



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 PM GMT

PDB ID : 4LNO  
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: form two of GS-1  
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.  
Deposited on : 2013-07-11  
Resolution : 2.90 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

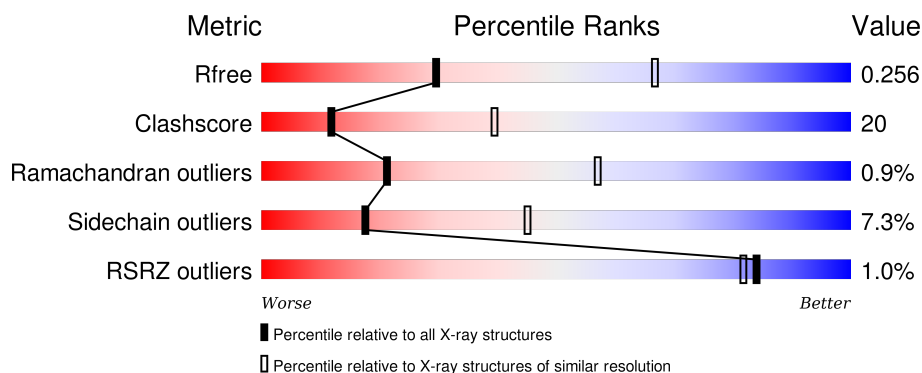
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	443	<div> <div></div> <div>65% 30% .</div> </div>
1	B	443	<div> <div></div> <div>58% 37% .</div> </div>
1	C	443	<div> <div></div> <div>61% 35% .</div> </div>
1	D	443	<div> <div></div> <div>62% 33% 5%</div> </div>
1	E	443	<div> <div></div> <div>59% 37% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	443	<div> <div></div> <div>%</div> <div>58%</div> <div>36%</div> <div>5%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	C	502	-	-	-	X
2	MG	E	502	-	-	-	X
3	GLN	A	503	-	-	-	X
3	GLN	B	503	-	-	-	X
3	GLN	E	503	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21993 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

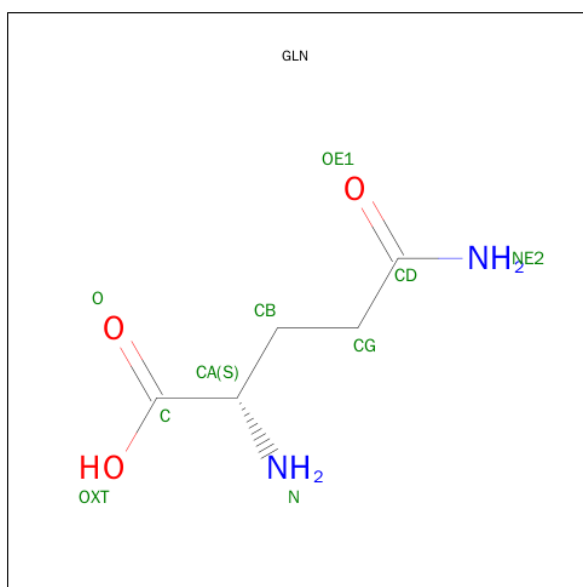
- Molecule 1 is a protein called Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	B	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	C	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	D	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	E	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	F	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	5	2	2		
3	B	1	Total	C	N	O	0	0
			9	5	2	2		
3	C	1	Total	C	N	O	0	0
			10	5	2	3		
3	D	1	Total	C	N	O	0	0
			10	5	2	3		
3	E	1	Total	C	N	O	0	0
			10	5	2	3		
3	F	1	Total	C	N	O	0	0
			10	5	2	3		

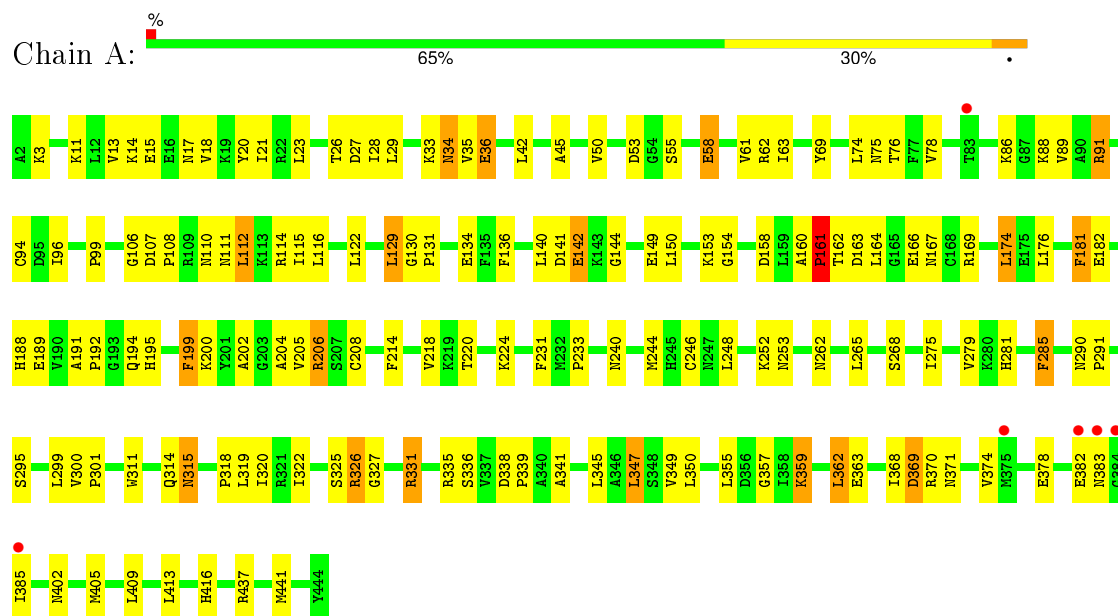
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	117	Total	O	0	0
			117	117		
4	C	123	Total	O	0	0
			123	123		
4	D	114	Total	O	0	0
			114	114		
4	E	134	Total	O	0	0
			134	134		
4	F	103	Total	O	0	0
			103	103		

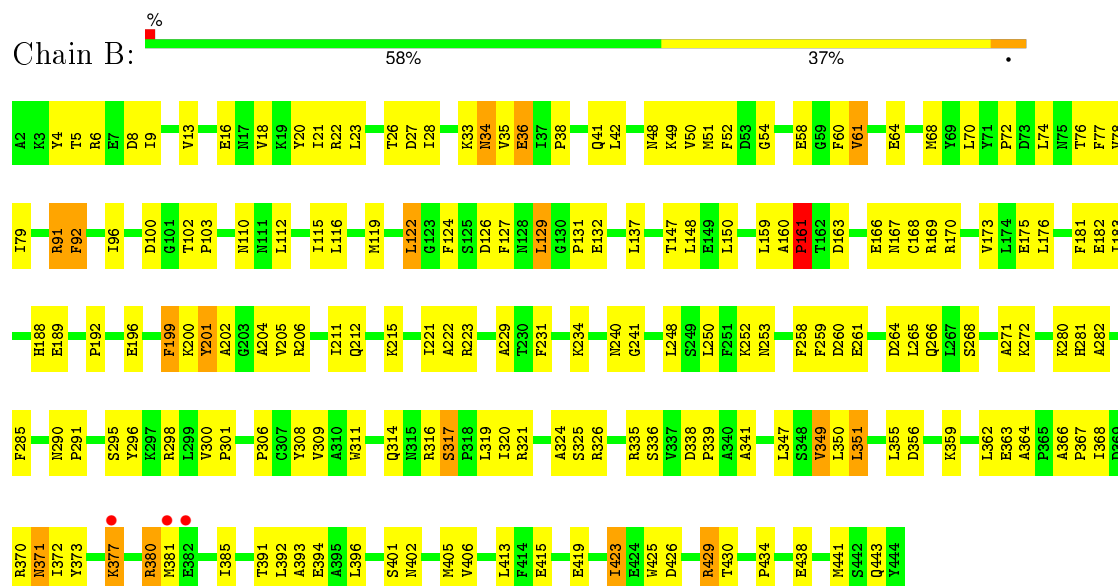
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

