Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:49 PM GMT

PDB ID	:	1M7R
Title	:	Crystal Structure of Myotubularin-related Protein-2 (MTMR2) Complexed with Phosphate
Authors	:	Begley, M.J.; Taylor, G.S.; Kim, S.-A.; Veine, D.M.; Dixon, J.E.; Stuckey, J.A.
Deposited on	:	2002-07-22
Resolution	:	2.60 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

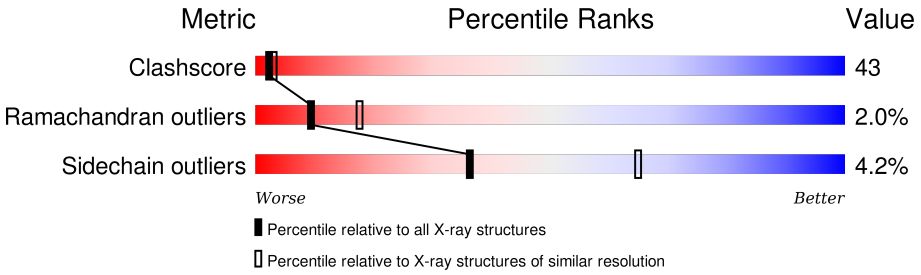
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	657	36% 37% 5% • 22%
1	B	657	30% 43% 5% 22%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	656	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8632 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 Myotubularin-related Protein-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	75	0	0
			4189	2679	729	764	17			
1	B	513	Total	C	N	O	S	114	0	0
			4189	2679	729	764	17			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	CLONING ARTIFACT	UNP Q13614
A	-1	ALA	-	CLONING ARTIFACT	UNP Q13614
A	0	SER	-	CLONING ARTIFACT	UNP Q13614
A	417	SER	CYS	ENGINEERED	UNP Q13614
A	644	ALA	-	EXPRESSION TAG	UNP Q13614
A	645	ALA	-	EXPRESSION TAG	UNP Q13614
A	646	ALA	-	EXPRESSION TAG	UNP Q13614
A	647	LEU	-	EXPRESSION TAG	UNP Q13614
A	648	GLU	-	EXPRESSION TAG	UNP Q13614
A	649	HIS	-	EXPRESSION TAG	UNP Q13614
A	650	HIS	-	EXPRESSION TAG	UNP Q13614
A	651	HIS	-	EXPRESSION TAG	UNP Q13614
A	652	HIS	-	EXPRESSION TAG	UNP Q13614
A	653	HIS	-	EXPRESSION TAG	UNP Q13614
A	654	HIS	-	EXPRESSION TAG	UNP Q13614
B	-2	MET	-	CLONING ARTIFACT	UNP Q13614
B	-1	ALA	-	CLONING ARTIFACT	UNP Q13614
B	0	SER	-	CLONING ARTIFACT	UNP Q13614
B	417	SER	CYS	ENGINEERED	UNP Q13614
B	644	ALA	-	EXPRESSION TAG	UNP Q13614
B	645	ALA	-	EXPRESSION TAG	UNP Q13614
B	646	ALA	-	EXPRESSION TAG	UNP Q13614
B	647	LEU	-	EXPRESSION TAG	UNP Q13614
B	648	GLU	-	EXPRESSION TAG	UNP Q13614
B	649	HIS	-	EXPRESSION TAG	UNP Q13614

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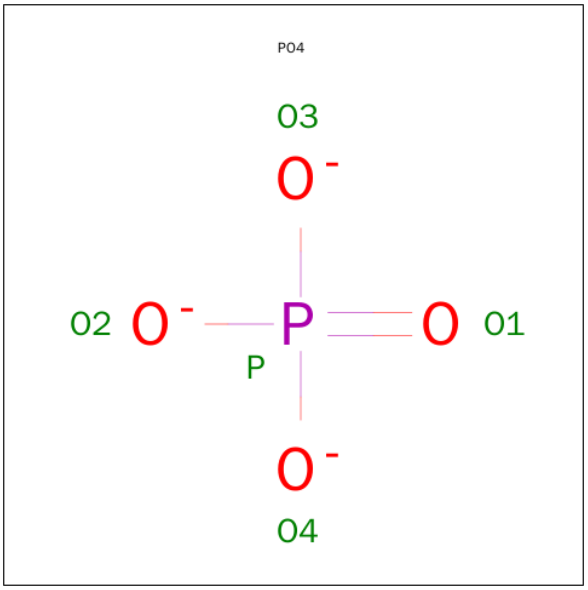
Chain	Residue	Modelled	Actual	Comment	Reference
B	650	HIS	-	EXPRESSION TAG	UNP Q13614
B	651	HIS	-	EXPRESSION TAG	UNP Q13614
B	652	HIS	-	EXPRESSION TAG	UNP Q13614
B	653	HIS	-	EXPRESSION TAG	UNP Q13614
B	654	HIS	-	EXPRESSION TAG	UNP Q13614

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	146	Total O 146 146	0	0
3	B	88	Total O 88 88	0	0

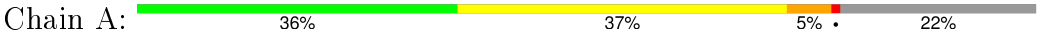
3 Residue-property plots (i)

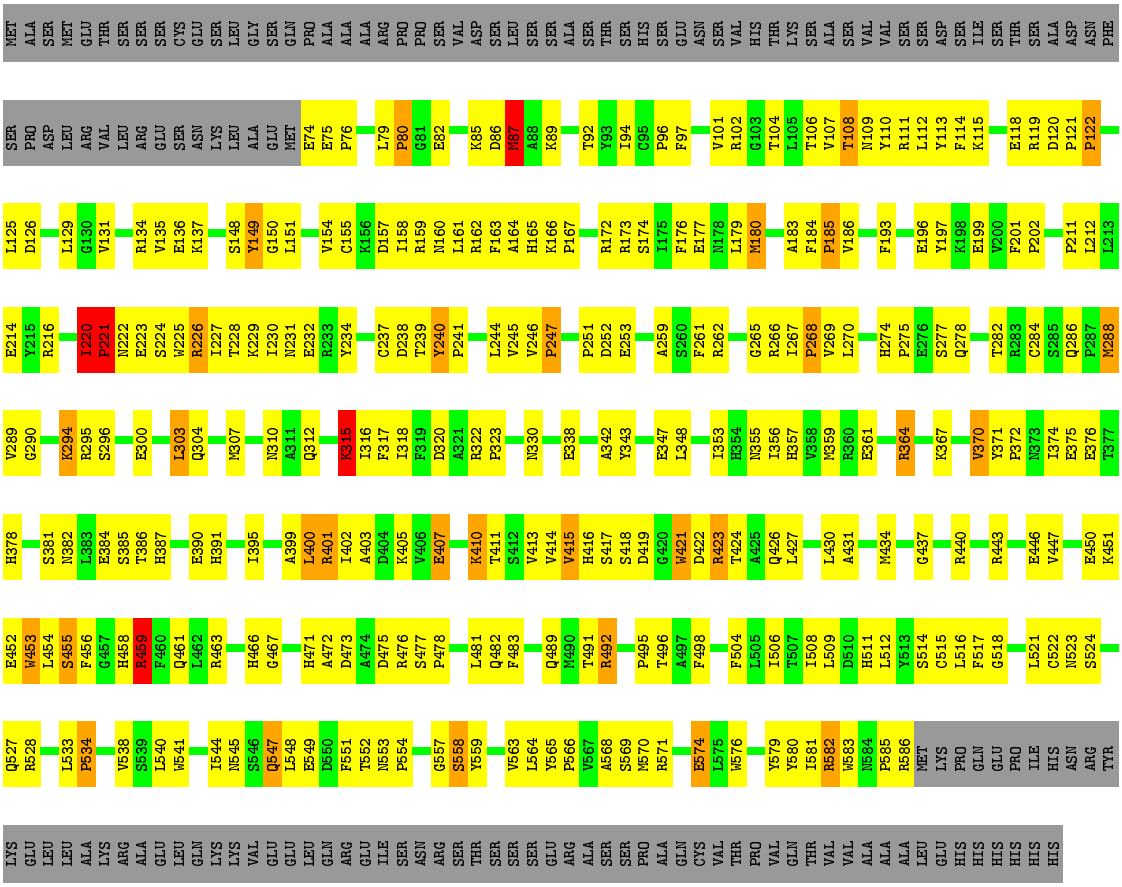
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: Myotubularin-related Protein-2

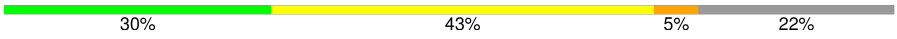
Chain A:

