



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:20 PM GMT

PDB ID : 1JSW  
Title : NATIVE L-ASPARTATE AMMONIA LYASE  
Authors : Shi, W.; Dunbar, J.; Farber, G.K.  
Deposited on : 1997-02-19  
Resolution : 2.70 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

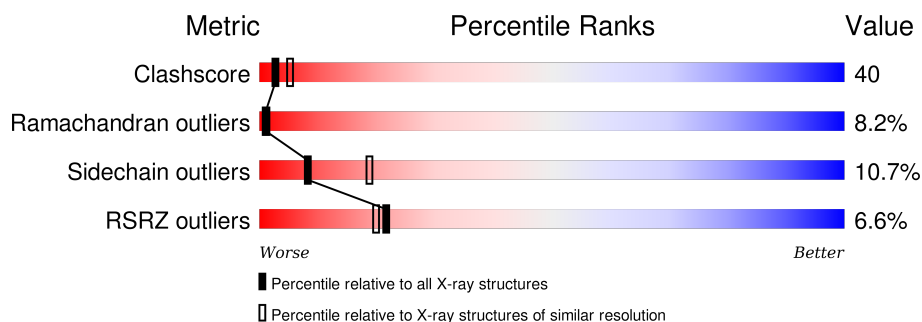
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	478	
1	B	478	
1	C	478	
1	D	478	

## 2 Entry composition [i](#)

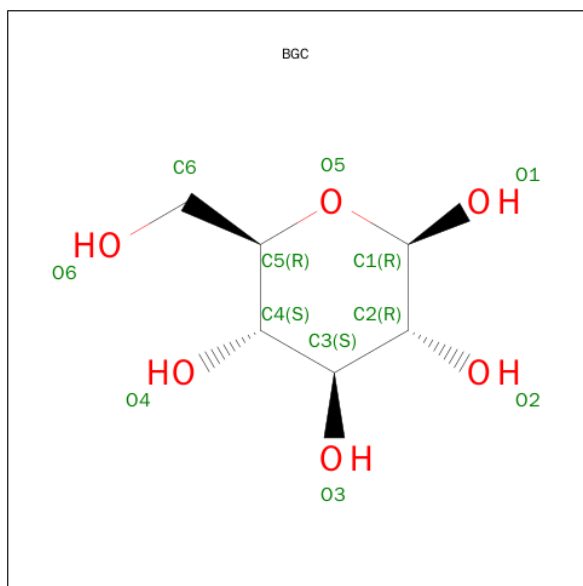
There are 4 unique types of molecules in this entry. The entry contains 13764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-ASPARTATE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3502	2205	595	676	26			
1	B	460	Total	C	N	O	S	0	0	0
			3511	2210	597	678	26			
1	C	413	Total	C	N	O	S	0	0	0
			3152	1988	534	606	24			
1	D	459	Total	C	N	O	S	0	0	0
			3502	2205	595	676	26			

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).

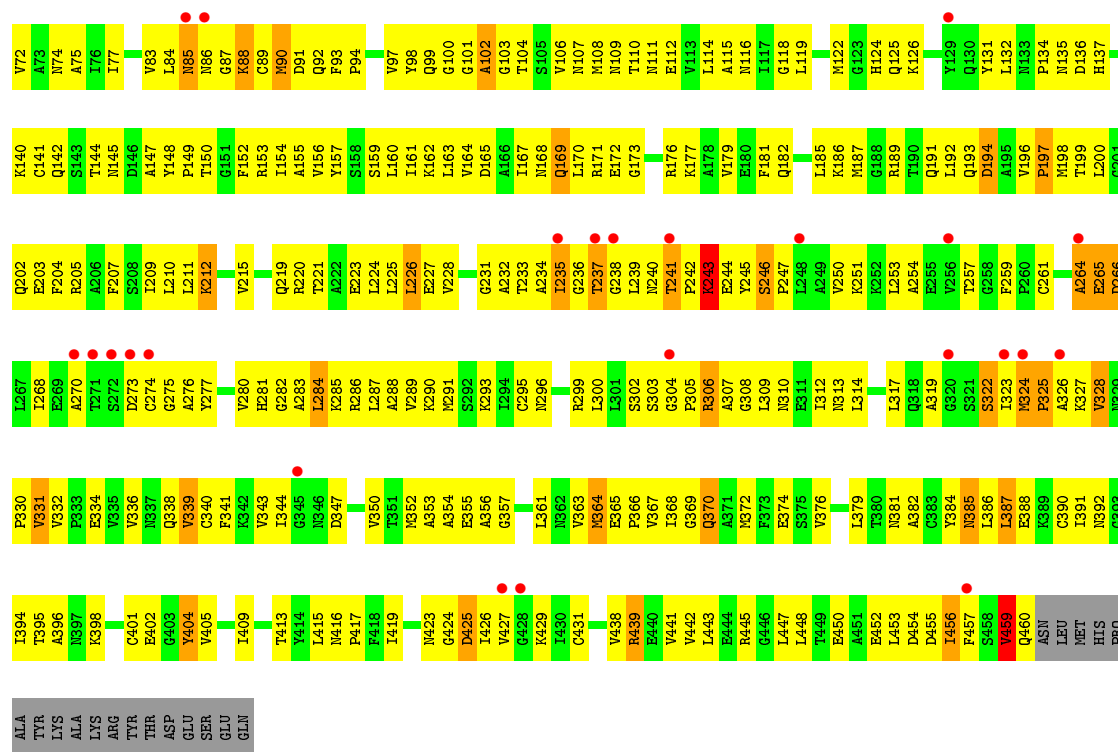


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

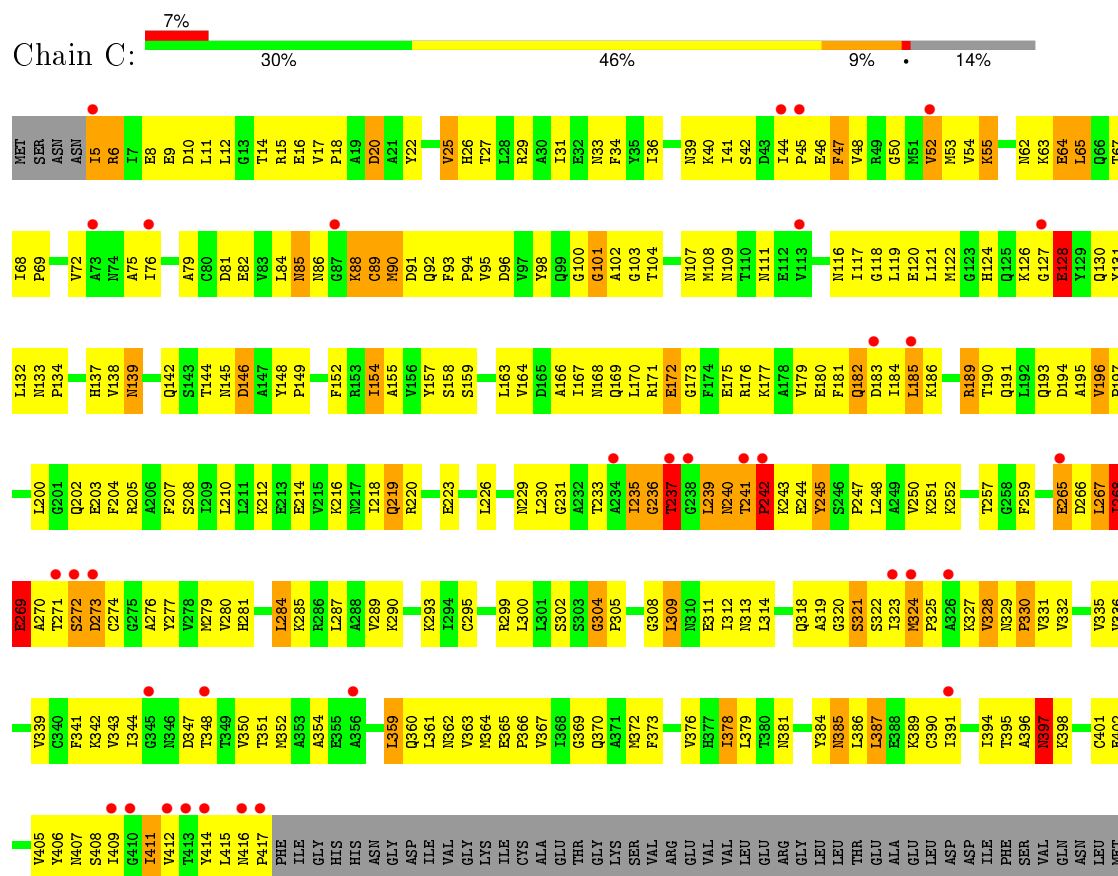
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	16	Total	O	0	0
			16	16		
4	C	11	Total	O	0	0
			11	11		
4	D	23	Total	O	0	0
			23	23		



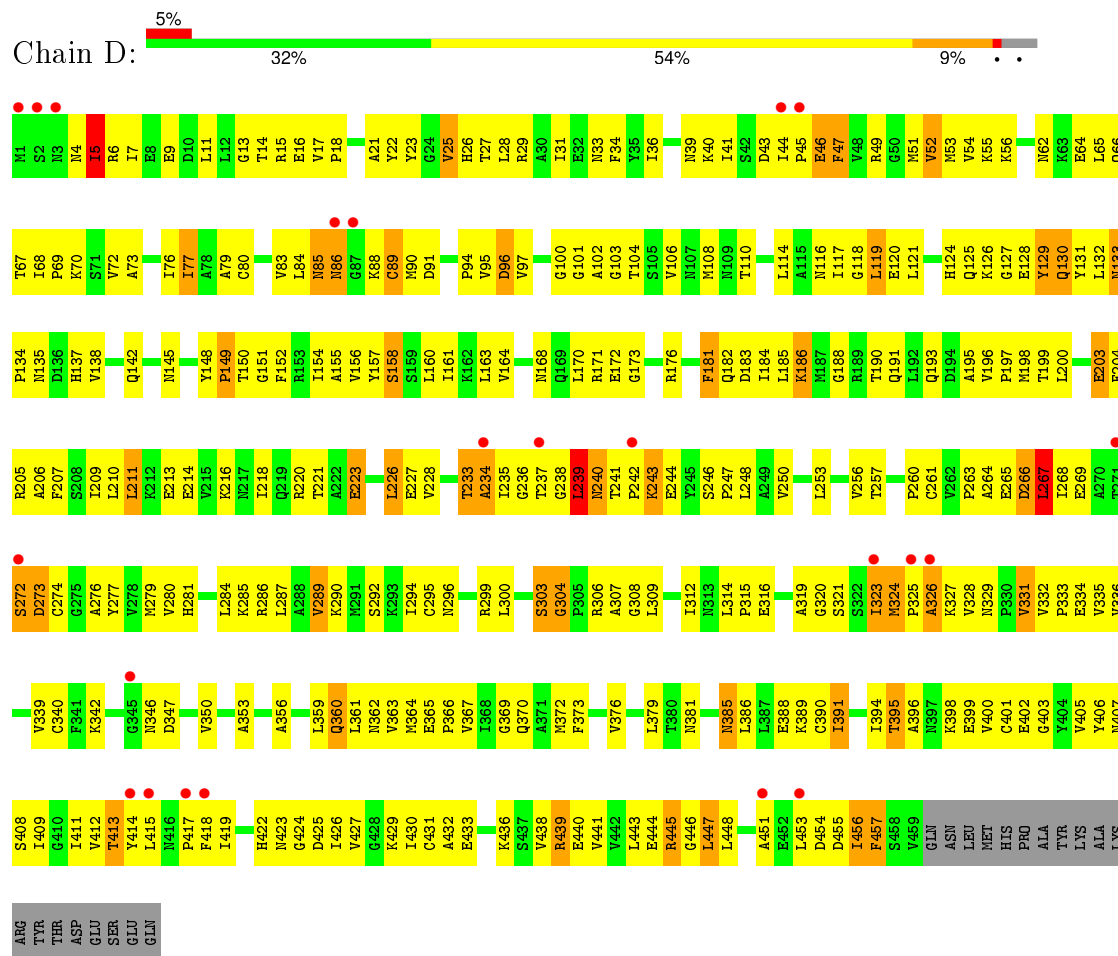


### • Molecule 1: L-ASPARTATE AMMONIA-LYASE



HIS  
PRO  
ALA  
TYR  
LYS  
ALA  
LYS  
ARG  
THR  
ASP  
GLU  
SER  
GLU  
GLN

• Molecule 1: L-ASPARTATE AMMONIA-LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.50Å 146.20Å 103.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 46.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 75.7 (46.38-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.216 , 0.371 0.252 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 112.5	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 43803 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	13764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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 [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.48	0/3553	0.76	1/4815 (0.0%)
1	B	0.47	0/3562	0.73	0/4827
1	C	0.47	0/3199	0.75	2/4338 (0.0%)
1	D	0.47	0/3553	0.74	0/4815
All	All	0.47	0/13867	0.74	3/18795 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	GLU	N-CA-C	5.93	127.02	111.00
1	C	240	ASN	N-CA-C	5.63	126.21	111.00
1	A	132	LEU	N-CA-C	-5.43	96.33	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3502	0	3539	338	0
1	B	3511	0	3547	299	0
1	C	3152	0	3191	268	0
1	D	3502	0	3539	318	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	4	0	3	0	0
4	A	19	0	0	1	0
4	B	16	0	0	0	0
4	C	11	0	0	0	0
4	D	23	0	0	1	0
All	All	13764	0	13843	1112	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 40.

