Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 10:25 PM EDT

PDB ID	:	3Q2V
Title	:	Crystal structure of mouse E-cadherin ectodomain
Authors	:	Jin, X.; Harrison, O.J.; Shapiro, L.
Deposited on	:	2010-12-20
Resolution	:	3.40 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

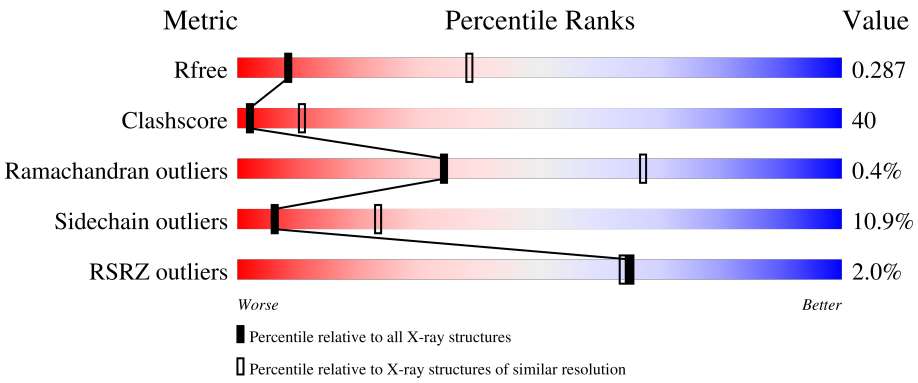
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	550	2% 41% 48% 8% •
1	B	550	2% 33% 41% 5% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	802	X	-	-	-
4	MAN	A	804	X	-	-	-
4	MAN	A	805	X	-	-	-
4	MAN	A	806	X	-	-	-
4	MAN	A	807	X	-	-	-
4	MAN	B	801	X	-	-	-
4	MAN	B	803	X	-	-	-
4	MAN	B	804	X	-	-	X
4	MAN	B	805	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7871 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 Cadherin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	532	4113	2581	683	838	11	0	1	0
1	B	440	3399	2138	553	701	7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	545	HIS	-	expression tag	UNP P09803
A	546	HIS	-	expression tag	UNP P09803
A	547	HIS	-	expression tag	UNP P09803
A	548	HIS	-	expression tag	UNP P09803
A	549	HIS	-	expression tag	UNP P09803
A	550	HIS	-	expression tag	UNP P09803
B	545	HIS	-	expression tag	UNP P09803
B	546	HIS	-	expression tag	UNP P09803
B	547	HIS	-	expression tag	UNP P09803
B	548	HIS	-	expression tag	UNP P09803
B	549	HIS	-	expression tag	UNP P09803
B	550	HIS	-	expression tag	UNP P09803

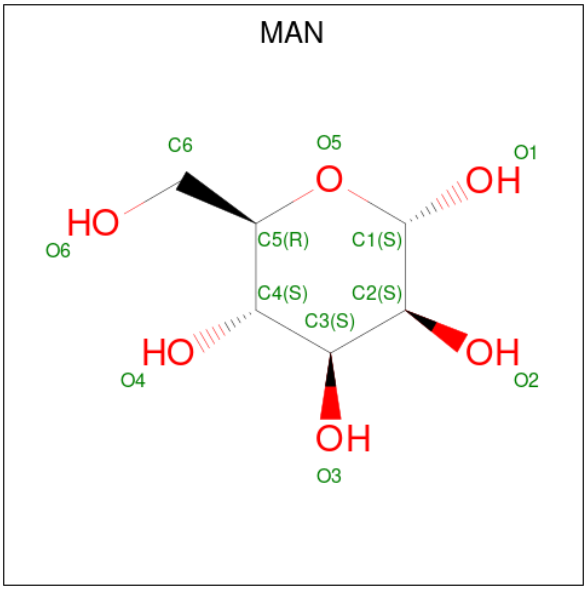
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	12	12	12	0	0
2	B	12	12	12	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	B	1	Total C O 11 6 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	11	6	5	0	0
			Total	C	O		
4	B	1	11	6	5	0	0
			Total	C	O		
4	B	1	11	6	5	0	0
			Total	C	O		
4	B	1	11	6	5	0	0
			Total	C	O		
4	B	1	11	6	5	0	0
			Total	C	O		
4	B	1	11	6	5	0	0
			Total	C	O		
4	B	1	11	6	5	0	0
			Total	C	O		
4	B	1	11	6	5	0	0

- Molecule 5 is water.

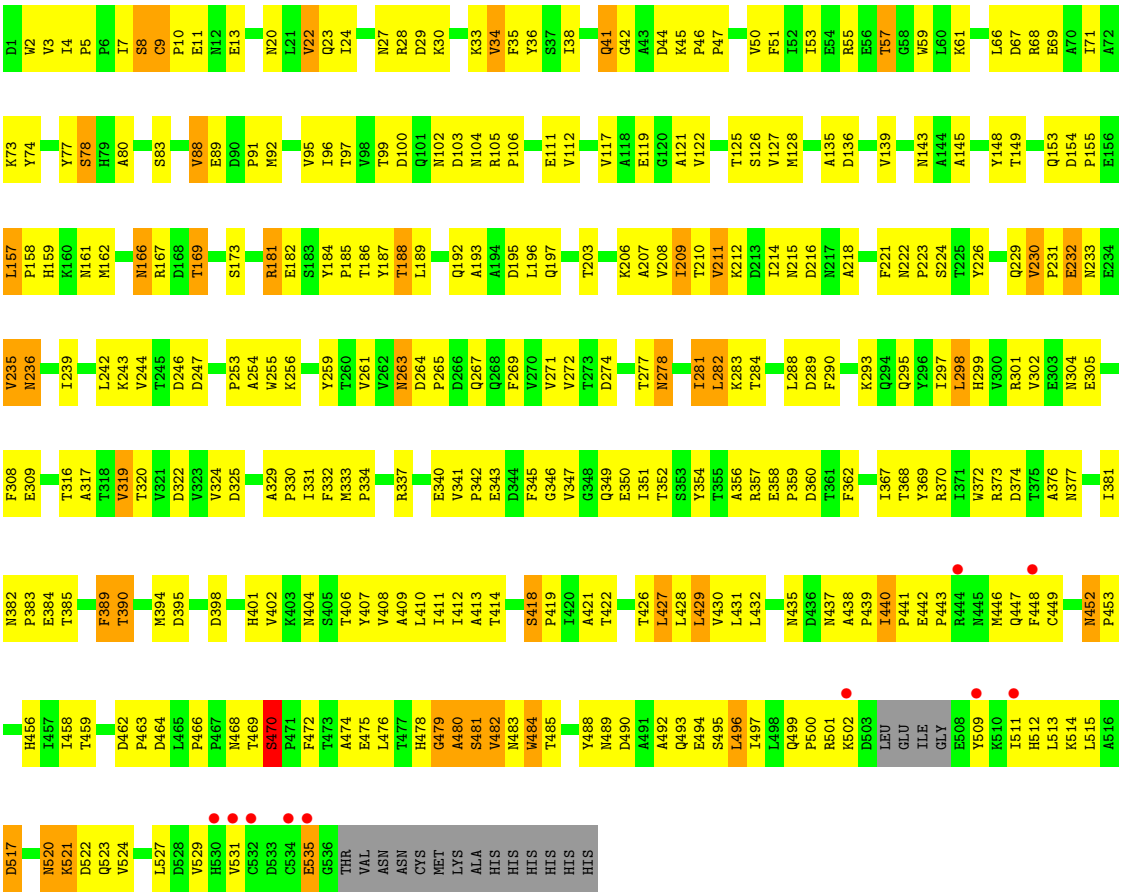
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	55	55	55	0	0
			Total	O		
5	B	80	80	80	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

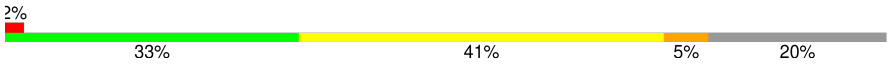
• Molecule 1: Cadherin-1

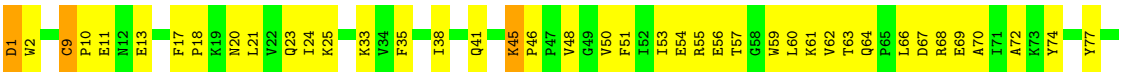
Chain A:

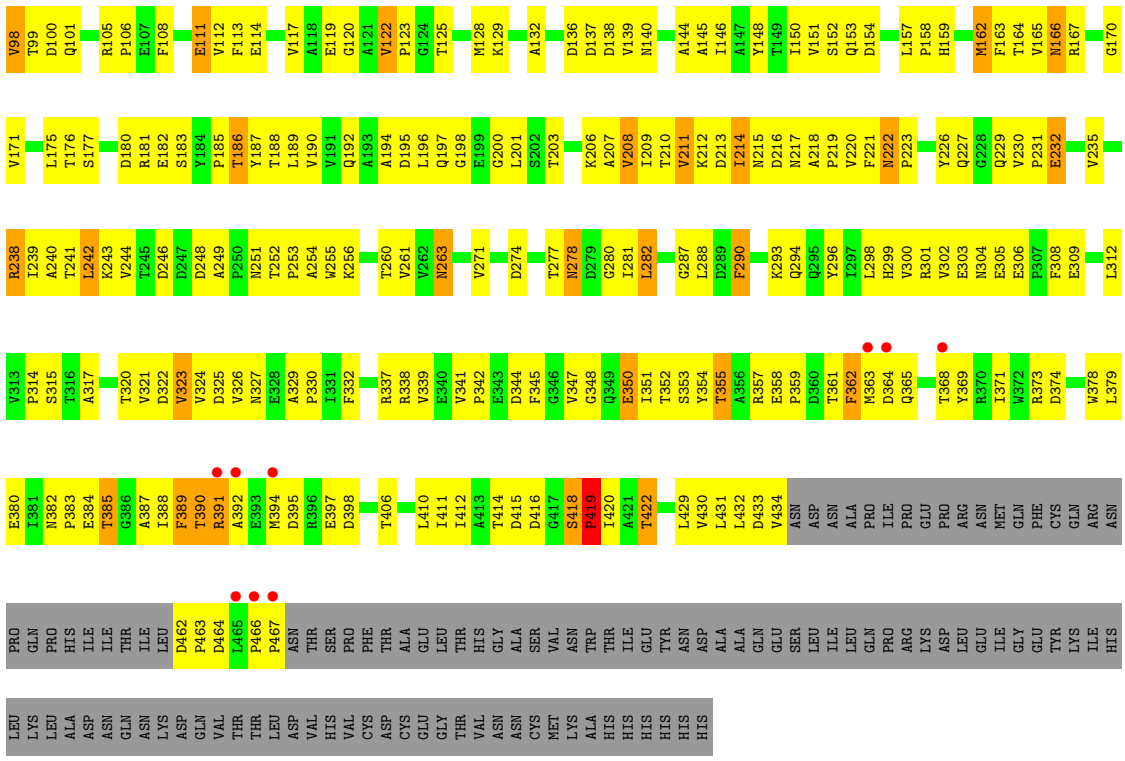


• Molecule 1: Cadherin-1

Chain B:






