



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:04 AM GMT

PDB ID : 3H32  
Title : Crystal structure of D-dimer from human fibrin complexed with Gly-His-Arg-Pro-Tyr-amide  
Authors : Doolittle, R.F.; Pandi, L.  
Deposited on : 2009-04-15  
Resolution : 3.60 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

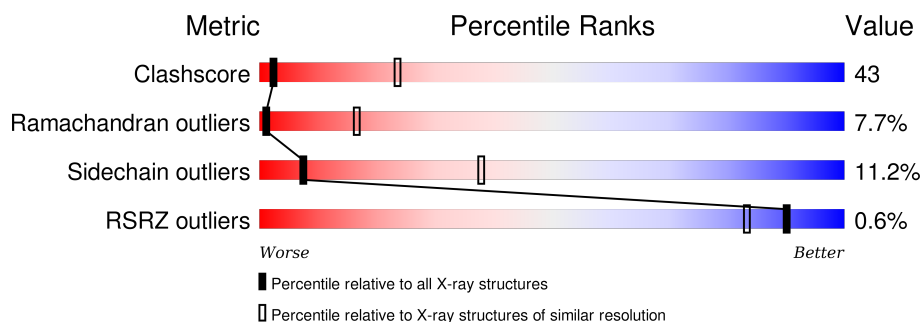
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	197	<div> <div>2%</div> <div>13% 19% 5% • 62%</div> </div>
1	D	197	<div> <div>%</div> <div>12% 21% • • 62%</div> </div>
2	B	458	<div> <div>26% 36% 5% • 33%</div> </div>
2	E	458	<div> <div>24% 37% 6% 33%</div> </div>
3	C	317	<div> <div>35% 44% 14% • 5%</div> </div>
3	F	317	<div> <div>30% 50% 12% • 7%</div> </div>
4	M	5	<div> <div>40% 60%</div> </div>

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Mol	Chain	Length	Quality of chain
4	N	5	 <div>60% 40%</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
6	NAG	B	471	X	-	-	-
6	MAN	B	473	X	-	-	-
6	NAG	B	477	X	-	-	-
6	NAG	E	471	X	-	-	-
6	NAG	E	477	X	-	-	-
6	SIA	E	479	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11246 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	D	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	308	Total	C	N	O	S	0	0	0
			2474	1544	434	474	22			
2	E	308	Total	C	N	O	S	0	0	0
			2474	1544	434	474	22			

- Molecule 3 is a protein called Fibrinogen gamma chain, isoform gamma-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	301	Total	C	N	O	S	0	0	0
			2404	1523	405	465	11			
3	F	296	Total	C	N	O	S	0	0	0
			2372	1504	400	457	11			

- Molecule 4 is a protein called Fibrin B knob pentapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	5	Total	C	N	O	0	0	0
			45	28	10	7			
4	N	5	Total	C	N	O	0	0	0
			45	28	10	7			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (8-MER).

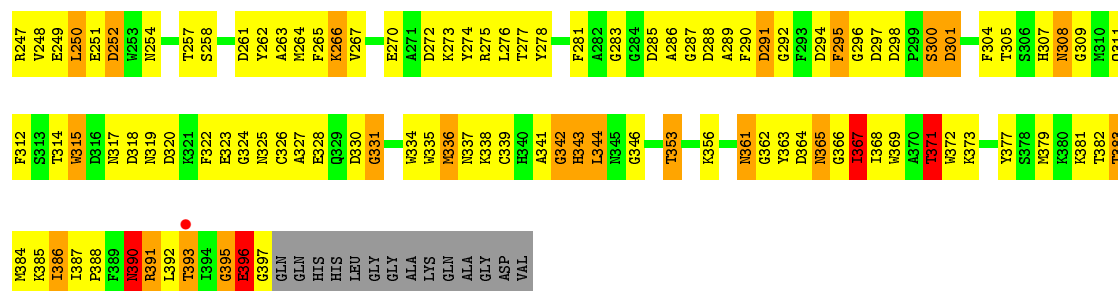
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	8	Total C N O 106 59 4 43	0	0
6	E	8	Total C N O 106 59 4 43	0	0



- Molecule 1: Fibrinogen alpha chain

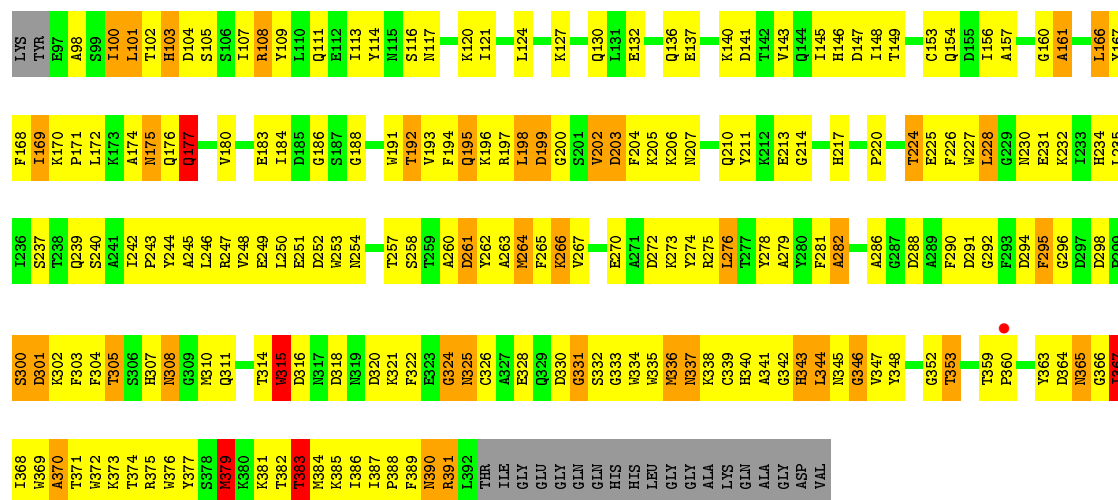






- Molecule 3: Fibrinogen gamma chain, isoform gamma-A

Chain F: 30% 50% 12% 7%



- Molecule 4: Fibrin B knob pentapeptide

Chain M: 40% 60%



- Molecule 4: Fibrin B knob pentapeptide

Chain N: 60% 40%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.72 Å   97.32 Å   132.49 Å 90.00°   122.78°   90.00°	Depositor
Resolution (Å)	50.00 – 3.60 29.72 – 3.60	Depositor EDS
% Data completeness (in resolution range)	75.5 (50.00-3.60) 75.7 (29.72-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	30.66 (at 3.55 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.263 ,      0.320 0.263 ,      (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	89.3	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 16.2	EDS
Estimated twinning fraction	0.016 for -h-2*k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 25002 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: CA, GAL, SIA, NAG, MAN

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	0.72	0/609	0.87	2/811 (0.2%)
1	D	0.64	0/609	0.82	1/811 (0.1%)
2	B	0.58	0/2536	0.71	0/3425
2	E	0.60	0/2536	0.72	1/3425 (0.0%)
3	C	0.59	0/2469	0.69	0/3339
3	F	0.55	0/2437	0.68	0/3296
4	M	0.56	0/47	0.67	0/61
4	N	0.58	0/47	0.50	0/61
All	All	0.59	0/11290	0.72	4/15229 (0.0%)

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
2	B	0	1
6	B	3	0
6	E	3	0
All	All	6	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	CYS	CA-CB-SG	-9.69	96.56	114.00
1	D	161	CYS	CA-CB-SG	6.66	125.98	114.00
2	E	152	TYR	N-CA-C	5.32	125.37	111.00
1	A	124	ARG	N-CA-C	5.11	124.81	111.00

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	471	NAG	C1
6	B	473	MAN	C1
6	B	477	NAG	C1
6	E	471	NAG	C1
6	E	477	NAG	C1
6	E	479	SIA	C2

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	192	TYR	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	608	0	649	62	0
1	D	608	0	649	61	0
2	B	2474	0	2336	196	0
2	E	2474	0	2336	224	0
3	C	2404	0	2249	228	0
3	F	2372	0	2219	251	0
4	M	45	0	41	5	0
4	N	45	0	41	5	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	B	106	0	89	5	0
6	E	106	0	89	6	0
All	All	11246	0	10698	941	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 43.