All (1112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:HG3	1:A:270:ALA:H	1.20	1.05
1:D:273:ASP:HB2	1:D:362:ASN:HD22	1.22	1.04
1:B:319:ALA:HB2	1:D:26:HIS:CE1	1.94	1.02
1:B:119:LEU:HG	1:B:132:LEU:HB3	1.42	1.01
1:A:83:VAL:HG13	1:A:90:MET:HB3	1.43	1.01
1:A:284:LEU:HD21	1:A:376:VAL:HG22	1.40	1.00
1:A:323:ILE:HB	1:A:324:MET:SD	2.02	0.99
1:A:241:THR:N	1:A:242:PRO:HD2	1.78	0.98
1:D:431:CYS:SG	1:D:441:VAL:HG21	2.05	0.95
1:B:314:LEU:HD12	1:B:390:CYS:SG	2.07	0.93
1:A:416:ASN:HD21	1:A:424:GLY:HA3	1.32	0.93
1:C:185:LEU:HB3	1:C:405:VAL:HG11	1.50	0.93
1:D:235:ILE:HD12	1:D:236:GLY:H	1.34	0.92
1:B:439:ARG:HH22	1:B:454:ASP:HB3	1.35	0.91
1:D:287:LEU:HD23	1:D:379:LEU:HD13	1.53	0.91
1:D:253:LEU:HD12	1:D:261:CYS:SG	2.11	0.91
1:C:200:LEU:HD22	1:C:401:CYS:SG	2.11	0.91
1:A:52:VAL:HG21	1:A:83:VAL:HG11	1.53	0.91
1:A:5:ILE:HG22	1:A:18:PRO:HA	1.53	0.89
1:A:226:LEU:HD11	1:A:259:PHE:HB3	1.52	0.89
1:D:323:ILE:HG12	1:D:324:MET:SD	2.12	0.89
1:C:185:LEU:HB2	1:C:402:GLU:HG2	1.54	0.89
1:B:93:PHE:HA	1:B:109:ASN:HD21	1.37	0.89
1:A:269:GLU:CG	1:A:270:ALA:H	1.87	0.88
1:D:445:ARG:HG2	1:D:445:ARG:HH11	1.36	0.88
1:D:233:THR:HA	1:D:238:GLY:HA2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:H	1:B:45:PRO:HD2	1.38	0.88
1:C:152:PHE:HE2	1:C:369:GLY:HA2	1.37	0.87
1:C:172:GLU:HB3	1:C:176:ARG:HH21	1.38	0.87
1:B:323:ILE:HB	1:B:324:MET:SD	2.16	0.86
1:B:12:LEU:HD13	1:D:319:ALA:HA	1.58	0.86
1:B:35:TYR:CE1	1:D:385:ASN:HA	2.11	0.85
1:A:135:ASN:HA	1:A:139:ASN:HB3	1.59	0.84
1:B:199:THR:HG23	1:B:202:GLN:H	1.41	0.84
1:B:35:TYR:HE1	1:D:385:ASN:HA	1.43	0.84
1:B:319:ALA:HB2	1:D:26:HIS:HE1	1.38	0.83
1:D:409:ILE:H	1:D:409:ILE:HD12	1.40	0.83
1:D:409:ILE:O	1:D:412:VAL:HG23	1.78	0.83
1:C:179:VAL:O	1:C:182:GLN:HG2	1.79	0.82
1:C:104:THR:HG22	1:C:144:THR:HG21	1.60	0.82
1:B:277:TYR:HA	1:B:280:VAL:HG22	1.61	0.82
1:C:408:SER:O	1:C:411:ILE:HG23	1.80	0.82
1:A:416:ASN:ND2	1:A:424:GLY:HA3	1.95	0.81
1:D:85:ASN:OD1	1:D:88:LYS:HB2	1.79	0.81
1:B:238:GLY:HA3	1:B:242:PRO:HG2	1.59	0.81
1:D:49:ARG:HG2	1:D:84:LEU:HD23	1.63	0.81
1:B:9:GLU:HB2	1:B:14:THR:HG22	1.62	0.80
1:B:104:THR:HA	1:B:144:THR:HG21	1.63	0.80
1:B:338:GLN:HE21	1:D:367:VAL:HB	1.46	0.80
1:A:6:ARG:HH11	1:A:17:VAL:HG13	1.47	0.79
1:C:119:LEU:HD23	1:C:132:LEU:HB3	1.64	0.79
1:C:247:PRO:O	1:C:251:LYS:HG2	1.83	0.79
1:A:270:ALA:HA	1:A:274:CYS:HG	1.47	0.79
1:C:152:PHE:CE2	1:C:369:GLY:HA2	2.18	0.79
1:A:270:ALA:HA	1:A:274:CYS:SG	2.23	0.78
1:B:239:LEU:O	1:B:242:PRO:HD2	1.83	0.78
1:D:40:LYS:HA	1:D:96:ASP:HA	1.65	0.78
1:C:8:GLU:HB2	1:C:25:VAL:HG13	1.63	0.78
1:C:412:VAL:HA	1:C:415:LEU:HB3	1.65	0.78
1:C:235:ILE:HA	1:C:360:GLN:HG2	1.66	0.78
1:D:207:PHE:O	1:D:210:LEU:HB3	1.84	0.77
1:B:243:LYS:HE3	1:B:244:GLU:H	1.49	0.77
1:A:215:VAL:HG12	1:A:219:GLN:HE21	1.49	0.77
1:B:439:ARG:HG3	1:B:439:ARG:HH11	1.49	0.77
1:B:364:MET:O	1:B:367:VAL:HG12	1.84	0.77
1:D:272:SER:HA	1:D:361:LEU:HA	1.66	0.77
1:A:204:PHE:HA	1:A:207:PHE:HD2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:PRO:HA	1:D:246:SER:OG	1.85	0.76
1:B:187:MET:HE3	1:B:405:VAL:HA	1.67	0.76
1:C:300:LEU:HD11	1:D:300:LEU:HD11	1.64	0.76
1:D:72:VAL:HB	1:D:132:LEU:HD13	1.67	0.76
1:A:99:GLN:OE1	1:A:105:SER:HB2	1.86	0.76
1:C:327:LYS:O	1:C:328:VAL:HG23	1.86	0.75
1:D:323:ILE:H	1:D:323:ILE:HD13	1.51	0.75
1:D:425:ASP:O	1:D:429:LYS:HG2	1.85	0.75
1:B:93:PHE:HA	1:B:109:ASN:ND2	2.01	0.75
1:D:414:TYR:O	1:D:417:PRO:HD2	1.87	0.75
1:A:217:ASN:HD21	1:D:279:MET:HG3	1.52	0.74
1:A:305:PRO:HD3	1:B:193:GLN:HE22	1.53	0.74
1:A:93:PHE:HA	1:A:109:ASN:HD21	1.52	0.74
1:B:150:THR:O	1:B:154:ILE:HG12	1.88	0.73
1:A:343:VAL:HG21	1:A:379:LEU:HG	1.67	0.73
1:B:49:ARG:HA	1:B:52:VAL:HG22	1.69	0.73
1:A:10:ASP:HB3	1:A:25:VAL:HG11	1.68	0.73
1:A:47:PHE:HE2	1:A:106:VAL:HG11	1.53	0.73
1:D:210:LEU:HD21	1:D:290:LYS:HB3	1.71	0.73
1:D:436:LYS:HB3	1:D:440:GLU:HG3	1.70	0.73
1:B:8:GLU:HB3	1:B:25:VAL:HG22	1.69	0.73
1:D:11:LEU:H	1:D:11:LEU:HD22	1.53	0.73
1:D:130:GLN:N	1:D:130:GLN:HE21	1.86	0.73
1:A:198:MET:HB3	1:D:235:ILE:HD13	1.71	0.72
1:D:204:PHE:HA	1:D:207:PHE:HD2	1.54	0.72
1:A:21:ALA:HA	1:A:92:GLN:OE1	1.90	0.72
1:A:152:PHE:O	1:A:156:VAL:HG23	1.89	0.72
1:C:324:MET:N	1:C:324:MET:SD	2.62	0.72
1:A:285:LYS:O	1:A:289:VAL:HG23	1.90	0.72
1:A:230:LEU:HD23	1:A:249:ALA:HB1	1.71	0.72
1:D:204:PHE:HA	1:D:207:PHE:CD2	2.25	0.72
1:D:28:LEU:HA	1:D:31:ILE:HD12	1.72	0.72
1:C:416:ASN:HB2	1:C:417:PRO:HD3	1.72	0.72
1:D:284:LEU:HD21	1:D:376:VAL:HG12	1.70	0.71
1:D:241:THR:N	1:D:242:PRO:HD2	2.05	0.71
1:B:5:ILE:HD13	1:B:5:ILE:H	1.54	0.71
1:C:152:PHE:HE2	1:C:369:GLY:CA	2.03	0.71
1:B:210:LEU:HD21	1:B:290:LYS:HD2	1.72	0.71
1:D:414:TYR:CD2	1:D:456:ILE:HG12	2.26	0.71
1:B:341:PHE:CE2	1:D:353:ALA:HA	2.26	0.71
1:C:202:GLN:O	1:C:205:ARG:HG2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLU:HB3	1:A:25:VAL:HG22	1.71	0.71
1:A:359:LEU:HD11	1:D:300:LEU:HD23	1.73	0.71
1:B:456:ILE:HG13	1:B:457:PHE:H	1.55	0.71
1:C:40:LYS:HD3	1:C:94:PRO:HA	1.71	0.71
1:B:51:MET:O	1:B:54:VAL:HG12	1.89	0.71
1:A:61:ALA:O	1:A:65:LEU:HB2	1.89	0.71
1:A:69:PRO:HB2	1:A:72:VAL:HG13	1.73	0.71
1:D:296:ASN:HA	1:D:299:ARG:HE	1.55	0.70
1:D:51:MET:O	1:D:54:VAL:HG12	1.91	0.70
1:A:449:THR:HG22	1:A:451:ALA:H	1.56	0.70
1:A:51:MET:O	1:A:55:LYS:HG2	1.92	0.70
1:C:182:GLN:HG3	1:C:183:ASP:H	1.57	0.70
1:A:230:LEU:HD22	1:A:253:LEU:HD12	1.72	0.70
1:D:56:LYS:HD3	1:D:256:VAL:HG21	1.73	0.70
1:B:63:LYS:HZ2	1:B:74:ASN:HD21	1.38	0.70
1:D:129:TYR:CD2	1:D:131:TYR:HE2	2.10	0.70
1:D:47:PHE:HA	1:D:155:ALA:CB	2.21	0.70
1:A:269:GLU:HG3	1:A:270:ALA:N	2.01	0.69
1:D:76:ILE:HG13	1:D:132:LEU:HD11	1.73	0.69
1:B:235:ILE:HG13	1:C:196:VAL:HG13	1.74	0.69
1:B:221:THR:O	1:B:224:LEU:HG	1.92	0.69
1:B:176:ARG:O	1:B:179:VAL:HG12	1.93	0.69
1:C:323:ILE:HG22	1:C:324:MET:SD	2.31	0.69
1:B:233:THR:HB	1:B:238:GLY:HA2	1.73	0.69
1:A:56:LYS:HB2	1:A:80:CYS:SG	2.31	0.69
1:A:339:VAL:HG21	1:A:382:ALA:HB2	1.74	0.69
1:D:250:VAL:HG21	1:D:263:PRO:HG3	1.74	0.69
1:D:130:GLN:HE21	1:D:130:GLN:CA	2.06	0.69
1:C:189:ARG:HH21	1:C:309:LEU:HD11	1.58	0.69
1:C:53:MET:SD	1:C:257:THR:HA	2.33	0.68
1:C:146:ASP:HB2	1:C:229:ASN:OD1	1.92	0.68
1:A:122:MET:SD	1:A:132:LEU:CD1	2.81	0.68
1:A:109:ASN:O	1:A:113:VAL:HG23	1.93	0.68
1:B:7:ILE:HA	1:B:16:GLU:HA	1.74	0.68
1:C:235:ILE:HD12	1:C:236:GLY:N	2.09	0.68
1:D:150:THR:O	1:D:154:ILE:HG12	1.94	0.68
1:D:6:ARG:NH1	1:D:127:GLY:HA2	2.07	0.68
1:B:341:PHE:HE2	1:D:353:ALA:HA	1.59	0.67
1:B:72:VAL:HG21	1:B:137:HIS:CD2	2.29	0.67
1:B:90:MET:HG3	1:B:91:ASP:H	1.58	0.67
1:C:182:GLN:HG3	1:C:183:ASP:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:VAL:HG21	1:C:219:GLN:OE1	1.95	0.67
1:D:23:TYR:HB2	1:D:27:THR:HB	1.76	0.67
1:C:22:TYR:HB2	1:C:92:GLN:HG3	1.76	0.67
1:A:11:LEU:HD22	1:A:11:LEU:H	1.60	0.67
1:A:215:VAL:HG12	1:A:219:GLN:NE2	2.10	0.67
1:A:336:VAL:HA	1:A:339:VAL:HG13	1.75	0.67
1:C:44:ILE:H	1:C:45:PRO:HD2	1.60	0.66
1:A:9:GLU:HG3	1:A:13:GLY:O	1.95	0.66
1:C:281:HIS:HA	1:C:284:LEU:HD22	1.76	0.66
1:B:322:SER:O	1:B:325:PRO:HG3	1.96	0.66
1:A:305:PRO:HD3	1:B:193:GLN:NE2	2.10	0.66
1:A:187:MET:SD	1:A:197:PRO:HD3	2.35	0.66
1:B:431:CYS:SG	1:B:441:VAL:HG21	2.35	0.66
1:A:212:LYS:O	1:A:216:LYS:HG3	1.96	0.66
1:C:273:ASP:HB2	1:C:362:ASN:HD22	1.61	0.66
1:A:318:GLN:HG3	1:A:319:ALA:H	1.61	0.66
1:A:34:PHE:HZ	1:C:331:VAL:HG22	1.60	0.66
1:D:414:TYR:CE2	1:D:456:ILE:HG12	2.30	0.66
1:C:409:ILE:HD11	1:D:306:ARG:HB2	1.77	0.66
1:C:101:GLY:O	1:C:104:THR:HG23	1.96	0.66
1:B:314:LEU:CD1	1:B:390:CYS:SG	2.83	0.65
1:A:318:GLN:CG	1:A:319:ALA:H	2.08	0.65
1:D:246:SER:HB2	1:D:247:PRO:HD3	1.76	0.65
1:B:63:LYS:NZ	1:B:74:ASN:HD21	1.93	0.65
1:D:188:GLY:O	1:D:195:ALA:HB3	1.96	0.65
1:B:439:ARG:HH21	1:B:450:GLU:HG3	1.62	0.65
1:B:44:ILE:H	1:B:45:PRO:CD	2.09	0.65
1:C:126:LYS:HG2	1:C:127:GLY:H	1.62	0.65
1:A:34:PHE:CZ	1:C:331:VAL:HG22	2.31	0.65
1:A:122:MET:SD	1:A:132:LEU:HD13	2.37	0.65
1:B:85:ASN:CG	1:B:86:ASN:H	2.00	0.65
1:A:241:THR:N	1:A:242:PRO:CD	2.58	0.65
1:D:323:ILE:HD13	1:D:323:ILE:N	2.12	0.65
1:D:210:LEU:HD13	1:D:294:ILE:HD11	1.77	0.65
1:D:158:SER:HA	1:D:161:ILE:HD12	1.79	0.65
1:D:285:LYS:O	1:D:289:VAL:HG23	1.97	0.65
1:B:220:ARG:O	1:B:223:GLU:HG2	1.96	0.65
1:B:425:ASP:O	1:B:429:LYS:HG2	1.97	0.64
1:D:332:VAL:O	1:D:335:VAL:HG12	1.96	0.64
1:A:68:ILE:HD12	1:A:72:VAL:HG23	1.78	0.64
1:B:34:PHE:HZ	1:D:331:VAL:HG22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:HH11	1:D:279:MET:HG2	1.63	0.64
1:A:214:GLU:O	1:A:218:ILE:HG12	1.97	0.64
1:C:267:LEU:HD23	1:C:267:LEU:H	1.63	0.64
1:A:92:GLN:O	1:A:94:PRO:HD3	1.98	0.64
1:B:163:LEU:O	1:B:167:ILE:HG13	1.96	0.64
1:B:381:ASN:O	1:B:385:ASN:HB2	1.98	0.64
1:D:47:PHE:HA	1:D:155:ALA:HB1	1.78	0.64
1:D:150:THR:HG23	1:D:228:VAL:HB	1.78	0.64
1:D:220:ARG:O	1:D:223:GLU:HB3	1.97	0.64
1:B:317:LEU:HB3	1:D:33:ASN:ND2	2.13	0.64
1:B:239:LEU:HD21	1:C:196:VAL:HG11	1.80	0.64
1:B:324:MET:N	1:B:324:MET:SD	2.71	0.64
1:A:63:LYS:HE3	1:A:70:LYS:HG3	1.79	0.64
1:B:443:LEU:HD13	1:B:453:LEU:HD22	1.79	0.63
1:B:235:ILE:CG1	1:C:196:VAL:HG13	2.28	0.63
1:D:145:ASN:O	1:D:149:PRO:HG2	1.97	0.63
1:C:189:ARG:NH2	1:C:309:LEU:HD11	2.13	0.63
1:D:323:ILE:CD1	1:D:323:ILE:H	2.11	0.63
1:A:379:LEU:O	1:A:382:ALA:HB3	1.99	0.63
1:C:407:ASN:ND2	1:D:306:ARG:HH21	1.97	0.63
1:D:158:SER:O	1:D:161:ILE:HB	1.99	0.63
1:A:332:VAL:O	1:A:335:VAL:HG12	1.99	0.63
1:B:87:GLY:C	1:B:89:CYS:H	2.02	0.63
1:C:402:GLU:HB3	1:C:406:TYR:HE2	1.62	0.63
1:C:372:MET:O	1:C:376:VAL:HG23	1.98	0.63
1:B:209:ILE:HG13	1:C:268:ILE:HD12	1.80	0.63
1:A:30:ALA:HA	1:A:33:ASN:HD22	1.63	0.63
1:B:275:GLY:HA3	1:C:290:LYS:HZ1	1.64	0.63
1:C:280:VAL:HG23	1:C:372:MET:SD	2.39	0.63
1:D:285:LYS:HD3	1:D:347:ASP:CG	2.19	0.63
1:B:231:GLY:HA2	1:B:241:THR:HG22	1.81	0.63
1:D:7:ILE:HA	1:D:16:GLU:HA	1.81	0.63
1:A:331:VAL:HG22	1:C:100:GLY:HA3	1.79	0.63
1:C:72:VAL:HG21	1:C:137:HIS:CD2	2.34	0.63
1:C:20:ASP:HA	1:C:126:LYS:HZ2	1.64	0.62
1:C:82:GLU:O	1:C:88:LYS:HB3	1.99	0.62
1:B:119:LEU:N	1:B:132:LEU:HD23	2.14	0.62
1:C:343:VAL:CG2	1:C:378:ILE:HD11	2.28	0.62
1:C:130:GLN:NE2	1:C:133:ASN:HA	2.14	0.62
1:A:207:PHE:CE1	1:A:294:ILE:HG23	2.34	0.62
1:A:145:ASN:HD22	1:A:234:ALA:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:HA	1:A:201:GLY:HA3	1.80	0.62
1:B:257:THR:HB	1:B:259:PHE:CD2	2.34	0.62
1:B:319:ALA:HB1	1:D:11:LEU:HD23	1.81	0.62
1:B:313:ASN:O	1:B:394:ILE:HA	2.00	0.62
1:D:184:ILE:O	1:D:200:LEU:N	2.31	0.62
1:B:141:CYS:HB3	1:B:245:TYR:CE2	2.34	0.62
1:A:409:ILE:HG23	1:B:306:ARG:HD2	1.81	0.62
1:B:415:LEU:HD22	1:B:448:LEU:HD21	1.81	0.62
1:D:31:ILE:HD11	1:D:94:PRO:HG2	1.82	0.62
1:D:52:VAL:HG13	1:D:114:LEU:HD11	1.82	0.62
1:B:416:ASN:HB2	1:B:417:PRO:HD3	1.81	0.62
1:C:212:LYS:O	1:C:216:LYS:HG2	2.00	0.61
1:D:221:THR:HG22	1:D:280:VAL:HG12	1.82	0.61
1:B:150:THR:HG23	1:B:228:VAL:HB	1.80	0.61
1:A:343:VAL:HG23	1:A:378:ILE:HD11	1.82	0.61
1:A:218:ILE:HD13	1:A:283:ALA:HB1	1.80	0.61
1:A:341:PHE:CD1	1:C:352:MET:HB3	2.36	0.61
1:D:156:VAL:O	1:D:160:LEU:HG	1.99	0.61
1:B:119:LEU:CG	1:B:132:LEU:HB3	2.24	0.61
1:D:11:LEU:H	1:D:11:LEU:CD2	2.14	0.61
1:C:128:GLU:O	1:C:130:GLN:HG2	2.01	0.61
1:D:173:GLY:O	1:D:176:ARG:HB3	2.00	0.61
1:D:323:ILE:HG12	1:D:324:MET:H	1.65	0.61
1:A:437:SER:OG	1:A:440:GLU:HG3	2.01	0.61
1:B:102:ALA:HB2	1:B:363:VAL:HA	1.82	0.61
1:D:119:LEU:HB2	1:D:124:HIS:HB2	1.83	0.61
1:C:53:MET:SD	1:C:257:THR:HG22	2.41	0.61
1:C:269:GLU:HA	1:C:272:SER:OG	2.00	0.61
1:B:225:LEU:HG	1:B:280:VAL:HG11	1.83	0.61
1:C:281:HIS:CD2	1:C:350:VAL:HG21	2.36	0.60
1:D:292:SER:HB2	1:D:340:CYS:SG	2.40	0.60
1:B:254:ALA:HB2	1:B:261:CYS:SG	2.41	0.60
1:D:423:ASN:HD22	1:D:447:LEU:HD11	1.66	0.60
1:B:363:VAL:O	1:B:366:PRO:HD2	2.01	0.60
1:B:6:ARG:HD2	1:B:17:VAL:CG1	2.31	0.60
1:A:416:ASN:O	1:A:420:GLY:N	2.34	0.60
1:C:218:ILE:HD11	1:C:287:LEU:HD22	1.83	0.60
1:B:211:LEU:O	1:B:215:VAL:HG23	2.01	0.60
1:A:47:PHE:HZ	1:A:148:TYR:CE1	2.18	0.60
1:A:119:LEU:CD1	1:A:126:LYS:HA	2.32	0.60
1:D:76:ILE:CG1	1:D:132:LEU:HD11	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:CE1	1:A:369:GLY:HA2	2.37	0.60
1:C:40:LYS:HD3	1:C:94:PRO:CA	2.32	0.60
1:A:318:GLN:HG3	1:A:319:ALA:N	2.17	0.60
1:A:176:ARG:O	1:A:180:GLU:HG3	2.01	0.60