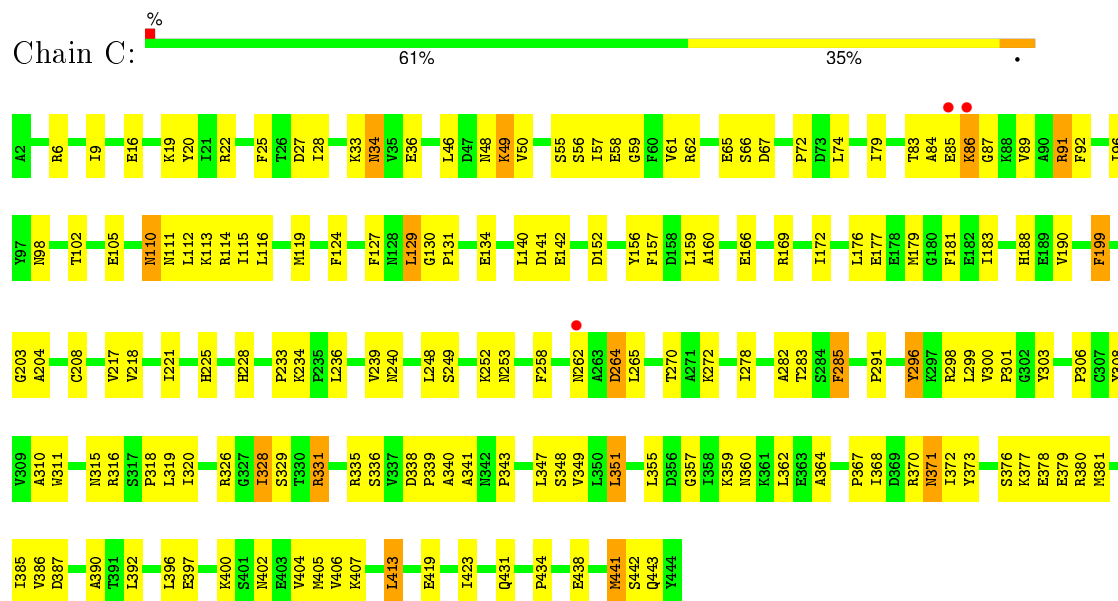
#### • Molecule 1: Glutamine synthetase



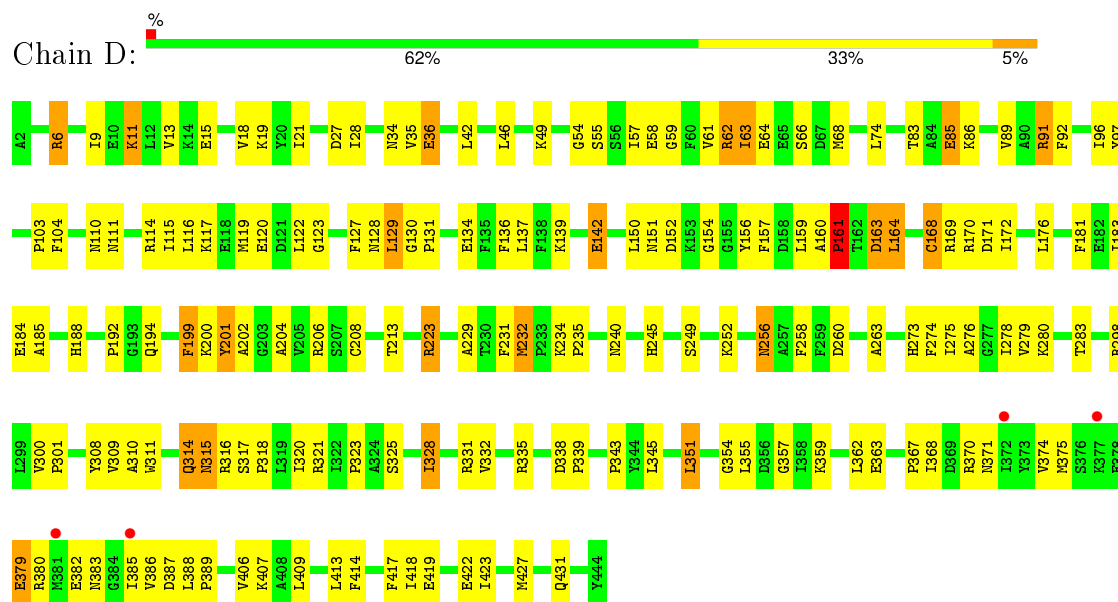
#### • Molecule 1: Glutamine synthetase



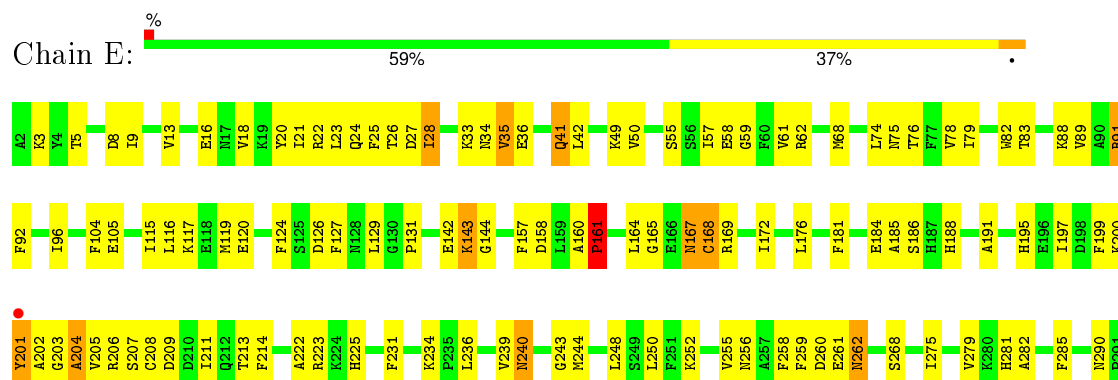
- Molecule 1: Glutamine synthetase

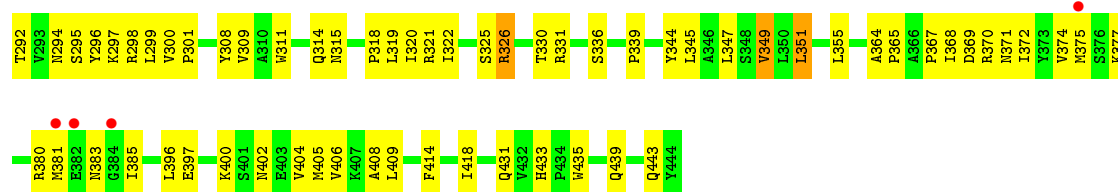


- Molecule 1: Glutamine synthetase

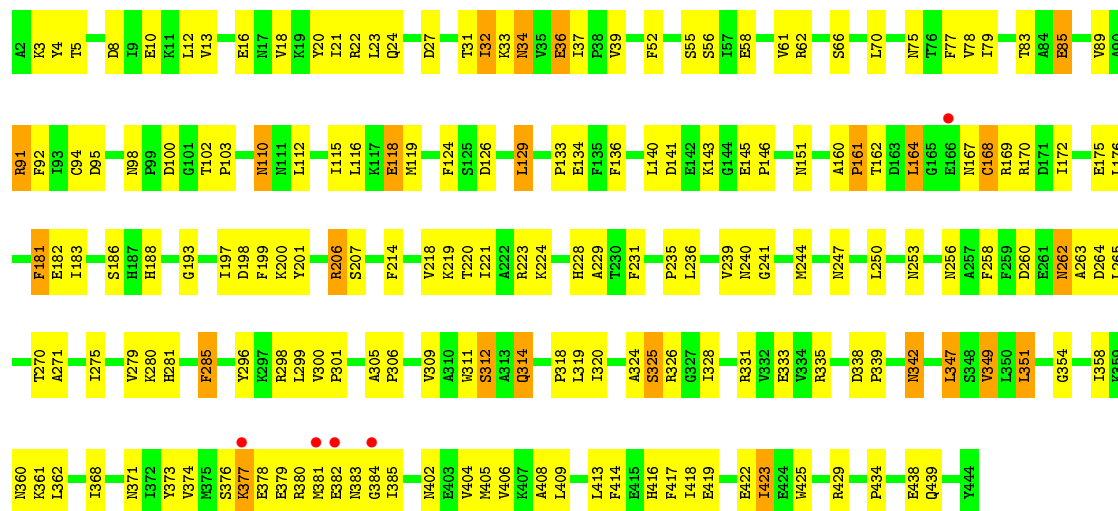


- Molecule 1: Glutamine synthetase





• Molecule 1: Glutamine synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.86Å 138.94Å 144.73Å 90.00° 125.17° 90.00°	Depositor
Resolution (Å)	71.68 – 2.90 71.68 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.68-2.90) 99.8 (71.68-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.88 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.196 , 0.256 0.195 , 0.256	Depositor DCC
$R_{free}$ test set	4565 reflections (6.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 75153 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21993	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

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	0.44	0/3618	0.61	0/4895
1	B	0.44	0/3618	0.61	0/4895
1	C	0.46	0/3618	0.62	0/4895
1	D	0.44	0/3618	0.61	0/4895
1	E	0.43	0/3618	0.62	0/4895
1	F	0.44	0/3618	0.61	0/4895
All	All	0.44	0/21708	0.61	0/29370

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	296	TYR	Sidechain
1	C	296	TYR	Sidechain
1	E	296	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	F	296	TYR	Sidechain

## 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	3535	0	3466	130	0
1	B	3535	0	3466	146	0
1	C	3535	0	3466	138	0
1	D	3535	0	3466	147	0
1	E	3535	0	3466	153	0
1	F	3535	0	3466	166	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	9	0	7	2	0
3	B	9	0	7	1	0
3	C	10	0	7	2	0
3	D	10	0	7	1	0
3	E	10	0	7	0	0
3	F	10	0	7	2	0
4	A	122	0	0	6	0
4	B	117	0	0	6	0
4	C	123	0	0	10	0
4	D	114	0	0	7	0
4	E	134	0	0	8	0
4	F	103	0	0	4	0
All	All	21993	0	20838	847	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 20.