V98 T99 D100 Q101 R105 P106 E107 F108 E111 V112 F113 E114 V117 A118 E119 G120 A121 V122 P123 G124 T125 M128 K129 A132 D136 D137 D138 V139 N140 A144 A145 I146 A147 Y148 T149 I150 V151 S152 Q153 D154 L157 P158 H159 M162 F163 T164 V165 N166 R167 G170
V171 L175 T176 S177 D180 R181 E182 S183 Y184 P185 T186 Y187 T188 L189 V190 V191 Q192 A193 A194 D195 L196 Q197 G198 E199 G200 L201 S202 T203 K206 A207 V208 I209 T210 V211 K212 D213 I214 N215 D216 N217 A218 P219 V220 F221 N222 P223 Y226 Q227 G228 Q229 V230 P231 E232 V235
R238 I239 A240 T241 L242 K243 V244 T245 D246 D247 D248 A249 P250 N251 T252 P253 A254 W255 K256 T260 V261 V262 N263 V271 D274 T277 N278 D279 G280 I281 L282 G287 L288 D289 F290 K293 Q294 Q295 Y296 I297 L298 H299 V300 R301 V302 E303 N304 E305 E306 P307 F308 E309 L312
V313 P314 S315 T316 A317 T320 V321 D322 V323 V324 D325 V326 N327 E328 A329 P330 I331 F332 R337 R338 V339 E340 V341 P342 E343 D344 F345 G346 V347 G348 G349 E350 I351 T352 S353 Y354 T355 A356 R357 E358 P359 D360 T361 F362 M363 D364 Q365 T368 Y369 R370 I371 W372 R373 D374 W378 L379
E380 I381 N382 P383 E384 T385 G386 A387 I388 F389 T390 R391 A392 E393 M394 D395 R396 E397 D398 T406 L410 I411 I412 A413 T414 D415 D416 G417 S418 P419 I420 A421 T422 L429 V430 L431 L432 D433 V434 ASN ASP ASN ALA PRO ILE PRO GLU PRO ARG ASN MET GLN PHE CYS GLN ARG ASN
PRO GLN PRO HIS ILE ILE THR ILE LEU D462 P463 D464 L465 P466 P467 ASN THR SER PRO PHE THR ALA GLU LEU THR HIS GLY ALA SER VAL ASN TRP THR ILE GLU TYR ASN ASP ALA ALA GLN GLU SER LEU ILE LEU GLN PRO ARG LYS ASP LEU GLU ILE GLY GLU TYR LYS ILE HIS
LEU LYS LEU ALA ASP ASN GLN ASN LYS ASP GLN VAL THR THR LEU ASP VAL HIS VAL CYS ASP CYS GLU GLY THR VAL ASN ASN CYS MET LYS ALA HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.14Å 79.70Å 176.00Å 90.00° 98.56° 90.00°	Depositor
Resolution (Å)	19.92 – 3.40 29.78 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.92-3.40) 99.6 (29.78-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.230 , 0.293 0.229 , 0.287	Depositor DCC
R_{free} test set	1254 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 71.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7871	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MAN, CA, MN

