Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 10:55 PM EDT

PDB ID	:	2IMO
Title	:	Crystal structure of allantoate amidohydrolase from Escherichia coli at pH 4.6
Authors	:	Agarwal, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2006-10-04
Resolution	:	2.80 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 ⓘ 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 ⓘ) were used in the production of this report:

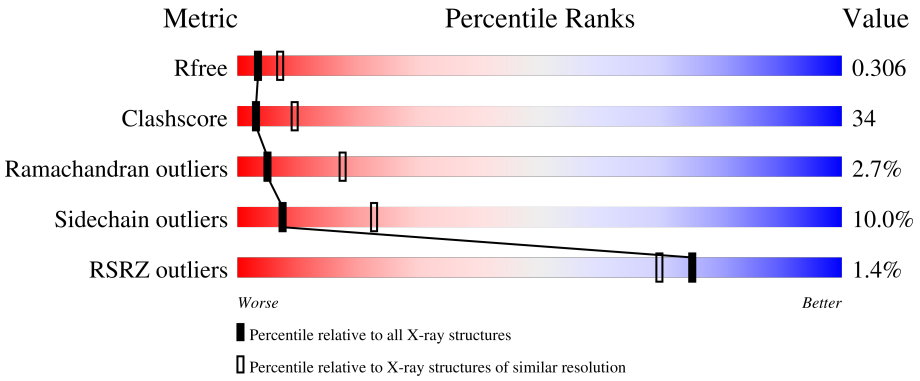
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

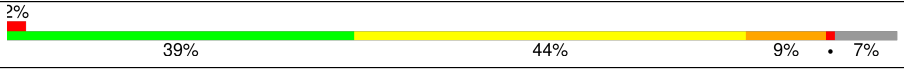
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	423	
1	B	423	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6265 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 Allantoate amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	Se	0	0	0
			3128	1975	541	592	7	13			
1	B	394	Total	C	N	O	S	Se	0	0	0
			3080	1946	535	579	7	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP P77425
A	2	SER	-	cloning artifact	UNP P77425
A	3	LEU	-	cloning artifact	UNP P77425
A	29	MSE	MET	modified residue	UNP P77425
A	49	MSE	MET	modified residue	UNP P77425
A	125	MSE	MET	modified residue	UNP P77425
A	167	MSE	MET	modified residue	UNP P77425
A	234	MSE	MET	modified residue	UNP P77425
A	258	MSE	MET	modified residue	UNP P77425
A	308	MSE	MET	modified residue	UNP P77425
A	315	MSE	MET	modified residue	UNP P77425
A	325	MSE	MET	modified residue	UNP P77425
A	332	MSE	MET	modified residue	UNP P77425
A	354	MSE	MET	modified residue	UNP P77425
A	373	MSE	MET	modified residue	UNP P77425
A	405	MSE	MET	modified residue	UNP P77425
A	414	GLU	-	expression tag	UNP P77425
A	415	GLY	-	expression tag	UNP P77425
A	416	GLY	-	expression tag	UNP P77425
A	417	SER	-	expression tag	UNP P77425
A	418	HIS	-	expression tag	UNP P77425
A	419	HIS	-	expression tag	UNP P77425
A	420	HIS	-	expression tag	UNP P77425
A	421	HIS	-	expression tag	UNP P77425
A	422	HIS	-	expression tag	UNP P77425

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Chain	Residue	Modelled	Actual	Comment	Reference
A	423	HIS	-	expression tag	UNP P77425
B	1	MSE	-	cloning artifact	UNP P77425
B	2	SER	-	cloning artifact	UNP P77425
B	3	LEU	-	cloning artifact	UNP P77425
B	29	MSE	MET	modified residue	UNP P77425
B	49	MSE	MET	modified residue	UNP P77425
B	125	MSE	MET	modified residue	UNP P77425
B	167	MSE	MET	modified residue	UNP P77425
B	234	MSE	MET	modified residue	UNP P77425
B	258	MSE	MET	modified residue	UNP P77425
B	308	MSE	MET	modified residue	UNP P77425
B	315	MSE	MET	modified residue	UNP P77425
B	325	MSE	MET	modified residue	UNP P77425
B	332	MSE	MET	modified residue	UNP P77425
B	354	MSE	MET	modified residue	UNP P77425
B	373	MSE	MET	modified residue	UNP P77425
B	405	MSE	MET	modified residue	UNP P77425
B	414	GLU	-	expression tag	UNP P77425
B	415	GLY	-	expression tag	UNP P77425
B	416	GLY	-	expression tag	UNP P77425
B	417	SER	-	expression tag	UNP P77425
B	418	HIS	-	expression tag	UNP P77425
B	419	HIS	-	expression tag	UNP P77425
B	420	HIS	-	expression tag	UNP P77425
B	421	HIS	-	expression tag	UNP P77425
B	422	HIS	-	expression tag	UNP P77425
B	423	HIS	-	expression tag	UNP P77425

- Molecule 2 is water.

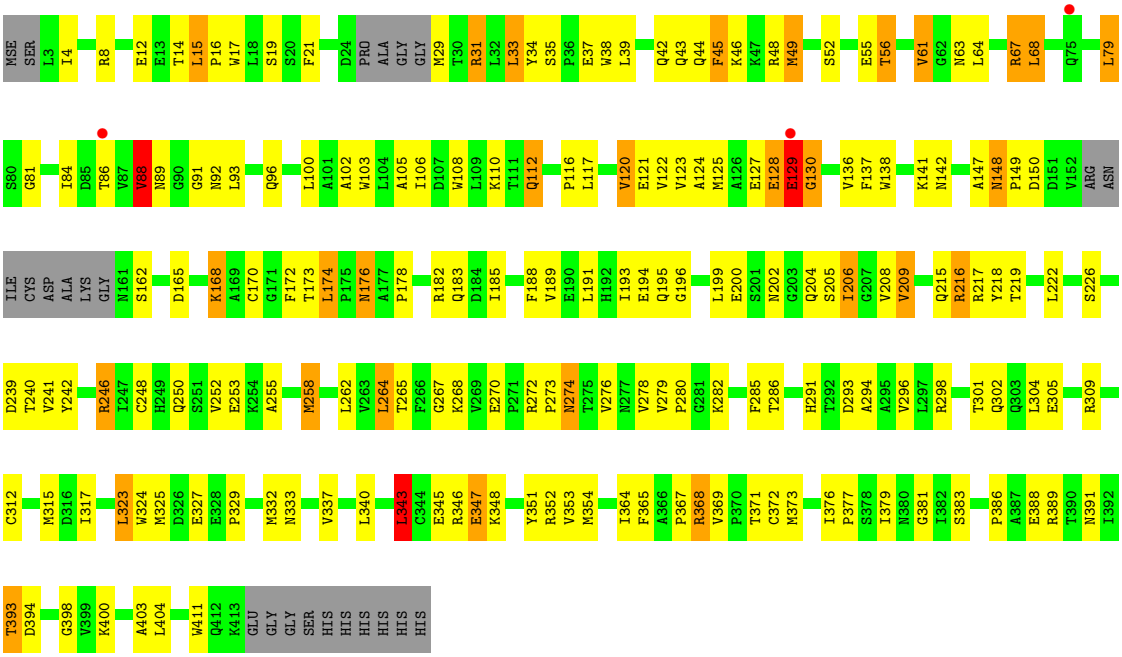
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	37	Total O 37 37	0	0
2	B	20	Total O 20 20	0	0