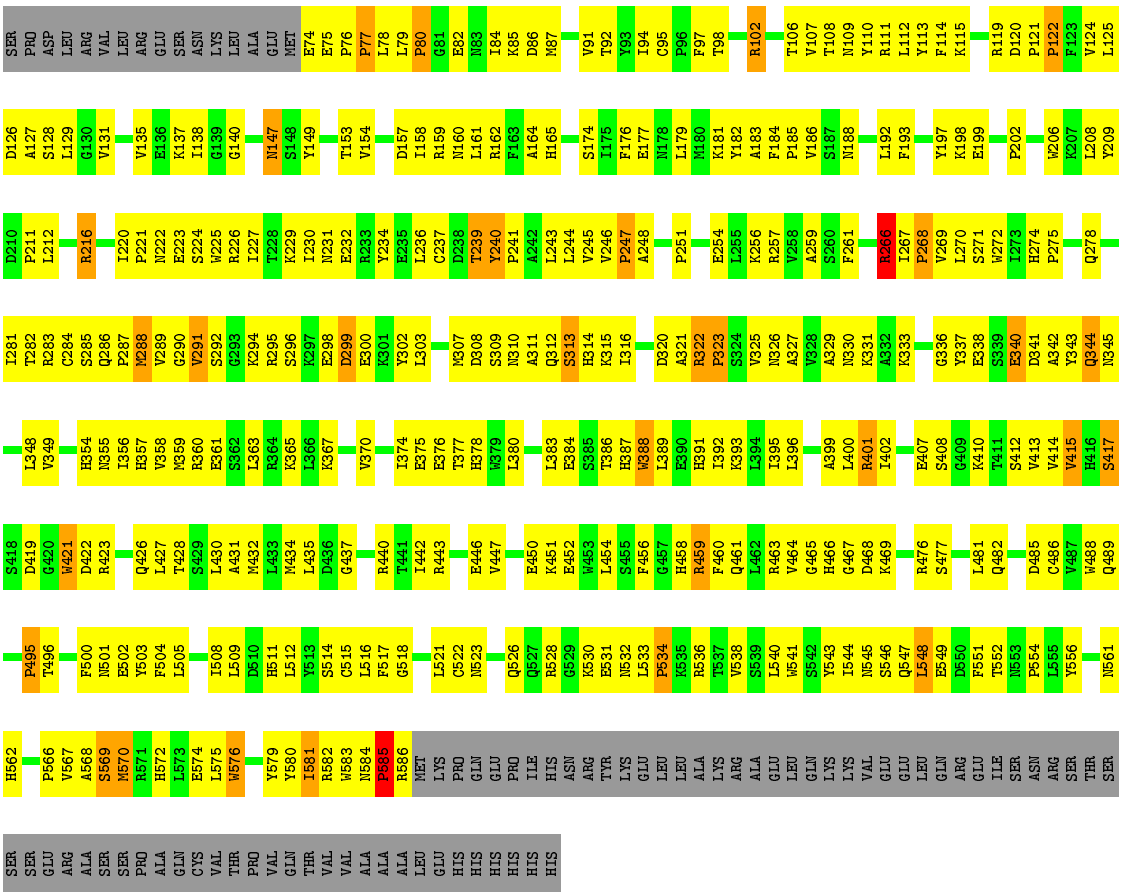




- Molecule 1: Myotubularin-related Protein-2

Chain B:




SER PRO ASP LEU ARG VAL LEU ARG GLU SER ASN LYS LEU ALA GLU MET E74 E75 P76 P77 L78 L79 P80 G81 E82 N83 I84 K85 D86 M87 V91 T92 Y93 I94 C95 P96 F97 T98 R102 T106 V107 T108 N109 Y110 R111 L112 Y113 F114 K115 R119 D120 P121 P122 F123 V124 L125
D126 A127 S128 L129 G130 V131 V135 E136 K137 I138 G139 G140 N147 S148 Y149 T153 V154 D157 I158 R159 N160 L161 R162 F163 A164 H165 S174 I175 F176 E177 N178 L179 M180 K181 Y182 A183 F184 P185 V186 S187 N188 L192 F193 Y197 K198 E199 P202 W206 K207 L208 Y209
D210 P211 L212 R216 I220 P221 N222 E223 S224 W225 R226 I227 T228 K229 I230 N231 E232 R233 Y234 E235 L236 C237 D238 T239 Y240 P241 A242 L243 L244 V245 V246 P247 A248 P251 E254 L255 K256 R257 V258 A259 S260 F261 R266 I267 P268 V269 L270 S271 W272 I273 H274 P275 Q278
I281 T282 R283 C284 S285 Q286 P287 M288 V289 G290 V291 S292 G293 K294 R295 S296 K297 E298 D299 E300 K301 Y302 L303 M307 D308 S309 N310 A311 Q312 S313 H314 K315 I316 D320 A321 R322 P323 S324 V325 N326 A327 V328 A329 N330 K331 A332 K333 G336 Y337 E338 S339 E340 D341 A342 Y343 Q344 N345
L348 V349 H354 N355 I356 H357 V358 M359 R360 E361 S362 L363 R364 K365 L366 K367 V370 I374 E375 E376 T377 H378 W379 L380 L383 E384 S385 T386 H387 W388 L389 E390 H391 I392 K393 L394 I395 L396 A399 L400 R401 I402 E407 S408 G409 K410 T411 S412 V413 V414 V415 H416 S417
S418 D419 G420 W421 D422 R423 Q426 L427 T428 S429 L430 A431 M432 L433 M434 L435 D436 G437 R440 T441 I442 R443 E446 V447 E450 K451 E452 W453 L454 S455 F456 G457 H458 R459 F460 Q461 L462 R463 V464 G465 H466 G467 D468 K469 R476 S477 L481 Q482 D485 C486 Y487 W488 Q489
P495 T496 F500 N501 E502 Y503 F504 L505 I508 L509 D510 H511 L512 Y513 S514 C515 L516 F517 G518 L521 C522 N523 Q526 Q527 R528 G529 K530 E531 N532 L533 P534 K535 R536 T537 V538 S539 L540 W541 S542 Y543 I544 N545 S546 Q547 L548 E549 D550 F551 T552 N553 P554 L555 Y556 N561
H562 P566 V567 A568 S569 M570 R571 H572 L573 E574 L575 W576 Y579 Y580 I581 R582 W583 N584 P585 R586 MET LYS PRO GLN GLU PRO ILE HIS ASN ARG TYR LYS GLU LEU LEU ALA LYS ARG ALA GLU LEU GLN LYS LYS VAL GLU GLU LEU GLN ARG GLU ILE SER ASN ARG SER THR SER
SER SER GLU ARG ALA SER SER PRO ALA GLN CYS VAL THR PRO VAL GLN THR VAL VAL ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.25Å 82.66Å 100.13Å 90.00° 117.93° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.1 (8.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8632	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.73	13/4300 (0.3%)	0.80	8/5829 (0.1%)
1	B	0.77	13/4300 (0.3%)	0.81	8/5829 (0.1%)
All	All	0.75	26/8600 (0.3%)	0.80	16/11658 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	2
All	All	0	9

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	554	PRO	N-CD	-18.06	1.22	1.47
1	A	220	ILE	CA-C	-6.00	1.37	1.52
1	B	323	PRO	N-CD	5.38	1.55	1.47
1	B	251	PRO	N-CD	5.37	1.55	1.47
1	B	585	PRO	N-CD	5.37	1.55	1.47
1	B	247	PRO	N-CD	5.36	1.55	1.47
1	B	77	PRO	N-CD	5.35	1.55	1.47
1	A	534	PRO	N-CD	5.34	1.55	1.47
1	A	585	PRO	N-CD	5.34	1.55	1.47
1	B	80	PRO	N-CD	5.34	1.55	1.47
1	A	122	PRO	N-CD	5.32	1.55	1.47
1	B	122	PRO	N-CD	5.32	1.55	1.47
1	A	323	PRO	N-CD	5.32	1.55	1.47
1	A	247	PRO	N-CD	5.31	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	PRO	N-CD	5.31	1.55	1.47
1	A	185	PRO	N-CD	5.31	1.55	1.47
1	A	268	PRO	N-CD	5.31	1.55	1.47
1	A	80	PRO	N-CD	5.30	1.55	1.47
1	A	211	PRO	N-CD	5.30	1.55	1.47
1	B	268	PRO	N-CD	5.30	1.55	1.47
1	A	251	PRO	N-CD	5.29	1.55	1.47
1	A	495	PRO	N-CD	5.29	1.55	1.47
1	A	221	PRO	N-CD	5.29	1.55	1.47
1	B	534	PRO	N-CD	5.28	1.55	1.47
1	B	211	PRO	N-CD	5.25	1.55	1.47
1	B	561	ASN	C-O	5.15	1.33	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	ILE	CB-CA-C	7.91	127.42	111.60
1	A	571	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	A	459	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	B	582	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	B	459	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	B	102	ARG	NE-CZ-NH2	6.47	123.53	120.30
1	A	87	MET	CG-SD-CE	5.85	109.56	100.20
1	B	570	MET	CG-SD-CE	5.74	109.39	100.20
1	B	288	MET	CG-SD-CE	5.72	109.35	100.20
1	A	288	MET	CG-SD-CE	5.71	109.34	100.20
1	B	532	ASN	O-C-N	-5.70	113.58	122.70
1	A	221	PRO	O-C-N	5.70	131.81	122.70
1	A	570	MET	CG-SD-CE	5.64	109.23	100.20
1	B	554	PRO	N-CD-CG	5.52	111.48	103.20
1	B	388	TRP	O-C-N	5.24	131.08	122.70
1	A	410	LYS	O-C-N	-5.07	114.60	122.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	TYR	Mainchain
1	A	180	MET	Mainchain
1	A	220	ILE	Mainchain,Peptide
1	A	315	LYS	Mainchain
1	A	453	TRP	Mainchain

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Mol	Chain	Res	Type	Group
1	A	547	GLN	Mainchain
1	B	266	ARG	Mainchain
1	B	562	HIS	Mainchain