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	0.45	0/4200	0.71	10/5755 (0.2%)
1	B	0.47	1/3469 (0.0%)	0.67	3/4752 (0.1%)
All	All	0.46	1/7669 (0.0%)	0.69	13/10507 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	419	PRO	N-CD	5.03	1.54	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	492	ALA	N-CA-CB	-11.52	93.98	110.10
1	A	452	ASN	N-CA-CB	7.71	124.47	110.60
1	A	452	ASN	N-CA-C	-7.34	91.18	111.00
1	B	419	PRO	N-CA-C	-6.72	94.62	112.10
1	B	418	SER	C-N-CD	-5.80	107.84	120.60
1	A	479	GLY	N-CA-C	5.72	127.40	113.10
1	B	419	PRO	CB-CA-C	5.68	126.21	112.00
1	A	232	GLU	N-CA-C	5.56	126.02	111.00
1	A	492	ALA	N-CA-C	5.40	125.59	111.00
1	A	470	SER	N-CA-C	5.18	124.97	111.00
1	A	235	VAL	CB-CA-C	-5.13	101.65	111.40
1	A	233	ASN	N-CA-C	5.08	124.71	111.00
1	A	236	ASN	N-CA-C	5.02	124.55	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	4113	0	3949	353	0
1	B	3399	0	3284	269	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	99	0	90	1	0
4	B	99	0	90	5	0
5	A	55	0	0	1	0
5	B	80	0	0	0	0
All	All	7871	0	7413	612	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 (612) 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:483:ASN:CG	1:A:502:LYS:HB2	1.46	1.33
1:A:483:ASN:OD1	1:A:502:LYS:HB2	1.23	1.31
1:B:418:SER:HB2	1:B:419:PRO:CD	1.61	1.30
1:A:483:ASN:OD1	1:A:502:LYS:CB	1.81	1.29
1:B:418:SER:HB2	1:B:419:PRO:HD2	1.23	1.15
1:B:418:SER:CB	1:B:419:PRO:HD3	1.76	1.15
1:A:483:ASN:ND2	1:A:502:LYS:HB2	1.60	1.13
1:B:232:GLU:O	1:B:288:LEU:O	1.65	1.11
1:B:314:PRO:HB2	4:B:804:MAN:O6	1.52	1.08
1:B:186:THR:HG22	1:B:210:THR:HG22	1.34	1.04
1:B:418:SER:CB	1:B:419:PRO:CD	2.24	1.03
1:A:222:ASN:HB3	1:A:223:PRO:HD3	1.39	1.02
1:A:483:ASN:ND2	1:A:502:LYS:CB	2.23	1.01
1:A:483:ASN:HD21	1:A:502:LYS:CB	1.74	0.99
1:B:186:THR:CG2	1:B:210:THR:HG22	1.94	0.97
1:A:27:ASN:HD21	1:B:1:ASP:N	1.60	0.97
1:A:28:ARG:HD3	1:A:88:VAL:HG13	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:THR:OG1	1:B:422:THR:HG23	1.64	0.97
1:A:483:ASN:HA	1:A:501:ARG:HB3	1.44	0.97
1:A:483:ASN:CG	1:A:502:LYS:CB	2.28	0.96
1:A:490:ASP:CB	1:A:494:GLU:HG2	1.96	0.96
1:A:435:ASN:OD1	1:A:468:ASN:HB3	1.69	0.93
1:A:36:TYR:O	1:A:55:ARG:HD2	1.68	0.92
1:B:358:GLU:OE2	1:B:365:GLN:OE1	1.88	0.92
1:A:340:GLU:HA	1:A:430:VAL:HG13	1.52	0.91
1:A:414:THR:HG22	1:A:422:THR:CG2	1.99	0.91
1:A:442:GLU:HB2	1:A:459:THR:HB	1.51	0.91
1:A:442:GLU:HB3	1:A:443:PRO:HD3	1.53	0.91
1:A:27:ASN:HD21	1:B:1:ASP:H2	1.03	0.91
1:B:418:SER:HB3	1:B:419:PRO:HD3	1.51	0.90
1:B:256:LYS:HB2	1:B:305:GLU:OE2	1.73	0.89
1:A:483:ASN:OD1	1:A:502:LYS:CG	2.19	0.88
1:A:484:TRP:CZ2	1:A:511:ILE:HD11	2.08	0.88
1:A:452:ASN:HB3	1:A:535:GLU:O	1.75	0.87
1:A:154:ASP:HB3	1:A:188:THR:HG22	1.55	0.86
1:A:189:LEU:HB2	1:A:207:ALA:HB3	1.56	0.86
1:B:120:GLY:H	1:B:214:ILE:HD12	1.40	0.85
1:B:68:ARG:HD3	1:B:100:ASP:OD1	1.75	0.85
1:A:509:TYR:CZ	1:A:529:VAL:HB	2.12	0.84
1:A:414:THR:HG22	1:A:422:THR:HG21	1.58	0.84
1:B:220:VAL:O	1:B:244:VAL:HA	1.79	0.83
1:A:301:ARG:HD3	4:A:804:MAN:H3	1.60	0.83
1:B:221:PHE:CZ	1:B:302:VAL:HG13	2.13	0.83
1:A:483:ASN:CG	1:A:502:LYS:H	1.82	0.83
1:A:232:GLU:O	1:A:288:LEU:O	1.97	0.82
1:B:119:GLU:HG3	1:B:181:ARG:H	1.42	0.82
1:B:406:THR:HG22	1:B:430:VAL:HG22	1.61	0.81
1:A:360:ASP:HB3	1:A:362:PHE:CE2	2.15	0.81
1:A:483:ASN:CG	1:A:502:LYS:N	2.34	0.81
1:A:119:GLU:HG3	1:A:181:ARG:H	1.46	0.80
1:B:137:ASP:HB2	1:B:139:VAL:HG12	1.64	0.80
1:B:263:ASN:H	1:B:263:ASN:HD22	1.26	0.80
1:A:46:PRO:HA	1:A:47:PRO:C	2.02	0.80
1:B:378:TRP:CE3	1:B:394:MET:HG2	2.17	0.80
1:A:478:HIS:HB2	1:A:512:HIS:HB2	1.64	0.80
1:A:3:VAL:HG22	1:A:4:ILE:H	1.47	0.79
1:A:480:ALA:O	1:A:484:TRP:HB2	1.81	0.79
1:B:158:PRO:HG2	1:B:162:MET:HE1	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:THR:HA	1:A:422:THR:HG22	1.65	0.79
1:B:21:LEU:HD12	1:B:60:LEU:HD22	1.65	0.78
1:A:483:ASN:ND2	1:A:502:LYS:CA	2.45	0.78
1:B:152:SER:HB3	1:B:190:VAL:HG12	1.65	0.78
1:A:483:ASN:HA	1:A:501:ARG:CB	2.14	0.77
1:B:277:THR:O	1:B:278:ASN:ND2	2.17	0.77
1:B:72:ALA:HA	1:B:98:VAL:HG13	1.67	0.77
1:B:314:PRO:CB	4:B:804:MAN:O6	2.33	0.77
1:A:112:VAL:HG22	1:A:206:LYS:HB2	1.65	0.77
1:A:27:ASN:ND2	1:B:1:ASP:N	2.32	0.76
1:A:340:GLU:HB3	1:A:432:LEU:HD11	1.66	0.76
1:A:347:VAL:O	1:A:390:THR:HB	1.85	0.76
1:A:483:ASN:OD1	1:A:502:LYS:HG3	1.86	0.76
1:A:489:ASN:HB2	1:A:497:ILE:HG13	1.66	0.76
1:A:484:TRP:HA	1:A:484:TRP:CE3	2.22	0.74
1:B:263:ASN:HD21	1:B:298:LEU:HB2	1.52	0.74
1:B:194:ALA:HB3	1:B:198:GLY:HA2	1.68	0.74
1:B:113:PHE:O	1:B:207:ALA:HA	1.88	0.74
1:B:351:ILE:HD12	1:B:388:ILE:HG22	1.69	0.74
1:B:215:ASN:O	1:B:309:GLU:HG3	1.87	0.74
1:A:483:ASN:O	1:A:484:TRP:CE3	2.40	0.74
1:B:242:LEU:HD12	1:B:280:GLY:HA3	1.70	0.73
1:A:474:ALA:HB2	1:A:515:LEU:HD23	1.70	0.73
1:A:232:GLU:CD	1:A:290:PHE:H	1.91	0.73
1:B:195:ASP:OD1	1:B:201:LEU:HB2	1.88	0.73
1:A:239:ILE:HD11	1:A:282:LEU:HD13	1.71	0.72
1:A:414:THR:HG22	1:A:422:THR:HG22	1.70	0.72
1:A:443:PRO:HD2	1:A:458:ILE:HG23	1.69	0.72
1:A:263:ASN:N	1:A:263:ASN:HD22	1.83	0.72
1:A:480:ALA:C	1:A:484:TRP:HB2	2.10	0.72
1:A:41[B]:GLN:CD	1:A:41[B]:GLN:H	1.91	0.72
1:B:263:ASN:H	1:B:263:ASN:ND2	1.88	0.72
1:A:128:MET:HE3	1:A:207:ALA:HB1	1.71	0.72
1:A:462:ASP:HB3	1:A:469:THR:HG23	1.72	0.71
1:A:480:ALA:HA	1:A:484:TRP:CD1	2.26	0.70
1:A:224:SER:O	1:A:317:ALA:HB1	1.91	0.70
1:B:217:ASN:HB2	1:B:248:ASP:OD1	1.91	0.70
1:B:232:GLU:O	1:B:288:LEU:C	2.29	0.70
1:B:185:PRO:HA	1:B:211:VAL:HG13	1.72	0.70
1:A:117:VAL:HB	1:A:127:VAL:HG13	1.73	0.70
1:A:341:VAL:HG13	1:A:342:PRO:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:MET:C	1:A:529:VAL:HG13	2.13	0.69
1:B:242:LEU:CD1	1:B:280:GLY:HA3	2.22	0.69
1:A:230:VAL:CG1	1:A:239:ILE:HG22	2.23	0.69
1:A:484:TRP:HA	1:A:484:TRP:HE3	1.54	0.69
1:B:117:VAL:O	1:B:212:LYS:HG2	1.93	0.69
1:B:176:THR:HG22	1:B:177:SER:H	1.57	0.69
1:A:155:PRO:HD2	1:A:187:TYR:CE1	2.28	0.69
1:A:372:TRP:HB2	1:A:412:ILE:HG23	1.74	0.69
1:B:72:ALA:HA	1:B:98:VAL:CG1	2.23	0.68
1:B:145:ALA:O	1:B:195:ASP:HA	1.92	0.68
1:B:186:THR:HG22	1:B:210:THR:CG2	2.18	0.68
1:A:476:LEU:HD22	1:A:511:ILE:HG22	1.74	0.68
1:A:442:GLU:CB	1:A:459:THR:HB	2.23	0.68
1:A:483:ASN:ND2	1:A:502:LYS:C	2.46	0.68
1:B:138:ASP:HB3	1:B:144:ALA:HB3	1.74	0.67
1:A:127:VAL:HG23	1:A:173:SER:HA	1.75	0.67
1:A:264:ASP:N	1:A:265:PRO:HD3	2.10	0.67
1:B:263:ASN:HD22	1:B:263:ASN:N	1.89	0.67
1:A:483:ASN:CG	1:A:502:LYS:CA	2.63	0.66
1:B:114:GLU:HB3	1:B:208:VAL:HG23	1.77	0.66
1:B:111:GLU:CD	1:B:111:GLU:H	2.00	0.65
1:A:57:THR:HB	1:A:59:TRP:CD1	2.31	0.65
1:A:214:ILE:HG12	1:A:309:GLU:HG3	1.78	0.65
1:A:3:VAL:HG22	1:A:4:ILE:N	2.12	0.65
1:A:74:TYR:HB2	1:A:96:ILE:HB	1.78	0.65
1:A:246:ASP:OD2	1:A:255:TRP:HA	1.95	0.65
1:A:446:MET:O	1:A:529:VAL:HG13	1.96	0.65
1:A:7:ILE:HD12	1:A:7:ILE:H	1.61	0.65
1:A:57:THR:HB	1:A:59:TRP:HD1	1.62	0.65
1:A:448:PHE:CE1	1:A:500:PRO:HD3	2.31	0.64
1:A:474:ALA:CB	1:A:515:LEU:HD23	2.27	0.64
1:B:152:SER:HB3	1:B:190:VAL:CG1	2.27	0.64
1:A:298:LEU:CD1	1:A:319:VAL:HG13	2.27	0.64
1:A:121:ALA:HB1	1:A:125:THR:HG21	1.79	0.64
1:A:480:ALA:HA	1:A:484:TRP:HB2	1.79	0.64