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.

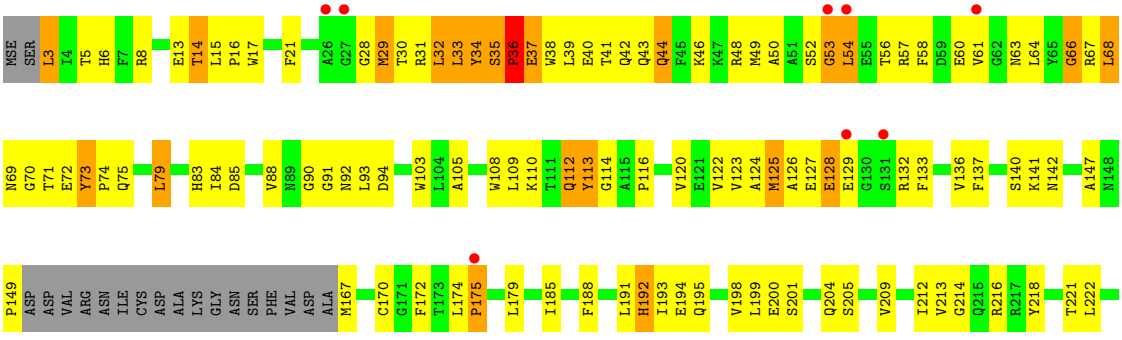
• Molecule 1: Allantoate amidohydrolase

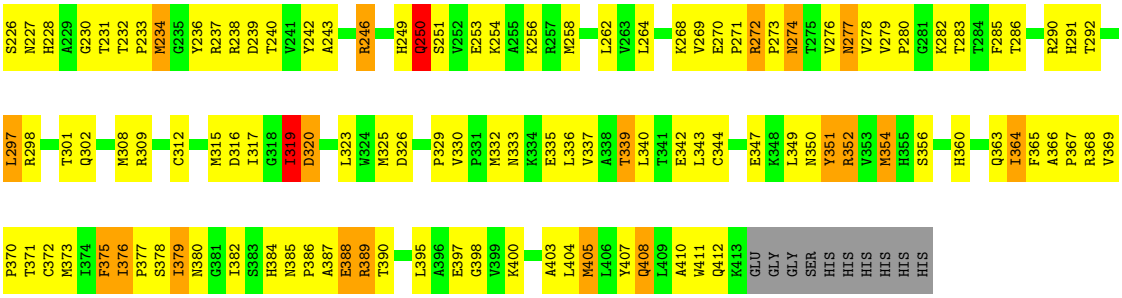
Chain A:



• Molecule 1: Allantoate amidohydrolase

Chain B:




S226 N227 H228 A229 G230 T231 T232 P233 M234 G235 Y236 R237 R238 D239 T240 V241 Y242 A243 R246 H249 Q250 S251 V252 E253 K254 A255 K256 R257 M258 L262 V263 L264 K268 V269 E270 P271 R272 P273 N274 T275 V276 N277 V278 V279 P280 G281 K282 T283 T284 F285 T286 R290 H291 T292
L297 R298 T301 Q302 M308 R309 C312 M315 D316 I317 G318 I319 D320 L323 W324 M325 D326 P329 V330 P331 M332 N333 K334 E335 L336 V337 A338 T339 L340 T341 E342 L343 C344 E347 K348 L349 N350 Y351 R352 V353 M354 H355 S356 H360 Q363 I364 F365 A366 P367 R368 V369
P370 T371 C372 M373 I374 F375 I376 P377 S378 I379 N380 G381 I382 S383 H384 N385 P386 A387 E388 R389 T390 L395 A396 E397 G398 V399 K400 A403 L404 M405 L406 Y407 Q408 L409 A410 W411 Q412 K413 GLU GLY GLY SER HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.75Å 183.92Å 48.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 2.80 48.78 – 2.77	Depositor EDS
% Data completeness (in resolution range)	90.0 (48.78-2.80) 88.5 (48.78-2.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.302 0.264 , 0.306	Depositor DCC
R_{free} test set	578 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6265	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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

5.1 Standard geometry

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	0.55	2/3183 (0.1%)	0.74	3/4302 (0.1%)
1	B	0.54	4/3136 (0.1%)	0.71	1/4239 (0.0%)
All	All	0.55	6/6319 (0.1%)	0.72	4/8541 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	MSE	CG-SE	-5.50	1.76	1.95
1	B	29	MSE	CG-SE	-5.45	1.76	1.95
1	B	354	MSE	CG-SE	-5.08	1.78	1.95
1	B	125	MSE	CG-SE	-5.07	1.78	1.95
1	A	49	MSE	CG-SE	-5.05	1.78	1.95
1	B	308	MSE	CG-SE	-5.05	1.78	1.95

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	LEU	CA-CB-CG	6.11	129.36	115.30
1	B	66	GLY	N-CA-C	-5.41	99.57	113.10
1	A	343	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	68	LEU	N-CA-C	-5.30	96.69	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3128	0	3064	180	0
1	B	3080	0	3028	247	0
2	A	37	0	0	6	0
2	B	20	0	0	3	0
All	All	6265	0	6092	419	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 34.