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	4189	0	4113	319	0
1	B	4189	0	4113	392	0
2	A	10	0	0	2	0
2	B	10	0	0	1	0
3	A	146	0	0	16	0
3	B	88	0	0	14	0
All	All	8632	0	8226	707	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 (707) 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:317:PHE:CE1	1:A:405:LYS:HD2	1.60	1.36
1:A:454:LEU:HD13	3:A:1207:HOH:O	1.38	1.23
1:B:393:LYS:HG3	1:B:568:ALA:O	1.37	1.20
1:A:261:PHE:O	1:A:288:MET:HG2	1.42	1.16
1:B:370:VAL:CG1	1:B:581:ILE:HG12	1.75	1.14
1:B:137:LYS:HE3	1:B:176:PHE:CD2	1.83	1.13
1:B:230:ILE:HD11	1:B:256:LYS:HE2	1.22	1.12
1:B:511:HIS:HD2	1:B:540:LEU:CD1	1.62	1.11
1:A:112:LEU:HD13	1:A:179:LEU:HD21	1.31	1.11
1:B:511:HIS:CD2	1:B:540:LEU:CD1	2.32	1.11
1:B:511:HIS:HD2	1:B:540:LEU:HD11	0.98	1.11
1:B:337:TYR:CD1	1:B:348:LEU:CD2	2.34	1.11
1:B:137:LYS:HE2	1:B:176:PHE:CG	1.86	1.10
1:A:74:GLU:HB3	1:A:115:LYS:HD3	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LYS:HE2	3:B:1093:HOH:O	0.92	1.09
1:B:94:ILE:HD11	1:B:147:ASN:HB3	1.28	1.07
1:A:544:ILE:HG23	1:A:551:PHE:CE1	1.89	1.07
1:B:337:TYR:HD1	1:B:348:LEU:CD2	1.67	1.06
1:B:511:HIS:CD2	1:B:540:LEU:HD11	1.88	1.06
1:A:317:PHE:CE1	1:A:405:LYS:CD	2.41	1.04
1:B:94:ILE:HD11	1:B:147:ASN:CB	1.90	1.02
1:A:274:HIS:CD2	1:A:275:PRO:HD2	1.96	0.99
1:B:337:TYR:CD1	1:B:348:LEU:HD21	1.96	0.98
1:B:314:HIS:CD2	1:B:315:LYS:HB2	1.97	0.98
1:B:370:VAL:HG13	1:B:581:ILE:HG12	1.45	0.98
1:B:261:PHE:O	1:B:288:MET:HG2	1.64	0.97
1:B:137:LYS:HE2	1:B:176:PHE:CB	1.94	0.97
1:B:91:VAL:HG22	1:B:165:HIS:ND1	1.78	0.96
1:B:137:LYS:CE	1:B:176:PHE:CD2	2.47	0.96
1:B:337:TYR:CD1	1:B:348:LEU:HD23	2.01	0.96
1:B:370:VAL:HG11	1:B:581:ILE:HG12	1.45	0.96
1:A:158:ILE:HG23	1:A:367:LYS:HG3	1.46	0.95
1:A:110:TYR:HB2	1:A:193:PHE:CD1	2.02	0.95
1:B:137:LYS:CE	1:B:176:PHE:CG	2.49	0.94
1:A:101:VAL:CG2	1:A:119:ARG:HH21	1.81	0.93
1:B:274:HIS:ND1	1:B:275:PRO:HD2	1.86	0.91
1:B:229:LYS:O	1:B:232:GLU:HG2	1.70	0.91
1:A:317:PHE:HE1	1:A:405:LYS:HD2	1.35	0.90
1:A:165:HIS:CD2	1:A:172:ARG:HG2	2.06	0.89
1:A:544:ILE:HG23	1:A:551:PHE:CD1	2.08	0.89
1:B:137:LYS:HG2	1:B:176:PHE:CD1	2.08	0.89
1:B:338:GLU:HB3	1:B:343:TYR:CD1	2.08	0.88
1:B:402:ILE:HG23	1:B:413:VAL:HG21	1.56	0.88
1:A:390:GLU:HG2	3:A:1037:HOH:O	1.74	0.87
1:B:432:MET:HE3	1:B:452:GLU:HG3	1.57	0.87
1:B:74:GLU:HB3	1:B:115:LYS:HD3	1.58	0.86
1:B:314:HIS:HD2	1:B:315:LYS:HB2	1.39	0.85
1:B:511:HIS:CD2	1:B:540:LEU:HD13	2.10	0.85
1:A:545:ASN:HA	1:A:548:LEU:HD21	1.59	0.84
1:A:74:GLU:CB	1:A:115:LYS:HD3	2.07	0.83
1:B:320:ASP:OD1	1:B:322:ARG:HG3	1.78	0.83
1:B:125:LEU:HD21	1:B:161:LEU:HD22	1.60	0.83
1:A:274:HIS:CG	1:A:275:PRO:HD2	2.13	0.82
1:B:138:ILE:HD13	1:B:162:ARG:NH1	1.94	0.82
1:B:400:LEU:HD23	1:B:434:MET:SD	2.19	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:O	1:A:269:VAL:HG13	1.80	0.82
1:B:120:ASP:HB3	1:B:121:PRO:HD3	1.60	0.82
1:B:231:ASN:HD22	1:B:236:LEU:H	1.27	0.81
1:A:387:HIS:O	1:A:391:HIS:CD2	2.33	0.81
1:B:432:MET:CE	1:B:452:GLU:HG3	2.09	0.81
1:A:378:HIS:HB2	1:A:382:ASN:HD21	1.46	0.80
1:A:277:SER:O	1:A:278:GLN:HB2	1.79	0.80
1:A:261:PHE:CE1	1:A:288:MET:O	2.34	0.80
1:B:338:GLU:HA	1:B:343:TYR:CE1	2.15	0.80
1:B:295:ARG:HH11	1:B:342:ALA:HA	1.48	0.79
1:A:353:ILE:HD13	1:A:395:ILE:HD13	1.64	0.79
1:A:359:MET:HE3	1:A:482:GLN:HE22	1.48	0.79
1:B:375:GLU:OE2	1:B:377:THR:HB	1.83	0.78
1:B:110:TYR:HB2	1:B:193:PHE:CD1	2.19	0.78
1:B:567:VAL:HG11	1:B:572:HIS:CD2	2.18	0.78
1:B:330:ASN:HA	1:B:333:LYS:HE3	1.64	0.78
1:B:138:ILE:CD1	1:B:162:ARG:NH1	2.46	0.78
1:A:518:GLY:HA2	1:A:521:LEU:CD1	2.13	0.78
1:B:466:HIS:CD2	1:B:521:LEU:HD23	2.17	0.78
1:B:393:LYS:CG	1:B:568:ALA:O	2.27	0.78
1:B:545:ASN:HA	1:B:548:LEU:HD21	1.64	0.78
1:B:137:LYS:HG3	1:B:176:PHE:CE1	2.19	0.77
1:A:317:PHE:CD1	1:A:405:LYS:HG2	2.19	0.77
1:A:259:ALA:HA	1:A:267:ILE:CG2	2.14	0.77
1:B:307:MET:CE	1:B:316:ILE:HG22	2.15	0.77
1:B:359:MET:HE2	1:B:482:GLN:HE22	1.50	0.76
1:A:212:LEU:O	1:A:216:ARG:HG3	1.85	0.76
1:B:110:TYR:HB2	1:B:193:PHE:CG	2.19	0.76
1:A:137:LYS:HD3	1:A:172:ARG:NH1	2.00	0.75
1:A:267:ILE:HG13	1:A:267:ILE:O	1.84	0.75
1:A:120:ASP:HB3	1:A:121:PRO:HD3	1.68	0.75
1:B:159:ARG:HB3	1:B:583:TRP:CD1	2.22	0.75
1:B:314:HIS:CG	1:B:315:LYS:N	2.55	0.75
1:B:504:PHE:CZ	1:B:508:ILE:HD11	2.21	0.75
1:B:135:VAL:HG22	1:B:153:THR:HG22	1.67	0.75
1:A:268:PRO:HA	1:A:284:CYS:HB3	1.69	0.74
1:B:461:GLN:HE22	1:B:466:HIS:HB2	1.53	0.74
1:B:340:GLU:HG2	3:B:1227:HOH:O	1.86	0.74
1:B:216:ARG:O	1:B:216:ARG:HD2	1.88	0.74
1:B:240:TYR:HE1	1:B:266:ARG:NH1	1.86	0.74
1:A:359:MET:CE	1:A:482:GLN:HE22	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ARG:NH1	1:B:342:ALA:HA	2.02	0.74
1:A:185:PRO:HD2	1:A:467:GLY:HA3	1.70	0.74
1:A:101:VAL:HG23	1:A:119:ARG:HH21	1.51	0.73
1:A:134:ARG:NH1	1:A:136:GLU:HG3	2.03	0.73
1:B:545:ASN:HA	1:B:548:LEU:CD2	2.19	0.73
1:B:340:GLU:HG3	1:B:341:ASP:N	2.04	0.73
1:A:509:LEU:HD12	1:A:579:TYR:CE1	2.24	0.73
1:B:337:TYR:HD1	1:B:348:LEU:HD23	1.40	0.73
1:A:374:ILE:HD11	1:A:581:ILE:HD13	1.69	0.73
1:A:166:LYS:HB3	1:A:167:PRO:HD2	1.71	0.73
1:B:137:LYS:CG	1:B:176:PHE:CD1	2.71	0.72
1:B:286:GLN:OE1	1:B:322:ARG:NH1	2.22	0.72
1:A:101:VAL:CG2	1:A:119:ARG:HE	2.02	0.72
1:A:186:VAL:HG22	1:A:467:GLY:O	1.89	0.72
1:B:343:TYR:O	1:B:345:ASN:N	2.22	0.72
1:B:526:GLN:HG2	1:B:530:LYS:HE3	1.69	0.72
1:A:101:VAL:CG2	1:A:119:ARG:NH2	2.53	0.72
1:A:387:HIS:O	1:A:391:HIS:HD2	1.72	0.72
1:B:383:LEU:HD11	1:B:575:LEU:HD13	1.72	0.72
1:A:511:HIS:HA	1:A:514:SER:OG	1.90	0.72
1:B:137:LYS:HE2	1:B:176:PHE:HB3	1.70	0.72
1:B:138:ILE:HD13	1:B:162:ARG:HH12	1.54	0.71
1:A:437:GLY:HA2	1:A:440:ARG:NH1	2.04	0.71
1:B:329:ALA:O	1:B:333:LYS:HG3	1.91	0.71
1:B:268:PRO:HA	1:B:284:CYS:HB3	1.71	0.71
1:B:340:GLU:CG	1:B:341:ASP:H	2.04	0.71
1:A:89:LYS:HG2	1:A:104:THR:OG1	1.90	0.71
1:B:185:PRO:CG	1:B:192:LEU:HD23	2.20	0.70
1:A:158:ILE:HG12	1:A:367:LYS:HB2	1.74	0.70
1:B:295:ARG:HD2	1:B:300:GLU:OE2	1.90	0.70
1:A:289:VAL:O	1:A:294:LYS:HG3	1.91	0.70
1:A:222:ASN:O	1:A:224:SER:N	2.25	0.70
1:A:158:ILE:HG22	1:A:158:ILE:O	1.92	0.70
1:B:518:GLY:HA2	1:B:521:LEU:CD1	2.21	0.70
1:B:86:ASP:OD1	1:B:87:MET:N	2.25	0.70
1:B:370:VAL:HG11	1:B:580:TYR:O	1.92	0.69
1:B:370:VAL:HG13	1:B:581:ILE:CG1	2.21	0.69
1:A:338:GLU:HB3	1:A:343:TYR:CD1	2.27	0.69
1:A:509:LEU:CD1	1:A:579:TYR:CE1	2.76	0.69
1:B:401:ARG:HD2	3:B:1197:HOH:O	1.89	0.69
1:B:400:LEU:HD21	1:B:566:PRO:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:GLY:HA2	1:B:521:LEU:HD12	1.75	0.69
1:B:431:ALA:HA	1:B:434:MET:HE3	1.75	0.69
1:B:458:HIS:NE2	1:B:463:ARG:HG3	2.08	0.69
1:A:125:LEU:HD21	1:A:161:LEU:HD13	1.75	0.69
1:A:491:THR:HG22	1:A:498:PHE:CD1	2.27	0.69
1:A:317:PHE:CZ	1:A:405:LYS:NZ	2.61	0.68
1:A:361:GLU:OE2	1:A:364:ARG:NH1	2.27	0.68
1:B:495:PRO:HD2	3:B:1217:HOH:O	1.93	0.68
1:A:422:ASP:OD1	1:A:458:HIS:CE1	2.47	0.68
1:B:220:ILE:HG23	1:B:221:PRO:HA	1.76	0.68
1:B:266:ARG:HD2	1:B:419:ASP:O	1.94	0.68
1:A:518:GLY:HA2	1:A:521:LEU:HD12	1.76	0.68
1:A:286:GLN:OE1	1:A:322:ARG:NH1	2.23	0.68
1:B:231:ASN:ND2	1:B:236:LEU:H	1.91	0.68
1:B:185:PRO:HG2	1:B:192:LEU:CD2	2.23	0.68
1:B:291:VAL:HG12	3:B:1211:HOH:O	1.93	0.68
1:B:322:ARG:NH2	1:B:336:GLY:O	2.22	0.68
1:B:338:GLU:HG3	1:B:343:TYR:CZ	2.29	0.67
1:A:220:ILE:HD12	1:A:225:TRP:HB2	1.75	0.67
1:B:314:HIS:CD2	1:B:315:LYS:N	2.62	0.67
1:A:356:ILE:HG13	1:A:357:HIS:N	2.08	0.67
1:B:91:VAL:CG2	1:B:165:HIS:ND1	2.56	0.67
1:B:79:LEU:HG	1:B:111:ARG:NH2	2.09	0.67
1:B:254:GLU:HG3	1:B:257:ARG:NH2	2.08	0.67
1:A:466:HIS:ND1	1:A:515:CYS:SG	2.68	0.67
1:A:296:SER:O	1:A:300:GLU:HG3	1.95	0.67
1:B:154:VAL:HA	1:B:160:ASN:OD1	1.93	0.67
1:A:101:VAL:HG22	1:A:119:ARG:HE	1.58	0.67
1:B:340:GLU:HG3	1:B:341:ASP:H	1.59	0.67
1:A:317:PHE:HB2	1:A:413:VAL:HG12	1.76	0.66
1:B:231:ASN:HD21	1:B:237:CYS:H	1.43	0.66
1:A:120:ASP:HB3	1:A:121:PRO:CD	2.24	0.66
1:B:359:MET:CE	1:B:482:GLN:HE22	2.08	0.66
1:B:356:ILE:HG13	1:B:357:HIS:N	2.10	0.66