1:A:239:ILE:HG12	1:A:282:LEU:HB3	1.80	0.64
1:B:290:PHE:CD2	1:B:325:ASP:CA	2.80	0.64
1:B:290:PHE:CE2	1:B:325:ASP:N	2.67	0.63
1:A:274:ASP:CG	1:A:277:THR:HG22	2.18	0.63
1:A:480:ALA:CA	1:A:484:TRP:HB2	2.28	0.63
1:A:111:GLU:CD	1:A:111:GLU:H	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:THR:HA	1:A:495:SER:HB3	1.81	0.63
1:B:290:PHE:CD2	1:B:325:ASP:N	2.66	0.63
1:A:185:PRO:HA	1:A:211:VAL:HG23	1.79	0.63
1:B:263:ASN:ND2	1:B:298:LEU:HB2	2.13	0.63
1:A:10:PRO:HA	1:A:99:THR:OG1	1.99	0.63
1:A:236:ASN:HA	1:A:284:THR:H	1.63	0.63
1:A:119:GLU:HB2	1:A:212:LYS:O	1.99	0.63
1:B:166:ASN:C	1:B:166:ASN:HD22	2.02	0.63
1:B:342:PRO:HB3	1:B:434:VAL:HG21	1.81	0.63
1:B:232:GLU:C	1:B:288:LEU:O	2.37	0.62
1:A:458:ILE:O	1:A:495:SER:HB2	1.99	0.62
1:A:231:PRO:HA	1:A:324:VAL:HB	1.80	0.62
1:B:148:TYR:HA	1:B:192:GLN:O	2.00	0.62
1:A:78:SER:O	1:A:91:PRO:HA	2.00	0.62
1:A:329:ALA:HA	1:A:421:ALA:HB1	1.82	0.62
1:A:483:ASN:HD21	1:A:502:LYS:C	2.04	0.62
1:B:10:PRO:HA	1:B:99:THR:OG1	2.00	0.61
1:A:483:ASN:OD1	1:A:502:LYS:N	2.32	0.61
1:A:483:ASN:HD21	1:A:502:LYS:CA	2.12	0.61
1:B:369:TYR:O	1:B:383:PRO:HA	1.99	0.61
1:B:11:GLU:HG3	1:B:68:ARG:H	1.64	0.61
1:B:395:ASP:HB3	1:B:398:ASP:HB2	1.83	0.61
1:A:159:HIS:HB3	5:A:586:HOH:O	2.00	0.61
1:A:230:VAL:HG11	1:A:239:ILE:HG22	1.83	0.61
1:B:290:PHE:CE2	1:B:325:ASP:HB2	2.36	0.61
1:A:38:ILE:HA	1:A:77:TYR:O	2.01	0.60
1:A:480:ALA:HA	1:A:484:TRP:CB	2.30	0.60
1:A:143:ASN:HD22	1:A:196:LEU:HD21	1.64	0.60
1:A:474:ALA:HA	1:A:514:LYS:O	2.01	0.60
1:B:290:PHE:HE1	1:B:294:GLN:HG3	1.66	0.60
1:B:128:MET:HE2	1:B:207:ALA:HB1	1.84	0.60
1:A:119:GLU:OE1	1:A:214:ILE:HG22	2.01	0.60
1:A:343:GLU:OE1	1:A:395:ASP:OD1	2.20	0.60
1:B:108:PHE:HA	1:B:132:ALA:HA	1.84	0.60
1:A:73:LYS:HD2	1:A:95:VAL:HG13	1.83	0.60
1:A:374:ASP:HB2	1:A:407:TYR:OH	2.01	0.60
1:A:221:PHE:CE2	1:A:302:VAL:HG12	2.37	0.60
1:A:448:PHE:HE1	1:A:500:PRO:HD3	1.67	0.60
1:A:122:VAL:HG23	1:A:125:THR:HB	1.82	0.60
1:A:298:LEU:HD12	1:A:319:VAL:O	2.02	0.60
1:A:480:ALA:HA	1:A:484:TRP:HD1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:CD	1:A:243:LYS:HB2	2.32	0.60
1:B:344:ASP:OD1	1:B:434:VAL:HG11	2.02	0.60
1:A:483:ASN:OD1	1:A:502:LYS:CA	2.50	0.60
1:A:119:GLU:OE2	1:A:182:GLU:OE2	2.21	0.59
1:A:145:ALA:O	1:A:195:ASP:HA	2.03	0.59
1:A:105:ARG:HD3	1:A:203:THR:HG22	1.84	0.59
1:A:222:ASN:HB3	1:A:223:PRO:CD	2.23	0.59
1:A:345:PHE:CE2	1:A:349:GLN:HB2	2.37	0.59
1:B:249:ALA:O	1:B:255:TRP:HB2	2.03	0.59
1:B:337:ARG:HB2	1:B:354:TYR:CE1	2.37	0.59
1:A:429:LEU:HD21	1:A:431:LEU:HD21	1.84	0.59
1:B:378:TRP:HA	1:B:392:ALA:HB3	1.84	0.59
1:B:226:TYR:CE1	1:B:242:LEU:HA	2.37	0.59
1:B:241:THR:HA	1:B:280:GLY:O	2.03	0.59
1:B:100:ASP:OD2	1:B:136:ASP:HB3	2.02	0.59
1:A:340:GLU:HA	1:A:430:VAL:CG1	2.31	0.58
1:B:218:ALA:HB2	1:B:308:PHE:HE2	1.68	0.58
1:A:376:ALA:HB2	1:A:401:HIS:CD2	2.39	0.58
1:A:382:ASN:ND2	1:A:385:THR:H	2.01	0.58
1:A:489:ASN:CG	1:A:497:ILE:HD11	2.23	0.58
1:B:68:ARG:NH1	1:B:100:ASP:OD1	2.36	0.58
1:B:288:LEU:HD22	1:B:296:TYR:CE2	2.38	0.58
1:B:361:THR:HG22	1:B:361:THR:O	2.03	0.58
1:A:381:ILE:O	1:A:383:PRO:HD3	2.03	0.58
1:A:511:ILE:O	1:A:527:LEU:HD12	2.03	0.57
1:B:68:ARG:NH1	1:B:69:GLU:OE2	2.37	0.57
1:B:235:VAL:HG22	1:B:287:GLY:N	2.19	0.57
1:B:344:ASP:OD1	1:B:434:VAL:CG1	2.52	0.57
1:A:513:LEU:O	1:A:523:GLN:HA	2.04	0.57
1:B:330:PRO:HA	1:B:359:PRO:CD	2.35	0.57
1:A:440:ILE:HG22	1:A:441:PRO:HD2	1.87	0.57
1:B:358:GLU:CD	1:B:365:GLN:OE1	2.43	0.57
1:B:112:VAL:HG22	1:B:206:LYS:HB2	1.87	0.57
1:B:246:ASP:OD2	1:B:304:ASN:ND2	2.35	0.57
1:A:409:ALA:HB3	1:A:427:LEU:HB3	1.86	0.56
1:A:186:THR:HG22	1:A:210:THR:HG22	1.88	0.56
1:A:297:ILE:HG12	1:A:320:THR:HG23	1.87	0.56
1:B:348:GLY:N	1:B:390:THR:O	2.38	0.56
1:A:402:VAL:HG12	1:A:404:ASN:O	2.06	0.56
1:A:472:PHE:HD2	1:A:493:GLN:O	1.88	0.56
1:B:290:PHE:CE1	1:B:294:GLN:HG3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ILE:HG23	1:B:422:THR:HG22	1.87	0.56
1:A:350:GLU:HA	1:A:389:PHE:HA	1.87	0.56
1:B:301:ARG:HD3	4:B:804:MAN:H61	1.88	0.56
1:A:341:VAL:O	1:A:431:LEU:HA	2.04	0.56
1:A:360:ASP:HB3	1:A:362:PHE:HE2	1.69	0.56
1:A:484:TRP:CE2	1:A:511:ILE:CD1	2.89	0.56
1:A:71:ILE:HG21	1:A:74:TYR:CE2	2.41	0.56
1:A:509:TYR:OH	1:A:529:VAL:HB	2.06	0.56
1:A:263:ASN:N	1:A:263:ASN:ND2	2.53	0.56
1:B:215:ASN:HB2	1:B:254:ALA:CB	2.36	0.56
1:B:368:THR:CG2	1:B:414:THR:HB	2.36	0.56
1:A:218:ALA:HA	1:A:308:PHE:HE1	1.71	0.56
1:A:382:ASN:HD22	1:A:385:THR:H	1.52	0.56
1:B:290:PHE:CD2	1:B:325:ASP:HA	2.41	0.56
1:A:489:ASN:HB2	1:A:497:ILE:CG1	2.36	0.55
1:A:478:HIS:CB	1:A:512:HIS:HB2	2.35	0.55
1:A:236:ASN:N	1:A:284:THR:O	2.39	0.55
1:A:447:GLN:O	1:A:447:GLN:HG2	2.04	0.55
1:B:374:ASP:OD2	1:B:379:LEU:HB2	2.05	0.55
1:A:239:ILE:HD11	1:A:282:LEU:HD22	1.89	0.55
1:B:229:GLN:HA	1:B:322:ASP:O	2.06	0.55
1:A:298:LEU:HD13	1:A:319:VAL:HG13	1.89	0.55
1:A:230:VAL:HG13	1:A:239:ILE:HG22	1.88	0.55
1:B:11:GLU:HG2	1:B:67:ASP:HA	1.88	0.55
1:B:122:VAL:HG23	1:B:125:THR:HB	1.89	0.55
1:A:418:SER:CB	1:A:419:PRO:HD3	2.37	0.55
1:A:274:ASP:O	1:A:278:ASN:N	2.34	0.55
1:A:370:ARG:HD2	1:A:412:ILE:HD11	1.89	0.55
1:B:299:HIS:CD2	4:B:805:MAN:H2	2.42	0.55
1:A:441:PRO:HD3	1:A:524:VAL:HG21	1.89	0.55
1:B:119:GLU:OE1	1:B:182:GLU:OE1	2.25	0.55
1:A:104:ASN:HB2	1:A:136:ASP:OD1	2.07	0.54
1:B:41:GLN:HG2	1:B:45:LYS:HB3	1.90	0.54
1:A:299:HIS:HB3	1:A:316:THR:HG21	1.88	0.54
1:A:341:VAL:HG13	1:A:345:PHE:CD1	2.42	0.54
1:A:229:GLN:HA	1:A:322:ASP:O	2.08	0.54
1:A:382:ASN:HD21	1:A:384:GLU:HB2	1.72	0.54
1:B:114:GLU:CB	1:B:208:VAL:HG23	2.38	0.54
1:A:332:PHE:HA	1:A:356:ALA:HA	1.89	0.54
1:A:488:TYR:HA	1:A:496:LEU:HB3	1.88	0.54
1:A:27:ASN:ND2	1:B:1:ASP:H3	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASN:N	1:B:222:ASN:HD22	2.06	0.54
1:A:517:ASP:OD2	1:A:517:ASP:N	2.41	0.54
1:A:346:GLY:HA3	1:A:349:GLN:HG3	1.89	0.54
1:A:382:ASN:ND2	1:A:384:GLU:HB2	2.22	0.54
1:A:126:SER:HA	1:A:173:SER:HB3	1.89	0.53
1:A:157:LEU:HA	1:A:159:HIS:N	2.22	0.53
1:A:189:LEU:CD1	1:A:209:ILE:HD11	2.37	0.53
1:A:337:ARG:HD3	1:A:352:THR:HG21	1.90	0.53
1:A:269:PHE:CD1	1:A:284:THR:HG22	2.42	0.53
1:A:269:PHE:HA	1:A:284:THR:HA	1.90	0.53
1:A:5:PRO:HG2	1:B:23:GLN:HG3	1.90	0.53
1:A:119:GLU:HG3	1:A:181:ARG:N	2.19	0.53
1:A:489:ASN:H	1:A:496:LEU:HA	1.74	0.53
1:A:329:ALA:CA	1:A:421:ALA:HB1	2.38	0.53
1:B:100:ASP:O	1:B:101:GLN:HG2	2.09	0.53
1:A:470:SER:O	1:A:472:PHE:N	2.41	0.53
1:B:209:ILE:N	1:B:209:ILE:HD12	2.24	0.53
1:B:362:PHE:C	1:B:364:ASP:H	2.09	0.53
1:B:21:LEU:HD12	1:B:60:LEU:CD2	2.36	0.53
1:B:239:ILE:HG21	1:B:321:VAL:HG22	1.89	0.53
1:A:47:PRO:HB2	1:A:50:VAL:HG21	1.90	0.52
1:B:17:PHE:CB	1:B:18:PRO:HA	2.40	0.52
1:A:274:ASP:HB3	1:A:277:THR:CG2	2.39	0.52
1:B:223:PRO:O	1:B:226:TYR:CE2	2.62	0.52
1:A:47:PRO:HB2	1:A:50:VAL:CG2	2.39	0.52
1:B:274:ASP:O	1:B:278:ASN:N	2.41	0.52
1:B:325:ASP:CG	1:B:362:PHE:HE1	2.13	0.52
1:A:369:TYR:O	1:A:383:PRO:HA	2.10	0.52
1:A:68:ARG:HD3	1:A:100:ASP:OD2	2.10	0.52
1:B:380:GLU:OE1	1:B:391:ARG:HG2	2.10	0.52
1:B:11:GLU:HB2	1:B:99:THR:O	2.10	0.52
1:B:153:GLN:NE2	1:B:159:HIS:O	2.43	0.52