All (419) 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:B:344:CYS:HA	1:B:349:LEU:HD12	1.42	1.02
1:A:365:PHE:HB3	1:A:371:THR:HG21	1.49	0.94
1:A:379:ILE:HD11	1:A:389:ARG:HB2	1.49	0.94
1:B:209:VAL:HG11	1:B:373:MSE:HE3	1.49	0.93
1:A:208:VAL:HG13	1:A:340:LEU:HD23	1.51	0.92
1:B:240:THR:HG22	1:B:280:PRO:O	1.75	0.87
1:B:228:HIS:O	1:B:232:THR:HG22	1.76	0.86
1:B:74:PRO:HG2	1:B:75:GLN:HE21	1.39	0.86
1:A:240:THR:HG22	1:A:280:PRO:O	1.76	0.85
1:A:149:PRO:HB3	1:A:174:LEU:HD23	1.57	0.84
1:B:340:LEU:HB2	1:B:405:MSE:HE2	1.58	0.84
1:B:228:HIS:HD2	1:B:230:GLY:H	1.23	0.83
1:B:379:ILE:HA	1:B:389:ARG:CZ	2.12	0.80
1:A:4:ILE:HG13	1:A:400:LYS:HD3	1.65	0.79
1:B:379:ILE:HD13	1:B:382:ILE:O	1.85	0.77
1:A:204:GLN:HB2	2:A:439:HOH:O	1.83	0.77
1:B:246:ARG:HH21	1:B:315:MSE:SE	2.17	0.76
1:B:142:ASN:ND2	1:B:147:ALA:HB3	2.01	0.75
1:B:277:ASN:H	1:B:277:ASN:HD22	1.33	0.75
1:A:199:LEU:HA	2:A:439:HOH:O	1.85	0.75
1:B:376:ILE:HG23	1:B:390:THR:HG21	1.67	0.74
1:B:68:LEU:HD21	1:B:110:LYS:HE2	1.69	0.73
1:B:379:ILE:HA	1:B:389:ARG:NH1	2.02	0.73
1:A:68:LEU:HD22	1:A:116:PRO:HD2	1.71	0.73
1:B:63:ASN:HD22	1:B:125:MSE:HA	1.54	0.72
1:B:39:LEU:HD13	1:B:170:CYS:HB3	1.72	0.71
1:B:376:ILE:HD11	1:B:398:GLY:HA3	1.71	0.71
1:B:116:PRO:HG3	1:B:120:VAL:HG23	1.72	0.70
1:B:379:ILE:H	1:B:379:ILE:HD12	1.57	0.70
1:A:332:MSE:SE	2:A:451:HOH:O	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:MSE:HE3	1:A:92:ASN:HB3	1.74	0.69
1:B:46:LYS:HG3	1:B:56:THR:OG1	1.91	0.69
1:A:14:THR:CG2	1:A:100:LEU:HD11	2.22	0.69
1:A:286:THR:HG23	2:B:427:HOH:O	1.92	0.69
1:A:274:ASN:HD21	1:B:269:VAL:H	1.40	0.69
1:B:61:VAL:HG11	1:B:142:ASN:OD1	1.93	0.69
1:A:272:ARG:HD3	1:A:282:LYS:HE2	1.74	0.68
1:A:369:VAL:O	1:A:371:THR:HG23	1.94	0.68
1:B:31:ARG:NH1	1:B:41:THR:HG21	2.07	0.68
1:A:202:ASN:HB3	1:A:204:GLN:HE21	1.59	0.68
1:A:204:GLN:NE2	1:A:352:ARG:HE	1.91	0.67
1:A:217:ARG:HB2	1:A:325:MSE:HB3	1.76	0.67
1:A:333:ASN:O	1:A:337:VAL:HG23	1.94	0.67
1:A:267:GLY:O	1:B:274:ASN:HA	1.95	0.67
1:B:83:HIS:CG	1:B:128:GLU:HG2	2.30	0.67
1:B:365:PHE:HB3	1:B:371:THR:HG21	1.77	0.67
1:B:360:HIS:O	1:B:363:GLN:HG2	1.95	0.66
1:A:185:ILE:HB	1:A:369:VAL:HG11	1.77	0.66
1:B:369:VAL:O	1:B:371:THR:HG23	1.95	0.66
1:B:34:TYR:OH	1:B:167:MSE:HE3	1.95	0.66
1:A:246:ARG:NH2	1:A:315:MSE:HE2	2.11	0.66
1:B:90:GLY:HA3	1:B:384:HIS:O	1.96	0.66
1:B:379:ILE:HD12	1:B:379:ILE:N	2.11	0.65
1:B:228:HIS:CD2	1:B:230:GLY:H	2.10	0.65
1:A:14:THR:HG22	1:A:100:LEU:HD11	1.79	0.65
1:B:385:ASN:HD21	1:B:387:ALA:HB3	1.62	0.64
1:A:246:ARG:HH21	1:A:315:MSE:HE2	1.61	0.64
1:A:368:ARG:HG3	1:A:368:ARG:HH11	1.63	0.64
1:B:116:PRO:HB3	1:B:411:TRP:CE2	2.33	0.64
1:A:49:MSE:HE1	1:A:122:VAL:HB	1.80	0.64
1:B:167:MSE:SE	1:B:174:LEU:HB3	2.48	0.63
1:B:312:CYS:HB3	1:B:317:ILE:O	1.99	0.63
1:B:8:ARG:HH11	1:B:8:ARG:HG2	1.64	0.63
1:B:277:ASN:H	1:B:277:ASN:ND2	1.95	0.63
1:B:63:ASN:ND2	1:B:126:ALA:H	1.96	0.62
1:A:248:CYS:O	1:A:252:VAL:HG23	2.00	0.61
1:B:49:MSE:O	1:B:54:LEU:HB2	2.00	0.61
1:B:309:ARG:HD3	1:B:319:ILE:HD13	1.82	0.61
1:A:194:GLU:O	1:A:195:GLN:HB2	2.01	0.61
1:B:36:PRO:O	1:B:37:GLU:HB2	1.99	0.61
1:B:60:GLU:H	1:B:60:GLU:CD	2.04	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD12	1:A:170:CYS:HA	1.82	0.61
1:A:343:LEU:HB3	1:A:346:ARG:HH22	1.65	0.61
1:B:185:ILE:HB	1:B:369:VAL:HG11	1.83	0.61
1:A:343:LEU:HB2	1:A:346:ARG:HH12	1.66	0.60
1:B:174:LEU:HD12	1:B:174:LEU:O	2.01	0.60
1:B:226:SER:HA	1:B:279:VAL:O	2.00	0.60
1:B:286:THR:HG23	2:B:425:HOH:O	2.02	0.60
1:B:408:GLN:HA	1:B:412:GLN:HG2	1.83	0.60
1:B:46:LYS:NZ	1:B:56:THR:HG23	2.16	0.60
1:B:319:ILE:HD12	1:B:319:ILE:H	1.66	0.60
1:B:109:LEU:O	1:B:113:TYR:HB2	2.02	0.59
1:B:205:SER:O	1:B:377:PRO:HD3	2.01	0.59