All (847) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:ALA:HB1	1:E:161:PRO:HD2	1.29	1.10
1:C:328:ILE:HD13	1:C:328:ILE:H	1.11	1.09
1:D:160:ALA:HB1	1:D:161:PRO:HD2	1.38	1.05
1:D:160:ALA:HB3	1:D:169:ARG:HH22	1.22	1.03
1:D:63:ILE:HG22	1:D:64:GLU:HG3	1.43	0.95
1:A:160:ALA:HB3	1:A:169:ARG:HH12	1.28	0.95
1:D:160:ALA:HB3	1:D:169:ARG:NH2	1.80	0.95
1:A:160:ALA:HB1	1:A:161:PRO:HD2	1.48	0.95
1:A:370:ARG:HG2	1:A:371:ASN:H	1.33	0.93
1:D:357:GLY:HA2	1:D:362:LEU:HD13	1.50	0.93
1:B:160:ALA:HB1	1:B:161:PRO:HD2	1.52	0.91
1:A:74:LEU:HD22	1:A:74:LEU:H	1.37	0.90
1:C:16:GLU:HG2	1:C:79:ILE:HD13	1.52	0.90
1:F:27:ASP:HB3	1:F:33:LYS:HD2	1.52	0.88
1:D:129:LEU:HD13	1:D:131:PRO:HD3	1.56	0.87
1:C:368:ILE:HG21	1:C:372:ILE:HD11	1.56	0.86
1:F:160:ALA:HB1	1:F:161:PRO:HD2	1.57	0.85
1:C:129:LEU:HD13	1:C:131:PRO:HD3	1.58	0.84
1:B:20:TYR:OH	1:B:36:GLU:HG3	1.77	0.84
1:E:57:ILE:HD11	1:E:96:ILE:HG12	1.60	0.83
1:D:256:ASN:HD22	1:D:258:PHE:H	1.26	0.83
1:C:328:ILE:CD1	1:C:328:ILE:H	1.91	0.83
1:F:338:ASP:HB2	1:F:339:PRO:HD2	1.61	0.82
1:B:5:THR:HG22	1:B:8:ASP:CG	2.00	0.81
1:D:328:ILE:HD13	1:D:328:ILE:H	1.44	0.81
1:B:380:ARG:HG3	1:B:385:ILE:HB	1.63	0.81
1:B:311:TRP:CZ2	1:B:367:PRO:HG3	2.17	0.80
1:D:164:LEU:HD21	1:E:223:ARG:HD3	1.65	0.79
1:B:160:ALA:HB2	1:B:188:HIS:HB2	1.66	0.77
1:F:13:VAL:HG13	1:F:18:VAL:HB	1.66	0.77
1:B:22:ARG:HB3	1:B:34:ASN:HD22	1.49	0.77
1:D:13:VAL:HG13	1:D:18:VAL:HB	1.67	0.77
1:C:20:TYR:OH	1:C:36:GLU:HG3	1.84	0.77
1:E:349:VAL:HG22	1:E:405:MET:SD	2.25	0.76
1:D:321:ARG:HD2	4:E:663:HOH:O	1.84	0.76
1:B:13:VAL:HG13	1:B:18:VAL:HB	1.66	0.76
1:C:57:ILE:HD11	1:C:96:ILE:HG12	1.68	0.76
1:B:58:GLU:HG2	4:B:627:HOH:O	1.87	0.75
1:F:244:MET:H	1:F:338:ASP:HA	1.52	0.74
1:C:58:GLU:HG2	4:C:615:HOH:O	1.87	0.74
1:A:338:ASP:HB2	1:A:339:PRO:HD2	1.68	0.74
1:E:281:HIS:CD2	1:E:402:ASN:HD21	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:VAL:HG22	1:B:405:MET:SD	2.28	0.74
1:C:328:ILE:HD13	1:C:328:ILE:N	1.96	0.74
1:F:182:GLU:HB3	1:F:200:LYS:HD3	1.70	0.74
1:D:351:LEU:HD22	1:D:355:LEU:HG	1.71	0.73
1:D:338:ASP:HB2	1:D:339:PRO:HD2	1.72	0.71
1:D:375:MET:HB3	1:D:379:GLU:HB3	1.73	0.71
1:A:220:THR:HG23	1:F:162:THR:HB	1.73	0.70
1:D:311:TRP:CZ2	1:D:367:PRO:HG3	2.26	0.70
1:E:13:VAL:HG13	1:E:18:VAL:HB	1.72	0.70
1:A:142:GLU:CD	1:A:142:GLU:H	1.94	0.70
1:C:172:ILE:HD13	1:C:218:VAL:HG22	1.73	0.70
1:D:142:GLU:CD	1:D:142:GLU:H	1.95	0.70
1:F:100:ASP:OD2	1:F:102:THR:HG22	1.91	0.69
1:A:129:LEU:HD13	1:A:131:PRO:HG3	1.74	0.69
1:E:176:LEU:O	1:E:181:PHE:HB2	1.92	0.69
1:D:283:THR:HG23	4:D:616:HOH:O	1.92	0.69
1:F:376:SER:HB3	1:F:379:GLU:OE1	1.91	0.69
1:E:9:ILE:HG13	1:E:74:LEU:HD12	1.75	0.69
1:B:176:LEU:O	1:B:181:PHE:HB2	1.92	0.68
1:C:338:ASP:HB2	1:C:339:PRO:HD2	1.74	0.68
1:C:208:CYS:SG	1:C:343:PRO:HB2	2.33	0.68
1:B:22:ARG:HB3	1:B:34:ASN:ND2	2.08	0.68
1:E:281:HIS:HD2	1:E:402:ASN:HD21	1.40	0.68
1:F:377:LYS:O	1:F:381:MET:HG2	1.94	0.68
1:E:160:ALA:HB1	1:E:161:PRO:CD	2.16	0.67
1:E:160:ALA:CB	1:E:161:PRO:HD2	2.14	0.67
1:B:131:PRO:HG2	1:B:199:PHE:CD1	2.30	0.67
1:F:349:VAL:HG22	1:F:405:MET:SD	2.35	0.67
1:A:114:ARG:HH21	1:A:115:ILE:HD11	1.60	0.66
1:B:252:LYS:HG2	1:B:253:ASN:ND2	2.10	0.66
1:F:402:ASN:O	1:F:406:VAL:HG23	1.95	0.66
1:E:259:PHE:CZ	1:E:261:GLU:HB2	2.31	0.66
1:D:328:ILE:HD13	1:D:328:ILE:N	2.12	0.65
1:C:265:LEU:O	1:C:326:ARG:NH1	2.28	0.65
1:E:168:CYS:SG	1:E:225:HIS:HD2	2.19	0.65
1:A:76:THR:O	1:A:91:ARG:NH1	2.29	0.65
1:A:345:LEU:HD22	1:A:409:LEU:HD22	1.78	0.65
1:C:402:ASN:OD1	1:C:404:VAL:HG12	1.95	0.65
1:C:349:VAL:HG22	1:C:405:MET:SD	2.37	0.65
1:D:11:LYS:HA	1:D:11:LYS:HE3	1.78	0.65
1:C:371:ASN:HD21	1:C:373:TYR:HB2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLU:HG2	1:C:79:ILE:CD1	2.27	0.65
1:F:300:VAL:HG13	1:F:301:PRO:HD2	1.77	0.65
1:E:185:ALA:HB2	1:F:37:ILE:HG22	1.79	0.64
1:E:371:ASN:ND2	1:E:374:VAL:HG23	2.12	0.64
1:D:275:ILE:O	1:D:279:VAL:HG23	1.96	0.64
1:F:311:TRP:HB3	1:F:320:ILE:HB	1.79	0.63
1:D:116:LEU:HD23	1:D:351:LEU:HD11	1.80	0.63
1:A:129:LEU:HD21	1:A:246:CYS:HB3	1.80	0.63
1:D:11:LYS:O	1:D:15:GLU:HG3	1.99	0.63
1:E:28:ILE:O	1:E:28:ILE:HD13	1.98	0.63
1:A:160:ALA:HB3	1:A:169:ARG:NH1	2.07	0.63
1:D:117:LYS:HD2	4:D:655:HOH:O	1.97	0.63
1:A:74:LEU:CD2	1:A:74:LEU:H	2.12	0.63
1:D:328:ILE:H	1:D:328:ILE:CD1	2.11	0.63
1:D:55:SER:O	1:D:62:ARG:HG2	1.98	0.63
1:C:141:ASP:HB2	1:C:142:GLU:OE1	1.99	0.63
1:A:176:LEU:O	1:A:181:PHE:HB2	1.98	0.63
1:E:314:GLN:HE22	1:F:66:SER:HB3	1.62	0.63
1:F:281:HIS:CD2	1:F:402:ASN:HD21	2.16	0.63
1:E:129:LEU:HD23	1:E:248:LEU:HD23	1.81	0.63
1:B:300:VAL:HG13	1:B:301:PRO:HD2	1.81	0.63
1:D:131:PRO:HG2	1:D:199:PHE:CD1	2.34	0.62
1:D:129:LEU:HD22	1:D:130:GLY:N	2.14	0.62
1:E:74:LEU:H	1:E:74:LEU:HD22	1.63	0.62
1:D:315:ASN:ND2	1:D:316:ARG:H	1.96	0.62
1:A:314:GLN:NE2	1:B:64:GLU:HB2	2.14	0.62
1:B:372:ILE:HD11	1:B:385:ILE:HG21	1.81	0.62
1:D:116:LEU:HD11	1:D:204:ALA:HB3	1.80	0.62
1:D:114:ARG:HH21	1:D:115:ILE:HD11	1.65	0.62
1:E:127:PHE:CE2	1:E:351:LEU:HG	2.35	0.62
1:F:83:THR:HG21	1:F:89:VAL:HB	1.81	0.62
1:B:338:ASP:HB2	1:B:339:PRO:HD2	1.82	0.62
1:E:311:TRP:CZ2	1:E:367:PRO:HG3	2.35	0.62
1:D:68:MET:CE	1:D:104:PHE:HB2	2.30	0.62
1:F:236:LEU:HB2	1:F:239:VAL:CG2	2.30	0.62
1:A:314:GLN:HE21	1:B:64:GLU:HB2	1.66	0.61
1:A:160:ALA:HB2	1:A:188:HIS:CD2	2.35	0.61
1:F:342:ASN:HD22	1:F:342:ASN:C	2.03	0.61
1:E:115:ILE:HG22	1:E:351:LEU:HD13	1.82	0.61
1:F:175:GLU:HG3	1:F:221:ILE:CD1	2.31	0.61
1:A:300:VAL:HG13	1:A:301:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:PHE:HB3	1:D:339:PRO:HB2	1.82	0.60
1:E:311:TRP:CB	1:E:320:ILE:HB	2.31	0.60
1:B:127:PHE:HE2	1:B:347:LEU:HD12	1.66	0.60
1:F:58:GLU:O	1:F:61:VAL:HG22	2.00	0.60
1:D:383:ASN:HB2	1:D:385:ILE:HG13	1.83	0.60
1:E:234:LYS:HD3	1:E:298:ARG:HA	1.82	0.60
1:A:281:HIS:CD2	1:A:402:ASN:HD21	2.18	0.60
1:D:58:GLU:O	1:D:61:VAL:HG22	2.00	0.60
1:D:160:ALA:HB2	1:D:188:HIS:CD2	2.36	0.60
1:F:201:TYR:CE2	1:F:331:ARG:HD2	2.35	0.60
1:A:208:CYS:SG	1:A:347:LEU:HD23	2.42	0.60
1:A:281:HIS:HD2	1:A:402:ASN:HD21	1.50	0.60
1:A:11:LYS:O	1:A:15:GLU:HB2	2.02	0.60
1:E:205:VAL:HG12	4:E:618:HOH:O	2.00	0.60
1:E:59:GLY:O	1:E:62:ARG:HG3	2.02	0.59
1:E:96:ILE:N	1:E:96:ILE:HD12	2.17	0.59
1:B:129:LEU:HD13	1:B:131:PRO:HD3	1.84	0.59
1:A:182:GLU:HB3	1:A:200:LYS:HD2	1.84	0.59
1:E:200:LYS:HE2	1:E:201:TYR:HD2	1.65	0.59
1:D:370:ARG:HG2	1:D:371:ASN:N	2.18	0.59
1:E:57:ILE:CD1	1:E:96:ILE:HG12	2.31	0.59
1:C:402:ASN:O	1:C:406:VAL:HG23	2.01	0.59
1:A:252:LYS:O	1:A:253:ASN:HB2	2.02	0.59
1:D:423:ILE:HD13	4:D:662:HOH:O	2.01	0.59
1:F:176:LEU:O	1:F:181:PHE:HB2	2.03	0.59
1:D:260:ASP:OD1	1:D:263:ALA:HB2	2.03	0.59
1:D:256:ASN:HD21	1:D:258:PHE:HB2	1.68	0.59
1:E:129:LEU:HD13	1:E:131:PRO:HD3	1.85	0.59
1:E:200:LYS:HG2	1:E:201:TYR:H	1.67	0.59
1:C:56:SER:HA	1:C:62:ARG:HD2	1.85	0.59
1:A:160:ALA:HB2	1:A:188:HIS:HB2	1.85	0.58
1:D:308:TYR:HA	1:D:387:ASP:HA	1.85	0.58
1:C:248:LEU:O	1:C:331:ARG:HB2	2.03	0.58
1:D:116:LEU:HD23	1:D:351:LEU:CD1	2.33	0.58
1:F:206:ARG:HG3	1:F:206:ARG:HH11	1.67	0.58
1:D:256:ASN:ND2	1:D:258:PHE:H	1.98	0.58
1:F:311:TRP:CB	1:F:320:ILE:HB	2.33	0.58
1:C:291:PRO:HG3	1:C:341:ALA:HA	1.84	0.58
1:E:160:ALA:HB2	1:E:188:HIS:HD2	1.68	0.58
1:A:74:LEU:N	1:A:74:LEU:HD22	2.13	0.58
1:C:152:ASP:HB2	4:C:649:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:GLU:HG3	1:F:221:ILE:HD13	1.86	0.58
1:F:265:LEU:O	1:F:326:ARG:NH1	2.36	0.58
1:F:22:ARG:HH11	1:F:22:ARG:HG2	1.67	0.58
1:C:176:LEU:O	1:C:181:PHE:HB2	2.03	0.58
1:A:129:LEU:HD23	1:A:248:LEU:HD23	1.85	0.58
1:A:169:ARG:NH2	1:A:195:HIS:ND1	2.50	0.57
1:F:182:GLU:CB	1:F:200:LYS:HD3	2.34	0.57
1:B:261:GLU:HG3	1:B:266:GLN:HE21	1.69	0.57
1:C:308:TYR:HD2	1:C:387:ASP:HB3	1.69	0.57
1:B:223:ARG:NH1	1:B:223:ARG:HG3	2.19	0.57
1:A:129:LEU:CD1	1:A:131:PRO:HG3	2.34	0.57
1:E:55:SER:O	1:E:62:ARG:HG2	2.04	0.57
1:F:56:SER:HA	1:F:62:ARG:HD2	1.86	0.57
1:B:371:ASN:HD22	1:B:372:ILE:N	2.03	0.57
1:A:13:VAL:HG13	1:A:18:VAL:HB	1.86	0.57
1:E:3:LYS:H	1:E:75:ASN:ND2	2.02	0.57
1:F:78:VAL:HG12	1:F:79:ILE:N	2.20	0.57
1:A:205:VAL:HG23	4:A:603:HOH:O	2.05	0.57
1:F:160:ALA:HB2	1:F:188:HIS:CD2	2.40	0.57
1:E:68:MET:HE1	1:E:104:PHE:HB2	1.87	0.57
1:E:311:TRP:HB3	1:E:320:ILE:HB	1.86	0.57
1:B:280:LYS:HD2	1:B:362:LEU:HD21	1.87	0.57
1:A:58:GLU:O	1:A:61:VAL:HG22	2.05	0.56
1:B:50:VAL:HB	4:B:633:HOH:O	2.05	0.56
1:B:115:ILE:HG22	1:B:351:LEU:HD13	1.87	0.56
1:D:311:TRP:HB3	1:D:320:ILE:HB	1.87	0.56
1:E:345:LEU:HD22	1:E:409:LEU:HD22	1.87	0.56
1:C:310:ALA:HB1	1:C:368:ILE:HD13	1.86	0.56
1:F:58:GLU:HG2	1:F:416:HIS:CD2	2.41	0.56
1:F:380:ARG:O	1:F:385:ILE:HB	2.05	0.56
1:D:163:ASP:HB2	1:E:82:TRP:HE1	1.70	0.56
1:D:256:ASN:HB2	1:D:328:ILE:HA	1.88	0.56
1:D:176:LEU:O	1:D:181:PHE:HB2	2.05	0.56
1:C:127:PHE:HE2	1:C:347:LEU:HD12	1.70	0.56
1:C:129:LEU:HG	1:C:347:LEU:HD21	1.85	0.56
1:C:55:SER:O	1:C:62:ARG:HG2	2.06	0.56
1:C:419:GLU:O	1:C:423:ILE:HG12	2.06	0.56
1:C:28:ILE:HD12	1:C:413:LEU:HD23	1.88	0.56
1:E:74:LEU:N	1:E:74:LEU:HD22	2.21	0.56
1:B:319:LEU:CD1	1:B:336:SER:HB3	2.36	0.56
1:B:35:VAL:O	1:B:35:VAL:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ASN:ND2	1:B:373:TYR:H	2.03	0.56
1:E:142:GLU:H	1:E:142:GLU:CD	2.10	0.56
1:D:160:ALA:CB	1:D:188:HIS:CD2	2.89	0.56
1:C:329:SER:O	1:C:331:ARG:HD3	2.06	0.56
1:C:111:ASN:O	1:C:115:ILE:HG12	2.06	0.56
1:C:252:LYS:HG2	1:C:253:ASN:ND2	2.20	0.56