1:C:205:ARG:HB2	1:C:205:ARG:NH1	2.17	0.60
1:B:312:ILE:HB	1:B:394:ILE:CG2	2.32	0.60
1:A:28:LEU:HA	1:A:31:ILE:HD12	1.84	0.60
1:A:346:ASN:O	1:A:350:VAL:HG23	2.02	0.60
1:D:73:ALA:O	1:D:77:ILE:HG23	2.02	0.60
1:D:39:ASN:O	1:D:97:VAL:HG22	2.02	0.59
1:D:127:GLY:O	1:D:129:TYR:N	2.35	0.59
1:A:119:LEU:HA	1:A:122:MET:HB2	1.85	0.59
1:D:148:TYR:HB3	1:D:149:PRO:HD3	1.84	0.59
1:A:369:GLY:O	1:A:373:PHE:HD1	1.84	0.59
1:C:248:LEU:O	1:C:252:LYS:HG2	2.02	0.59
1:B:295:CYS:O	1:B:299:ARG:HG3	2.02	0.59
1:A:8:GLU:OE1	1:A:17:VAL:HG11	2.03	0.59
1:D:49:ARG:O	1:D:53:MET:HG3	2.02	0.59
1:B:149:PRO:O	1:B:153:ARG:HG3	2.02	0.59
1:D:314:LEU:HD23	1:D:394:ILE:HD12	1.83	0.59
1:D:226:LEU:HD23	1:D:260:PRO:HG2	1.84	0.59
1:C:364:MET:O	1:C:367:VAL:HG12	2.03	0.59
1:A:306:ARG:NE	1:A:306:ARG:HA	2.18	0.59
1:C:69:PRO:O	1:C:72:VAL:HG22	2.02	0.59
1:C:68:ILE:HD12	1:C:72:VAL:HG23	1.85	0.59
1:A:241:THR:H	1:A:242:PRO:HD2	1.66	0.59
1:C:130:GLN:NE2	1:C:130:GLN:HA	2.17	0.59
1:A:244:GLU:HB3	1:A:248:LEU:HD22	1.85	0.59
1:C:327:LYS:NZ	1:C:329:ASN:HD21	2.00	0.58
1:B:62:ASN:HB3	1:B:68:ILE:HG12	1.85	0.58
1:A:223:GLU:HA	1:A:226:LEU:HD23	1.85	0.58
1:B:233:THR:CB	1:B:238:GLY:HA2	2.34	0.58
1:A:370:GLN:HG3	1:A:371:ALA:N	2.16	0.58
1:A:334:GLU:O	1:A:337:ASN:HB2	2.03	0.58
1:B:324:MET:N	1:B:325:PRO:HD3	2.18	0.58
1:B:343:VAL:HG21	1:B:379:LEU:HD21	1.84	0.58
1:A:65:LEU:HD22	1:A:245:TYR:HD1	1.68	0.58
1:D:234:ALA:CB	1:D:239:LEU:HD23	2.33	0.58
1:C:343:VAL:HG21	1:C:379:LEU:HG	1.85	0.58
1:B:314:LEU:HD13	1:B:394:ILE:HG12	1.86	0.58
1:D:186:LYS:HA	1:D:401:CYS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:GLU:HA	1:D:405:VAL:HG12	1.84	0.58
1:A:405:VAL:HG23	1:A:406:TYR:N	2.18	0.58
1:D:427:VAL:HG11	1:D:438:VAL:HG13	1.86	0.58
1:D:221:THR:CG2	1:D:280:VAL:HA	2.34	0.58
1:B:6:ARG:HD2	1:B:17:VAL:HG13	1.85	0.58
1:C:241:THR:O	1:C:243:LYS:N	2.37	0.58
1:D:129:TYR:C	1:D:130:GLN:HE21	2.07	0.58
1:D:132:LEU:O	1:D:137:HIS:HB2	2.03	0.58
1:A:72:VAL:O	1:A:76:ILE:HG12	2.03	0.58
1:B:181:PHE:CZ	1:B:395:THR:HA	2.39	0.58
1:B:353:ALA:O	1:B:356:ALA:HB3	2.03	0.58
1:D:426:ILE:O	1:D:430:ILE:HG12	2.03	0.58
1:C:20:ASP:HA	1:C:126:LYS:NZ	2.19	0.57
1:D:130:GLN:HG3	1:D:133:ASN:HA	1.85	0.57
1:A:146:ASP:HB2	1:A:229:ASN:O	2.04	0.57
1:B:35:TYR:OH	1:D:389:LYS:HG2	2.04	0.57
1:A:441:VAL:O	1:A:445:ARG:HG3	2.04	0.57
1:B:285:LYS:O	1:B:288:ALA:HB3	2.04	0.57
1:A:330:PRO:O	1:A:333:PRO:HD2	2.04	0.57
1:A:389:LYS:NZ	1:C:33:ASN:HA	2.19	0.57
1:C:313:ASN:N	1:C:395:THR:O	2.34	0.57
1:D:221:THR:HG21	1:D:280:VAL:HA	1.85	0.57
1:A:204:PHE:HA	1:A:207:PHE:CD2	2.36	0.57
1:C:189:ARG:HB2	1:C:189:ARG:HH11	1.68	0.57
1:B:98:TYR:CD2	1:D:339:VAL:HG12	2.40	0.57
1:C:11:LEU:HD22	1:C:11:LEU:H	1.69	0.57
1:C:45:PRO:HB2	1:C:159:SER:OG	2.04	0.57
1:A:97:VAL:HG23	1:A:98:TYR:CE1	2.38	0.57
1:D:295:CYS:SG	1:D:336:VAL:HB	2.43	0.57
1:A:162:LYS:HD2	4:A:709:HOH:O	2.04	0.57
1:B:452:GLU:O	1:B:455:ASP:HB2	2.05	0.57
1:C:177:LYS:HE3	1:C:391:ILE:O	2.04	0.57
1:D:445:ARG:NH1	1:D:445:ARG:HG2	2.14	0.57
1:B:235:ILE:HG12	1:C:196:VAL:O	2.04	0.57
1:C:214:GLU:OE1	1:C:287:LEU:HA	2.05	0.57
1:D:52:VAL:HG21	1:D:83:VAL:HG11	1.87	0.57
1:D:233:THR:OG1	1:D:234:ALA:N	2.37	0.57
1:D:346:ASN:O	1:D:350:VAL:HG23	2.05	0.57
1:D:124:HIS:HB3	1:D:129:TYR:HD2	1.70	0.57
1:B:365:GLU:N	1:B:366:PRO:HD2	2.20	0.57
1:A:21:ALA:HB1	1:A:23:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:HD12	1:A:251:LYS:HD3	1.86	0.56
1:B:104:THR:HA	1:B:144:THR:CG2	2.34	0.56
1:C:94:PRO:HD2	1:C:109:ASN:HD21	1.69	0.56
1:B:107:ASN:ND2	1:B:147:ALA:HB3	2.19	0.56
1:D:200:LEU:HD21	1:D:312:ILE:CG2	2.36	0.56
1:B:200:LEU:HD11	1:B:204:PHE:HE1	1.70	0.56
1:A:56:LYS:HB2	1:A:80:CYS:CB	2.35	0.56
1:B:273:ASP:O	1:C:290:LYS:NZ	2.38	0.56
1:C:241:THR:O	1:C:243:LYS:HG2	2.05	0.56
1:A:79:ALA:O	1:A:82:GLU:HB2	2.05	0.56
1:A:358:GLN:NE2	1:C:299:ARG:HH12	2.03	0.56
1:C:311:GLU:HB3	1:C:401:CYS:SG	2.46	0.56
1:D:119:LEU:HD23	1:D:132:LEU:HB3	1.87	0.56
1:D:120:GLU:HA	1:D:124:HIS:O	2.05	0.56
1:D:127:GLY:C	1:D:129:TYR:H	2.09	0.56
1:A:234:ALA:O	1:A:235:ILE:HG23	2.05	0.56
1:D:419:ILE:HD11	1:D:424:GLY:HA2	1.88	0.56
1:B:88:LYS:C	1:B:89:CYS:SG	2.84	0.56
1:B:161:ILE:O	1:B:164:VAL:HG22	2.05	0.56
1:B:159:SER:HB3	1:B:376:VAL:HG11	1.87	0.56
1:D:204:PHE:HZ	1:D:312:ILE:HD13	1.71	0.56
1:B:350:VAL:HG13	1:B:368:ILE:HG12	1.86	0.56
1:D:391:ILE:HA	1:D:394:ILE:HG12	1.88	0.56
1:B:108:MET:O	1:B:112:GLU:HG3	2.05	0.56
1:A:391:ILE:HA	1:A:394:ILE:HG13	1.88	0.56
1:A:257:THR:HB	1:A:259:PHE:CD2	2.40	0.56
1:D:6:ARG:O	1:D:17:VAL:N	2.39	0.56
1:A:11:LEU:HD23	1:C:319:ALA:HA	1.87	0.56
1:C:247:PRO:HA	1:C:250:VAL:HG22	1.87	0.56
1:A:34:PHE:HZ	1:C:331:VAL:CG2	2.19	0.56
1:B:189:ARG:HB2	1:C:359:LEU:HD12	1.86	0.56
1:D:295:CYS:SG	1:D:336:VAL:CG1	2.94	0.56
1:D:6:ARG:HG2	1:D:17:VAL:O	2.06	0.55
1:A:40:LYS:HD3	1:A:94:PRO:O	2.06	0.55
1:A:237:THR:HA	1:A:267:LEU:HD23	1.88	0.55
1:A:107:ASN:OD1	1:A:147:ALA:HB3	2.05	0.55
1:D:13:GLY:HA3	1:D:15:ARG:HH12	1.70	0.55
1:A:419:ILE:O	1:A:423:ASN:HB2	2.06	0.55
1:C:11:LEU:HD22	1:C:11:LEU:N	2.21	0.55
1:A:196:VAL:HG23	1:D:235:ILE:HG12	1.87	0.55
1:C:173:GLY:O	1:C:177:LYS:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ASN:O	1:A:426:ILE:HG23	2.07	0.55
1:C:302:SER:HB3	1:C:314:LEU:HD13	1.87	0.55
1:C:329:ASN:O	1:C:331:VAL:N	2.39	0.55
1:B:268:ILE:HD13	1:C:205:ARG:HD3	1.88	0.55
1:C:90:MET:O	1:C:92:GLN:N	2.38	0.55
1:D:168:ASN:HD22	1:D:171:ARG:HD3	1.71	0.55
1:C:81:ASP:O	1:C:85:ASN:HB3	2.06	0.55
1:D:356:ALA:HB3	1:D:364:MET:HG3	1.88	0.55
1:A:97:VAL:HG23	1:A:98:TYR:CD1	2.41	0.55
1:B:350:VAL:HG13	1:B:368:ILE:HG23	1.87	0.55
1:C:241:THR:OG1	1:C:242:PRO:HD3	2.06	0.55
1:B:419:ILE:HG21	1:B:448:LEU:HD21	1.87	0.55
1:D:315:PRO:HD3	1:D:394:ILE:HD13	1.87	0.55
1:A:119:LEU:HD12	1:A:126:LYS:HA	1.88	0.55
1:A:314:LEU:HD21	1:A:333:PRO:HG2	1.89	0.55
1:B:288:ALA:HB1	1:B:344:ILE:HG13	1.89	0.55
1:A:328:VAL:HG12	1:A:328:VAL:O	2.06	0.55
1:D:11:LEU:N	1:D:11:LEU:HD22	2.20	0.55
1:C:402:GLU:HB3	1:C:406:TYR:CE2	2.41	0.55
1:D:385:ASN:C	1:D:385:ASN:HD22	2.10	0.55
1:C:267:LEU:O	1:C:268:ILE:HG23	2.06	0.55
1:B:116:ASN:CG	1:B:126:LYS:HB2	2.27	0.55
1:B:156:VAL:O	1:B:160:LEU:HG	2.07	0.55
1:B:327:LYS:O	1:B:328:VAL:HG23	2.07	0.55
1:B:116:ASN:OD1	1:B:126:LYS:HB2	2.06	0.55
1:A:207:PHE:O	1:A:211:LEU:HG	2.08	0.55
1:D:281:HIS:CD2	1:D:350:VAL:HG21	2.42	0.55
1:A:364:MET:HG2	1:C:341:PHE:CE2	2.42	0.55
1:A:332:VAL:O	1:A:336:VAL:HG23	2.07	0.54
1:B:431:CYS:SG	1:B:441:VAL:CG2	2.95	0.54
1:C:267:LEU:CD2	1:C:267:LEU:H	2.21	0.54
1:C:134:PRO:HA	1:C:138:VAL:HG23	1.90	0.54
1:B:370:GLN:O	1:B:374:GLU:HB2	2.08	0.54
1:A:110:THR:HG22	1:A:114:LEU:HD11	1.89	0.54
1:D:170:LEU:HD23	1:D:211:LEU:HG	1.90	0.54
1:D:40:LYS:HE2	1:D:94:PRO:O	2.06	0.54
1:D:241:THR:N	1:D:242:PRO:CD	2.66	0.54
1:D:168:ASN:O	1:D:172:GLU:HG3	2.07	0.54
1:C:386:LEU:O	1:C:390:CYS:HB3	2.06	0.54
1:B:102:ALA:HB2	1:B:363:VAL:HG12	1.90	0.54
1:B:36:ILE:HG12	1:D:339:VAL:HG11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LEU:O	1:A:419:ILE:HG12	2.08	0.54
1:D:126:LYS:HZ3	1:D:126:LYS:HB3	1.73	0.54
1:B:23:TYR:HB2	1:B:27:THR:HG21	1.90	0.54
1:B:308:GLY:O	1:B:310:ASN:N	2.40	0.54
1:A:115:ALA:O	1:A:119:LEU:HG	2.08	0.54
1:B:243:LYS:CE	1:B:244:GLU:H	2.18	0.54
1:D:246:SER:HB2	1:D:247:PRO:CD	2.37	0.54
1:A:378:ILE:HG13	1:A:379:LEU:N	2.23	0.54
1:B:423:ASN:O	1:B:426:ILE:HG22	2.06	0.54
1:A:281:HIS:CD2	1:A:350:VAL:HG21	2.43	0.54
1:B:339:VAL:O	1:B:343:VAL:HG23	2.08	0.54
1:A:272:SER:HA	1:A:362:ASN:N	2.22	0.54
1:A:237:THR:HA	1:A:267:LEU:CD2	2.38	0.53
1:D:152:PHE:CE1	1:D:369:GLY:HA2	2.43	0.53
1:B:88:LYS:O	1:B:89:CYS:SG	2.66	0.53
1:A:331:VAL:HG13	1:C:34:PHE:HE1	1.72	0.53
1:B:363:VAL:CG1	1:C:191:GLN:HG2	2.38	0.53
1:B:439:ARG:HG3	1:B:439:ARG:NH1	2.22	0.53
1:A:34:PHE:HA	1:C:385:ASN:OD1	2.08	0.53
1:C:6:ARG:HH11	1:C:127:GLY:HA3	1.73	0.53
1:D:321:SER:OG	1:D:325:PRO:HA	2.09	0.53
1:C:325:PRO:O	1:D:409:ILE:HD13	2.09	0.53
1:D:280:VAL:HG23	1:D:281:HIS:N	2.24	0.53
1:A:295:CYS:O	1:A:299:ARG:HG3	2.08	0.53
1:A:451:ALA:C	1:A:453:LEU:H	2.11	0.53
1:A:153:ARG:HD3	1:A:228:VAL:HG12	1.91	0.53
1:A:324:MET:N	1:A:324:MET:SD	2.82	0.53
1:B:52:VAL:HG12	1:B:114:LEU:HD21	1.90	0.53
1:B:5:ILE:HD13	1:B:5:ILE:N	2.22	0.53
1:B:205:ARG:O	1:B:209:ILE:HG12	2.07	0.53
1:C:27:THR:O	1:C:31:ILE:HG13	2.08	0.53
1:C:154:ILE:HG13	1:C:259:PHE:HD2	1.73	0.53
1:C:62:ASN:HD22	1:C:67:THR:HG21	1.72	0.53
1:D:246:SER:O	1:D:250:VAL:HG13	2.09	0.53
1:A:359:LEU:HD12	1:A:359:LEU:N	2.23	0.53
1:B:191:GLN:O	1:B:192:LEU:HB2	2.09	0.53
1:C:200:LEU:O	1:C:203:GLU:HB3	2.09	0.53
1:D:22:TYR:O	1:D:116:ASN:ND2	2.40	0.53
1:C:193:GLN:HB2	1:D:327:LYS:NZ	2.23	0.53
1:B:45:PRO:O	1:B:46:GLU:HB2	2.09	0.52
1:A:299:ARG:HB3	1:B:192:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLN:HG3	1:A:371:ALA:H	1.75	0.52
1:A:327:LYS:O	1:A:328:VAL:HG23	2.09	0.52
1:A:35:TYR:HE1	1:C:389:LYS:HD2	1.73	0.52
1:D:185:LEU:HA	1:D:198:MET:O	2.09	0.52
1:D:28:LEU:O	1:D:31:ILE:HB	2.09	0.52
1:D:210:LEU:HD22	1:D:294:ILE:HD11	1.91	0.52
1:D:296:ASN:HA	1:D:299:ARG:NE	2.24	0.52
1:D:46:GLU:OE2	1:D:155:ALA:HA	2.09	0.52
1:C:276:ALA:O	1:C:280:VAL:HG13	2.09	0.52
1:B:181:PHE:HZ	1:B:395:THR:HA	1.73	0.52
1:D:101:GLY:O	1:D:104:THR:HG23	2.09	0.52
1:A:275:GLY:HA3	1:D:286:ARG:NE	2.24	0.52
1:D:439:ARG:HA	1:D:453:LEU:HD21	1.91	0.52
1:B:323:ILE:C	1:B:325:PRO:HD3	2.30	0.52
1:B:199:THR:HG23	1:B:202:GLN:N	2.18	0.52
1:A:294:ILE:O	1:A:298:LEU:HG	2.09	0.52
1:B:305:PRO:O	1:B:306:ARG:HB3	2.09	0.52
1:D:365:GLU:N	1:D:366:PRO:CD	2.72	0.52
1:D:247:PRO:O	1:D:250:VAL:HG22	2.09	0.52
1:B:189:ARG:HA	1:B:193:GLN:O	2.09	0.52
1:A:235:ILE:HD13	1:D:196:VAL:HG23	1.91	0.52
1:A:322:SER:CB	1:B:429:LYS:HZ1	2.23	0.52
1:D:314:LEU:HD23	1:D:394:ILE:CD1	2.40	0.52
1:A:188:GLY:HA2	1:D:360:GLN:OE1	2.10	0.52
1:D:119:LEU:HD22	1:D:129:TYR:O	2.09	0.52
1:C:44:ILE:HB	1:C:45:PRO:HD3	1.91	0.52
1:A:267:LEU:N	1:A:267:LEU:HD22	2.24	0.52
1:A:327:LYS:HG2	1:A:328:VAL:H	1.73	0.52
1:A:275:GLY:HA3	1:D:286:ARG:CZ	2.39	0.52
1:C:148:TYR:HB3	1:C:149:PRO:HD3	1.92	0.52
1:B:196:VAL:O	1:C:235:ILE:HG21	2.10	0.52
1:D:117:ILE:O	1:D:121:LEU:HG	2.10	0.52
1:A:350:VAL:HG13	1:A:368:ILE:HG23	1.92	0.52
1:C:391:ILE:HA	1:C:394:ILE:HG13	1.90	0.52
1:C:332:VAL:O	1:C:335:VAL:HG12	2.10	0.52
1:B:31:ILE:HG22	1:B:31:ILE:O	2.10	0.52
1:D:55:LYS:HG3	1:D:110:THR:CG2	2.39	0.52
1:D:415:LEU:HA	1:D:418:PHE:HD2	1.74	0.52
1:A:68:ILE:HD11	1:A:73:ALA:HA	1.92	0.52
1:D:295:CYS:SG	1:D:336:VAL:HG11	2.50	0.52
1:C:11:LEU:H	1:C:11:LEU:CD2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HD13	1:A:5:ILE:N	2.25	0.51
1:C:88:LYS:C	1:C:90:MET:H	2.14	0.51
1:C:149:PRO:O	1:C:152:PHE:HB3	2.10	0.51
1:A:359:LEU:HD11	1:D:300:LEU:CD2	2.40	0.51
1:B:83:VAL:HA	1:B:87:GLY:HA2	1.92	0.51
1:A:74:ASN:O	1:A:78:ALA:HB2	2.10	0.51
1:A:434:THR:HB	1:A:436:LYS:HG3	1.92	0.51
1:A:365:GLU:N	1:A:366:PRO:HD2	2.25	0.51
1:C:119:LEU:CD2	1:C:132:LEU:HB3	2.37	0.51
1:B:185:LEU:HB3	1:B:405:VAL:HG21	1.93	0.51
1:A:458:SER:O	1:A:459:VAL:HB	2.09	0.51
1:B:41:ILE:HD11	1:B:99:GLN:HE22	1.74	0.51
1:B:302:SER:HB3	1:B:312:ILE:HG13	1.92	0.51
1:B:281:HIS:O	1:B:284:LEU:N	2.43	0.51
1:D:415:LEU:O	1:D:419:ILE:HG23	2.10	0.51
1:A:286:ARG:HH11	1:D:279:MET:CG	2.22	0.51
1:B:413:THR:HA	1:B:416:ASN:OD1	2.11	0.51
1:A:364:MET:HG2	1:C:341:PHE:HE2	1.74	0.51
1:A:342:LYS:NZ	1:C:342:LYS:NZ	2.58	0.51
1:C:220:ARG:O	1:C:223:GLU:HG3	2.09	0.51
1:A:125:GLN:NE2	1:A:129:TYR:HB2	2.25	0.51
1:A:389:LYS:HZ3	1:C:33:ASN:HA	1.75	0.51
1:A:240:ASN:C	1:A:242:PRO:HD2	2.31	0.51
1:C:402:GLU:O	1:C:405:VAL:HG12	2.10	0.51
1:C:175:GLU:O	1:C:179:VAL:HG23	2.10	0.51
1:A:271:THR:HG23	1:A:272:SER:N	2.25	0.51
1:D:55:LYS:HG3	1:D:110:THR:HG21	1.93	0.51
1:D:323:ILE:HG12	1:D:324:MET:N	2.25	0.51
1:A:163:LEU:O	1:A:167:ILE:HG13	2.10	0.51
1:A:269:GLU:CG	1:A:270:ALA:N	2.63	0.51
1:A:23:TYR:HB2	1:A:27:THR:HG21	1.92	0.51
1:D:235:ILE:CD1	1:D:236:GLY:H	2.13	0.51
1:B:186:LYS:HE3	1:B:203:GLU:OE1	2.10	0.51
1:B:69:PRO:HB2	1:B:72:VAL:HG13	1.93	0.51
1:A:387:LEU:HA	1:A:391:ILE:HG13	1.93	0.51
1:B:445:ARG:HB3	1:B:447:LEU:HD13	1.93	0.51
1:B:200:LEU:CD2	1:B:396:ALA:HB2	2.41	0.50
1:C:139:ASN:ND2	1:C:142:GLN:HB2	2.27	0.50
1:C:168:ASN:O	1:C:171:ARG:HB2	2.11	0.50