1:B:268:LYS:H	1:B:286:THR:HG22	1.67	0.59
1:A:61:VAL:HG21	1:A:142:ASN:CG	2.23	0.59
1:A:168:LYS:HB2	1:A:168:LYS:HZ3	1.67	0.59
1:B:141:LYS:HB3	1:B:147:ALA:HB2	1.83	0.59
1:B:271:PRO:HG2	1:B:274:ASN:HB2	1.84	0.59
1:B:277:ASN:HD22	1:B:277:ASN:N	1.95	0.59
1:B:379:ILE:HG12	1:B:388:GLU:HA	1.85	0.59
1:A:8:ARG:HG2	1:A:8:ARG:NH1	2.18	0.58
1:A:31:ARG:HH12	1:A:96:GLN:HG3	1.68	0.58
1:A:273:PRO:HG3	1:A:278:VAL:HG11	1.86	0.58
1:B:271:PRO:HG2	1:B:274:ASN:HD22	1.69	0.58
1:B:333:ASN:O	1:B:337:VAL:HG23	2.02	0.58
1:A:136:VAL:O	1:A:137:PHE:HB2	2.04	0.58
1:A:205:SER:O	1:A:377:PRO:HD3	2.03	0.58
1:B:175:PRO:HG2	1:B:179:LEU:HD11	1.85	0.58
1:A:46:LYS:HG3	1:A:56:THR:HB	1.84	0.58
1:A:204:GLN:OE1	1:A:352:ARG:HB2	2.03	0.58
1:B:33:LEU:HG	1:B:127:GLU:HB2	1.84	0.58
1:B:213:VAL:HG21	1:B:290:ARG:HB3	1.85	0.58
1:B:214:GLY:HA3	1:B:329:PRO:HG3	1.86	0.58
1:A:174:LEU:O	1:A:174:LEU:HD22	2.04	0.57
1:A:218:TYR:CZ	1:A:323:LEU:HG	2.40	0.57
1:B:120:VAL:HG21	1:B:411:TRP:CZ3	2.40	0.57
1:A:274:ASN:ND2	1:B:268:LYS:HA	2.20	0.57
1:A:147:ALA:O	1:A:148:ASN:HB3	2.05	0.57
1:A:209:VAL:HA	1:A:354:MSE:O	2.03	0.57
1:A:8:ARG:HG2	1:A:8:ARG:HH11	1.69	0.57
1:A:268:LYS:HB3	1:A:286:THR:HG22	1.87	0.57
1:A:365:PHE:CB	1:A:371:THR:HG21	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ASN:ND2	1:B:370:PRO:HB3	2.20	0.57
1:A:196:GLY:O	1:A:381:GLY:HA2	2.04	0.57
1:A:218:TYR:CE2	1:A:323:LEU:HG	2.39	0.57
1:B:132:ARG:HD3	1:B:133:PHE:CE1	2.40	0.57
1:B:367:PRO:HB2	1:B:368:ARG:NH1	2.19	0.57
1:A:188:PHE:HB3	1:A:371:THR:HG22	1.86	0.56
1:B:93:LEU:HB3	1:B:193:ILE:HG21	1.85	0.56
1:B:105:ALA:O	1:B:109:LEU:HB2	2.05	0.56
1:A:264:LEU:H	1:B:234:MSE:HE1	1.71	0.56
1:B:8:ARG:HG2	1:B:8:ARG:NH1	2.18	0.56
1:B:239:ASP:HB3	1:B:242:TYR:HB3	1.86	0.56
1:B:268:LYS:HB3	1:B:286:THR:CG2	2.34	0.56
1:B:116:PRO:HB3	1:B:411:TRP:CD2	2.40	0.56
1:B:179:LEU:HD12	1:B:179:LEU:H	1.70	0.56
1:B:71:THR:O	1:B:72:GLU:HB3	2.06	0.56
1:B:379:ILE:CG1	1:B:389:ARG:H	2.19	0.56
1:A:128:GLU:O	1:A:129:GLU:HG3	2.06	0.56
1:A:168:LYS:HZ1	1:A:173:THR:HG23	1.69	0.56
1:A:33:LEU:HD22	1:A:34:TYR:CD1	2.40	0.56
1:B:347:GLU:HB2	1:B:349:LEU:HG	1.88	0.56
1:B:222:LEU:HD13	1:B:285:PHE:HE2	1.69	0.56
1:B:228:HIS:CD2	1:B:231:THR:HG23	2.41	0.56
1:B:191:LEU:HD21	1:B:376:ILE:HD13	1.86	0.56
1:B:228:HIS:CD2	1:B:231:THR:H	2.24	0.56
1:A:272:ARG:HD3	1:A:282:LYS:CE	2.35	0.55
1:A:204:GLN:NE2	1:A:352:ARG:HH21	2.04	0.55
1:A:15:LEU:O	1:A:19:SER:HB2	2.06	0.55
1:A:14:THR:O	1:A:17:TRP:HB3	2.07	0.55
1:A:116:PRO:HG3	1:A:120:VAL:HG22	1.87	0.55
1:B:29:MSE:HB2	1:B:90:GLY:O	2.06	0.55
1:A:137:PHE:HB3	1:A:141:LYS:HG3	1.89	0.55
1:A:216:ARG:HA	1:A:325:MSE:O	2.07	0.55
1:B:83:HIS:CD2	1:B:128:GLU:HG2	2.42	0.55
1:B:250:GLN:O	1:B:254:LYS:HG3	2.06	0.55
1:A:209:VAL:HG13	1:A:373:MSE:HB2	1.89	0.55
1:B:52:SER:C	1:B:54:LEU:H	2.09	0.55
1:A:37:GLU:CD	1:A:37:GLU:H	2.10	0.55
1:A:268:LYS:HB3	1:A:286:THR:CG2	2.37	0.55
1:A:345:GLU:HA	1:A:345:GLU:OE2	2.06	0.55
1:B:273:PRO:HG3	1:B:278:VAL:HG11	1.88	0.55
1:B:352:ARG:HG2	1:B:352:ARG:HH11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:HD2	1:A:84:ILE:O	2.06	0.54
1:A:226:SER:HA	1:A:279:VAL:O	2.07	0.54
1:B:204:GLN:HA	1:B:350:ASN:ND2	2.22	0.54
1:A:68:LEU:HD22	1:A:116:PRO:CD	2.35	0.54
1:A:67:ARG:HA	1:A:120:VAL:O	2.08	0.54
1:A:103:TRP:HA	1:A:122:VAL:HG21	1.89	0.54
1:A:130:GLY:H	1:A:136:VAL:HG12	1.72	0.54
1:B:63:ASN:HD22	1:B:125:MSE:CA	2.20	0.54
1:B:216:ARG:HG2	1:B:323:LEU:HD21	1.88	0.54
1:B:188:PHE:HB3	1:B:371:THR:HG22	1.89	0.54
1:B:193:ILE:O	1:B:195:GLN:N	2.34	0.54
1:B:368:ARG:HH11	1:B:368:ARG:HG3	1.73	0.53
1:B:379:ILE:HG13	1:B:389:ARG:O	2.08	0.53
1:A:294:ALA:HB2	1:A:329:PRO:HD2	1.91	0.53