All (941) 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)
3:F:228:LEU:HG	3:F:232:LYS:HD2	1.22	1.15
2:E:415:ARG:H	2:E:434:GLY:HA2	0.98	1.14
3:F:338:LYS:N	3:F:339:CYS:HA	1.70	1.07
3:C:305:THR:HB	3:C:341:ALA:HB2	1.37	1.07
3:C:166:LEU:HD12	3:C:166:LEU:H	1.20	1.07
2:B:415:ARG:H	2:B:434:GLY:HA2	1.20	1.05
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.37	1.02
3:C:338:LYS:N	3:C:339:CYS:HA	1.78	0.98
2:E:300:SER:HA	2:E:331:VAL:HG23	1.44	0.98
3:F:196:LYS:HD2	3:F:383:THR:HB	1.47	0.97
2:B:203:ILE:H	2:B:203:ILE:HD12	1.29	0.94
2:E:415:ARG:N	2:E:434:GLY:HA2	1.82	0.94
3:F:197:ARG:HA	3:F:225:GLU:HG2	1.50	0.93
1:A:123:LYS:HZ2	2:B:151:LEU:HB3	1.34	0.92
1:A:123:LYS:NZ	2:B:151:LEU:HB3	1.84	0.92
6:B:478:GAL:H4	6:B:479:SIA:H8	1.51	0.92
6:E:478:GAL:H4	6:E:479:SIA:H6	1.51	0.92
3:C:174:ALA:HB2	3:C:235:LEU:HD22	1.49	0.92
2:B:309:GLU:HB3	2:B:327:GLY:HA2	1.52	0.91
2:E:203:ILE:H	2:E:203:ILE:HD12	1.34	0.91
3:F:305:THR:HB	3:F:341:ALA:HB2	1.53	0.91
2:E:228:GLN:HE22	3:F:177:GLN:HE22	1.19	0.89
2:B:380:ARG:NH2	2:B:382:ASN:HD21	1.70	0.89
1:D:147:MET:HE1	3:F:121:ILE:HD11	1.55	0.89
1:D:181:GLN:NE2	2:E:171:ILE:HA	1.88	0.88
2:B:300:SER:HA	2:B:331:VAL:HG23	1.53	0.88
1:D:154:ILE:O	1:D:158:ILE:HG12	1.73	0.87
1:D:169:LEU:H	2:E:189:GLN:HE22	1.20	0.87
3:C:197:ARG:HA	3:C:225:GLU:HG2	1.55	0.87
2:B:252:ILE:HD11	2:B:299:ILE:HG12	1.57	0.86
3:C:325:ASN:HD21	3:C:328:GLU:HB2	1.40	0.86
1:D:186:GLU:HA	1:D:189:ILE:HD11	1.57	0.86
2:B:158:ASN:O	2:B:162:PRO:HG2	1.75	0.85
3:C:191:TRP:HA	3:C:387:ILE:HD13	1.60	0.84
3:F:249:GLU:HB3	3:F:383:THR:HG23	1.60	0.84
6:E:472:MAN:H4	6:E:473:MAN:H2	1.61	0.83
1:D:169:LEU:H	2:E:189:GLN:NE2	1.76	0.83
3:F:367:ILE:HD13	3:F:367:ILE:H	1.44	0.83
3:C:107:ILE:HA	3:C:110:LEU:HD23	1.62	0.82
1:D:120:GLU:HG2	1:D:124:ARG:HD2	1.58	0.82
3:C:287:GLY:HA3	3:C:371:THR:HB	1.59	0.82
2:B:293:TRP:HE1	2:B:296:ASN:ND2	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:251:GLU:HB2	3:F:257:THR:HG22	1.61	0.82
2:E:191:GLU:O	2:E:194:ARG:HG2	1.79	0.82
3:C:166:LEU:HD12	3:C:166:LEU:N	1.95	0.82
2:E:386:LEU:H	2:E:386:LEU:HD23	1.43	0.81
3:C:288:ASP:OD2	3:C:291:ASP:HB2	1.79	0.81
3:F:240:SER:HB2	3:F:242:ILE:HG12	1.62	0.81
3:C:110:LEU:HD22	3:C:110:LEU:H	1.43	0.81
1:D:181:GLN:HE21	2:E:171:ILE:HA	1.43	0.80
3:F:166:LEU:N	3:F:166:LEU:HD12	1.95	0.80
2:E:436:VAL:HG12	2:E:445:TYR:O	1.80	0.80
2:B:315:GLU:HB3	2:B:321:LYS:HG2	1.64	0.80
1:A:186:GLU:HA	1:A:189:ILE:HD11	1.64	0.80
3:C:192:THR:HG23	3:C:386:ILE:HG23	1.61	0.80
1:D:151:GLU:HG3	1:D:173:VAL:HG13	1.63	0.79
2:B:370:HIS:CE1	2:B:402:TRP:HE1	1.99	0.79
3:C:338:LYS:H	3:C:339:CYS:HA	1.45	0.79
2:B:386:LEU:HD23	2:B:386:LEU:H	1.47	0.79
2:B:359:GLN:C	2:B:360:LEU:HD12	2.02	0.79
1:D:159:ARG:HG2	1:D:159:ARG:HH11	1.48	0.78
2:B:318:LYS:HD2	2:B:320:ASP:OD2	1.83	0.78
2:E:252:ILE:HD11	2:E:299:ILE:HG12	1.66	0.78
3:F:192:THR:HG23	3:F:386:ILE:O	1.84	0.77
2:B:180:GLN:HA	2:B:183:GLU:OE2	1.85	0.77
3:C:367:ILE:H	3:C:367:ILE:HD13	1.49	0.77
3:C:110:LEU:HD22	3:C:110:LEU:N	1.99	0.77
2:E:295:GLY:O	2:E:299:ILE:HG13	1.84	0.76
2:B:295:GLY:O	2:B:299:ILE:HG13	1.85	0.76
2:B:201:CYS:O	3:C:143:VAL:HG21	1.86	0.76
3:C:98:ALA:O	3:C:101:LEU:HG	1.85	0.76
3:C:286:ALA:O	3:C:372:TRP:HB2	1.86	0.76
3:F:338:LYS:H	3:F:339:CYS:HA	1.48	0.75
3:F:171:PRO:HA	3:F:239:GLN:HE22	1.50	0.75
2:E:309:GLU:HB3	2:E:327:GLY:HA2	1.67	0.75
2:E:415:ARG:H	2:E:434:GLY:CA	1.90	0.75
2:E:313:GLU:HA	2:E:323:LYS:HB3	1.69	0.75
2:E:406:ARG:HG3	4:N:3:ARG:HB2	1.69	0.74
2:B:389:ASP:OD2	2:B:392:LYS:HG3	1.86	0.74
1:A:149:ARG:HD3	2:B:427:ALA:O	1.88	0.74
2:E:238:VAL:HG22	2:E:239:TYR:H	1.52	0.74
2:E:270:LYS:HG3	2:E:338:TYR:OH	1.88	0.73
2:B:440:TRP:O	2:B:441:LYS:HE2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:GLU:OE1	3:C:100:ILE:HG12	1.89	0.73
2:E:414:GLY:H	2:E:435:VAL:HG23	1.54	0.73
2:E:406:ARG:N	2:E:407:CYS:HA	2.03	0.72
2:E:242:MET:SD	2:E:248:GLY:HA2	2.28	0.72
2:B:230:ASP:HB3	2:B:233:VAL:HG12	1.71	0.72
3:C:228:LEU:HG	3:C:232:LYS:HD2	1.70	0.72
2:E:343:ASN:ND2	2:E:344:LYS:HG2	2.05	0.72
3:F:166:LEU:H	3:F:166:LEU:HD12	1.52	0.72
2:E:333:ASN:ND2	2:E:335:ALA:HB3	2.04	0.72
3:C:251:GLU:HB2	3:C:257:THR:HG22	1.72	0.72
3:F:382:THR:HG22	3:F:383:THR:H	1.54	0.72
2:E:315:GLU:HB3	2:E:321:LYS:HG2	1.71	0.72
3:F:311:GLN:O	3:F:335:TRP:HA	1.90	0.71
3:C:367:ILE:HG12	3:C:379:MET:H	1.55	0.71
2:B:203:ILE:H	2:B:203:ILE:CD1	2.02	0.71
2:B:412:PRO:O	2:B:413:ASN:HB2	1.88	0.71
2:B:351:ASN:HD21	2:B:354:MET:HG2	1.55	0.71
3:F:156:ILE:HG22	3:F:161:ALA:CB	2.19	0.71
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.72	0.71
2:B:406:ARG:N	2:B:407:CYS:HA	2.04	0.71
2:B:203:ILE:N	2:B:203:ILE:HD12	2.04	0.71
3:C:214:GLY:HA3	3:C:228:LEU:O	1.90	0.71
2:B:308:THR:HG22	2:B:309:GLU:N	2.06	0.70
2:B:351:ASN:ND2	2:B:354:MET:HG2	2.07	0.70
3:F:321:LYS:HB2	3:F:337:ASN:OD1	1.90	0.70
2:E:389:ASP:OD2	2:E:392:LYS:HG3	1.90	0.70
6:B:472:MAN:H2	6:B:474:MAN:O6	1.91	0.70
3:C:132:GLU:O	3:C:136:GLN:HB2	1.92	0.70
3:F:244:TYR:HA	3:F:388:PRO:HA	1.72	0.69
2:B:424:TRP:CH2	6:B:479:SIA:H92	2.27	0.69
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.72	0.69
2:E:182:LEU:O	2:E:186:VAL:HG23	1.92	0.69
2:E:316:ASP:OD1	2:E:318:LYS:HB3	1.92	0.69
1:A:123:LYS:HZ2	2:B:151:LEU:HD13	1.56	0.69
3:C:169:ILE:O	3:C:177:GLN:HB3	1.92	0.69
3:F:276:LEU:O	3:F:276:LEU:HD23	1.92	0.69
3:F:171:PRO:HA	3:F:239:GLN:NE2	2.08	0.69
6:E:471:NAG:H3	6:E:471:NAG:H83	1.73	0.69
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.74	0.69
3:C:195:GLN:OE1	3:C:197:ARG:HG3	1.93	0.68
1:D:150:LEU:HD11	3:F:121:ILE:HG23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:GLU:HG3	2:B:194:ARG:NH2	2.08	0.68
3:F:180:VAL:HG12	3:F:228:LEU:HD11	1.75	0.68
1:A:128:GLU:HG3	1:A:129:LYS:HD3	1.74	0.68
1:A:129:LYS:O	1:A:132:HIS:ND1	2.27	0.68
3:C:145:ILE:HD12	3:C:145:ILE:O	1.94	0.68
6:E:478:GAL:H4	6:E:479:SIA:C6	2.21	0.68
2:E:238:VAL:HG22	2:E:239:TYR:N	2.08	0.68
2:E:397:GLU:HB3	2:E:431:THR:HG21	1.76	0.68
3:F:305:THR:HB	3:F:341:ALA:CB	2.24	0.68
2:E:359:GLN:C	2:E:360:LEU:HD12	2.13	0.68
3:F:192:THR:HG23	3:F:386:ILE:HG23	1.75	0.68
3:F:294:ASP:HA	3:F:301:ASP:HB3	1.76	0.68
3:F:191:TRP:CZ3	3:F:387:ILE:HB	2.29	0.68
3:C:373:LYS:HB3	3:C:377:TYR:HD2	1.58	0.67
2:E:406:ARG:CG	4:N:3:ARG:HB2	2.24	0.67
2:E:414:GLY:H	2:E:435:VAL:CG2	2.07	0.67
6:B:479:SIA:H6	6:B:479:SIA:H112	1.76	0.67
3:F:325:ASN:HD21	3:F:328:GLU:HB2	1.59	0.67
2:E:412:PRO:O	2:E:413:ASN:HB2	1.93	0.67
3:F:109:TYR:O	3:F:113:ILE:HG23	1.95	0.67
1:D:140:VAL:HG21	1:D:185:LEU:HD21	1.77	0.67
2:E:324:ALA:HB1	2:E:326:TYR:HE1	1.59	0.67
2:B:189:GLN:OE1	2:B:192:TYR:HB2	1.94	0.67
2:B:343:ASN:ND2	2:B:344:LYS:HG2	2.10	0.67
2:E:237:ARG:HD3	2:E:276:VAL:HG21	1.77	0.67
3:C:276:LEU:HB2	3:C:335:TRP:NE1	2.09	0.67
3:C:190:GLY:O	3:C:387:ILE:HD11	1.95	0.67
2:E:176:ARG:HG2	3:F:120:LYS:NZ	2.10	0.67
2:E:255:ARG:HA	2:E:291:GLU:HG2	1.77	0.66
3:C:304:PHE:O	3:C:338:LYS:HB2	1.96	0.66
2:B:277:ALA:HA	2:B:289:PRO:O	1.95	0.66
3:F:246:LEU:HD12	3:F:247:ARG:N	2.10	0.66
3:C:326:CYS:HB2	3:C:336:MET:HG3	1.77	0.66
3:F:308:ASN:HD22	3:F:308:ASN:C	1.99	0.66
2:E:228:GLN:HB2	2:E:235:PRO:HG3	1.78	0.66
3:F:338:LYS:N	3:F:339:CYS:CA	2.56	0.65
3:F:387:ILE:HG13	3:F:388:PRO:HD2	1.78	0.65
3:F:343:HIS:ND1	3:F:343:HIS:O	2.29	0.65
3:F:270:GLU:HB2	3:F:274:TYR:CZ	2.31	0.65
3:F:195:GLN:NE2	3:F:384:MET:HG3	2.11	0.65
3:C:110:LEU:CD2	3:C:110:LEU:H	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ASN:HA	2:B:299:ILE:HD12	1.78	0.65
3:F:336:MET:HB3	3:F:339:CYS:HB3	1.77	0.65
3:C:166:LEU:H	3:C:166:LEU:CD1	2.02	0.65
2:E:203:ILE:HG21	2:E:226:LEU:HD22	1.79	0.65
3:F:251:GLU:CB	3:F:257:THR:HG22	2.27	0.65
2:E:333:ASN:HD21	2:E:335:ALA:HB3	1.62	0.65
1:D:189:ILE:H	1:D:191:LYS:NZ	1.93	0.64
3:C:211:TYR:HB3	3:C:230:ASN:HD21	1.61	0.64
2:B:238:VAL:HG22	2:B:239:TYR:N	2.12	0.64
3:C:153:CYS:HB2	3:C:192:THR:HB	1.77	0.64
2:B:415:ARG:N	2:B:434:GLY:HA2	2.04	0.64
3:C:334:TRP:CH2	3:C:344:LEU:HG	2.33	0.64
3:F:324:GLY:O	3:F:326:CYS:N	2.29	0.64
1:A:128:GLU:HG3	1:A:129:LYS:CD	2.28	0.64
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.80	0.64
2:B:211:CYS:SG	2:B:250:THR:HA	2.38	0.64
2:E:380:ARG:NH2	2:E:382:ASN:HD21	1.96	0.64
1:A:186:GLU:O	1:A:189:ILE:HG12	1.97	0.64
3:F:192:THR:O	3:F:386:ILE:HG22	1.98	0.64
3:F:153:CYS:SG	3:F:192:THR:HB	2.37	0.64
3:F:107:ILE:HB	3:F:108:ARG:HH12	1.63	0.63
2:E:310:LEU:HD12	2:E:453:LYS:O	1.97	0.63
1:D:123:LYS:HD3	2:E:151:LEU:N	2.13	0.63
3:C:356:LYS:HG3	3:C:362:GLY:O	1.98	0.63
3:C:174:ALA:HB2	3:C:235:LEU:CD2	2.25	0.63
1:A:189:ILE:HG22	1:A:190:ALA:N	2.12	0.63
3:C:392:LEU:HD13	3:C:397:GLY:HA2	1.81	0.63
2:E:454:ILE:HD12	2:E:454:ILE:C	2.19	0.63
1:D:169:LEU:HD12	1:D:171:ARG:HG2	1.80	0.63
3:C:346:GLY:HA3	3:C:366:GLY:H	1.64	0.62
2:B:252:ILE:HD12	2:B:294:LEU:HB3	1.80	0.62
2:E:318:LYS:HD2	2:E:320:ASP:OD2	1.99	0.62
2:B:314:MET:HA	2:B:449:LYS:O	1.99	0.62
1:D:140:VAL:CG2	1:D:185:LEU:HD21	2.29	0.62
3:F:170:LYS:HE3	3:F:175:ASN:HA	1.82	0.62
2:E:421:GLN:HG3	2:E:422:TYR:N	2.14	0.62
2:E:415:ARG:HH12	2:E:428:LYS:HB2	1.64	0.62
3:C:382:THR:HG22	3:C:383:THR:N	2.15	0.62
2:B:386:LEU:HD23	2:B:386:LEU:N	2.13	0.62
2:E:213:GLU:O	2:E:217:LYS:HG3	1.99	0.62
3:F:234:HIS:HA	3:F:267:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:PHE:CD2	3:C:232:LYS:HD3	2.35	0.61
3:C:166:LEU:HD11	3:C:220:PRO:HG3	1.81	0.61
2:B:172:LEU:HD22	3:C:113:ILE:HG13	1.79	0.61
2:B:265:LYS:HB3	2:B:379:ASP:OD2	2.00	0.61
2:B:415:ARG:HH11	2:B:415:ARG:HG3	1.64	0.61
2:E:351:ASN:ND2	2:E:354:MET:HG2	2.15	0.61
2:B:345:TYR:O	2:B:346:ARG:HG3	2.00	0.61
3:C:263:ALA:O	3:C:278:TYR:HB2	2.00	0.61
3:C:270:GLU:HB2	3:C:274:TYR:OH	2.00	0.61
3:F:143:VAL:HA	3:F:220:PRO:HG2	1.83	0.61
2:B:296:ASN:HD22	2:B:299:ILE:HD12	1.66	0.61
3:C:258:SER:HA	3:C:285:ASP:OD1	2.00	0.61
3:F:205:LYS:HG2	3:F:331:GLY:O	2.01	0.61
2:B:191:GLU:O	2:B:194:ARG:HG2	2.00	0.61
3:C:265:PHE:O	3:C:266:LYS:HB3	2.00	0.61
3:F:156:ILE:HG22	3:F:161:ALA:HB2	1.82	0.61
3:C:323:GLU:HG2	3:C:324:GLY:H	1.65	0.61
2:E:246:ASN:HB3	2:E:455:ARG:HH12	1.66	0.61
2:E:163:THR:O	2:E:167:VAL:HG23	2.00	0.61
3:F:368:ILE:HG13	3:F:368:ILE:O	1.99	0.61
3:C:344:LEU:CA	3:C:367:ILE:HG22	2.31	0.60
3:C:149:THR:HG23	3:C:168:PHE:C	2.22	0.60
3:C:143:VAL:HA	3:C:220:PRO:HG2	1.83	0.60
1:A:148:LYS:HZ2	1:A:182:GLN:HE22	1.49	0.60
1:D:181:GLN:HE22	2:E:174:ASN:HB3	1.64	0.60
3:F:197:ARG:HG3	3:F:382:THR:HB	1.83	0.60
3:F:264:MET:HG2	3:F:264:MET:O	2.01	0.60
3:F:156:ILE:O	3:F:161:ALA:HB3	2.01	0.60
