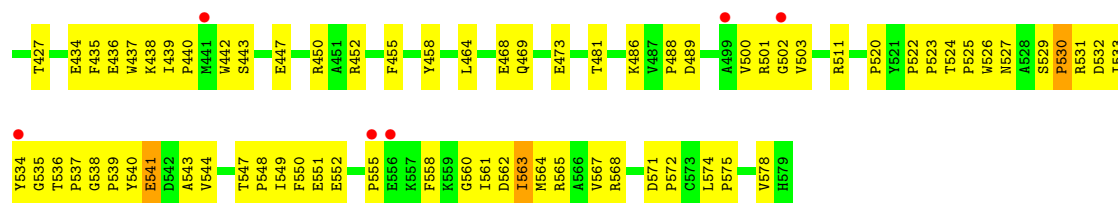


• Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG

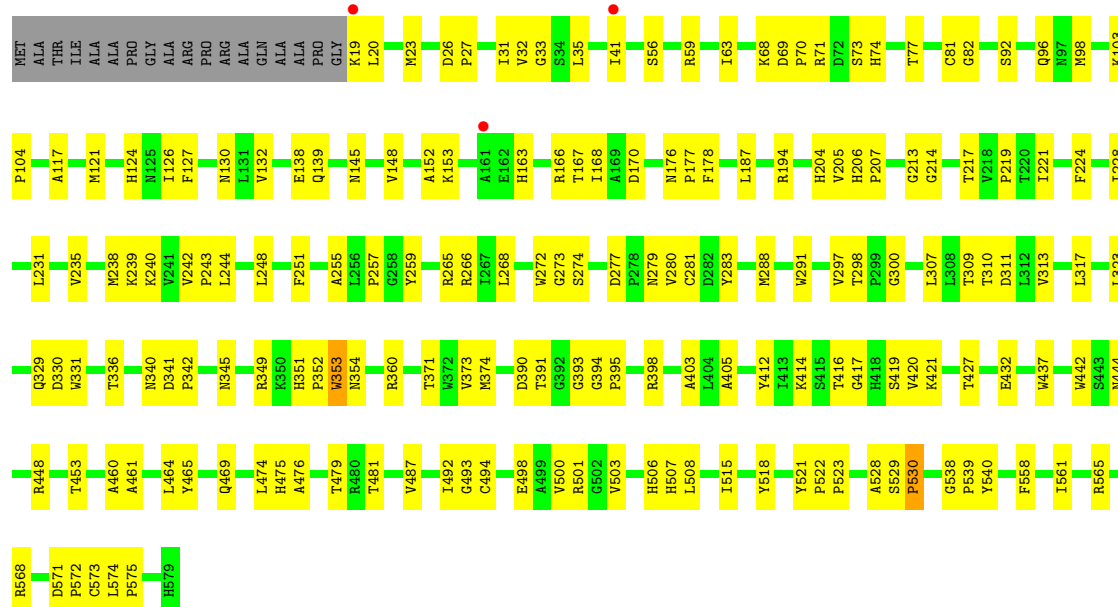


• Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG

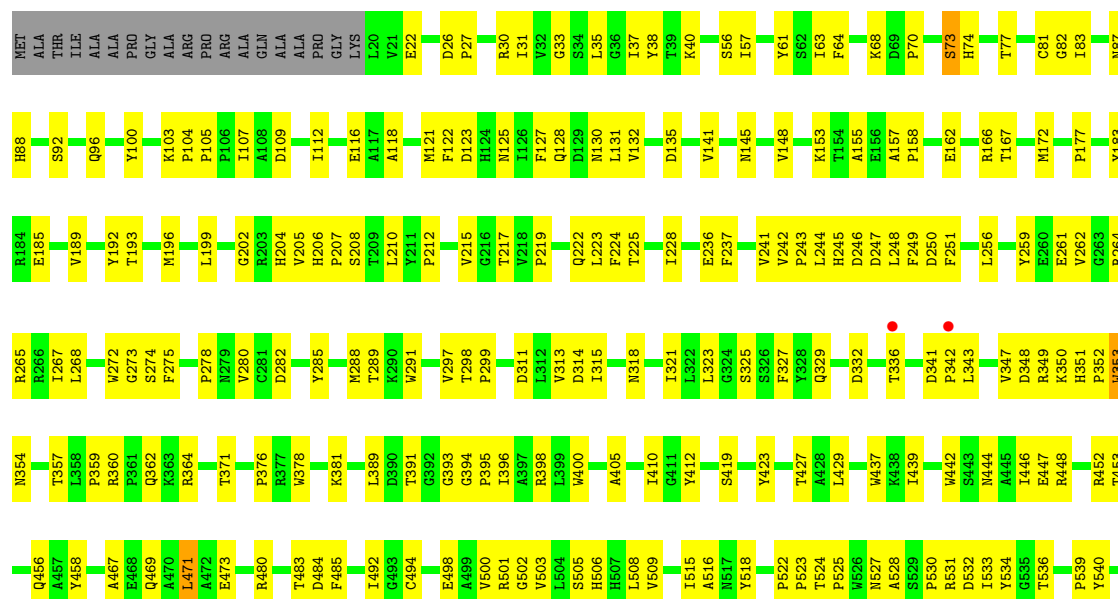




• Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG



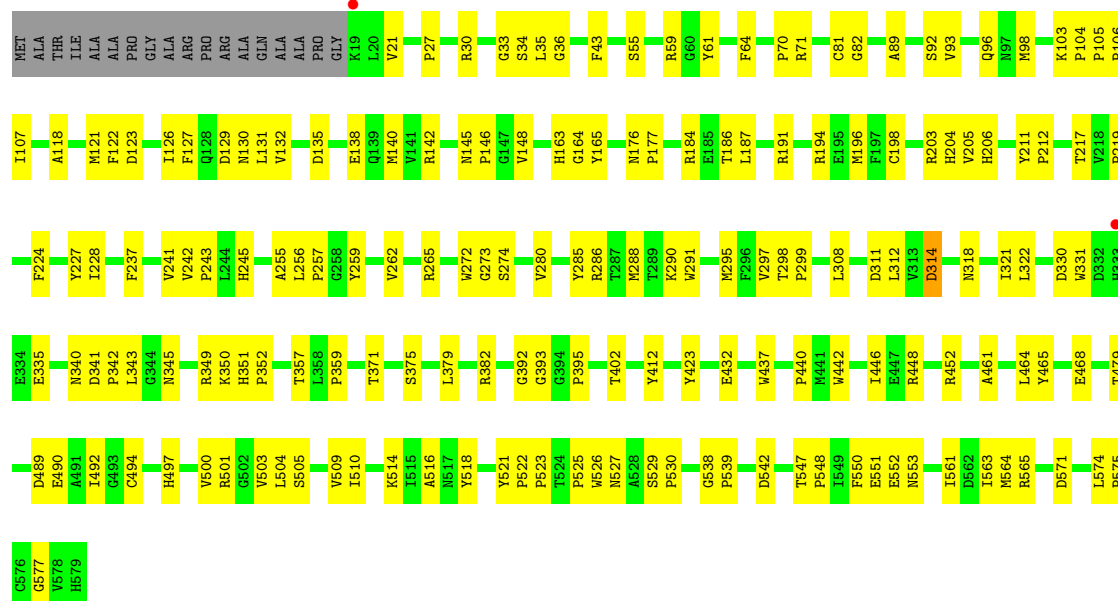
• Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG





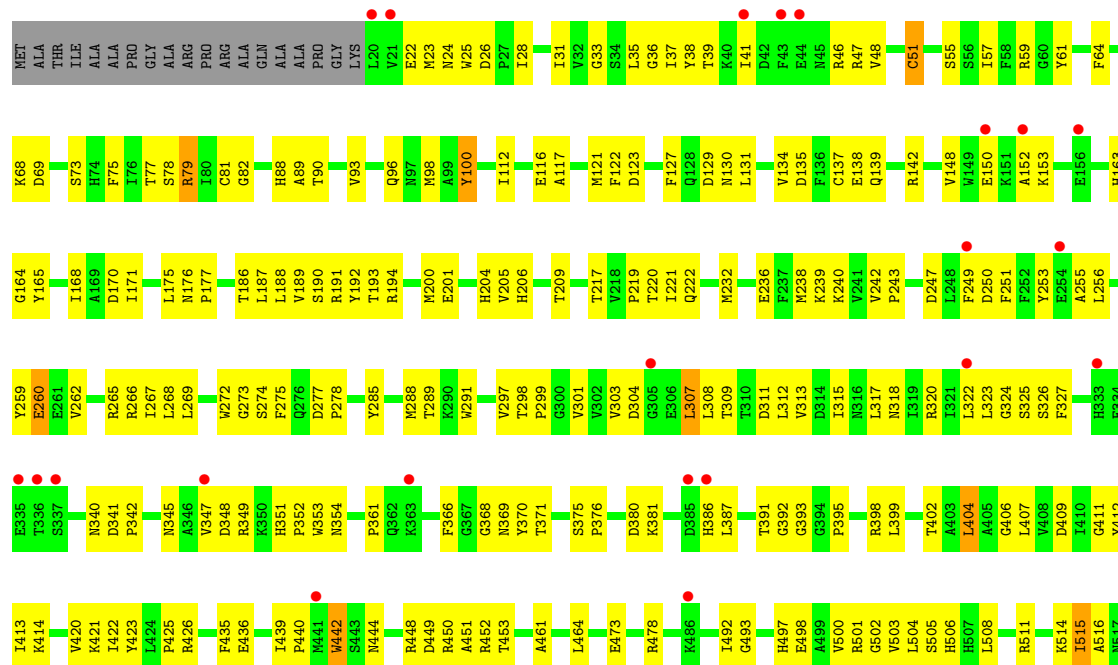
• Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG

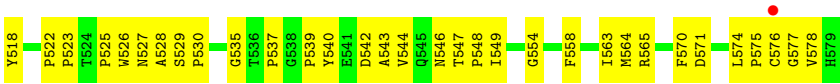
Chain K: 67% 30%



• Molecule 2: NIFE-HYDROGENASE LARGE SUBUNIT, HOFG

Chain L: 4% 54% 42%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.78Å 267.97Å 144.69Å 90.00° 106.58° 90.00°	Depositor
Resolution (Å)	45.97 – 2.50 48.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (45.97-2.50) 97.4 (48.18-2.50)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.187 , 0.242 0.201 , 0.250	Depositor DCC
$R_{free}$ test set	10023 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	42867	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: SF4, MLA, NFU

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	0.27	0/2694	0.46	0/3683
1	B	0.28	0/2694	0.48	0/3683
1	D	0.27	0/2694	0.47	0/3683
1	F	0.27	0/2694	0.45	0/3683
1	H	0.27	0/2694	0.45	0/3683
1	M	0.27	0/2694	0.45	0/3683
2	C	0.28	0/4629	0.44	0/6296
2	E	0.26	0/4612	0.46	0/6274
2	G	0.29	0/4629	0.47	0/6296
2	I	0.26	0/4620	0.43	0/6285
2	K	0.27	0/4629	0.44	0/6296
2	L	0.25	0/4620	0.42	0/6285
All	All	0.27	0/43903	0.45	0/59830

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2616	0	2571	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2616	0	2571	120	0
1	D	2616	0	2571	113	0
1	F	2616	0	2571	123	0
1	H	2616	0	2571	120	0
1	M	2616	0	2571	105	0
2	C	4495	0	4337	173	0
2	E	4478	0	4313	294	0
2	G	4495	0	4337	147	0
2	I	4486	0	4324	196	0
2	K	4495	0	4337	152	0
2	L	4486	0	4324	254	0
3	A	24	0	0	1	0
3	B	24	0	0	2	0
3	D	24	0	0	0	0
3	F	24	0	0	1	0
3	H	24	0	0	2	0
3	M	24	0	0	3	0
4	A	21	2	6	0	0
4	D	7	0	2	2	0
4	F	7	0	2	0	0
4	M	7	0	2	1	0
5	C	8	0	0	3	0
5	E	8	0	0	2	0
5	G	8	0	0	1	0
5	I	8	0	0	3	0
5	K	8	0	0	0	0
5	L	8	0	0	2	0
All	All	42865	2	41410	1740	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 21.