1:D:170:ARG:NH1	1:D:171:ASP:OD2	2.39	0.56
1:E:160:ALA:HB3	1:E:169:ARG:NH1	2.22	0.55
1:F:20:TYR:HB3	1:F:89:VAL:HG22	1.88	0.55
1:C:156:TYR:HB2	1:C:190:VAL:HA	1.88	0.55
1:E:311:TRP:CH2	1:E:367:PRO:HG3	2.41	0.55
1:E:205:VAL:HG13	1:E:206:ARG:N	2.22	0.55
1:B:116:LEU:HD11	1:B:204:ALA:HB3	1.87	0.55
1:E:58:GLU:O	1:E:61:VAL:HG22	2.07	0.55
1:B:76:THR:O	1:B:78:VAL:HG23	2.05	0.55
1:A:265:LEU:O	1:A:326:ARG:NH1	2.39	0.55
1:F:419:GLU:O	1:F:423:ILE:HG23	2.06	0.55
1:D:6:ARG:HG2	1:D:46:LEU:HD13	1.88	0.55
1:D:160:ALA:CB	1:D:161:PRO:HD2	2.19	0.55
1:F:160:ALA:HB3	1:F:169:ARG:NH2	2.22	0.55
1:E:402:ASN:OD1	1:E:404:VAL:HG12	2.07	0.55
1:B:314:GLN:HE22	1:C:66:SER:HB2	1.71	0.55
1:C:91:ARG:C	1:C:91:ARG:HD2	2.27	0.55
1:B:4:TYR:HB3	1:B:9:ILE:CD1	2.37	0.55
1:B:147:THR:HG22	1:B:148:LEU:N	2.21	0.55
1:C:115:ILE:HG13	1:C:348:SER:HB3	1.88	0.55
1:F:270:THR:HG23	1:F:358:ILE:HD12	1.88	0.55
1:F:172:ILE:HD12	1:F:218:VAL:HA	1.87	0.55
1:C:311:TRP:CB	1:C:320:ILE:HB	2.37	0.55
1:E:252:LYS:O	1:E:255:VAL:HG22	2.07	0.55
1:A:370:ARG:HG2	1:A:371:ASN:N	2.14	0.55
1:C:300:VAL:HG13	1:C:301:PRO:HD2	1.88	0.55
1:A:202:ALA:HB1	1:A:206:ARG:HG2	1.89	0.55
1:B:434:PRO:O	1:B:438:GLU:HG3	2.07	0.55
1:D:150:LEU:HD13	1:D:192:PRO:HB2	1.89	0.55
1:F:167:ASN:HD22	1:F:170:ARG:H	1.53	0.55
1:C:318:PRO:O	1:C:335:ARG:HD3	2.07	0.55
1:B:169:ARG:NH1	1:C:36:GLU:OE1	2.40	0.54
1:E:68:MET:HE2	1:E:96:ILE:HG22	1.89	0.54
1:E:5:THR:H	1:E:8:ASP:HB2	1.71	0.54
1:C:431:GLN:HG3	4:C:646:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:SER:HB2	4:B:687:HOH:O	2.07	0.54
1:E:116:LEU:O	1:E:119:MET:HB3	2.07	0.54
1:E:164:LEU:HD13	1:F:224:LYS:HB2	1.89	0.54
1:F:91:ARG:HD2	1:F:92:PHE:N	2.22	0.54
1:B:282:ALA:HA	1:B:285:PHE:CZ	2.42	0.54
1:D:68:MET:HE1	1:D:104:PHE:HB2	1.88	0.54
1:F:236:LEU:HB2	1:F:239:VAL:HG21	1.89	0.54
1:F:140:LEU:HD21	1:F:228:HIS:HB2	1.89	0.54
1:E:160:ALA:HB2	1:E:188:HIS:CD2	2.43	0.54
1:B:119:MET:HB2	1:B:355:LEU:HD11	1.90	0.54
1:F:371:ASN:ND2	1:F:374:VAL:HG13	2.23	0.54
1:F:91:ARG:HD2	1:F:91:ARG:C	2.27	0.54
1:F:264:ASP:O	1:F:265:LEU:HB2	2.06	0.54
1:D:163:ASP:HB3	1:E:83:THR:HG22	1.90	0.54
1:E:319:LEU:CD1	1:E:336:SER:HB3	2.37	0.54
1:E:16:GLU:O	1:E:88:LYS:HD2	2.07	0.54
1:B:285:PHE:HB2	1:B:349:VAL:HG11	1.89	0.54
1:E:383:ASN:HB2	1:E:385:ILE:HG12	1.90	0.54
1:C:376:SER:HB3	1:C:379:GLU:HG3	1.90	0.54
1:A:69:TYR:CE1	1:A:99:PRO:HA	2.43	0.54
1:B:96:ILE:HD12	1:B:96:ILE:N	2.22	0.54
1:C:377:LYS:HD2	1:C:380:ARG:HH12	1.73	0.54
1:F:32:ILE:HD13	4:F:652:HOH:O	2.07	0.53
1:B:122:LEU:HD11	1:B:359:LYS:HG3	1.89	0.53
1:C:298:ARG:NH1	3:C:501:GLN:O	2.40	0.53
1:E:300:VAL:HG13	1:E:301:PRO:HD2	1.90	0.53
1:A:136:PHE:CE2	1:A:194:GLN:HB2	2.43	0.53
1:D:278:ILE:CG2	1:D:320:ILE:HD11	2.38	0.53
1:F:281:HIS:HD2	1:F:402:ASN:HD21	1.56	0.53
1:A:166:GLU:HB3	4:A:670:HOH:O	2.08	0.53
1:D:300:VAL:HG13	1:D:301:PRO:HD2	1.91	0.53
1:E:68:MET:CE	1:E:104:PHE:HB2	2.39	0.53
1:F:262:ASN:ND2	1:F:262:ASN:H	2.06	0.53
1:A:189:GLU:HB3	1:A:194:GLN:NE2	2.23	0.53
1:D:61:VAL:O	1:D:63:ILE:HD12	2.08	0.53
1:E:294:ASN:HA	1:E:297:LYS:HG2	1.89	0.53
1:F:256:ASN:HB2	1:F:328:ILE:HA	1.89	0.53
1:A:26:THR:HG22	1:A:27:ASP:O	2.09	0.53
1:F:20:TYR:OH	1:F:36:GLU:HG3	2.08	0.53
1:E:160:ALA:O	1:E:161:PRO:C	2.46	0.53
1:B:23:LEU:HD13	1:B:70:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:GLU:HG2	1:F:79:ILE:HD12	1.91	0.53
1:A:357:GLY:HA2	1:A:362:LEU:HD22	1.91	0.53
1:A:378:GLU:O	1:A:382:GLU:HG2	2.09	0.53
1:D:223:ARG:HG2	1:D:223:ARG:HH11	1.74	0.52
1:B:160:ALA:HB3	1:B:169:ARG:HH22	1.73	0.52
1:E:74:LEU:H	1:E:74:LEU:CD2	2.23	0.52
1:B:281:HIS:CD2	1:B:402:ASN:HD21	2.27	0.52
1:B:402:ASN:O	1:B:406:VAL:HG23	2.09	0.52
1:B:223:ARG:HH11	1:B:223:ARG:HG3	1.73	0.52
1:A:160:ALA:CB	1:A:161:PRO:HD2	2.28	0.52
1:C:282:ALA:HA	1:C:285:PHE:CZ	2.45	0.52
1:F:231:PHE:O	1:F:339:PRO:HG2	2.08	0.52
1:B:129:LEU:HD23	1:B:248:LEU:HD23	1.91	0.52
1:E:119:MET:HG2	1:E:124:PHE:HB2	1.92	0.52
1:A:319:LEU:CD1	1:A:336:SER:HB3	2.40	0.52
1:E:169:ARG:HE	1:E:195:HIS:HD2	1.57	0.52
1:B:122:LEU:HD21	1:B:359:LYS:HG2	1.91	0.52
1:D:176:LEU:HD13	1:D:183:ILE:HD11	1.90	0.52
1:B:380:ARG:HG2	1:B:380:ARG:HH11	1.73	0.52
1:D:170:ARG:HH11	1:D:170:ARG:HG2	1.75	0.52
1:E:321:ARG:HD2	4:E:630:HOH:O	2.09	0.52
1:B:28:ILE:HD12	1:B:413:LEU:HD23	1.90	0.52
1:F:168:CYS:O	1:F:172:ILE:HG12	2.10	0.52
1:F:183:ILE:HG23	1:F:198:ASP:O	2.10	0.52
1:B:419:GLU:O	1:B:423:ILE:HD12	2.09	0.52
1:C:59:GLY:O	1:C:62:ARG:HG3	2.09	0.52
1:B:9:ILE:HD11	1:B:74:LEU:HB3	1.91	0.52
1:A:86:LYS:HD3	4:A:669:HOH:O	2.10	0.52
1:C:351:LEU:HD22	1:C:355:LEU:HG	1.92	0.51
1:D:19:LYS:HG3	1:D:86:LYS:O	2.10	0.51
1:F:77:PHE:HB2	1:F:92:PHE:CE2	2.46	0.51
1:C:169:ARG:HH11	1:D:36:GLU:CD	2.14	0.51
1:A:322:ILE:N	1:A:322:ILE:HD12	2.25	0.51
1:D:278:ILE:HG22	1:D:320:ILE:HD11	1.91	0.51
1:B:9:ILE:CD1	1:B:74:LEU:HB3	2.40	0.51
1:A:69:TYR:HE1	1:A:99:PRO:HA	1.74	0.51
1:F:136:PHE:CD1	1:F:235:PRO:HG2	2.45	0.51
1:D:159:LEU:HD11	1:E:22:ARG:HD3	1.92	0.51
1:F:167:ASN:ND2	1:F:170:ARG:H	2.08	0.51
1:C:28:ILE:HG12	1:C:57:ILE:O	2.09	0.51
1:F:360:ASN:HB2	1:F:362:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ALA:HB1	1:D:206:ARG:HD3	1.93	0.51
1:D:345:LEU:HD22	1:D:409:LEU:HD22	1.92	0.51
1:C:199:PHE:CD2	1:C:199:PHE:N	2.77	0.51
1:E:91:ARG:HD2	1:E:92:PHE:N	2.25	0.51
1:A:58:GLU:HG2	1:A:416:HIS:CD2	2.45	0.51
1:C:22:ARG:HH11	1:C:34:ASN:HD21	1.57	0.51
3:A:503:GLN:N	4:A:609:HOH:O	2.42	0.51
1:F:231:PHE:HB3	1:F:339:PRO:HB2	1.92	0.51
1:E:24:GLN:OE1	1:E:91:ARG:HD3	2.11	0.51
1:E:200:LYS:HG2	1:E:201:TYR:N	2.26	0.51
1:B:119:MET:HG2	1:B:124:PHE:HB2	1.92	0.51
1:E:282:ALA:HA	1:E:285:PHE:CZ	2.45	0.51
1:A:111:ASN:O	1:A:115:ILE:HG12	2.10	0.51
1:D:9:ILE:HG21	1:D:92:PHE:HZ	1.76	0.51
1:F:21:ILE:HD12	1:F:39:VAL:HA	1.93	0.51
1:E:208:CYS:SG	1:E:347:LEU:HD12	2.50	0.51
1:F:285:PHE:HB3	1:F:405:MET:SD	2.51	0.51
1:F:418:ILE:O	1:F:422:GLU:HB2	2.11	0.51
1:A:36:GLU:HG2	1:F:186:SER:O	2.11	0.51
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.92	0.51
1:C:134:GLU:OE1	3:C:501:GLN:N	2.43	0.50
1:D:137:LEU:HD23	1:D:229:ALA:HA	1.93	0.50
1:C:166:GLU:HG3	1:C:225:HIS:HD1	1.75	0.50
1:D:91:ARG:HD2	1:D:91:ARG:C	2.32	0.50
1:C:208:CYS:SG	1:C:343:PRO:C	2.90	0.50
1:F:133:PRO:HD2	1:F:197:ILE:O	2.10	0.50
1:D:232:MET:HB3	1:D:235:PRO:HG3	1.92	0.50
1:A:3:LYS:HG2	1:A:3:LYS:O	2.10	0.50
1:C:65:GLU:O	1:C:65:GLU:HG3	2.10	0.50
1:E:351:LEU:HD22	1:E:355:LEU:HG	1.93	0.50
1:F:384:GLY:O	1:F:385:ILE:HD13	2.11	0.50
1:D:200:LYS:HE3	1:E:41:GLN:OE1	2.11	0.50
1:F:425:TRP:HE1	1:F:429:ARG:HD3	1.77	0.50
1:C:380:ARG:HB3	1:C:385:ILE:HB	1.93	0.50
1:E:375:MET:HG3	1:E:375:MET:O	2.12	0.50
1:D:59:GLY:O	1:D:62:ARG:HG3	2.12	0.50
1:E:372:ILE:HD13	1:E:375:MET:HE3	1.94	0.50
1:C:22:ARG:HB3	1:C:34:ASN:HD22	1.77	0.50
1:F:409:LEU:O	1:F:413:LEU:HB2	2.11	0.50
1:F:85:GLU:N	1:F:85:GLU:CD	2.65	0.50
1:C:58:GLU:O	1:C:61:VAL:HG22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:THR:HG23	4:F:630:HOH:O	2.12	0.50
1:B:290:ASN:HB3	1:B:295:SER:HB3	1.94	0.50
1:D:260:ASP:CG	1:D:263:ALA:HB2	2.32	0.50
1:C:278:ILE:O	1:C:282:ALA:HB2	2.11	0.50
1:A:275:ILE:O	1:A:279:VAL:HG23	2.12	0.50
1:B:182:GLU:HB3	1:B:200:LYS:CD	2.42	0.50
1:D:380:ARG:O	1:D:385:ILE:HB	2.12	0.49
1:C:156:TYR:O	1:C:157:PHE:HB2	2.12	0.49
1:B:77:PHE:HB2	1:B:92:PHE:CE2	2.47	0.49
1:C:217:VAL:O	1:C:221:ILE:HG12	2.11	0.49
1:B:100:ASP:OD1	1:B:102:THR:HG23	2.11	0.49
1:E:285:PHE:HB3	1:E:405:MET:SD	2.51	0.49
1:C:306:PRO:HG2	1:C:335:ARG:C	2.33	0.49
1:B:21:ILE:HD13	1:B:42:LEU:HD13	1.94	0.49
1:D:152:ASP:HB2	4:D:701:HOH:O	2.11	0.49
1:F:318:PRO:O	1:F:335:ARG:HD3	2.11	0.49
1:A:248:LEU:O	1:A:331:ARG:HB2	2.12	0.49
1:C:169:ARG:HH22	1:C:188:HIS:HB2	1.76	0.49
1:B:168:CYS:SG	1:B:222:ALA:HA	2.52	0.49
1:B:429:ARG:HD3	1:B:430:THR:HG23	1.93	0.49
1:A:53:ASP:CG	1:A:55:SER:HG	2.16	0.49
1:E:158:ASP:OD1	1:F:33:LYS:HE3	2.13	0.49
1:D:383:ASN:C	1:D:385:ILE:H	2.14	0.49
1:B:351:LEU:HD22	1:B:355:LEU:HG	1.94	0.49
1:A:21:ILE:HD13	1:A:42:LEU:HD13	1.94	0.49
1:F:24:GLN:HB2	1:F:32:ILE:HD11	1.94	0.49
1:F:206:ARG:NH1	1:F:206:ARG:HG3	2.28	0.49
1:C:311:TRP:HB3	1:C:320:ILE:HB	1.94	0.49
1:A:27:ASP:HB3	1:A:33:LYS:HE3	1.93	0.49
1:D:331:ARG:HH21	1:D:331:ARG:HG2	1.76	0.49
1:B:160:ALA:O	1:B:161:PRO:C	2.51	0.49
1:D:131:PRO:HG2	1:D:199:PHE:HD1	1.77	0.49
1:F:116:LEU:HD23	1:F:351:LEU:HD11	1.94	0.49
1:B:160:ALA:HB3	1:B:169:ARG:HH12	1.77	0.49
1:E:433:HIS:HB3	4:E:640:HOH:O	2.12	0.49
1:D:249:SER:HA	1:D:258:PHE:CE1	2.47	0.49
1:F:22:ARG:NH1	1:F:22:ARG:HG2	2.28	0.49
1:F:423:ILE:C	1:F:423:ILE:HD12	2.33	0.49
1:A:231:PHE:HB3	1:A:339:PRO:HB2	1.94	0.49
1:C:264:ASP:O	1:C:265:LEU:HB2	2.13	0.49
1:C:234:LYS:HD3	1:C:298:ARG:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASP:O	1:B:266:GLN:HA	2.13	0.48
1:E:21:ILE:HD13	1:E:42:LEU:HD13	1.94	0.48
1:C:357:GLY:HA2	1:C:362:LEU:HD12	1.95	0.48
1:C:441:MET:O	1:C:441:MET:HG3	2.12	0.48
1:E:405:MET:O	1:E:408:ALA:HB3	2.13	0.48
1:F:236:LEU:HB2	1:F:239:VAL:HG22	1.94	0.48
1:B:260:ASP:HB2	1:B:268:SER:HB3	1.95	0.48
1:F:3:LYS:HB3	1:F:75:ASN:OD1	2.13	0.48
4:E:704:HOH:O	1:F:223:ARG:HD3	2.14	0.48
1:D:314:GLN:O	1:D:314:GLN:HG3	2.11	0.48
1:C:377:LYS:HD2	1:C:380:ARG:NH1	2.28	0.48
1:F:169:ARG:NH2	1:F:188:HIS:HB2	2.29	0.48
1:A:27:ASP:HB3	1:A:33:LYS:CE	2.43	0.48
1:B:272:LYS:O	1:B:364:ALA:HB2	2.13	0.48
1:D:116:LEU:O	1:D:119:MET:HB3	2.13	0.48