2:B:237:ARG:HD3	2:B:276:VAL:HG21	1.81	0.60
3:C:305:THR:HG23	3:C:338:LYS:HD2	1.84	0.60
3:F:196:LYS:CD	3:F:383:THR:HB	2.28	0.60
1:D:185:LEU:HD23	2:E:171:ILE:HD13	1.84	0.60
3:F:154:GLN:HB2	3:F:387:ILE:HD11	1.83	0.60
2:E:158:ASN:O	2:E:162:PRO:HG2	2.02	0.60
2:E:393:GLN:O	2:E:397:GLU:HG2	2.00	0.59
1:D:166:SER:HB3	2:E:195:THR:O	2.01	0.59
2:E:175:LEU:O	2:E:179:ILE:HG13	2.03	0.59
4:M:2:HIS:O	4:M:3:ARG:HD3	2.03	0.59
2:B:377:THR:C	2:B:379:ASP:H	2.04	0.59
3:F:305:THR:CB	3:F:341:ALA:HB2	2.30	0.59
3:C:323:GLU:HG2	3:C:324:GLY:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:SER:HB3	2:B:195:THR:O	2.03	0.59
2:E:340:ILE:HG23	2:E:340:ILE:O	2.02	0.59
2:E:326:TYR:HA	2:E:344:LYS:O	2.03	0.59
1:D:140:VAL:HG11	2:E:168:LEU:HD22	1.84	0.59
2:B:357:ALA:HB3	2:B:360:LEU:HD13	1.84	0.59
2:B:385:TRP:CH2	2:B:392:LYS:HB3	2.38	0.59
2:B:345:TYR:CG	2:B:346:ARG:N	2.71	0.59
3:F:252:ASP:HB3	3:F:373:LYS:NZ	2.18	0.59
3:F:108:ARG:HH11	3:F:108:ARG:H	1.50	0.59
1:A:126:VAL:HG22	2:B:154:ASP:HA	1.84	0.59
2:E:421:GLN:HG3	2:E:422:TYR:H	1.67	0.59
1:D:147:MET:CE	2:E:179:ILE:HD11	2.33	0.59
2:B:293:TRP:NE1	2:B:296:ASN:ND2	2.48	0.59
3:C:234:HIS:HA	3:C:267:VAL:HG23	1.85	0.59
2:B:300:SER:HA	2:B:331:VAL:CG2	2.31	0.58
1:D:169:LEU:N	2:E:189:GLN:HE22	1.96	0.58
1:A:171:ARG:NH1	1:A:173:VAL:HG22	2.18	0.58
1:A:127:ILE:O	1:A:130:VAL:HG22	2.04	0.58
2:E:177:SER:O	2:E:180:GLN:HG3	2.02	0.58
2:B:380:ARG:HH11	2:B:380:ARG:HG2	1.68	0.58
3:C:193:VAL:HG12	3:C:385:LYS:HG2	1.85	0.58
3:C:149:THR:HG23	3:C:168:PHE:O	2.04	0.58
3:F:246:LEU:HD12	3:F:247:ARG:H	1.69	0.58
3:C:342:GLY:HA2	3:C:368:ILE:HD12	1.85	0.58
3:C:197:ARG:O	3:C:381:LYS:HA	2.03	0.58
2:E:199:VAL:O	3:F:141:ASP:HA	2.04	0.58
2:E:304:ARG:HD3	2:E:332:GLN:NE2	2.19	0.58
2:E:357:ALA:HB3	2:E:360:LEU:HD13	1.85	0.58
2:B:310:LEU:HD12	2:B:311:LEU:H	1.68	0.58
3:C:338:LYS:HG2	3:C:338:LYS:O	2.04	0.58
1:A:123:LYS:NZ	2:B:151:LEU:HD13	2.19	0.58
2:B:300:SER:CA	2:B:331:VAL:HG23	2.28	0.58
1:A:159:ARG:HG2	1:A:159:ARG:HH11	1.68	0.58
2:B:255:ARG:HE	2:B:435:VAL:HG21	1.69	0.57
3:C:198:LEU:O	3:C:199:ASP:C	2.43	0.57
1:D:147:MET:HE1	2:E:179:ILE:HD11	1.87	0.57
3:C:191:TRP:CZ3	3:C:387:ILE:HB	2.38	0.57
2:B:199:VAL:O	3:C:141:ASP:HA	2.03	0.57
2:B:354:MET:HA	2:B:369:ILE:HG23	1.86	0.57
3:C:276:LEU:HB2	3:C:335:TRP:CE2	2.40	0.57
3:F:365:ASN:C	3:F:365:ASN:HD22	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:263:ALA:O	3:F:278:TYR:HB2	2.03	0.57
1:A:123:LYS:HZ2	2:B:151:LEU:CB	2.12	0.57
3:C:334:TRP:CD1	3:C:335:TRP:N	2.71	0.57
2:E:215:ILE:HG23	2:E:216:ARG:N	2.20	0.57
2:E:351:ASN:HD21	2:E:354:MET:HG2	1.70	0.57
2:B:256:GLN:N	2:B:291:GLU:OE2	2.36	0.57
3:C:246:LEU:O	3:C:261:ASP:HA	2.04	0.56
1:D:186:GLU:O	1:D:189:ILE:HG12	2.05	0.56
2:B:265:LYS:O	2:B:377:THR:HG21	2.05	0.56
3:F:249:GLU:HB3	3:F:383:THR:CG2	2.34	0.56
2:B:172:LEU:HD13	3:C:113:ILE:HD11	1.88	0.56
2:E:310:LEU:HD21	2:E:312:ILE:HD11	1.87	0.56
2:E:301:GLN:O	2:E:305:MET:HG3	2.05	0.56
3:C:344:LEU:C	3:C:367:ILE:HG22	2.26	0.56
2:E:420:GLY:O	2:E:445:TYR:HA	2.06	0.56
2:E:236:TYR:CE2	2:E:294:LEU:HD21	2.41	0.56
3:F:114:TYR:O	3:F:117:ASN:HB2	2.06	0.56
3:F:338:LYS:CG	3:F:338:LYS:O	2.54	0.56
1:D:159:ARG:HG2	1:D:159:ARG:NH1	2.17	0.56
3:F:197:ARG:O	3:F:381:LYS:HA	2.05	0.56
2:E:161:ILE:HB	2:E:162:PRO:HD3	1.88	0.56
3:C:246:LEU:HD12	3:C:247:ARG:N	2.21	0.56
1:D:164:SER:O	2:E:196:PRO:HA	2.05	0.56
3:F:103:HIS:HD2	3:F:104:ASP:H	1.54	0.56
2:B:331:VAL:O	2:B:331:VAL:HG23	2.06	0.55
2:B:293:TRP:HE1	2:B:296:ASN:HD21	1.51	0.55
2:B:310:LEU:HD12	2:B:311:LEU:N	2.21	0.55
3:F:300:SER:HB3	3:F:304:PHE:HD2	1.71	0.55
3:F:338:LYS:HG2	3:F:338:LYS:O	2.06	0.55
2:E:310:LEU:CD2	2:E:312:ILE:HD11	2.37	0.55
2:B:408:HIS:CE1	4:M:1:GLY:H3	2.24	0.55
3:C:160:GLY:O	3:C:161:ALA:O	2.23	0.55
2:B:210:GLU:OE1	2:B:456:PRO:HG3	2.06	0.55
2:B:230:ASP:HB3	2:B:233:VAL:CG1	2.35	0.55
3:F:325:ASN:ND2	3:F:328:GLU:HB2	2.21	0.55
1:D:125:LYS:O	1:D:129:LYS:HG2	2.07	0.55
3:C:240:SER:HB2	3:C:242:ILE:HG12	1.87	0.55
3:F:348:TYR:HA	3:F:367:ILE:HD11	1.88	0.55
3:C:334:TRP:CD2	3:C:343:HIS:HB2	2.41	0.55
2:B:385:TRP:CZ2	2:B:392:LYS:HB3	2.41	0.55
3:F:367:ILE:HG12	3:F:379:MET:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:THR:HB	2:B:454:ILE:HG13	1.87	0.55
3:C:297:ASP:O	3:C:298:ASP:HB2	2.05	0.55
3:C:318:ASP:OD1	3:C:325:ASN:HA	2.07	0.55
3:F:246:LEU:O	3:F:261:ASP:HA	2.07	0.55
2:E:373:MET:HG3	2:E:405:ASN:HB2	1.88	0.55
3:F:174:ALA:HB2	3:F:235:LEU:HD22	1.88	0.55
1:D:127:ILE:O	1:D:130:VAL:HG22	2.06	0.55
3:C:225:GLU:O	3:C:226:PHE:HB3	2.06	0.55
2:B:177:SER:O	2:B:180:GLN:HG3	2.07	0.55
3:C:100:ILE:O	3:C:102:THR:N	2.40	0.55
2:E:370:HIS:O	2:E:373:MET:HG2	2.06	0.55
2:B:212:GLU:O	2:B:215:ILE:HG22	2.06	0.55
3:C:205:LYS:HG2	3:C:331:GLY:O	2.06	0.55
1:A:133:ILE:HG23	3:C:107:ILE:HD11	1.88	0.55
2:E:217:LYS:HD3	3:F:213:GLU:HG3	1.88	0.55
3:F:270:GLU:HB2	3:F:274:TYR:OH	2.06	0.55
3:F:252:ASP:HB3	3:F:373:LYS:HZ1	1.72	0.54
3:F:253:TRP:CD1	3:F:352:GLY:HA3	2.42	0.54
2:E:252:ILE:HD11	2:E:299:ILE:CG1	2.36	0.54
3:C:211:TYR:HB3	3:C:230:ASN:ND2	2.23	0.54
2:E:230:ASP:HB3	2:E:233:VAL:HG12	1.87	0.54
3:C:270:GLU:HB2	3:C:274:TYR:CZ	2.43	0.54
2:B:252:ILE:CD1	2:B:294:LEU:HB3	2.37	0.54
3:C:390:ASN:HD22	3:C:391:ARG:N	2.05	0.54
3:F:207:ASN:HB2	3:F:316:ASP:OD2	2.05	0.54
2:B:326:TYR:C	2:B:328:GLY:H	2.10	0.54
2:E:250:THR:HB	2:E:454:ILE:HG13	1.89	0.54
3:F:169:ILE:O	3:F:177:GLN:HB3	2.07	0.54
3:F:334:TRP:CD2	3:F:343:HIS:HB2	2.43	0.54
2:E:345:TYR:CG	2:E:346:ARG:N	2.75	0.54
3:F:198:LEU:H	3:F:225:GLU:CG	2.20	0.54
3:F:262:TYR:HD2	3:F:278:TYR:CE1	2.25	0.54
2:E:402:TRP:CG	2:E:403:TRP:N	2.76	0.54
1:D:126:VAL:HG22	2:E:154:ASP:HA	1.88	0.54
1:A:148:LYS:NZ	1:A:182:GLN:HE22	2.06	0.54
2:E:340:ILE:HG12	2:E:342:VAL:HG13	1.90	0.54
1:A:147:MET:HE1	2:B:179:ILE:HD11	1.89	0.54
2:B:203:ILE:HB	3:C:179:LEU:HD22	1.90	0.54
3:F:117:ASN:O	3:F:121:ILE:HG13	2.08	0.54
2:B:360:LEU:HB2	2:B:365:ARG:HB2	1.89	0.54
3:C:184:ILE:HG23	3:C:189:ASN:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:OE2	1:A:125:LYS:HE3	2.08	0.53
2:E:435:VAL:O	2:E:446:SER:HA	2.07	0.53
2:E:405:ASN:O	2:E:405:ASN:CG	2.43	0.53
2:B:300:SER:HB2	2:B:331:VAL:O	2.09	0.53
3:C:200:GLY:HA2	3:C:225:GLU:OE2	2.07	0.53
2:E:346:ARG:O	2:E:347:GLY:O	2.27	0.53
3:C:387:ILE:HG13	3:C:388:PRO:HD2	1.89	0.53
3:F:205:LYS:HE2	3:F:331:GLY:HA2	1.90	0.53
2:E:438:MET:HG3	2:E:443:SER:N	2.23	0.53
2:E:412:PRO:O	2:E:413:ASN:CB	2.57	0.53
3:F:197:ARG:HB2	3:F:382:THR:OG1	2.08	0.53
3:C:101:LEU:O	3:C:104:ASP:OD1	2.26	0.53
3:C:252:ASP:OD1	3:C:254:ASN:HB3	2.09	0.53
3:C:251:GLU:CB	3:C:257:THR:HG22	2.39	0.53
1:A:184:GLN:O	1:A:188:VAL:HG22	2.09	0.53
3:F:382:THR:HG22	3:F:383:THR:N	2.21	0.53
1:D:169:LEU:C	1:D:169:LEU:HD13	2.28	0.53
2:E:431:THR:OG1	2:E:432:ASP:N	2.39	0.53
3:C:314:THR:OG1	3:C:317:ASN:HB2	2.09	0.53
3:F:294:ASP:HA	3:F:301:ASP:CB	2.38	0.53
4:N:5:TYR:CD1	4:N:5:TYR:N	2.77	0.53
3:F:305:THR:HG23	3:F:338:LYS:HD2	1.90	0.53
1:A:123:LYS:HZ3	2:B:151:LEU:HB3	1.69	0.53
2:B:309:GLU:CB	2:B:327:GLY:HA2	2.32	0.53
2:E:224:MET:O	2:E:224:MET:HG3	2.09	0.53
3:F:325:ASN:CG	3:F:325:ASN:O	2.47	0.53
2:E:236:TYR:HE2	2:E:294:LEU:HD21	1.74	0.53
3:F:192:THR:CG2	3:F:386:ILE:O	2.55	0.53
2:E:354:MET:HA	2:E:369:ILE:HG23	1.91	0.53
2:B:378:TYR:N	2:B:395:SER:OG	2.41	0.52
2:E:172:LEU:CD2	3:F:114:TYR:HB2	2.40	0.52
3:F:314:THR:O	3:F:316:ASP:N	2.42	0.52
3:C:298:ASP:C	3:C:300:SER:H	2.12	0.52
2:B:176:ARG:HG3	2:B:176:ARG:HH11	1.73	0.52
3:C:113:ILE:HG13	3:C:114:TYR:N	2.23	0.52
3:C:353:THR:HG1	3:C:377:TYR:HD1	1.57	0.52
2:E:176:ARG:HH22	3:F:113:ILE:HG22	1.73	0.52
2:E:436:VAL:HG12	2:E:445:TYR:C	2.30	0.52
3:C:166:LEU:HD11	3:C:220:PRO:CG	2.38	0.52
3:F:116:SER:O	3:F:120:LYS:HG3	2.09	0.52
2:B:414:GLY:H	2:B:435:VAL:HG23	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:CG2	1:A:185:LEU:HD21	2.40	0.52
3:C:365:ASN:N	3:C:365:ASN:HD22	2.07	0.52
3:F:214:GLY:HA3	3:F:228:LEU:O	2.10	0.52
2:E:226:LEU:HD12	2:E:236:TYR:O	2.10	0.52
1:A:119:ILE:O	1:A:119:ILE:HG22	2.09	0.52
3:C:195:GLN:HA	3:C:226:PHE:O	2.10	0.52
2:B:360:LEU:N	2:B:360:LEU:HD12	2.25	0.52
3:C:205:LYS:HE2	3:C:331:GLY:HA3	1.92	0.52
3:F:204:PHE:HB3	3:F:211:TYR:OH	2.09	0.52
1:A:126:VAL:HG21	2:B:153:ILE:HG12	1.92	0.52
3:F:224:THR:HG23	3:F:224:THR:O	2.08	0.52
2:E:308:THR:HG22	2:E:309:GLU:N	2.25	0.51
2:E:311:LEU:HG	2:E:453:LYS:HD3	1.92	0.51
2:E:345:TYR:O	2:E:346:ARG:HG3	2.10	0.51
2:E:357:ALA:O	2:E:365:ARG:HG3	2.10	0.51
3:F:252:ASP:OD1	3:F:254:ASN:HB3	2.10	0.51
3:F:207:ASN:OD1	3:F:210:GLN:HG3	2.10	0.51
3:C:166:LEU:CD1	3:C:220:PRO:HG3	2.40	0.51
1:A:123:LYS:HZ2	2:B:151:LEU:CD1	2.22	0.51
3:C:344:LEU:HA	3:C:367:ILE:HA	1.91	0.51
2:E:413:ASN:N	2:E:435:VAL:HG22	2.25	0.51
3:F:334:TRP:CG	3:F:343:HIS:HB2	2.45	0.51
3:F:300:SER:O	3:F:302:LYS:N	2.43	0.51
2:E:211:CYS:SG	2:E:250:THR:HA	2.51	0.51
3:C:252:ASP:C	3:C:254:ASN:H	2.14	0.51
3:F:288:ASP:CG	3:F:291:ASP:HB2	2.30	0.51
1:A:132:HIS:HD1	1:A:132:HIS:H	1.59	0.51
2:E:203:ILE:HD12	2:E:203:ILE:N	2.15	0.51
3:F:292:GLY:O	3:F:302:LYS:HA	2.10	0.51
2:B:308:THR:CG2	2:B:309:GLU:N	2.74	0.51
1:A:126:VAL:HG22	2:B:154:ASP:CA	2.40	0.51
3:F:334:TRP:HE3	3:F:345:ASN:ND2	2.09	0.51
2:E:386:LEU:H	2:E:386:LEU:CD2	2.20	0.51
3:F:166:LEU:HD11	3:F:220:PRO:HG3	1.92	0.51
3:C:264:MET:CE	3:C:266:LYS:NZ	2.74	0.51
2:E:308:THR:HG22	2:E:309:GLU:H	1.76	0.50
2:E:326:TYR:C	2:E:328:GLY:H	2.13	0.50
1:D:184:GLN:O	1:D:188:VAL:HG22	2.11	0.50
3:C:202:VAL:HG11	3:C:225:GLU:HB3	1.93	0.50
3:F:211:TYR:HB3	3:F:230:ASN:HD21	1.75	0.50
2:B:340:ILE:HG23	2:B:340:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:ARG:NH1	2:B:415:ARG:HG3	2.25	0.50
2:B:348:THR:O	2:B:349:ALA:HB2	2.12	0.50
2:E:228:GLN:HE22	3:F:177:GLN:NE2	1.98	0.50
2:E:385:TRP:CE3	4:N:3:ARG:HG3	2.47	0.50
1:A:148:LYS:HZ2	1:A:179:GLU:HG3	1.77	0.50
3:C:184:ILE:HG22	3:C:186:GLY:H	1.76	0.50
3:F:149:THR:HA	3:F:168:PHE:O	2.11	0.50
6:E:471:NAG:C8	6:E:471:NAG:H3	2.41	0.50
1:D:158:ILE:O	1:D:161:CYS:HB2	2.12	0.50
1:D:154:ILE:HD11	3:F:124:LEU:HD21	1.94	0.50
2:E:224:MET:HB2	2:E:238:VAL:O	2.11	0.50
2:B:254:ASN:O	2:B:291:GLU:HA	2.12	0.50
3:C:174:ALA:CB	3:C:235:LEU:HD13	2.41	0.50
3:C:258:SER:HB2	3:C:286:ALA:HB2	1.93	0.50
3:F:132:GLU:O	3:F:136:GLN:HB2	2.11	0.50
3:F:359:THR:HG21	3:F:363:TYR:O	2.12	0.50
3:F:334:TRP:CE3	3:F:345:ASN:ND2	2.79	0.50
3:F:108:ARG:HH11	3:F:108:ARG:N	2.09	0.50
3:F:320:ASP:OD2	3:F:322:PHE:O	2.29	0.50
3:C:325:ASN:ND2	3:C:328:GLU:HB2	2.20	0.50
2:E:176:ARG:HH22	3:F:113:ILE:CG2	2.25	0.50
3:C:392:LEU:O	3:C:395:GLY:N	2.44	0.50