1:A:5:ILE:HG13	1:A:16:GLU:HB3	1.93	0.50
1:C:274:CYS:HB2	1:C:277:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:H	1:A:402:GLU:HG2	1.75	0.50
1:D:273:ASP:CB	1:D:362:ASN:HD22	2.08	0.50
1:D:431:CYS:SG	1:D:441:VAL:CG2	2.91	0.50
1:D:381:ASN:O	1:D:385:ASN:HB2	2.10	0.50
1:A:113:VAL:O	1:A:117:ILE:HG13	2.10	0.50
1:C:26:HIS:ND1	1:C:108:MET:HG2	2.26	0.50
1:B:415:LEU:HB3	1:B:419:ILE:CD1	2.40	0.50
1:B:231:GLY:HA2	1:B:241:THR:CG2	2.41	0.50
1:D:413:THR:O	1:D:417:PRO:HD3	2.10	0.50
1:B:157:TYR:O	1:B:161:ILE:HG13	2.10	0.50
1:B:40:LYS:O	1:B:42:SER:N	2.44	0.50
1:B:401:CYS:O	1:B:404:TYR:HB2	2.11	0.50
1:D:244:GLU:OE2	1:D:248:LEU:HD22	2.12	0.50
1:B:250:VAL:HA	1:B:253:LEU:CB	2.42	0.50
1:A:339:VAL:HG21	1:A:382:ALA:CB	2.40	0.50
1:D:214:GLU:OE1	1:D:287:LEU:HA	2.12	0.50
1:C:120:GLU:C	1:C:122:MET:H	2.15	0.50
1:B:250:VAL:HA	1:B:253:LEU:HB3	1.92	0.50
1:A:131:TYR:O	1:A:132:LEU:HD12	2.11	0.50
1:A:302:SER:OG	1:A:314:LEU:HD13	2.11	0.50
1:D:126:LYS:HZ3	1:D:126:LYS:CB	2.24	0.50
1:D:444:GLU:HG3	1:D:445:ARG:N	2.27	0.50
1:D:130:GLN:HE21	1:D:130:GLN:HA	1.76	0.50
1:B:85:ASN:ND2	1:B:88:LYS:NZ	2.60	0.50
1:A:172:GLU:O	1:A:176:ARG:HG3	2.11	0.50
1:C:10:ASP:HB3	1:C:29:ARG:HH21	1.77	0.50
1:D:85:ASN:O	1:D:86:ASN:HB3	2.12	0.50
1:D:210:LEU:HD22	1:D:294:ILE:CD1	2.42	0.50
1:A:216:LYS:O	1:A:220:ARG:HB2	2.12	0.50
1:B:439:ARG:HG2	1:B:453:LEU:HD21	1.94	0.49
1:B:72:VAL:O	1:B:75:ALA:HB3	2.11	0.49
1:D:134:PRO:HG2	1:D:135:ASN:H	1.77	0.49
1:C:117:ILE:O	1:C:121:LEU:HG	2.11	0.49
1:D:445:ARG:CG	1:D:445:ARG:HH11	2.12	0.49
1:A:152:PHE:CZ	1:A:369:GLY:HA2	2.47	0.49
1:B:275:GLY:HA3	1:C:290:LYS:NZ	2.25	0.49
1:C:108:MET:HA	1:C:111:ASN:HD22	1.78	0.49
1:A:413:THR:O	1:A:413:THR:HG22	2.12	0.49
1:A:222:ALA:O	1:A:224:LEU:N	2.45	0.49
1:D:323:ILE:CG1	1:D:324:MET:SD	2.94	0.49
1:C:45:PRO:HG2	1:C:373:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:VAL:O	1:C:52:VAL:HG12	2.12	0.49
1:A:192:LEU:HD13	1:B:300:LEU:HA	1.93	0.49
1:A:247:PRO:O	1:A:250:VAL:HG22	2.13	0.49
1:D:373:PHE:HA	1:D:376:VAL:HG22	1.94	0.49
1:B:456:ILE:O	1:B:457:PHE:HB2	2.12	0.49
1:A:68:ILE:HD12	1:A:72:VAL:CG2	2.40	0.49
1:A:235:ILE:HG22	1:D:188:GLY:HA3	1.94	0.49
1:A:199:THR:C	1:A:201:GLY:H	2.16	0.49
1:A:110:THR:O	1:A:114:LEU:HG	2.12	0.49
1:C:304:GLY:HA2	1:D:193:GLN:HA	1.93	0.49
1:A:122:MET:C	1:A:124:HIS:H	2.14	0.49
1:B:331:VAL:HG23	1:D:101:GLY:N	2.28	0.49
1:A:191:GLN:HG2	1:D:363:VAL:CG1	2.42	0.49
1:B:442:VAL:HG11	1:B:448:LEU:HD23	1.93	0.49
1:C:205:ARG:CZ	1:C:205:ARG:HB2	2.43	0.49
1:C:257:THR:HB	1:C:259:PHE:CD2	2.47	0.49
1:A:126:LYS:HG3	1:A:127:GLY:N	2.28	0.49
1:B:85:ASN:HD22	1:B:88:LYS:HZ1	1.61	0.49
1:B:336:VAL:HA	1:B:339:VAL:HG13	1.94	0.49
1:A:191:GLN:HG2	1:D:363:VAL:HG11	1.95	0.49
1:D:303:SER:HG	1:D:309:LEU:HB2	1.78	0.49
1:B:354:ALA:CB	1:C:289:VAL:HG11	2.42	0.49
1:C:196:VAL:HG23	1:C:197:PRO:HD2	1.94	0.49
1:C:119:LEU:O	1:C:122:MET:HB2	2.13	0.49
1:A:296:ASN:O	1:A:300:LEU:HB2	2.13	0.49
1:D:161:ILE:O	1:D:164:VAL:HG22	2.13	0.49
1:C:69:PRO:HB2	1:C:72:VAL:HG13	1.94	0.49
1:D:269:GLU:HA	1:D:272:SER:OG	2.13	0.49
1:D:241:THR:H	1:D:242:PRO:HD2	1.78	0.49
1:B:5:ILE:HA	1:B:19:ALA:HB2	1.95	0.49
1:B:85:ASN:ND2	1:B:88:LYS:HZ1	2.11	0.49
1:A:405:VAL:CG2	1:A:406:TYR:N	2.76	0.49
1:A:322:SER:HA	1:B:429:LYS:HZ3	1.78	0.49
1:A:272:SER:HA	1:A:362:ASN:H	1.78	0.49
1:D:274:CYS:SG	1:D:276:ALA:HB3	2.53	0.49
1:B:324:MET:O	1:B:326:ALA:N	2.46	0.48
1:A:125:GLN:HE22	1:A:131:TYR:HE1	1.61	0.48
1:A:327:LYS:HG2	1:A:328:VAL:N	2.28	0.48
1:D:83:VAL:HG22	1:D:89:CYS:HB2	1.95	0.48
1:B:52:VAL:HG23	1:B:84:LEU:HD21	1.95	0.48
1:A:145:ASN:HB2	1:A:233:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:TYR:C	1:C:408:SER:H	2.15	0.48
1:D:129:TYR:CD2	1:D:131:TYR:CE2	2.97	0.48
1:A:93:PHE:HA	1:A:109:ASN:ND2	2.24	0.48
1:D:56:LYS:HB2	1:D:80:CYS:SG	2.53	0.48
1:A:36:ILE:HG23	1:C:378:ILE:HB	1.93	0.48
1:B:108:MET:CE	1:B:111:ASN:HD22	2.26	0.48
1:B:58:ALA:HB1	1:B:142:GLN:HE22	1.79	0.48
1:D:273:ASP:HB2	1:D:362:ASN:ND2	2.07	0.48
1:A:343:VAL:HG22	1:A:375:SER:HA	1.94	0.48
1:D:47:PHE:N	1:D:155:ALA:HB1	2.27	0.48
1:C:272:SER:HA	1:C:362:ASN:N	2.29	0.48
1:D:13:GLY:HA3	1:D:15:ARG:NH1	2.28	0.48
1:A:307:ALA:HB3	1:B:194:ASP:OD2	2.13	0.48
1:B:419:ILE:CG2	1:B:448:LEU:HD21	2.43	0.48
1:D:79:ALA:HB1	1:D:117:ILE:HB	1.95	0.48
1:A:290:LYS:HZ3	1:D:273:ASP:CG	2.17	0.48
1:D:23:TYR:HB2	1:D:27:THR:CB	2.43	0.48
1:B:387:LEU:HG	1:B:388:GLU:N	2.29	0.48
1:B:293:LYS:HA	1:B:296:ASN:HB2	1.95	0.48
1:A:226:LEU:CD1	1:A:259:PHE:HB3	2.35	0.48
1:B:49:ARG:HA	1:B:52:VAL:CG2	2.43	0.48
1:B:177:LYS:HE3	1:B:391:ILE:O	2.13	0.48
1:A:98:TYR:N	1:A:98:TYR:CD1	2.80	0.48
1:A:146:ASP:CG	1:A:231:GLY:H	2.17	0.48
1:B:227:GLU:HB3	1:B:264:ALA:HA	1.96	0.48
1:C:5:ILE:HG22	1:C:18:PRO:HA	1.93	0.48
1:A:184:ILE:HG23	1:A:398:LYS:HA	1.95	0.48
1:D:264:ALA:C	1:D:266:ASP:H	2.15	0.48
1:D:41:ILE:HG13	1:D:95:VAL:O	2.13	0.48
1:B:241:THR:HB	1:B:242:PRO:HD3	1.95	0.48
1:B:459:VAL:HG22	1:B:460:GLN:H	1.77	0.48
1:D:325:PRO:O	1:D:326:ALA:HB2	2.14	0.48
1:A:47:PHE:CZ	1:A:148:TYR:CE1	3.01	0.48
1:B:173:GLY:C	1:B:391:ILE:HD12	2.34	0.48
1:B:176:ARG:NH2	1:B:392:ASN:ND2	2.62	0.48
1:A:126:LYS:HG3	1:A:127:GLY:H	1.79	0.48
1:D:274:CYS:SG	1:D:276:ALA:CB	3.02	0.48
1:A:242:PRO:O	1:A:243:LYS:HB3	2.14	0.48
1:D:234:ALA:HB2	1:D:239:LEU:HD23	1.96	0.48
1:B:124:HIS:HD2	1:B:131:TYR:CE1	2.32	0.48
1:D:190:THR:O	1:D:191:GLN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HG13	1:A:236:GLY:H	1.79	0.47
1:A:364:MET:O	1:A:367:VAL:HG12	2.14	0.47
1:C:285:LYS:HD3	1:C:347:ASP:CB	2.44	0.47
1:D:26:HIS:HD2	1:D:108:MET:HG3	1.79	0.47
1:C:126:LYS:HG2	1:C:127:GLY:N	2.28	0.47
1:C:8:GLU:HA	1:C:128:GLU:HG2	1.96	0.47
1:B:87:GLY:C	1:B:89:CYS:N	2.67	0.47
1:A:331:VAL:HG13	1:C:34:PHE:CE1	2.49	0.47
1:C:241:THR:N	1:C:242:PRO:HD2	2.30	0.47
1:C:166:ALA:HA	1:C:384:TYR:CE1	2.49	0.47
1:D:9:GLU:HB2	1:D:14:THR:HG22	1.97	0.47
1:A:368:ILE:O	1:A:372:MET:HB2	2.13	0.47
1:A:369:GLY:O	1:A:372:MET:HB3	2.14	0.47
1:D:423:ASN:O	1:D:427:VAL:HG23	2.14	0.47
1:D:185:LEU:HA	1:D:199:THR:HA	1.96	0.47
1:C:295:CYS:SG	1:C:336:VAL:HG11	2.54	0.47
1:C:8:GLU:HB2	1:C:25:VAL:CG1	2.39	0.47
1:A:185:LEU:HD22	1:A:406:TYR:HE1	1.78	0.47
1:D:423:ASN:HD22	1:D:447:LEU:HD21	1.80	0.47
1:C:79:ALA:HB2	1:C:118:GLY:CA	2.43	0.47
1:C:323:ILE:C	1:C:324:MET:SD	2.92	0.47
1:C:378:ILE:HD13	1:C:379:LEU:H	1.80	0.47
1:A:342:LYS:HZ2	1:C:342:LYS:NZ	2.12	0.47
1:B:152:PHE:CE1	1:B:369:GLY:HA2	2.48	0.47
1:B:415:LEU:HD13	1:B:442:VAL:HG21	1.97	0.47
1:D:214:GLU:O	1:D:218:ILE:HG13	2.15	0.47
1:B:225:LEU:CG	1:B:280:VAL:HG11	2.44	0.47
1:D:204:PHE:CZ	1:D:312:ILE:HD13	2.49	0.47
1:B:187:MET:HE2	1:B:405:VAL:HG22	1.95	0.47
1:D:456:ILE:O	1:D:457:PHE:CG	2.67	0.47
1:A:9:GLU:HG3	1:A:13:GLY:C	2.34	0.47
1:D:102:ALA:HB2	1:D:363:VAL:HB	1.94	0.47
1:C:47:PHE:O	1:C:50:GLY:N	2.47	0.47
1:D:399:GLU:O	1:D:403:GLY:N	2.48	0.47
1:A:56:LYS:HB2	1:A:80:CYS:HB3	1.96	0.47
1:C:280:VAL:O	1:C:284:LEU:HD13	2.15	0.47
1:A:194:ASP:OD2	1:B:305:PRO:O	2.33	0.47
1:A:419:ILE:O	1:A:423:ASN:ND2	2.47	0.47
1:A:205:ARG:HH21	1:A:209:ILE:HD11	1.80	0.47
1:A:83:VAL:CG1	1:A:90:MET:HB3	2.31	0.47
1:C:299:ARG:HG2	1:C:330:PRO:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ILE:HD13	1:D:5:ILE:N	2.30	0.47
1:C:170:LEU:HA	1:C:387:LEU:HD13	1.96	0.47
1:C:104:THR:HG22	1:C:144:THR:CG2	2.37	0.47
1:B:51:MET:HB3	1:B:110:THR:HG21	1.97	0.47
1:A:145:ASN:ND2	1:A:234:ALA:HB2	2.30	0.47
1:D:168:ASN:ND2	1:D:171:ARG:HD3	2.30	0.47
1:A:243:LYS:HG2	1:A:244:GLU:N	2.30	0.46
1:A:196:VAL:HG23	1:D:235:ILE:CG1	2.44	0.46
1:B:439:ARG:NH2	1:B:450:GLU:HG3	2.28	0.46
1:D:54:VAL:HG13	1:D:55:LYS:N	2.30	0.46
1:B:323:ILE:C	1:B:324:MET:SD	2.93	0.46
1:B:9:GLU:CG	1:B:10:ASP:N	2.78	0.46
1:D:27:THR:O	1:D:31:ILE:HG13	2.15	0.46
1:C:327:LYS:HE2	1:C:329:ASN:OD1	2.15	0.46
1:A:164:VAL:HB	1:A:215:VAL:HG13	1.97	0.46
1:A:45:PRO:O	1:A:46:GLU:HB2	2.15	0.46
1:D:372:MET:O	1:D:376:VAL:HG13	2.15	0.46
1:B:63:LYS:HG3	1:B:64:GLU:N	2.30	0.46
1:A:330:PRO:O	1:A:334:GLU:HG3	2.16	0.46
1:A:35:TYR:CE1	1:C:389:LYS:HD2	2.51	0.46
1:C:157:TYR:CE2	1:C:226:LEU:HD11	2.51	0.46
1:D:197:PRO:HB3	1:D:405:VAL:HG23	1.97	0.46
1:B:99:GLN:HE22	1:B:106:VAL:CG2	2.29	0.46
1:B:118:GLY:O	1:B:122:MET:HG3	2.15	0.46
1:A:241:THR:O	1:A:242:PRO:O	2.33	0.46
1:D:324:MET:N	1:D:324:MET:SD	2.88	0.46
1:B:45:PRO:HB2	1:B:159:SER:OG	2.16	0.46
1:B:280:VAL:O	1:B:284:LEU:HD22	2.14	0.46
1:B:61:ALA:O	1:B:64:GLU:HB3	2.16	0.46
1:B:281:HIS:HA	1:B:284:LEU:CD2	2.46	0.46
1:C:365:GLU:HB2	1:C:366:PRO:HD3	1.98	0.46
1:A:290:LYS:NZ	1:D:273:ASP:CG	2.69	0.46
1:D:207:PHE:CD1	1:D:294:ILE:HG23	2.50	0.46
1:D:250:VAL:HG21	1:D:263:PRO:CG	2.45	0.46
1:D:116:ASN:O	1:D:120:GLU:HB2	2.15	0.46
1:D:69:PRO:O	1:D:72:VAL:HG22	2.15	0.46
1:D:186:LYS:O	1:D:405:VAL:HB	2.15	0.46
1:B:330:PRO:O	1:B:334:GLU:HG3	2.16	0.46
1:B:101:GLY:O	1:B:104:THR:HG23	2.15	0.46
1:C:312:ILE:HG13	1:C:312:ILE:O	2.15	0.46
1:D:439:ARG:HH22	1:D:454:ASP:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:PHE:O	1:A:207:PHE:HB2	2.16	0.46
1:B:186:LYS:HG2	1:B:187:MET:N	2.29	0.46
1:A:175:GLU:O	1:A:179:VAL:HG23	2.15	0.46
1:B:431:CYS:SG	1:B:438:VAL:HA	2.56	0.46
1:C:231:GLY:CA	1:C:241:THR:HG21	2.46	0.46
1:A:35:TYR:CD1	1:A:35:TYR:N	2.84	0.46
1:C:223:GLU:O	1:C:226:LEU:HB2	2.16	0.46
1:A:273:ASP:OD1	1:A:274:CYS:N	2.49	0.45
1:B:326:ALA:O	1:B:327:LYS:HG3	2.16	0.45
1:D:436:LYS:HZ1	1:D:440:GLU:HB2	1.80	0.45
1:A:355:GLU:C	1:A:357:GLY:H	2.19	0.45
1:C:233:THR:HB	1:C:237:THR:O	2.16	0.45
1:D:253:LEU:CD1	1:D:261:CYS:SG	2.94	0.45
1:C:186:LYS:HD3	1:C:200:LEU:HA	1.99	0.45
1:C:116:ASN:O	1:C:120:GLU:HG3	2.16	0.45
1:B:170:LEU:HD12	1:B:391:ILE:HD13	1.97	0.45
1:C:277:TYR:HA	1:C:280:VAL:HG22	1.98	0.45
1:B:49:ARG:CA	1:B:52:VAL:HG22	2.43	0.45
1:A:46:GLU:HG2	1:A:49:ARG:HD3	1.97	0.45
1:C:92:GLN:O	1:C:94:PRO:HD3	2.17	0.45
1:A:318:GLN:O	1:C:12:LEU:HD22	2.16	0.45
1:D:25:VAL:O	1:D:29:ARG:N	2.41	0.45
1:A:170:LEU:HD11	1:A:386:LEU:HD23	1.99	0.45
1:D:53:MET:SD	1:D:257:THR:HG22	2.57	0.45
1:C:328:VAL:HG12	1:C:328:VAL:O	2.16	0.45
1:C:273:ASP:N	1:C:362:ASN:HB2	2.31	0.45
1:A:322:SER:HA	1:B:429:LYS:NZ	2.32	0.45
1:B:324:MET:C	1:B:326:ALA:H	2.20	0.45
1:B:241:THR:CB	1:B:242:PRO:HD3	2.47	0.45
1:C:339:VAL:HB	1:C:378:ILE:HG12	1.98	0.45
1:A:225:LEU:HD21	1:A:280:VAL:HG11	1.98	0.45
1:C:348:THR:O	1:C:351:THR:HB	2.15	0.45
1:A:6:ARG:HG2	1:A:7:ILE:N	2.31	0.45
1:C:194:ASP:OD1	1:D:307:ALA:HB3	2.16	0.45
1:D:138:VAL:O	1:D:142:GLN:NE2	2.49	0.45
1:D:239:LEU:HB3	1:D:240:ASN:H	1.64	0.45
1:D:406:TYR:HE1	1:D:457:PHE:HB3	1.82	0.45
1:A:245:TYR:CD2	1:A:246:SER:N	2.85	0.45
1:A:212:LYS:HG3	1:A:213:GLU:N	2.31	0.45
1:C:409:ILE:CD1	1:D:306:ARG:HB2	2.47	0.45
1:B:209:ILE:HG13	1:C:268:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LEU:O	1:D:163:LEU:HB3	2.17	0.45
1:D:336:VAL:O	1:D:340:CYS:SG	2.62	0.45
1:A:142:GLN:O	1:A:143:SER:HB3	2.16	0.45
1:A:207:PHE:CD1	1:A:294:ILE:HG23	2.52	0.45
1:A:336:VAL:HA	1:A:339:VAL:CG1	2.46	0.45
1:D:151:GLY:O	1:D:154:ILE:HB	2.16	0.45
1:D:65:LEU:O	1:D:66:GLN:HB2	2.16	0.45
1:A:6:ARG:HD3	1:A:8:GLU:HG3	1.99	0.45
1:A:92:GLN:C	1:A:94:PRO:HD3	2.37	0.45
1:C:416:ASN:CB	1:C:417:PRO:HD3	2.42	0.45
1:A:312:ILE:HB	1:A:394:ILE:CG2	2.47	0.45
1:A:279:MET:O	1:A:282:GLY:N	2.49	0.45
1:B:442:VAL:HG11	1:B:453:LEU:HD13	1.99	0.44
1:B:85:ASN:CG	1:B:86:ASN:N	2.69	0.44
1:A:70:LYS:HG2	1:A:74:ASN:ND2	2.31	0.44
1:C:50:GLY:O	1:C:54:VAL:HG23	2.16	0.44
1:B:251:LYS:HA	1:B:251:LYS:HD2	1.83	0.44
1:B:198:MET:HB2	1:B:198:MET:HE3	1.91	0.44
1:C:323:ILE:CG2	1:C:324:MET:SD	3.03	0.44
1:B:204:PHE:HA	1:B:207:PHE:CD2	2.52	0.44
1:C:93:PHE:HA	1:C:109:ASN:HD21	1.82	0.44
1:B:423:ASN:O	1:B:427:VAL:HG23	2.17	0.44
1:C:62:ASN:ND2	1:C:245:TYR:HE1	2.15	0.44
1:A:32:GLU:HG2	1:A:32:GLU:H	1.56	0.44
1:B:442:VAL:CG1	1:B:448:LEU:HD23	2.47	0.44
1:B:235:ILE:CD1	1:B:236:GLY:N	2.81	0.44
1:C:116:ASN:ND2	1:C:127:GLY:HA2	2.32	0.44
1:D:132:LEU:O	1:D:133:ASN:O	2.34	0.44
1:D:72:VAL:HB	1:D:132:LEU:CD1	2.41	0.44
1:A:122:MET:SD	1:A:132:LEU:HD11	2.57	0.44
1:D:423:ASN:ND2	1:D:447:LEU:HD11	2.32	0.44
1:A:323:ILE:HG12	1:B:425:ASP:OD1	2.17	0.44
1:D:181:PHE:CD1	1:D:184:ILE:HD12	2.52	0.44