1:A:122:LEU:CD1	1:A:355:LEU:HD22	2.44	0.48
1:F:279:VAL:HG13	1:F:309:VAL:HG12	1.96	0.48
1:E:23:LEU:HB2	1:E:35:VAL:HG13	1.94	0.48
1:D:27:ASP:C	1:D:27:ASP:OD2	2.50	0.48
1:B:264:ASP:OD2	1:B:265:LEU:HD13	2.13	0.48
1:E:223:ARG:HG3	1:E:223:ARG:NH1	2.28	0.48
1:A:114:ARG:NH2	1:A:115:ILE:HD11	2.28	0.48
1:F:58:GLU:HB3	1:F:61:VAL:HG23	1.96	0.48
1:B:16:GLU:HG2	1:B:79:ILE:HD13	1.96	0.48
1:B:137:LEU:HD23	1:B:229:ALA:HA	1.95	0.48
1:A:14:LYS:HE2	4:A:676:HOH:O	2.14	0.48
1:C:392:LEU:O	1:C:396:LEU:HG	2.13	0.48
1:E:76:THR:O	1:E:78:VAL:HG23	2.13	0.48
1:E:396:LEU:O	1:E:400:LYS:HG3	2.14	0.48
1:D:317:SER:HB2	1:D:335:ARG:HH22	1.79	0.48
1:F:20:TYR:CZ	1:F:36:GLU:HB2	2.49	0.48
1:D:379:GLU:HA	1:D:382:GLU:OE1	2.14	0.48
1:E:157:PHE:O	1:F:33:LYS:HB3	2.14	0.47
1:C:129:LEU:HD23	1:C:248:LEU:HD23	1.95	0.47
1:C:96:ILE:N	1:C:96:ILE:HD12	2.29	0.47
1:C:169:ARG:NH2	1:C:188:HIS:HB2	2.29	0.47
1:B:259:PHE:CD1	1:B:326:ARG:HG3	2.49	0.47
1:A:359:LYS:NZ	1:A:359:LYS:HB2	2.28	0.47
1:B:202:ALA:HB1	1:B:206:ARG:HD3	1.96	0.47
1:D:274:PHE:CD2	1:D:332:VAL:HG11	2.49	0.47
1:E:91:ARG:HH12	1:E:213:THR:CG2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:LEU:HB2	1:F:220:THR:CG2	2.44	0.47
1:F:85:GLU:H	1:F:85:GLU:CD	2.18	0.47
1:C:49:LYS:HE3	4:C:610:HOH:O	2.13	0.47
1:E:435:TRP:O	1:E:439:GLN:HG2	2.14	0.47
1:E:370:ARG:HD3	1:E:375:MET:HE1	1.95	0.47
1:C:434:PRO:O	1:C:438:GLU:HG3	2.14	0.47
1:D:160:ALA:HB2	1:D:188:HIS:CG	2.50	0.47
1:D:68:MET:HE2	1:D:104:PHE:HB2	1.95	0.47
1:D:223:ARG:HG2	1:D:223:ARG:NH1	2.29	0.47
1:B:321:ARG:HH22	1:C:67:ASP:CG	2.17	0.47
1:A:23:LEU:HB3	1:A:94:CYS:SG	2.54	0.47
1:C:377:LYS:O	1:C:381:MET:HG2	2.15	0.47
1:A:164:LEU:C	1:A:166:GLU:H	2.16	0.47
1:E:116:LEU:HD11	1:E:204:ALA:HB3	1.95	0.47
1:F:3:LYS:HE2	1:F:4:TYR:CE2	2.49	0.47
1:C:83:THR:HG21	1:C:89:VAL:HG23	1.97	0.47
1:F:241:GLY:HA3	1:F:298:ARG:HG2	1.96	0.47
1:A:160:ALA:CB	1:A:188:HIS:HD2	2.28	0.47
1:C:27:ASP:HB2	1:C:57:ILE:O	2.15	0.47
1:A:162:THR:O	1:A:164:LEU:N	2.47	0.47
1:F:55:SER:O	1:F:62:ARG:HG2	2.15	0.47
1:B:38:PRO:HD2	1:B:41:GLN:HG3	1.95	0.47
1:E:418:ILE:HD12	1:E:418:ILE:N	2.30	0.47
1:F:32:ILE:HD12	1:F:33:LYS:N	2.30	0.47
1:B:311:TRP:HB3	1:B:320:ILE:HB	1.95	0.47
1:C:308:TYR:CD2	1:C:387:ASP:HB3	2.48	0.47
1:A:164:LEU:HD21	1:B:223:ARG:HG2	1.95	0.47
1:B:309:VAL:HA	1:B:319:LEU:HD22	1.96	0.47
1:A:140:LEU:HD22	1:A:144:GLY:O	2.14	0.47
1:A:20:TYR:HB3	1:A:89:VAL:HG22	1.97	0.47
1:D:120:GLU:C	1:D:122:LEU:H	2.17	0.47
1:B:429:ARG:CD	1:B:430:THR:HG23	2.45	0.47
1:C:110:ASN:O	1:C:113:LYS:HB2	2.14	0.47
1:C:177:GLU:C	1:C:179:MET:H	2.18	0.47
1:F:160:ALA:O	1:F:161:PRO:O	2.33	0.47
1:E:184:GLU:O	1:E:185:ALA:HB2	2.15	0.47
1:E:290:ASN:HB3	1:E:295:SER:HB3	1.96	0.47
1:A:160:ALA:HB2	1:A:188:HIS:HD2	1.78	0.46
1:A:169:ARG:HD3	1:A:195:HIS:HB3	1.97	0.46
1:F:285:PHE:CD1	1:F:285:PHE:C	2.87	0.46
1:B:4:TYR:HB3	1:B:9:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:ALA:CB	1:F:188:HIS:CD2	2.98	0.46
1:F:378:GLU:O	1:F:381:MET:HB2	2.15	0.46
1:C:33:LYS:O	1:C:34:ASN:HB3	2.15	0.46
1:B:205:VAL:HG22	4:B:631:HOH:O	2.15	0.46
1:A:233:PRO:HG2	1:A:295:SER:OG	2.15	0.46
1:F:170:ARG:HG2	1:F:170:ARG:HH11	1.80	0.46
1:A:182:GLU:CB	1:A:200:LYS:HD2	2.45	0.46
1:B:78:VAL:HG12	1:B:79:ILE:N	2.31	0.46
1:C:6:ARG:HD2	1:C:46:LEU:HD13	1.97	0.46
1:E:185:ALA:CB	1:F:37:ILE:HG22	2.44	0.46
1:C:49:LYS:HE2	1:C:49:LYS:HA	1.97	0.46
1:E:377:LYS:HB2	4:E:682:HOH:O	2.15	0.46
1:B:52:PHE:CE2	1:B:54:GLY:HA2	2.51	0.46
1:D:273:HIS:O	1:D:276:ALA:HB3	2.15	0.46
1:C:234:LYS:HE3	1:C:239:VAL:O	2.16	0.46
1:C:20:TYR:CZ	1:C:36:GLU:HG3	2.50	0.46
1:B:5:THR:HG23	1:B:8:ASP:H	1.80	0.46
1:E:322:ILE:HG22	1:E:326:ARG:HH21	1.80	0.46
1:A:96:ILE:N	1:A:96:ILE:HD12	2.30	0.46
1:F:379:GLU:HA	1:F:382:GLU:OE1	2.16	0.46
1:E:370:ARG:HG2	1:E:370:ARG:HH11	1.81	0.46
1:B:116:LEU:HD23	1:B:351:LEU:HD11	1.98	0.46
1:E:279:VAL:HG13	1:E:309:VAL:HG12	1.97	0.46
1:E:368:ILE:HD13	1:E:385:ILE:HD11	1.98	0.46
1:A:116:LEU:HD11	1:A:204:ALA:HB3	1.97	0.46
1:D:91:ARG:HH12	1:D:213:THR:HG23	1.81	0.46
1:E:78:VAL:HG12	1:E:79:ILE:N	2.31	0.46
1:A:318:PRO:O	1:A:335:ARG:HD3	2.15	0.46
1:B:258:PHE:HA	1:B:271:ALA:HB2	1.96	0.46
1:C:48:ASN:OD1	1:C:72:PRO:HD2	2.16	0.46
1:F:134:GLU:OE2	3:F:503:GLN:HG3	2.15	0.46
1:F:219:LYS:HA	1:F:229:ALA:HB3	1.98	0.46
1:B:170:ARG:HG3	1:C:20:TYR:CD2	2.51	0.46
1:C:372:ILE:CG2	1:C:380:ARG:HD3	2.45	0.46
1:E:371:ASN:HD21	1:E:374:VAL:HG23	1.80	0.46
1:E:25:PHE:HE2	1:E:35:VAL:HG12	1.79	0.46
1:D:97:TYR:HA	1:D:103:PRO:HA	1.97	0.46
1:A:291:PRO:HG3	1:A:341:ALA:HA	1.98	0.46
1:D:279:VAL:HG13	1:D:309:VAL:HG12	1.98	0.46
1:D:139:LYS:HE2	1:E:143:LYS:HE3	1.97	0.46
1:E:20:TYR:HB3	1:E:89:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ILE:HD12	1:C:183:ILE:N	2.30	0.45
1:A:106:GLY:O	1:A:413:LEU:HD21	2.15	0.45
1:D:418:ILE:HD12	1:D:418:ILE:N	2.31	0.45
1:B:150:LEU:HD13	1:B:192:PRO:HB2	1.98	0.45
1:A:199:PHE:N	1:A:199:PHE:CD2	2.83	0.45
1:E:260:ASP:HB2	1:E:268:SER:HB3	1.99	0.45
1:B:170:ARG:HG3	1:C:20:TYR:CE2	2.51	0.45
1:D:311:TRP:CB	1:D:320:ILE:HB	2.45	0.45
1:E:168:CYS:SG	1:E:225:HIS:CD2	3.06	0.45
1:F:16:GLU:HG2	1:F:79:ILE:CD1	2.46	0.45
1:E:164:LEU:HD23	1:E:165:GLY:N	2.30	0.45
1:A:378:GLU:H	1:A:378:GLU:CD	2.19	0.45
1:C:116:LEU:HD23	1:C:351:LEU:CD1	2.46	0.45
1:B:58:GLU:O	1:B:61:VAL:HG23	2.15	0.45
1:A:129:LEU:HD22	1:A:130:GLY:N	2.31	0.45
1:E:186:SER:O	1:F:36:GLU:HG2	2.16	0.45
1:A:191:ALA:H	1:A:194:GLN:NE2	2.15	0.45
1:A:220:THR:HG23	1:F:162:THR:CB	2.45	0.45
1:D:123:GLY:O	1:D:252:LYS:HG3	2.17	0.45
1:B:234:LYS:HD3	1:B:298:ARG:HA	1.99	0.45
1:E:27:ASP:HB3	1:E:33:LYS:HD3	1.98	0.45
1:F:103:PRO:HB3	1:F:110:ASN:HD21	1.81	0.45
1:A:325:SER:HB3	1:B:51:MET:CE	2.47	0.45
1:D:418:ILE:HG23	1:D:422:GLU:HG3	1.98	0.45
1:F:260:ASP:OD1	1:F:263:ALA:HB2	2.17	0.45
1:B:173:VAL:HG13	1:B:183:ILE:CD1	2.47	0.45
1:A:17:ASN:O	1:A:88:LYS:HB2	2.17	0.45
1:A:28:ILE:HG13	1:A:29:LEU:N	2.30	0.45
1:F:118:GLU:HG2	1:F:118:GLU:H	1.53	0.45
1:F:281:HIS:CE1	1:F:404:VAL:HG11	2.52	0.45
1:F:78:VAL:CG1	1:F:79:ILE:N	2.80	0.45
1:F:417:PHE:HD2	1:F:418:ILE:HD12	1.82	0.45
1:E:191:ALA:HB2	1:E:240:ASN:HB2	1.99	0.45
1:C:270:THR:HG21	4:C:631:HOH:O	2.16	0.45
1:C:378:GLU:H	1:C:378:GLU:CD	2.20	0.45
1:D:256:ASN:ND2	1:D:258:PHE:HB2	2.32	0.45
1:E:275:ILE:O	1:E:279:VAL:HG23	2.15	0.45
1:E:431:GLN:HG3	4:E:639:HOH:O	2.16	0.45
1:C:22:ARG:HH11	1:C:22:ARG:HG2	1.82	0.44
1:C:19:LYS:HB2	1:C:87:GLY:HA3	1.99	0.44
1:B:131:PRO:HG2	1:B:199:PHE:HD1	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:HA	1:B:92:PHE:HE2	1.81	0.44
1:F:116:LEU:HD23	1:F:351:LEU:CD1	2.46	0.44
1:B:173:VAL:HG13	1:B:183:ILE:HD12	1.99	0.44
1:B:392:LEU:O	1:B:396:LEU:HG	2.17	0.44
1:F:175:GLU:HG3	1:F:221:ILE:HD11	1.99	0.44
1:C:308:TYR:HA	1:C:387:ASP:HA	2.00	0.44
1:B:319:LEU:HD12	1:B:336:SER:HB3	1.99	0.44
1:B:4:TYR:HB3	1:B:9:ILE:HD11	1.98	0.44
1:E:199:PHE:HZ	1:E:214:PHE:CG	2.36	0.44
1:D:156:TYR:CZ	1:D:157:PHE:HE1	2.35	0.44
1:E:169:ARG:HE	1:E:195:HIS:CD2	2.34	0.44
1:D:131:PRO:HG2	1:D:199:PHE:CE1	2.51	0.44
1:B:124:PHE:CE2	1:B:250:LEU:HD13	2.53	0.44
1:C:203:GLY:O	1:C:204:ALA:C	2.56	0.44
1:A:311:TRP:CB	1:A:320:ILE:HB	2.47	0.44
1:A:134:GLU:OE2	3:A:503:GLN:HB3	2.17	0.44
1:B:241:GLY:HA3	1:B:298:ARG:HG3	2.00	0.44
1:A:150:LEU:HD13	1:A:192:PRO:HB2	1.99	0.44
1:A:154:GLY:O	1:A:188:HIS:CE1	2.70	0.44
1:C:160:ALA:O	1:C:169:ARG:NH2	2.50	0.44
1:A:285:PHE:C	1:A:285:PHE:CD1	2.91	0.44
1:F:129:LEU:HD13	1:F:207:SER:OG	2.18	0.44
1:A:370:ARG:CG	1:A:371:ASN:H	2.11	0.44
1:B:285:PHE:HB2	1:B:349:VAL:CG1	2.48	0.44
1:D:127:PHE:CD2	1:D:351:LEU:HG	2.53	0.44
1:C:85:GLU:O	1:C:86:LYS:C	2.55	0.44
1:C:233:PRO:HD3	1:C:340:ALA:HB2	1.99	0.44
1:B:160:ALA:HB2	1:B:188:HIS:CD2	2.53	0.44
1:E:168:CYS:SG	1:E:222:ALA:HA	2.58	0.44
1:F:260:ASP:HB3	1:F:263:ALA:HB3	1.99	0.44
1:C:119:MET:HG2	1:C:124:PHE:HB2	1.99	0.44
1:C:272:LYS:O	1:C:364:ALA:HB2	2.18	0.44
1:F:434:PRO:O	1:F:438:GLU:HG3	2.18	0.44
1:E:169:ARG:HH12	1:E:188:HIS:HB2	1.83	0.44
1:D:274:PHE:CE1	1:D:354:GLY:HA3	2.53	0.44
1:D:111:ASN:O	1:D:115:ILE:HG12	2.18	0.44
1:B:122:LEU:HD13	1:B:355:LEU:HD22	1.99	0.44
1:D:159:LEU:HD13	1:E:34:ASN:CG	2.37	0.44
1:F:418:ILE:N	1:F:418:ILE:HD12	2.33	0.44
1:E:197:ILE:HB	1:E:214:PHE:CZ	2.53	0.44
1:D:114:ARG:NH2	1:D:407:LYS:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:ASP:OD2	1:E:344:TYR:OH	2.25	0.43
1:A:368:ILE:HG21	1:A:385:ILE:HD11	1.99	0.43
1:E:236:LEU:HB2	1:E:239:VAL:HG22	2.00	0.43
1:F:312:SER:HB2	1:F:368:ILE:O	2.18	0.43
1:F:314:GLN:HE21	1:F:314:GLN:HB3	1.58	0.43
1:A:244:MET:HE2	1:A:339:PRO:HA	1.98	0.43
1:F:402:ASN:OD1	1:F:404:VAL:HG12	2.18	0.43
1:B:91:ARG:HD2	1:B:92:PHE:N	2.32	0.43
1:E:368:ILE:CD1	1:E:385:ILE:HD11	2.49	0.43
1:E:27:ASP:C	1:E:27:ASP:OD2	2.55	0.43
1:D:28:ILE:HD11	1:D:417:PHE:CA	2.48	0.43
1:D:28:ILE:HD11	1:D:417:PHE:HA	2.00	0.43
1:F:201:TYR:OH	1:F:331:ARG:NE	2.46	0.43
1:A:33:LYS:O	1:A:34:ASN:HB3	2.18	0.43
1:B:425:TRP:O	1:B:429:ARG:HG3	2.18	0.43
1:B:291:PRO:HG3	1:B:341:ALA:HA	2.00	0.43
1:B:26:THR:HG22	1:B:27:ASP:O	2.18	0.43
1:A:220:THR:O	1:A:224:LYS:HG3	2.19	0.43
1:F:285:PHE:HD1	1:F:285:PHE:C	2.22	0.43
1:C:91:ARG:HD2	1:C:92:PHE:N	2.33	0.43
1:F:5:THR:H	1:F:8:ASP:HB2	1.83	0.43
1:B:212:GLN:OE1	1:B:215:LYS:NZ	2.52	0.43
1:D:21:ILE:HD13	1:D:42:LEU:HD13	2.01	0.43
1:D:274:PHE:O	1:D:278:ILE:HD13	2.19	0.43
1:C:160:ALA:HB3	1:C:188:HIS:CD2	2.53	0.43