2:E:377:THR:C	2:E:379:ASP:H	2.14	0.50
3:F:367:ILE:HD13	3:F:367:ILE:N	2.21	0.49
2:E:253:GLN:NE2	2:E:452:MET:HG3	2.27	0.49
2:E:360:LEU:HD23	2:E:364:ASN:HB3	1.93	0.49
1:A:181:GLN:HE22	2:B:174:ASN:HB3	1.77	0.49
3:C:154:GLN:O	3:C:158:ASN:HB2	2.12	0.49
3:C:289:ALA:HB3	3:C:369:TRP:CE2	2.48	0.49
2:B:384:GLY:H	2:B:405:ASN:HA	1.77	0.49
3:C:367:ILE:CG1	3:C:379:MET:H	2.25	0.49
3:C:204:PHE:O	3:C:206:LYS:N	2.40	0.49
2:E:418:TRP:HD1	2:E:419:GLY:H	1.60	0.49
2:E:380:ARG:HH11	2:E:380:ARG:HG2	1.78	0.49
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.13	0.49
2:B:436:VAL:HG12	2:B:446:SER:HA	1.94	0.49
3:F:346:GLY:HA3	3:F:366:GLY:HA2	1.95	0.49
2:E:203:ILE:CD1	2:E:203:ILE:H	2.11	0.49
3:C:196:LYS:HD2	3:C:382:THR:O	2.13	0.49
3:C:344:LEU:O	3:C:344:LEU:HD12	2.13	0.49
3:C:193:VAL:HA	3:C:385:LYS:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:PRO:O	2:B:413:ASN:CB	2.57	0.49
3:C:365:ASN:N	3:C:365:ASN:ND2	2.60	0.49
1:D:160:SER:OG	2:E:261:ASP:HB2	2.13	0.49
2:E:385:TRP:CZ3	4:N:3:ARG:HG3	2.47	0.49
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.31	0.49
3:F:300:SER:HB3	3:F:304:PHE:CD2	2.48	0.49
2:B:422:TYR:O	2:B:444:TRP:HB3	2.13	0.49
3:F:166:LEU:CD1	3:F:166:LEU:N	2.68	0.49
2:E:411:ASN:O	2:E:435:VAL:HA	2.13	0.49
3:C:117:ASN:N	3:C:117:ASN:HD22	2.09	0.49
2:B:205:VAL:HG22	3:C:218:LEU:HD11	1.94	0.49
2:B:411:ASN:O	2:B:435:VAL:HA	2.13	0.49
2:B:418:TRP:O	2:B:420:GLY:N	2.42	0.49
1:A:183:LYS:O	1:A:187:GLN:HB2	2.12	0.49
3:F:166:LEU:HD11	3:F:220:PRO:CA	2.43	0.48
3:C:251:GLU:HG2	3:C:252:ASP:N	2.27	0.48
2:B:192:TYR:C	2:B:194:ARG:H	2.15	0.48
3:C:346:GLY:HA3	3:C:366:GLY:N	2.28	0.48
3:C:322:PHE:CD2	3:C:323:GLU:N	2.81	0.48
2:E:437:TRP:O	2:E:439:ASN:N	2.42	0.48
3:F:228:LEU:CG	3:F:232:LYS:HD2	2.15	0.48
3:F:366:GLY:O	3:F:368:ILE:HG23	2.13	0.48
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.95	0.48
3:C:249:GLU:HB3	3:C:383:THR:CG2	2.43	0.48
3:C:325:ASN:HD21	3:C:328:GLU:CB	2.20	0.48
2:E:164:ASN:HD22	2:E:164:ASN:N	2.10	0.48
3:F:146:HIS:HB2	3:F:167:TYR:CD2	2.48	0.48
3:C:166:LEU:HD11	3:C:220:PRO:CA	2.42	0.48
1:A:156:ILE:HD13	2:B:415:ARG:HB3	1.96	0.48
2:E:398:ASP:HA	2:E:433:ASP:CB	2.27	0.48
3:F:172:LEU:H	3:F:239:GLN:HE21	1.61	0.48
3:C:275:ARG:HA	3:C:311:GLN:HA	1.94	0.48
3:F:231:GLU:O	3:F:234:HIS:HB3	2.13	0.48
1:D:157:LYS:HE3	3:F:132:GLU:CD	2.33	0.48
2:B:249:TRP:HB3	2:B:453:LYS:HB2	1.96	0.48
3:F:275:ARG:HG3	3:F:310:MET:O	2.13	0.48
2:E:300:SER:OG	2:E:301:GLN:N	2.47	0.48
2:E:252:ILE:HD11	2:E:299:ILE:CD1	2.43	0.48
2:E:252:ILE:CD1	2:E:299:ILE:HG12	2.41	0.48
3:F:251:GLU:CG	3:F:257:THR:HG22	2.43	0.48
2:E:212:GLU:O	2:E:215:ILE:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:315:GLU:HB3	2:E:321:LYS:CG	2.39	0.48
3:C:304:PHE:O	3:C:338:LYS:CB	2.62	0.48
3:C:265:PHE:O	3:C:266:LYS:CB	2.62	0.48
2:E:157:VAL:HG13	2:E:161:ILE:HD12	1.96	0.48
3:F:145:ILE:HD12	3:F:145:ILE:O	2.14	0.48
2:B:377:THR:C	2:B:379:ASP:N	2.66	0.48
3:F:203:ASP:OD2	3:F:204:PHE:N	2.46	0.48
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.95	0.48
2:E:238:VAL:CG2	2:E:239:TYR:N	2.77	0.48
3:F:191:TRP:CG	3:F:385:LYS:HD3	2.48	0.48
2:B:238:VAL:CG2	2:B:239:TYR:N	2.76	0.48
1:A:144:LEU:HD23	2:B:175:LEU:HD11	1.94	0.48
1:A:164:SER:O	2:B:196:PRO:HA	2.14	0.48
3:C:197:ARG:HH11	3:C:367:ILE:HG23	1.78	0.48
2:E:215:ILE:HB	2:E:242:MET:CE	2.43	0.48
2:E:381:ASP:HB2	2:E:393:GLN:NE2	2.29	0.47
3:F:326:CYS:O	3:F:330:ASP:N	2.46	0.47
2:E:311:LEU:HB3	2:E:453:LYS:HG2	1.95	0.47
3:C:181:TYR:O	3:C:193:VAL:HG22	2.14	0.47
2:E:380:ARG:CZ	2:E:380:ARG:HB3	2.44	0.47
2:B:437:TRP:CD1	2:B:439:ASN:HB2	2.49	0.47
3:F:250:LEU:HD13	3:F:379:MET:HE3	1.96	0.47
2:E:309:GLU:CB	2:E:327:GLY:HA2	2.40	0.47
3:C:200:GLY:CA	3:C:225:GLU:OE2	2.62	0.47
3:C:224:THR:O	3:C:226:PHE:HD2	1.98	0.47
2:B:253:GLN:NE2	2:B:452:MET:HG3	2.29	0.47
3:C:153:CYS:CB	3:C:192:THR:HB	2.43	0.47
2:E:291:GLU:O	2:E:292:TYR:HB3	2.15	0.47
3:F:169:ILE:HD12	3:F:171:PRO:HD3	1.95	0.47
2:E:434:GLY:O	2:E:436:VAL:HG22	2.15	0.47
3:C:166:LEU:HD11	3:C:220:PRO:N	2.29	0.47
3:F:149:THR:HG23	3:F:168:PHE:O	2.14	0.47
2:B:377:THR:O	2:B:379:ASP:N	2.48	0.47
3:F:258:SER:OG	3:F:286:ALA:HB2	2.14	0.47
3:F:347:VAL:HG12	3:F:348:TYR:N	2.29	0.47
3:C:114:TYR:C	3:C:114:TYR:CD1	2.88	0.47
1:D:169:LEU:CD1	1:D:171:ARG:HG2	2.45	0.47
2:B:402:TRP:CH2	2:B:412:PRO:HG2	2.49	0.47
2:B:406:ARG:HG2	4:M:3:ARG:HB2	1.97	0.47
2:B:424:TRP:HA	2:B:444:TRP:CH2	2.50	0.47
2:E:228:GLN:NE2	3:F:177:GLN:HE22	2.00	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:O	1:D:185:LEU:HD13	2.15	0.47
2:B:360:LEU:CB	2:B:365:ARG:HB2	2.45	0.47
3:C:294:ASP:HA	3:C:301:ASP:CB	2.45	0.47
3:F:171:PRO:CA	3:F:239:GLN:NE2	2.76	0.47
2:E:238:VAL:CG2	2:E:239:TYR:H	2.25	0.47
3:F:261:ASP:HB2	3:F:282:ALA:HB3	1.96	0.47
1:D:123:LYS:O	1:D:126:VAL:HG23	2.14	0.47
3:C:365:ASN:H	3:C:365:ASN:HD22	1.62	0.47
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.12	0.47
3:C:234:HIS:O	3:C:236:ILE:N	2.48	0.47
2:B:348:THR:OG1	2:B:348:THR:O	2.28	0.47
2:B:437:TRP:HD1	2:B:439:ASN:HB2	1.79	0.47
3:F:184:ILE:HG22	3:F:186:GLY:H	1.80	0.47
3:C:248:VAL:HG12	3:C:250:LEU:HD21	1.96	0.47
3:F:248:VAL:HB	3:F:260:ALA:HB3	1.97	0.47
3:C:264:MET:O	3:C:266:LYS:HG2	2.14	0.46
3:F:373:LYS:HB3	3:F:377:TYR:HD2	1.80	0.46
3:F:375:ARG:HD2	3:F:376:TRP:CZ3	2.50	0.46
3:C:151:LYS:HD2	3:C:172:LEU:HD21	1.96	0.46
2:B:200:SER:CB	3:C:142:THR:HG1	2.28	0.46
2:B:313:GLU:HA	2:B:323:LYS:HB3	1.95	0.46
2:B:414:GLY:H	2:B:435:VAL:CG2	2.28	0.46
1:A:147:MET:CE	2:B:179:ILE:HD11	2.44	0.46
2:B:428:LYS:HE3	2:B:429:HIS:CD2	2.50	0.46
3:C:276:LEU:C	3:C:276:LEU:HD23	2.35	0.46
2:E:191:GLU:HG3	2:E:194:ARG:CZ	2.45	0.46
2:B:315:GLU:HB3	2:B:321:LYS:CG	2.40	0.46
1:A:161:CYS:HB3	1:A:165:CYS:HB2	1.58	0.46
3:C:161:ALA:O	3:C:162:LYS:HD3	2.15	0.46
2:E:438:MET:SD	2:E:443:SER:HB3	2.54	0.46
2:E:437:TRP:CD1	2:E:439:ASN:HB2	2.50	0.46
3:F:186:GLY:C	3:F:188:GLY:H	2.19	0.46
3:C:238:THR:O	3:C:239:GLN:C	2.53	0.46
3:F:270:GLU:O	3:F:270:GLU:HG2	2.15	0.46
2:B:238:VAL:HG22	2:B:239:TYR:H	1.79	0.46
3:C:392:LEU:O	3:C:393:THR:C	2.52	0.46
1:A:126:VAL:CG2	2:B:154:ASP:HA	2.45	0.46
1:D:159:ARG:NH1	1:D:159:ARG:CG	2.78	0.46
2:E:215:ILE:C	2:E:217:LYS:H	2.19	0.46
3:F:387:ILE:HG23	3:F:388:PRO:O	2.16	0.46
3:C:203:ASP:HB3	3:C:206:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:234:LYS:NZ	3:F:145:ILE:HD11	2.30	0.46
2:B:172:LEU:HD22	3:C:113:ILE:CG1	2.45	0.46
1:D:140:VAL:O	1:D:143:GLN:HB3	2.15	0.46
1:D:147:MET:HG2	2:E:175:LEU:HD22	1.98	0.46
3:F:154:GLN:HB2	3:F:387:ILE:CD1	2.46	0.46
1:D:169:LEU:HD13	1:D:170:ALA:N	2.30	0.46
3:C:143:VAL:O	3:C:143:VAL:HG23	2.15	0.46
1:A:132:HIS:HB2	3:C:107:ILE:HD13	1.98	0.46
2:E:454:ILE:O	2:E:455:ARG:HB2	2.16	0.46
3:F:191:TRP:CE3	3:F:385:LYS:HB3	2.51	0.46
3:C:373:LYS:HZ3	3:C:377:TYR:HE2	1.64	0.46
3:C:390:ASN:ND2	3:C:391:ARG:N	2.63	0.46
2:E:377:THR:HA	2:E:395:SER:OG	2.16	0.46
2:B:397:GLU:HB3	2:B:431:THR:HG21	1.97	0.46
2:B:332:GLN:NE2	2:B:332:GLN:HA	2.31	0.46
3:C:262:TYR:CZ	3:C:290:PHE:HD1	2.34	0.46
3:F:166:LEU:CD1	3:F:220:PRO:HG3	2.46	0.46
2:E:239:TYR:OH	2:E:287:GLY:O	2.30	0.46
2:B:445:TYR:HD1	2:B:447:MET:HE2	1.81	0.46
2:E:428:LYS:HE3	2:E:429:HIS:CD2	2.51	0.46
2:E:172:LEU:HD22	3:F:114:TYR:HB2	1.98	0.46
1:D:166:SER:CB	2:E:195:THR:O	2.64	0.46
3:F:243:PRO:HB2	3:F:389:PHE:CB	2.46	0.46
3:F:344:LEU:CB	3:F:367:ILE:HG22	2.46	0.45
1:D:161:CYS:O	1:D:165:CYS:HB2	2.16	0.45
3:C:196:LYS:HD2	3:C:383:THR:HB	1.99	0.45
3:C:326:CYS:SG	3:C:336:MET:HB3	2.56	0.45
3:F:252:ASP:C	3:F:254:ASN:H	2.19	0.45
3:F:265:PHE:O	3:F:266:LYS:HB3	2.16	0.45
2:E:252:ILE:HG13	2:E:252:ILE:O	2.16	0.45
2:B:375:PHE:CE2	2:B:402:TRP:N	2.84	0.45
3:F:343:HIS:CG	3:F:343:HIS:O	2.68	0.45
1:A:154:ILE:HD12	2:B:182:LEU:HD13	1.96	0.45
3:F:197:ARG:HA	3:F:225:GLU:CG	2.35	0.45
3:C:224:THR:HG23	3:C:224:THR:O	2.15	0.45
2:B:408:HIS:O	4:M:1:GLY:N	2.50	0.45
2:E:321:LYS:O	2:E:322:VAL:HG13	2.16	0.45
2:B:393:GLN:O	2:B:397:GLU:HG2	2.17	0.45
3:F:276:LEU:CD2	3:F:307:HIS:O	2.65	0.45
3:F:195:GLN:O	3:F:383:THR:HA	2.16	0.45
2:B:203:ILE:O	3:C:218:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:O	2:B:172:LEU:HB2	2.17	0.45
3:C:382:THR:CG2	3:C:383:THR:N	2.79	0.45
3:F:318:ASP:OD1	3:F:320:ASP:OD2	2.35	0.45
1:D:126:VAL:HG22	2:E:154:ASP:CA	2.47	0.45
2:E:332:GLN:NE2	2:E:332:GLN:HA	2.31	0.45
3:C:361:ASN:ND2	3:C:363:TYR:HB2	2.32	0.45
1:D:156:ILE:HG21	2:E:415:ARG:HE	1.82	0.45
3:F:198:LEU:O	3:F:199:ASP:C	2.54	0.45
3:C:110:LEU:O	3:C:113:ILE:HG12	2.17	0.45
3:C:195:GLN:HE22	3:C:382:THR:HG22	1.82	0.45
3:C:346:GLY:C	3:C:366:GLY:HA2	2.37	0.45
3:C:366:GLY:O	3:C:368:ILE:HG13	2.17	0.45
3:C:266:LYS:HG3	3:F:303:PHE:CE2	2.51	0.45
3:C:174:ALA:HB2	3:C:235:LEU:HD13	1.99	0.45
3:F:149:THR:HG23	3:F:169:ILE:HA	1.98	0.45
2:B:406:ARG:CG	4:M:3:ARG:HB2	2.47	0.45
2:E:182:LEU:N	2:E:182:LEU:HD23	2.31	0.45
3:C:278:TYR:CE1	3:C:308:ASN:OD1	2.70	0.45
3:F:375:ARG:HB3	3:F:376:TRP:CE3	2.51	0.45
3:C:373:LYS:HB3	3:C:377:TYR:CD2	2.45	0.45
3:F:186:GLY:C	3:F:188:GLY:N	2.69	0.45
2:B:361:MET:O	2:B:364:ASN:HB2	2.17	0.45
2:E:316:ASP:HB2	2:E:445:TYR:OH	2.16	0.45
2:E:422:TYR:HE1	2:E:445:TYR:N	2.15	0.45
1:D:189:ILE:HG22	1:D:190:ALA:N	2.31	0.45
3:C:100:ILE:C	3:C:102:THR:H	2.20	0.45
3:C:294:ASP:HA	3:C:301:ASP:HB3	1.97	0.45
3:F:127:LYS:O	3:F:130:GLN:HB2	2.17	0.45
2:B:316:ASP:OD2	2:B:316:ASP:N	2.50	0.45
2:E:178:LYS:O	2:E:181:LYS:HB3	2.18	0.45
3:C:312:PHE:CE1	3:C:334:TRP:HA	2.52	0.44
3:C:169:ILE:O	3:C:169:ILE:HG13	2.16	0.44
3:C:396:GLU:CG	3:C:397:GLY:H	2.30	0.44
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.51	0.44
3:F:98:ALA:O	3:F:101:LEU:HG	2.17	0.44
6:B:478:GAL:H5	6:B:479:SIA:O6	2.17	0.44
3:C:223:THR:O	3:C:224:THR:HB	2.17	0.44
3:C:334:TRP:CG	3:C:343:HIS:HB2	2.51	0.44
1:A:140:VAL:HG21	1:A:185:LEU:HD21	2.00	0.44
1:A:125:LYS:O	1:A:129:LYS:HG2	2.17	0.44
2:B:172:LEU:HD22	3:C:113:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:ARG:O	2:E:406:ARG:HG2	2.17	0.44
3:F:205:LYS:HE2	3:F:331:GLY:CA	2.47	0.44
3:F:243:PRO:HB2	3:F:389:PHE:HB2	1.98	0.44
1:A:134:GLN:O	1:A:137:GLN:HB3	2.17	0.44
2:B:262:PHE:O	2:B:400:GLY:HA2	2.18	0.44
3:F:382:THR:C	3:F:383:THR:HG22	2.38	0.44
3:F:191:TRP:CD1	3:F:385:LYS:HD3	2.52	0.44
3:C:373:LYS:CB	3:C:377:TYR:HD2	2.27	0.44
1:D:130:VAL:O	1:D:133:ILE:HG13	2.18	0.44
2:E:279:ASN:O	2:E:288:LEU:HD12	2.17	0.44
1:D:144:LEU:O	1:D:147:MET:HB3	2.17	0.44
1:A:189:ILE:CG2	1:A:190:ALA:N	2.75	0.44
3:C:258:SER:CB	3:C:286:ALA:HB2	2.48	0.44
2:E:380:ARG:HH22	2:E:382:ASN:HD21	1.66	0.44