All (1740) 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)
2:C:392:GLY:HA2	2:C:396:ILE:HG22	1.31	1.11
2:L:39:THR:HG22	2:L:51:CYS:HB2	1.22	1.11
2:E:262:VAL:HG23	2:E:547:THR:HG23	1.30	1.08
1:A:234:ALA:HB3	1:F:234:ALA:HB3	1.35	1.06
2:C:280:VAL:HG23	2:C:290:LYS:HE3	1.34	1.06
2:I:105:PRO:HD3	2:I:483:THR:HG23	1.31	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:77:THR:HG21	2:L:506:HIS:HE1	1.22	1.02
2:L:77:THR:HG22	2:L:88:HIS:HB3	1.39	1.02
2:L:163:HIS:HB2	2:L:165:TYR:H	1.24	1.01
2:L:307:LEU:HG	2:L:404:LEU:HD13	1.43	0.99
2:C:220:THR:HG22	2:C:222:GLN:H	1.24	0.97
2:L:515:ILE:HD11	2:L:518:TYR:HB2	1.46	0.97
1:A:345:LEU:HD13	1:F:104:ILE:HD13	1.46	0.95
1:B:15:THR:HG21	1:B:19:LYS:HE2	1.49	0.94
2:E:286:ARG:HA	2:E:343:LEU:HD11	1.50	0.93
2:K:280:VAL:HG23	2:K:290:LYS:HE3	1.51	0.92
2:L:220:THR:HG22	2:L:222:GLN:H	1.29	0.92
2:L:412:TYR:HB3	2:L:461:ALA:HB1	1.52	0.92
1:M:227:VAL:HG13	1:M:267:PRO:HG3	1.48	0.91
2:E:267:ILE:HB	2:E:304:ASP:HB2	1.53	0.91
1:A:227:VAL:HG13	1:A:267:PRO:HG2	1.52	0.89
2:I:527:ASN:HA	2:I:539:PRO:HG2	1.51	0.89
2:L:33:GLY:HA3	2:L:575:PRO:HD3	1.52	0.88
2:L:148:VAL:HG13	2:L:255:ALA:HB1	1.56	0.88
2:C:70:PRO:HA	2:C:515:ILE:HD11	1.55	0.88
1:A:254:LYS:HE2	1:A:311:SER:HB2	1.54	0.88
2:I:311:ASP:HB3	2:I:314:ASP:HB2	1.56	0.87
2:E:238:MET:HE1	2:E:241:VAL:HB	1.57	0.87
2:L:301:VAL:HG23	2:L:308:LEU:HB2	1.56	0.87
1:F:313:LEU:HG	1:F:315:LYS:HG3	1.54	0.87
1:F:99:ILE:HD11	1:F:164:LEU:HD12	1.58	0.86
2:C:88:HIS:HE1	2:C:522:PRO:HG3	1.41	0.86
2:E:531:ARG:HG2	2:E:537:PRO:HA	1.58	0.85
2:I:88:HIS:HE1	2:I:522:PRO:HG3	1.41	0.85
1:B:308:VAL:O	1:B:312:ASN:ND2	2.10	0.85
1:D:59:PRO:HD3	1:D:205:ALA:HB2	1.57	0.85
1:H:77:MET:HE3	2:K:27:PRO:HD2	1.59	0.85
2:E:273:GLY:HA3	2:E:295:MET:HE3	1.59	0.84
1:H:178:LEU:HD11	1:H:203:GLN:HE22	1.41	0.84
1:B:158:PRO:HG3	2:G:63:ILE:HG21	1.57	0.83
2:E:145:ASN:HB3	2:E:148:VAL:HG23	1.59	0.83
2:E:242:VAL:HB	2:E:243:PRO:HD3	1.60	0.83
1:H:19:LYS:HG2	1:H:20:GLU:HG3	1.59	0.83
1:B:301:MET:HE3	2:G:71:ARG:HB3	1.61	0.83
1:F:188:VAL:HG21	1:F:193:PHE:HB2	1.58	0.83
2:E:527:ASN:HA	2:E:539:PRO:HB2	1.61	0.82
2:E:380:ASP:HB3	2:E:383:THR:HG22	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:163:HIS:HB2	2:L:165:TYR:N	1.93	0.82
2:C:265:ARG:NH2	2:C:388:ALA:O	2.13	0.82
1:H:278:CYS:HB2	1:H:279:PRO:HD3	1.61	0.82
1:B:347:THR:HG22	1:D:156:GLY:H	1.44	0.82
1:F:106:GLY:N	1:F:107:GLU:HB2	1.95	0.82
2:L:77:THR:HG21	2:L:506:HIS:CE1	2.13	0.81
2:E:312:LEU:HA	2:E:315:ILE:HG22	1.61	0.81
2:E:277:ASP:HB3	2:E:280:VAL:HG22	1.60	0.81
2:K:527:ASN:HA	2:K:539:PRO:HG2	1.62	0.81
1:M:77:MET:CE	1:M:113:MET:HG2	2.11	0.81
2:G:70:PRO:HA	2:G:515:ILE:HD11	1.61	0.81
2:I:22:GLU:HG2	2:I:40:LYS:HG2	1.63	0.81
1:A:314:ILE:HD11	1:H:316:SER:HB3	1.61	0.81
2:L:232:MET:HA	2:L:232:MET:HE2	1.60	0.81
2:L:268:LEU:HD23	2:L:303:VAL:HG12	1.62	0.80
2:C:316:ASN:HB2	2:C:496:PHE:CZ	2.16	0.80
2:C:220:THR:HG22	2:C:222:GLN:N	1.95	0.80
1:H:301:MET:HE2	2:K:71:ARG:HB3	1.62	0.80
2:C:118:ALA:HA	2:C:121:MET:HE3	1.62	0.79
1:M:185:GLY:HA2	1:M:289:THR:HG22	1.64	0.79
2:C:33:GLY:HA3	2:C:575:PRO:HD3	1.64	0.79
1:A:254:LYS:CE	1:A:311:SER:HB2	2.12	0.79
2:L:77:THR:CG2	2:L:88:HIS:HB3	2.12	0.79
1:A:278:CYS:HB2	1:A:279:PRO:CD	2.13	0.79
2:I:33:GLY:HA3	2:I:575:PRO:HD3	1.64	0.79
2:C:280:VAL:CG2	2:C:290:LYS:HE3	2.13	0.79
2:G:152:ALA:HB1	2:G:168:ILE:HG22	1.64	0.79
1:M:77:MET:HE1	1:M:113:MET:HG2	1.66	0.78
2:E:273:GLY:HA3	2:E:295:MET:CE	2.14	0.78
2:E:55:SER:OG	2:E:574:LEU:HD13	1.82	0.78
2:E:21:VAL:HG21	2:E:43:PHE:CE2	2.18	0.78
2:G:166:ARG:HG3	2:G:167:THR:HG23	1.64	0.78
2:E:323:LEU:HD21	2:E:331:TRP:CZ3	2.18	0.78
2:G:98:MET:HE2	2:G:494:CYS:N	2.00	0.77
1:M:15:THR:HG21	1:M:19:LYS:HE2	1.66	0.77
1:A:119:THR:HG22	1:A:121:GLN:HG3	1.66	0.77
2:L:163:HIS:CB	2:L:165:TYR:H	1.96	0.77
1:D:185:GLY:HA2	1:D:289:THR:HG22	1.66	0.77
2:K:98:MET:HE1	2:K:285:TYR:HD2	1.50	0.77
1:A:332:LEU:HD12	1:F:261:VAL:HG12	1.68	0.76
1:F:278:CYS:HB2	1:F:279:PRO:CD	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:288:MET:HA	2:I:291:TRP:CE2	2.20	0.76
2:E:33:GLY:HA3	2:E:575:PRO:HD3	1.67	0.76
2:G:33:GLY:HA3	2:G:575:PRO:HD3	1.65	0.76
2:K:280:VAL:CG2	2:K:290:LYS:HE3	2.15	0.76
2:K:280:VAL:HG22	2:K:291:TRP:HB3	1.67	0.76
2:L:307:LEU:CG	2:L:404:LEU:HD13	2.15	0.76
2:C:37:ILE:HD12	2:C:567:VAL:HG21	1.68	0.75
2:L:122:PHE:HB2	2:L:193:THR:HG23	1.66	0.75
2:K:163:HIS:HB2	2:K:165:TYR:H	1.51	0.75
2:E:371:THR:HG21	2:E:530:PRO:HG3	1.68	0.75
2:K:393:GLY:HA3	2:K:452:ARG:HH21	1.51	0.75
2:E:262:VAL:HG23	2:E:547:THR:CG2	2.14	0.74
2:E:301:VAL:HG13	2:E:389:LEU:HD21	1.68	0.74
2:I:480:ARG:HH22	2:I:483:THR:HG22	1.52	0.74
2:K:55:SER:HB2	2:K:574:LEU:HD23	1.69	0.74
2:C:360:ARG:O	2:C:362:GLN:HG3	1.87	0.74
1:F:82:LYS:HG2	1:F:87:GLU:HB2	1.68	0.74
1:D:227:VAL:HG13	1:D:267:PRO:HG2	1.70	0.74
2:E:298:THR:HG21	2:E:405:ALA:HB2	1.69	0.74
2:I:242:VAL:HB	2:I:243:PRO:HD3	1.70	0.74
2:L:220:THR:HG22	2:L:222:GLN:N	2.03	0.74
2:L:353:TRP:CH2	2:L:492:ILE:HG12	2.23	0.74
2:L:68:LYS:O	2:L:515:ILE:HG22	1.87	0.73
1:H:317:TYR:CE2	1:M:313:LEU:HG	2.23	0.73
2:G:266:ARG:HD3	2:G:268:LEU:HD21	1.69	0.73
1:A:30:LEU:HB2	1:A:98:SER:HB2	1.70	0.73
1:H:278:CYS:HB2	1:H:279:PRO:CD	2.18	0.73
2:K:322:LEU:HD23	2:K:350:LYS:HD3	1.71	0.73
1:F:39:ILE:HD12	1:F:194:MET:CE	2.19	0.73
1:A:328:THR:HG22	1:F:261:VAL:HG11	1.71	0.73
1:F:315:LYS:HB3	1:F:317:TYR:CE1	2.23	0.73
2:E:286:ARG:HB3	2:E:343:LEU:HD21	1.71	0.72
2:E:259:TYR:O	2:E:262:VAL:HG12	1.89	0.72
2:I:391:THR:HG21	2:I:523:PRO:HB3	1.71	0.72
2:K:273:GLY:HA3	2:K:295:MET:CE	2.20	0.72
2:G:19:LYS:HG2	2:G:20:LEU:H	1.54	0.72
1:B:12:THR:HG21	2:E:412:TYR:CZ	2.25	0.71
1:B:185:GLY:HA2	1:B:289:THR:HG22	1.72	0.71
2:L:262:VAL:HA	2:L:547:THR:HG23	1.72	0.71
2:C:122:PHE:HB2	2:C:193:THR:HG23	1.72	0.71
1:M:253:VAL:HA	1:M:257:CYS:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:88:HIS:CE1	2:I:522:PRO:HG3	2.24	0.71
2:G:98:MET:HE2	2:G:494:CYS:H	1.55	0.71
2:L:163:HIS:HB2	2:L:164:GLY:HA2	1.73	0.71
2:L:515:ILE:CD1	2:L:518:TYR:HB2	2.21	0.70
1:F:185:GLY:HA2	1:F:289:THR:HG22	1.71	0.70
1:H:185:GLY:HA2	1:H:289:THR:HG22	1.72	0.70
2:L:542:ASP:O	2:L:546:ASN:ND2	2.24	0.70
1:B:103:ARG:NH2	1:D:343:PRO:HG3	2.06	0.70
2:G:288:MET:HA	2:G:291:TRP:CE2	2.26	0.70
1:B:227:VAL:HG13	1:B:267:PRO:HG2	1.71	0.70
2:C:342:PRO:HD3	2:C:492:ILE:HD11	1.73	0.70
2:C:392:GLY:HA3	2:C:394:GLY:HA2	1.73	0.70
2:L:204:HIS:CG	2:L:205:VAL:HA	2.27	0.70
1:F:187:PRO:HD3	2:L:206:HIS:CD2	2.26	0.70
2:K:288:MET:HA	2:K:291:TRP:CE2	2.25	0.70
2:C:392:GLY:N	2:C:393:GLY:HA2	2.05	0.70
2:E:35:LEU:HB2	2:E:574:LEU:HD11	1.72	0.70
2:G:398:ARG:NH2	2:G:500:VAL:O	2.25	0.70
2:L:376:PRO:HG2	2:L:526:TRP:HA	1.72	0.70
2:L:259:TYR:CZ	2:L:262:VAL:HG21	2.27	0.69
2:L:88:HIS:CE1	2:L:522:PRO:HG3	2.27	0.69
2:L:35:LEU:HD13	2:L:574:LEU:HD21	1.74	0.69
1:A:345:LEU:HD13	1:F:104:ILE:CD1	2.19	0.69
1:F:318:GLY:O	1:F:321:ILE:HG22	1.91	0.69
2:E:48:VAL:HG23	2:E:549:ILE:HD11	1.73	0.69
2:L:288:MET:HE2	2:L:312:LEU:HB3	1.73	0.69
2:E:88:HIS:HE1	2:E:522:PRO:HG3	1.56	0.69
2:C:358:LEU:HB3	2:C:360:ARG:HH12	1.57	0.69
1:B:310:SER:HA	1:D:321:ILE:HD11	1.73	0.69
2:I:112:ILE:HD12	2:I:210:LEU:HD21	1.74	0.69
1:M:278:CYS:HB2	1:M:279:PRO:HD3	1.75	0.69
2:L:340:ASN:HA	2:L:347:VAL:HG23	1.75	0.69
1:D:32:CYS:HB2	2:E:82:GLY:N	2.07	0.69
1:H:41:ALA:HB2	2:K:194:ARG:NH1	2.08	0.69
2:E:523:PRO:HD2	5:E:701:NFU:N2	2.08	0.68
2:G:238:MET:HA	2:G:238:MET:HE2	1.74	0.68
1:F:254:LYS:HE2	1:F:311:SER:HB3	1.74	0.68
2:G:139:GLN:H	2:G:176:ASN:HD21	1.39	0.68
1:A:320:LEU:HD23	1:B:320:LEU:HD13	1.76	0.68
2:G:204:HIS:CG	2:G:205:VAL:HA	2.29	0.68
2:L:288:MET:HA	2:L:291:TRP:CE2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:242:PHE:HD2	1:H:254:LYS:HZ2	1.42	0.68
1:M:117:PRO:HB2	1:M:118:GLN:NE2	2.09	0.68
1:B:12:THR:HG21	2:E:412:TYR:CE2	2.29	0.68
1:D:105:ASN:HB3	1:D:106:GLY:HA3	1.76	0.68
2:E:127:PHE:HD1	2:E:131:LEU:HD12	1.59	0.68
2:E:42:ASP:HB3	2:E:47:ARG:HG2	1.75	0.68
1:F:315:LYS:HD2	1:F:317:TYR:HE1	1.58	0.68
2:G:98:MET:HE3	2:G:493:GLY:HA2	1.76	0.68
2:I:480:ARG:NH2	2:I:483:THR:HG22	2.08	0.67
1:D:71:GLU:HB3	1:D:75:GLU:HG3	1.75	0.67
2:E:523:PRO:HD2	5:E:701:NFU:C2	2.24	0.67
2:I:527:ASN:HA	2:I:539:PRO:CG	2.24	0.67
1:M:278:CYS:HB2	1:M:279:PRO:CD	2.24	0.67
1:H:301:MET:CE	2:K:71:ARG:HB3	2.23	0.67
1:A:278:CYS:HB2	1:A:279:PRO:HD3	1.73	0.67
1:B:119:THR:O	1:B:121:GLN:NE2	2.27	0.67
2:K:118:ALA:HA	2:K:121:MET:HE3	1.75	0.67
2:L:301:VAL:HG22	2:L:309:THR:HG22	1.77	0.67
1:H:332:LEU:HD22	1:M:297:PHE:CZ	2.29	0.67
2:E:548:PRO:C	2:E:549:ILE:HD12	2.15	0.67
2:E:25:TRP:HB2	2:E:564:MET:HE1	1.76	0.67
2:L:398:ARG:HE	2:L:498:GLU:HG2	1.59	0.67
2:C:88:HIS:CE1	2:C:522:PRO:HG3	2.27	0.67
2:E:297:VAL:HG11	2:E:398:ARG:HG2	1.77	0.67
2:K:98:MET:HE2	2:K:494:CYS:H	1.60	0.67
2:L:371:THR:HG21	2:L:530:PRO:HB3	1.77	0.67
1:H:338:TRP:CZ2	1:M:155:GLU:HB2	2.30	0.66
2:L:421:LYS:HG3	2:L:436:GLU:HG3	1.76	0.66
2:C:392:GLY:CA	2:C:394:GLY:HA2	2.25	0.66
1:D:30:LEU:HG	1:D:100:PRO:HG3	1.78	0.66
1:D:24:LEU:HD12	1:D:91:PHE:CD2	2.29	0.66
2:L:272:TRP:CD2	2:L:503:VAL:HB	2.30	0.66
2:E:242:VAL:HG11	2:E:435:PHE:CD1	2.30	0.66
1:B:342:GLN:HB3	1:B:343:PRO:HD2	1.77	0.66
2:C:392:GLY:N	2:C:394:GLY:HA2	2.11	0.66
2:E:371:THR:HG21	2:E:530:PRO:CG	2.26	0.66
1:F:32:CYS:HB2	2:L:81:CYS:HA	1.78	0.66
2:K:286:ARG:HG2	2:K:343:LEU:HD21	1.76	0.66
1:A:271:TRP:CD1	1:A:272:ILE:HG13	2.31	0.66
1:F:253:VAL:HA	1:F:257:CYS:HB3	1.76	0.66
2:I:87:ASN:ND2	2:I:116:GLU:OE1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:VAL:CG2	1:D:264:CYS:HB3	2.26	0.65
2:E:284:ASN:OD1	2:E:286:ARG:HG2	1.94	0.65
1:B:278:CYS:HB2	1:B:279:PRO:CD	2.26	0.65
1:H:338:TRP:CH2	1:M:155:GLU:HB2	2.31	0.65
2:C:358:LEU:HB3	2:C:360:ARG:NH1	2.10	0.65
2:L:163:HIS:HB2	2:L:164:GLY:CA	2.26	0.65
2:C:114:LEU:HD22	2:C:227:TYR:CE1	2.32	0.65
2:K:55:SER:CB	2:K:574:LEU:HD23	2.25	0.65
2:E:272:TRP:CD2	2:E:503:VAL:HB	2.31	0.65
2:E:35:LEU:CB	2:E:574:LEU:HD11	2.26	0.65
2:L:90:THR:O	2:L:93:VAL:HG22	1.96	0.65
2:E:288:MET:HA	2:E:291:TRP:CE2	2.31	0.65
2:E:288:MET:HE3	2:E:312:LEU:HB3	1.78	0.65
1:F:95:LEU:HD23	1:F:164:LEU:CD1	2.27	0.65
1:H:180:ILE:HB	1:H:217:LEU:HD13	1.79	0.65
2:L:23:MET:HG3	2:L:41:ILE:HD12	1.79	0.65
2:E:41:ILE:HG12	2:E:48:VAL:HG22	1.78	0.65
2:G:416:THR:H	2:G:417:GLY:HA2	1.62	0.65
1:H:119:THR:HG22	1:H:121:GLN:HB2	1.78	0.65
2:E:380:ASP:HB3	2:E:383:THR:CG2	2.26	0.65
2:I:64:PHE:O	2:I:68:LYS:NZ	2.30	0.65
2:K:423:TYR:OH	2:K:432:GLU:OE1	2.15	0.65
1:B:15:THR:CG2	1:B:19:LYS:HE2	2.26	0.64
2:C:288:MET:HA	2:C:291:TRP:CE2	2.32	0.64
1:A:314:ILE:HD11	1:H:316:SER:CB	2.27	0.64
2:L:163:HIS:O	2:L:240:LYS:HE3	1.97	0.64
2:L:168:ILE:CD1	2:L:251:PHE:HB2	2.27	0.64
1:M:30:LEU:HB2	1:M:98:SER:HB2	1.79	0.64
2:E:21:VAL:HG22	2:E:41:ILE:O	1.96	0.64
2:K:392:GLY:HA2	2:K:448:ARG:HD3	1.78	0.64
2:L:28:ILE:HD11	2:L:37:ILE:HG12	1.78	0.64
1:D:301:MET:CE	2:E:71:ARG:HB3	2.28	0.64
2:E:274:SER:HB3	2:E:297:VAL:HB	1.80	0.64
2:C:511:ARG:HB2	2:C:516:ALA:HB2	1.77	0.64
2:E:285:TYR:O	2:E:288:MET:HB3	1.98	0.64
2:I:342:PRO:HD3	2:I:492:ILE:HD11	1.80	0.64
1:B:119:THR:HG22	1:B:121:GLN:HE21	1.62	0.64
1:B:271:TRP:CD1	1:B:272:ILE:HG13	2.33	0.64
1:A:195:GLU:OE1	2:L:222:GLN:HG2	1.97	0.64
1:D:247:GLY:HA3	2:E:481:THR:CG2	2.28	0.64
2:E:268:LEU:HB3	2:E:389:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:273:GLY:HA3	2:K:295:MET:HE3	1.79	0.64
2:K:33:GLY:HA3	2:K:575:PRO:HD3	1.79	0.64
2:K:163:HIS:HB2	2:K:165:TYR:N	2.13	0.64
2:L:288:MET:HE2	2:L:312:LEU:CB	2.28	0.64
2:E:34:SER:C	2:E:574:LEU:HD12	2.19	0.63
2:K:318:ASN:ND2	2:K:379:LEU:O	2.32	0.63
2:I:522:PRO:HB3	5:I:701:NFU:C3	2.28	0.63
1:M:227:VAL:HG22	1:M:264:CYS:HB3	1.80	0.63
2:I:236:GLU:HB2	2:I:427:THR:HG21	1.80	0.63
2:E:259:TYR:CE1	2:E:262:VAL:HG11	2.33	0.63
2:L:88:HIS:HE1	2:L:522:PRO:HG3	1.64	0.63
2:G:391:THR:HG21	2:G:523:PRO:HB3	1.79	0.63
2:L:325:SER:HA	2:L:369:ASN:HA	1.80	0.63
2:C:394:GLY:N	2:C:395:PRO:CD	2.62	0.63
2:E:88:HIS:CE1	2:E:522:PRO:HG3	2.32	0.63
1:A:318:GLY:O	1:A:321:ILE:HG22	1.97	0.63
1:B:59:PRO:HD3	1:B:205:ALA:HB2	1.81	0.63
2:C:40:LYS:HD2	2:C:50:GLU:OE2	1.98	0.63
1:D:301:MET:HE3	2:E:71:ARG:HB3	1.81	0.63
2:L:46:ARG:HD2	2:L:549:ILE:O	1.98	0.63
1:A:167:TYR:HD2	1:A:168:LEU:HD23	1.63	0.63
2:E:238:MET:HE1	2:E:241:VAL:CB	2.27	0.63
2:K:432:GLU:OE2	1:M:10:ARG:NH2	2.27	0.63
1:A:309:LEU:HB3	1:H:320:LEU:CD2	2.29	0.62
2:E:538:GLY:H	2:E:541:GLU:HG3	1.63	0.62
1:H:76:PHE:HD2	1:H:77:MET:HE2	1.64	0.62
2:I:162:GLU:OE1	2:I:162:GLU:N	2.30	0.62
2:E:312:LEU:HA	2:E:315:ILE:CG2	2.30	0.62
2:E:551:GLU:HG3	2:E:552:GLU:N	2.14	0.62
2:I:554:GLY:O	2:I:558:PHE:HB2	2.00	0.62
2:I:27:PRO:HD3	1:M:77:MET:CE	2.29	0.62
2:C:335:GLU:OE1	2:C:335:GLU:N	2.22	0.62
1:B:347:THR:HG22	1:D:156:GLY:N	2.13	0.62
1:F:24:LEU:HB3	1:F:80:PHE:CE2	2.35	0.62
1:H:69:ALA:O	2:K:30:ARG:HD3	1.99	0.62
2:I:204:HIS:CG	2:I:205:VAL:HA	2.34	0.62
2:I:272:TRP:CD2	2:I:503:VAL:HB	2.33	0.62
2:I:329:GLN:OE1	2:I:360:ARG:NH2	2.32	0.62
1:B:32:CYS:HB2	2:G:81:CYS:HA	1.82	0.62
2:E:236:GLU:HB2	2:E:427:THR:HG21	1.81	0.62
1:F:152:HIS:CD2	2:L:59:ARG:HD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ASP:OD1	1:D:118:GLN:HB2	1.99	0.62
2:E:145:ASN:HB3	2:E:148:VAL:CG2	2.27	0.62
2:E:421:LYS:HG2	2:E:436:GLU:HG3	1.82	0.62
1:F:187:PRO:HD3	2:L:206:HIS:HD2	1.63	0.62
2:E:551:GLU:HG3	2:E:552:GLU:H	1.65	0.62
2:G:19:LYS:CG	2:G:20:LEU:H	2.13	0.62
2:G:297:VAL:HG11	2:G:398:ARG:HG2	1.81	0.62
1:D:307:ALA:HB2	4:D:701:MLA:HC22	1.82	0.62
1:F:162:MET:HG3	1:F:166:ASP:HB2	1.81	0.62
2:K:395:PRO:HG2	2:K:452:ARG:HA	1.82	0.62
2:L:444:ASN:O	2:L:448:ARG:HG3	1.99	0.62
1:A:308:VAL:HG13	1:A:309:LEU:HD22	1.81	0.61
1:B:302:ASP:OD1	2:G:71:ARG:NH2	2.33	0.61
2:I:206:HIS:ND1	1:M:187:PRO:HD3	2.15	0.61
1:D:51:VAL:HG21	2:E:178:PHE:CD2	2.34	0.61
2:E:103:LYS:HD2	2:E:282:ASP:HA	1.83	0.61
1:B:41:ALA:HB2	2:G:194:ARG:CZ	2.30	0.61
2:G:416:THR:N	2:G:417:GLY:HA2	2.15	0.61
1:B:301:MET:CE	2:G:71:ARG:HB3	2.30	0.61
1:H:309:LEU:O	1:H:313:LEU:HD23	2.00	0.61
2:L:307:LEU:CD1	2:L:404:LEU:HD13	2.30	0.61
2:E:536:THR:CG2	2:E:537:PRO:HD2	2.31	0.61
1:B:185:GLY:CA	1:B:289:THR:HG22	2.29	0.61
1:D:72:ASN:O	1:D:75:GLU:HG2	2.01	0.61
2:G:298:THR:HG21	2:G:405:ALA:CB	2.30	0.61
2:I:30:ARG:NH2	2:I:135:ASP:OD1	2.33	0.61
2:I:371:THR:CG2	2:I:530:PRO:HG3	2.31	0.61
2:L:238:MET:HA	2:L:238:MET:CE	2.30	0.61
2:I:217:THR:O	2:I:219:PRO:HD3	2.01	0.61
2:K:35:LEU:HD13	2:K:574:LEU:HD21	1.81	0.61
2:G:272:TRP:CE3	2:G:503:VAL:HB	2.35	0.61
2:G:242:VAL:HB	2:G:243:PRO:HD3	1.83	0.61
2:G:74:HIS:HD2	2:G:96:GLN:HE22	1.48	0.61
2:L:148:VAL:HG13	2:L:255:ALA:CB	2.29	0.61
1:H:296:LYS:NZ	1:M:331:THR:O	2.30	0.61
2:L:260:GLU:O	2:L:260:GLU:HG2	1.99	0.61
1:H:317:TYR:CD2	1:M:313:LEU:HG	2.36	0.61
2:C:398:ARG:HD3	2:C:498:GLU:HG2	1.81	0.60
2:C:522:PRO:HD2	2:C:525:PRO:HG2	1.82	0.60
1:H:45:PRO:HD2	1:H:194:MET:HB3	1.83	0.60
2:L:250:ASP:OD1	2:L:450:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6:VAL:HG23	1:M:10:ARG:CZ	2.31	0.60
2:E:148:VAL:HA	2:E:151:LYS:HD2	1.82	0.60
1:H:30:LEU:HD11	1:H:159:THR:HG21	1.83	0.60
1:B:243:ALA:HB1	1:B:248:ASN:HB3	1.81	0.60
1:B:295:ASP:HA	1:B:298:MET:HE2	1.82	0.60
2:C:280:VAL:HG22	2:C:291:TRP:HB3	1.83	0.60
2:C:444:ASN:O	2:C:448:ARG:HG3	2.00	0.60
1:H:187:PRO:HD3	2:K:206:HIS:CD2	2.36	0.60
2:C:163:HIS:HA	2:C:240:LYS:HG3	1.82	0.60
2:E:538:GLY:O	2:E:541:GLU:N	2.34	0.60
1:F:151:ILE:HD12	2:L:79:ARG:HD2	1.83	0.60
2:K:204:HIS:CG	2:K:205:VAL:HA	2.36	0.60
2:L:266:ARG:NH2	2:L:304:ASP:OD2	2.34	0.60
2:C:391:THR:HG21	2:C:523:PRO:HB3	1.84	0.60
2:I:145:ASN:HB3	2:I:148:VAL:CG2	2.32	0.60
1:F:152:HIS:NE2	2:L:59:ARG:HD2	2.17	0.60
1:B:89:ASP:OD1	1:B:89:ASP:N	2.34	0.60
2:L:348:ASP:OD1	2:L:349:ARG:N	2.34	0.60
2:G:501:ARG:N	2:G:501:ARG:HD2	2.17	0.60
1:H:116:ASP:HB3	1:H:119:THR:HB	1.82	0.60
2:I:509:VAL:HG12	2:I:516:ALA:HB3	1.82	0.60
2:L:69:ASP:HA	2:L:514:LYS:HD3	1.84	0.60
1:M:157:ASN:OD1	1:M:160:GLY:N	2.32	0.60
2:E:34:SER:O	2:E:574:LEU:HD12	2.02	0.60
2:K:127:PHE:O	2:K:132:VAL:HG12	2.02	0.60
2:K:295:MET:HE3	2:K:299:PRO:HG3	1.83	0.60
2:L:31:ILE:HD11	2:L:35:LEU:HB3	1.84	0.60
2:C:204:HIS:CG	2:C:205:VAL:HA	2.36	0.60
1:H:238:GLU:HG2	1:H:239:GLN:N	2.17	0.60
2:I:351:HIS:ND1	2:I:353:TRP:HB2	2.17	0.60
2:L:171:ILE:O	2:L:175:LEU:HD13	2.02	0.60
1:H:297:PHE:CZ	1:M:332:LEU:HD22	2.37	0.60
2:I:311:ASP:HB3	2:I:314:ASP:CB	2.31	0.59
2:I:311:ASP:OD1	2:I:313:VAL:HG12	2.02	0.59
2:I:81:CYS:SG	2:I:82:GLY:N	2.75	0.59
1:M:168:LEU:HD12	1:M:180:ILE:HD11	1.82	0.59
2:I:148:VAL:CG2	2:I:256:LEU:HD21	2.32	0.59
1:M:125:ILE:HB	1:M:126:PRO:HD3	1.83	0.59
2:C:398:ARG:CD	2:C:498:GLU:HG2	2.32	0.59
2:C:527:ASN:HA	2:C:539:PRO:HG2	1.84	0.59
2:E:551:GLU:OE1	2:E:561:ILE:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:446:ILE:H	2:K:446:ILE:HD12	1.66	0.59
2:C:37:ILE:CD1	2:C:567:VAL:HG21	2.33	0.59
2:E:147:GLY:O	2:E:151:LYS:HG3	2.01	0.59
2:K:265:ARG:HG2	2:K:542:ASP:OD2	2.03	0.59
2:E:387:LEU:H	2:E:387:LEU:HD22	1.66	0.59
1:F:59:PRO:HD3	1:F:205:ALA:HB2	1.84	0.59
1:H:55:ILE:HD11	1:H:202:TYR:OH	2.03	0.59
1:M:228:HIS:HB2	1:M:260:PRO:HA	1.83	0.59
2:E:145:ASN:HD22	2:E:148:VAL:HG21	1.68	0.59
2:K:123:ASP:CG	2:K:500:VAL:HG11	2.23	0.59
1:A:254:LYS:HE2	1:A:311:SER:CB	2.27	0.59
2:I:37:ILE:CD1	2:I:567:VAL:HG21	2.33	0.59
2:L:232:MET:HE1	2:L:464:LEU:HD21	1.85	0.59
2:I:391:THR:HG21	2:I:523:PRO:CB	2.33	0.59
2:C:341:ASP:HB2	2:C:342:PRO:HD2	1.84	0.59
2:G:465:TYR:O	2:G:469:GLN:HG2	2.03	0.59
1:M:266:VAL:O	1:M:270:GLY:N	2.32	0.59
1:A:125:ILE:HB	1:A:126:PRO:HD3	1.84	0.59
2:E:267:ILE:HB	2:E:304:ASP:CB	2.32	0.59
2:E:541:GLU:HA	2:E:544:VAL:HG12	1.85	0.59
2:E:51:CYS:SG	2:E:544:VAL:HG11	2.43	0.59
2:I:148:VAL:HG21	2:I:256:LEU:HD21	1.83	0.59
2:I:398:ARG:HE	2:I:498:GLU:HG2	1.68	0.59
1:M:77:MET:HE3	1:M:113:MET:HG2	1.84	0.59
2:E:288:MET:CE	2:E:312:LEU:HB3	2.32	0.58
1:H:119:THR:CG2	1:H:121:GLN:HB2	2.33	0.58
1:H:15:THR:HG23	1:H:16:PRO:HD2	1.85	0.58
2:K:280:VAL:HG23	2:K:290:LYS:CE	2.31	0.58
2:K:272:TRP:CE3	2:K:503:VAL:HB	2.39	0.58
2:C:272:TRP:CZ3	2:C:505:SER:HB3	2.37	0.58
1:D:248:ASN:ND2	1:D:249:PRO:HD2	2.18	0.58
1:D:320:LEU:HD22	1:H:313:LEU:HD21	1.85	0.58
1:H:246:TYR:CE1	1:H:255:LEU:HB3	2.38	0.58
2:I:480:ARG:HH12	2:I:483:THR:HG22	1.68	0.58
2:L:272:TRP:CE2	2:L:503:VAL:HB	2.39	0.58
2:L:497:HIS:O	2:L:504:LEU:HB3	2.03	0.58
2:G:166:ARG:HG2	2:G:170:ASP:OD2	2.03	0.58
1:H:295:ASP:HA	1:H:298:MET:CE	2.33	0.58
2:K:148:VAL:CG2	2:K:256:LEU:HD21	2.33	0.58
1:F:165:ALA:HB1	1:F:170:TRP:CD2	2.39	0.58
2:L:168:ILE:HD13	2:L:251:PHE:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:307:LEU:HG	2:L:404:LEU:CD1	2.26	0.58
1:A:99:ILE:CD1	1:A:129:LEU:HD11	2.33	0.58
2:I:236:GLU:OE2	2:I:429:LEU:HB2	2.04	0.58
2:K:259:TYR:CZ	2:K:262:VAL:HG21	2.38	0.58
2:L:35:LEU:HB2	2:L:574:LEU:HD22	1.86	0.58
2:E:341:ASP:OD1	2:E:345:ASN:N	2.36	0.58
2:E:393:GLY:N	2:E:394:GLY:HA2	2.18	0.58
1:F:278:CYS:HB2	1:F:279:PRO:HD2	1.85	0.58
2:G:307:LEU:HD21	2:G:310:THR:CG2	2.33	0.58
2:E:522:PRO:HD2	2:E:525:PRO:HG2	1.85	0.58
1:F:46:SER:O	1:F:49:ASP:HB2	2.04	0.58
1:H:148:TYR:OH	1:H:216:ALA:HB1	2.04	0.58
2:C:231:LEU:O	2:C:235:VAL:HG23	2.04	0.58
1:F:278:CYS:CB	1:F:279:PRO:CD	2.82	0.58
1:M:288:CYS:HA	1:M:293:PHE:CD1	2.39	0.58
2:C:305:GLY:HA2	2:C:400:TRP:CZ3	2.38	0.58
1:H:234:ALA:HB3	1:M:234:ALA:HB3	1.86	0.58
1:M:313:LEU:O	1:M:313:LEU:HD13	2.03	0.58