1:D:159:LEU:HD13	1:E:34:ASN:CB	2.49	0.43
1:B:393:ALA:HB2	1:B:425:TRP:CE2	2.54	0.43
1:B:211:ILE:O	1:B:215:LYS:HG3	2.19	0.43
1:E:167:ASN:C	1:E:167:ASN:HD22	2.21	0.43
1:E:9:ILE:HG21	1:E:92:PHE:HZ	1.84	0.43
1:A:402:ASN:HB3	1:A:405:MET:HB2	2.00	0.43
1:F:201:TYR:CD1	1:F:201:TYR:N	2.86	0.43
1:F:119:MET:HG2	1:F:124:PHE:HB2	2.00	0.43
1:C:396:LEU:O	1:C:400:LYS:HG3	2.17	0.43
1:A:62:ARG:O	1:A:63:ILE:HD13	2.18	0.43
1:D:85:GLU:H	1:D:85:GLU:CD	2.20	0.43
1:D:117:LYS:HG2	4:D:706:HOH:O	2.19	0.43
1:D:28:ILE:HD11	1:D:417:PHE:N	2.34	0.43
1:A:437:ARG:O	1:A:441:MET:HB3	2.18	0.43
1:D:136:PHE:CE2	1:D:194:GLN:HB2	2.54	0.43
1:B:367:PRO:C	1:B:368:ILE:HD12	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:ASN:ND2	1:F:342:ASN:C	2.69	0.43
1:E:124:PHE:CE2	1:E:250:LEU:HD13	2.54	0.43
1:E:300:VAL:CG1	1:E:301:PRO:HD2	2.49	0.43
1:E:377:LYS:HA	1:E:380:ARG:HB2	2.01	0.43
1:E:326:ARG:HD3	1:E:330:THR:OG1	2.18	0.43
1:E:20:TYR:OH	1:E:36:GLU:HG3	2.19	0.43
1:C:249:SER:HA	1:C:258:PHE:CE1	2.54	0.43
1:C:300:VAL:CG1	1:C:301:PRO:HD2	2.49	0.43
1:E:203:GLY:O	1:E:204:ALA:C	2.57	0.43
1:F:197:ILE:HB	1:F:214:PHE:CZ	2.54	0.43
1:B:182:GLU:HB3	1:B:200:LYS:HD3	2.01	0.43
1:A:141:ASP:HB2	1:A:142:GLU:OE2	2.19	0.42
1:D:9:ILE:HD13	1:D:92:PHE:CZ	2.54	0.42
1:C:84:ALA:O	1:C:85:GLU:HG3	2.20	0.42
1:A:383:ASN:O	1:A:385:ILE:N	2.48	0.42
1:D:280:LYS:HD2	1:D:362:LEU:CD2	2.49	0.42
1:E:223:ARG:HG3	1:E:223:ARG:HH11	1.84	0.42
1:F:331:ARG:HG2	1:F:331:ARG:HH21	1.84	0.42
1:F:354:GLY:O	1:F:358:ILE:HG12	2.19	0.42
1:C:351:LEU:CD2	1:C:355:LEU:HG	2.49	0.42
1:B:112:LEU:HD23	1:B:205:VAL:HG12	2.00	0.42
1:F:324:ALA:O	1:F:325:SER:C	2.57	0.42
1:B:306:PRO:HG2	1:B:335:ARG:C	2.40	0.42
1:E:211:ILE:HD13	1:E:244:MET:HE3	2.01	0.42
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.84	0.42
1:D:156:TYR:O	1:D:157:PHE:HB2	2.19	0.42
1:C:283:THR:HG23	4:C:619:HOH:O	2.20	0.42
1:F:405:MET:O	1:F:408:ALA:HB3	2.18	0.42
1:C:116:LEU:HD11	1:C:204:ALA:HB3	2.01	0.42
1:F:309:VAL:HA	1:F:319:LEU:HD23	2.01	0.42
1:E:211:ILE:HD13	1:E:244:MET:CE	2.49	0.42
1:F:280:LYS:HE3	1:F:280:LYS:HB2	1.85	0.42
1:D:184:GLU:O	1:D:185:ALA:HB2	2.20	0.42
1:C:127:PHE:CE2	1:C:347:LEU:HD12	2.52	0.42
1:B:316:ARG:HD2	1:B:371:ASN:ND2	2.34	0.42
1:F:311:TRP:HA	1:F:320:ILE:O	2.19	0.42
1:F:201:TYR:CZ	1:F:331:ARG:HD2	2.53	0.42
1:D:370:ARG:HG2	1:D:371:ASN:H	1.85	0.42
1:D:388:LEU:HB3	1:D:389:PRO:HD2	2.01	0.42
1:C:114:ARG:NH2	1:C:407:LYS:O	2.51	0.42
1:D:427:MET:O	1:D:431:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:HD3	4:B:697:HOH:O	2.19	0.42
1:A:164:LEU:HD22	1:B:223:ARG:HD3	2.02	0.42
1:D:91:ARG:HG2	1:D:91:ARG:HH11	1.84	0.42
1:F:258:PHE:HA	1:F:271:ALA:HB2	2.02	0.42
3:B:503:GLN:HG2	4:C:607:HOH:O	2.20	0.42
1:E:282:ALA:HA	1:E:285:PHE:CE2	2.55	0.42
1:D:122:LEU:HD12	1:D:355:LEU:HD22	2.00	0.42
1:F:383:ASN:O	1:F:385:ILE:N	2.52	0.42
1:C:22:ARG:HG2	1:C:22:ARG:NH1	2.34	0.42
1:B:27:ASP:OD1	1:B:33:LYS:HE3	2.19	0.42
1:F:129:LEU:HG	1:F:347:LEU:HD21	2.02	0.42
1:F:145:GLU:HA	1:F:146:PRO:HD3	1.95	0.42
1:F:275:ILE:O	1:F:279:VAL:HG23	2.19	0.42
1:E:202:ALA:HB3	1:E:207:SER:HB2	2.02	0.42
1:B:201:TYR:HD2	1:B:201:TYR:H	1.68	0.42
1:F:406:VAL:HG13	1:F:414:PHE:CD1	2.55	0.42
1:D:309:VAL:HG23	1:D:386:VAL:O	2.18	0.42
1:A:281:HIS:HD2	1:A:402:ASN:ND2	2.15	0.42
1:A:3:LYS:HB3	1:A:75:ASN:ND2	2.35	0.42
1:D:318:PRO:O	1:D:335:ARG:HD3	2.20	0.42
1:C:140:LEU:HD21	1:C:228:HIS:HB2	2.00	0.42
1:E:117:LYS:HA	1:E:120:GLU:OE1	2.20	0.42
1:B:391:THR:OG1	1:B:394:GLU:HG3	2.20	0.42
1:A:370:ARG:CG	1:A:371:ASN:N	2.80	0.41
1:B:366:ALA:O	1:B:368:ILE:HD12	2.20	0.41
1:B:176:LEU:HD12	1:B:183:ILE:HD11	2.01	0.41
1:D:371:ASN:ND2	1:D:374:VAL:HG13	2.34	0.41
1:F:183:ILE:N	1:F:183:ILE:HD12	2.35	0.41
1:C:65:GLU:HG2	4:C:623:HOH:O	2.20	0.41
1:D:323:PRO:HG2	4:D:626:HOH:O	2.20	0.41
1:C:98:ASN:HD22	1:C:102:THR:HG23	1.84	0.41
1:D:154:GLY:O	1:D:188:HIS:CE1	2.73	0.41
1:F:33:LYS:O	1:F:34:ASN:HB3	2.20	0.41
1:F:161:PRO:HB2	1:F:167:ASN:OD1	2.20	0.41
1:B:359:LYS:CB	1:B:359:LYS:NZ	2.82	0.41
1:E:26:THR:HG22	1:E:27:ASP:O	2.20	0.41
1:B:349:VAL:CG1	1:B:350:LEU:N	2.82	0.41
1:D:351:LEU:HD22	1:D:355:LEU:CG	2.44	0.41
1:A:129:LEU:HD22	1:A:130:GLY:H	1.86	0.41
1:D:315:ASN:ND2	1:D:316:ARG:N	2.66	0.41
1:E:164:LEU:HD11	1:F:224:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LYS:O	1:B:381:MET:HG2	2.20	0.41
1:C:9:ILE:CD1	1:C:74:LEU:HD22	2.50	0.41
1:C:129:LEU:HD22	1:C:130:GLY:N	2.36	0.41
1:A:231:PHE:O	1:A:339:PRO:HG2	2.20	0.41
1:A:220:THR:CG2	1:F:162:THR:HB	2.48	0.41
1:A:34:ASN:C	1:A:34:ASN:ND2	2.73	0.41
1:A:311:TRP:HE3	1:A:322:ILE:HD13	1.85	0.41
1:C:33:LYS:O	1:C:34:ASN:CB	2.68	0.41
1:A:290:ASN:HB3	1:A:295:SER:HB3	2.02	0.41
1:C:303:TYR:HB2	4:C:613:HOH:O	2.19	0.41
1:F:373:TYR:HE2	4:F:610:HOH:O	2.03	0.41
1:B:166:GLU:O	1:B:167:ASN:C	2.59	0.41
1:E:315:ASN:HB3	1:E:318:PRO:HD3	2.02	0.41
1:D:201:TYR:H	1:D:201:TYR:HD2	1.67	0.41
1:D:310:ALA:HB1	1:D:368:ILE:HD13	2.02	0.41
1:A:160:ALA:O	1:A:161:PRO:C	2.59	0.41
1:A:154:GLY:C	1:A:188:HIS:CE1	2.94	0.41
1:F:24:GLN:NE2	1:F:91:ARG:HH11	2.19	0.41
1:D:54:GLY:HA3	1:D:68:MET:SD	2.60	0.41
1:F:115:ILE:HG22	1:F:351:LEU:HD13	2.02	0.41
1:E:292:THR:O	1:E:295:SER:HB2	2.20	0.41
1:B:175:GLU:HG2	1:B:221:ILE:HD11	2.02	0.41
1:C:296:TYR:HB3	1:C:390:ALA:O	2.20	0.41
1:B:282:ALA:HA	1:B:285:PHE:CE2	2.56	0.41
1:C:142:GLU:H	1:C:142:GLU:CD	2.17	0.41
1:F:134:GLU:OE1	3:F:503:GLN:N	2.53	0.41
1:D:134:GLU:OE2	3:D:503:GLN:OE1	2.39	0.41
1:F:305:ALA:HA	1:F:306:PRO:HD3	1.97	0.41
1:E:169:ARG:NH1	1:E:188:HIS:HB2	2.34	0.41
1:A:112:LEU:HD11	1:A:204:ALA:HB1	2.03	0.41
1:E:199:PHE:HZ	1:E:214:PHE:HB2	1.85	0.41
1:A:149:GLU:HG2	4:A:713:HOH:O	2.20	0.41
1:E:256:ASN:OD1	1:E:258:PHE:HB2	2.20	0.41
1:C:208:CYS:SG	1:C:343:PRO:O	2.78	0.41
1:A:78:VAL:HG12	1:A:91:ARG:NH1	2.36	0.41
1:D:54:GLY:HA3	1:D:68:MET:HG3	2.03	0.41
1:B:102:THR:HA	1:B:103:PRO:HD3	1.95	0.41
1:F:116:LEU:O	1:F:119:MET:HB3	2.21	0.41
1:F:23:LEU:HB3	1:F:94:CYS:SG	2.60	0.41
1:A:107:ASP:HA	1:A:108:PRO:HD3	1.91	0.41
1:A:36:GLU:OE2	1:F:169:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ARG:HH12	1:E:213:THR:HG23	1.86	0.41
1:B:176:LEU:CD1	1:B:183:ILE:HD11	2.51	0.41
1:A:347:LEU:HD13	1:A:347:LEU:HA	1.87	0.41
1:C:236:LEU:HB2	1:C:239:VAL:CG2	2.51	0.41
1:D:245:HIS:CE1	1:D:335:ARG:HE	2.39	0.41
1:F:8:ASP:O	1:F:12:LEU:HG	2.21	0.41
1:E:315:ASN:HD22	1:E:369:ASP:HA	1.85	0.41
1:D:74:LEU:HG	4:D:639:HOH:O	2.21	0.41
1:C:25:PHE:CD2	1:C:25:PHE:N	2.88	0.41
1:F:247:ASN:ND2	1:F:333:GLU:HB2	2.35	0.41
1:C:319:LEU:HD12	1:C:336:SER:HB3	2.03	0.41
1:C:315:ASN:ND2	1:C:370:ARG:O	2.54	0.41
1:B:160:ALA:HB2	1:B:188:HIS:CB	2.43	0.41
1:F:27:ASP:HB3	1:F:33:LYS:CD	2.37	0.41
1:F:98:ASN:HB2	1:F:102:THR:HG22	2.02	0.41
1:C:386:VAL:HG12	1:C:387:ASP:N	2.35	0.41
1:A:45:ALA:HA	1:A:50:VAL:HG23	2.03	0.41
1:E:325:SER:HB2	1:E:331:ARG:HH22	1.86	0.41
1:F:151:ASN:OD1	1:F:193:GLY:HA2	2.21	0.41
1:C:316:ARG:CZ	1:D:63:ILE:HG23	2.50	0.40
1:E:309:VAL:HA	1:E:319:LEU:HD22	2.03	0.40
1:B:206:ARG:HB2	4:B:612:HOH:O	2.21	0.40
1:A:158:ASP:OD2	1:B:33:LYS:HE2	2.22	0.40
1:F:52:PHE:CD1	1:F:70:LEU:HD13	2.56	0.40
1:F:70:LEU:HG	1:F:94:CYS:HB2	2.03	0.40
1:E:406:VAL:HG22	1:E:414:PHE:CE1	2.56	0.40
1:E:231:PHE:HB3	1:E:339:PRO:HB2	2.03	0.40
1:C:50:VAL:HB	4:C:606:HOH:O	2.21	0.40
1:B:311:TRP:CH2	1:B:367:PRO:HG3	2.54	0.40
1:B:176:LEU:HB3	1:B:181:PHE:CB	2.51	0.40
1:F:201:TYR:H	1:F:201:TYR:HD1	1.69	0.40
1:A:326:ARG:HB3	1:A:327:GLY:H	1.60	0.40
1:D:128:ASN:HA	1:D:202:ALA:O	2.21	0.40
1:C:319:LEU:CD1	1:C:336:SER:HB3	2.51	0.40
1:D:234:LYS:HD2	1:D:298:ARG:HA	2.04	0.40
1:A:326:ARG:HD3	1:A:326:ARG:HA	1.78	0.40
1:C:355:LEU:O	1:C:359:LYS:HG2	2.22	0.40
1:B:324:ALA:O	1:B:325:SER:C	2.59	0.40
1:E:50:VAL:HB	4:E:612:HOH:O	2.21	0.40
1:D:83:THR:HG21	1:D:89:VAL:HB	2.02	0.40
1:A:214:PHE:O	1:A:218:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:VAL:HG22	1:D:414:PHE:CE1	2.56	0.40
1:B:48:ASN:OD1	1:B:72:PRO:HD2	2.21	0.40
1:D:208:CYS:SG	1:D:343:PRO:C	3.00	0.40
1:B:316:ARG:O	1:B:317:SER:HB3	2.22	0.40
1:E:370:ARG:HG2	1:E:371:ASN:H	1.86	0.40
1:E:351:LEU:CD2	1:E:355:LEU:HG	2.50	0.40
1:D:419:GLU:O	1:D:423:ILE:HG12	2.21	0.40
1:C:311:TRP:CZ2	1:C:367:PRO:HD3	2.55	0.40
1:B:281:HIS:CE1	1:B:356:ASP:OD2	2.74	0.40
1:A:359:LYS:HB2	1:A:359:LYS:HZ2	1.87	0.40
1:B:52:PHE:CZ	1:B:54:GLY:HA2	2.56	0.40
1:F:52:PHE:CE1	1:F:70:LEU:HD13	2.55	0.40
1:D:208:CYS:SG	1:D:343:PRO:O	2.80	0.40
1:A:349:VAL:HG23	1:A:350:LEU:N	2.37	0.40
1:D:57:ILE:CD1	1:D:96:ILE:HG13	2.52	0.40
1:B:132:GLU:HB3	1:B:196:GLU:OE1	2.22	0.40
1:B:189:GLU:OE1	1:B:196:GLU:OE2	2.38	0.40
1:F:199:PHE:N	1:F:199:PHE:CD2	2.86	0.40
1:A:315:ASN:ND2	1:A:369:ASP:HA	2.36	0.40
1:F:162:THR:C	1:F:164:LEU:H	2.25	0.40
1:B:231:PHE:O	1:B:339:PRO:HG2	2.21	0.40
1:F:206:ARG:HB2	4:F:624:HOH:O	2.21	0.40
1:A:150:LEU:HD13	1:A:192:PRO:O	2.21	0.40
1:E:243:GLY:C	1:E:339:PRO:HD3	2.42	0.40
1:E:364:ALA:HA	1:E:365:PRO:HD3	1.99	0.40
1:D:168:CYS:O	1:D:172:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/443 (100%)	397 (90%)	39 (9%)	5 (1%)	17	51
1	B	441/443 (100%)	412 (93%)	25 (6%)	4 (1%)	21	57
1	C	441/443 (100%)	404 (92%)	36 (8%)	1 (0%)	52	84
1	D	441/443 (100%)	403 (91%)	33 (8%)	5 (1%)	17	51
1	E	441/443 (100%)	401 (91%)	35 (8%)	5 (1%)	17	51
1	F	441/443 (100%)	418 (95%)	20 (4%)	3 (1%)	26	63
All	All	2646/2658 (100%)	2435 (92%)	188 (7%)	23 (1%)	21	57