1:A:122:MET:HB3	1:A:124:HIS:ND1	2.32	0.44
1:B:247:PRO:O	1:B:251:LYS:HG2	2.17	0.44
1:B:382:ALA:HA	1:D:36:ILE:HD12	1.99	0.44
1:D:323:ILE:O	1:D:325:PRO:HD3	2.17	0.44
1:C:116:ASN:HA	1:C:119:LEU:HD12	1.98	0.44
1:D:47:PHE:CE2	1:D:106:VAL:HG11	2.53	0.44
1:D:157:TYR:CE2	1:D:226:LEU:HD22	2.53	0.44
1:D:226:LEU:HA	1:D:226:LEU:HD12	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:SER:CB	1:B:247:PRO:HD3	2.48	0.44
1:D:451:ALA:O	1:D:455:ASP:N	2.50	0.44
1:B:171:ARG:NH2	1:B:212:LYS:NZ	2.65	0.44
1:B:118:GLY:HA3	1:B:132:LEU:HD21	2.00	0.44
1:A:323:ILE:HG12	1:B:425:ASP:OD2	2.17	0.44
1:B:281:HIS:C	1:B:283:ALA:N	2.70	0.44
1:D:205:ARG:O	1:D:209:ILE:HG12	2.18	0.44
1:A:56:LYS:CA	1:A:80:CYS:SG	3.05	0.44
1:A:116:ASN:HB3	1:A:126:LYS:HD2	1.99	0.44
1:A:36:ILE:HD12	1:C:339:VAL:HG11	1.99	0.44
1:C:239:LEU:O	1:C:242:PRO:HD2	2.17	0.44
1:C:285:LYS:HD2	1:C:344:ILE:HG23	2.00	0.44
1:C:47:PHE:HA	1:C:155:ALA:CB	2.47	0.44
1:C:230:LEU:HD12	1:C:230:LEU:HA	1.59	0.44
1:A:245:TYR:O	1:A:249:ALA:N	2.46	0.44
1:B:386:LEU:HD12	1:B:390:CYS:HB3	2.00	0.44
1:B:8:GLU:HB3	1:B:25:VAL:CG2	2.41	0.44
1:C:55:LYS:HD2	1:C:55:LYS:N	2.32	0.44
1:D:44:ILE:N	1:D:45:PRO:CD	2.81	0.44
1:A:402:GLU:O	1:A:405:VAL:HG22	2.18	0.44
1:B:285:LYS:HD3	1:B:347:ASP:CG	2.37	0.44
1:C:47:PHE:HA	1:C:155:ALA:HB1	1.99	0.44
1:A:244:GLU:O	1:A:248:LEU:HB2	2.17	0.43
1:A:111:ASN:CG	1:A:139:ASN:HB2	2.38	0.43
1:C:324:MET:HB2	1:D:409:ILE:CG2	2.48	0.43
1:D:49:ARG:NH2	4:D:490:HOH:O	2.48	0.43
1:A:158:SER:O	1:A:161:ILE:HB	2.18	0.43
1:A:117:ILE:O	1:A:121:LEU:HD23	2.18	0.43
1:B:49:ARG:HB3	1:B:49:ARG:HH11	1.82	0.43
1:C:181:PHE:O	1:C:184:ILE:N	2.50	0.43
1:A:430:ILE:HD13	1:A:430:ILE:HA	1.84	0.43
1:A:313:ASN:HB2	1:A:395:THR:OG1	2.17	0.43
1:D:54:VAL:HA	1:D:253:LEU:HD23	2.00	0.43
1:A:449:THR:HB	1:A:452:GLU:HG2	2.00	0.43
1:B:97:VAL:HG23	1:B:98:TYR:CD1	2.52	0.43
1:A:380:THR:O	1:A:383:CYS:HB2	2.19	0.43
1:A:421:HIS:H	1:A:421:HIS:CD2	2.36	0.43
1:A:246:SER:O	1:A:250:VAL:HG13	2.18	0.43
1:C:327:LYS:HD2	1:D:193:GLN:CB	2.48	0.43
1:A:179:VAL:O	1:A:182:GLN:HG2	2.19	0.43
1:B:306:ARG:O	1:B:306:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:SER:HB3	1:A:324:MET:HE3	2.00	0.43
1:D:49:ARG:HG3	1:D:90:MET:CE	2.47	0.43
1:B:57:ALA:HB2	1:B:253:LEU:HA	2.00	0.43
1:C:40:LYS:O	1:C:42:SER:N	2.51	0.43
1:C:86:ASN:OD1	1:C:88:LYS:HB2	2.18	0.43
1:D:332:VAL:HB	1:D:333:PRO:HD3	2.00	0.43
1:A:297:ASP:OD2	1:D:359:LEU:HD23	2.18	0.43
1:B:439:ARG:NH1	1:B:439:ARG:CG	2.81	0.43
1:A:259:PHE:HA	1:A:260:PRO:HD3	1.79	0.43
1:B:281:HIS:HB2	1:B:372:MET:CE	2.48	0.43
1:B:150:THR:CG2	1:B:253:LEU:HD21	2.48	0.43
1:C:84:LEU:O	1:C:86:ASN:N	2.51	0.43
1:A:185:LEU:HD23	1:A:405:VAL:HG21	1.99	0.43
1:B:92:GLN:O	1:B:94:PRO:HD3	2.19	0.43
1:C:6:ARG:HE	1:C:6:ARG:HB3	1.63	0.43
1:D:130:GLN:N	1:D:130:GLN:NE2	2.60	0.43
1:D:429:LYS:O	1:D:432:ALA:HB3	2.18	0.43
1:B:424:GLY:O	1:B:427:VAL:HB	2.19	0.43
1:A:271:THR:HG23	1:A:272:SER:H	1.82	0.43
1:A:62:ASN:OD1	1:A:245:TYR:HE1	2.02	0.43
1:A:17:VAL:HG23	1:A:18:PRO:HD2	1.99	0.43
1:A:45:PRO:HB2	1:A:373:PHE:HD2	1.83	0.43
1:C:302:SER:CB	1:C:314:LEU:HD13	2.48	0.43
1:D:152:PHE:CZ	1:D:369:GLY:HA2	2.53	0.43
1:A:163:LEU:HG	1:A:167:ILE:HD11	1.99	0.43
1:B:40:LYS:HD3	1:B:94:PRO:O	2.18	0.43
1:B:115:ALA:HB2	1:B:134:PRO:HB3	2.01	0.43
1:D:304:GLY:O	1:D:308:GLY:N	2.52	0.43
1:D:456:ILE:HG23	1:D:456:ILE:O	2.19	0.43
1:D:436:LYS:NZ	1:D:440:GLU:HB2	2.33	0.43
1:B:285:LYS:HG3	1:B:344:ILE:HA	2.01	0.43
1:C:63:LYS:O	1:C:65:LEU:N	2.42	0.43
1:A:322:SER:CA	1:B:429:LYS:NZ	2.81	0.43
1:A:196:VAL:CB	1:A:197:PRO:HD2	2.49	0.43
1:B:323:ILE:O	1:B:323:ILE:HG22	2.19	0.43
1:D:210:LEU:HD13	1:D:294:ILE:CD1	2.48	0.43
1:C:327:LYS:HD2	1:D:193:GLN:HB2	2.01	0.43
1:C:193:GLN:HG3	1:D:329:ASN:OD1	2.18	0.43
1:C:279:MET:CE	1:C:279:MET:HA	2.49	0.43
1:A:248:LEU:O	1:A:251:LYS:HB3	2.19	0.43
1:C:45:PRO:HG2	1:C:373:PHE:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLY:O	1:C:279:MET:HE3	2.18	0.43
1:B:169:GLN:HG2	1:B:384:TYR:HE1	1.84	0.43
1:C:204:PHE:O	1:C:207:PHE:HB2	2.18	0.43
1:A:243:LYS:O	1:A:244:GLU:C	2.56	0.42
1:D:110:THR:HG22	1:D:114:LEU:HD13	2.01	0.42
1:A:161:ILE:O	1:A:164:VAL:HG22	2.19	0.42
1:A:40:LYS:O	1:A:42:SER:N	2.45	0.42
1:C:145:ASN:O	1:C:271:THR:HB	2.18	0.42
1:A:65:LEU:HD21	1:A:245:TYR:HB2	2.01	0.42
1:A:65:LEU:HB3	1:A:67:THR:HG23	2.01	0.42
1:B:419:ILE:HG21	1:B:448:LEU:CD2	2.49	0.42
1:C:169:GLN:O	1:C:172:GLU:HB3	2.19	0.42
1:D:119:LEU:HD13	1:D:129:TYR:O	2.20	0.42
1:B:354:ALA:HB1	1:C:289:VAL:HG11	2.00	0.42
1:C:65:LEU:HD13	1:C:244:GLU:HB2	2.01	0.42
1:D:388:GLU:O	1:D:389:LYS:HD2	2.20	0.42
1:C:130:GLN:HE21	1:C:133:ASN:HA	1.84	0.42
1:A:56:LYS:HA	1:A:80:CYS:SG	2.59	0.42
1:C:44:ILE:N	1:C:45:PRO:HD2	2.31	0.42
1:C:272:SER:HB3	1:C:361:LEU:HA	2.01	0.42
1:A:70:LYS:NZ	1:A:74:ASN:HD21	2.17	0.42
1:B:336:VAL:O	1:B:339:VAL:HG13	2.19	0.42
1:C:139:ASN:HD22	1:C:142:GLN:HB2	1.84	0.42
1:C:265:GLU:HG3	1:C:265:GLU:H	1.49	0.42
1:A:144:THR:O	1:A:149:PRO:HD2	2.19	0.42
1:A:359:LEU:HD12	1:A:359:LEU:H	1.83	0.42
1:C:280:VAL:O	1:C:284:LEU:HD22	2.20	0.42
1:A:318:GLN:CG	1:A:319:ALA:N	2.75	0.42
1:D:103:GLY:HA3	1:D:148:TYR:CD2	2.55	0.42
1:B:370:GLN:OE1	1:D:342:LYS:HE2	2.19	0.42
1:C:62:ASN:HB3	1:C:67:THR:OG1	2.18	0.42
1:A:284:LEU:HD21	1:A:376:VAL:CG2	2.30	0.42
1:C:45:PRO:O	1:C:159:SER:OG	2.36	0.42
1:B:140:LYS:O	1:B:141:CYS:HB2	2.19	0.42
1:A:334:GLU:OE1	1:C:363:VAL:HB	2.19	0.42
1:C:332:VAL:O	1:C:336:VAL:HG23	2.19	0.42
1:B:103:GLY:HA3	1:B:148:TYR:CD2	2.54	0.42
1:D:272:SER:O	1:D:273:ASP:CB	2.68	0.42
1:C:304:GLY:HA2	1:C:305:PRO:HD3	1.84	0.42
1:D:170:LEU:HD11	1:D:386:LEU:HD23	2.01	0.42
1:D:439:ARG:CZ	1:D:453:LEU:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ALA:C	1:D:266:ASP:N	2.72	0.42
1:B:124:HIS:CD2	1:B:131:TYR:CD1	3.07	0.42
1:D:18:PRO:HB2	1:D:21:ALA:HB2	2.00	0.42
1:B:415:LEU:HB3	1:B:419:ILE:HD13	2.01	0.42
1:A:304:GLY:HA2	1:A:305:PRO:HD2	1.94	0.42
1:C:378:ILE:HD13	1:C:379:LEU:N	2.34	0.42
1:D:453:LEU:HA	1:D:453:LEU:HD12	1.81	0.42
1:C:9:GLU:HA	1:C:14:THR:HG22	2.00	0.42
1:B:10:ASP:OD2	1:D:319:ALA:HB2	2.20	0.42
1:B:281:HIS:O	1:B:283:ALA:N	2.53	0.42
1:A:300:LEU:O	1:A:303:SER:HB3	2.20	0.42
1:A:56:LYS:CB	1:A:80:CYS:SG	3.06	0.42
1:C:241:THR:N	1:C:242:PRO:CD	2.83	0.42
1:C:313:ASN:OD1	1:C:397:ASN:ND2	2.53	0.42
1:A:5:ILE:HB	1:A:17:VAL:O	2.19	0.42
1:D:76:ILE:O	1:D:79:ALA:HB3	2.19	0.42
1:A:99:GLN:HG3	1:A:99:GLN:O	2.20	0.42
1:A:303:SER:HB2	1:B:192:LEU:HB3	2.02	0.42
1:B:150:THR:CG2	1:B:228:VAL:HB	2.50	0.42
1:B:365:GLU:O	1:B:368:ILE:HB	2.20	0.42
1:D:157:TYR:CD2	1:D:226:LEU:HD13	2.55	0.42
1:A:312:ILE:HA	1:A:396:ALA:HA	2.02	0.42
1:B:231:GLY:O	1:B:241:THR:HB	2.20	0.42
1:A:93:PHE:CA	1:A:109:ASN:HD21	2.29	0.42
1:A:44:ILE:N	1:A:45:PRO:CD	2.83	0.42
1:B:5:ILE:N	1:B:5:ILE:CD1	2.82	0.42
1:B:391:ILE:HG13	1:B:392:ASN:N	2.34	0.42
1:B:273:ASP:OD1	1:C:290:LYS:NZ	2.46	0.42
1:B:226:LEU:HA	1:B:226:LEU:HD12	1.87	0.42
1:A:400:VAL:HG12	1:A:401:CYS:N	2.34	0.42
1:B:198:MET:HG2	1:B:199:THR:N	2.35	0.41
1:C:175:GLU:HG2	1:C:208:SER:CB	2.49	0.41
1:C:101:GLY:O	1:C:103:GLY:N	2.53	0.41
1:A:374:GLU:O	1:A:378:ILE:HG12	2.20	0.41
1:B:100:GLY:HA3	1:D:331:VAL:O	2.20	0.41
1:A:194:ASP:H	1:B:305:PRO:HD2	1.85	0.41
1:D:277:TYR:HA	1:D:280:VAL:HG22	2.02	0.41
1:D:280:VAL:HG23	1:D:281:HIS:H	1.84	0.41
1:B:363:VAL:HG11	1:C:191:GLN:HG2	2.01	0.41
1:A:310:ASN:O	1:A:400:VAL:HG11	2.20	0.41
1:D:395:THR:HG22	1:D:396:ALA:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASP:HB3	1:C:98:TYR:O	2.19	0.41
1:D:213:GLU:HA	1:D:216:LYS:HD3	2.02	0.41
1:B:286:ARG:O	1:B:289:VAL:HG22	2.20	0.41
1:A:74:ASN:O	1:A:78:ALA:CB	2.68	0.41
1:A:36:ILE:HG21	1:A:98:TYR:CG	2.55	0.41
1:D:126:LYS:CB	1:D:126:LYS:NZ	2.83	0.41
1:B:445:ARG:CB	1:B:447:LEU:HD13	2.50	0.41
1:D:267:LEU:HG	1:D:268:ILE:HG23	2.02	0.41
1:A:153:ARG:NH2	1:A:274:CYS:SG	2.94	0.41
1:B:44:ILE:N	1:B:45:PRO:CD	2.79	0.41
1:B:46:GLU:CG	1:B:47:PHE:H	2.33	0.41
1:C:324:MET:HB2	1:D:409:ILE:HB	2.02	0.41
1:B:281:HIS:HA	1:B:284:LEU:HD22	2.02	0.41
1:C:235:ILE:CD1	1:C:236:GLY:N	2.81	0.41
1:A:27:THR:O	1:A:31:ILE:HG13	2.20	0.41
1:C:88:LYS:HG3	1:C:89:CYS:N	2.35	0.41
1:B:387:LEU:HA	1:B:391:ILE:HG12	2.02	0.41
1:D:226:LEU:CD2	1:D:260:PRO:HG2	2.49	0.41
1:D:403:GLY:O	1:D:407:ASN:HB2	2.19	0.41
1:D:203:GLU:O	1:D:206:ALA:HB3	2.20	0.41
1:C:190:THR:HG23	1:C:195:ALA:HB2	2.02	0.41
1:A:239:LEU:O	1:A:242:PRO:HD2	2.20	0.41
1:D:242:PRO:O	1:D:243:LYS:HB2	2.20	0.41
1:B:200:LEU:O	1:B:203:GLU:HB3	2.20	0.41
1:D:130:GLN:CA	1:D:130:GLN:NE2	2.78	0.41
1:D:172:GLU:O	1:D:176:ARG:HB2	2.19	0.41
1:D:295:CYS:SG	1:D:336:VAL:CB	3.09	0.41
1:A:315:PRO:HG3	1:A:390:CYS:O	2.21	0.41
1:B:97:VAL:HG23	1:B:98:TYR:N	2.35	0.41
1:A:415:LEU:O	1:A:419:ILE:N	2.47	0.41
1:C:63:LYS:NZ	1:C:63:LYS:HB3	2.35	0.41
1:C:146:ASP:C	1:C:149:PRO:HD2	2.41	0.41
1:B:331:VAL:CG1	1:B:332:VAL:N	2.84	0.41
1:C:6:ARG:NH1	1:C:127:GLY:HA3	2.34	0.41
1:D:127:GLY:C	1:D:129:TYR:N	2.74	0.41
1:D:414:TYR:O	1:D:418:PHE:CE2	2.74	0.41
1:B:340:CYS:O	1:B:343:VAL:HB	2.20	0.41
1:C:75:ALA:HB1	1:C:132:LEU:HD22	2.03	0.41
1:C:158:SER:HB3	1:C:259:PHE:CZ	2.56	0.41
1:C:390:CYS:O	1:C:394:ILE:HG13	2.21	0.41
1:A:1:MET:SD	1:A:2:SER:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:THR:O	1:A:245:TYR:HB3	2.20	0.41
1:A:23:TYR:O	1:A:23:TYR:CD2	2.74	0.41
1:A:405:VAL:CG2	1:A:406:TYR:H	2.34	0.41
1:C:312:ILE:HD12	1:C:394:ILE:HG21	2.02	0.41
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.79	0.41
1:A:322:SER:CA	1:B:429:LYS:HZ3	2.34	0.41
1:C:323:ILE:HB	1:C:324:MET:SD	2.61	0.41
1:B:87:GLY:O	1:B:89:CYS:N	2.54	0.41
1:A:199:THR:C	1:A:201:GLY:N	2.73	0.41
1:B:17:VAL:HG23	1:B:18:PRO:HD2	2.03	0.41
1:B:17:VAL:HA	1:B:18:PRO:HD3	1.90	0.41
1:D:186:LYS:O	1:D:197:PRO:HA	2.20	0.41
1:D:62:ASN:HB3	1:D:68:ILE:HG12	2.02	0.41
1:B:398:LYS:HG2	1:B:402:GLU:HG3	2.02	0.41
1:D:62:ASN:HB3	1:D:67:THR:HG1	1.86	0.41
1:C:320:GLY:O	1:C:322:SER:N	2.54	0.41
1:A:48:VAL:C	1:A:50:GLY:N	2.72	0.41
1:B:357:GLY:O	1:C:293:LYS:HG2	2.20	0.41
1:A:196:VAL:HB	1:A:197:PRO:HD2	2.02	0.41
1:A:303:SER:O	1:A:308:GLY:HA3	2.20	0.41
1:A:312:ILE:HB	1:A:394:ILE:HG21	2.03	0.41
1:A:312:ILE:HD12	1:A:394:ILE:HD13	2.03	0.41
1:A:35:TYR:O	1:C:381:ASN:HB3	2.20	0.41
1:D:100:GLY:C	1:D:102:ALA:H	2.24	0.41
1:A:323:ILE:HG12	1:B:425:ASP:CG	2.42	0.40
1:A:243:LYS:CG	1:A:244:GLU:N	2.84	0.40
1:D:54:VAL:CG1	1:D:55:LYS:N	2.84	0.40
1:C:272:SER:HA	1:C:362:ASN:H	1.85	0.40
1:C:163:LEU:O	1:C:167:ILE:HG13	2.21	0.40
1:C:130:GLN:NE2	1:C:132:LEU:O	2.54	0.40
1:D:243:LYS:HD3	1:D:244:GLU:H	1.86	0.40
1:A:89:CYS:HB3	1:A:117:ILE:HD13	2.03	0.40
1:C:414:TYR:O	1:C:417:PRO:HD2	2.21	0.40
1:C:93:PHE:HA	1:C:109:ASN:ND2	2.36	0.40
1:C:343:VAL:HG22	1:C:378:ILE:HD11	2.03	0.40
1:C:181:PHE:HZ	1:C:394:ILE:O	2.05	0.40
1:B:264:ALA:O	1:B:266:ASP:N	2.54	0.40
1:A:317:LEU:N	1:A:317:LEU:CD2	2.84	0.40
1:B:199:THR:HG22	1:B:202:GLN:CG	2.51	0.40
1:B:276:ALA:O	1:B:280:VAL:HG13	2.22	0.40
1:D:242:PRO:HA	1:D:246:SER:HG	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:TYR:O	1:D:414:TYR:CD1	2.75	0.40
1:A:303:SER:O	1:A:304:GLY:O	2.39	0.40
1:B:74:ASN:HA	1:B:77:ILE:HG12	2.03	0.40
1:B:6:ARG:HH21	1:B:126:LYS:HZ2	1.68	0.40
1:A:314:LEU:HG	1:A:390:CYS:SG	2.61	0.40
1:A:317:LEU:N	1:A:317:LEU:HD23	2.37	0.40
1:A:325:PRO:HG2	1:B:409:ILE:CD1	2.52	0.40
1:C:172:GLU:CB	1:C:176:ARG:HH21	2.22	0.40
1:A:164:VAL:HG23	1:A:165:ASP:N	2.37	0.40
1:D:168:ASN:HD22	1:D:168:ASN:HA	1.70	0.40
1:B:343:VAL:HG21	1:B:379:LEU:CD2	2.49	0.40
1:B:108:MET:HE2	1:B:111:ASN:ND2	2.37	0.40
1:C:124:HIS:CD2	1:C:131:TYR:CE1	3.10	0.40
1:B:287:LEU:CD1	1:B:291:MET:HG3	2.52	0.40
1:A:290:LYS:NZ	1:D:273:ASP:OD2	2.55	0.40
1:D:114:LEU:HD12	1:D:114:LEU:N	2.37	0.40
1:A:125:GLN:H	1:A:125:GLN:CD	2.25	0.40
1:C:177:LYS:O	1:C:180:GLU:HB3	2.22	0.40
1:A:387:LEU:O	1:A:392:ASN:HB2	2.22	0.40
1:D:25:VAL:HB	1:D:29:ARG:HH11	1.87	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	457/478 (96%)	341 (75%)	82 (18%)	34 (7%)	1	1
1	B	458/478 (96%)	352 (77%)	70 (15%)	36 (8%)	1	1
1	C	411/478 (86%)	295 (72%)	77 (19%)	39 (10%)	1	1
1	D	457/478 (96%)	356 (78%)	63 (14%)	38 (8%)	1	1
All	All	1783/1912 (93%)	1344 (75%)	292 (16%)	147 (8%)	1	1