2:E:286:ARG:CB	2:E:343:LEU:HD21	2.33	0.58
1:F:15:THR:HG21	1:F:19:LYS:HE2	1.84	0.58
2:I:265:ARG:HH12	2:I:539:PRO:HG3	1.69	0.57
2:L:123:ASP:HB3	2:L:500:VAL:HG11	1.86	0.57
1:B:8:TYR:HB2	2:E:421:LYS:NZ	2.19	0.57
1:H:30:LEU:HG	1:H:100:PRO:HG3	1.86	0.57
2:L:398:ARG:NE	2:L:498:GLU:HG2	2.19	0.57
2:L:232:MET:CE	2:L:464:LEU:HD21	2.35	0.57
1:B:318:GLY:N	1:B:319:PRO:HD2	2.19	0.57
2:C:412:TYR:HB3	2:C:461:ALA:HB1	1.85	0.57
2:C:528:ALA:HB2	2:C:540:TYR:CE2	2.40	0.57
2:E:204:HIS:CG	2:E:205:VAL:HA	2.39	0.57
2:E:295:MET:CE	2:E:299:PRO:HG3	2.34	0.57
2:L:341:ASP:OD2	2:L:345:ASN:HB2	2.04	0.57
2:E:536:THR:HG23	2:E:537:PRO:HD2	1.87	0.57
1:F:123:ILE:HD12	1:F:128:TRP:CZ2	2.40	0.57
1:F:35:ASP:O	1:F:39:ILE:HG23	2.05	0.57
2:E:238:MET:HA	2:E:238:MET:CE	2.34	0.57
2:E:273:GLY:HA2	2:E:297:VAL:O	2.04	0.57
2:E:322:LEU:HD12	2:E:532:ASP:CB	2.34	0.57
2:I:311:ASP:CB	2:I:314:ASP:HB2	2.33	0.57
2:I:444:ASN:O	2:I:448:ARG:HG3	2.05	0.57
1:A:320:LEU:HD21	1:B:320:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:TRP:CD1	1:F:272:ILE:HG13	2.40	0.57
2:I:506:HIS:ND1	2:I:518:TYR:OH	2.30	0.57
1:D:252:ILE:HG22	1:D:255:LEU:HD12	1.86	0.57
1:D:45:PRO:HD2	1:D:194:MET:HB3	1.85	0.57
2:E:303:VAL:N	2:E:306:GLU:O	2.36	0.57
2:L:285:TYR:OH	2:L:313:VAL:HG13	2.04	0.57
2:E:301:VAL:HG23	2:E:315:ILE:HD12	1.86	0.57
2:G:475:HIS:O	2:G:476:ALA:HB3	2.04	0.57
1:H:180:ILE:O	1:H:217:LEU:HB3	2.05	0.57
2:I:522:PRO:O	2:I:525:PRO:HD2	2.05	0.57
2:K:335:GLU:N	2:K:335:GLU:OE1	2.37	0.57
2:I:484:ASP:OD1	2:I:485:PHE:N	2.36	0.57
2:K:393:GLY:O	2:K:501:ARG:HA	2.05	0.57
1:D:183:VAL:HG12	1:D:188:VAL:CG2	2.35	0.57
2:I:289:THR:HG23	2:I:311:ASP:CG	2.25	0.57
2:L:55:SER:HB2	2:L:574:LEU:HD23	1.87	0.57
2:C:447:GLU:OE2	2:C:450:ARG:NH1	2.38	0.56
1:F:99:ILE:HG23	1:F:125:ILE:CG2	2.34	0.56
2:L:288:MET:HA	2:L:291:TRP:NE1	2.20	0.56
1:F:316:SER:HB3	1:M:313:LEU:HD23	1.87	0.56
1:D:151:ILE:O	1:D:154:MET:HB2	2.05	0.56
2:I:245:HIS:ND1	2:I:453:THR:OG1	2.35	0.56
2:I:393:GLY:O	2:I:501:ARG:HA	2.05	0.56
2:L:28:ILE:HD12	2:L:35:LEU:HD23	1.86	0.56
2:L:127:PHE:CZ	2:L:571:ASP:HA	2.39	0.56
1:A:310:SER:HA	1:A:313:LEU:HB2	1.87	0.56
1:B:269:ARG:HH12	2:E:222:GLN:HB3	1.71	0.56
2:K:561:ILE:O	2:K:565:ARG:HG3	2.06	0.56
2:E:288:MET:HA	2:E:291:TRP:CZ2	2.40	0.56
1:F:252:ILE:HG22	1:F:255:LEU:HD12	1.88	0.56
1:H:59:PRO:HD3	1:H:205:ALA:HB2	1.86	0.56
2:L:73:SER:HB2	2:L:96:GLN:NE2	2.20	0.56
2:C:508:LEU:HD21	2:C:510:ILE:HD11	1.86	0.56
2:E:126:ILE:O	2:E:130:ASN:HB2	2.06	0.56
2:E:286:ARG:O	2:E:289:THR:HG22	2.05	0.56
1:F:15:THR:HG23	1:F:16:PRO:HD2	1.88	0.56
2:L:265:ARG:HD3	2:L:542:ASP:HB3	1.87	0.56
1:A:315:LYS:HD3	1:A:317:TYR:OH	2.05	0.56
2:L:127:PHE:HD1	2:L:131:LEU:HD22	1.71	0.56
2:E:286:ARG:HG3	2:E:287:THR:HG23	1.88	0.56
2:K:286:ARG:HG2	2:K:343:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:351:HIS:CG	2:K:352:PRO:HD2	2.41	0.56
2:L:366:PHE:HA	2:L:370:TYR:CD2	2.40	0.56
2:E:302:VAL:HG22	2:E:307:LEU:HD13	1.88	0.56
2:K:98:MET:HE1	2:K:285:TYR:CD2	2.38	0.56
1:D:95:LEU:HD23	1:D:164:LEU:HG	1.88	0.56
2:I:118:ALA:HA	2:I:121:MET:HE3	1.87	0.56
2:K:187:LEU:O	2:K:191:ARG:HG3	2.05	0.56
2:E:239:LYS:NZ	2:E:427:THR:HG23	2.21	0.55
1:F:26:ILE:CD1	1:F:93:LEU:HD11	2.36	0.55
1:H:266:VAL:N	1:H:267:PRO:HD2	2.21	0.55
2:K:237:PHE:CE2	2:K:241:VAL:HG21	2.41	0.55
1:A:305:PRO:O	1:A:308:VAL:HG12	2.06	0.55
2:C:272:TRP:HZ3	2:C:505:SER:HB3	1.71	0.55
2:E:42:ASP:HB3	2:E:47:ARG:CG	2.37	0.55
2:G:98:MET:CE	2:G:493:GLY:HA2	2.36	0.55
1:B:17:ALA:HB3	1:B:204:LEU:O	2.06	0.55
2:E:264:ARG:HG2	2:E:265:ARG:N	2.21	0.55
2:E:263:GLY:N	2:E:547:THR:OG1	2.38	0.55
2:E:555:PRO:HA	2:E:558:PHE:HB3	1.89	0.55
2:I:272:TRP:CE3	2:I:503:VAL:HB	2.41	0.55
2:L:268:LEU:HD23	2:L:303:VAL:CG1	2.34	0.55
2:E:265:ARG:HB2	2:E:265:ARG:NH1	2.22	0.55
2:E:336:THR:HG23	2:E:354:ASN:OD1	2.06	0.55
1:B:154:MET:SD	2:G:68:LYS:HE2	2.47	0.55
1:H:178:LEU:HD11	1:H:203:GLN:NE2	2.16	0.55
1:H:32:CYS:HB2	2:K:81:CYS:HA	1.87	0.55
2:I:480:ARG:NH1	2:I:483:THR:HG22	2.20	0.55
2:L:89:ALA:O	2:L:93:VAL:HG13	2.06	0.55
2:C:351:HIS:ND1	2:C:353:TRP:HB2	2.21	0.55
2:I:237:PHE:CE2	2:I:241:VAL:HG21	2.41	0.55
2:L:129:ASP:CB	2:L:186:THR:HG21	2.36	0.55
1:M:227:VAL:HG13	1:M:267:PRO:CG	2.30	0.55
1:B:34:GLY:CA	2:G:82:GLY:HA3	2.36	0.55
1:D:31:GLY:HA2	1:D:152:HIS:CE1	2.41	0.55
1:F:127:GLU:O	1:F:131:ARG:HG3	2.06	0.55
1:F:128:TRP:CE3	1:F:132:LEU:HD11	2.41	0.55
1:H:95:LEU:HD23	1:H:164:LEU:HG	1.89	0.55
1:H:178:LEU:HD13	1:H:210:MET:SD	2.47	0.55
1:H:193:PHE:HD2	1:H:194:MET:CE	2.19	0.55
2:I:318:ASN:HD21	2:I:381:LYS:HE2	1.72	0.55
1:A:332:LEU:HD12	1:F:261:VAL:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:259:TYR:CZ	2:C:262:VAL:HG21	2.41	0.55
1:D:304:PRO:HG2	1:D:307:ALA:HB2	1.89	0.55
1:B:103:ARG:HH21	1:D:343:PRO:HG3	1.70	0.55
2:G:231:LEU:HD21	2:G:464:LEU:HD23	1.88	0.55
2:G:272:TRP:CD2	2:G:503:VAL:HB	2.42	0.55
1:B:187:PRO:HD3	2:G:206:HIS:CD2	2.42	0.55
2:K:321:ILE:HG12	2:K:521:TYR:CZ	2.42	0.55
2:K:437:TRP:CZ2	2:K:440:PRO:HD3	2.42	0.55
2:K:446:ILE:N	2:K:446:ILE:HD12	2.22	0.55
2:L:380:ASP:HB2	2:L:387:LEU:HD11	1.89	0.55
2:L:391:THR:HG21	2:L:502:GLY:HA3	1.89	0.55
2:C:316:ASN:HB2	2:C:496:PHE:HZ	1.66	0.54
2:E:87:ASN:ND2	2:E:116:GLU:OE1	2.40	0.54
1:F:167:TYR:HD2	1:F:168:LEU:HD12	1.72	0.54
2:L:55:SER:CB	2:L:574:LEU:HD23	2.37	0.54
1:B:295:ASP:HA	1:B:298:MET:CE	2.36	0.54
2:C:394:GLY:H	2:C:395:PRO:HD3	1.73	0.54
2:I:141:VAL:HG21	2:I:172:MET:CE	2.37	0.54
1:A:138:ALA:HB2	1:A:178:LEU:HD22	1.89	0.54
2:E:447:GLU:OE1	2:E:450:ARG:HD2	2.06	0.54
2:E:527:ASN:HB3	2:E:540:TYR:CE1	2.42	0.54
2:L:75:PHE:O	2:L:79:ARG:NH1	2.40	0.54
1:D:278:CYS:CB	1:D:279:PRO:CD	2.86	0.54
1:F:315:LYS:HB3	1:F:317:TYR:CD1	2.42	0.54
2:I:130:ASN:C	2:I:131:LEU:HD23	2.27	0.54
1:F:124:THR:OG1	1:F:127:GLU:HG3	2.07	0.54
2:G:19:LYS:HG2	2:G:20:LEU:N	2.22	0.54
2:G:277:ASP:OD1	2:G:279:ASN:HB2	2.08	0.54
1:H:243:ALA:HB1	1:H:248:ASN:HB3	1.89	0.54
2:K:357:THR:HG22	2:K:359:PRO:HD3	1.90	0.54
2:L:298:THR:OG1	2:L:402:THR:HA	2.06	0.54
1:M:39:ILE:HB	1:M:194:MET:HE2	1.90	0.54
1:D:158:PRO:HG3	2:E:63:ILE:HG21	1.88	0.54
2:E:107:ILE:O	2:E:111:ILE:HG13	2.07	0.54
1:H:288:CYS:HA	1:H:293:PHE:CD1	2.43	0.54
2:K:371:THR:CG2	2:K:530:PRO:HG3	2.37	0.54
2:L:297:VAL:CG1	2:L:398:ARG:HB3	2.38	0.54
1:A:318:GLY:O	1:A:322:ARG:HG3	2.07	0.54
1:D:227:VAL:HG22	1:D:264:CYS:HB3	1.89	0.54
2:E:531:ARG:CG	2:E:537:PRO:HA	2.33	0.54
1:F:77:MET:CE	1:F:77:MET:HA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:255:ALA:O	2:G:257:PRO:HD3	2.08	0.54
2:G:69:ASP:OD2	2:G:71:ARG:NH1	2.41	0.54
2:E:264:ARG:HA	2:E:443:SER:O	2.08	0.54
2:G:98:MET:HG3	2:G:283:TYR:O	2.08	0.54
2:L:31:ILE:CD1	2:L:35:LEU:HB3	2.38	0.54
1:D:178:LEU:HD23	1:D:210:MET:SD	2.48	0.54
2:E:25:TRP:CZ3	2:E:563:ILE:HD13	2.43	0.54
1:F:240:ALA:HA	1:F:242:PHE:CE2	2.43	0.54
1:F:27:THR:HG22	1:F:96:GLU:OE1	2.08	0.54
2:I:540:TYR:O	2:I:544:VAL:HG23	2.08	0.54
2:K:163:HIS:N	2:K:164:GLY:HA2	2.22	0.54
1:F:25:TRP:CD1	1:F:27:THR:HG23	2.43	0.53
2:G:528:ALA:HB2	2:G:540:TYR:CE2	2.43	0.53
1:H:227:VAL:HG13	1:H:267:PRO:HG3	1.90	0.53
2:G:414:LYS:HB3	2:G:421:LYS:HB2	1.90	0.53
2:I:548:PRO:HG2	2:I:550:PHE:HE1	1.74	0.53
2:L:380:ASP:HB2	2:L:387:LEU:CD1	2.38	0.53
1:B:26:ILE:HG23	1:B:113:MET:HE2	1.91	0.53
2:G:474:LEU:HD12	2:G:479:THR:CG2	2.38	0.53
1:H:76:PHE:CD2	1:H:77:MET:HE2	2.44	0.53
2:I:285:TYR:OH	2:I:313:VAL:HG23	2.09	0.53
2:L:242:VAL:N	2:L:243:PRO:HD2	2.23	0.53
2:C:403:ALA:HB2	2:C:420:VAL:HG23	1.88	0.53
2:K:163:HIS:HB2	2:K:164:GLY:CA	2.39	0.53
2:L:265:ARG:HG2	2:L:543:ALA:HB2	1.90	0.53
1:M:299:PRO:HG2	1:M:302:ASP:OD2	2.07	0.53
1:B:314:ILE:HG22	1:D:317:TYR:OH	2.07	0.53
2:E:147:GLY:C	2:E:151:LYS:HE3	2.29	0.53
1:B:269:ARG:NH1	2:E:222:GLN:OE1	2.42	0.53
2:E:502:GLY:C	2:E:523:PRO:HG3	2.29	0.53
2:E:272:TRP:CE3	2:E:503:VAL:HB	2.44	0.53
1:B:41:ALA:HB2	2:G:194:ARG:NH1	2.23	0.53
2:E:237:PHE:CE2	2:E:241:VAL:HG21	2.44	0.53
2:G:117:ALA:O	2:G:121:MET:HG3	2.09	0.53
2:L:325:SER:HA	2:L:368:GLY:O	2.07	0.53
2:L:123:ASP:CG	2:L:500:VAL:HG11	2.29	0.53
1:D:278:CYS:HB2	1:D:279:PRO:CD	2.39	0.53
2:I:348:ASP:OD1	2:I:350:LYS:N	2.37	0.53
2:I:528:ALA:HA	2:I:540:TYR:CD2	2.44	0.53
2:L:285:TYR:CE2	2:L:341:ASP:HB2	2.43	0.53
2:C:267:ILE:O	2:C:268:LEU:HD23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:406:GLY:HA2	2:C:415:SER:OG	2.09	0.53
2:C:71:ARG:HD2	2:C:487:VAL:HG21	1.90	0.53
2:E:538:GLY:N	2:E:541:GLU:HG3	2.23	0.53
1:A:133:ALA:N	1:A:134:PRO:HD2	2.24	0.53
1:B:199:TYR:CE2	1:B:211:ILE:HA	2.43	0.53
1:B:278:CYS:HB2	1:B:279:PRO:HD3	1.89	0.53
1:D:111:ALA:HA	2:E:56:SER:O	2.09	0.53
2:E:298:THR:HG21	2:E:405:ALA:CB	2.37	0.53
2:E:31:ILE:CG2	2:E:572:PRO:HG2	2.39	0.53
2:E:135:ASP:O	2:E:565:ARG:NH2	2.42	0.53
2:G:265:ARG:NH1	2:G:539:PRO:HG3	2.24	0.53
2:I:38:TYR:OH	2:I:364:ARG:NH2	2.42	0.53
2:L:348:ASP:O	2:L:354:ASN:ND2	2.42	0.53
2:C:392:GLY:H	2:C:394:GLY:HA2	1.73	0.53
2:G:391:THR:HG21	2:G:523:PRO:CB	2.39	0.53
2:I:112:ILE:CD1	2:I:210:LEU:HD21	2.38	0.53
2:L:28:ILE:HD11	2:L:37:ILE:CG1	2.39	0.53
1:A:30:LEU:HD12	1:A:161:CYS:HB3	1.91	0.52
2:C:126:ILE:O	2:C:130:ASN:HB2	2.09	0.52
2:E:35:LEU:HB2	2:E:574:LEU:CD1	2.38	0.52
1:F:6:VAL:HG22	1:F:10:ARG:HH21	1.74	0.52
2:G:393:GLY:N	2:G:394:GLY:HA2	2.22	0.52
1:B:152:HIS:NE2	2:G:59:ARG:HD2	2.25	0.52
1:H:67:VAL:O	2:K:30:ARG:HA	2.09	0.52
1:H:77:MET:CE	2:K:27:PRO:HD2	2.34	0.52
2:K:61:TYR:HA	2:K:64:PHE:CZ	2.45	0.52
2:L:272:TRP:C	2:L:299:PRO:HB3	2.29	0.52
2:C:508:LEU:HD11	2:C:515:ILE:HD13	1.91	0.52
2:E:253:TYR:OH	2:E:447:GLU:HG2	2.10	0.52
2:E:308:LEU:HD23	2:E:308:LEU:N	2.24	0.52
2:E:262:VAL:HA	2:E:548:PRO:HD2	1.91	0.52
2:I:393:GLY:HA3	2:I:395:PRO:HD2	1.90	0.52
2:L:163:HIS:H	2:L:164:GLY:HA2	1.74	0.52
1:A:232:ASP:HB2	1:F:230:GLY:HA2	1.91	0.52
1:B:7:PRO:HB3	2:E:434:GLU:OE1	2.08	0.52
1:D:30:LEU:HD12	1:D:161:CYS:HB3	1.91	0.52
2:E:531:ARG:HA	2:E:536:THR:O	2.10	0.52
1:H:105:ASN:HB3	1:H:106:GLY:HA3	1.92	0.52
2:I:280:VAL:O	2:I:291:TRP:HB3	2.09	0.52
2:K:273:GLY:HA2	2:K:297:VAL:O	2.09	0.52
2:K:509:VAL:HG12	2:K:516:ALA:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:318:ASN:OD1	2:L:381:LYS:HE3	2.09	0.52
2:C:392:GLY:O	2:C:448:ARG:HD3	2.09	0.52
2:E:25:TRP:CB	2:E:564:MET:HE1	2.39	0.52
1:D:47:VAL:HG23	1:D:194:MET:HE3	1.91	0.52
2:E:529:SER:O	2:E:538:GLY:HA3	2.08	0.52
2:G:163:HIS:CD2	2:G:244:LEU:HA	2.44	0.52
2:K:259:TYR:CE1	2:K:262:VAL:HG21	2.45	0.52
2:L:320:ARG:HG3	2:L:386:HIS:CE1	2.45	0.52
2:C:371:THR:CG2	2:C:530:PRO:HG3	2.39	0.52
1:H:30:LEU:HB2	1:H:98:SER:HB2	1.91	0.52
2:L:392:GLY:HA2	2:L:448:ARG:HD3	1.90	0.52
1:H:185:GLY:CA	1:H:289:THR:HG22	2.39	0.52
2:L:137:CYS:SG	2:L:176:ASN:HA	2.49	0.52
2:L:527:ASN:HB3	2:L:540:TYR:CE1	2.45	0.52
1:M:15:THR:HG22	1:M:16:PRO:O	2.09	0.52
2:E:21:VAL:HG11	2:E:43:PHE:CD2	2.45	0.52
1:F:26:ILE:HD12	1:F:93:LEU:HD11	1.92	0.52
1:H:77:MET:HE3	2:K:27:PRO:CD	2.37	0.52
2:I:313:VAL:HG21	2:I:343:LEU:HD12	1.92	0.52
2:L:35:LEU:CD1	2:L:574:LEU:HD21	2.38	0.52
1:M:144:THR:HA	1:M:147:THR:OG1	2.10	0.52
2:G:508:LEU:HD13	2:G:518:TYR:HD2	1.75	0.52
2:G:92:SER:O	2:G:96:GLN:HG3	2.09	0.52
2:L:134:VAL:HA	2:L:137:CYS:HB2	1.91	0.52
2:L:393:GLY:O	2:L:501:ARG:HA	2.10	0.52
1:A:238:GLU:OE1	1:A:239:GLN:HG3	2.09	0.52
1:A:185:GLY:HA2	1:A:289:THR:HG22	1.91	0.52
1:B:7:PRO:HB3	2:E:434:GLU:CD	2.30	0.52
2:L:117:ALA:O	2:L:121:MET:HG3	2.09	0.52
1:B:278:CYS:CB	1:B:279:PRO:CD	2.88	0.51
1:F:99:ILE:HG23	1:F:125:ILE:HG22	1.91	0.51
2:K:130:ASN:C	2:K:131:LEU:HD12	2.30	0.51
1:A:246:TYR:CE1	1:A:255:LEU:HB3	2.45	0.51
2:C:105:PRO:HG2	2:C:481:THR:C	2.31	0.51
2:E:127:PHE:O	2:E:132:VAL:HG22	2.10	0.51
2:L:152:ALA:HB2	2:L:251:PHE:CZ	2.46	0.51
1:A:271:TRP:HD1	1:A:272:ILE:HG13	1.72	0.51
1:D:119:THR:OG1	1:D:121:GLN:HB2	2.10	0.51
2:E:348:ASP:OD1	2:E:349:ARG:N	2.44	0.51
2:E:391:THR:HG21	2:E:523:PRO:HB3	1.91	0.51
2:G:127:PHE:CZ	2:G:571:ASP:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:295:MET:CE	2:K:299:PRO:HG3	2.39	0.51
2:K:34:SER:O	2:K:574:LEU:HD22	2.10	0.51
1:A:167:TYR:CD2	1:A:168:LEU:HD23	2.45	0.51
1:B:9:GLY:HA3	2:E:423:TYR:CG	2.46	0.51
2:C:264:ARG:HG3	2:C:265:ARG:N	2.25	0.51
1:D:247:GLY:HA3	2:E:481:THR:HG21	1.90	0.51
1:D:91:PHE:CE2	1:D:136:ALA:HB2	2.46	0.51
2:E:96:GLN:HB3	2:E:100:TYR:CE2	2.45	0.51
2:I:321:ILE:HD12	2:I:376:PRO:HB3	1.91	0.51
2:L:266:ARG:HD3	2:L:268:LEU:HD11	1.92	0.51
1:M:84:ALA:O	1:M:135:LYS:HE3	2.11	0.51
1:B:266:VAL:HG21	3:B:502:SF4:S1	2.50	0.51
1:D:266:VAL:HB	1:D:267:PRO:HD3	1.91	0.51
2:E:272:TRP:HE1	2:E:315:ILE:HD11	1.76	0.51
2:G:23:MET:HG3	2:G:41:ILE:HD12	1.92	0.51
1:D:178:LEU:HD21	1:D:203:GLN:NE2	2.25	0.51
1:F:340:HIS:CE1	1:F:342:GLN:HB2	2.46	0.51
2:I:145:ASN:HB3	2:I:148:VAL:HB	1.93	0.51
1:D:95:LEU:HB3	1:D:164:LEU:HD11	1.92	0.51
2:E:312:LEU:HD23	2:E:315:ILE:HG21	1.92	0.51
2:E:269:LEU:HD13	2:E:397:ALA:HA	1.91	0.51
2:G:121:MET:HE1	2:G:460:ALA:HA	1.92	0.51
2:I:112:ILE:HD11	2:I:215:VAL:CG1	2.40	0.51
2:I:31:ILE:HD11	2:I:35:LEU:HB3	1.93	0.51
2:L:473:GLU:OE1	2:L:478:ARG:HD2	2.11	0.51
1:M:26:ILE:HD12	1:M:93:LEU:HD11	1.93	0.51
2:C:160:ALA:HA	2:C:163:HIS:CE1	2.45	0.51
2:C:311:ASP:OD1	2:C:313:VAL:HG12	2.11	0.51
2:C:336:THR:HB	2:C:354:ASN:OD1	2.11	0.51
1:D:25:TRP:CD1	1:D:27:THR:HG23	2.46	0.51
2:E:127:PHE:CD1	2:E:131:LEU:HD12	2.41	0.51
2:G:341:ASP:HB2	2:G:342:PRO:HD2	1.93	0.51
1:D:10:ARG:NH2	2:G:432:GLU:OE2	2.28	0.51
2:I:127:PHE:CZ	2:I:132:VAL:HG23	2.45	0.51
2:I:467:ALA:O	2:I:471:LEU:HB2	2.11	0.51
2:K:196:MET:HB3	2:K:227:TYR:CE2	2.46	0.51
1:M:227:VAL:CG2	1:M:264:CYS:HB3	2.40	0.51
1:D:76:PHE:O	1:D:79:PRO:HD2	2.10	0.51
2:I:272:TRP:CZ3	2:I:505:SER:HB3	2.46	0.51
2:I:533:ILE:HD11	2:I:534:TYR:CE2	2.46	0.51
2:I:56:SER:O	1:M:111:ALA:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:399:LEU:HB3	2:C:437:TRP:CE3	2.46	0.51
2:E:303:VAL:CG1	2:E:308:LEU:HD21	2.41	0.51
2:G:300:GLY:HA2	2:G:309:THR:O	2.11	0.51
2:G:494:CYS:HA	2:G:506:HIS:O	2.11	0.51
2:I:285:TYR:CZ	2:I:313:VAL:HG23	2.46	0.51
2:I:480:ARG:HH12	2:I:483:THR:HA	1.75	0.51
1:H:187:PRO:HD3	2:K:206:HIS:HD2	1.76	0.51
2:K:146:PRO:HD2	2:K:552:GLU:OE1	2.11	0.51
2:E:289:THR:HA	2:E:311:ASP:OD1	2.10	0.50
2:E:265:ARG:CD	2:E:543:ALA:HB2	2.41	0.50
2:G:273:GLY:HA2	2:G:297:VAL:O	2.11	0.50
2:I:273:GLY:HA3	2:I:299:PRO:HG3	1.93	0.50
2:I:351:HIS:CG	2:I:352:PRO:HD2	2.46	0.50
2:K:490:GLU:HA	2:K:510:ILE:O	2.11	0.50
1:M:24:LEU:HD12	1:M:91:PHE:CD2	2.46	0.50
1:M:278:CYS:CB	1:M:279:PRO:CD	2.89	0.50
1:A:186:CYS:HB3	1:A:288:CYS:HB2	1.92	0.50
1:B:26:ILE:HG12	1:B:113:MET:HE1	1.93	0.50
2:C:292:GLY:HA3	2:C:312:LEU:HD22	1.93	0.50
2:E:439:ILE:HG23	2:E:440:PRO:HD2	1.93	0.50
2:G:280:VAL:HG23	2:G:291:TRP:HB3	1.93	0.50
2:G:508:LEU:HD13	2:G:518:TYR:CD2	2.44	0.50
1:H:211:ILE:HG23	1:H:213:LEU:HD21	1.93	0.50
2:K:138:GLU:OE2	2:K:142:ARG:NH1	2.45	0.50
2:K:548:PRO:HG2	2:K:550:PHE:HE1	1.75	0.50
1:M:189:GLN:O	1:M:192:ASN:HB2	2.11	0.50
1:A:278:CYS:CB	1:A:279:PRO:CD	2.88	0.50
2:C:311:ASP:HB3	2:C:314:ASP:HB3	1.93	0.50
2:E:250:ASP:O	2:E:254:GLU:HG3	2.11	0.50
2:E:380:ASP:CB	2:E:383:THR:HG22	2.37	0.50
2:G:340:ASN:HA	2:G:345:ASN:O	2.12	0.50
2:G:132:VAL:HG22	2:G:568:ARG:HB3	1.93	0.50
2:I:336:THR:HG23	2:I:354:ASN:OD1	2.11	0.50
2:C:302:VAL:HG11	2:C:400:TRP:CE3	2.46	0.50
2:E:138:GLU:HB2	2:E:149:TRP:CZ3	2.47	0.50
2:I:398:ARG:NH2	2:I:500:VAL:O	2.44	0.50
2:L:232:MET:CA	2:L:232:MET:HE2	2.38	0.50
1:A:155:GLU:HB2	1:F:338:TRP:CZ2	2.46	0.50
2:E:303:VAL:HG13	2:E:308:LEU:HD21	1.93	0.50
2:E:132:VAL:HG12	2:E:568:ARG:HB3	1.93	0.50
2:G:126:ILE:O	2:G:130:ASN:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:73:SER:HB2	2:G:96:GLN:NE2	2.26	0.50
1:H:242:PHE:HD2	1:H:254:LYS:NZ	2.10	0.50
2:I:351:HIS:CD2	2:I:352:PRO:HD2	2.45	0.50
2:L:398:ARG:O	2:L:402:THR:HG22	2.11	0.50
1:B:119:THR:CG2	1:B:121:GLN:HG2	2.41	0.50
2:C:144:THR:CG2	2:C:559:LYS:HD3	2.41	0.50
2:C:322:LEU:HD12	2:C:377:ARG:HG3	1.94	0.50
2:C:71:ARG:HD2	2:C:487:VAL:CG2	2.42	0.50
2:E:210:LEU:HD12	2:E:215:VAL:HG12	1.94	0.50
2:E:238:MET:HA	2:E:238:MET:HE2	1.93	0.50
2:E:21:VAL:HG11	2:E:43:PHE:HD2	1.76	0.50
2:E:531:ARG:HG3	2:E:531:ARG:HH11	1.77	0.50
1:F:33:ASP:HA	1:F:96:GLU:OE2	2.12	0.50
2:I:37:ILE:HD11	2:I:567:VAL:HG11	1.93	0.50
2:L:165:TYR:HB3	2:L:170:ASP:HB2	1.93	0.50
1:D:116:ASP:CG	1:D:118:GLN:HB2	2.31	0.50
1:D:271:TRP:HB3	1:D:276:GLY:HA3	1.93	0.50
1:D:78:ALA:HB3	1:D:79:PRO:HD3	1.93	0.50
1:B:8:TYR:HB2	2:E:421:LYS:HZ3	1.77	0.50
1:F:55:ILE:HD11	1:F:202:TYR:OH	2.12	0.50
1:F:248:ASN:CG	1:F:249:PRO:HD2	2.32	0.50
1:H:105:ASN:HB3	1:H:106:GLY:CA	2.42	0.50
2:K:551:GLU:HG2	2:K:553:ASN:HB2	1.94	0.50
2:L:267:ILE:O	2:L:303:VAL:HA	2.11	0.50
2:L:351:HIS:CG	2:L:352:PRO:HD2	2.46	0.50
2:L:242:VAL:HA	2:L:453:THR:CG2	2.41	0.50
2:L:522:PRO:HB3	5:L:701:NFU:C3	2.42	0.50
2:C:288:MET:HG3	2:C:291:TRP:CH2	2.47	0.50
1:D:271:TRP:CD1	1:D:272:ILE:HG13	2.46	0.50
2:E:124:HIS:NE2	2:E:395:PRO:HG3	2.27	0.50
2:E:526:TRP:O	2:E:529:SER:OG	2.16	0.50
2:G:23:MET:HE2	2:G:558:PHE:HD2	1.76	0.50
2:I:551:GLU:OE2	2:I:553:ASN:ND2	2.33	0.50
2:I:544:VAL:HG13	2:I:563:ILE:HG23	1.94	0.50
2:K:198:CYS:SG	2:K:203:ARG:HA	2.52	0.50
2:L:61:TYR:HA	2:L:64:PHE:CZ	2.46	0.50
1:B:189:GLN:O	1:B:192:ASN:HB2	2.12	0.50
2:C:282:ASP:N	2:C:282:ASP:OD1	2.44	0.50
2:E:348:ASP:O	2:E:354:ASN:ND2	2.41	0.50
1:F:261:VAL:O	1:F:261:VAL:HG12	2.11	0.50
1:H:36:SER:O	1:H:39:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:128:GLN:OE1	2:I:452:ARG:HD2	2.12	0.50
2:L:409:ASP:OD2	2:L:414:LYS:HD3	2.12	0.50
2:C:242:VAL:N	2:C:243:PRO:HD2	2.27	0.49
1:D:85:ARG:NE	1:D:87:GLU:OE2	2.35	0.49
2:E:159:HIS:HB2	2:E:247:ASP:OD2	2.11	0.49
2:E:387:LEU:HD23	2:E:387:LEU:O	2.12	0.49
2:G:288:MET:HA	2:G:291:TRP:NE1	2.27	0.49
2:I:103:LYS:HD2	2:I:282:ASP:HA	1.93	0.49
2:E:267:ILE:HD13	2:E:400:TRP:CZ2	2.46	0.49
1:H:30:LEU:CD1	1:H:159:THR:HG21	2.42	0.49
2:K:163:HIS:CB	2:K:164:GLY:HA2	2.42	0.49
2:K:259:TYR:CD2	2:K:446:ILE:HD11	2.47	0.49
2:K:274:SER:HB3	2:K:297:VAL:HB	1.93	0.49
1:A:309:LEU:O	1:A:313:LEU:HD13	2.12	0.49
2:E:325:SER:HB2	2:E:530:PRO:HB2	1.95	0.49
1:H:279:PRO:C	1:H:281:VAL:H	2.15	0.49
2:I:261:GLU:OE2	2:I:264:ARG:NH1	2.34	0.49
2:K:273:GLY:HA3	2:K:295:MET:HE1	1.95	0.49
2:K:98:MET:HE2	2:K:494:CYS:N	2.26	0.49
2:L:442:TRP:HB2	2:L:444:ASN:HD22	1.78	0.49
2:C:528:ALA:HA	2:C:540:TYR:CD2	2.46	0.49
2:C:564:MET:HA	2:C:564:MET:CE	2.42	0.49
1:H:237:TYR:HA	1:H:242:PHE:HE1	1.77	0.49
1:B:183:VAL:HG12	1:B:188:VAL:HG23	1.94	0.49
2:E:337:SER:O	2:E:511:ARG:NH2	2.45	0.49
2:E:531:ARG:HD3	2:E:535:GLY:O	2.12	0.49
2:G:214:GLY:HA3	2:G:481:THR:O	2.11	0.49
2:L:138:GLU:O	2:L:142:ARG:HG3	2.12	0.49
1:B:90:ASN:HA	1:B:137:LEU:HD11	1.95	0.49
2:C:351:HIS:CG	2:C:352:PRO:HD2	2.47	0.49
2:K:564:MET:HA	2:K:564:MET:HE2	1.94	0.49
2:L:163:HIS:CB	2:L:164:GLY:HA2	2.39	0.49
2:E:43:PHE:CE1	2:E:555:PRO:HD3	2.47	0.49
1:H:253:VAL:HA	1:H:257:CYS:HB3	1.94	0.49
2:I:185:GLU:O	2:I:189:VAL:HG23	2.11	0.49
2:I:273:GLY:HA2	2:I:297:VAL:O	2.13	0.49
2:L:259:TYR:CE1	2:L:262:VAL:HG21	2.47	0.49
2:L:317:LEU:HD21	2:L:341:ASP:OD2	2.13	0.49
1:A:67:VAL:O	2:C:30:ARG:HA	2.11	0.49
2:E:271:CYS:O	2:E:300:GLY:N	2.36	0.49
2:E:341:ASP:CG	2:E:345:ASN:HB2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:LYS:HD2	1:F:317:TYR:CE1	2.44	0.49
1:F:78:ALA:N	1:F:79:PRO:HD2	2.27	0.49
2:K:288:MET:HA	2:K:291:TRP:NE1	2.28	0.49
2:L:123:ASP:CB	2:L:500:VAL:HG11	2.43	0.49
2:L:297:VAL:HG11	2:L:398:ARG:HB3	1.95	0.49