1:A:44:ASP:OD1	1:A:45:LYS:N	2.42	0.52
1:A:478:HIS:CG	1:A:512:HIS:HB2	2.45	0.52
1:A:484:TRP:CZ2	1:A:511:ILE:CD1	2.89	0.52
1:A:511:ILE:HB	1:A:527:LEU:HD13	1.91	0.52
1:B:368:THR:HG23	1:B:368:THR:O	2.10	0.52
1:A:330:PRO:HG3	1:A:358:GLU:OE2	2.10	0.52
1:A:479:GLY:O	1:A:480:ALA:HB3	2.10	0.52
1:B:299:HIS:HA	1:B:317:ALA:O	2.10	0.52
1:A:36:TYR:O	1:A:55:ARG:CD	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:HG3	1:A:337:ARG:HH11	1.75	0.51
1:B:244:VAL:HG11	1:B:302:VAL:HG11	1.92	0.51
1:A:264:ASP:CG	1:A:264:ASP:O	2.46	0.51
1:A:345:PHE:CD2	1:A:349:GLN:HB2	2.46	0.51
1:B:119:GLU:HB2	1:B:212:LYS:O	2.10	0.51
1:A:254:ALA:C	1:A:304:ASN:OD1	2.49	0.51
1:B:238:ARG:NH1	1:B:281:ILE:HD12	2.25	0.51
1:A:439:PRO:HB2	1:A:515:LEU:HB2	1.92	0.51
1:A:480:ALA:O	1:A:482:VAL:N	2.44	0.51
1:B:17:PHE:HB3	1:B:18:PRO:HA	1.91	0.51
1:B:232:GLU:HB2	1:B:288:LEU:O	2.10	0.51
1:B:290:PHE:CD1	1:B:290:PHE:C	2.83	0.51
1:A:41[A]:GLN:HA	1:A:45:LYS:O	2.10	0.51
1:B:345:PHE:HZ	1:B:350:GLU:O	1.94	0.51
1:A:476:LEU:HD22	1:A:511:ILE:CG2	2.39	0.51
1:A:51:PHE:CZ	1:A:66:LEU:HD11	2.46	0.51
1:A:232:GLU:HG3	1:A:289:ASP:HA	1.91	0.51
1:A:442:GLU:N	1:A:459:THR:O	2.44	0.51
1:B:145:ALA:HB1	1:B:197:GLN:HG3	1.92	0.51
1:B:327:ASN:ND2	1:B:415:ASP:OD1	2.43	0.51
1:A:186:THR:HA	1:A:210:THR:HA	1.92	0.50
1:A:376:ALA:HB2	1:A:401:HIS:NE2	2.25	0.50
1:B:119:GLU:OE1	1:B:216:ASP:OD2	2.30	0.50
1:B:314:PRO:HB2	4:B:804:MAN:HO6	1.73	0.50
1:A:11:GLU:OE1	1:A:103:ASP:OD1	2.29	0.50
1:A:226:TYR:HB2	1:A:319:VAL:HB	1.93	0.50
1:A:232:GLU:CG	1:A:289:ASP:HA	2.41	0.50
1:B:23:GLN:HB3	1:B:59:TRP:CD2	2.46	0.50
1:B:414:THR:OG1	1:B:422:THR:CG2	2.50	0.50
1:B:181:ARG:HD2	1:B:213:ASP:HA	1.94	0.50
1:A:256:LYS:O	1:A:304:ASN:ND2	2.45	0.50
1:A:223:PRO:HD2	1:A:243:LYS:HB2	1.94	0.50
1:A:215:ASN:ND2	1:A:308:PHE:HA	2.27	0.50
1:A:157:LEU:HA	1:A:158:PRO:C	2.32	0.49
1:B:371:ILE:HG13	1:B:410:LEU:O	2.12	0.49
1:A:236:ASN:HB2	1:A:283:LYS:HD3	1.93	0.49
1:A:390:THR:HG23	1:A:394:MET:HE3	1.94	0.49
1:B:151:VAL:HG23	1:B:190:VAL:HG13	1.94	0.49
1:B:176:THR:HG22	1:B:177:SER:N	2.26	0.49
1:B:230:VAL:O	1:B:323:VAL:HA	2.12	0.49
1:A:166:ASN:O	1:A:167:ARG:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ILE:HG22	1:B:412:ILE:N	2.28	0.49
1:A:128:MET:CE	1:A:207:ALA:HB1	2.41	0.49
1:A:242:LEU:HD12	1:A:271:VAL:HG21	1.95	0.49
1:B:327:ASN:OD1	1:B:415:ASP:OD1	2.31	0.49
1:A:35:PHE:HE2	1:A:83:SER:HB3	1.78	0.49
1:B:214:ILE:O	1:B:216:ASP:N	2.45	0.49
1:B:341:VAL:O	1:B:431:LEU:HA	2.12	0.49
1:B:352:THR:HG22	1:B:353:SER:N	2.27	0.49
1:B:373:ARG:HB3	1:B:410:LEU:H	1.78	0.49
1:A:22:VAL:HG12	1:A:23:GLN:H	1.77	0.49
1:A:277:THR:O	1:A:278:ASN:ND2	2.32	0.49
1:A:438:ALA:HB2	1:A:520:ASN:ND2	2.28	0.49
1:B:9:CYS:SG	1:B:13:GLU:OE2	2.71	0.49
1:B:220:VAL:O	1:B:244:VAL:CA	2.56	0.49
1:A:468:ASN:O	1:A:517:ASP:OD1	2.31	0.49
1:A:489:ASN:ND2	1:A:497:ILE:HD11	2.28	0.49
1:B:120:GLY:N	1:B:214:ILE:HD12	2.20	0.49
1:A:346:GLY:CA	1:A:349:GLN:HG3	2.42	0.48
1:A:484:TRP:CE2	1:A:511:ILE:HD11	2.47	0.48
1:B:271:VAL:HA	1:B:281:ILE:O	2.13	0.48
1:A:224:SER:O	1:A:317:ALA:CB	2.60	0.48
1:A:350:GLU:HA	1:A:389:PHE:HB3	1.96	0.48
1:A:521:LYS:HD3	1:A:521:LYS:N	2.28	0.48
1:A:3:VAL:CG2	1:A:4:ILE:H	2.22	0.48
1:A:437:ASN:HB2	1:A:464:ASP:OD2	2.13	0.48
1:B:358:GLU:HA	1:B:358:GLU:OE1	2.11	0.48
1:B:24:ILE:HD11	1:B:53:ILE:CD1	2.44	0.48
1:B:67:ASP:O	1:B:70:ALA:HB3	2.14	0.48
1:A:214:ILE:HG23	1:A:216:ASP:HB3	1.96	0.48
1:A:264:ASP:OD2	1:A:267:GLN:HA	2.13	0.48
1:A:409:ALA:O	1:A:410:LEU:HD23	2.14	0.48
1:B:215:ASN:HB2	1:B:254:ALA:HB1	1.95	0.48
1:B:221:PHE:HA	1:B:243:LYS:O	2.13	0.48
1:A:20:ASN:HA	1:A:61:LYS:HB3	1.95	0.48
1:A:223:PRO:HD2	1:A:226:TYR:OH	2.14	0.48
1:A:298:LEU:HD12	1:A:298:LEU:H	1.78	0.48
1:A:481:SER:O	1:A:483:ASN:N	2.46	0.48
1:A:121:ALA:CB	1:A:125:THR:HG21	2.45	0.47
1:A:432:LEU:H	1:A:432:LEU:HD12	1.79	0.47
1:A:484:TRP:CE2	1:A:511:ILE:HD13	2.49	0.47
1:A:330:PRO:HA	1:A:359:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:HA	1:B:77:TYR:O	2.14	0.47
1:B:395:ASP:OD2	1:B:397:GLU:HB2	2.14	0.47
1:B:150:ILE:HG21	1:B:189:LEU:HD22	1.94	0.47
1:B:290:PHE:C	1:B:290:PHE:HD1	2.17	0.47
1:B:300:VAL:CG2	1:B:317:ALA:HB3	2.44	0.47
1:A:166:ASN:HB3	1:A:169:THR:HB	1.97	0.47
1:A:239:ILE:CD1	1:A:282:LEU:HD22	2.45	0.47
1:A:453:PRO:CB	1:A:500:PRO:HG2	2.45	0.47
1:A:474:ALA:HB2	1:A:515:LEU:CD2	2.43	0.47
1:B:263:ASN:OD1	1:B:298:LEU:HA	2.14	0.47
1:B:290:PHE:CD2	1:B:325:ASP:HB2	2.49	0.47
1:A:8:SER:HA	1:A:97:THR:O	2.15	0.47
1:A:184:TYR:O	1:A:211:VAL:HG21	2.15	0.47
1:B:62:VAL:HG21	1:B:66:LEU:HD11	1.97	0.47
1:A:80:ALA:HB3	1:A:89:GLU:HB2	1.96	0.47
1:A:148:TYR:HA	1:A:192:GLN:O	2.15	0.47
1:A:411:ILE:N	1:A:411:ILE:HD12	2.30	0.47
1:A:480:ALA:O	1:A:481:SER:C	2.52	0.47
1:B:303:GLU:HA	1:B:308:PHE:HE1	1.80	0.47
1:A:53:ILE:HG23	1:A:55:ARG:HH11	1.80	0.47
1:B:53:ILE:HA	1:B:59:TRP:O	2.14	0.47
1:A:53:ILE:HA	1:A:59:TRP:O	2.15	0.47
1:A:345:PHE:CE2	1:A:349:GLN:CB	2.98	0.47
1:A:475:GLU:O	1:A:513:LEU:HD12	2.14	0.46
1:A:509:TYR:CE2	1:A:511:ILE:HD11	2.49	0.46
1:B:114:GLU:HB3	1:B:208:VAL:CG2	2.43	0.46
1:B:187:TYR:N	1:B:209:ILE:O	2.39	0.46
1:B:312:LEU:N	1:B:312:LEU:HD12	2.30	0.46
1:A:232:GLU:HG3	1:A:290:PHE:N	2.30	0.46
1:B:122:VAL:O	1:B:125:THR:HB	2.16	0.46
1:B:339:VAL:HG23	1:B:429:LEU:HD12	1.97	0.46
1:B:341:VAL:HG21	1:B:429:LEU:HD11	1.97	0.46
1:A:166:ASN:C	1:A:166:ASN:HD22	2.19	0.46
1:B:148:TYR:CD2	1:B:170:GLY:HA2	2.51	0.46
1:B:414:THR:CG2	1:B:420:ILE:HG23	2.46	0.46
1:A:244:VAL:HG11	1:A:302:VAL:HG11	1.96	0.46
1:B:20:ASN:HA	1:B:61:LYS:HG2	1.96	0.46
1:B:119:GLU:HA	1:B:211:VAL:HG23	1.98	0.46
1:B:122:VAL:O	1:B:123:PRO:C	2.52	0.46
1:B:380:GLU:HB3	1:B:389:PHE:CE1	2.51	0.46
1:B:108:PHE:HE1	1:B:203:THR:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:PRO:HA	1:B:324:VAL:HG23	1.97	0.46
1:B:290:PHE:HE2	1:B:325:ASP:H	1.62	0.46
1:B:332:PHE:HD1	1:B:355:THR:O	1.99	0.46
1:A:24:ILE:HD12	1:B:2:TRP:CH2	2.51	0.46
1:A:192:GLN:HG2	1:A:193:ALA:N	2.31	0.46
1:B:46:PRO:HA	1:B:48:VAL:N	2.31	0.46
1:B:325:ASP:C	1:B:325:ASP:OD2	2.54	0.46
1:A:3:VAL:HG13	1:B:25:LYS:HD3	1.97	0.46
1:A:41[B]:GLN:H	1:A:41[B]:GLN:NE2	2.13	0.46
1:A:153:GLN:HE22	1:A:162:MET:HG2	1.81	0.46
1:A:236:ASN:HA	1:A:284:THR:O	2.16	0.45
1:A:350:GLU:HB2	1:A:389:PHE:HD2	1.81	0.45
1:A:29:ASP:HA	1:A:34:VAL:HG22	1.97	0.45
1:A:274:ASP:HB3	1:A:277:THR:HG22	1.98	0.45
1:A:485:THR:HG22	1:A:499:GLN:O	2.17	0.45
1:B:261:VAL:HG12	1:B:300:VAL:HG12	1.98	0.45
1:A:263:ASN:HD22	1:A:263:ASN:H	1.63	0.45
1:B:11:GLU:OE1	1:B:67:ASP:OD2	2.35	0.45
1:B:219:PRO:O	1:B:302:VAL:HG21	2.17	0.45
1:A:102:ASN:HA	1:A:136:ASP:OD2	2.16	0.45
1:A:374:ASP:OD1	1:A:377:ASN:HA	2.16	0.45
1:A:449:CYS:HB3	1:A:453:PRO:HA	1.97	0.45
1:B:145:ALA:HB3	1:B:197:GLN:H	1.80	0.45
1:A:67:ASP:OD2	1:A:69:GLU:N	2.50	0.44
1:B:119:GLU:HB3	1:B:214:ILE:HB	1.99	0.44
1:B:24:ILE:HD11	1:B:53:ILE:HD11	1.98	0.44
1:B:466:PRO:HA	1:B:467:PRO:C	2.37	0.44
1:A:67:ASP:OD2	1:A:67:ASP:C	2.55	0.44
1:B:347:VAL:HG12	1:B:392:ALA:O	2.18	0.44
1:A:45:LYS:O	1:A:47:PRO:O	2.35	0.44