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO
1	B	161	PRO
1	D	161	PRO
1	E	143	LYS
1	E	161	PRO
1	F	161	PRO
1	A	163	ASP
1	A	369	ASP
1	B	163	ASP
1	D	325	SER
1	E	262	ASN
1	F	325	SER
1	B	60	PHE
1	D	62	ARG
1	D	163	ASP
1	E	204	ALA
1	F	141	ASP
1	A	268	SER
1	C	86	LYS
1	A	374	VAL
1	E	144	GLY
1	B	317	SER
1	D	63	ILE

### 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	382/382 (100%)	355 (93%)	27 (7%)	18	47
1	B	382/382 (100%)	352 (92%)	30 (8%)	15	41
1	C	382/382 (100%)	358 (94%)	24 (6%)	22	54
1	D	382/382 (100%)	352 (92%)	30 (8%)	15	41
1	E	382/382 (100%)	360 (94%)	22 (6%)	25	58
1	F	382/382 (100%)	349 (91%)	33 (9%)	13	36
All	All	2292/2292 (100%)	2126 (93%)	166 (7%)	17	46

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	35	VAL
1	A	36	GLU
1	A	58	GLU
1	A	91	ARG
1	A	110	ASN
1	A	112	LEU
1	A	129	LEU
1	A	142	GLU
1	A	153	LYS
1	A	161	PRO
1	A	167	ASN
1	A	174	LEU
1	A	181	PHE
1	A	199	PHE
1	A	206	ARG
1	A	240	ASN
1	A	262	ASN
1	A	285	PHE
1	A	299	LEU
1	A	315	ASN
1	A	326	ARG
1	A	331	ARG
1	A	347	LEU
1	A	359	LYS
1	A	362	LEU
1	A	363	GLU