1:A:378:HIS:CB	1:A:382:ASN:ND2	2.59	0.66
1:A:378:HIS:CB	1:A:382:ASN:HD21	2.09	0.66
1:A:226:ARG:NE	3:A:1130:HOH:O	2.29	0.66
1:A:74:GLU:HB3	1:A:115:LYS:CD	2.17	0.66
1:B:230:ILE:CD1	1:B:256:LYS:HE2	2.14	0.66
1:A:452:GLU:O	1:A:456:PHE:HB2	1.96	0.66
1:B:137:LYS:CG	1:B:176:PHE:CE1	2.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:HD2	1:A:419:ASP:O	1.95	0.66
1:A:284:CYS:O	1:A:416:HIS:HB2	1.96	0.66
1:B:232:GLU:OE2	1:B:243:LEU:CD2	2.43	0.65
1:A:268:PRO:HG3	1:A:284:CYS:SG	2.36	0.65
1:A:400:LEU:HD11	1:A:566:PRO:O	1.96	0.65
1:B:266:ARG:CD	1:B:419:ASP:O	2.44	0.65
1:B:341:ASP:O	1:B:344:GLN:HG2	1.96	0.65
1:A:159:ARG:HD3	1:A:583:TRP:CE2	2.31	0.65
1:A:110:TYR:HB2	1:A:193:PHE:CE1	2.31	0.65
1:A:461:GLN:HB3	1:A:522:CYS:O	1.95	0.65
1:B:340:GLU:CG	1:B:341:ASP:N	2.60	0.65
1:A:107:VAL:HG22	1:A:112:LEU:HD12	1.79	0.65
1:B:307:MET:CE	1:B:316:ILE:CG2	2.75	0.65
1:A:431:ALA:HA	1:A:434:MET:HE3	1.79	0.65
1:A:150:GLY:HA3	1:A:163:PHE:O	1.97	0.64
1:B:338:GLU:CA	1:B:343:TYR:CE1	2.80	0.64
1:B:91:VAL:O	1:B:102:ARG:HA	1.98	0.64
1:B:287:PRO:HG2	1:B:337:TYR:HA	1.79	0.64
1:A:545:ASN:HA	1:A:548:LEU:CD2	2.27	0.64
1:B:138:ILE:CD1	1:B:162:ARG:HH12	2.08	0.64
1:B:159:ARG:HB3	1:B:583:TRP:NE1	2.13	0.64
1:B:137:LYS:HE3	1:B:176:PHE:CE2	2.32	0.63
1:A:426:GLN:O	1:A:430:LEU:HG	1.98	0.63
1:A:378:HIS:HB2	1:A:382:ASN:ND2	2.12	0.63
1:B:450:GLU:HA	1:B:454:LEU:HD12	1.80	0.63
1:B:292:SER:HB2	1:B:294:LYS:NZ	2.14	0.63
1:B:232:GLU:OE2	1:B:243:LEU:HD23	1.97	0.63
1:A:317:PHE:CZ	1:A:405:LYS:HD2	2.30	0.63
1:A:135:VAL:HG12	1:A:176:PHE:CE1	2.33	0.63
1:A:371:TYR:CD1	1:A:372:PRO:HA	2.33	0.63
1:B:547:GLN:O	1:B:549:GLU:N	2.31	0.63
1:B:181:LYS:HA	1:B:188:ASN:ND2	2.14	0.63
1:B:239:THR:HG22	3:B:1170:HOH:O	1.97	0.63
1:B:185:PRO:HD2	1:B:467:GLY:HA3	1.80	0.63
1:A:489:GLN:NE2	1:A:574:GLU:O	2.31	0.63
1:B:208:LEU:HD21	1:B:446:GLU:OE1	1.98	0.63
1:A:481:LEU:HD12	1:A:481:LEU:O	1.99	0.63
1:A:317:PHE:CD1	1:A:405:LYS:CG	2.81	0.62
1:B:458:HIS:CE1	1:B:463:ARG:HG3	2.34	0.62
1:B:450:GLU:CD	1:B:454:LEU:HD12	2.19	0.62
1:B:222:ASN:OD1	1:B:224:SER:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ASN:HA	1:B:333:LYS:CE	2.28	0.62
1:A:295:ARG:NH2	1:A:342:ALA:HA	2.15	0.62
1:B:120:ASP:HB3	1:B:121:PRO:CD	2.29	0.62
1:A:509:LEU:HD12	1:A:579:TYR:CD1	2.33	0.62
1:B:308:ASP:OD1	1:B:312:GLN:HG2	2.00	0.62
1:B:231:ASN:ND2	1:B:237:CYS:H	1.96	0.62
1:A:112:LEU:CD1	1:A:179:LEU:HD21	2.19	0.62
1:B:92:THR:HB	1:B:164:ALA:HB3	1.82	0.62
1:B:365:LYS:HB2	1:B:386:THR:HG22	1.82	0.62
1:B:407:GLU:HB3	3:B:1124:HOH:O	2.00	0.62
1:B:516:LEU:O	1:B:516:LEU:HD23	1.99	0.62
1:B:511:HIS:HA	1:B:514:SER:OG	1.99	0.61
1:B:426:GLN:NE2	1:B:482:GLN:HB3	2.15	0.61
1:B:338:GLU:N	1:B:338:GLU:OE1	2.33	0.61
1:A:261:PHE:O	1:A:288:MET:CG	2.34	0.61
1:A:375:GLU:O	1:A:375:GLU:OE1	2.19	0.61
1:A:268:PRO:CA	1:A:284:CYS:HB3	2.30	0.61
1:B:387:HIS:O	1:B:391:HIS:CD2	2.54	0.61
1:B:338:GLU:CB	1:B:343:TYR:CE1	2.83	0.61
1:B:185:PRO:HG2	1:B:192:LEU:HD23	1.83	0.61
1:B:363:LEU:HB2	1:B:388:TRP:CZ3	2.34	0.61
1:B:290:GLY:HA2	1:B:331:LYS:O	2.00	0.61
1:B:267:ILE:O	1:B:269:VAL:HG13	2.01	0.61
1:B:323:PRO:HD2	1:B:326:ASN:CG	2.21	0.61
1:B:85:LYS:HB3	1:B:182:TYR:CE1	2.36	0.61
1:A:402:ILE:HG23	1:A:413:VAL:HG21	1.82	0.60
1:A:317:PHE:CZ	1:A:405:LYS:CE	2.84	0.60
1:B:85:LYS:HG3	1:B:182:TYR:CE1	2.37	0.60
1:A:227:ILE:HG12	1:A:245:VAL:HG22	1.82	0.60
1:B:321:ALA:HB2	1:B:427:LEU:HD11	1.83	0.60
1:B:138:ILE:HD13	1:B:162:ARG:CZ	2.31	0.60
1:B:157:ASP:OD1	1:B:159:ARG:HG2	2.01	0.60
1:B:340:GLU:HG3	1:B:341:ASP:OD1	2.02	0.60
1:B:246:VAL:HB	1:B:247:PRO:CD	2.32	0.60
1:A:426:GLN:HG2	1:A:453:TRP:HH2	1.67	0.60
1:A:201:PHE:HB3	1:A:202:PRO:HD2	1.83	0.60
1:B:400:LEU:CD2	1:B:566:PRO:HD2	2.32	0.60
1:A:135:VAL:HB	1:A:180:MET:SD	2.41	0.59
1:A:303:LEU:CD2	1:A:318:ILE:HD11	2.32	0.59
1:B:261:PHE:O	1:B:288:MET:CG	2.46	0.59
1:B:323:PRO:HD2	1:B:326:ASN:ND2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:HG3	1:A:75:GLU:N	2.17	0.59
1:A:399:ALA:O	1:A:434:MET:HE1	2.03	0.59
1:B:291:VAL:CG1	3:B:1211:HOH:O	2.50	0.59
1:B:91:VAL:HG22	1:B:165:HIS:CE1	2.37	0.58
1:B:307:MET:HE3	1:B:316:ILE:CG2	2.33	0.58
1:B:240:TYR:CE1	1:B:266:ARG:NH1	2.69	0.58
1:B:396:LEU:HD21	1:B:486:CYS:HB3	1.85	0.58
1:A:149:TYR:CE2	1:A:172:ARG:HG3	2.38	0.58
1:A:92:THR:OG1	1:A:102:ARG:HG2	2.03	0.58
1:B:423:ARG:O	1:B:427:LEU:HG	2.04	0.58
1:B:377:THR:HG22	1:B:378:HIS:CD2	2.38	0.58
1:B:220:ILE:CD1	1:B:222:ASN:ND2	2.67	0.58
1:B:422:ASP:OD1	1:B:458:HIS:CE1	2.57	0.58
1:A:303:LEU:HD13	1:A:343:TYR:CE2	2.39	0.57
1:B:307:MET:HE3	1:B:316:ILE:HB	1.85	0.57
1:B:289:VAL:O	1:B:294:LYS:HG2	2.04	0.57
1:B:286:GLN:HB3	1:B:417:SER:O	2.04	0.57
1:A:266:ARG:O	1:A:284:CYS:HB2	2.04	0.57
1:B:159:ARG:HD3	1:B:583:TRP:CE2	2.38	0.57
1:A:241:PRO:HD2	1:A:244:LEU:HD21	1.85	0.57
1:B:115:LYS:HG3	1:B:124:VAL:HG22	1.85	0.57
1:B:549:GLU:HB2	3:B:1064:HOH:O	2.05	0.57
1:A:229:LYS:HD3	1:A:232:GLU:OE2	2.04	0.57
1:A:461:GLN:CB	1:A:522:CYS:O	2.53	0.57
1:B:186:VAL:HB	1:B:467:GLY:O	2.05	0.57
1:B:94:ILE:CD1	1:B:147:ASN:HB3	2.19	0.56
1:A:101:VAL:HG22	1:A:119:ARG:HH21	1.69	0.56
1:A:196:GLU:HG3	3:A:1159:HOH:O	2.05	0.56
1:A:241:PRO:HG2	1:A:244:LEU:HD23	1.87	0.56
1:B:375:GLU:C	1:B:375:GLU:OE1	2.43	0.56
1:B:338:GLU:HA	1:B:343:TYR:HE1	1.68	0.56
1:B:270:LEU:C	1:B:270:LEU:HD23	2.25	0.56
1:A:96:PRO:HG2	1:A:97:PHE:CE1	2.41	0.56
1:B:567:VAL:HG11	1:B:572:HIS:HD2	1.70	0.56
1:B:268:PRO:CA	1:B:284:CYS:HB3	2.36	0.56
1:B:126:ASP:OD1	1:B:127:ALA:N	2.38	0.56
1:B:357:HIS:ND1	1:B:360:ARG:NH2	2.54	0.56
1:B:129:LEU:HB3	1:B:183:ALA:HA	1.88	0.56
1:A:382:ASN:O	1:A:385:SER:OG	2.23	0.56
1:A:282:THR:OG1	1:A:414:VAL:HG22	2.05	0.56
1:A:86:ASP:OD2	1:A:174:SER:OG	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:GLN:O	1:B:530:LYS:HG3	2.05	0.56
1:A:504:PHE:O	1:A:508:ILE:HG13	2.06	0.56
1:A:82:GLU:HG3	1:A:108:THR:OG1	2.06	0.56
1:A:154:VAL:HA	1:A:160:ASN:OD1	2.06	0.56
1:A:443:ARG:HD3	3:A:1075:HOH:O	2.06	0.56
1:B:348:LEU:HD12	1:B:349:VAL:N	2.21	0.55
1:A:107:VAL:HG22	1:A:112:LEU:CD1	2.36	0.55
1:B:185:PRO:CG	1:B:192:LEU:CD2	2.83	0.55
1:A:159:ARG:HD3	1:A:583:TRP:CZ2	2.41	0.55
1:B:533:LEU:N	1:B:534:PRO:CD	2.69	0.55
1:B:340:GLU:HG3	1:B:341:ASP:CG	2.25	0.55
1:A:111:ARG:HD3	1:A:126:ASP:OD1	2.06	0.55
1:B:226:ARG:HD3	1:B:248:ALA:HA	1.88	0.55
1:A:586:ARG:HG3	3:A:1195:HOH:O	2.07	0.55
1:B:338:GLU:CB	1:B:343:TYR:CD1	2.86	0.55
1:B:78:LEU:HD22	1:B:82:GLU:HG2	1.89	0.55
1:A:246:VAL:HB	1:A:247:PRO:CD	2.37	0.55
1:B:338:GLU:HB3	1:B:343:TYR:CE1	2.42	0.54
1:B:220:ILE:HD13	1:B:222:ASN:ND2	2.22	0.54
1:B:181:LYS:HA	1:B:188:ASN:HD22	1.72	0.54
1:A:294:LYS:HE3	3:A:1106:HOH:O	2.07	0.54
1:B:337:TYR:CE1	1:B:348:LEU:HD23	2.41	0.54
1:A:101:VAL:CG2	1:A:119:ARG:NE	2.69	0.54
1:B:312:GLN:O	1:B:313:SER:C	2.45	0.54
1:B:567:VAL:CG1	1:B:572:HIS:CD2	2.90	0.54
1:B:184:PHE:CG	1:B:469:LYS:HG2	2.43	0.54
1:B:502:GLU:HG3	1:B:576:TRP:HZ2	1.72	0.54
1:A:322:ARG:NH1	1:A:330:ASN:HD22	2.06	0.54
1:B:296:SER:HB3	1:B:299:ASP:HB2	1.89	0.54
1:A:407:GLU:HA	1:A:407:GLU:OE1	2.07	0.54
1:A:415:VAL:HG22	1:A:424:THR:HG23	1.89	0.54
1:A:214:GLU:OE1	1:A:214:GLU:HA	2.07	0.54
1:B:209:TYR:CD1	1:B:447:VAL:HG13	2.41	0.54
1:A:110:TYR:CZ	1:A:516:LEU:HD13	2.42	0.54
1:A:547:GLN:O	1:A:547:GLN:HG3	2.08	0.54
1:A:521:LEU:O	1:A:522:CYS:HB2	2.08	0.53
1:B:266:ARG:HH21	1:B:421:TRP:HE3	1.56	0.53
1:A:511:HIS:CE1	1:A:517:PHE:HE1	2.27	0.53
1:A:245:VAL:HG11	1:A:270:LEU:HD23	1.89	0.53
1:A:496:THR:HG21	1:A:558:SER:HB2	1.91	0.53
1:A:517:PHE:HB3	1:A:538:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:HD12	1:B:343:TYR:CD2	2.43	0.53
1:B:79:LEU:HG	1:B:111:ARG:HH22	1.73	0.53
1:B:325:VAL:HG23	3:B:1005:HOH:O	2.08	0.53
1:B:112:LEU:HD13	1:B:179:LEU:HD13	1.91	0.53
1:A:528:ARG:CG	1:A:533:LEU:HD12	2.38	0.53
1:B:314:HIS:CG	1:B:315:LYS:H	2.25	0.53
1:B:485:ASP:O	1:B:489:GLN:HG2	2.08	0.53
1:A:238:ASP:OD1	1:A:239:THR:HG23	2.09	0.53
1:B:266:ARG:CD	1:B:285:SER:HB3	2.39	0.53