3:C:264:MET:CE	3:C:266:LYS:HZ3	2.29	0.44
3:C:149:THR:HA	3:C:168:PHE:O	2.16	0.44
3:F:374:THR:C	3:F:376:TRP:H	2.21	0.44
2:E:231:SER:HB2	3:F:176:GLN:OE1	2.18	0.44
3:F:369:TRP:O	3:F:370:ALA:C	2.56	0.44
3:F:196:LYS:HD2	3:F:382:THR:O	2.18	0.44
3:F:172:LEU:H	3:F:239:GLN:NE2	2.16	0.44
2:B:370:HIS:HE1	2:B:408:HIS:HB2	1.82	0.44
2:B:175:LEU:O	2:B:179:ILE:HG13	2.17	0.44
3:C:365:ASN:HD22	3:C:365:ASN:C	2.21	0.44
2:E:319:GLY:O	2:E:320:ASP:C	2.56	0.44
3:F:298:ASP:C	3:F:300:SER:H	2.19	0.44
3:F:148:ILE:O	3:F:156:ILE:HD12	2.17	0.44
3:F:194:PHE:CZ	3:F:384:MET:HB3	2.53	0.44
3:C:277:THR:HB	3:C:309:GLY:HA2	2.00	0.44
3:F:264:MET:SD	3:F:279:ALA:HB2	2.58	0.44
1:A:188:VAL:HG23	1:A:188:VAL:O	2.17	0.44
2:B:417:TYR:HB2	2:B:446:SER:CB	2.48	0.44
2:B:217:LYS:HB3	3:C:213:GLU:HG3	2.00	0.44
3:C:305:THR:CG2	3:C:338:LYS:HD2	2.47	0.43
2:B:418:TRP:HD1	2:B:419:GLY:H	1.65	0.43
2:B:380:ARG:HH11	2:B:380:ARG:CG	2.30	0.43
3:C:245:ALA:O	3:C:386:ILE:HA	2.17	0.43
3:C:356:LYS:O	3:C:362:GLY:HA2	2.18	0.43
2:B:182:LEU:O	2:B:186:VAL:HG23	2.18	0.43
2:B:308:THR:HG22	2:B:309:GLU:H	1.82	0.43
3:C:219:SER:HB2	3:C:224:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:141:ASP:CG	3:F:143:VAL:HG22	2.38	0.43
1:A:159:ARG:NH1	1:A:159:ARG:HG2	2.31	0.43
3:F:262:TYR:CZ	3:F:290:PHE:HD1	2.37	0.43
1:D:130:VAL:O	1:D:133:ILE:CG1	2.66	0.43
2:E:234:LYS:HZ1	3:F:145:ILE:CD1	2.30	0.43
2:B:163:THR:O	2:B:167:VAL:HG23	2.19	0.43
1:A:124:ARG:O	1:A:128:GLU:HG2	2.19	0.43
3:C:113:ILE:CG1	3:C:114:TYR:N	2.81	0.43
2:E:309:GLU:HA	2:E:326:TYR:O	2.19	0.43
3:F:136:GLN:HG2	3:F:136:GLN:O	2.18	0.43
2:B:249:TRP:CZ2	2:B:455:ARG:NH2	2.86	0.43
1:D:134:GLN:O	1:D:137:GLN:HB3	2.18	0.43
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.99	0.43
1:D:148:LYS:HA	1:D:178:TYR:CE2	2.52	0.43
3:C:202:VAL:HG11	3:C:225:GLU:CB	2.48	0.43
3:C:273:LYS:HB2	3:C:311:GLN:OE1	2.18	0.43
3:F:137:GLU:OE1	3:F:137:GLU:HA	2.17	0.43
3:C:338:LYS:N	3:C:339:CYS:CA	2.65	0.43
2:B:309:GLU:HA	2:B:326:TYR:O	2.18	0.43
2:B:176:ARG:HG3	2:B:176:ARG:NH1	2.34	0.43
2:B:365:ARG:O	2:B:367:MET:N	2.52	0.43
3:C:246:LEU:HD12	3:C:247:ARG:H	1.83	0.43
1:A:124:ARG:HG3	1:A:124:ARG:HH11	1.84	0.43
2:E:250:THR:O	2:E:453:LYS:HA	2.18	0.43
2:E:169:ARG:NH1	3:F:109:TYR:CE2	2.86	0.43
3:C:320:ASP:OD1	3:C:326:CYS:SG	2.77	0.43
1:D:166:SER:N	2:E:195:THR:O	2.50	0.43
3:F:206:LYS:HB3	3:F:210:GLN:CB	2.49	0.43
1:D:188:VAL:O	1:D:188:VAL:HG23	2.19	0.43
2:B:381:ASP:OD2	2:B:383:ASP:CG	2.57	0.43
1:D:147:MET:CE	3:F:121:ILE:HD11	2.38	0.43
3:C:154:GLN:HB2	3:C:387:ILE:HD11	2.00	0.43
3:F:141:ASP:OD2	3:F:143:VAL:HG22	2.19	0.43
1:D:126:VAL:CG2	2:E:154:ASP:HA	2.48	0.43
2:B:449:LYS:HB2	2:B:449:LYS:HE3	1.74	0.43
3:F:174:ALA:CB	3:F:235:LEU:HD13	2.48	0.43
2:B:152:TYR:O	2:B:154:ASP:N	2.52	0.43
3:F:365:ASN:ND2	3:F:365:ASN:C	2.72	0.43
3:F:391:ARG:HD3	3:F:391:ARG:HA	1.41	0.43
3:F:382:THR:O	3:F:383:THR:HB	2.19	0.43
2:E:326:TYR:N	2:E:326:TYR:CD1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:281:PHE:CE2	3:C:288:ASP:HB2	2.54	0.43
3:C:153:CYS:SG	3:C:192:THR:HB	2.59	0.43
1:D:123:LYS:HG2	2:E:151:LEU:O	2.18	0.43
1:A:148:LYS:NZ	1:A:179:GLU:HG3	2.34	0.43
1:A:159:ARG:NH2	2:B:418:TRP:CE3	2.87	0.43
3:F:102:THR:O	3:F:105:SER:HB2	2.18	0.43
3:C:230:ASN:HA	3:C:233:ILE:HD12	2.00	0.42
2:B:182:LEU:HD23	2:B:182:LEU:N	2.33	0.42
3:F:390:ASN:N	3:F:390:ASN:HD22	2.17	0.42
3:F:370:ALA:O	3:F:372:TRP:N	2.51	0.42
2:B:157:VAL:HG13	2:B:161:ILE:HD12	2.01	0.42
2:E:215:ILE:CG2	2:E:216:ARG:N	2.81	0.42
1:A:154:ILE:O	1:A:158:ILE:HG12	2.18	0.42
2:B:178:LYS:O	2:B:182:LEU:HG	2.19	0.42
3:C:124:LEU:HD23	3:C:125:LYS:N	2.34	0.42
2:B:228:GLN:HE22	3:C:177:GLN:HE22	1.67	0.42
1:A:165:CYS:HA	2:B:193:CYS:HA	2.02	0.42
3:F:374:THR:C	3:F:376:TRP:N	2.72	0.42
2:E:440:TRP:CE3	2:E:441:LYS:HG2	2.54	0.42
3:C:338:LYS:H	3:C:339:CYS:CA	2.25	0.42
3:C:367:ILE:HG12	3:C:367:ILE:O	2.20	0.42
2:E:386:LEU:N	2:E:386:LEU:HD23	2.22	0.42
3:F:111:GLN:O	3:F:114:TYR:HB3	2.19	0.42
3:C:191:TRP:CE3	3:C:387:ILE:HB	2.54	0.42
3:C:192:THR:O	3:C:192:THR:OG1	2.29	0.42
3:F:333:GLY:O	3:F:334:TRP:HB2	2.19	0.42
3:F:205:LYS:HB3	3:F:205:LYS:NZ	2.35	0.42
2:E:398:ASP:O	2:E:399:GLY:C	2.58	0.42
2:E:310:LEU:O	2:E:325:HIS:HA	2.19	0.42
2:B:380:ARG:CZ	2:B:380:ARG:HB3	2.49	0.42
3:C:311:GLN:O	3:C:335:TRP:HA	2.18	0.42
6:E:472:MAN:H4	6:E:473:MAN:C2	2.43	0.42
3:C:298:ASP:C	3:C:300:SER:N	2.73	0.42
3:F:202:VAL:HG13	3:F:203:ASP:N	2.34	0.42
3:F:341:ALA:O	3:F:370:ALA:HB2	2.19	0.42
3:C:307:HIS:HE1	3:C:341:ALA:HB3	1.83	0.42
2:E:294:LEU:O	2:E:299:ILE:HD11	2.20	0.42
2:E:296:ASN:O	2:E:297:ASP:C	2.57	0.42
3:C:344:LEU:HD11	3:C:384:MET:SD	2.60	0.42
2:E:191:GLU:HG3	2:E:194:ARG:NH2	2.35	0.42
2:B:365:ARG:C	2:B:367:MET:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLN:HB2	2:B:171:ILE:HD11	2.01	0.42
3:F:307:HIS:HE1	3:F:341:ALA:HB3	1.85	0.42
3:F:347:VAL:N	3:F:366:GLY:HA2	2.34	0.42
3:C:273:LYS:O	3:C:274:TYR:C	2.58	0.42
1:D:159:ARG:NH2	2:E:418:TRP:CE3	2.88	0.42
3:F:311:GLN:O	3:F:335:TRP:CD1	2.73	0.42
1:A:140:VAL:HG23	1:A:185:LEU:HD21	2.02	0.42
3:C:315:TRP:N	3:C:327:ALA:HB1	2.35	0.42
3:F:227:TRP:O	3:F:228:LEU:C	2.59	0.42
2:E:454:ILE:HD12	2:E:455:ARG:N	2.34	0.42
1:A:155:ASP:HB2	1:A:173:VAL:HG21	2.02	0.42
3:F:166:LEU:HD11	3:F:220:PRO:CG	2.50	0.42
2:E:218:GLY:HA3	3:F:210:GLN:HG2	2.02	0.42
3:F:145:ILE:HG13	3:F:145:ILE:H	1.75	0.42
2:E:205:VAL:HG21	3:F:226:PHE:HB2	2.02	0.42
3:F:193:VAL:HG23	3:F:226:PHE:HZ	1.84	0.42
2:E:348:THR:O	2:E:349:ALA:HB2	2.20	0.42
2:B:204:PRO:HA	3:C:217:HIS:HA	2.01	0.42
3:F:338:LYS:H	3:F:339:CYS:CA	2.25	0.41
3:F:339:CYS:HB2	3:F:340:HIS:H	1.67	0.41
3:F:344:LEU:HD13	3:F:382:THR:HG21	2.02	0.41
3:F:239:GLN:O	3:F:240:SER:HB2	2.20	0.41
3:C:385:LYS:O	3:C:386:ILE:HB	2.20	0.41
2:B:408:HIS:CD2	2:B:411:ASN:HB2	2.55	0.41
2:B:373:MET:HE3	2:B:373:MET:HA	2.03	0.41
2:E:359:GLN:O	2:E:360:LEU:HD12	2.20	0.41
2:E:176:ARG:HG2	3:F:120:LYS:HZ2	1.84	0.41
2:B:161:ILE:N	2:B:162:PRO:CD	2.83	0.41
1:D:128:GLU:OE2	1:D:129:LYS:HE2	2.21	0.41
3:C:391:ARG:HA	3:C:391:ARG:HD2	1.82	0.41
2:B:253:GLN:HE21	2:B:452:MET:HG3	1.85	0.41
3:C:277:THR:HG23	3:F:303:PHE:HD2	1.84	0.41
3:C:297:ASP:O	3:C:298:ASP:CB	2.69	0.41
3:F:100:ILE:C	3:F:102:THR:H	2.23	0.41
1:D:145:VAL:HG12	1:D:149:ARG:NH1	2.35	0.41
2:B:230:ASP:O	2:B:233:VAL:HG12	2.19	0.41
3:F:308:ASN:C	3:F:308:ASN:ND2	2.72	0.41
3:C:346:GLY:HA3	3:C:366:GLY:CA	2.51	0.41
2:B:265:LYS:C	2:B:377:THR:HG21	2.41	0.41
3:C:264:MET:O	3:C:264:MET:HG2	2.19	0.41
1:A:148:LYS:HZ2	1:A:182:GLN:NE2	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:ASP:O	2:E:379:ASP:OD1	2.39	0.41
3:F:315:TRP:C	3:F:315:TRP:CD1	2.94	0.41
3:F:157:ALA:HA	3:F:160:GLY:O	2.20	0.41
2:B:199:VAL:O	3:C:141:ASP:OD2	2.38	0.41
3:F:253:TRP:NE1	3:F:379:MET:O	2.53	0.41
2:B:326:TYR:CZ	2:B:353:LEU:HD12	2.55	0.41
2:E:336:ASN:O	2:E:338:TYR:N	2.53	0.41
3:F:140:LYS:HD3	3:F:141:ASP:N	2.35	0.41
3:F:166:LEU:H	3:F:166:LEU:CD1	2.28	0.41
3:F:205:LYS:HG2	3:F:331:GLY:C	2.41	0.41
1:A:126:VAL:HG22	2:B:154:ASP:CB	2.50	0.41
2:E:352:ALA:O	2:E:370:HIS:HD2	2.03	0.41
3:F:204:PHE:O	3:F:332:SER:HA	2.20	0.41
3:F:272:ASP:O	3:F:273:LYS:HB2	2.20	0.41
3:C:304:PHE:HB3	3:C:338:LYS:HG3	2.01	0.41
2:E:172:LEU:HD21	3:F:114:TYR:HD2	1.86	0.41
2:B:413:ASN:N	2:B:435:VAL:HG22	2.34	0.41
2:E:412:PRO:HA	2:E:435:VAL:HG13	2.01	0.41
2:B:406:ARG:O	2:B:406:ARG:HG2	2.21	0.41
3:F:170:LYS:HE3	3:F:175:ASN:CA	2.49	0.41
1:A:165:CYS:O	1:A:166:SER:C	2.59	0.41
2:E:177:SER:HA	2:E:180:GLN:HG2	2.02	0.41
2:B:362:GLY:O	2:B:363:GLU:C	2.59	0.41
2:B:229:PRO:HG3	2:B:236:TYR:OH	2.21	0.41
3:F:304:PHE:HB3	3:F:338:LYS:HB2	2.03	0.41
3:F:367:ILE:H	3:F:367:ILE:CD1	2.19	0.41
2:E:309:GLU:HG2	2:E:455:ARG:O	2.21	0.41
2:E:162:PRO:O	2:E:165:LEU:HB2	2.21	0.41
2:E:438:MET:HA	2:E:442:GLY:CA	2.51	0.41
2:B:301:GLN:HE21	2:B:301:GLN:HB3	1.53	0.41
3:F:196:LYS:O	3:F:225:GLU:HA	2.20	0.41
2:E:172:LEU:HD21	3:F:114:TYR:HB2	2.02	0.41
3:C:344:LEU:HA	3:C:367:ILE:HG22	2.03	0.41
3:F:245:ALA:O	3:F:386:ILE:HA	2.21	0.41
2:E:169:ARG:NH1	3:F:109:TYR:CD2	2.89	0.41
2:E:254:ASN:O	2:E:291:GLU:HA	2.21	0.41
3:F:234:HIS:CG	3:F:235:LEU:N	2.87	0.41
1:A:147:MET:O	1:A:150:LEU:HB2	2.21	0.41
2:E:449:LYS:HE3	2:E:449:LYS:HB2	1.88	0.41
3:F:352:GLY:O	3:F:353:THR:HB	2.21	0.41
2:E:452:MET:C	2:E:453:LYS:HD2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:272:ASP:O	3:C:273:LYS:HB2	2.19	0.41
3:C:100:ILE:O	3:C:103:HIS:CD2	2.73	0.41
2:E:176:ARG:CG	3:F:120:LYS:NZ	2.82	0.41
3:C:205:LYS:HE2	3:C:331:GLY:CA	2.51	0.41
3:F:186:GLY:O	3:F:188:GLY:N	2.54	0.41
2:E:421:GLN:HE21	2:E:421:GLN:HB2	1.50	0.40
2:E:253:GLN:HG3	2:E:293:TRP:HE3	1.84	0.40
2:E:236:TYR:CD2	2:E:294:LEU:HD11	2.56	0.40
2:B:438:MET:SD	2:B:443:SER:HB3	2.61	0.40
2:E:225:TYR:HD2	2:E:240:CYS:HB2	1.86	0.40
2:E:168:LEU:O	2:E:172:LEU:HB2	2.22	0.40
2:B:180:GLN:HG3	2:B:181:LYS:N	2.35	0.40
2:B:228:GLN:HB2	2:B:235:PRO:HG3	2.03	0.40
3:C:277:THR:CG2	3:F:303:PHE:HD2	2.34	0.40
3:C:148:ILE:O	3:C:148:ILE:HG22	2.21	0.40
3:C:305:THR:HB	3:C:341:ALA:CB	2.28	0.40
2:E:253:GLN:HE21	2:E:253:GLN:HB3	1.56	0.40
1:D:126:VAL:HG21	2:E:153:ILE:HG12	2.04	0.40
2:B:325:HIS:HB3	2:B:346:ARG:HB2	2.02	0.40
2:B:322:VAL:HB	2:B:349:ALA:HB2	2.03	0.40
3:F:359:THR:HA	3:F:360:PRO:HD3	1.88	0.40
3:C:175:ASN:O	3:C:176:GLN:O	2.39	0.40
2:B:209:LYS:HD2	2:B:213:GLU:OE2	2.21	0.40
3:F:305:THR:CG2	3:F:338:LYS:HD2	2.51	0.40
3:C:141:ASP:CG	3:C:143:VAL:HG22	2.42	0.40
1:A:123:LYS:HE2	1:A:124:ARG:HH22	1.86	0.40
2:E:249:TRP:HH2	2:E:325:HIS:CE1	2.39	0.40
3:C:311:GLN:HB2	3:C:319:ASN:O	2.21	0.40
2:B:373:MET:HG3	2:B:405:ASN:CB	2.46	0.40
3:F:334:TRP:CE2	3:F:343:HIS:HA	2.57	0.40
3:F:373:LYS:HZ3	3:F:377:TYR:HE2	1.69	0.40
1:A:176:LYS:O	1:A:180:ASP:HB2	2.21	0.40
2:E:367:MET:HG3	2:E:367:MET:O	2.20	0.40
3:F:198:LEU:O	3:F:200:GLY:N	2.55	0.40
2:E:296:ASN:HD22	2:E:299:ILE:HD12	1.87	0.40
2:E:296:ASN:HA	2:E:299:ILE:HD12	2.03	0.40
3:C:342:GLY:HA2	3:C:368:ILE:CD1	2.52	0.40
2:E:265:LYS:C	2:E:268:PRO:HD2	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	72/197 (36%)	62 (86%)	6 (8%)	4 (6%)	2	26
1	D	72/197 (36%)	62 (86%)	7 (10%)	3 (4%)	3	33
2	B	306/458 (67%)	230 (75%)	57 (19%)	19 (6%)	2	24
2	E	306/458 (67%)	226 (74%)	63 (21%)	17 (6%)	2	26
3	C	299/317 (94%)	199 (67%)	67 (22%)	33 (11%)	0	9
3	F	294/317 (93%)	211 (72%)	54 (18%)	29 (10%)	1	12
4	M	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
4	N	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	1355/1954 (69%)	994 (73%)	256 (19%)	105 (8%)	1	16