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Mol	Chain	Res	Type
1	B	34	ASN
1	B	36	GLU
1	B	49	LYS
1	B	61	VAL
1	B	68	MET
1	B	91	ARG
1	B	92	PHE
1	B	110	ASN
1	B	122	LEU
1	B	126	ASP
1	B	129	LEU
1	B	159	LEU
1	B	161	PRO
1	B	199	PHE
1	B	201	TYR
1	B	240	ASN
1	B	308	TYR
1	B	349	VAL
1	B	351	LEU
1	B	363	GLU
1	B	370	ARG
1	B	371	ASN
1	B	377	LYS
1	B	380	ARG
1	B	415	GLU
1	B	423	ILE
1	B	426	ASP
1	B	429	ARG
1	B	441	MET
1	B	443	GLN
1	C	34	ASN
1	C	49	LYS
1	C	91	ARG
1	C	105	GLU
1	C	110	ASN
1	C	112	LEU
1	C	129	LEU
1	C	159	LEU
1	C	199	PHE
1	C	240	ASN
1	C	262	ASN
1	C	264	ASP

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Mol	Chain	Res	Type
1	C	285	PHE
1	C	299	LEU
1	C	328	ILE
1	C	331	ARG
1	C	351	LEU
1	C	360	ASN
1	C	371	ASN
1	C	397	GLU
1	C	413	LEU
1	C	441	MET
1	C	442	SER
1	C	443	GLN
1	D	6	ARG
1	D	11	LYS
1	D	34	ASN
1	D	35	VAL
1	D	36	GLU
1	D	49	LYS
1	D	66	SER
1	D	85	GLU
1	D	91	ARG
1	D	110	ASN
1	D	129	LEU
1	D	142	GLU
1	D	151	ASN
1	D	161	PRO
1	D	164	LEU
1	D	168	CYS
1	D	199	PHE
1	D	201	TYR
1	D	223	ARG
1	D	232	MET
1	D	240	ASN
1	D	256	ASN
1	D	314	GLN
1	D	315	ASN
1	D	328	ILE
1	D	351	LEU
1	D	359	LYS
1	D	363	GLU
1	D	379	GLU
1	D	413	LEU

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Mol	Chain	Res	Type
1	E	28	ILE
1	E	35	VAL
1	E	41	GLN
1	E	49	LYS
1	E	91	ARG
1	E	105	GLU
1	E	126	ASP
1	E	161	PRO
1	E	167	ASN
1	E	168	CYS
1	E	172	ILE
1	E	201	TYR
1	E	240	ASN
1	E	262	ASN
1	E	299	LEU
1	E	308	TYR
1	E	326	ARG
1	E	349	VAL
1	E	351	LEU
1	E	381	MET
1	E	397	GLU
1	E	443	GLN
1	F	10	GLU
1	F	32	ILE
1	F	34	ASN
1	F	36	GLU
1	F	85	GLU
1	F	91	ARG
1	F	95	ASP
1	F	110	ASN
1	F	112	LEU
1	F	118	GLU
1	F	126	ASP
1	F	129	LEU
1	F	143	LYS
1	F	164	LEU
1	F	168	CYS
1	F	181	PHE
1	F	206	ARG
1	F	240	ASN
1	F	250	LEU
1	F	253	ASN

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Mol	Chain	Res	Type
1	F	262	ASN
1	F	285	PHE
1	F	299	LEU
1	F	312	SER
1	F	314	GLN
1	F	342	ASN
1	F	347	LEU
1	F	349	VAL
1	F	351	LEU
1	F	361	LYS
1	F	377	LYS
1	F	423	ILE
1	F	439	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	75	ASN
1	A	110	ASN
1	A	128	ASN
1	A	167	ASN
1	A	194	GLN
1	A	240	ASN
1	A	253	ASN
1	A	281	HIS
1	A	290	ASN
1	A	315	ASN
1	A	360	ASN
1	A	431	GLN
1	A	443	GLN
1	B	17	ASN
1	B	34	ASN
1	B	128	ASN
1	B	194	GLN
1	B	225	HIS
1	B	240	ASN
1	B	253	ASN
1	B	262	ASN
1	B	266	GLN
1	B	281	HIS
1	B	290	ASN

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Mol	Chain	Res	Type
1	B	314	GLN
1	B	371	ASN
1	B	383	ASN
1	C	24	GLN
1	C	34	ASN
1	C	98	ASN
1	C	128	ASN
1	C	194	GLN
1	C	240	ASN
1	C	253	ASN
1	C	281	HIS
1	C	290	ASN
1	C	360	ASN
1	C	371	ASN
1	C	383	ASN
1	C	443	GLN
1	D	128	ASN
1	D	194	GLN
1	D	240	ASN
1	D	245	HIS
1	D	253	ASN
1	D	256	ASN
1	D	281	HIS
1	D	290	ASN
1	D	314	GLN
1	D	315	ASN
1	E	17	ASN
1	E	34	ASN
1	E	75	ASN
1	E	110	ASN
1	E	167	ASN
1	E	195	HIS
1	E	225	HIS
1	E	262	ASN
1	E	281	HIS
1	E	290	ASN
1	E	314	GLN
1	F	24	GLN
1	F	110	ASN
1	F	128	ASN
1	F	167	ASN
1	F	194	GLN

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Mol	Chain	Res	Type
1	F	225	HIS
1	F	247	ASN
1	F	253	ASN
1	F	262	ASN
1	F	281	HIS
1	F	290	ASN
1	F	314	GLN
1	F	342	ASN
1	F	439	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](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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	GLN	A	503	-	7,8,9	1.05	1 (14%)	6,9,11	0.79	0
3	GLN	B	503	2	7,8,9	0.48	0	6,9,11	0.78	0
3	GLN	C	501	-	6,9,9	0.39	0	5,11,11	0.13	0
3	GLN	D	503	2	6,9,9	0.30	0	5,11,11	0.11	0
3	GLN	E	503	2	6,9,9	0.24	0	5,11,11	0.21	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLN	F	503	-	6,9,9	0.29	0	5,11,11	0.26	0

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	GLN	A	503	-	-	0/5/7/9	0/0/0/0
3	GLN	B	503	2	-	0/5/7/9	0/0/0/0
3	GLN	C	501	-	-	0/5/9/9	0/0/0/0
3	GLN	D	503	2	-	0/5/9/9	0/0/0/0
3	GLN	E	503	2	-	0/5/9/9	0/0/0/0
3	GLN	F	503	-	-	0/5/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	GLN	CB-CA	-2.05	1.51	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	GLN	2	0
3	B	503	GLN	1	0
3	C	501	GLN	2	0
3	D	503	GLN	1	0
3	F	503	GLN	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	443/443 (100%)	-0.04	6 (1%) 78 76	19, 37, 66, 98	0
1	B	443/443 (100%)	-0.10	3 (0%) 89 88	18, 36, 61, 93	0
1	C	443/443 (100%)	-0.13	3 (0%) 89 88	19, 35, 62, 91	0
1	D	443/443 (100%)	-0.09	4 (0%) 85 84	19, 36, 62, 96	0
1	E	443/443 (100%)	-0.09	5 (1%) 82 80	14, 35, 63, 94	0
1	F	443/443 (100%)	-0.05	5 (1%) 82 80	19, 37, 66, 101	0
All	All	2658/2658 (100%)	-0.08	26 (0%) 84 82	14, 36, 64, 101	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	384	GLY	4.1
1	C	86	LYS	4.0
1	A	384	GLY	3.1
1	B	377	LYS	2.9
1	D	385	ILE	2.9
1	E	201	TYR	2.9
1	F	381	MET	2.8
1	D	377	LYS	2.8
1	A	83	THR	2.7
1	F	382	GLU	2.7
1	B	382	GLU	2.6
1	A	385	ILE	2.6
1	C	85	GLU	2.6
1	E	381	MET	2.5
1	E	382	GLU	2.4
1	C	262	ASN	2.3
1	F	166	GLU	2.1
1	A	382	GLU	2.1
1	E	375	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	383	ASN	2.0
1	E	384	GLY	2.0
1	F	377	LYS	2.0
1	A	375	MET	2.0
1	D	372	ILE	2.0
1	B	381	MET	2.0
1	D	381	MET	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
2	MG	C	502	1/1	0.93	0.26	6.38	31,31,31,31	0
3	GLN	A	503	9/10	0.93	0.26	3.28	28,32,33,35	0
3	GLN	E	503	10/10	0.93	0.25	3.25	38,41,42,43	0
3	GLN	B	503	9/10	0.91	0.22	2.77	27,29,31,32	0
2	MG	E	502	1/1	0.90	0.19	2.20	27,27,27,27	0
2	MG	D	501	1/1	0.98	0.21	1.65	16,16,16,16	0
3	GLN	D	503	10/10	0.97	0.21	1.49	34,36,39,42	0
3	GLN	C	501	10/10	0.96	0.19	0.72	25,27,29,34	0
2	MG	F	501	1/1	0.98	0.18	0.62	24,24,24,24	0
3	GLN	F	503	10/10	0.95	0.17	0.25	28,32,34,36	0
2	MG	D	502	1/1	0.98	0.17	-0.16	14,14,14,14	0
2	MG	B	501	1/1	0.97	0.14	-0.55	18,18,18,18	0
2	MG	F	502	1/1	0.98	0.12	-1.53	18,18,18,18	0
2	MG	E	501	1/1	0.97	0.14	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	502	1/1	0.98	0.24	-	32,32,32,32	0
2	MG	C	503	1/1	0.98	0.18	-	13,13,13,13	0
2	MG	A	502	1/1	0.94	0.18	-	17,17,17,17	0
2	MG	A	501	1/1	0.92	0.17	-	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.