1:B:243:ALA:HB2	1:B:315:MSE:HE2	1.90	0.53
1:A:383:SER:HA	1:A:388:GLU:OE1	2.09	0.53
1:B:91:GLY:O	1:B:388:GLU:HG3	2.09	0.53
1:B:240:THR:HG21	1:B:282:LYS:N	2.22	0.53
1:B:366:ALA:HB3	1:B:367:PRO:HD3	1.90	0.53
1:B:379:ILE:HD11	1:B:389:ARG:H	1.73	0.53
1:B:319:ILE:HG22	1:B:320:ASP:H	1.72	0.53
1:B:68:LEU:HD12	1:B:116:PRO:HD2	1.91	0.53
1:B:213:VAL:CG2	1:B:290:ARG:HB3	2.39	0.53
1:A:130:GLY:CA	1:A:136:VAL:HG12	2.39	0.52
1:A:204:GLN:HE22	1:A:352:ARG:NH2	2.07	0.52
1:B:54:LEU:HD22	1:B:68:LEU:HD23	1.90	0.52
1:B:385:ASN:ND2	1:B:387:ALA:H	2.08	0.52
1:A:130:GLY:N	1:A:136:VAL:HG12	2.25	0.52
1:B:218:TYR:OH	1:B:301:THR:HB	2.10	0.52
1:B:70:GLY:O	1:B:74:PRO:HB3	2.10	0.52
1:A:91:GLY:HA3	1:A:388:GLU:CG	2.39	0.52
1:A:255:ALA:O	1:A:258:MSE:HB2	2.10	0.52
1:B:28:GLY:HA3	1:B:386:PRO:HG3	1.92	0.52
1:B:68:LEU:CD2	1:B:110:LYS:HE2	2.39	0.52
1:B:379:ILE:HA	1:B:389:ARG:NH2	2.26	0.51
1:B:60:GLU:HB2	1:B:179:LEU:HD21	1.92	0.51
1:B:128:GLU:O	1:B:128:GLU:HG3	2.07	0.51
1:A:368:ARG:HD2	1:A:368:ARG:N	2.25	0.51
1:B:53:GLY:H	1:B:110:LYS:HZ1	1.57	0.51
1:B:315:MSE:HE2	1:B:317:ILE:HD12	1.91	0.51
1:A:8:ARG:O	1:A:12:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:CD1	1:A:170:CYS:HA	2.39	0.51
1:B:216:ARG:HH21	1:B:298:ARG:HG3	1.76	0.51
1:A:268:LYS:HE2	1:A:270:GLU:OE1	2.10	0.51
1:B:40:GLU:O	1:B:44:GLN:HG2	2.10	0.51
1:B:227:ASN:CB	1:B:232:THR:HG21	2.41	0.51
1:B:291:HIS:ND1	1:B:292:THR:N	2.59	0.51
1:A:106:ILE:HD12	1:A:122:VAL:CG2	2.41	0.51
1:A:200:GLU:OE2	1:A:379:ILE:HA	2.11	0.50
1:B:149:PRO:HB3	1:B:174:LEU:HD13	1.92	0.50
1:B:368:ARG:NH1	1:B:368:ARG:HG3	2.26	0.50
1:A:55:GLU:O	1:A:55:GLU:HG2	2.11	0.50
1:B:319:ILE:O	1:B:320:ASP:HB2	2.09	0.50
1:B:323:LEU:HD11	1:B:326:ASP:HB2	1.94	0.50
1:A:367:PRO:HG2	1:A:368:ARG:HD2	1.91	0.50
1:B:194:GLU:HG3	1:B:375:PHE:CD2	2.46	0.50
1:B:194:GLU:HA	1:B:375:PHE:CE2	2.46	0.50
1:A:79:LEU:HD23	1:A:121:GLU:O	2.11	0.50
1:A:298:ARG:O	1:A:302:GLN:HG3	2.10	0.50
1:B:33:LEU:HD23	1:B:34:TYR:H	1.77	0.50
1:A:128:GLU:C	1:A:129:GLU:HG3	2.32	0.50
1:A:219:THR:HG1	1:A:324:TRP:HD1	1.58	0.50
1:A:45:PHE:O	1:A:49:MSE:HG3	2.12	0.50
1:A:206:ILE:HD11	1:A:398:GLY:HA2	1.94	0.50
1:B:85:ASP:OD1	1:B:127:GLU:HA	2.12	0.50
1:B:39:LEU:HG	1:B:43:GLN:HE21	1.77	0.50
1:B:212:ILE:HG12	1:B:356:SER:HB3	1.92	0.50
1:A:42:GLN:NE2	1:A:84:ILE:HG12	2.27	0.50
1:B:232:THR:HG23	1:B:232:THR:O	2.11	0.50
1:A:347:GLU:HB2	2:A:427:HOH:O	2.11	0.49
1:B:233:PRO:O	1:B:237:ARG:HG3	2.13	0.49
1:B:340:LEU:HD13	1:B:405:MSE:HG3	1.94	0.49
1:B:340:LEU:O	1:B:343:LEU:HB3	2.12	0.49
1:A:15:LEU:N	1:A:16:PRO:HD2	2.27	0.49
1:A:168:LYS:HB2	1:A:168:LYS:NZ	2.27	0.49
1:B:21:PHE:CE2	1:B:44:GLN:HG3	2.47	0.49
1:A:204:GLN:NE2	1:A:352:ARG:NE	2.60	0.49
1:B:227:ASN:HB3	1:B:232:THR:HG21	1.93	0.49
1:B:379:ILE:HG22	1:B:380:ASN:N	2.26	0.49
1:B:68:LEU:HD12	1:B:116:PRO:CD	2.42	0.49
1:B:71:THR:O	1:B:72:GLU:CB	2.61	0.49
1:B:200:GLU:HG3	1:B:201:SER:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HG22	1:A:351:TYR:HB2	1.93	0.49
1:B:199:LEU:HD21	1:B:352:ARG:HB3	1.94	0.49
1:B:382:ILE:HG21	1:B:387:ALA:HB3	1.93	0.49
1:B:53:GLY:H	1:B:110:LYS:NZ	2.10	0.49
1:B:216:ARG:HA	1:B:325:MSE:O	2.13	0.49
1:A:130:GLY:HA3	1:A:136:VAL:HG12	1.94	0.49
1:B:50:ALA:C	1:B:52:SER:H	2.15	0.48
1:B:269:VAL:O	1:B:270:GLU:HG3	2.12	0.48
1:A:148:ASN:HD21	1:A:150:ASP:HB2	1.77	0.48
1:A:182:ARG:NE	1:A:185:ILE:HD11	2.28	0.48
1:B:15:LEU:N	1:B:16:PRO:HD2	2.27	0.48
1:A:391:ASN:O	1:A:394:ASP:HB2	2.14	0.48
1:B:52:SER:HB3	1:B:110:LYS:HZ1	1.78	0.48
1:B:57:ARG:O	1:B:64:LEU:HD12	2.12	0.48
1:B:60:GLU:OE1	1:B:179:LEU:HD23	2.14	0.48
1:B:214:GLY:O	1:B:297:LEU:HD12	2.14	0.48
1:B:404:LEU:O	1:B:407:TYR:HB3	2.13	0.48
1:B:90:GLY:HA2	1:B:386:PRO:HA	1.95	0.48