1:A:284:CYS:O	1:A:416:HIS:CB	2.56	0.53
1:A:456:PHE:CE1	3:A:1020:HOH:O	2.54	0.53
1:B:584:ASN:OD1	1:B:585:PRO:HD2	2.09	0.53
1:B:220:ILE:CG2	1:B:221:PRO:HA	2.40	0.52
1:B:461:GLN:O	1:B:465:GLY:HA2	2.08	0.52
1:B:361:GLU:O	1:B:365:LYS:HG3	2.10	0.52
1:B:137:LYS:HG3	1:B:176:PHE:CZ	2.45	0.52
1:B:135:VAL:HG12	1:B:176:PHE:CE1	2.45	0.52
1:B:259:ALA:HA	1:B:267:ILE:HG22	1.90	0.52
1:A:79:LEU:HD11	1:A:111:ARG:NH2	2.25	0.52
1:B:459:ARG:HB3	1:B:523:ASN:OD1	2.08	0.52
1:B:468:ASP:HB3	1:B:476:ARG:NH2	2.24	0.52
1:A:451:LYS:O	1:A:456:PHE:HD1	1.92	0.52
1:B:521:LEU:O	1:B:522:CYS:HB2	2.10	0.52
1:B:422:ASP:HB2	2:B:656:PO4:O2	2.09	0.52
1:A:122:PRO:HD2	3:A:1152:HOH:O	2.09	0.52
1:B:466:HIS:CD2	1:B:521:LEU:CD2	2.90	0.52
1:B:468:ASP:HB3	1:B:476:ARG:HH21	1.75	0.52
1:A:129:LEU:HB3	1:A:183:ALA:HA	1.92	0.52
1:B:197:TYR:O	1:B:198:LYS:HD3	2.09	0.52
1:A:430:LEU:HD23	1:A:483:PHE:HE1	1.74	0.52
1:B:432:MET:HE1	1:B:452:GLU:HG3	1.88	0.52
1:B:375:GLU:O	1:B:375:GLU:OE1	2.28	0.52
1:A:472:ALA:O	1:A:473:ASP:C	2.47	0.52
1:A:304:GLN:HE22	1:A:307:MET:HE3	1.74	0.52
1:B:240:TYR:CZ	1:B:266:ARG:HB3	2.46	0.51
1:A:240:TYR:HE1	1:A:266:ARG:NH1	2.08	0.51
1:B:246:VAL:HB	1:B:247:PRO:HD2	1.91	0.51
1:B:272:TRP:CZ3	1:B:435:LEU:HD13	2.45	0.51
1:A:390:GLU:CG	3:A:1037:HOH:O	2.45	0.51
1:B:526:GLN:CG	1:B:530:LYS:HE3	2.38	0.51
1:A:137:LYS:HD3	1:A:172:ARG:HH12	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:TRP:CE2	1:B:576:TRP:CD1	2.99	0.51
1:B:84:ILE:HA	1:B:108:THR:HG22	1.92	0.51
1:B:85:LYS:HG3	1:B:182:TYR:CZ	2.45	0.51
1:A:430:LEU:HD23	1:A:483:PHE:CE1	2.45	0.51
1:A:149:TYR:O	1:A:165:HIS:N	2.42	0.51
1:A:239:THR:HG23	3:A:1032:HOH:O	2.10	0.51
1:A:370:VAL:HG11	1:A:580:TYR:O	2.09	0.51
1:A:461:GLN:HB3	1:A:523:ASN:OD1	2.11	0.51
1:A:185:PRO:HD2	1:A:467:GLY:CA	2.39	0.51
1:A:131:VAL:HG21	1:A:157:ASP:OD2	2.10	0.51
1:B:584:ASN:C	1:B:586:ARG:H	2.14	0.51
1:A:173:ARG:O	1:A:177:GLU:HG2	2.10	0.51
1:A:183:ALA:O	1:A:184:PHE:CD2	2.63	0.51
1:A:410:LYS:HG3	3:A:1073:HOH:O	2.10	0.51
1:A:315:LYS:NZ	1:A:347:GLU:OE1	2.23	0.51
1:A:317:PHE:CE1	1:A:411:THR:HG21	2.45	0.51
1:A:150:GLY:HA2	1:A:165:HIS:HD2	1.75	0.51
1:B:504:PHE:CE2	1:B:508:ILE:CD1	2.94	0.51
1:B:547:GLN:C	1:B:549:GLU:H	2.14	0.51
1:B:338:GLU:HB3	1:B:343:TYR:CG	2.46	0.50
1:A:186:VAL:CG2	1:A:467:GLY:O	2.58	0.50
1:B:422:ASP:OD1	1:B:458:HIS:HE1	1.94	0.50
1:B:292:SER:HB2	1:B:294:LYS:HZ2	1.76	0.50
1:A:101:VAL:HG21	1:A:119:ARG:NE	2.27	0.50
1:A:518:GLY:CA	1:A:521:LEU:HD12	2.40	0.50
1:A:547:GLN:O	1:A:549:GLU:N	2.44	0.50
1:B:283:ARG:NH1	1:B:452:GLU:OE1	2.43	0.50
1:A:303:LEU:HD21	1:A:318:ILE:HD11	1.93	0.50
1:B:407:GLU:HA	1:B:407:GLU:OE1	2.10	0.50
1:A:443:ARG:O	1:A:447:VAL:HG23	2.11	0.50
1:A:86:ASP:OD1	1:A:87:MET:N	2.44	0.50
1:B:428:THR:O	1:B:432:MET:HE2	2.11	0.50
1:B:548:LEU:O	1:B:552:THR:OG1	2.16	0.50
1:B:206:TRP:CE2	1:B:534:PRO:HA	2.47	0.50
1:B:338:GLU:CG	1:B:343:TYR:CZ	2.95	0.49
1:B:76:PRO:HG3	1:B:106:THR:HG21	1.94	0.49
1:A:401:ARG:HH11	1:A:401:ARG:HB3	1.76	0.49
1:B:500:PHE:CE1	1:B:505:LEU:HD21	2.47	0.49
1:A:421:TRP:CD1	1:A:422:ASP:OD2	2.66	0.49
1:B:446:GLU:HG2	1:B:541:TRP:CE3	2.46	0.49
1:B:186:VAL:HG23	1:B:192:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PHE:HB3	1:A:125:LEU:HB3	1.94	0.49
1:A:240:TYR:HB3	1:A:241:PRO:HD2	1.95	0.49
1:A:131:VAL:HG13	1:A:155:CYS:HB3	1.94	0.49
1:B:310:ASN:O	1:B:311:ALA:HB3	2.13	0.49
1:A:259:ALA:CA	1:A:267:ILE:CG2	2.89	0.49
1:B:323:PRO:HB2	1:B:326:ASN:HD22	1.78	0.49
1:B:85:LYS:CB	1:B:182:TYR:CE1	2.96	0.49
1:A:582:ARG:O	1:A:582:ARG:HG3	2.12	0.49
1:A:259:ALA:HA	1:A:267:ILE:HG22	1.92	0.48
1:A:262:ARG:HG3	1:A:267:ILE:HA	1.95	0.48
1:A:527:GLN:HG3	3:A:1234:HOH:O	2.13	0.48
1:B:241:PRO:HG2	1:B:244:LEU:HD23	1.95	0.48
1:A:516:LEU:HD23	1:A:517:PHE:CE1	2.49	0.48
1:A:378:HIS:HB3	1:A:382:ASN:ND2	2.27	0.48
1:B:355:ASN:O	1:B:359:MET:HG2	2.13	0.48
1:B:234:TYR:CD2	1:B:526:GLN:HB2	2.47	0.48
1:A:126:ASP:C	1:A:126:ASP:OD1	2.51	0.48
1:A:101:VAL:HG21	1:A:119:ARG:HE	1.74	0.48
1:B:119:ARG:O	1:B:120:ASP:C	2.52	0.48
1:B:78:LEU:HD11	1:B:84:ILE:HG13	1.95	0.48
1:B:153:THR:OG1	1:B:161:LEU:HB2	2.13	0.48
1:B:75:GLU:HB3	1:B:76:PRO:HD2	1.95	0.48
1:A:267:ILE:O	1:A:268:PRO:C	2.51	0.48
1:A:430:LEU:O	1:A:434:MET:HG3	2.13	0.48
1:A:416:HIS:C	1:A:416:HIS:CD2	2.85	0.48
1:B:528:ARG:HD3	1:B:533:LEU:HD12	1.94	0.48
1:A:317:PHE:CD1	1:A:411:THR:HG21	2.49	0.48
1:B:283:ARG:NH2	1:B:456:PHE:HB3	2.29	0.48
1:B:340:GLU:CG	3:B:1227:HOH:O	2.54	0.48
1:A:102:ARG:HB2	1:A:118:GLU:OE2	2.14	0.48
1:A:113:TYR:CE1	1:A:126:ASP:HB2	2.49	0.47
1:A:304:GLN:HE22	1:A:307:MET:CE	2.27	0.47
1:A:522:CYS:SG	1:A:533:LEU:HD11	2.54	0.47
1:A:318:ILE:O	1:A:348:LEU:HA	2.14	0.47
1:B:135:VAL:HG11	1:B:179:LEU:HD23	1.96	0.47
1:B:316:ILE:HG13	1:B:412:SER:O	2.14	0.47
1:A:563:VAL:HG12	1:A:565:TYR:CE1	2.49	0.47
1:B:450:GLU:OE2	1:B:454:LEU:CD1	2.62	0.47
1:A:85:LYS:O	1:A:86:ASP:HB2	2.15	0.47
1:B:149:TYR:O	1:B:164:ALA:HA	2.15	0.47
1:A:381:SER:HB3	1:B:384:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LEU:HD13	1:A:579:TYR:CE1	2.48	0.47
1:B:282:THR:HG23	3:B:1110:HOH:O	2.14	0.47
1:A:446:GLU:HG2	1:A:541:TRP:CE3	2.50	0.47
1:A:541:TRP:CE3	1:A:544:ILE:HD12	2.50	0.47
1:A:197:TYR:CE2	1:A:199:GLU:HB3	2.50	0.47
1:A:220:ILE:CG2	1:A:221:PRO:N	2.78	0.47
1:B:220:ILE:HD12	1:B:225:TRP:HB2	1.96	0.47
1:B:292:SER:HB2	1:B:294:LYS:HZ1	1.80	0.47
1:B:85:LYS:HD2	1:B:182:TYR:OH	2.14	0.47
1:A:79:LEU:CD1	1:A:111:ARG:NH2	2.78	0.47
1:A:423:ARG:HH21	2:A:656:PO4:P	2.38	0.47
1:A:150:GLY:HA2	1:A:165:HIS:CD2	2.49	0.47
1:B:399:ALA:O	1:B:434:MET:HE1	2.15	0.47
1:A:303:LEU:HD13	1:A:343:TYR:HE2	1.80	0.47
1:B:259:ALA:HA	1:B:267:ILE:CG2	2.45	0.47
1:A:76:PRO:HB3	1:A:113:TYR:CG	2.50	0.47
1:B:388:TRP:O	1:B:392:ILE:HG12	2.15	0.47
1:A:76:PRO:HG3	1:A:106:THR:HG21	1.96	0.47
1:B:502:GLU:HG3	1:B:576:TRP:CZ2	2.49	0.47
1:B:531:GLU:O	1:B:536:ARG:HD3	2.14	0.47
1:B:222:ASN:OD1	1:B:225:TRP:N	2.41	0.47
1:A:422:ASP:O	1:A:426:GLN:HG3	2.16	0.46
1:B:383:LEU:HD13	1:B:575:LEU:HD22	1.98	0.46
1:A:320:ASP:HB2	1:A:348:LEU:HD11	1.96	0.46
1:A:237:CYS:HB2	1:A:265:GLY:O	2.15	0.46
1:B:504:PHE:CE2	1:B:508:ILE:HD11	2.49	0.46
1:B:296:SER:CB	1:B:299:ASP:HB2	2.45	0.46
1:B:415:VAL:HG11	1:B:428:THR:HG22	1.97	0.46
1:B:206:TRP:CD1	1:B:534:PRO:HA	2.50	0.46
1:B:543:TYR:O	1:B:546:SER:OG	2.23	0.46
1:B:91:VAL:CG2	1:B:165:HIS:CE1	2.98	0.46
1:A:511:HIS:CD2	1:A:540:LEU:CD1	2.99	0.46
1:A:524:SER:O	1:A:528:ARG:HG3	2.14	0.46
1:B:307:MET:HE2	1:B:316:ILE:N	2.30	0.46
1:B:426:GLN:HE21	1:B:482:GLN:HB3	1.78	0.46
1:B:321:ALA:HB2	1:B:427:LEU:CD1	2.46	0.46
1:A:511:HIS:CD2	1:A:540:LEU:HD11	2.50	0.46
1:B:212:LEU:HD21	1:B:243:LEU:HD13	1.96	0.46
1:B:545:ASN:ND2	1:B:548:LEU:HD21	2.31	0.46
1:A:159:ARG:NE	1:A:583:TRP:CZ2	2.84	0.46
1:B:245:VAL:HB	1:B:270:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:THR:OG1	1:B:414:VAL:HG22	2.15	0.46
1:A:231:ASN:HD21	1:A:237:CYS:H	1.63	0.46
1:B:158:ILE:HG23	1:B:367:LYS:HG3	1.96	0.46
1:A:112:LEU:HD13	1:A:179:LEU:CD2	2.22	0.46
1:A:418:SER:HB2	2:A:656:PO4:O3	2.16	0.46
1:B:287:PRO:HG2	1:B:337:TYR:CA	2.46	0.46
1:A:137:LYS:HE3	1:A:176:PHE:CE2	2.51	0.46
1:A:220:ILE:HG22	1:A:221:PRO:N	2.30	0.46
1:A:222:ASN:O	1:A:222:ASN:OD1	2.33	0.46
1:B:138:ILE:HD13	1:B:162:ARG:NH2	2.31	0.46
1:A:399:ALA:O	1:A:434:MET:CE	2.63	0.46
1:B:396:LEU:HD23	1:B:430:LEU:HD13	1.98	0.46
1:B:270:LEU:HD23	1:B:271:SER:N	2.30	0.46
1:A:423:ARG:O	1:A:427:LEU:HG	2.15	0.46
1:A:295:ARG:HH21	1:A:300:GLU:CD	2.19	0.46
1:A:113:TYR:CD1	1:A:126:ASP:HB2	2.51	0.46
1:B:310:ASN:OD1	1:B:310:ASN:O	2.34	0.46
1:B:437:GLY:HA2	1:B:440:ARG:NH1	2.30	0.46
1:A:159:ARG:CD	1:A:583:TRP:CZ2	2.99	0.45
1:B:85:LYS:CG	1:B:182:TYR:CE1	2.99	0.45
1:B:307:MET:CE	1:B:316:ILE:HB	2.46	0.45
1:A:316:ILE:HG23	1:A:316:ILE:O	2.16	0.45
1:B:95:CYS:O	1:B:98:THR:O	2.34	0.45
1:A:85:LYS:HB2	1:A:107:VAL:O	2.17	0.45
1:B:94:ILE:HD11	1:B:147:ASN:HB2	1.90	0.45