2:C:221:ILE:O	2:C:225:THR:HG23	2.13	0.49
2:E:396:ILE:HG23	2:E:397:ALA:N	2.28	0.49
1:H:310:SER:O	1:H:313:LEU:HB2	2.13	0.49
2:I:480:ARG:CZ	2:I:483:THR:HG22	2.42	0.49
2:I:563:ILE:O	2:I:567:VAL:HG23	2.13	0.49
2:K:504:LEU:HD12	2:K:505:SER:N	2.28	0.49
2:L:322:LEU:C	2:L:323:LEU:HD12	2.33	0.49
1:M:99:ILE:HD11	1:M:164:LEU:HD23	1.94	0.49
2:E:128:GLN:HA	2:E:132:VAL:CG2	2.43	0.49
2:E:35:LEU:CD1	2:E:574:LEU:HD11	2.42	0.49
2:L:393:GLY:O	2:L:395:PRO:HD3	2.13	0.49
2:L:554:GLY:O	2:L:558:PHE:HB2	2.13	0.49
1:M:228:HIS:CB	1:M:260:PRO:HA	2.43	0.49
1:A:24:LEU:HD12	1:A:91:PHE:CD2	2.48	0.48
2:G:163:HIS:HA	2:G:240:LYS:HG3	1.95	0.48
2:I:265:ARG:HH11	2:I:539:PRO:HB3	1.78	0.48
1:M:188:VAL:HG21	1:M:193:PHE:HB2	1.95	0.48
1:A:52:LEU:O	2:L:426:ARG:NH2	2.45	0.48
2:C:300:GLY:HA2	2:C:309:THR:O	2.13	0.48
1:F:213:LEU:O	1:F:220:LYS:HE2	2.13	0.48
2:G:444:ASN:O	2:G:448:ARG:HG3	2.12	0.48
1:M:186:CYS:HB3	1:M:288:CYS:HB2	1.96	0.48
1:D:180:ILE:HB	1:D:217:LEU:HD13	1.95	0.48
1:D:286:ILE:HB	1:D:300:PHE:CD1	2.49	0.48
2:E:322:LEU:HD12	2:E:532:ASP:HB2	1.96	0.48
2:E:25:TRP:HB2	2:E:564:MET:CE	2.42	0.48
2:E:31:ILE:HG21	2:E:572:PRO:HG2	1.96	0.48
1:F:124:THR:HB	1:F:126:PRO:HD2	1.93	0.48
1:F:44:GLN:NE2	1:F:191:ASP:OD2	2.34	0.48
1:F:266:VAL:O	1:F:270:GLY:N	2.46	0.48
1:F:185:GLY:CA	1:F:289:THR:HG22	2.40	0.48
1:H:347:THR:HG21	1:M:160:GLY:HA2	1.95	0.48
2:I:391:THR:HG21	2:I:502:GLY:HA3	1.94	0.48
2:L:340:ASN:HA	2:L:345:ASN:O	2.13	0.48
1:F:186:CYS:SG	2:L:79:ARG:HD3	2.53	0.48
2:C:522:PRO:O	2:C:525:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:301:VAL:O	2:E:307:LEU:HD12	2.14	0.48
1:F:294:PRO:O	1:F:298:MET:HG3	2.14	0.48
2:G:103:LYS:HE2	2:G:281:CYS:O	2.13	0.48
2:I:525:PRO:HG3	2:I:577:GLY:HA2	1.96	0.48
2:K:272:TRP:CZ3	2:K:503:VAL:HB	2.48	0.48
2:L:535:GLY:O	2:L:537:PRO:HD3	2.13	0.48
1:M:105:ASN:HB3	1:M:106:GLY:HA3	1.93	0.48
1:D:304:PRO:HG2	1:D:307:ALA:CB	2.44	0.48
2:E:286:ARG:HA	2:E:343:LEU:CD1	2.34	0.48
2:G:329:GLN:O	2:G:330:ASP:HB3	2.14	0.48
1:H:346:THR:O	1:H:346:THR:HG22	2.14	0.48
2:I:158:PRO:HD2	2:I:247:ASP:HB2	1.95	0.48
1:A:18:LEU:HG	1:A:20:GLU:O	2.14	0.48
1:B:26:ILE:HD12	1:B:93:LEU:HD11	1.95	0.48
2:C:138:GLU:O	2:C:142:ARG:HG3	2.13	0.48
2:E:259:TYR:CE2	2:E:550:PHE:HB2	2.49	0.48
2:I:27:PRO:HD3	1:M:77:MET:HE2	1.96	0.48
2:I:289:THR:HG23	2:I:311:ASP:OD1	2.13	0.48
2:K:349:ARG:O	2:K:349:ARG:HD2	2.13	0.48
2:L:238:MET:HE1	2:L:238:MET:HA	1.95	0.48
2:L:26:ASP:OD2	2:L:36:GLY:HA3	2.14	0.48
2:L:366:PHE:HA	2:L:370:TYR:HD2	1.76	0.48
2:L:406:GLY:O	2:L:407:LEU:HD12	2.14	0.48
2:L:501:ARG:HG2	2:L:571:ASP:HB3	1.95	0.48
1:A:155:GLU:HB2	1:F:338:TRP:CH2	2.49	0.48
2:C:512:ASP:O	2:C:514:LYS:HG3	2.13	0.48
2:E:331:TRP:HB2	2:E:334:GLU:HB2	1.95	0.48
2:K:242:VAL:N	2:K:243:PRO:HD2	2.29	0.48
2:L:122:PHE:HA	2:L:193:THR:HG21	1.96	0.48
2:L:130:ASN:C	2:L:131:LEU:HD12	2.34	0.48
2:C:190:SER:HA	2:C:193:THR:CG2	2.44	0.48
1:D:138:ALA:HB2	1:D:178:LEU:HD12	1.95	0.48
2:E:79:ARG:HA	2:E:206:HIS:CE1	2.49	0.48
2:L:127:PHE:CD1	2:L:131:LEU:HD22	2.49	0.48
2:L:301:VAL:CG2	2:L:308:LEU:HB2	2.37	0.48
2:L:242:VAL:HA	2:L:453:THR:HG21	1.95	0.48
1:M:45:PRO:HD2	1:M:194:MET:HB3	1.96	0.48
1:D:187:PRO:HD3	2:E:206:HIS:CD2	2.47	0.48
2:E:501:ARG:HG3	2:E:501:ARG:HH11	1.79	0.48
2:G:342:PRO:HD3	2:G:492:ILE:HD11	1.95	0.48
2:I:70:PRO:O	2:I:73:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:224:PHE:O	2:K:228:ILE:HG13	2.14	0.48
2:L:324:GLY:O	2:L:325:SER:HB3	2.14	0.48
1:B:155:GLU:HB2	1:D:338:TRP:CZ2	2.49	0.48
2:E:524:THR:N	2:E:525:PRO:HD2	2.29	0.48
1:F:105:ASN:HB3	1:F:106:GLY:H	1.46	0.48
1:H:47:VAL:HG13	1:H:48:GLU:N	2.28	0.48
2:L:163:HIS:HB3	2:L:165:TYR:CD2	2.48	0.48
1:A:309:LEU:HB3	1:H:320:LEU:HD21	1.96	0.47
1:B:32:CYS:O	1:B:33:ASP:HB2	2.13	0.47
2:C:398:ARG:HE	2:C:498:GLU:HG3	1.79	0.47
2:E:286:ARG:HG3	2:E:287:THR:N	2.29	0.47
2:E:398:ARG:HD2	2:E:455:PHE:CE1	2.48	0.47
2:G:313:VAL:O	2:G:317:LEU:HG	2.13	0.47
1:B:243:ALA:CB	1:B:248:ASN:HB3	2.44	0.47
2:C:118:ALA:HA	2:C:121:MET:CE	2.38	0.47
1:D:326:LYS:HA	1:D:326:LYS:HE2	1.96	0.47
2:K:393:GLY:HA3	2:K:452:ARG:NH2	2.23	0.47
2:L:265:ARG:NH1	2:L:539:PRO:HA	2.29	0.47
2:C:576:CYS:CB	5:C:701:NFU:C2	2.92	0.47
1:D:260:PRO:HG2	4:D:701:MLA:HC21	1.97	0.47
2:E:265:ARG:HB2	2:E:265:ARG:HH11	1.79	0.47
2:E:440:PRO:C	2:E:442:TRP:H	2.17	0.47
1:F:105:ASN:HD21	2:L:361:PRO:HG2	1.79	0.47
2:G:336:THR:CG2	2:G:354:ASN:HB3	2.45	0.47
2:G:501:ARG:NH1	2:G:573:CYS:HB2	2.29	0.47
2:G:71:ARG:HD3	2:G:487:VAL:HG21	1.95	0.47
2:I:27:PRO:HD3	1:M:77:MET:HE1	1.95	0.47
2:I:325:SER:HB2	2:I:530:PRO:HB2	1.97	0.47
2:K:127:PHE:CZ	2:K:571:ASP:HA	2.49	0.47
2:L:285:TYR:CD2	2:L:342:PRO:HD2	2.49	0.47
1:A:119:THR:CG2	1:A:121:GLN:HG3	2.39	0.47
1:A:41:ALA:HB2	2:C:194:ARG:NH1	2.29	0.47
2:E:398:ARG:NH2	2:E:500:VAL:O	2.46	0.47
1:F:119:THR:O	1:F:121:GLN:N	2.47	0.47
1:F:227:VAL:HG13	1:F:267:PRO:HG3	1.95	0.47
2:G:31:ILE:HD11	2:G:35:LEU:HB3	1.96	0.47
2:G:351:HIS:CG	2:G:352:PRO:HD2	2.49	0.47
2:G:561:ILE:O	2:G:565:ARG:HG3	2.15	0.47
2:I:68:LYS:O	2:I:515:ILE:HG13	2.14	0.47
2:L:256:LEU:O	2:L:259:TYR:HB2	2.14	0.47
2:L:61:TYR:OH	2:L:79:ARG:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:MET:O	2:C:217:THR:OG1	2.30	0.47
1:D:6:VAL:HG13	1:D:10:ARG:NH1	2.30	0.47
2:E:250:ASP:OD1	2:E:450:ARG:NH2	2.47	0.47
1:F:167:TYR:HD2	1:F:168:LEU:CD1	2.27	0.47
1:H:187:PRO:HB3	3:H:503:SF4:S2	2.54	0.47
1:H:213:LEU:HA	1:H:218:ARG:O	2.15	0.47
2:I:564:MET:HA	2:I:564:MET:CE	2.44	0.47
2:K:341:ASP:HB2	2:K:342:PRO:HD2	1.97	0.47
1:B:133:ALA:N	1:B:134:PRO:HD2	2.29	0.47
1:B:347:THR:HG21	1:D:157:ASN:H	1.79	0.47
2:C:122:PHE:HB2	2:C:193:THR:CG2	2.43	0.47
2:C:322:LEU:HD23	2:C:350:LYS:HD3	1.96	0.47
1:D:51:VAL:HG23	1:D:52:LEU:N	2.29	0.47
2:E:148:VAL:HA	2:E:151:LYS:CD	2.44	0.47
2:E:163:HIS:CE1	2:E:165:TYR:HB2	2.50	0.47
1:F:41:ALA:HB2	2:L:194:ARG:CZ	2.44	0.47
2:I:398:ARG:NE	2:I:498:GLU:HG2	2.29	0.47
2:L:353:TRP:HH2	2:L:493:GLY:H	1.63	0.47
1:A:111:ALA:HA	2:C:56:SER:O	2.15	0.47
2:C:190:SER:HA	2:C:193:THR:HG22	1.96	0.47
1:D:22:HIS:O	1:D:91:PHE:HA	2.14	0.47
2:E:274:SER:CB	2:E:297:VAL:HB	2.44	0.47
2:E:303:VAL:HA	2:E:304:ASP:HA	1.58	0.47
2:G:127:PHE:CZ	2:G:132:VAL:HG23	2.50	0.47
1:H:119:THR:O	1:H:120:HIS:HB2	2.15	0.47
1:H:41:ALA:HB2	2:K:194:ARG:CZ	2.45	0.47
2:K:163:HIS:HB2	2:K:164:GLY:HA2	1.96	0.47
1:B:119:THR:HG22	1:B:121:GLN:HG2	1.97	0.47
1:B:258:TRP:O	1:B:262:VAL:HG23	2.15	0.47
2:E:371:THR:CG2	2:E:530:PRO:CG	2.92	0.47
1:F:154:MET:HG2	1:F:155:GLU:N	2.28	0.47
1:F:197:LEU:HD12	1:F:197:LEU:O	2.14	0.47
1:F:320:LEU:HD11	1:H:321:ILE:CD1	2.44	0.47
1:H:321:ILE:HD11	1:M:310:SER:HB3	1.97	0.47
1:H:70:TYR:CE2	2:K:140:MET:HE2	2.49	0.47
2:I:549:ILE:N	2:I:549:ILE:HD12	2.30	0.47
2:K:129:ASP:HB2	2:K:186:THR:HG21	1.96	0.47
2:L:122:PHE:HB2	2:L:193:THR:CG2	2.42	0.47
2:L:528:ALA:HB2	2:L:540:TYR:CE2	2.50	0.47
2:E:558:PHE:CZ	2:E:560:GLY:HA2	2.50	0.47
1:F:32:CYS:HB2	2:L:81:CYS:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:571:ASP:N	2:G:572:PRO:HD3	2.29	0.47
1:H:295:ASP:HA	1:H:298:MET:HE3	1.94	0.47
2:K:311:ASP:HB3	2:K:314:ASP:HB2	1.95	0.47
2:L:150:GLU:OE1	2:L:153:LYS:HE2	2.15	0.47
2:L:273:GLY:HA2	2:L:297:VAL:O	2.15	0.47
2:L:413:ILE:CD1	2:L:422:ILE:HG23	2.45	0.47
2:L:511:ARG:HB2	2:L:516:ALA:HB2	1.96	0.47
1:F:72:ASN:ND2	2:L:564:MET:SD	2.88	0.47
1:B:180:ILE:HB	1:B:217:LEU:HD13	1.97	0.47
2:C:378:TRP:HB2	2:C:389:LEU:HD12	1.96	0.47
1:D:48:GLU:HA	1:D:51:VAL:HG22	1.97	0.47
2:G:274:SER:HB3	2:G:297:VAL:HB	1.97	0.47
2:K:21:VAL:HG21	2:K:43:PHE:CE1	2.50	0.47
1:M:238:GLU:OE1	1:M:239:GLN:HG3	2.14	0.47
1:A:152:HIS:NE2	2:C:59:ARG:HD2	2.30	0.47
1:B:288:CYS:HA	1:B:293:PHE:CG	2.50	0.47
2:C:392:GLY:HA3	2:C:394:GLY:CA	2.45	0.47
2:C:394:GLY:H	2:C:395:PRO:CD	2.28	0.47
1:D:107:GLU:O	2:E:363:LYS:N	2.49	0.47
1:D:183:VAL:HG12	1:D:188:VAL:HG22	1.97	0.47
2:E:242:VAL:HG11	2:E:435:PHE:CE1	2.49	0.47
1:F:6:VAL:HG13	1:F:10:ARG:HE	1.80	0.47
2:G:265:ARG:NH1	2:G:390:ASP:HB3	2.30	0.47
1:H:152:HIS:CD2	2:K:59:ARG:HD2	2.51	0.47
1:H:152:HIS:NE2	2:K:59:ARG:HD2	2.29	0.47
2:L:341:ASP:HB2	2:L:342:PRO:HD2	1.97	0.47
1:D:105:ASN:CB	1:D:106:GLY:HA3	2.40	0.46
2:G:311:ASP:OD1	2:G:313:VAL:HG22	2.16	0.46
2:I:371:THR:HG21	2:I:530:PRO:HG3	1.96	0.46
2:K:412:TYR:HB3	2:K:461:ALA:HB1	1.97	0.46
2:C:399:LEU:HD13	2:C:437:TRP:CG	2.51	0.46
2:E:33:GLY:HA3	2:E:574:LEU:HB2	1.97	0.46
2:G:77:THR:HG21	2:G:518:TYR:CE1	2.50	0.46
2:I:92:SER:O	2:I:96:GLN:HG3	2.16	0.46
2:K:30:ARG:NH2	2:K:135:ASP:OD1	2.48	0.46
2:L:187:LEU:O	2:L:191:ARG:HG3	2.15	0.46
2:L:564:MET:CE	2:L:564:MET:HA	2.45	0.46
1:A:288:CYS:HA	1:A:293:PHE:CD1	2.50	0.46
1:B:119:THR:HB	1:B:121:GLN:HG2	1.97	0.46
1:B:185:GLY:HA2	1:B:289:THR:CG2	2.45	0.46
2:E:377:ARG:HD2	2:E:388:ALA:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:529:SER:O	2:G:538:GLY:HA3	2.16	0.46
2:K:55:SER:OG	2:K:574:LEU:HD23	2.15	0.46
2:L:523:PRO:HD2	5:L:701:NFU:C2	2.44	0.46
2:L:79:ARG:HA	2:L:206:HIS:CE1	2.51	0.46
1:M:78:ALA:N	1:M:79:PRO:HD2	2.31	0.46
1:B:82:LYS:HG3	1:B:87:GLU:HB2	1.98	0.46
2:C:385:ASP:N	2:C:385:ASP:OD1	2.47	0.46
2:E:35:LEU:CA	2:E:574:LEU:HD11	2.46	0.46
1:F:32:CYS:HB2	2:L:82:GLY:N	2.30	0.46
1:H:286:ILE:HB	1:H:300:PHE:CD1	2.50	0.46
2:K:274:SER:CB	2:K:297:VAL:HB	2.46	0.46
2:C:371:THR:HG21	2:C:530:PRO:HG3	1.97	0.46
2:C:69:ASP:O	2:C:72:ASP:HB2	2.16	0.46
1:D:324:LEU:HD21	1:M:320:LEU:HD11	1.98	0.46
2:E:21:VAL:HG21	2:E:43:PHE:HE2	1.78	0.46
2:I:158:PRO:HD2	2:I:247:ASP:CB	2.46	0.46
2:I:247:ASP:HA	2:I:250:ASP:HB2	1.98	0.46
2:K:145:ASN:HB3	2:K:148:VAL:HG23	1.96	0.46
1:A:183:VAL:HG12	1:A:188:VAL:CG2	2.46	0.46
1:B:94:VAL:HG22	1:B:140:VAL:HB	1.97	0.46
2:C:430:LYS:HD3	2:C:430:LYS:HA	1.82	0.46
1:B:313:LEU:HD11	1:D:317:TYR:CD1	2.50	0.46
2:E:192:TYR:O	2:E:196:MET:HG3	2.15	0.46
2:E:265:ARG:NH2	2:E:268:LEU:HD12	2.30	0.46
2:E:273:GLY:HA3	2:E:295:MET:HE1	1.94	0.46
1:F:115:THR:HA	1:F:121:GLN:O	2.16	0.46
2:G:412:TYR:HB3	2:G:461:ALA:HB1	1.97	0.46
2:L:323:LEU:HD12	2:L:323:LEU:N	2.31	0.46
2:C:341:ASP:HB2	2:C:342:PRO:CD	2.46	0.46
2:C:380:ASP:HB2	2:C:387:LEU:HD13	1.96	0.46
2:E:265:ARG:HD2	2:E:543:ALA:N	2.30	0.46
2:E:323:LEU:N	2:E:323:LEU:HD12	2.31	0.46
1:F:89:ASP:N	1:F:89:ASP:OD1	2.31	0.46
2:L:28:ILE:HD12	2:L:35:LEU:CD2	2.46	0.46
2:I:206:HIS:HE1	3:M:704:SF4:S2	2.39	0.46
1:B:253:VAL:HA	1:B:257:CYS:HB3	1.98	0.46
1:B:78:ALA:HB3	1:B:79:PRO:HD3	1.97	0.46
2:C:348:ASP:OD1	2:C:349:ARG:N	2.48	0.46
1:D:215:GLU:H	1:D:215:GLU:CD	2.19	0.46
1:F:55:ILE:HD11	1:F:202:TYR:CZ	2.50	0.46
1:F:34:GLY:CA	2:L:82:GLY:HA3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:GLY:HA2	2:K:211:TYR:OH	2.16	0.46
2:L:253:TYR:CE1	2:L:260:GLU:HB2	2.51	0.46
2:L:525:PRO:HD3	2:L:577:GLY:HA2	1.96	0.46
1:B:234:ALA:HB3	1:D:234:ALA:HB3	1.98	0.46
2:E:263:GLY:HA2	2:E:543:ALA:O	2.15	0.46
2:G:265:ARG:HH11	2:G:390:ASP:HB3	1.81	0.46
2:G:574:LEU:N	2:G:575:PRO:CD	2.79	0.46
1:H:228:HIS:HB2	1:H:260:PRO:HA	1.98	0.46
2:I:177:PRO:HA	2:I:183:TYR:CD2	2.50	0.46
2:I:193:THR:O	2:I:196:MET:HB2	2.16	0.46
1:M:325:ARG:NE	4:M:705:MLA:O1A	2.32	0.46
1:B:258:TRP:CE2	1:B:304:PRO:HB3	2.50	0.46
1:D:286:ILE:HB	1:D:300:PHE:CE1	2.50	0.46
2:E:336:THR:HG22	2:E:337:SER:N	2.31	0.46
2:E:33:GLY:CA	2:E:575:PRO:HD3	2.43	0.46
1:H:24:LEU:HB3	1:H:80:PHE:CE1	2.51	0.46
1:H:253:VAL:HB	3:H:501:SF4:S4	2.56	0.46
2:I:189:VAL:HA	2:I:192:TYR:CE2	2.51	0.46
2:I:30:ARG:HD3	1:M:69:ALA:O	2.15	0.46
2:K:89:ALA:O	2:K:93:VAL:HG23	2.16	0.46
2:L:272:TRP:CZ3	2:L:505:SER:HB3	2.51	0.46
2:L:303:VAL:CG2	2:L:308:LEU:HD11	2.46	0.46
1:M:280:ASN:N	1:M:280:ASN:OD1	2.48	0.46
1:D:320:LEU:O	1:D:324:LEU:HD23	2.16	0.45
1:F:239:GLN:HB2	1:F:239:GLN:HE21	1.54	0.45
1:H:125:ILE:HB	1:H:126:PRO:HD3	1.97	0.45
2:K:330:ASP:OD1	2:K:349:ARG:NH1	2.32	0.45
2:K:81:CYS:SG	2:K:82:GLY:N	2.89	0.45
2:L:163:HIS:N	2:L:164:GLY:HA2	2.30	0.45
2:E:290:LYS:HD3	2:E:293:ARG:NH1	2.32	0.45
2:E:307:LEU:HD22	2:E:404:LEU:HB2	1.97	0.45
2:G:266:ARG:CD	2:G:268:LEU:HD21	2.44	0.45
1:H:105:ASN:CB	1:H:106:GLY:HA3	2.47	0.45
1:H:77:MET:O	1:H:80:PHE:HB2	2.16	0.45
2:L:100:TYR:CD1	2:L:100:TYR:N	2.84	0.45
1:A:233:ARG:O	1:A:236:SER:HB3	2.16	0.45
1:A:266:VAL:HB	1:A:267:PRO:HD3	1.98	0.45
1:B:347:THR:HG21	1:D:157:ASN:N	2.32	0.45
1:D:320:LEU:HD22	1:H:313:LEU:CD2	2.47	0.45
2:E:286:ARG:HG3	2:E:287:THR:H	1.81	0.45
2:E:61:TYR:HA	2:E:64:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:217:THR:O	2:G:219:PRO:HD3	2.17	0.45
1:H:307:ALA:O	1:H:311:SER:N	2.42	0.45
1:H:331:THR:O	1:M:296:LYS:NZ	2.35	0.45
2:I:259:TYR:CZ	2:I:262:VAL:HG21	2.51	0.45
2:I:378:TRP:HB2	2:I:389:LEU:HD12	1.98	0.45
2:I:83:ILE:HG12	2:I:123:ASP:OD2	2.16	0.45
2:K:145:ASN:HB3	2:K:148:VAL:CG2	2.46	0.45
2:K:321:ILE:HD12	2:K:321:ILE:N	2.31	0.45
2:L:112:ILE:O	2:L:116:GLU:HG2	2.16	0.45
2:L:249:PHE:CZ	2:L:449:ASP:HB3	2.51	0.45
1:M:109:TYR:CZ	1:M:122:PRO:HG2	2.51	0.45
1:A:180:ILE:HB	1:A:217:LEU:HD13	1.98	0.45
2:C:235:VAL:HG13	2:C:424:LEU:HD22	1.97	0.45
1:D:113:MET:HG3	1:D:128:TRP:HE1	1.82	0.45
2:E:265:ARG:NH1	2:E:390:ASP:OD1	2.49	0.45
2:G:239:LYS:NZ	2:G:427:THR:HG23	2.31	0.45
2:G:475:HIS:O	2:G:476:ALA:CB	2.64	0.45
2:I:249:PHE:HB3	2:I:446:ILE:CG2	2.47	0.45
2:K:335:GLU:H	2:K:335:GLU:CD	2.19	0.45
2:L:412:TYR:HA	2:L:423:TYR:HB3	1.99	0.45
2:L:61:TYR:HA	2:L:64:PHE:CE2	2.51	0.45
2:L:79:ARG:HG3	2:L:79:ARG:HH11	1.80	0.45
2:L:78:SER:HB2	2:L:89:ALA:HB2	1.99	0.45
1:A:78:ALA:N	1:A:79:PRO:HD2	2.31	0.45
2:C:273:GLY:HA2	2:C:297:VAL:O	2.16	0.45
2:E:242:VAL:HB	2:E:243:PRO:CD	2.40	0.45
1:F:254:LYS:CE	1:F:311:SER:HB3	2.45	0.45
2:G:206:HIS:HA	2:G:207:PRO:HD3	1.77	0.45
2:I:157:ALA:H	2:I:167:THR:H	1.65	0.45
2:I:274:SER:HB3	2:I:297:VAL:HB	1.97	0.45
2:I:74:HIS:CE1	2:I:212:PRO:HD3	2.52	0.45
2:K:126:ILE:O	2:K:130:ASN:HB2	2.15	0.45
2:L:57:ILE:O	2:L:578:VAL:HG11	2.17	0.45
1:B:111:ALA:HA	2:G:56:SER:O	2.17	0.45
2:C:241:VAL:HG13	2:C:245:HIS:CE1	2.52	0.45
1:D:165:ALA:HB1	1:D:170:TRP:CD2	2.52	0.45
2:E:395:PRO:HG2	2:E:452:ARG:HG3	1.97	0.45
1:F:140:VAL:HG22	1:F:181:VAL:HB	1.98	0.45
1:H:78:ALA:N	1:H:79:PRO:HD2	2.32	0.45
2:I:360:ARG:O	2:I:362:GLN:HG2	2.17	0.45
2:I:452:ARG:O	2:I:456:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:353:TRP:HZ3	2:L:508:LEU:O	2.00	0.45
1:A:234:ALA:HB3	1:F:234:ALA:CB	2.26	0.45
2:C:105:PRO:HG2	2:C:482:PHE:N	2.31	0.45
2:C:132:VAL:HG22	2:C:568:ARG:HB3	1.98	0.45
2:C:359:PRO:O	2:C:360:ARG:HD3	2.16	0.45
2:C:45:ASN:HB3	2:C:47:ARG:HG2	1.98	0.45
1:D:71:GLU:OE1	1:D:71:GLU:N	2.47	0.45
2:I:155:ALA:O	2:I:167:THR:HA	2.17	0.45
2:I:256:LEU:O	2:I:259:TYR:HB2	2.16	0.45
2:L:200:MET:O	2:L:217:THR:OG1	2.30	0.45
2:L:393:GLY:HA2	2:L:570:PHE:O	2.16	0.45
2:C:139:GLN:O	2:C:143:GLU:HG3	2.17	0.45
2:E:80:ILE:HD11	2:E:520:PRO:HG3	1.97	0.45
2:G:248:LEU:O	2:G:251:PHE:HB3	2.17	0.45
1:H:269:ARG:NH1	2:I:222:GLN:OE1	2.50	0.45
2:I:357:THR:HG22	2:I:359:PRO:HD3	1.99	0.45
2:I:410:ILE:O	2:I:412:TYR:N	2.48	0.45
2:I:63:ILE:HD12	1:M:158:PRO:HG3	1.99	0.45
2:K:375:SER:HA	2:K:529:SER:HB2	1.98	0.45
2:L:549:ILE:HD13	2:L:558:PHE:CZ	2.52	0.45
1:M:246:TYR:CE1	1:M:255:LEU:HB3	2.52	0.45
1:D:99:ILE:HA	1:D:100:PRO:HD3	1.85	0.45
1:D:246:TYR:CE1	1:D:255:LEU:HB3	2.52	0.45
2:E:398:ARG:NH1	2:E:455:PHE:CE2	2.85	0.45
1:A:310:SER:OG	1:F:321:ILE:HD11	2.17	0.45
2:I:224:PHE:O	2:I:228:ILE:HG13	2.17	0.45
1:M:191:ASP:O	1:M:195:GLU:HG3	2.17	0.45
1:A:183:VAL:HG12	1:A:188:VAL:HG23	1.98	0.45
2:C:107:ILE:HG23	2:C:481:THR:HG22	1.98	0.45
1:D:138:ALA:HB2	1:D:178:LEU:CD1	2.47	0.45
1:F:116:ASP:O	1:F:120:HIS:HA	2.17	0.45
1:H:105:ASN:HB3	1:H:106:GLY:O	2.16	0.45
1:H:278:CYS:CB	1:H:279:PRO:CD	2.91	0.45
2:L:188:LEU:HD23	2:L:191:ARG:NH1	2.32	0.45
2:L:413:ILE:HD11	2:L:422:ILE:HG23	1.99	0.45
1:M:185:GLY:CA	1:M:289:THR:HG22	2.41	0.45
1:M:318:GLY:O	1:M:321:ILE:HG22	2.17	0.45
1:B:178:LEU:N	1:B:178:LEU:HD12	2.33	0.44
2:C:190:SER:C	2:C:193:THR:HG22	2.38	0.44
2:E:150:GLU:HA	2:E:153:LYS:HE2	1.99	0.44
1:F:25:TRP:HD1	1:F:27:THR:HG23	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:277:ASP:HA	2:L:278:PRO:HD2	1.84	0.44
1:B:78:ALA:HB3	1:B:79:PRO:CD	2.47	0.44
2:C:156:GLU:HA	2:C:167:THR:HA	1.99	0.44
1:A:41:ALA:HB2	2:C:194:ARG:CZ	2.48	0.44
2:E:387:LEU:H	2:E:387:LEU:CD2	2.28	0.44
2:E:400:TRP:CZ2	2:E:439:ILE:HG23	2.53	0.44
2:E:541:GLU:CA	2:E:544:VAL:HG12	2.46	0.44
1:F:106:GLY:HA2	1:F:107:GLU:O	2.17	0.44
2:I:419:SER:HB2	2:I:437:TRP:O	2.17	0.44
2:L:412:TYR:O	2:L:422:ILE:HA	2.18	0.44
1:B:298:MET:HA	1:B:299:PRO:C	2.37	0.44
2:C:187:LEU:HD23	2:C:187:LEU:HA	1.89	0.44
2:E:24:ASN:HB3	2:E:38:TYR:HA	1.97	0.44
2:G:124:HIS:CE1	2:G:500:VAL:HG13	2.52	0.44
2:I:206:HIS:HA	2:I:207:PRO:HD2	1.82	0.44
2:L:190:SER:C	2:L:193:THR:HG22	2.38	0.44
2:L:375:SER:HA	2:L:529:SER:HB2	1.99	0.44
2:C:533:ILE:HG13	2:C:534:TYR:CD1	2.53	0.44
2:E:311:ASP:HB3	2:E:314:ASP:HB2	2.00	0.44
1:F:307:ALA:O	1:F:311:SER:OG	2.27	0.44
2:G:104:PRO:HB3	2:G:213:GLY:O	2.18	0.44
2:I:109:ASP:HB3	2:I:278:PRO:HG3	2.00	0.44
2:I:522:PRO:HB3	5:I:701:NFU:O3	2.17	0.44
2:L:549:ILE:HD13	2:L:558:PHE:HZ	1.82	0.44
1:M:32:CYS:O	1:M:33:ASP:HB2	2.17	0.44
1:A:228:HIS:HB3	1:A:260:PRO:HA	1.99	0.44
1:B:271:TRP:HD1	1:B:272:ILE:HG13	1.79	0.44
2:C:127:PHE:HD1	2:C:131:LEU:HD12	1.82	0.44
2:E:522:PRO:C	2:E:525:PRO:HD2	2.38	0.44
2:L:391:THR:HG21	2:L:503:VAL:H	1.82	0.44
2:C:211:TYR:HB3	2:C:212:PRO:HD2	2.00	0.44
1:D:293:PHE:CD1	1:D:294:PRO:HA	2.53	0.44
1:F:27:THR:OG1	1:F:66:PRO:HG2	2.18	0.44
2:K:295:MET:HE2	2:K:312:LEU:HD11	1.98	0.44
2:L:69:ASP:HA	2:L:514:LYS:CD	2.46	0.44
1:M:143:GLY:O	1:M:147:THR:HG23	2.18	0.44
1:A:32:CYS:O	1:A:33:ASP:HB2	2.18	0.44
1:B:165:ALA:HB1	1:B:170:TRP:CD2	2.52	0.44
2:C:395:PRO:HG2	2:C:452:ARG:HA	1.99	0.44
2:G:231:LEU:O	2:G:235:VAL:HG23	2.18	0.44
1:H:308:VAL:O	1:H:312:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:ASP:N	1:H:89:ASP:OD1	2.41	0.44
2:I:576:CYS:CB	5:I:701:NFU:C2	2.96	0.44
2:K:92:SER:O	2:K:96:GLN:HG3	2.17	0.44
1:M:15:THR:CG2	1:M:19:LYS:HE2	2.42	0.44
1:A:154:MET:HG2	1:A:155:GLU:N	2.32	0.44
1:A:248:ASN:CG	1:A:249:PRO:HD2	2.37	0.44
1:A:288:CYS:HA	1:A:293:PHE:CG	2.53	0.44
2:C:288:MET:HA	2:C:291:TRP:NE1	2.32	0.44
2:C:127:PHE:CZ	2:C:571:ASP:HA	2.52	0.44
2:E:261:GLU:HB3	2:E:548:PRO:CG	2.48	0.44
2:E:548:PRO:O	2:E:549:ILE:HD12	2.18	0.44
1:F:99:ILE:HG23	1:F:125:ILE:HG21	1.99	0.44
2:K:138:GLU:HB3	2:K:176:ASN:HD21	1.83	0.44
2:L:189:VAL:HA	2:L:192:TYR:CE2	2.52	0.44
2:L:79:ARG:HH11	2:L:79:ARG:CG	2.30	0.44
1:M:119:THR:O	1:M:120:HIS:HB2	2.17	0.44
1:M:304:PRO:HG2	1:M:307:ALA:HB2	1.99	0.44
1:B:116:ASP:O	1:B:120:HIS:HA	2.18	0.44
1:B:187:PRO:HD3	2:G:206:HIS:HD2	1.81	0.44
1:B:211:ILE:HG23	1:B:213:LEU:HD11	1.99	0.44
2:C:522:PRO:HB3	5:C:701:NFU:C3	2.48	0.44
1:D:89:ASP:N	1:D:89:ASP:OD1	2.49	0.44
2:E:378:TRP:O	2:E:386:HIS:HA	2.17	0.44
2:E:394:GLY:N	2:E:395:PRO:HD3	2.33	0.44
2:G:323:LEU:N	2:G:323:LEU:HD12	2.32	0.44
2:G:329:GLN:OE1	2:G:360:ARG:NH2	2.50	0.44
2:G:398:ARG:NE	2:G:498:GLU:HG2	2.33	0.44
1:H:137:LEU:O	1:H:176:ALA:HB3	2.18	0.44
1:M:39:ILE:HD12	1:M:194:MET:HE2	1.99	0.44
1:M:253:VAL:HB	3:M:702:SF4:S4	2.58	0.44
1:A:78:ALA:HB3	1:A:79:PRO:CD	2.47	0.43
1:B:101:ASN:OD1	1:B:104:ILE:HG23	2.18	0.43
2:C:272:TRP:CH2	2:C:319:ILE:HD11	2.53	0.43
2:E:189:VAL:HA	2:E:192:TYR:CE2	2.53	0.43
2:E:406:GLY:HA2	2:E:415:SER:HB3	1.99	0.43
2:E:412:TYR:OH	2:E:468:GLU:OE2	2.30	0.43
2:E:469:GLN:O	2:E:473:GLU:HG2	2.17	0.43
1:F:105:ASN:C	1:F:107:GLU:HB2	2.36	0.43