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	153	ILE
2	B	238	VAL
2	B	289	PRO
2	B	349	ALA
3	C	98	ALA
3	C	101	LEU
3	C	161	ALA
3	C	199	ASP
3	C	336	MET
3	C	386	ILE
3	C	396	GLU
1	D	191	LYS
2	E	337	LYS
2	E	349	ALA
3	F	161	ALA
3	F	199	ASP
3	F	301	ASP

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Mol	Chain	Res	Type
3	F	371	THR
2	B	256	GLN
2	B	366	THR
2	B	405	ASN
2	B	416	TYR
3	C	202	VAL
3	C	235	LEU
3	C	266	LYS
3	C	295	PHE
3	C	300	SER
3	C	393	THR
2	E	153	ILE
2	E	245	GLU
2	E	256	GLN
2	E	289	PRO
2	E	347	GLY
2	E	399	GLY
2	E	433	ASP
3	F	177	GLN
3	F	202	VAL
3	F	315	TRP
3	F	324	GLY
3	F	325	ASN
3	F	336	MET
3	F	367	ILE
3	F	370	ALA
1	A	189	ILE
2	B	237	ARG
2	B	243	ASN
2	B	245	GLU
2	B	291	GLU
2	B	399	GLY
2	B	404	TYR
2	B	457	PHE
3	C	136	GLN
3	C	176	GLN
3	C	224	THR
3	C	228	LEU
3	C	330	ASP
3	C	342	GLY
3	C	353	THR
3	C	371	THR