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.35	0.44
1:A:480:ALA:HA	1:A:484:TRP:CG	2.53	0.44
1:B:11:GLU:CG	1:B:67:ASP:HA	2.46	0.44
1:B:129:LYS:HD3	1:B:171:VAL:HG22	2.00	0.44
1:B:406:THR:CG2	1:B:430:VAL:HG22	2.38	0.44
1:A:30:LYS:HD2	1:A:30:LYS:HA	1.84	0.44
1:A:38:ILE:HG23	1:A:53:ILE:HG21	1.99	0.44
1:A:155:PRO:HD2	1:A:187:TYR:CD1	2.53	0.44
1:A:188:THR:OG1	1:A:208:VAL:HG22	2.18	0.44
1:A:253:PRO:HB3	1:A:305:GLU:HG2	1.99	0.44
1:A:143:ASN:ND2	1:A:196:LEU:HD21	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLN:N	1:A:529:VAL:HG13	2.32	0.44
1:B:11:GLU:CG	1:B:68:ARG:H	2.28	0.44
1:B:332:PHE:CD1	1:B:355:THR:O	2.71	0.44
1:B:414:THR:HA	1:B:422:THR:HA	1.99	0.44
1:B:150:ILE:HG13	1:B:165:VAL:HG12	2.00	0.44
1:B:166:ASN:HD22	1:B:167:ARG:N	2.14	0.44
1:B:180:ASP:HB3	1:B:183:SER:HB3	2.00	0.44
1:B:214:ILE:O	1:B:214:ILE:HG22	2.18	0.44
1:B:232:GLU:O	1:B:288:LEU:N	2.51	0.44
1:A:274:ASP:CB	1:A:277:THR:HG22	2.48	0.44
1:A:331:ILE:CD1	1:A:359:PRO:HG3	2.48	0.44
1:A:358:GLU:HA	1:A:359:PRO:HD3	1.81	0.44
1:A:263:ASN:OD1	1:A:298:LEU:HA	2.18	0.44
1:A:472:PHE:H	1:A:493:GLN:CB	2.30	0.44
1:B:246:ASP:HB3	1:B:255:TRP:CD1	2.53	0.44
1:B:60:LEU:HD23	1:B:61:LYS:N	2.33	0.43
1:B:105:ARG:HB3	1:B:201:LEU:HD13	2.00	0.43
1:B:357:ARG:O	1:B:359:PRO:HD3	2.17	0.43
1:A:102:ASN:HB2	1:A:143:ASN:ND2	2.34	0.43
1:B:18:PRO:HB3	1:B:63:THR:HA	1.98	0.43
1:B:337:ARG:HA	1:B:337:ARG:HD2	1.88	0.43
1:B:379:LEU:N	1:B:379:LEU:HD12	2.32	0.43
1:A:456:HIS:O	1:A:497:ILE:HA	2.18	0.43
1:B:368:THR:HG23	1:B:414:THR:HB	1.99	0.43
1:A:2:TRP:CZ3	1:B:24:ILE:HD12	2.53	0.43
1:A:89:GLU:OE2	1:B:1:ASP:HA	2.18	0.43
1:A:89:GLU:HG2	1:B:2:TRP:CD1	2.53	0.43
1:A:221:PHE:HA	1:A:243:LYS:O	2.19	0.43
1:A:264:ASP:N	1:A:265:PRO:CD	2.78	0.43
1:B:50:VAL:HG22	1:B:64:GLN:NE2	2.33	0.43
1:B:253:PRO:HB2	1:B:306:GLU:HB2	2.01	0.43
1:A:341:VAL:HG21	1:A:351:ILE:HG23	2.00	0.43
1:B:337:ARG:HH22	1:B:352:THR:HG21	1.83	0.43
1:A:41[B]:GLN:HA	1:A:45:LYS:O	2.18	0.43
1:A:111:GLU:CD	1:A:111:GLU:N	2.69	0.43
1:A:483:ASN:HD21	1:A:502:LYS:HB3	1.74	0.43
1:A:106:PRO:O	1:A:203:THR:HG21	2.19	0.43
1:A:196:LEU:O	1:A:197:GLN:HB2	2.19	0.43
1:A:395:ASP:HB3	1:A:398:ASP:HB2	2.01	0.43
1:B:159:HIS:CD2	1:B:162:MET:CE	3.02	0.43
1:B:162:MET:HB3	1:B:163:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ALA:O	1:B:282:LEU:HB2	2.18	0.43
1:B:462:ASP:HA	1:B:463:PRO:HD3	1.79	0.43
1:A:77:TYR:HA	1:A:92:MET:O	2.18	0.43
1:A:186:THR:CG2	1:A:210:THR:HG22	2.49	0.43
1:A:290:PHE:CG	1:A:325:ASP:HB2	2.54	0.43
1:A:333:MET:HA	1:A:334:PRO:HA	1.85	0.43
1:B:63:THR:OG1	1:B:64:GLN:HG2	2.19	0.43
1:A:42:GLY:HA2	1:A:47:PRO:O	2.19	0.43
1:A:253:PRO:C	1:A:255:TRP:H	2.22	0.43
1:A:290:PHE:CD1	1:A:290:PHE:C	2.92	0.43
1:A:290:PHE:CD2	1:A:325:ASP:HB2	2.54	0.43
1:B:218:ALA:HA	1:B:219:PRO:HD3	1.77	0.43
1:B:255:TRP:C	1:B:304:ASN:ND2	2.71	0.43
1:B:290:PHE:HD2	1:B:325:ASP:N	2.16	0.43
1:A:148:TYR:N	1:A:167:ARG:O	2.51	0.42
1:A:154:ASP:HA	1:A:155:PRO:HA	1.71	0.42
1:A:370:ARG:HG3	1:A:412:ILE:HG12	2.01	0.42
1:A:439:PRO:HB2	1:A:515:LEU:CB	2.48	0.42
1:B:229:GLN:CA	1:B:322:ASP:O	2.66	0.42
1:B:239:ILE:HG21	1:B:321:VAL:CG2	2.48	0.42
1:B:327:ASN:HB3	1:B:419:PRO:HD2	2.00	0.42
1:B:120:GLY:H	1:B:214:ILE:CD1	2.22	0.42
1:A:438:ALA:HB1	1:A:522:ASP:HB2	2.01	0.42
1:B:152:SER:O	1:B:189:LEU:HD23	2.19	0.42
1:B:54:GLU:HB2	1:B:57:THR:OG1	2.19	0.42
1:B:51:PHE:CE2	1:B:74:TYR:CD2	3.07	0.42
1:B:432:LEU:HA	1:B:432:LEU:HD12	1.77	0.42
1:A:104:ASN:ND2	1:A:135:ALA:HB3	2.35	0.42
1:A:341:VAL:CG1	1:A:345:PHE:CD1	3.02	0.42
1:B:150:ILE:CG2	1:B:189:LEU:HD22	2.50	0.42
1:B:362:PHE:C	1:B:364:ASP:N	2.72	0.42
1:A:332:PHE:CZ	1:A:411:ILE:HG22	2.55	0.42
1:B:55:ARG:H	1:B:55:ARG:HG3	1.52	0.42
1:A:51:PHE:HZ	1:A:66:LEU:HD11	1.83	0.42
1:A:71:ILE:HG21	1:A:74:TYR:CZ	2.55	0.42
1:A:272:VAL:HG23	1:A:281:ILE:HG13	2.01	0.42
1:A:351:ILE:HD11	1:A:394:MET:HE1	2.02	0.42
1:B:215:ASN:CB	1:B:254:ALA:HB1	2.49	0.42
1:B:412:ILE:HG23	1:B:422:THR:CG2	2.50	0.42
1:A:274:ASP:HB3	1:A:277:THR:HG23	2.01	0.42
1:B:232:GLU:HG3	1:B:326:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:HD12	1:B:280:GLY:CA	2.44	0.42
1:A:9:CYS:SG	1:A:13:GLU:OE1	2.76	0.42
1:A:329:ALA:HA	1:A:330:PRO:HD3	1.81	0.42
1:A:414:THR:CG2	1:A:422:THR:HG22	2.45	0.41
1:B:45:LYS:N	1:B:45:LYS:HD2	2.35	0.41
1:B:282:LEU:HA	1:B:282:LEU:HD23	1.76	0.41
1:B:382:ASN:HB3	1:B:387:ALA:HB3	2.01	0.41
1:A:244:VAL:HG22	1:A:259:TYR:OH	2.20	0.41
1:B:242:LEU:HD11	1:B:280:GLY:HA3	1.98	0.41
1:B:382:ASN:N	1:B:387:ALA:O	2.43	0.41
1:A:367:ILE:HG22	1:A:413:ALA:HB1	2.01	0.41
1:A:462:ASP:HA	1:A:463:PRO:HD3	1.70	0.41
1:B:33:LYS:HG3	1:B:35:PHE:CE1	2.55	0.41
1:B:215:ASN:HB2	1:B:254:ALA:HB2	2.02	0.41
1:B:221:PHE:CD2	1:B:244:VAL:HG12	2.55	0.41
1:A:7:ILE:HD12	1:A:7:ILE:N	2.32	0.41
1:A:38:ILE:HG12	1:A:53:ILE:HG22	2.03	0.41
1:A:111:GLU:HG2	1:A:112:VAL:N	2.35	0.41
1:A:189:LEU:HA	1:A:189:LEU:HD23	1.84	0.41
1:A:406:THR:HG22	1:A:407:TYR:O	2.21	0.41
1:B:196:LEU:HB2	1:B:200:GLY:N	2.36	0.41
1:A:33:LYS:O	1:A:83:SER:N	2.54	0.41
1:A:466:PRO:HA	1:A:468:ASN:N	2.35	0.41
1:A:476:LEU:HD23	1:A:513:LEU:HA	2.01	0.41
1:B:304:ASN:O	1:B:305:GLU:C	2.59	0.41
1:B:66:LEU:HD12	1:B:66:LEU:H	1.85	0.41
1:B:164:THR:HG23	1:B:175:LEU:HD22	2.03	0.41
1:B:185:PRO:O	1:B:210:THR:HA	2.20	0.41
1:B:301:ARG:HA	1:B:315:SER:O	2.21	0.41
1:B:373:ARG:HB3	1:B:410:LEU:HB2	2.01	0.41
1:B:390:THR:HG22	1:B:392:ALA:O	2.21	0.41
1:B:411:ILE:CG2	1:B:412:ILE:N	2.83	0.41
1:A:408:VAL:HG22	1:A:428:LEU:HD23	2.03	0.41
1:A:488:TYR:N	1:A:488:TYR:CD2	2.89	0.41
1:B:166:ASN:C	1:B:166:ASN:ND2	2.72	0.41
1:B:232:GLU:O	1:B:288:LEU:CA	2.69	0.41
1:A:295:GLN:OE1	1:A:322:ASP:OD1	2.39	0.41
1:A:410:LEU:HD23	1:A:426:THR:HG23	2.01	0.41
1:A:442:GLU:HB3	1:A:443:PRO:CD	2.36	0.41
1:A:453:PRO:HB3	1:A:500:PRO:HG2	2.03	0.41
1:A:494:GLU:HG3	1:A:495:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:O	1:A:521:LYS:HA	2.21	0.41
1:B:217:ASN:HB2	1:B:248:ASP:CG	2.41	0.41
1:B:232:GLU:HG2	1:B:324:VAL:O	2.21	0.41
1:B:415:ASP:OD2	1:B:416:ASP:N	2.51	0.41
1:A:29:ASP:HA	1:A:34:VAL:CG2	2.51	0.41
1:A:372:TRP:HB2	1:A:412:ILE:CG2	2.47	0.41
1:A:441:PRO:CD	1:A:524:VAL:HG21	2.51	0.41
1:B:51:PHE:HE2	1:B:74:TYR:CG	2.37	0.41
1:B:105:ARG:HA	1:B:106:PRO:HD3	1.88	0.41
1:B:298:LEU:H	1:B:298:LEU:HD23	1.86	0.41
1:B:382:ASN:ND2	1:B:385:THR:H	2.19	0.41
1:B:152:SER:O	1:B:189:LEU:HA	2.20	0.40
1:B:373:ARG:HD3	1:B:410:LEU:HD13	2.02	0.40
1:A:414:THR:CA	1:A:422:THR:HG22	2.42	0.40
1:B:157:LEU:HA	1:B:158:PRO:C	2.42	0.40
1:B:252:THR:O	1:B:255:TRP:N	2.49	0.40
1:A:51:PHE:CE2	1:A:96:ILE:HD13	2.56	0.40
1:A:281:ILE:H	1:A:281:ILE:HG12	1.72	0.40
1:A:418:SER:HB2	1:A:419:PRO:HD3	2.04	0.40
1:B:128:MET:CE	1:B:207:ALA:HB1	2.51	0.40
1:B:329:ALA:O	1:B:359:PRO:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	529/550 (96%)	454 (86%)	72 (14%)	3 (1%)	25 57
1	B	436/550 (79%)	387 (89%)	48 (11%)	1 (0%)	47 78
All	All	965/1100 (88%)	841 (87%)	120 (12%)	4 (0%)	34 67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	ALA
1	A	481	SER
1	A	482	VAL
1	B	419	PRO