1:B:270:LEU:HA	1:B:282:THR:HG22	1.97	0.45
1:A:82:GLU:CG	1:A:108:THR:OG1	2.64	0.45
1:B:459:ARG:NH1	1:B:523:ASN:ND2	2.64	0.45
1:B:266:ARG:HD2	1:B:285:SER:HB3	1.97	0.45
1:A:274:HIS:CG	1:A:275:PRO:CD	2.93	0.45
1:A:353:ILE:CD1	1:A:395:ILE:HD13	2.41	0.45
1:A:452:GLU:HB2	1:A:453:TRP:CD1	2.52	0.45
1:A:318:ILE:O	1:A:348:LEU:HD12	2.16	0.45
1:A:419:ASP:HB2	1:A:421:TRP:NE1	2.31	0.45
1:B:383:LEU:CD1	1:B:575:LEU:HD22	2.47	0.45
1:A:290:GLY:HA3	3:A:1106:HOH:O	2.17	0.45
1:B:220:ILE:HD13	1:B:222:ASN:HD22	1.81	0.45
1:B:460:PHE:O	1:B:464:VAL:HG23	2.16	0.45
1:B:229:LYS:HB3	1:B:232:GLU:CG	2.46	0.45
1:B:461:GLN:HB2	1:B:522:CYS:O	2.17	0.45
1:B:320:ASP:CG	1:B:322:ARG:HE	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:GLN:O	1:B:465:GLY:N	2.47	0.45
1:B:307:MET:HE3	1:B:316:ILE:CB	2.46	0.45
1:A:135:VAL:HG12	1:A:176:PHE:CD1	2.52	0.45
1:B:113:TYR:CE2	1:B:115:LYS:HB2	2.52	0.45
1:A:353:ILE:HD13	1:A:395:ILE:CD1	2.41	0.45
1:B:528:ARG:CG	1:B:533:LEU:HD12	2.46	0.45
1:A:506:ILE:CG2	1:A:582:ARG:NH1	2.80	0.45
1:B:125:LEU:HD21	1:B:161:LEU:CD2	2.41	0.44
1:A:557:GLY:O	1:A:558:SER:C	2.55	0.44
1:A:231:ASN:ND2	1:A:234:TYR:HA	2.31	0.44
1:B:365:LYS:CB	1:B:386:THR:HG22	2.48	0.44
1:A:473:ASP:OD1	1:A:475:ASP:HB2	2.17	0.44
1:A:450:GLU:CD	1:A:454:LEU:HD12	2.37	0.44
1:A:74:GLU:CG	1:A:115:LYS:HD3	2.47	0.44
1:B:113:TYR:CZ	1:B:124:VAL:HG13	2.52	0.44
1:B:544:ILE:HG23	1:B:551:PHE:CD1	2.52	0.44
1:A:246:VAL:HB	1:A:247:PRO:HD2	2.00	0.44
1:B:517:PHE:HB3	1:B:538:VAL:O	2.17	0.44
1:B:466:HIS:CG	1:B:515:CYS:SG	3.11	0.44
1:B:224:SER:HB3	1:B:309:SER:HB2	2.00	0.44
1:A:544:ILE:CG2	1:A:551:PHE:CD1	2.91	0.44
1:A:134:ARG:NH1	1:A:136:GLU:CG	2.78	0.44
1:A:576:TRP:CD1	1:A:576:TRP:O	2.70	0.44
1:A:74:GLU:CG	1:A:75:GLU:N	2.80	0.44
1:A:266:ARG:NH2	1:A:456:PHE:O	2.43	0.44
1:B:374:ILE:HD11	1:B:581:ILE:HG21	2.00	0.44
1:A:359:MET:HE2	1:A:482:GLN:HE22	1.80	0.44
1:B:185:PRO:HG3	1:B:192:LEU:HD23	1.98	0.44
1:B:356:ILE:HB	1:B:477:SER:HB2	2.00	0.44
1:A:110:TYR:CE1	1:A:516:LEU:HD13	2.53	0.44
1:A:528:ARG:HG2	1:A:533:LEU:HD12	1.99	0.44
1:A:466:HIS:HE1	1:A:512:LEU:O	2.00	0.44
1:B:85:LYS:HE2	1:B:109:ASN:HB3	1.99	0.44
1:A:431:ALA:HA	1:A:434:MET:CE	2.46	0.43
1:B:267:ILE:HG13	1:B:269:VAL:HG13	1.99	0.43
1:B:460:PHE:CD2	1:B:512:LEU:HD11	2.53	0.43
1:B:348:LEU:C	1:B:348:LEU:HD12	2.38	0.43
1:B:241:PRO:HD2	1:B:244:LEU:HD21	2.00	0.43
1:A:423:ARG:HE	1:A:423:ARG:HB2	1.49	0.43
1:A:134:ARG:NH2	3:A:1200:HOH:O	2.51	0.43
1:B:234:TYR:HB2	1:B:526:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:LEU:N	1:B:534:PRO:HD3	2.34	0.43
1:A:231:ASN:ND2	1:A:237:CYS:H	2.15	0.43
1:B:504:PHE:CE2	1:B:508:ILE:HD12	2.53	0.43
1:A:440:ARG:HE	1:A:564:LEU:HD12	1.83	0.43
1:B:410:LYS:CE	3:B:1093:HOH:O	1.83	0.43
1:A:471:HIS:HA	1:A:476:ARG:NH1	2.33	0.43
1:A:459:ARG:O	1:A:463:ARG:HG2	2.19	0.43
1:A:374:ILE:CD1	1:A:581:ILE:HD13	2.43	0.43
1:B:509:LEU:HD12	1:B:579:TYR:CD1	2.53	0.43
1:B:432:MET:CE	1:B:452:GLU:CG	2.90	0.43
1:B:547:GLN:C	1:B:549:GLU:N	2.72	0.43
1:B:92:THR:OG1	1:B:102:ARG:HG2	2.19	0.43
1:B:451:LYS:O	1:B:456:PHE:HD1	2.02	0.43
1:A:403:ALA:HB2	1:A:434:MET:HE3	2.01	0.43
1:A:430:LEU:CD2	1:A:483:PHE:CE1	3.01	0.43
1:A:533:LEU:N	1:A:534:PRO:CD	2.82	0.43
1:B:460:PHE:CE2	1:B:512:LEU:HD11	2.53	0.43
1:B:298:GLU:CD	1:B:298:GLU:H	2.22	0.43
1:B:511:HIS:CG	1:B:540:LEU:HD13	2.51	0.43
1:A:322:ARG:HH11	1:A:330:ASN:ND2	2.16	0.43
1:A:295:ARG:NE	1:A:300:GLU:OE2	2.40	0.43
1:B:314:HIS:CD2	1:B:315:LYS:CB	2.85	0.42
1:B:323:PRO:HB2	1:B:326:ASN:ND2	2.34	0.42
1:B:298:GLU:O	1:B:302:TYR:N	2.45	0.42
1:A:317:PHE:CE1	1:A:405:LYS:CE	2.98	0.42
1:A:437:GLY:CA	1:A:440:ARG:NH1	2.79	0.42
1:B:481:LEU:HD13	1:B:509:LEU:HD13	2.02	0.42
1:A:92:THR:HB	1:A:164:ALA:HB3	2.02	0.42
1:A:234:TYR:HB3	1:A:238:ASP:HA	2.01	0.42
1:B:128:SER:O	1:B:131:VAL:HG12	2.20	0.42
1:B:114:PHE:HB3	1:B:125:LEU:HB3	2.00	0.42
1:B:461:GLN:O	1:B:465:GLY:CA	2.68	0.42
1:B:401:ARG:HH11	1:B:401:ARG:HB3	1.83	0.42
1:B:97:PHE:CD1	1:B:585:PRO:HD3	2.55	0.42
1:A:101:VAL:HG22	1:A:119:ARG:NE	2.30	0.42
1:B:322:ARG:NH1	1:B:327:ALA:HA	2.35	0.42
1:B:544:ILE:HG22	1:B:545:ASN:HD22	1.84	0.42
1:A:82:GLU:HA	1:A:109:ASN:OD1	2.20	0.42
1:B:209:TYR:HB3	3:B:1182:HOH:O	2.19	0.42
1:A:177:GLU:HA	1:A:177:GLU:OE1	2.20	0.42
1:B:354:HIS:CG	1:B:358:VAL:HG11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLU:HA	1:B:177:GLU:OE1	2.20	0.42
1:A:338:GLU:CG	1:A:343:TYR:CE1	3.03	0.42
1:A:563:VAL:CG1	1:A:565:TYR:CE1	3.03	0.42
1:B:545:ASN:HD22	1:B:548:LEU:HD21	1.85	0.42
1:A:378:HIS:HA	1:B:384:GLU:OE1	2.20	0.42
1:B:316:ILE:O	1:B:316:ILE:HG23	2.19	0.42
1:A:568:ALA:O	1:A:569:SER:OG	2.33	0.42
1:A:399:ALA:HB1	1:A:434:MET:HE2	2.02	0.41
1:A:395:ILE:HG22	1:A:430:LEU:CD1	2.50	0.41
1:B:185:PRO:HG2	1:B:192:LEU:HD21	2.01	0.41
1:A:492:ARG:CD	1:A:574:GLU:OE2	2.67	0.41
1:A:295:ARG:HB2	3:A:1141:HOH:O	2.19	0.41
1:B:584:ASN:O	1:B:586:ARG:N	2.50	0.41
1:A:75:GLU:OE1	1:A:75:GLU:HA	2.20	0.41
1:B:501:ASN:O	1:B:504:PHE:HB3	2.20	0.41
1:A:492:ARG:HD3	1:A:574:GLU:OE2	2.20	0.41
1:B:391:HIS:O	1:B:395:ILE:HG13	2.21	0.41
1:B:226:ARG:HD3	1:B:248:ALA:O	2.21	0.41
1:B:107:VAL:HG22	1:B:112:LEU:HD12	2.01	0.41
1:B:232:GLU:OE1	1:B:232:GLU:HA	2.20	0.41
1:B:303:LEU:HD12	1:B:343:TYR:HD2	1.85	0.41
1:B:320:ASP:OD2	1:B:322:ARG:NE	2.53	0.41
1:A:459:ARG:O	1:A:463:ARG:CG	2.68	0.41
1:A:477:SER:OG	1:A:478:PRO:HD2	2.19	0.41
1:A:101:VAL:CG2	1:A:119:ARG:CZ	2.98	0.41
1:A:416:HIS:CD2	1:A:417:SER:N	2.89	0.41
1:A:422:ASP:OD1	1:A:458:HIS:HE1	1.99	0.41
1:A:458:HIS:NE2	1:A:463:ARG:HG3	2.35	0.41
1:B:503:TYR:CD2	1:B:551:PHE:CE2	3.09	0.41
1:B:383:LEU:HD11	1:B:575:LEU:CD1	2.47	0.41
1:B:401:ARG:CG	1:B:401:ARG:HH11	2.33	0.41
1:A:79:LEU:H	1:A:82:GLU:HB3	1.86	0.41
1:B:442:ILE:HG12	1:B:500:PHE:HB3	2.03	0.41
1:A:576:TRP:C	1:A:576:TRP:CD1	2.92	0.41
1:A:553:ASN:OD1	1:A:554:PRO:HD2	2.20	0.41
1:B:223:GLU:HA	1:B:223:GLU:OE1	2.20	0.41
1:B:389:LEU:HB2	1:B:570:MET:CE	2.51	0.41
1:A:148:SER:HB2	1:A:162:ARG:NH2	2.36	0.41
1:A:267:ILE:O	1:A:267:ILE:CG1	2.61	0.41
1:A:386:THR:O	1:A:387:HIS:HB2	2.21	0.41
1:A:317:PHE:CE1	1:A:405:LYS:CG	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:HG3	1:B:75:GLU:H	1.86	0.41
1:A:136:GLU:OE1	1:A:136:GLU:HA	2.20	0.41
1:A:222:ASN:O	1:A:225:TRP:N	2.52	0.41
1:A:400:LEU:CD2	1:A:565:TYR:HD2	2.34	0.41
1:A:375:GLU:OE1	1:A:375:GLU:C	2.59	0.41
1:B:270:LEU:HD23	1:B:271:SER:C	2.41	0.41
1:B:227:ILE:HG12	1:B:245:VAL:HG22	2.03	0.41
1:A:576:TRP:O	1:A:576:TRP:CG	2.73	0.41
1:A:384:GLU:HB2	1:B:380:LEU:HB2	2.02	0.41
1:B:428:THR:C	1:B:432:MET:HE2	2.42	0.41
1:A:355:ASN:O	1:A:359:MET:HG2	2.21	0.41
1:B:197:TYR:CZ	1:B:199:GLU:HB2	2.56	0.41
1:A:135:VAL:CG1	1:A:176:PHE:CD1	3.04	0.40
1:B:76:PRO:HA	1:B:77:PRO:HD3	1.95	0.40
1:B:461:GLN:NE2	1:B:466:HIS:HB2	2.28	0.40
1:B:82:GLU:OE1	1:B:111:ARG:NH2	2.54	0.40
1:A:94:ILE:HD12	1:A:162:ARG:HD3	2.02	0.40
1:A:228:THR:OG1	1:A:252:ASP:OD1	2.30	0.40
1:B:281:ILE:HG12	1:B:413:VAL:HG22	2.03	0.40
1:A:157:ASP:OD1	1:A:159:ARG:CG	2.70	0.40
1:B:363:LEU:HD12	1:B:363:LEU:O	2.20	0.40
1:A:376:GLU:OE2	1:B:569:SER:HB2	2.21	0.40
1:B:278:GLN:OE1	1:B:278:GLN:HA	2.22	0.40
1:B:188:ASN:OD1	1:B:469:LYS:HE3	2.22	0.40
1:B:443:ARG:O	1:B:447:VAL:HG23	2.21	0.40
1:A:582:ARG:O	1:A:582:ARG:CG	2.70	0.40
1:B:496:THR:O	1:B:556:TYR:HA	2.21	0.40
1:B:376:GLU:HA	1:B:376:GLU:OE1	2.20	0.40
1:A:450:GLU:O	1:A:455:SER:HB3	2.22	0.40
1:B:370:VAL:CG1	1:B:580:TYR:O	2.66	0.40
1:B:236:LEU:CD1	1:B:256:LYS:HD3	2.51	0.40
1:A:149:TYR:CZ	1:A:172:ARG:HG3	2.57	0.40
1:A:524:SER:OG	1:A:527:GLN:HB2	2.21	0.40
1:B:206:TRP:CD2	1:B:534:PRO:HA	2.56	0.40
1:A:230:ILE:HD12	1:A:252:ASP:HB3	2.04	0.40
1:B:237:CYS:HB3	1:B:240:TYR:HB2	2.04	0.40
1:A:193:PHE:HE2	1:A:197:TYR:CD1	2.39	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	511/657 (78%)	460 (90%)	44 (9%)	7 (1%)	14 28
1	B	511/657 (78%)	462 (90%)	36 (7%)	13 (2%)	7 12
All	All	1022/1314 (78%)	922 (90%)	80 (8%)	20 (2%)	9 18