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Mol	Chain	Res	Type
2	E	238	VAL
2	E	243	ASN
2	E	304	ARG
2	E	363	GLU
2	E	416	TYR
3	F	101	LEU
3	F	337	ASN
3	F	342	GLY
3	F	346	GLY
3	F	383	THR
1	A	164	SER
1	A	166	SER
3	C	203	ASP
3	C	367	ILE
3	C	390	ASN
2	E	291	GLU
3	F	203	ASP
3	F	224	THR
3	F	295	PHE
3	F	296	GLY
3	F	300	SER
3	F	331	GLY
3	F	353	THR
1	A	190	ALA
2	B	193	CYS
2	B	265	LYS
2	B	378	TYR
3	C	183	GLU
3	C	234	HIS
3	C	301	ASP
3	C	337	ASN
3	F	147	ASP
3	F	266	LYS
3	F	282	ALA
3	F	379	MET
3	F	228	LEU
3	C	283	GLY
3	C	292	GLY
3	C	296	GLY
3	C	331	GLY
3	C	395	GLY
2	B	196	PRO

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Mol	Chain	Res	Type
1	D	126	VAL
2	E	340	ILE
1	D	189	ILE
2	E	435	VAL

### 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	69/179 (38%)	58 (84%)	11 (16%)	3	21
1	D	69/179 (38%)	58 (84%)	11 (16%)	3	21
2	B	266/393 (68%)	239 (90%)	27 (10%)	9	42
2	E	266/393 (68%)	240 (90%)	26 (10%)	10	44
3	C	252/263 (96%)	223 (88%)	29 (12%)	7	36
3	F	249/263 (95%)	221 (89%)	28 (11%)	7	38
4	M	4/4 (100%)	4 (100%)	0	100	100
4	N	4/4 (100%)	4 (100%)	0	100	100
All	All	1179/1678 (70%)	1047 (89%)	132 (11%)	7	38

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	123	LYS
1	A	124	ARG
1	A	131	GLN
1	A	153	ASP
1	A	159	ARG
1	A	162	ARG
1	A	171	ARG
1	A	174	ASP
1	A	185	LEU
1	A	187	GLN

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Mol	Chain	Res	Type
2	B	152	TYR
2	B	153	ILE
2	B	159	SER
2	B	163	THR
2	B	193	CYS
2	B	197	CYS
2	B	206	VAL
2	B	237	ARG
2	B	253	GLN
2	B	260	VAL
2	B	276	VAL
2	B	301	GLN
2	B	314	MET
2	B	322	VAL
2	B	323	LYS
2	B	330	THR
2	B	341	SER
2	B	351	ASN
2	B	355	ASP
2	B	377	THR
2	B	378	TYR
2	B	386	LEU
2	B	418	TRP
2	B	421	GLN
2	B	451	SER
2	B	453	LYS
2	B	457	PHE
3	C	100	ILE
3	C	103	HIS
3	C	104	ASP
3	C	110	LEU
3	C	114	TYR
3	C	166	LEU
3	C	175	ASN
3	C	177	GLN
3	C	180	VAL
3	C	192	THR
3	C	195	GLN
3	C	217	HIS
3	C	250	LEU
3	C	252	ASP
3	C	291	ASP