All (147) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	25	VAL
1	A	84	LEU
1	A	88	LYS
1	A	232	ALA
1	A	235	ILE
1	A	242	PRO
1	A	244	GLU
1	A	245	TYR
1	A	267	LEU
1	A	304	GLY
1	A	319	ALA
1	A	328	VAL
1	A	456	ILE
1	A	457	PHE
1	B	41	ILE
1	B	46	GLU
1	B	85	ASN
1	B	237	THR
1	B	264	ALA
1	B	266	ASP
1	B	322	SER
1	B	328	VAL
1	B	459	VAL
1	C	47	PHE
1	C	85	ASN
1	C	90	MET
1	C	91	ASP
1	C	182	GLN
1	C	237	THR
1	C	239	LEU
1	C	242	PRO
1	C	245	TYR
1	C	268	ILE
1	C	328	VAL
1	C	398	LYS
1	D	47	PHE
1	D	86	ASN
1	D	128	GLU
1	D	133	ASN
1	D	233	THR
1	D	239	LEU

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Mol	Chain	Res	Type
1	D	243	LYS
1	D	273	ASP
1	D	303	SER
1	D	326	ALA
1	D	457	PHE
1	A	46	GLU
1	A	223	GLU
1	A	234	ALA
1	A	356	ALA
1	B	4	ASN
1	B	19	ALA
1	B	88	LYS
1	B	135	ASN
1	B	182	GLN
1	B	197	PRO
1	B	235	ILE
1	B	303	SER
1	B	307	ALA
1	B	309	LEU
1	B	325	PRO
1	B	364	MET
1	C	64	GLU
1	C	89	CYS
1	C	240	ASN
1	C	304	GLY
1	C	309	LEU
1	C	321	SER
1	C	396	ALA
1	D	46	GLU
1	D	64	GLU
1	D	234	ALA
1	D	267	LEU
1	D	304	GLY
1	D	320	GLY
1	D	391	ILE
1	D	446	GLY
1	A	145	ASN
1	A	237	THR
1	A	398	LYS
1	B	102	ALA
1	B	234	ALA
1	B	243	LYS