1:F:84:ALA:O	1:F:135:LYS:HE3	2.18	0.43
2:G:574:LEU:N	2:G:574:LEU:HD22	2.33	0.43
2:I:249:PHE:HB3	2:I:446:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:531:ARG:HH11	2:I:531:ARG:HG3	1.83	0.43
2:K:492:ILE:O	2:K:492:ILE:HG13	2.18	0.43
2:L:134:VAL:HG22	2:L:177:PRO:HG3	2.00	0.43
2:L:259:TYR:CE2	2:L:262:VAL:HG21	2.52	0.43
2:L:35:LEU:HB2	2:L:574:LEU:CD2	2.47	0.43
1:B:345:LEU:HD23	1:B:347:THR:H	1.83	0.43
1:D:324:LEU:CD2	1:M:320:LEU:HD11	2.48	0.43
1:B:73:GLY:HA2	2:G:27:PRO:O	2.18	0.43
1:H:256:GLY:HA2	1:H:302:ASP:O	2.18	0.43
1:H:65:ASN:HA	1:H:66:PRO:HD3	1.89	0.43
2:I:444:ASN:HD21	2:I:447:GLU:HG2	1.83	0.43
2:K:563:ILE:HG22	2:K:564:MET:CE	2.48	0.43
2:E:29:THR:O	2:E:568:ARG:NH2	2.46	0.43
2:G:419:SER:HB2	2:G:437:TRP:O	2.19	0.43
1:H:133:ALA:N	1:H:134:PRO:HD2	2.33	0.43
1:H:183:VAL:HG12	1:H:188:VAL:CG2	2.48	0.43
2:L:168:ILE:HD13	2:L:247:ASP:O	2.18	0.43
2:L:274:SER:HB2	2:L:498:GLU:HB3	2.00	0.43
2:L:522:PRO:CB	2:L:576:CYS:HB3	2.48	0.43
2:L:527:ASN:HA	2:L:539:PRO:HG2	2.00	0.43
1:M:309:LEU:N	1:M:309:LEU:HD12	2.34	0.43
1:A:55:ILE:O	1:A:58:LEU:HD12	2.17	0.43
1:B:45:PRO:HD2	1:B:194:MET:HB3	2.01	0.43
1:B:327:LEU:O	1:B:330:ASP:HB2	2.18	0.43
2:C:191:ARG:O	2:C:195:GLU:HG3	2.17	0.43
2:E:321:ILE:HD13	2:E:352:PRO:HD3	2.00	0.43
2:E:486:LYS:O	2:E:488:PRO:HD3	2.17	0.43
1:F:313:LEU:HD23	1:F:315:LYS:HD3	2.00	0.43
1:H:266:VAL:O	1:H:270:GLY:N	2.43	0.43
2:I:244:LEU:O	2:I:244:LEU:HD23	2.18	0.43
2:I:77:THR:HG21	2:I:518:TYR:CE1	2.52	0.43
2:K:525:PRO:CD	2:K:577:GLY:HA2	2.49	0.43
2:L:274:SER:H	2:L:297:VAL:HB	1.83	0.43
2:L:325:SER:CA	2:L:369:ASN:HA	2.47	0.43
2:L:439:ILE:HA	2:L:440:PRO:HD3	1.82	0.43
2:L:371:THR:CG2	2:L:530:PRO:HB3	2.45	0.43
1:M:127:GLU:O	1:M:131:ARG:HG2	2.18	0.43
1:B:99:ILE:HA	1:B:100:PRO:HD3	1.84	0.43
1:B:266:VAL:HB	1:B:267:PRO:HD3	2.00	0.43
2:C:122:PHE:HA	2:C:193:THR:HG21	2.00	0.43
2:C:574:LEU:N	2:C:575:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ALA:N	1:D:134:PRO:HD2	2.33	0.43
1:F:82:LYS:CG	1:F:87:GLU:HB2	2.45	0.43
2:G:221:ILE:HD12	2:G:221:ILE:HA	1.78	0.43
2:G:26:ASP:HA	2:G:27:PRO:HA	1.89	0.43
2:K:341:ASP:HB2	2:K:342:PRO:CD	2.48	0.43
2:C:307:LEU:HD21	2:C:310:THR:CG2	2.49	0.43
2:E:312:LEU:HD23	2:E:315:ILE:CG2	2.47	0.43
2:E:407:LEU:C	2:E:407:LEU:HD23	2.39	0.43
2:E:57:ILE:O	2:E:578:VAL:HG11	2.18	0.43
1:F:278:CYS:HB2	1:F:279:PRO:HD3	1.95	0.43
2:I:524:THR:HA	2:I:527:ASN:HD22	1.82	0.43
2:K:308:LEU:HD21	2:K:382:ARG:NH1	2.33	0.43
2:L:55:SER:OG	2:L:574:LEU:HD23	2.18	0.43
1:M:39:ILE:HB	1:M:194:MET:CE	2.47	0.43
1:A:191:ASP:O	1:A:195:GLU:HG3	2.19	0.43
1:B:166:ASP:N	1:B:166:ASP:OD1	2.51	0.43
1:B:211:ILE:O	1:B:211:ILE:HG23	2.18	0.43
2:C:392:GLY:HA2	2:C:396:ILE:CG2	2.23	0.43
2:E:277:ASP:HB3	2:E:280:VAL:CG2	2.41	0.43
2:E:524:THR:HB	2:E:525:PRO:HD3	2.00	0.43
2:E:541:GLU:HA	2:E:544:VAL:CG1	2.49	0.43
2:G:19:LYS:CG	2:G:20:LEU:N	2.81	0.43
2:G:394:GLY:N	2:G:395:PRO:CD	2.81	0.43
1:H:252:ILE:HG22	1:H:255:LEU:HD12	2.00	0.43
2:I:130:ASN:O	2:I:131:LEU:HD23	2.18	0.43
2:I:166:ARG:O	2:I:166:ARG:HG3	2.19	0.43
2:K:176:ASN:HA	2:K:177:PRO:HD3	1.89	0.43
2:L:546:ASN:O	2:L:548:PRO:HD3	2.18	0.43
1:M:15:THR:HG23	1:M:16:PRO:HD2	2.00	0.43
1:A:157:ASN:OD1	1:A:160:GLY:N	2.50	0.43
1:B:227:VAL:HB	1:B:259:GLY:HA2	2.01	0.43
2:C:298:THR:HA	2:C:299:PRO:HD3	1.88	0.43
1:D:110:TRP:CD2	1:D:159:THR:HG22	2.54	0.43
2:E:30:ARG:HD2	2:E:131:LEU:O	2.19	0.43
2:E:341:ASP:OD2	2:E:345:ASN:HB2	2.18	0.43
2:E:322:LEU:CD1	2:E:532:ASP:HB2	2.48	0.43
2:G:521:TYR:HA	2:G:522:PRO:HD2	1.70	0.43
2:G:522:PRO:HB2	2:G:523:PRO:HD2	2.01	0.43
2:I:400:TRP:CZ2	2:I:439:ILE:HG23	2.53	0.43
2:L:540:TYR:O	2:L:544:VAL:HG23	2.17	0.43
1:A:237:TYR:HD2	1:A:251:CYS:SG	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:HIS:CD2	2:G:59:ARG:HD2	2.54	0.43
2:C:532:ASP:OD1	2:C:536:THR:HG22	2.19	0.43
2:E:351:HIS:CG	2:E:352:PRO:HD2	2.53	0.43
2:E:371:THR:OG1	2:E:373:VAL:HG23	2.19	0.43
1:F:95:LEU:HD23	1:F:164:LEU:HD11	2.00	0.43
2:G:138:GLU:HB3	2:G:176:ASN:OD1	2.18	0.43
2:G:341:ASP:HB2	2:G:342:PRO:CD	2.49	0.43
1:H:318:GLY:N	1:H:319:PRO:HD2	2.34	0.43
2:I:274:SER:O	2:I:275:PHE:HB2	2.19	0.43
2:I:127:PHE:CZ	2:I:571:ASP:HA	2.53	0.43
2:K:395:PRO:CG	2:K:452:ARG:HA	2.48	0.43
2:K:371:THR:HG21	2:K:530:PRO:HG3	2.00	0.43
2:L:204:HIS:CD2	2:L:205:VAL:HA	2.52	0.43
2:L:399:LEU:HD12	2:L:451:ALA:HB1	2.00	0.43
1:M:230:GLY:HA3	1:M:268:LYS:HB2	1.99	0.43
1:D:35:ASP:O	1:D:39:ILE:HG23	2.19	0.43
2:E:551:GLU:CG	2:E:552:GLU:N	2.81	0.43
2:G:32:VAL:HG12	2:G:575:PRO:HG2	2.00	0.43
2:G:353:TRP:CD1	2:G:507:HIS:HB3	2.53	0.43
2:G:371:THR:CG2	2:G:530:PRO:HG3	2.49	0.43
2:I:396:ILE:O	2:I:400:TRP:HB2	2.19	0.43
2:I:81:CYS:HA	1:M:32:CYS:HB2	2.01	0.43
2:K:255:ALA:C	2:K:257:PRO:HD3	2.39	0.43
2:L:267:ILE:HG23	2:L:269:LEU:HD12	2.01	0.43
2:L:353:TRP:HH2	2:L:493:GLY:C	2.22	0.43
1:B:195:GLU:OE1	2:E:222:GLN:HG2	2.18	0.42
2:C:393:GLY:HA2	2:C:394:GLY:HA2	1.61	0.42
1:D:90:ASN:OD1	1:D:90:ASN:N	2.52	0.42
1:H:286:ILE:HB	1:H:300:PHE:CE1	2.54	0.42
2:I:236:GLU:CB	2:I:427:THR:HG21	2.48	0.42
2:K:465:TYR:O	2:K:468:GLU:HB2	2.19	0.42
2:L:236:GLU:O	2:L:239:LYS:HG2	2.19	0.42
1:H:230:GLY:O	1:M:232:ASP:HB2	2.20	0.42
1:M:262:VAL:HG13	1:M:290:MET:HG2	2.01	0.42
1:F:323:SER:OG	1:M:309:LEU:HD21	2.18	0.42
1:M:41:ALA:HB1	1:M:272:ILE:HD13	2.00	0.42
1:A:6:VAL:HA	1:A:7:PRO:HD3	1.80	0.42
1:B:68:LEU:HA	1:B:68:LEU:HD12	1.86	0.42
2:C:339:LYS:HA	2:C:339:LYS:HD3	1.83	0.42
2:C:45:ASN:ND2	2:C:47:ARG:HD3	2.33	0.42
2:C:523:PRO:O	2:C:527:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LEU:HD23	1:D:129:LEU:HA	1.75	0.42
1:D:321:ILE:HA	1:D:324:LEU:HD21	2.00	0.42
2:E:70:PRO:HB2	2:E:100:TYR:OH	2.19	0.42
2:G:403:ALA:HB2	2:G:420:VAL:HG23	2.01	0.42
2:I:318:ASN:ND2	2:I:381:LYS:HE2	2.33	0.42
1:H:9:GLY:HA3	2:I:423:TYR:CG	2.53	0.42
2:I:61:TYR:HA	2:I:64:PHE:CZ	2.54	0.42
1:M:212:PRO:HB2	1:M:220:LYS:HD2	2.01	0.42
2:C:392:GLY:CA	2:C:396:ILE:HG22	2.24	0.42
1:B:296:LYS:NZ	1:D:331:THR:O	2.28	0.42
2:E:322:LEU:HD12	2:E:532:ASP:HB3	2.01	0.42
2:E:437:TRP:CH2	2:E:440:PRO:HD3	2.54	0.42
1:D:301:MET:HE2	2:E:71:ARG:HB3	1.99	0.42
2:I:244:LEU:C	2:I:244:LEU:HD23	2.39	0.42
2:I:332:ASP:OD1	2:I:332:ASP:N	2.51	0.42
2:I:349:ARG:HG3	2:I:350:LYS:N	2.34	0.42
2:I:393:GLY:N	2:I:394:GLY:HA2	2.33	0.42
2:K:351:HIS:CD2	2:K:352:PRO:HD2	2.54	0.42
1:A:13:GLN:OE1	2:L:425:PRO:HB3	2.20	0.42
2:C:120:TYR:CD2	2:C:455:PHE:HE2	2.37	0.42
1:D:125:ILE:N	1:D:126:PRO:CD	2.82	0.42
2:G:145:ASN:HB3	2:G:148:VAL:HG23	2.02	0.42
2:G:394:GLY:N	2:G:395:PRO:HD3	2.34	0.42
2:G:474:LEU:HD12	2:G:479:THR:HG21	2.01	0.42
2:I:262:VAL:HG13	2:I:547:THR:HG23	2.00	0.42
2:L:325:SER:C	2:L:369:ASN:HA	2.39	0.42
1:M:125:ILE:N	1:M:126:PRO:CD	2.83	0.42
1:M:47:VAL:HG13	1:M:48:GLU:N	2.35	0.42
2:C:239:LYS:NZ	2:C:427:THR:HG23	2.35	0.42
1:D:51:VAL:HG21	2:E:178:PHE:CE2	2.54	0.42
2:E:23:MET:HB3	2:E:25:TRP:CH2	2.54	0.42
2:G:238:MET:HA	2:G:238:MET:CE	2.47	0.42
2:I:248:LEU:O	2:I:251:PHE:HB3	2.20	0.42
2:I:532:ASP:OD1	2:I:536:THR:N	2.53	0.42
2:K:273:GLY:HA3	2:K:299:PRO:HG3	2.01	0.42
2:K:497:HIS:O	2:K:504:LEU:HB3	2.18	0.42
2:K:574:LEU:N	2:K:574:LEU:HD12	2.34	0.42
2:L:48:VAL:HG11	2:L:544:VAL:O	2.19	0.42
1:M:325:ARG:O	1:M:329:LYS:HB2	2.19	0.42
1:A:169:GLY:H	1:A:172:TRP:HB2	1.85	0.42
1:A:253:VAL:HG13	1:A:254:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:THR:HG23	2:C:311:ASP:OD1	2.19	0.42
2:C:336:THR:HG22	2:C:354:ASN:HB3	2.00	0.42
1:D:247:GLY:HA3	2:E:481:THR:HG22	2.02	0.42
2:E:153:LYS:HA	2:E:169:ALA:CB	2.50	0.42
2:E:524:THR:N	2:E:525:PRO:CD	2.83	0.42
1:F:6:VAL:HA	1:F:7:PRO:HD3	1.82	0.42
2:G:501:ARG:HH11	2:G:573:CYS:HB2	1.83	0.42
2:I:153:LYS:HB2	2:I:153:LYS:HE3	1.71	0.42
2:I:35:LEU:HB2	2:I:574:LEU:CD2	2.50	0.42
2:I:298:THR:HG21	2:I:405:ALA:CB	2.49	0.42
2:L:25:TRP:CH2	2:L:563:ILE:HD12	2.54	0.42
2:L:492:ILE:HG12	2:L:493:GLY:H	1.85	0.42
1:M:110:TRP:HA	1:M:110:TRP:CE3	2.55	0.42
1:A:200:LEU:O	1:A:204:LEU:HG	2.20	0.42
2:C:323:LEU:O	2:C:533:ILE:HG23	2.20	0.42
2:C:42:ASP:CG	2:C:45:ASN:HB2	2.39	0.42
1:D:278:CYS:CB	1:D:279:PRO:HD3	2.50	0.42
2:E:377:ARG:CD	2:E:388:ALA:HA	2.50	0.42
1:F:106:GLY:HA2	1:F:107:GLU:C	2.39	0.42
1:F:125:ILE:N	1:F:126:PRO:CD	2.82	0.42
1:F:327:LEU:O	1:F:331:THR:HG23	2.19	0.42
2:I:57:ILE:HG12	1:M:111:ALA:HB1	2.01	0.42
2:K:527:ASN:HA	2:K:539:PRO:CG	2.40	0.42
2:L:38:TYR:O	2:L:51:CYS:HA	2.19	0.42
1:F:152:HIS:HE2	2:L:61:TYR:HH	1.59	0.42
1:M:94:VAL:HG22	1:M:140:VAL:HB	2.01	0.42
1:B:301:MET:HE1	2:G:71:ARG:HG2	2.00	0.42
1:B:304:PRO:HG2	1:B:307:ALA:HB2	2.01	0.42
1:D:27:THR:HG22	1:D:96:GLU:OE1	2.19	0.42
2:G:224:PHE:O	2:G:228:ILE:HG13	2.20	0.42
2:G:522:PRO:HB3	5:G:701:NFU:O3	2.20	0.42
2:I:202:GLY:HA3	2:I:208:SER:OG	2.20	0.42
2:I:236:GLU:CA	2:I:427:THR:HG21	2.50	0.42
2:L:201:GLU:HA	2:L:209:THR:OG1	2.19	0.42
2:L:242:VAL:HG11	2:L:435:PHE:CD1	2.55	0.42
1:B:294:PRO:HG2	1:B:298:MET:HE1	2.02	0.42
1:D:133:ALA:N	1:D:134:PRO:CD	2.83	0.42
2:E:239:LYS:HZ2	2:E:427:THR:HG23	1.84	0.42
2:E:242:VAL:CB	2:E:243:PRO:HD3	2.40	0.42
2:E:272:TRP:NE1	2:E:315:ILE:HD11	2.34	0.42
2:G:68:LYS:O	2:G:515:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:265:ARG:NH1	2:I:539:PRO:CB	2.83	0.42
2:L:217:THR:O	2:L:219:PRO:HD3	2.18	0.42
1:F:316:SER:HB3	1:M:313:LEU:CD2	2.49	0.42
2:C:73:SER:HB2	2:C:518:TYR:CE2	2.55	0.42
2:E:323:LEU:HD21	2:E:331:TRP:HZ3	1.81	0.42
2:E:549:ILE:HG22	2:E:549:ILE:O	2.20	0.42
1:B:247:GLY:HA3	2:G:481:THR:OG1	2.18	0.42
2:I:311:ASP:O	2:I:315:ILE:HG13	2.20	0.42
2:I:469:GLN:O	2:I:473:GLU:HG2	2.20	0.42
2:K:262:VAL:HA	2:K:547:THR:HG23	2.02	0.42
1:M:287:GLY:O	1:M:293:PHE:HB2	2.20	0.42
1:A:314:ILE:HG12	1:A:314:ILE:H	1.64	0.41
2:C:549:ILE:N	2:C:549:ILE:HD12	2.34	0.41
2:C:540:TYR:HE1	2:C:570:PHE:CB	2.33	0.41
2:C:81:CYS:SG	2:C:82:GLY:N	2.93	0.41
1:D:19:LYS:HG2	1:D:20:GLU:HG3	2.02	0.41
2:E:138:GLU:HG2	2:E:139:GLN:N	2.34	0.41
2:E:260:GLU:OE2	2:E:264:ARG:HD2	2.20	0.41
1:F:89:ASP:O	1:F:175:ARG:NH2	2.53	0.41
1:F:77:MET:HE2	1:F:80:PHE:CD1	2.55	0.41
1:H:8:TYR:O	1:H:11:LYS:HG2	2.20	0.41
2:I:494:CYS:HA	2:I:506:HIS:O	2.19	0.41
2:I:522:PRO:HD2	2:I:525:PRO:HG2	2.01	0.41
2:I:528:ALA:HB2	2:I:540:TYR:CE2	2.55	0.41
2:K:529:SER:O	2:K:538:GLY:HA3	2.19	0.41
2:L:240:LYS:HG2	2:L:240:LYS:O	2.19	0.41
2:L:311:ASP:O	2:L:315:ILE:HG13	2.19	0.41
2:L:398:ARG:HE	2:L:498:GLU:CG	2.29	0.41
2:L:98:MET:SD	2:L:493:GLY:HA2	2.60	0.41
2:E:142:ARG:HD2	2:E:149:TRP:CE2	2.55	0.41
2:E:336:THR:HG23	2:E:354:ASN:CG	2.40	0.41
2:E:35:LEU:HA	2:E:574:LEU:HD11	2.02	0.41
1:M:116:ASP:O	1:M:120:HIS:N	2.43	0.41
1:B:258:TRP:CZ2	1:B:304:PRO:HB3	2.55	0.41
1:B:90:ASN:HA	1:B:137:LEU:CD1	2.50	0.41
2:C:490:GLU:O	2:C:491:ALA:HB2	2.20	0.41
2:C:510:ILE:O	2:C:511:ARG:HD2	2.20	0.41
2:E:290:LYS:HA	2:E:290:LYS:HD3	1.83	0.41
2:E:511:ARG:HG3	2:E:511:ARG:HH11	1.84	0.41
1:H:94:VAL:HG22	1:H:140:VAL:HB	2.02	0.41
2:I:112:ILE:HD11	2:I:215:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:242:VAL:CB	2:I:243:PRO:HD3	2.46	0.41
2:I:285:TYR:CE1	2:I:313:VAL:HG23	2.55	0.41
2:K:129:ASP:CB	2:K:186:THR:HG21	2.50	0.41
2:K:237:PHE:O	2:K:241:VAL:HG23	2.20	0.41
1:A:234:ALA:HA	3:A:501:SF4:S1	2.61	0.41
1:B:188:VAL:HG21	1:B:193:PHE:HB2	2.03	0.41
2:C:105:PRO:HA	2:C:106:PRO:HD3	1.98	0.41
2:C:81:CYS:SG	2:C:83:ILE:HG22	2.60	0.41
2:E:210:LEU:HD12	2:E:210:LEU:HA	1.78	0.41
2:E:267:ILE:CB	2:E:304:ASP:HB2	2.35	0.41
2:E:452:ARG:HH21	2:E:571:ASP:HB2	1.86	0.41
1:F:313:LEU:CG	1:F:315:LYS:HG3	2.37	0.41
1:M:288:CYS:HA	1:M:293:PHE:CG	2.55	0.41
1:M:323:SER:O	1:M:327:LEU:HG	2.20	0.41
1:A:319:PRO:HA	1:A:322:ARG:NH1	2.35	0.41
1:A:345:LEU:HG	1:A:347:THR:HG23	2.02	0.41
2:C:261:GLU:OE2	2:C:264:ARG:NH1	2.53	0.41
2:C:523:PRO:HD2	5:C:701:NFU:C2	2.51	0.41
1:D:118:GLN:HA	1:D:118:GLN:OE1	2.20	0.41
1:B:347:THR:CG2	1:D:156:GLY:H	2.22	0.41
2:E:341:ASP:HB2	2:E:342:PRO:HD2	2.02	0.41
2:I:323:LEU:C	2:I:323:LEU:HD12	2.41	0.41
2:I:508:LEU:HD12	2:I:509:VAL:H	1.85	0.41
2:K:70:PRO:HD3	2:K:514:LYS:HA	2.01	0.41
2:L:82:GLY:O	2:L:205:VAL:HG11	2.21	0.41
2:L:501:ARG:NE	2:L:571:ASP:OD1	2.53	0.41
1:A:317:TYR:O	1:A:320:LEU:HB3	2.21	0.41
2:E:103:LYS:HA	2:E:104:PRO:HD3	1.86	0.41
1:F:186:CYS:HA	1:F:187:PRO:HA	1.81	0.41
2:I:70:PRO:HB2	2:I:100:TYR:OH	2.20	0.41
2:I:103:LYS:HA	2:I:104:PRO:HD3	1.95	0.41
2:I:264:ARG:HA	2:I:444:ASN:HA	2.02	0.41
2:I:26:ASP:HA	2:I:27:PRO:HA	1.79	0.41
2:I:288:MET:HA	2:I:291:TRP:CZ2	2.56	0.41
2:I:378:TRP:CB	2:I:389:LEU:HD12	2.51	0.41
2:I:242:VAL:HA	2:I:453:THR:HG21	2.02	0.41
2:I:564:MET:O	2:I:568:ARG:HG3	2.20	0.41
2:I:135:ASP:OD2	2:I:568:ARG:HD2	2.20	0.41
2:L:398:ARG:CD	2:L:498:GLU:HG2	2.50	0.41
1:B:105:ASN:HA	1:B:106:GLY:HA3	1.84	0.41
2:C:145:ASN:N	2:C:146:PRO:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:SD	2:C:68:LYS:HE2	2.61	0.41
1:D:25:TRP:HD1	1:D:27:THR:HG23	1.85	0.41
2:E:128:GLN:HA	2:E:132:VAL:HG22	2.03	0.41
2:E:277:ASP:HA	2:E:278:PRO:HD2	1.91	0.41
2:E:329:GLN:O	2:E:329:GLN:HG2	2.21	0.41
1:F:289:THR:HG23	3:F:703:SF4:S2	2.61	0.41
2:G:336:THR:HG21	2:G:349:ARG:HG2	2.03	0.41
2:G:74:HIS:CD2	2:G:74:HIS:H	2.38	0.41
1:H:90:ASN:OD1	1:H:90:ASN:N	2.53	0.41
2:I:268:LEU:HB3	2:I:389:LEU:HD23	2.01	0.41
2:I:400:TRP:CE2	2:I:439:ILE:HG23	2.55	0.41
2:L:395:PRO:CG	2:L:452:ARG:HA	2.51	0.41
1:B:119:THR:HG22	1:B:121:GLN:CG	2.51	0.41
2:C:142:ARG:O	2:C:146:PRO:HG3	2.20	0.41
2:C:277:ASP:HA	2:C:278:PRO:HD3	1.93	0.41
1:D:107:GLU:HB3	2:E:363:LYS:HE2	2.03	0.41
2:G:323:LEU:HD11	2:G:331:TRP:CZ3	2.55	0.41
1:H:143:GLY:O	1:H:147:THR:HG23	2.21	0.41
1:H:155:GLU:HB2	1:M:338:TRP:CZ2	2.56	0.41
2:I:145:ASN:HB3	2:I:148:VAL:CB	2.51	0.41
2:I:341:ASP:HB2	2:I:342:PRO:HD2	2.02	0.41
2:K:105:PRO:HA	2:K:106:PRO:HD3	1.97	0.41
2:K:321:ILE:HG22	2:K:331:TRP:HH2	1.85	0.41
2:K:123:ASP:CB	2:K:500:VAL:HG11	2.51	0.41
2:L:285:TYR:CZ	2:L:313:VAL:HG13	2.56	0.41
1:M:9:GLY:O	1:M:12:THR:HG23	2.20	0.41
1:M:189:GLN:HB3	1:M:192:ASN:ND2	2.35	0.41
1:M:211:ILE:HG23	1:M:211:ILE:O	2.20	0.41
1:M:258:TRP:O	1:M:262:VAL:HG23	2.21	0.41
1:A:299:PRO:HA	2:C:72:ASP:OD2	2.20	0.41
1:A:308:VAL:HA	1:A:311:SER:OG	2.20	0.41
1:B:185:GLY:N	1:B:289:THR:HG22	2.35	0.41
1:B:35:ASP:OD2	1:B:96:GLU:HG3	2.20	0.41
2:C:288:MET:HG3	2:C:291:TRP:CZ2	2.55	0.41
1:D:125:ILE:HB	1:D:126:PRO:HD3	2.03	0.41
1:D:228:HIS:CB	1:D:260:PRO:HA	2.50	0.41
1:H:253:VAL:HG13	1:H:254:LYS:N	2.36	0.41
1:H:316:SER:O	1:H:319:PRO:HD2	2.21	0.41
2:K:522:PRO:O	2:K:525:PRO:HD2	2.21	0.41
2:K:525:PRO:HD3	2:K:577:GLY:HA2	2.03	0.41
2:K:574:LEU:N	2:K:575:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:28:ILE:CD1	2:L:37:ILE:HG12	2.49	0.41
1:A:119:THR:O	1:A:120:HIS:HB2	2.21	0.41
1:A:169:GLY:N	1:A:172:TRP:HB2	2.36	0.41
2:C:232:MET:CE	2:C:464:LEU:HD21	2.51	0.41
2:C:120:TYR:HD1	2:C:500:VAL:HG22	1.85	0.41
2:C:61:TYR:O	2:C:65:MET:HG3	2.21	0.41
1:D:185:GLY:CA	1:D:289:THR:HG22	2.44	0.41
1:D:32:CYS:HB2	2:E:82:GLY:H	1.82	0.41
2:E:298:THR:HA	2:E:299:PRO:HD3	1.90	0.41
2:E:375:SER:HA	2:E:529:SER:HB2	2.03	0.41
2:E:549:ILE:N	2:E:549:ILE:HD12	2.35	0.41
2:K:123:ASP:HB3	2:K:500:VAL:HG11	2.02	0.41
2:K:129:ASP:OD1	2:K:245:HIS:NE2	2.48	0.41
2:L:221:ILE:HA	2:L:221:ILE:HD12	1.91	0.41
2:L:135:ASP:HB3	2:L:565:ARG:HG2	2.02	0.41
2:L:574:LEU:N	2:L:575:PRO:CD	2.84	0.41
1:A:12:THR:CG2	2:L:411:GLY:HA3	2.51	0.41
1:B:20:GLU:HG2	1:B:60:LYS:HB3	2.03	0.41
1:D:113:MET:O	1:D:113:MET:HG3	2.21	0.41
1:D:248:ASN:CG	1:D:249:PRO:HD2	2.41	0.41
2:E:277:ASP:OD1	2:E:279:ASN:HB2	2.21	0.41
2:E:31:ILE:HG21	2:E:572:PRO:CG	2.51	0.41
2:E:533:ILE:HG13	2:E:534:TYR:N	2.36	0.41
1:A:234:ALA:CB	1:F:234:ALA:HB3	2.26	0.41
1:F:95:LEU:HD12	1:F:96:GLU:H	1.85	0.41
2:G:349:ARG:HD2	2:G:349:ARG:O	2.21	0.41
2:G:373:VAL:HG12	2:G:374:MET:O	2.21	0.41
1:H:345:LEU:HD21	1:H:347:THR:OG1	2.21	0.41
2:I:574:LEU:N	2:I:575:PRO:CD	2.84	0.41
2:K:523:PRO:O	2:K:526:TRP:HB2	2.21	0.41
2:L:544:VAL:HG13	2:L:563:ILE:HG23	2.03	0.41
1:M:278:CYS:CB	1:M:279:PRO:HD3	2.45	0.41
1:B:154:MET:HG2	1:B:155:GLU:N	2.36	0.40
1:B:253:VAL:HB	3:B:501:SF4:S4	2.61	0.40
1:B:186:CYS:HB3	1:B:288:CYS:HB2	2.04	0.40
1:B:26:ILE:CD1	1:B:93:LEU:HD11	2.51	0.40
2:C:375:SER:HA	2:C:529:SER:HB2	2.03	0.40
2:C:387:LEU:N	2:C:387:LEU:HD12	2.35	0.40
2:C:70:PRO:HB2	2:C:100:TYR:OH	2.21	0.40
2:E:244:LEU:O	2:E:244:LEU:HD23	2.20	0.40
2:E:501:ARG:NH1	2:E:501:ARG:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:ILE:O	1:F:250:ASN:HB3	2.21	0.40
1:F:258:TRP:O	1:F:262:VAL:HG23	2.20	0.40
2:G:126:ILE:CD1	2:G:187:LEU:HD23	2.51	0.40
2:G:239:LYS:HZ1	2:G:427:THR:HG23	1.86	0.40
1:H:288:CYS:HA	1:H:293:PHE:CG	2.56	0.40
2:I:298:THR:HA	2:I:299:PRO:HD3	1.87	0.40
2:I:347:VAL:HG12	2:I:354:ASN:ND2	2.36	0.40
2:K:382:ARG:H	2:K:382:ARG:HG3	1.65	0.40
1:M:189:GLN:HB3	1:M:192:ASN:HB2	2.03	0.40
1:A:133:ALA:HB3	1:A:134:PRO:HD3	2.02	0.40
2:C:259:TYR:CE1	2:C:262:VAL:HG21	2.57	0.40
2:C:335:GLU:CD	2:C:335:GLU:H	2.18	0.40
1:D:259:GLY:N	1:D:260:PRO:CD	2.84	0.40
2:G:259:TYR:OH	2:G:565:ARG:HD2	2.22	0.40
2:K:103:LYS:HA	2:K:104:PRO:HD3	1.89	0.40
2:K:93:VAL:HG13	2:K:212:PRO:HA	2.02	0.40
1:M:234:ALA:HA	3:M:702:SF4:S1	2.61	0.40
1:B:23:ILE:N	1:B:23:ILE:HD12	2.37	0.40
2:C:226:ASP:O	2:C:229:THR:HG22	2.21	0.40
1:A:152:HIS:CD2	2:C:59:ARG:HD2	2.56	0.40
2:E:522:PRO:O	2:E:525:PRO:HD2	2.21	0.40
2:E:370:TYR:OH	2:E:530:PRO:HB3	2.21	0.40
1:F:32:CYS:O	1:F:33:ASP:HB2	2.21	0.40
2:G:126:ILE:HD12	2:G:130:ASN:OD1	2.21	0.40
2:K:217:THR:O	2:K:219:PRO:HD3	2.22	0.40
2:K:298:THR:HB	2:K:402:THR:HA	2.03	0.40
2:K:340:ASN:HA	2:K:345:ASN:O	2.21	0.40
2:K:35:LEU:HG	2:K:36:GLY:N	2.37	0.40
2:L:24:ASN:OD1	2:L:24:ASN:N	2.55	0.40
2:L:341:ASP:CG	2:L:345:ASN:HB2	2.42	0.40
1:B:34:GLY:HA2	2:G:82:GLY:HA3	2.03	0.40
1:B:65:ASN:HA	1:B:66:PRO:HD3	1.83	0.40
2:C:272:TRP:HZ3	2:C:505:SER:CB	2.32	0.40
1:D:46:SER:O	1:D:49:ASP:HB2	2.21	0.40
2:E:302:VAL:CG2	2:E:307:LEU:HD13	2.51	0.40
2:E:315:ILE:HG13	2:E:378:TRP:HE1	1.87	0.40
2:G:177:PRO:O	2:G:178:PHE:HB2	2.21	0.40
2:I:199:LEU:O	2:I:223:LEU:HD11	2.21	0.40
2:I:265:ARG:NH1	2:I:539:PRO:HA	2.37	0.40
2:K:148:VAL:HG22	2:K:256:LEU:HD21	2.00	0.40
2:K:461:ALA:O	2:K:464:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:47:ARG:HG2	2:L:48:VAL:N	2.36	0.40
2:L:272:TRP:HZ3	2:L:505:SER:N	2.19	0.40
1:A:188:VAL:HG21	1:A:193:PHE:HB2	2.04	0.40
1:B:116:ASP:HA	1:B:117:PRO:HD3	1.97	0.40
2:C:256:LEU:O	2:C:259:TYR:HB2	2.22	0.40
2:E:159:HIS:N	2:E:247:ASP:OD2	2.54	0.40
2:E:339:LYS:HA	2:E:339:LYS:HD3	1.66	0.40
2:E:416:THR:HB	2:E:418:HIS:CE1	2.57	0.40
1:F:157:ASN:OD1	1:F:160:GLY:N	2.50	0.40
1:H:32:CYS:O	1:H:33:ASP:HB2	2.22	0.40
1:H:6:VAL:HA	1:H:7:PRO:HD3	1.91	0.40
2:L:288:MET:CE	2:L:312:LEU:HB3	2.45	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	343/351 (98%)	323 (94%)	19 (6%)	1 (0%)	44	66
1	B	343/351 (98%)	321 (94%)	21 (6%)	1 (0%)	44	66
1	D	343/351 (98%)	321 (94%)	20 (6%)	2 (1%)	28	48
1	F	343/351 (98%)	316 (92%)	25 (7%)	2 (1%)	28	48
1	H	343/351 (98%)	327 (95%)	14 (4%)	2 (1%)	28	48
1	M	343/351 (98%)	324 (94%)	18 (5%)	1 (0%)	44	66
2	C	559/579 (96%)	528 (94%)	30 (5%)	1 (0%)	51	73
2	E	557/579 (96%)	516 (93%)	37 (7%)	4 (1%)	25	43
2	G	559/579 (96%)	537 (96%)	21 (4%)	1 (0%)	51	73
2	I	558/579 (96%)	520 (93%)	36 (6%)	2 (0%)	38	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	559/579 (96%)	523 (94%)	36 (6%)	0	100	100
2	L	558/579 (96%)	516 (92%)	40 (7%)	2 (0%)	38	59
All	All	5408/5580 (97%)	5072 (94%)	317 (6%)	19 (0%)	38	59