1:A:168:LYS:HA	1:A:172:PHE:O	2.14	0.48
1:A:193:ILE:HA	1:A:376:ILE:HG13	1.96	0.48
1:B:379:ILE:CD1	1:B:389:ARG:H	2.27	0.47
1:A:182:ARG:CZ	1:A:185:ILE:HD11	2.44	0.47
1:A:305:GLU:O	1:A:309:ARG:HD2	2.13	0.47
1:B:85:ASP:CG	1:B:127:GLU:HA	2.34	0.47
1:B:379:ILE:HG23	1:B:389:ARG:NH1	2.29	0.47
1:A:353:VAL:HG13	1:A:353:VAL:O	2.13	0.47
1:B:271:PRO:O	1:B:272:ARG:HD2	2.15	0.47
1:B:198:VAL:HB	1:B:354:MSE:HE1	1.96	0.47
1:A:21:PHE:CE2	1:A:44:GLN:HG3	2.49	0.47
1:A:39:LEU:HD12	1:A:170:CYS:CA	2.45	0.47
1:A:174:LEU:HD13	1:A:174:LEU:H	1.79	0.47
1:A:246:ARG:O	1:A:250:GLN:HB2	2.14	0.47
1:B:330:VAL:HG21	1:B:363:GLN:HB2	1.97	0.47
1:A:372:CYS:HB2	2:A:446:HOH:O	2.15	0.47
1:A:52:SER:O	1:A:110:LYS:HE3	2.15	0.47
1:B:14:THR:O	1:B:17:TRP:CD1	2.68	0.47
1:B:57:ARG:HH11	1:B:57:ARG:HG2	1.78	0.47
1:B:140:SER:C	1:B:364:ILE:HD11	2.35	0.46
1:B:120:VAL:HG22	1:B:410:ALA:CB	2.45	0.46
1:B:333:ASN:HB3	1:B:336:LEU:HB2	1.97	0.46
1:B:335:GLU:O	1:B:339:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ARG:HG3	1:B:298:ARG:HH11	1.80	0.46
1:B:379:ILE:HG13	1:B:389:ARG:H	1.81	0.46
1:A:343:LEU:HB2	1:A:346:ARG:NH1	2.30	0.46
1:B:5:THR:HA	1:B:8:ARG:HB3	1.98	0.46
1:A:343:LEU:HD12	1:A:343:LEU:C	2.36	0.46
1:B:298:ARG:O	1:B:302:GLN:HB2	2.16	0.46
1:A:63:ASN:HD22	1:A:125:MSE:HA	1.81	0.46
1:B:112:GLN:HE21	1:B:112:GLN:HB3	1.53	0.46
1:B:249:HIS:O	1:B:250:GLN:HB2	2.16	0.46
1:A:8:ARG:HD2	1:A:393:THR:HG23	1.97	0.46
1:B:42:GLN:HE21	1:B:84:ILE:HG12	1.80	0.46
1:B:141:LYS:N	1:B:364:ILE:HD11	2.31	0.46
1:B:179:LEU:H	1:B:179:LEU:CD1	2.28	0.46
1:A:174:LEU:H	1:A:174:LEU:CD1	2.28	0.46
1:B:268:LYS:HB3	1:B:286:THR:HG22	1.96	0.46
1:A:67:ARG:H	1:A:121:GLU:HA	1.80	0.45
1:A:209:VAL:CG1	1:A:373:MSE:HB2	2.46	0.45
1:B:92:ASN:HB3	1:B:388:GLU:CD	2.36	0.45
1:A:35:SER:H	1:A:38:TRP:HB3	1.80	0.45
1:A:162:SER:HB3	1:A:165:ASP:HB2	1.98	0.45
1:A:206:ILE:O	1:A:351:TYR:HA	2.17	0.45
1:A:293:ASP:OD2	1:A:296:VAL:HG23	2.15	0.45
1:A:239:ASP:HB3	1:A:242:TYR:HB3	1.99	0.45
1:B:14:THR:HG21	1:B:103:TRP:HZ3	1.80	0.45
1:B:376:ILE:CG2	1:B:390:THR:HG21	2.42	0.45
1:A:206:ILE:HG22	1:A:351:TYR:CB	2.46	0.45
1:B:79:LEU:HD21	1:B:123:VAL:HB	1.98	0.45
1:B:199:LEU:CD2	1:B:352:ARG:HB3	2.46	0.45
1:A:176:ASN:OD1	1:A:176:ASN:N	2.50	0.45
1:A:324:TRP:CZ3	1:A:325:MSE:HB2	2.51	0.45
1:B:52:SER:O	1:B:54:LEU:N	2.50	0.45
1:B:94:ASP:OD1	1:B:192:HIS:HE1	2.00	0.45
1:B:35:SER:OG	1:B:36:PRO:HD2	2.17	0.44
1:B:179:LEU:HD12	1:B:179:LEU:N	2.31	0.44
1:B:274:ASN:CG	1:B:274:ASN:O	2.55	0.44
1:A:204:GLN:HE22	1:A:352:ARG:NE	2.15	0.44
1:A:39:LEU:O	1:A:43:GLN:HG2	2.17	0.44
1:A:91:GLY:HA3	1:A:388:GLU:HG2	1.98	0.44
1:A:148:ASN:HA	1:A:178:PRO:HG3	1.99	0.44
1:B:63:ASN:HD22	1:B:126:ALA:H	1.64	0.44
1:B:309:ARG:CD	1:B:319:ILE:HD13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:MSE:HE3	1:B:372:CYS:HA	1.98	0.44
1:B:36:PRO:O	1:B:37:GLU:CB	2.63	0.44
1:B:332:MSE:HE3	1:B:372:CYS:CA	2.47	0.44
1:B:48:ARG:HB3	1:B:103:TRP:CZ2	2.52	0.44
1:A:364:ILE:O	1:A:368:ARG:HD3	2.18	0.44
1:B:216:ARG:NH2	1:B:298:ARG:HG3	2.33	0.44
1:B:390:THR:HB	1:B:395:LEU:HD21	2.00	0.44
1:A:368:ARG:HG3	1:A:368:ARG:NH1	2.32	0.44
1:B:66:GLY:O	1:B:122:VAL:HG12	2.18	0.44
1:B:221:THR:HB	1:B:320:ASP:HB3	2.00	0.44
1:A:120:VAL:HG11	1:A:411:TRP:HZ3	1.83	0.43
1:B:32:LEU:O	1:B:38:TRP:HB2	2.18	0.43
1:B:105:ALA:HB1	1:B:403:ALA:HA	2.00	0.43
1:B:251:SER:O	1:B:254:LYS:HB2	2.18	0.43
1:A:105:ALA:HB1	1:A:403:ALA:HA	2.00	0.43
1:A:199:LEU:HB3	1:A:377:PRO:HG3	1.99	0.43
1:A:216:ARG:HG2	1:A:323:LEU:HD21	2.00	0.43
1:A:218:TYR:OH	1:A:301:THR:HB	2.18	0.43
1:A:343:LEU:O	1:A:347:GLU:HB3	2.17	0.43
1:A:39:LEU:HD12	1:A:170:CYS:CB	2.48	0.43
1:A:149:PRO:CB	1:A:174:LEU:HD23	2.39	0.43