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PRO
1	A	223	GLU
1	A	559	TYR
1	B	344	GLN
1	B	548	LEU
1	A	558	SER
1	B	576	TRP
1	A	220	ILE
1	A	407	GLU
1	B	313	SER
1	B	174	SER
1	B	80	PRO
1	B	147	ASN
1	B	340	GLU
1	B	581	ILE
1	A	80	PRO
1	B	585	PRO
1	B	122	PRO
1	B	140	GLY
1	B	495	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	456/584 (78%)	432 (95%)	24 (5%)	28 53
1	B	456/584 (78%)	442 (97%)	14 (3%)	47 76
All	All	912/1168 (78%)	874 (96%)	38 (4%)	36 65

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	MET
1	A	108	THR
1	A	151	LEU
1	A	226	ARG
1	A	240	TYR
1	A	253	GLU
1	A	294	LYS
1	A	303	LEU
1	A	310	ASN
1	A	312	GLN
1	A	315	LYS
1	A	364	ARG
1	A	370	VAL
1	A	400	LEU
1	A	401	ARG
1	A	415	VAL
1	A	421	TRP
1	A	423	ARG
1	A	455	SER
1	A	459	ARG
1	A	492	ARG
1	A	552	THR
1	A	574	GLU
1	A	582	ARG
1	B	216	ARG
1	B	239	THR
1	B	240	TYR
1	B	266	ARG
1	B	291	VAL
1	B	299	ASP
1	B	322	ARG