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	CYS
1	B	278	CYS
1	D	278	CYS
1	F	120	HIS
1	F	278	CYS
1	H	278	CYS
1	M	278	CYS
2	C	267	ILE
2	E	368	GLY
1	H	280	ASN
2	G	530	PRO
2	I	327	PHE
2	L	327	PHE
1	D	116	ASP
2	I	267	ILE
2	L	275	PHE
2	E	267	ILE
2	E	393	GLY
2	E	530	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	277/281 (99%)	272 (98%)	5 (2%)	64	86
1	B	277/281 (99%)	271 (98%)	6 (2%)	57	82
1	D	277/281 (99%)	271 (98%)	6 (2%)	57	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	277/281 (99%)	266 (96%)	11 (4%)	36	62
1	H	277/281 (99%)	271 (98%)	6 (2%)	57	82
1	M	277/281 (99%)	275 (99%)	2 (1%)	87	96
2	C	476/485 (98%)	467 (98%)	9 (2%)	62	85
2	E	474/485 (98%)	455 (96%)	19 (4%)	36	62
2	G	476/485 (98%)	472 (99%)	4 (1%)	85	95
2	I	475/485 (98%)	464 (98%)	11 (2%)	56	81
2	K	476/485 (98%)	468 (98%)	8 (2%)	66	87
2	L	475/485 (98%)	462 (97%)	13 (3%)	50	77
All	All	4514/4596 (98%)	4414 (98%)	100 (2%)	57	82