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Mol	Chain	Res	Type
3	C	295	PHE
3	C	308	ASN
3	C	315	TRP
3	C	343	HIS
3	C	344	LEU
3	C	361	ASN
3	C	364	ASP
3	C	365	ASN
3	C	367	ILE
3	C	371	THR
3	C	383	THR
3	C	390	ASN
3	C	391	ARG
3	C	396	GLU
1	D	124	ARG
1	D	132	HIS
1	D	135	LEU
1	D	153	ASP
1	D	159	ARG
1	D	161	CYS
1	D	162	ARG
1	D	171	ARG
1	D	174	ASP
1	D	185	LEU
1	D	192	ASP
2	E	152	TYR
2	E	153	ILE
2	E	163	THR
2	E	180	GLN
2	E	184	SER
2	E	193	CYS
2	E	197	CYS
2	E	206	VAL
2	E	224	MET
2	E	237	ARG
2	E	253	GLN
2	E	276	VAL
2	E	280	THR
2	E	301	GLN
2	E	323	LYS
2	E	326	TYR
2	E	330	THR

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Mol	Chain	Res	Type
2	E	331	VAL
2	E	351	ASN
2	E	377	THR
2	E	378	TYR
2	E	386	LEU
2	E	418	TRP
2	E	421	GLN
2	E	423	THR
2	E	453	LYS
3	F	100	ILE
3	F	103	HIS
3	F	108	ARG
3	F	166	LEU
3	F	169	ILE
3	F	175	ASN
3	F	177	GLN
3	F	192	THR
3	F	195	GLN
3	F	198	LEU
3	F	217	HIS
3	F	237	SER
3	F	261	ASP
3	F	264	MET
3	F	276	LEU
3	F	295	PHE
3	F	305	THR
3	F	308	ASN
3	F	315	TRP
3	F	343	HIS
3	F	344	LEU
3	F	364	ASP
3	F	365	ASN
3	F	367	ILE
3	F	379	MET
3	F	383	THR
3	F	390	ASN
3	F	391	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN

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Mol	Chain	Res	Type
1	A	139	ASN
1	A	143	GLN
1	A	181	GLN
1	A	182	GLN
1	A	187	GLN
2	B	158	ASN
2	B	160	ASN
2	B	164	ASN
2	B	180	GLN
2	B	228	GLN
2	B	253	GLN
2	B	296	ASN
2	B	301	GLN
2	B	332	GLN
2	B	339	GLN
2	B	351	ASN
2	B	370	HIS
2	B	382	ASN
2	B	408	HIS
2	B	421	GLN
3	C	103	HIS
3	C	117	ASN
3	C	158	ASN
3	C	177	GLN
3	C	195	GLN
3	C	230	ASN
3	C	239	GLN
3	C	254	ASN
3	C	307	HIS
3	C	308	ASN
3	C	325	ASN
3	C	361	ASN
3	C	365	ASN
3	C	390	ASN
1	D	134	GLN
1	D	181	GLN
1	D	182	GLN
1	D	187	GLN
2	E	158	ASN
2	E	160	ASN
2	E	164	ASN
2	E	189	GLN

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Mol	Chain	Res	Type
2	E	253	GLN
2	E	296	ASN
2	E	301	GLN
2	E	332	GLN
2	E	333	ASN
2	E	336	ASN
2	E	351	ASN
2	E	382	ASN
2	E	393	GLN
2	E	408	HIS
2	E	421	GLN
2	E	429	HIS
3	F	103	HIS
3	F	117	ASN
3	F	118	ASN
3	F	119	GLN
3	F	177	GLN
3	F	189	ASN
3	F	195	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	308	ASN
3	F	317	ASN
3	F	319	ASN
3	F	350	GLN
3	F	361	ASN
3	F	390	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

16 carbohydrates 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	$\# Z  > 2$
6	NAG	B	470	2,6	14,14,15	0.62	0	15,19,21	1.09	1 (6%)
6	NAG	B	471	6	14,14,15	1.02	1 (7%)	15,19,21	1.31	2 (13%)
6	MAN	B	472	6	11,11,12	0.92	0	14,15,17	1.42	2 (14%)
6	MAN	B	473	6	11,11,12	0.74	0	14,15,17	1.16	2 (14%)
6	MAN	B	474	6	11,11,12	1.16	1 (9%)	14,15,17	0.84	0
6	NAG	B	477	6	14,14,15	1.40	1 (7%)	15,19,21	1.68	3 (20%)
6	GAL	B	478	6	11,11,12	1.10	0	14,15,17	0.82	0
6	SIA	B	479	6	16,20,21	1.29	2 (12%)	18,28,31	1.11	1 (5%)
6	NAG	E	470	2,6	14,14,15	0.65	0	15,19,21	1.07	2 (13%)
6	NAG	E	471	6	14,14,15	1.08	0	15,19,21	1.28	2 (13%)
6	MAN	E	472	6	11,11,12	1.22	0	14,15,17	0.83	0
6	MAN	E	473	6	11,11,12	0.89	0	14,15,17	1.12	2 (14%)
6	MAN	E	474	6	11,11,12	1.75	1 (9%)	14,15,17	1.67	3 (21%)
6	NAG	E	477	6	14,14,15	1.62	2 (14%)	15,19,21	0.89	0
6	GAL	E	478	6	11,11,12	1.06	1 (9%)	14,15,17	0.76	0
6	SIA	E	479	6	16,20,21	2.38	4 (25%)	18,28,31	1.88	5 (27%)

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
6	NAG	B	470	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	471	6	1/1/5/7	0/6/23/26	0/1/1/1
6	MAN	B	472	6	-	0/2/19/22	0/1/1/1
6	MAN	B	473	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	B	474	6	-	0/2/19/22	0/1/1/1
6	NAG	B	477	6	1/1/5/7	0/6/23/26	0/1/1/1
6	GAL	B	478	6	-	0/2/19/22	0/1/1/1
6	SIA	B	479	6	-	0/14/34/38	0/1/1/1
6	NAG	E	470	2,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	471	6	1/1/5/7	0/6/23/26	0/1/1/1
6	MAN	E	472	6	-	0/2/19/22	0/1/1/1
6	MAN	E	473	6	-	0/2/19/22	0/1/1/1
6	MAN	E	474	6	-	0/2/19/22	0/1/1/1
6	NAG	E	477	6	1/1/5/7	0/6/23/26	0/1/1/1
6	GAL	E	478	6	-	0/2/19/22	0/1/1/1
6	SIA	E	479	6	1/1/8/9	1/14/34/38	1/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	471	NAG	C4-C5	2.05	1.57	1.53
6	E	477	NAG	C3-C2	2.15	1.57	1.52
6	B	474	MAN	C2-C3	2.19	1.55	1.52
6	E	478	GAL	C1-C2	2.21	1.57	1.52
6	E	479	SIA	C8-C7	2.31	1.58	1.53
6	B	479	SIA	C7-C6	2.40	1.56	1.52
6	B	477	NAG	C1-C2	3.39	1.57	1.52
6	B	479	SIA	O6-C6	3.45	1.49	1.43
6	E	479	SIA	O6-C6	3.83	1.50	1.43
6	E	477	NAG	C1-C2	4.65	1.58	1.52
6	E	479	SIA	C6-C5	4.72	1.60	1.53
6	E	474	MAN	C2-C3	4.92	1.59	1.52
6	E	479	SIA	C7-C6	6.24	1.60	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	470	NAG	C2-N2-C7	-3.70	118.28	123.04
6	E	479	SIA	C7-C6-C5	-3.44	109.11	114.32
6	B	471	NAG	C2-N2-C7	-2.40	119.95	123.04
6	E	470	NAG	C2-N2-C7	-2.17	120.25	123.04
6	B	477	NAG	C2-N2-C7	-2.08	120.36	123.04
6	E	479	SIA	O10-C10-C11	-2.02	118.36	122.06
6	E	470	NAG	C4-C3-C2	2.03	114.39	111.23
6	E	473	MAN	C1-C2-C3	2.18	112.12	109.54
6	E	474	MAN	C3-C4-C5	2.24	114.10	110.20
6	B	479	SIA	O6-C6-C5	2.45	112.49	108.48
6	B	472	MAN	C1-O5-C5	2.48	115.39	112.25
6	E	474	MAN	C1-C2-C3	2.66	112.68	109.54
6	E	479	SIA	O6-C6-C5	2.69	112.88	108.48
6	B	473	MAN	C1-C2-C3	2.70	112.73	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	473	MAN	C1-O5-C5	2.73	115.71	112.25
6	B	477	NAG	C3-C4-C5	2.81	115.10	110.20
6	E	479	SIA	C3-C4-C5	2.91	114.72	111.47
6	E	471	NAG	C4-C3-C2	2.95	115.82	111.23
6	E	473	MAN	C1-O5-C5	3.04	116.11	112.25
6	E	471	NAG	C3-C4-C5	3.08	115.57	110.20
6	B	471	NAG	C3-C4-C5	3.29	115.94	110.20
6	B	472	MAN	C3-C4-C5	3.50	116.30	110.20
6	E	474	MAN	C2-C3-C4	3.99	117.82	111.04
6	B	477	NAG	C4-C3-C2	4.66	118.47	111.23
6	E	479	SIA	O6-C2-C3	4.95	119.36	109.86

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	477	NAG	C1
6	E	471	NAG	C1
6	E	477	NAG	C1
6	B	473	MAN	C1
6	B	471	NAG	C1
6	E	479	SIA	C2

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	479	SIA	O10-C10-N5-C5

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	479	SIA	C2-C3-C4-C5-C6-O6

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	472	MAN	1	0
6	B	474	MAN	1	0
6	B	478	GAL	2	0
6	B	479	SIA	4	0
6	E	471	NAG	2	0
6	E	472	MAN	2	0
6	E	473	MAN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	478	GAL	2	0
6	E	479	SIA	2	0

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	74/197 (37%)	-0.16	4 (5%)	29	20	77, 91, 103, 108	0
1	D	74/197 (37%)	-0.33	2 (2%)	58	43	79, 93, 104, 108	0
2	B	308/458 (67%)	-0.50	0	100	100	65, 82, 98, 108	0
2	E	308/458 (67%)	-0.50	0	100	100	64, 83, 97, 106	0
3	C	301/317 (94%)	-0.48	1 (0%)	94	90	67, 84, 98, 105	0
3	F	296/317 (93%)	-0.49	1 (0%)	94	90	67, 85, 97, 105	0
4	M	5/5 (100%)	-0.52	0	100	100	76, 80, 84, 85	0
4	N	5/5 (100%)	-0.22	0	100	100	83, 87, 91, 93	0
All	All	1371/1954 (70%)	-0.46	8 (0%)	90	83	64, 85, 100, 108	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	126	VAL	3.1
1	A	121	VAL	3.0
1	A	127	ILE	3.0
1	A	126	VAL	2.7
3	F	360	PRO	2.3
1	A	124	ARG	2.2
3	C	393	THR	2.2
1	D	127	ILE	2.0

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

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



### 6.3 Carbohydrates ⓘ

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
6	NAG	E	470	14/15	0.92	0.16	-0.49	90,94,97,101	0
6	MAN	B	474	11/12	0.77	0.53	-	115,115,116,116	0
6	NAG	B	477	14/15	0.72	0.50	-	107,114,115,117	0
6	NAG	E	471	14/15	0.73	0.38	-	104,108,112,114	0
6	NAG	B	470	14/15	0.90	0.18	-	85,91,95,99	0
6	NAG	E	477	14/15	0.80	0.63	-	103,109,112,112	0
6	GAL	B	478	11/12	0.84	0.60	-	116,117,118,119	0
6	GAL	E	478	11/12	0.83	0.76	-	107,110,112,112	0
6	MAN	E	472	11/12	0.71	0.49	-	117,118,120,121	0
6	MAN	B	472	11/12	0.71	0.35	-	111,113,114,115	0
6	SIA	B	479	20/21	0.78	0.54	-	107,111,117,118	0
6	MAN	E	474	11/12	0.70	0.48	-	111,116,119,120	0
6	MAN	B	473	11/12	0.79	0.44	-	106,110,112,115	0
6	MAN	E	473	11/12	0.58	0.50	-	114,117,119,122	0
6	NAG	B	471	14/15	0.93	0.23	-	95,105,108,111	0
6	SIA	E	479	20/21	0.58	0.96	-	104,113,114,114	0

### 6.4 Ligands ⓘ

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
5	CA	E	502	1/1	0.96	0.14	-1.26	26,26,26,26	0
5	CA	B	502	1/1	0.99	0.07	-1.88	40,40,40,40	0
5	CA	C	501	1/1	0.94	0.07	-2.11	74,74,74,74	0
5	CA	F	501	1/1	0.96	0.14	-	108,108,108,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.