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Mol	Chain	Res	Type
1	B	401	ARG
1	B	408	SER
1	B	415	VAL
1	B	417	SER
1	B	421	TRP
1	B	569	SER
1	B	574	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	HIS
1	A	231	ASN
1	A	304	GLN
1	A	310	ASN
1	A	330	ASN
1	A	345	ASN
1	A	373	ASN
1	A	382	ASN
1	A	426	GLN
1	A	482	GLN
1	B	231	ASN
1	B	314	HIS
1	B	326	ASN
1	B	354	HIS
1	B	378	HIS
1	B	426	GLN
1	B	461	GLN
1	B	482	GLN
1	B	511	HIS
1	B	526	GLN
1	B	532	ASN
1	B	545	ASN
1	B	572	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	A	655	-	4,4,4	1.22	0	6,6,6	0.27	0
2	PO4	A	656	-	4,4,4	1.23	0	6,6,6	0.27	0
2	PO4	B	655	-	4,4,4	1.23	0	6,6,6	0.27	0
2	PO4	B	656	-	4,4,4	1.23	0	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	655	-	-	0/0/0/0	0/0/0/0
2	PO4	A	656	-	-	0/0/0/0	0/0/0/0
2	PO4	B	655	-	-	0/0/0/0	0/0/0/0
2	PO4	B	656	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	656	PO4	2	0
2	B	656	PO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.