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	99	ILE
1	A	238	GLU
1	A	244	THR
1	A	314	ILE
1	B	47	VAL
1	B	49	ASP
1	B	68	LEU
1	B	166	ASP
1	B	311	SER
1	B	313	LEU
2	C	83	ILE
2	C	122	PHE
2	C	269	LEU
2	C	309	THR
2	C	353	TRP
2	C	385	ASP
2	C	442	TRP
2	C	459	SER
2	C	512	ASP
1	D	118	GLN
1	D	120	HIS
1	D	188	VAL
1	D	320	LEU
1	D	324	LEU

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Mol	Chain	Res	Type
1	D	326	LYS
2	E	156	GLU
2	E	256	LEU
2	E	289	THR
2	E	309	THR
2	E	323	LEU
2	E	353	TRP
2	E	365	ASN
2	E	369	ASN
2	E	379	LEU
2	E	387	LEU
2	E	402	THR
2	E	438	LYS
2	E	458	TYR
2	E	464	LEU
2	E	489	ASP
2	E	541	GLU
2	E	562	ASP
2	E	563	ILE
2	E	567	VAL
1	F	11	LYS
1	F	55	ILE
1	F	89	ASP
1	F	116	ASP
1	F	118	GLN
1	F	119	THR
1	F	120	HIS
1	F	151	ILE
1	F	168	LEU
1	F	239	GLN
1	F	252	ILE
2	G	153	LYS
2	G	353	TRP
2	G	442	TRP
2	G	453	THR
1	H	55	ILE
1	H	154	MET
1	H	188	VAL
1	H	238	GLU
1	H	281	VAL
1	H	313	LEU
2	I	73	SER