5.3.2 Protein sidechains (i)

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	458/482 (95%)	410 (90%)	48 (10%)	7	25
1	B	381/482 (79%)	337 (88%)	44 (12%)	5	20
All	All	839/964 (87%)	747 (89%)	92 (11%)	6	23

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	9	CYS
1	A	22	VAL
1	A	34	VAL
1	A	41[A]	GLN
1	A	41[B]	GLN
1	A	57	THR
1	A	78	SER
1	A	88	VAL
1	A	139	VAL
1	A	149	THR
1	A	157	LEU
1	A	161	ASN
1	A	166	ASN
1	A	169	THR
1	A	181	ARG
1	A	188	THR
1	A	209	ILE
1	A	211	VAL

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Mol	Chain	Res	Type
1	A	230	VAL
1	A	235	VAL
1	A	247	ASP
1	A	261	VAL
1	A	263	ASN
1	A	278	ASN
1	A	281	ILE
1	A	282	LEU
1	A	293	LYS
1	A	298	LEU
1	A	319	VAL
1	A	354	TYR
1	A	357	ARG
1	A	368	THR
1	A	373	ARG
1	A	389	PHE
1	A	390	THR
1	A	418	SER
1	A	427	LEU
1	A	429	LEU
1	A	440	ILE
1	A	470	SER
1	A	484	TRP
1	A	496	LEU
1	A	517	ASP
1	A	520	ASN
1	A	521	LYS
1	A	531	VAL
1	A	535	GLU
1	B	1	ASP
1	B	9	CYS
1	B	45	LYS
1	B	56	GLU
1	B	98	VAL
1	B	111	GLU
1	B	122	VAL
1	B	140	ASN
1	B	146	ILE
1	B	154	ASP
1	B	162	MET
1	B	166	ASN
1	B	186	THR