1:B:35:SER:HB2	1:B:132:ARG:NH2	2.33	0.43
1:A:14:THR:HG21	1:A:100:LEU:HD11	2.00	0.43
1:A:33:LEU:HG	1:A:127:GLU:HB3	2.00	0.43
1:B:90:GLY:HA2	1:B:386:PRO:CA	2.49	0.43
1:B:258:MSE:HB2	1:B:262:LEU:HD23	2.00	0.43
1:A:33:LEU:HD22	1:A:34:TYR:CG	2.53	0.43
1:B:83:HIS:HB2	1:B:85:ASP:OD1	2.19	0.43
1:A:147:ALA:O	1:A:148:ASN:CB	2.67	0.43
1:B:238:ARG:HD3	1:B:316:ASP:HB3	2.01	0.43
1:B:351:TYR:H	1:B:351:TYR:HD2	1.65	0.43
1:B:64:LEU:HB3	1:B:124:ALA:HB3	1.99	0.43
1:A:276:VAL:HA	1:B:286:THR:HG21	2.01	0.43
1:A:345:GLU:C	1:A:347:GLU:N	2.71	0.43
1:A:253:GLU:HA	1:A:253:GLU:OE1	2.19	0.42
1:B:74:PRO:CG	1:B:75:GLN:HE21	2.21	0.42
1:A:106:ILE:HD12	1:A:122:VAL:HG22	2.01	0.42
1:B:3:LEU:HD12	1:B:400:LYS:NZ	2.34	0.42
1:B:3:LEU:O	1:B:6:HIS:HB3	2.18	0.42
1:B:46:LYS:HZ1	1:B:56:THR:HG23	1.84	0.42
1:B:50:ALA:HB2	1:B:56:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HB	1:A:280:PRO:HG3	2.01	0.42
1:A:315:MSE:HG3	1:A:317:ILE:CD1	2.49	0.42
1:B:64:LEU:O	1:B:123:VAL:HA	2.19	0.42
1:B:240:THR:HG21	1:B:282:LYS:H	1.84	0.42
1:B:379:ILE:HG13	1:B:389:ARG:HG3	2.00	0.42
1:A:61:VAL:HG21	1:A:142:ASN:ND2	2.34	0.42
1:B:35:SER:HB2	1:B:132:ARG:HH22	1.84	0.42
1:B:68:LEU:CG	1:B:110:LYS:HG3	2.50	0.42
1:B:68:LEU:HD11	1:B:110:LYS:HG3	2.00	0.42
1:B:253:GLU:OE2	1:B:256:LYS:HD3	2.19	0.42
1:A:64:LEU:HB3	1:A:124:ALA:HB3	2.02	0.42
1:A:81:GLY:HA3	1:A:123:VAL:O	2.20	0.42
1:B:343:LEU:HD13	1:B:343:LEU:O	2.19	0.42
1:A:204:GLN:HE22	1:A:352:ARG:CZ	2.33	0.42
1:B:108:TRP:O	1:B:112:GLN:HB2	2.20	0.42
1:B:174:LEU:HA	1:B:175:PRO:HD3	1.88	0.42
1:B:388:GLU:HG3	2:B:424:HOH:O	2.19	0.42
1:A:15:LEU:O	1:A:19:SER:CB	2.68	0.42
1:B:194:GLU:O	1:B:195:GLN:HB2	2.20	0.42
1:A:194:GLU:O	1:A:195:GLN:CB	2.66	0.41
1:B:240:THR:HG23	1:B:283:THR:OG1	2.19	0.41
1:A:89:ASN:O	1:A:386:PRO:HD3	2.20	0.41
1:A:222:LEU:HD13	1:A:285:PHE:HE2	1.85	0.41
1:A:400:LYS:O	1:A:404:LEU:HG	2.20	0.41
1:B:29:MSE:H	1:B:90:GLY:H	1.68	0.41
1:B:46:LYS:HD2	1:B:58:PHE:CE1	2.55	0.41
1:A:61:VAL:HG22	1:A:138:TRP:NE1	2.35	0.41
1:B:129:GLU:O	1:B:129:GLU:HG2	2.20	0.41
1:A:102:ALA:HB3	1:A:122:VAL:HG13	2.02	0.41
1:A:189:VAL:O	1:A:189:VAL:HG23	2.19	0.41
1:B:323:LEU:HD13	1:B:323:LEU:O	2.20	0.41
1:A:68:LEU:HB3	1:A:120:VAL:HG23	2.02	0.41
1:A:88:VAL:HG23	1:A:89:ASN:H	1.86	0.41
1:A:217:ARG:HD3	1:B:276:VAL:HG21	2.03	0.41
1:A:312:CYS:HB3	1:A:317:ILE:O	2.20	0.41
1:B:60:GLU:CD	1:B:60:GLU:N	2.72	0.41
1:B:136:VAL:O	1:B:137:PHE:HB2	2.21	0.41
1:B:339:THR:HA	1:B:342:GLU:OE1	2.21	0.41
1:A:108:TRP:O	1:A:112:GLN:HB2	2.21	0.41
1:B:35:SER:H	1:B:132:ARG:HH12	1.68	0.41
1:B:110:LYS:O	1:B:114:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:MSE:HG2	1:B:172:PHE:O	2.21	0.41
1:B:175:PRO:HG2	1:B:179:LEU:CD1	2.50	0.41
1:B:336:LEU:HB3	1:B:372:CYS:HB3	2.03	0.41
1:A:174:LEU:HD13	1:A:174:LEU:N	2.36	0.41
1:B:30:THR:HG23	1:B:88:VAL:HA	2.03	0.41
1:A:106:ILE:HD12	1:A:122:VAL:HG23	2.03	0.40
1:A:264:LEU:N	1:B:234:MSE:HE1	2.34	0.40
1:B:64:LEU:O	1:B:123:VAL:HG23	2.21	0.40
1:A:262:LEU:HB2	1:A:291:HIS:HD2	1.86	0.40
1:A:365:PHE:HB3	1:A:371:THR:CG2	2.36	0.40
1:B:240:THR:HG22	1:B:280:PRO:C	2.39	0.40
1:B:364:ILE:O	1:B:364:ILE:HG13	2.21	0.40
1:A:240:THR:HG22	1:A:280:PRO:C	2.39	0.40
1:A:273:PRO:CG	1:A:278:VAL:HG11	2.51	0.40
1:B:57:ARG:HG2	1:B:57:ARG:NH1	2.37	0.40
1:B:379:ILE:N	1:B:379:ILE:CD1	2.81	0.40
1:B:67:ARG:O	1:B:67:ARG:HG3	2.21	0.40
1:B:73:TYR:N	1:B:74:PRO:CD	2.84	0.40
1:A:183:GLN:HA	2:A:443:HOH:O	2.21	0.40
1:A:286:THR:HG21	1:B:276:VAL:HA	2.04	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	393/423 (93%)	350 (89%)	35 (9%)	8 (2%)	7 24
1	B	390/423 (92%)	328 (84%)	49 (13%)	13 (3%)	4 13
All	All	783/846 (93%)	678 (87%)	84 (11%)	21 (3%)	5 17