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Mol	Chain	Res	Type
2	I	107	ILE
2	I	122	PHE
2	I	125	ASN
2	I	225	THR
2	I	246	ASP
2	I	353	TRP
2	I	442	TRP
2	I	458	TYR
2	I	471	LEU
2	I	556	GLU
2	K	107	ILE
2	K	122	PHE
2	K	184	ARG
2	K	314	ASP
2	K	442	TRP
2	K	479	THR
2	K	489	ASP
2	K	518	TYR
2	L	22	GLU
2	L	51	CYS
2	L	79	ARG
2	L	100	TYR
2	L	139	GLN
2	L	260	GLU
2	L	289	THR
2	L	307	LEU
2	L	326	SER
2	L	404	LEU
2	L	420	VAL
2	L	442	TRP
2	L	515	ILE
1	M	36	SER
1	M	118	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	121	GLN
2	E	362	GLN
1	F	105	ASN
2	G	45	ASN
2	G	74	HIS

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Mol	Chain	Res	Type
2	G	176	ASN
2	G	545	GLN
1	H	203	GLN
2	I	206	HIS
2	L	96	GLN
1	M	118	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

30 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	SF4	A	501	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	A	502	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	A	503	-	0,12,12	0.00	-	0,24,24	0.00	-
4	MLA	A	504	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLA	A	505	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLA	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SF4	B	501	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	B	502	-	0,12,12	0.00	-	0,24,24	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SF4	B	503	-	0,12,12	0.00	-	0,24,24	0.00	-
5	NFU	C	701	-	2,7,7	0.15	0	0,9,9	0.00	-
4	MLA	D	701	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SF4	D	702	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	D	703	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	D	704	-	0,12,12	0.00	-	0,24,24	0.00	-
5	NFU	E	701	-	2,7,7	0.08	0	0,9,9	0.00	-
4	MLA	F	701	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SF4	F	702	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	F	703	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	F	704	-	0,12,12	0.00	-	0,24,24	0.00	-
5	NFU	G	701	-	2,7,7	0.13	0	0,9,9	0.00	-
3	SF4	H	501	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	H	502	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	H	503	-	0,12,12	0.00	-	0,24,24	0.00	-
5	NFU	I	701	-	2,7,7	0.43	0	0,9,9	0.00	-
5	NFU	K	701	-	2,7,7	0.09	0	0,9,9	0.00	-
5	NFU	L	701	-	2,7,7	0.42	0	0,9,9	0.00	-
3	SF4	M	702	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	M	703	-	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	M	704	-	0,12,12	0.00	-	0,24,24	0.00	-
4	MLA	M	705	-	0,6,6	0.00	-	0,7,7	0.00	-

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	SF4	A	501	-	-	0/0/48/48	0/6/5/5
3	SF4	A	502	-	-	0/0/48/48	0/6/5/5
3	SF4	A	503	-	-	0/0/48/48	0/6/5/5
4	MLA	A	504	-	-	0/0/4/4	0/0/0/0
4	MLA	A	505	-	-	0/0/4/4	0/0/0/0
4	MLA	A	701	-	-	0/0/4/4	0/0/0/0
3	SF4	B	501	-	-	0/0/48/48	0/6/5/5
3	SF4	B	502	-	-	0/0/48/48	0/6/5/5
3	SF4	B	503	-	-	0/0/48/48	0/6/5/5
5	NFU	C	701	-	-	0/0/9/9	0/0/0/0
4	MLA	D	701	-	-	0/0/4/4	0/0/0/0
3	SF4	D	702	-	-	0/0/48/48	0/6/5/5
3	SF4	D	703	-	-	0/0/48/48	0/6/5/5
3	SF4	D	704	-	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NFU	E	701	-	-	0/0/9/9	0/0/0/0
4	MLA	F	701	-	-	0/0/4/4	0/0/0/0
3	SF4	F	702	-	-	0/0/48/48	0/6/5/5
3	SF4	F	703	-	-	0/0/48/48	0/6/5/5
3	SF4	F	704	-	-	0/0/48/48	0/6/5/5
5	NFU	G	701	-	-	0/0/9/9	0/0/0/0
3	SF4	H	501	-	-	0/0/48/48	0/6/5/5
3	SF4	H	502	-	-	0/0/48/48	0/6/5/5
3	SF4	H	503	-	-	0/0/48/48	0/6/5/5
5	NFU	I	701	-	-	0/0/9/9	0/0/0/0
5	NFU	K	701	-	-	0/0/9/9	0/0/0/0
5	NFU	L	701	-	-	0/0/9/9	0/0/0/0
3	SF4	M	702	-	-	0/0/48/48	0/6/5/5
3	SF4	M	703	-	-	0/0/48/48	0/6/5/5
3	SF4	M	704	-	-	0/0/48/48	0/6/5/5
4	MLA	M	705	-	-	0/0/4/4	0/0/0/0

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.

15 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	SF4	1	0
3	B	501	SF4	1	0
3	B	502	SF4	1	0
5	C	701	NFU	3	0
4	D	701	MLA	2	0
5	E	701	NFU	2	0
3	F	703	SF4	1	0
5	G	701	NFU	1	0
3	H	501	SF4	1	0
3	H	503	SF4	1	0
5	I	701	NFU	3	0
5	L	701	NFU	2	0
3	M	702	SF4	2	0
3	M	704	SF4	1	0
4	M	705	MLA	1	0

## 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	345/351 (98%)	-0.33	7 (2%) 65 67	14, 31, 67, 122	0
1	B	345/351 (98%)	-0.24	3 (0%) 84 85	16, 35, 73, 101	0
1	D	345/351 (98%)	-0.30	4 (1%) 79 80	16, 38, 77, 148	0
1	F	345/351 (98%)	-0.21	5 (1%) 75 76	19, 41, 77, 124	0
1	H	345/351 (98%)	-0.26	6 (1%) 70 72	18, 34, 77, 107	0
1	M	345/351 (98%)	-0.24	6 (1%) 70 72	19, 38, 73, 115	0
2	C	561/579 (96%)	-0.19	3 (0%) 90 91	23, 42, 63, 87	0
2	E	559/579 (96%)	0.32	28 (5%) 30 31	20, 61, 94, 141	0
2	G	561/579 (96%)	-0.31	3 (0%) 90 91	15, 32, 54, 78	0
2	I	560/579 (96%)	-0.10	2 (0%) 92 92	22, 49, 78, 112	0
2	K	561/579 (96%)	-0.22	2 (0%) 92 92	19, 43, 65, 90	0
2	L	560/579 (96%)	0.28	23 (4%) 38 40	21, 64, 92, 123	0
All	All	5432/5580 (97%)	-0.12	92 (1%) 70 72	14, 42, 80, 148	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	314	ILE	7.9
1	A	309	LEU	5.3
2	E	49	ALA	4.7
2	I	342	PRO	4.6
1	H	309	LEU	4.5
2	E	441	MET	4.4
2	E	555	PRO	4.3
1	H	311	SER	4.2
2	E	52	TYR	4.1
2	E	41	ILE	4.0
2	L	44	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	106	GLY	4.0
1	D	115	THR	4.0
1	F	314	ILE	3.9
2	L	41	ILE	3.9
1	D	117	PRO	3.9
2	E	23	MET	3.5
1	A	312	ASN	3.5
2	L	363	LYS	3.3
2	E	50	GLU	3.3
2	E	302	VAL	3.2
2	E	43	PHE	3.2
2	E	393	GLY	3.1
1	A	308	VAL	3.1
2	L	347	VAL	3.1
2	L	336	THR	3.1
2	L	21	VAL	3.1
2	L	249	PHE	3.0
1	A	6	VAL	3.0
2	E	269	LEU	3.0
2	E	499	ALA	2.9
2	L	152	ALA	2.9
2	L	385	ASP	2.9
1	B	5	ALA	2.9
2	L	333	HIS	2.8
1	M	5	ALA	2.8
2	L	337	SER	2.8
1	B	6	VAL	2.7
2	E	382	ARG	2.7
2	L	20	LEU	2.7
2	E	42	ASP	2.7
2	G	41	ILE	2.7
2	E	392	GLY	2.7
2	G	19	LYS	2.7
2	E	154	THR	2.6
2	L	322	LEU	2.6
2	E	257	PRO	2.6
1	M	316	SER	2.6
1	D	107	GLU	2.6
1	F	118	GLN	2.6
2	L	305	GLY	2.6
2	L	335	GLU	2.6
2	C	274	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	336	THR	2.5
1	H	312	ASN	2.5
1	M	315	LYS	2.5
1	H	314	ILE	2.5
1	A	311	SER	2.5
2	L	43	PHE	2.4
1	A	5	ALA	2.4
2	E	502	GLY	2.4
2	K	19	LYS	2.4
1	F	6	VAL	2.4
2	E	534	TYR	2.4
2	L	150	GLU	2.3
2	L	441	MET	2.3
1	F	317	TYR	2.3
1	M	313	LEU	2.3
2	E	333	HIS	2.3
2	I	336	THR	2.3
1	M	317	TYR	2.3
2	L	156	GLU	2.2
1	D	317	TYR	2.2
1	A	343	PRO	2.2
2	L	486	LYS	2.2
2	E	556	GLU	2.2
2	L	386	HIS	2.2
1	B	17	ALA	2.2
2	L	576	CYS	2.2
2	E	303	VAL	2.2
2	L	254	GLU	2.2
2	C	339	LYS	2.2
2	E	48	VAL	2.1
1	H	320	LEU	2.1
2	E	44	GLU	2.1
2	E	274	SER	2.1
2	G	161	ALA	2.1
1	H	308	VAL	2.1
2	K	333	HIS	2.0
2	E	272	TRP	2.0
2	E	310	THR	2.0
2	E	253	TYR	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
3	SF4	B	501	8/8	0.92	0.17	3.50	28,37,63,88	0
4	MLA	A	505	7/7	0.85	0.20	2.22	53,56,66,66	0
3	SF4	M	703	8/8	0.99	0.16	1.91	20,24,33,42	0
3	SF4	F	703	8/8	0.98	0.15	1.91	15,20,31,33	0
3	SF4	B	502	8/8	0.98	0.14	1.68	14,20,25,25	0
3	SF4	D	702	8/8	0.98	0.12	0.94	17,21,23,26	0
3	SF4	D	703	8/8	0.98	0.14	0.84	13,17,18,31	0
3	SF4	H	502	8/8	0.98	0.14	0.64	17,19,24,28	0
3	SF4	M	704	8/8	0.98	0.18	0.28	30,33,37,40	0
4	MLA	A	701	7/7	0.94	0.17	0.24	44,50,56,57	0
5	NFU	K	701	8/8	0.98	0.19	0.16	32,41,48,57	0
3	SF4	A	502	8/8	0.99	0.13	0.15	15,20,27,31	0
3	SF4	F	704	8/8	0.99	0.16	0.07	22,24,36,39	0
3	SF4	D	704	8/8	0.99	0.14	0.01	19,21,29,30	0
3	SF4	F	702	8/8	0.98	0.11	-0.02	17,22,25,28	0
4	MLA	F	701	7/7	0.96	0.13	-0.12	35,36,39,41	0
3	SF4	A	503	8/8	0.98	0.14	-0.22	15,19,22,30	0
3	SF4	H	503	8/8	0.99	0.15	-0.23	17,21,23,24	0
4	MLA	A	504	7/7	0.96	0.12	-0.31	45,47,49,50	0
3	SF4	H	501	8/8	0.99	0.11	-0.35	24,25,28,29	0
5	NFU	L	701	8/8	0.98	0.19	-0.37	24,60,72,72	0
3	SF4	B	503	8/8	0.99	0.13	-0.46	12,19,21,24	0
4	MLA	M	705	7/7	0.94	0.12	-0.55	37,38,41,42	0
3	SF4	A	501	8/8	0.99	0.09	-0.56	14,21,30,35	0
3	SF4	M	702	8/8	0.99	0.11	-0.57	25,28,31,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NFU	G	701	8/8	0.99	0.18	-1.00	26,40,50,51	0
5	NFU	C	701	8/8	0.98	0.16	-1.01	26,33,60,62	0
4	MLA	D	701	7/7	0.97	0.09	-1.06	32,34,36,37	0
5	NFU	I	701	8/8	0.98	0.17	-1.13	33,44,53,59	0
5	NFU	E	701	8/8	0.99	0.15	-1.49	40,46,64,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.