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Mol	Chain	Res	Type
1	B	270	ALA
1	C	102	ALA
1	C	236	GLY
1	C	270	ALA
1	C	359	LEU
1	C	397	ASN
1	D	85	ASN
1	D	186	LYS
1	D	390	CYS
1	D	398	LYS
1	A	4	ASN
1	A	33	ASN
1	A	89	CYS
1	A	128	GLU
1	A	143	SER
1	A	222	ALA
1	A	387	LEU
1	B	18	PRO
1	B	155	ALA
1	B	232	ALA
1	B	265	GLU
1	B	387	LEU
1	C	25	VAL
1	C	65	LEU
1	C	318	GLN
1	C	387	LEU
1	D	237	THR
1	D	411	ILE
1	D	443	LEU
1	A	94	PRO
1	B	44	ILE
1	B	45	PRO
1	B	304	GLY
1	B	456	ILE
1	C	128	GLU
1	C	269	GLU
1	C	273	ASP
1	C	330	PRO
1	D	70	LYS
1	D	181	PHE
1	D	266	ASP
1	D	289	VAL

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Mol	Chain	Res	Type
1	D	328	VAL
1	D	439	ARG
1	A	127	GLY
1	A	372	MET
1	B	90	MET
1	C	235	ILE
1	C	354	ALA
1	D	43	ASP
1	D	149	PRO
1	D	182	GLN
1	A	231	GLY
1	C	41	ILE
1	A	41	ILE
1	C	76	ILE
1	C	101	GLY
1	D	118	GLY
1	B	31	ILE
1	C	308	GLY
1	D	5	ILE
1	C	36	ILE
1	D	456	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	385/402 (96%)	345 (90%)	40 (10%)	9	20
1	B	386/402 (96%)	347 (90%)	39 (10%)	9	21
1	C	346/402 (86%)	306 (88%)	40 (12%)	7	16
1	D	385/402 (96%)	343 (89%)	42 (11%)	8	18
All	All	1502/1608 (93%)	1341 (89%)	161 (11%)	8	19