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Mol	Chain	Res	Type
1	B	188	THR
1	B	208	VAL
1	B	211	VAL
1	B	214	ILE
1	B	222	ASN
1	B	227	GLN
1	B	232	GLU
1	B	238	ARG
1	B	242	LEU
1	B	251	ASN
1	B	260	THR
1	B	263	ASN
1	B	278	ASN
1	B	282	LEU
1	B	290	PHE
1	B	293	LYS
1	B	320	THR
1	B	323	VAL
1	B	338	ARG
1	B	350	GLU
1	B	355	THR
1	B	362	PHE
1	B	363	MET
1	B	384	GLU
1	B	385	THR
1	B	389	PHE
1	B	390	THR
1	B	391	ARG
1	B	422	THR
1	B	433	ASP
1	B	464	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	23	GLN
1	A	27	ASN
1	A	64	GLN
1	A	84	ASN
1	A	104	ASN
1	A	110	GLN

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Mol	Chain	Res	Type
1	A	143	ASN
1	A	161	ASN
1	A	166	ASN
1	A	263	ASN
1	A	299	HIS
1	A	382	ASN
1	A	452	ASN
1	A	489	ASN
1	A	512	HIS
1	A	520	ASN
1	B	64	GLN
1	B	110	GLN
1	B	143	ASN
1	B	166	ASN
1	B	197	GLN
1	B	222	ASN
1	B	227	GLN
1	B	263	ASN
1	B	299	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 26 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MAN	A	803	1	11,11,12	0.70	0	15,15,17	0.80	1 (6%)
4	MAN	A	801	1	11,11,12	0.53	0	15,15,17	1.12	1 (6%)
4	MAN	A	802	1	11,11,12	0.62	0	15,15,17	0.76	0
4	MAN	B	804	1	11,11,12	0.71	0	15,15,17	1.17	1 (6%)
4	MAN	B	808	1	11,11,12	0.61	0	15,15,17	0.65	0
4	MAN	B	809	1	11,11,12	0.57	0	15,15,17	0.73	0
4	MAN	A	805	1	11,11,12	0.58	0	15,15,17	0.68	0
4	MAN	B	806	1	11,11,12	0.61	0	15,15,17	0.80	0
4	MAN	A	808	1	11,11,12	0.55	0	15,15,17	0.90	1 (6%)
4	MAN	A	807	1	11,11,12	0.56	0	15,15,17	1.03	2 (13%)
4	MAN	B	803	1	11,11,12	0.67	0	15,15,17	0.72	0
4	MAN	A	806	1	11,11,12	0.55	0	15,15,17	0.81	1 (6%)
4	MAN	A	804	1	11,11,12	0.54	0	15,15,17	0.87	1 (6%)
4	MAN	B	801	1	11,11,12	0.62	0	15,15,17	0.61	0
4	MAN	B	805	1	11,11,12	0.59	0	15,15,17	0.65	0
4	MAN	A	809	1	11,11,12	0.56	0	15,15,17	0.86	1 (6%)
4	MAN	B	807	1	11,11,12	0.64	0	15,15,17	0.72	0
4	MAN	B	802	1	11,11,12	0.55	0	15,15,17	0.85	1 (6%)

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
4	MAN	A	801	1	-	2/2/19/22	0/1/1/1
4	MAN	A	803	1	-	2/2/19/22	0/1/1/1
4	MAN	A	802	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	804	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	808	1	-	0/2/19/22	0/1/1/1
4	MAN	B	809	1	-	2/2/19/22	0/1/1/1
4	MAN	A	805	1	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	B	806	1	-	2/2/19/22	0/1/1/1
4	MAN	A	808	1	-	0/2/19/22	0/1/1/1
4	MAN	A	807	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	803	1	1/1/4/5	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	A	806	1	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	A	804	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	801	1	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	B	805	1	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	809	1	-	2/2/19/22	0/1/1/1
4	MAN	B	807	1	-	2/2/19/22	0/1/1/1
4	MAN	B	802	1	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	801	MAN	C1-O5-C5	3.77	117.24	112.19
4	B	804	MAN	C1-C2-C3	3.27	114.41	109.64
4	A	808	MAN	C1-O5-C5	2.57	115.63	112.19
4	A	809	MAN	C1-O5-C5	2.52	115.57	112.19
4	B	802	MAN	C1-O5-C5	2.38	115.37	112.19
4	A	806	MAN	C1-O5-C5	2.35	115.34	112.19
4	A	807	MAN	C1-O5-C5	2.30	115.26	112.19
4	A	804	MAN	C1-O5-C5	2.27	115.23	112.19
4	A	807	MAN	C3-C4-C5	2.09	114.02	110.23
4	A	803	MAN	C1-C2-C3	2.08	112.67	109.64

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	802	MAN	C1
4	A	804	MAN	C1
4	A	805	MAN	C1
4	A	806	MAN	C1
4	A	807	MAN	C1
4	B	801	MAN	C1
4	B	803	MAN	C1
4	B	804	MAN	C1
4	B	805	MAN	C1

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	807	MAN	O5-C5-C6-O6
4	A	806	MAN	C4-C5-C6-O6
4	A	805	MAN	C4-C5-C6-O6
4	B	806	MAN	O5-C5-C6-O6
4	B	807	MAN	C4-C5-C6-O6
4	B	802	MAN	C4-C5-C6-O6
4	A	805	MAN	O5-C5-C6-O6
4	B	809	MAN	C4-C5-C6-O6
4	A	801	MAN	O5-C5-C6-O6
4	B	802	MAN	O5-C5-C6-O6
4	B	809	MAN	O5-C5-C6-O6
4	B	803	MAN	C4-C5-C6-O6
4	B	803	MAN	O5-C5-C6-O6
4	B	806	MAN	C4-C5-C6-O6
4	A	801	MAN	C4-C5-C6-O6
4	B	801	MAN	C4-C5-C6-O6
4	A	809	MAN	C4-C5-C6-O6
4	A	803	MAN	C4-C5-C6-O6
4	B	801	MAN	O5-C5-C6-O6
4	A	809	MAN	O5-C5-C6-O6
4	A	803	MAN	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	804	MAN	4	0
4	A	804	MAN	1	0
4	B	805	MAN	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	532/550 (96%)	-0.23	10 (1%)	66	65	25, 59, 123, 157	0
1	B	440/550 (80%)	-0.16	9 (2%)	65	64	32, 61, 112, 131	0
All	All	972/1100 (88%)	-0.19	19 (1%)	65	64	25, 60, 116, 157	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	TYR	4.9
1	A	448	PHE	3.2
1	A	532	CYS	3.0
1	A	534	CYS	3.0
1	B	467	PRO	2.9
1	A	535	GLU	2.9
1	A	531	VAL	2.8
1	B	392	ALA	2.8
1	B	368	THR	2.6
1	B	394	MET	2.5
1	A	530	HIS	2.4
1	A	511	ILE	2.3
1	A	444	ARG	2.3
1	B	391	ARG	2.3
1	B	466	PRO	2.2
1	B	364	ASP	2.2
1	A	502	LYS	2.2
1	B	363	MET	2.1
1	B	465	LEU	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
4	MAN	B	804	11/12	0.69	0.46	91,100,120,132	0
4	MAN	B	806	11/12	0.79	0.28	99,109,124,129	0
2	CA	B	609	1/1	0.80	0.12	105,105,105,105	0
4	MAN	A	806	11/12	0.80	0.32	73,88,105,107	0
2	CA	B	610	1/1	0.81	0.09	93,93,93,93	0
4	MAN	A	808	11/12	0.81	0.23	72,85,90,98	0
2	CA	B	611	1/1	0.82	0.17	104,104,104,104	0
2	CA	B	612	1/1	0.82	0.09	89,89,89,89	0
2	CA	A	610	1/1	0.82	0.16	74,74,74,74	0
4	MAN	A	807	11/12	0.83	0.26	74,85,90,91	0
2	CA	A	605	1/1	0.83	0.16	31,31,31,31	0
4	MAN	B	807	11/12	0.83	0.33	106,117,122,129	0
2	CA	A	608	1/1	0.84	0.11	58,58,58,58	0
4	MAN	B	805	11/12	0.85	0.27	79,84,96,96	0
2	CA	B	607	1/1	0.85	0.07	87,87,87,87	0
4	MAN	A	805	11/12	0.85	0.28	66,69,89,95	0
4	MAN	B	808	11/12	0.87	0.21	114,123,126,127	0
4	MAN	B	802	11/12	0.88	0.18	67,71,81,83	0
4	MAN	A	802	11/12	0.88	0.42	59,63,79,91	0
4	MAN	A	803	11/12	0.88	0.21	50,69,77,78	0
4	MAN	B	809	11/12	0.88	0.19	95,99,112,113	0
4	MAN	A	809	11/12	0.89	0.38	87,91,98,112	0
2	CA	A	607	1/1	0.89	0.10	72,72,72,72	0
4	MAN	B	803	11/12	0.90	0.31	72,93,114,121	0
2	CA	A	612	1/1	0.91	0.16	74,74,74,74	0
4	MAN	B	801	11/12	0.91	0.19	55,60,72,73	0
2	CA	B	602	1/1	0.92	0.12	38,38,38,38	0
2	CA	B	605	1/1	0.93	0.14	38,38,38,38	0
2	CA	B	606	1/1	0.93	0.07	55,55,55,55	0
2	CA	B	601	1/1	0.93	0.18	44,44,44,44	0
2	CA	B	608	1/1	0.93	0.10	81,81,81,81	0
2	CA	A	606	1/1	0.94	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	A	801	11/12	0.94	0.20	44,48,59,71	0
2	CA	A	603	1/1	0.94	0.11	39,39,39,39	0
2	CA	A	604	1/1	0.95	0.20	35,35,35,35	0
4	MAN	A	804	11/12	0.95	0.18	47,60,76,80	0
2	CA	A	601	1/1	0.96	0.22	41,41,41,41	0
2	CA	A	609	1/1	0.96	0.04	87,87,87,87	0
2	CA	A	611	1/1	0.97	0.09	81,81,81,81	0
2	CA	B	604	1/1	0.97	0.12	37,37,37,37	0
2	CA	B	603	1/1	0.98	0.09	38,38,38,38	0
2	CA	A	602	1/1	0.98	0.13	35,35,35,35	0
3	MN	B	901	1/1	0.98	0.22	54,54,54,54	0
3	MN	A	901	1/1	0.99	0.26	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.