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	5	ILE
1	A	11	LEU
1	A	14	THR
1	A	15	ARG
1	A	20	ASP
1	A	32	GLU
1	A	35	TYR
1	A	65	LEU
1	A	77	ILE
1	A	86	ASN
1	A	94	PRO
1	A	107	ASN
1	A	125	GLN
1	A	145	ASN
1	A	186	LYS
1	A	189	ARG
1	A	212	LYS
1	A	221	THR
1	A	240	ASN
1	A	265	GLU
1	A	267	LEU
1	A	273	ASP
1	A	293	LYS
1	A	306	ARG
1	A	309	LEU
1	A	314	LEU
1	A	317	LEU
1	A	318	GLN
1	A	324	MET
1	A	331	VAL
1	A	337	ASN
1	A	339	VAL
1	A	352	MET
1	A	360	GLN
1	A	385	ASN
1	A	392	ASN
1	A	422	HIS
1	A	448	LEU
1	B	5	ILE
1	B	43	ASP
1	B	46	GLU

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Mol	Chain	Res	Type
1	B	47	PHE
1	B	49	ARG
1	B	125	GLN
1	B	136	ASP
1	B	145	ASN
1	B	162	LYS
1	B	165	ASP
1	B	168	ASN
1	B	169	GLN
1	B	172	GLU
1	B	194	ASP
1	B	197	PRO
1	B	212	LYS
1	B	219	GLN
1	B	226	LEU
1	B	237	THR
1	B	240	ASN
1	B	241	THR
1	B	243	LYS
1	B	246	SER
1	B	265	GLU
1	B	274	CYS
1	B	284	LEU
1	B	306	ARG
1	B	324	MET
1	B	331	VAL
1	B	339	VAL
1	B	352	MET
1	B	355	GLU
1	B	361	LEU
1	B	370	GLN
1	B	385	ASN
1	B	404	TYR
1	B	425	ASP
1	B	439	ARG
1	B	459	VAL
1	C	5	ILE
1	C	6	ARG
1	C	15	ARG
1	C	16	GLU
1	C	17	VAL
1	C	20	ASP

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Mol	Chain	Res	Type
1	C	39	ASN
1	C	52	VAL
1	C	55	LYS
1	C	64	GLU
1	C	88	LYS
1	C	95	VAL
1	C	107	ASN
1	C	128	GLU
1	C	139	ASN
1	C	146	ASP
1	C	154	ILE
1	C	172	GLU
1	C	185	LEU
1	C	189	ARG
1	C	196	VAL
1	C	210	LEU
1	C	219	GLN
1	C	237	THR
1	C	241	THR
1	C	242	PRO
1	C	265	GLU
1	C	266	ASP
1	C	267	LEU
1	C	268	ILE
1	C	269	GLU
1	C	272	SER
1	C	284	LEU
1	C	321	SER
1	C	324	MET
1	C	370	GLN
1	C	378	ILE
1	C	385	ASN
1	C	397	ASN
1	C	411	ILE
1	D	4	ASN
1	D	5	ILE
1	D	25	VAL
1	D	34	PHE
1	D	52	VAL
1	D	77	ILE
1	D	89	CYS
1	D	91	ASP

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Mol	Chain	Res	Type
1	D	96	ASP
1	D	119	LEU
1	D	125	GLN
1	D	129	TYR
1	D	130	GLN
1	D	158	SER
1	D	183	ASP
1	D	203	GLU
1	D	211	LEU
1	D	223	GLU
1	D	226	LEU
1	D	227	GLU
1	D	239	LEU
1	D	240	ASN
1	D	265	GLU
1	D	267	LEU
1	D	272	SER
1	D	316	GLU
1	D	323	ILE
1	D	324	MET
1	D	331	VAL
1	D	334	GLU
1	D	360	GLN
1	D	370	GLN
1	D	385	ASN
1	D	395	THR
1	D	400	VAL
1	D	408	SER
1	D	413	THR
1	D	422	HIS
1	D	433	GLU
1	D	445	ARG
1	D	447	LEU
1	D	448	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	62	ASN
1	A	74	ASN
1	A	85	ASN

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Mol	Chain	Res	Type
1	A	109	ASN
1	A	124	HIS
1	A	137	HIS
1	A	191	GLN
1	A	202	GLN
1	A	217	ASN
1	A	219	GLN
1	A	229	ASN
1	A	310	ASN
1	A	313	ASN
1	A	329	ASN
1	A	358	GLN
1	A	360	GLN
1	A	416	ASN
1	A	421	HIS
1	A	422	HIS
1	B	38	ASN
1	B	62	ASN
1	B	66	GLN
1	B	74	ASN
1	B	85	ASN
1	B	99	GLN
1	B	111	ASN
1	B	124	HIS
1	B	135	ASN
1	B	142	GLN
1	B	145	ASN
1	B	168	ASN
1	B	191	GLN
1	B	193	GLN
1	B	281	HIS
1	B	346	ASN
1	B	360	GLN
1	B	377	HIS
1	B	421	HIS
1	C	62	ASN
1	C	107	ASN
1	C	109	ASN
1	C	111	ASN
1	C	124	HIS
1	C	125	GLN
1	C	130	GLN

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Mol	Chain	Res	Type
1	C	137	HIS
1	C	139	ASN
1	C	168	ASN
1	C	219	GLN
1	C	313	ASN
1	C	329	ASN
1	C	338	GLN
1	C	346	ASN
1	C	397	ASN
1	C	407	ASN
1	C	416	ASN
1	D	4	ASN
1	D	26	HIS
1	D	62	ASN
1	D	130	GLN
1	D	168	ASN
1	D	310	ASN
1	D	313	ASN
1	D	338	GLN
1	D	362	ASN
1	D	370	GLN
1	D	377	HIS
1	D	397	ASN
1	D	423	ASN

### 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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	BGC	A	601	-	12,12,12	0.52	0	17,17,17	0.81	1 (5%)
3	ACT	A	701	-	1,3,3	3.01	1 (100%)	0,3,3	0.00	-
2	BGC	B	701	-	12,12,12	0.22	0	17,17,17	0.45	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
2	BGC	A	601	-	-	0/2/22/22	0/1/1/1
3	ACT	A	701	-	-	0/0/0/0	0/0/0/0
2	BGC	B	701	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ACT	CH3-C	3.01	1.53	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	BGC	C1-C2-C3	-2.61	106.54	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

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	459/478 (96%)	0.33	29 (6%) 23 22	2, 23, 50, 79	0
1	B	460/478 (96%)	0.31	33 (7%) 18 16	4, 22, 50, 69	0
1	C	413/478 (86%)	0.44	34 (8%) 14 11	3, 23, 46, 81	0
1	D	459/478 (96%)	0.28	22 (4%) 34 33	4, 21, 49, 100	0
All	All	1791/1912 (93%)	0.34	118 (6%) 22 20	2, 22, 49, 100	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	87	GLY	11.2
1	A	87	GLY	8.6
1	C	413	THR	8.3
1	C	412	VAL	7.3
1	B	237	THR	6.2
1	B	323	ILE	5.7
1	C	324	MET	5.7
1	D	1	MET	5.5
1	B	3	ASN	5.5
1	A	323	ILE	5.4
1	A	272	SER	5.3
1	A	44	ILE	5.2
1	C	414	TYR	5.2
1	C	45	PRO	5.0
1	B	86	ASN	4.9
1	C	410	GLY	4.9
1	C	323	ILE	4.8
1	B	272	SER	4.6
1	D	326	ALA	4.5
1	D	453	LEU	4.4
1	C	326	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	238	GLY	4.3
1	C	44	ILE	4.3
1	C	87	GLY	4.1
1	B	273	ASP	4.1
1	C	409	ILE	4.0
1	C	416	ASN	4.0
1	C	76	ILE	3.9
1	B	1	MET	3.9
1	D	86	ASN	3.9
1	D	2	SER	3.9
1	A	129	TYR	3.7
1	B	44	ILE	3.7
1	A	273	ASP	3.7
1	A	86	ASN	3.7
1	A	2	SER	3.7
1	D	418	PHE	3.7
1	D	45	PRO	3.7
1	A	45	PRO	3.6
1	D	237	THR	3.6
1	D	272	SER	3.5
1	A	185	LEU	3.5
1	C	271	THR	3.4
1	A	1	MET	3.4
1	D	3	ASN	3.4
1	B	45	PRO	3.3
1	B	2	SER	3.3
1	A	348	THR	3.2
1	C	242	PRO	3.1
1	C	417	PRO	3.1
1	B	428	GLY	3.1
1	B	274	CYS	3.1
1	A	77	ILE	3.1
1	B	324	MET	3.0
1	D	417	PRO	3.0
1	C	73	ALA	3.0
1	A	236	GLY	3.0
1	D	323	ILE	3.0
1	B	4	ASN	3.0
1	A	21	ALA	2.9
1	B	129	TYR	2.9
1	C	5	ILE	2.9
1	C	237	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	52	VAL	2.7
1	D	44	ILE	2.7
1	A	347	ASP	2.7
1	D	325	PRO	2.6
1	C	183	ASP	2.6
1	D	271	THR	2.6
1	D	414	TYR	2.6
1	B	320	GLY	2.6
1	A	5	ILE	2.6
1	B	457	PHE	2.6
1	C	241	THR	2.5
1	B	427	VAL	2.5
1	C	273	ASP	2.5
1	C	348	THR	2.5
1	C	391	ILE	2.5
1	C	127	GLY	2.5
1	D	451	ALA	2.4
1	B	248	LEU	2.4
1	A	3	ASN	2.4
1	B	25	VAL	2.4
1	A	237	THR	2.4
1	A	248	LEU	2.4
1	B	238	GLY	2.3
1	B	304	GLY	2.3
1	C	265	GLU	2.3
1	C	185	LEU	2.3
1	B	271	THR	2.3
1	B	241	THR	2.3
1	C	345	GLY	2.3
1	B	17	VAL	2.3
1	A	128	GLU	2.3
1	B	85	ASN	2.3
1	B	264	ALA	2.3
1	C	234	ALA	2.3
1	C	272	SER	2.2
1	C	113	VAL	2.2
1	B	256	VAL	2.2
1	B	270	ALA	2.2
1	D	415	LEU	2.2
1	A	234	ALA	2.2
1	A	244	GLU	2.2
1	C	52	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	414	TYR	2.2
1	B	345	GLY	2.1
1	B	235	ILE	2.1
1	A	90	MET	2.1
1	B	326	ALA	2.1
1	A	352	MET	2.1
1	C	356	ALA	2.1
1	A	17	VAL	2.1
1	D	242	PRO	2.1
1	D	345	GLY	2.1
1	A	68	ILE	2.0
1	B	28	LEU	2.0
1	D	234	ALA	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( $\text{\AA}^2$ )	Q<0.9
2	BGC	B	701	12/12	0.83	0.23	1.29	43,43,43,43	0
3	ACT	A	701	4/4	0.86	0.19	0.03	31,31,31,31	0
2	BGC	A	601	12/12	0.82	0.19	-	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.