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	TYR
1	B	36	PRO
1	B	320	ASP
1	B	379	ILE
1	A	129	GLU
1	B	32	LEU
1	B	250	GLN
1	B	37	GLU
1	B	175	PRO
1	A	31	ARG
1	A	67	ARG
1	A	348	LYS
1	A	148	ASN
1	A	112	GLN
1	B	33	LEU
1	B	73	TYR
1	B	113	TYR
1	A	88	VAL
1	B	319	ILE
1	B	53	GLY
1	A	130	GLY

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	338/341 (99%)	306 (90%)	32 (10%)	8 25
1	B	331/341 (97%)	296 (89%)	35 (11%)	6 20
All	All	669/682 (98%)	602 (90%)	67 (10%)	7 22

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	33	LEU
1	A	45	PHE

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Mol	Chain	Res	Type
1	A	48	ARG
1	A	56	THR
1	A	61	VAL
1	A	79	LEU
1	A	86	THR
1	A	88	VAL
1	A	93	LEU
1	A	120	VAL
1	A	128	GLU
1	A	129	GLU
1	A	168	LYS
1	A	174	LEU
1	A	176	ASN
1	A	191	LEU
1	A	206	ILE
1	A	209	VAL
1	A	215	GLN
1	A	216	ARG
1	A	246	ARG
1	A	264	LEU
1	A	265	THR
1	A	274	ASN
1	A	304	LEU
1	A	323	LEU
1	A	327	GLU
1	A	343	LEU
1	A	347	GLU
1	A	368	ARG
1	A	393	THR
1	B	3	LEU
1	B	13	GLU
1	B	14	THR
1	B	35	SER
1	B	36	PRO
1	B	44	GLN
1	B	54	LEU
1	B	68	LEU
1	B	69	ASN
1	B	79	LEU
1	B	112	GLN
1	B	128	GLU
1	B	192	HIS

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Mol	Chain	Res	Type
1	B	234	MSE
1	B	236	TYR
1	B	246	ARG
1	B	250	GLN
1	B	264	LEU
1	B	272	ARG
1	B	274	ASN
1	B	277	ASN
1	B	297	LEU
1	B	319	ILE
1	B	339	THR
1	B	351	TYR
1	B	352	ARG
1	B	364	ILE
1	B	375	PHE
1	B	376	ILE
1	B	378	SER
1	B	388	GLU
1	B	389	ARG
1	B	397	GLU
1	B	405	MSE
1	B	408	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	63	ASN
1	A	148	ASN
1	A	195	GLN
1	A	202	ASN
1	A	204	GLN
1	A	274	ASN
1	A	303	GLN
1	A	363	GLN
1	B	42	GLN
1	B	43	GLN
1	B	44	GLN
1	B	63	ASN
1	B	75	GLN
1	B	89	ASN
1	B	92	ASN

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Mol	Chain	Res	Type
1	B	96	GLN
1	B	112	GLN
1	B	195	GLN
1	B	228	HIS
1	B	277	ASN
1	B	303	GLN
1	B	360	HIS
1	B	363	GLN
1	B	384	HIS
1	B	385	ASN
1	B	391	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	386/423 (91%)	-0.15	3 (0%)	86	81	26, 45, 66, 84	0
1	B	381/423 (90%)	0.11	8 (2%)	63	54	32, 59, 91, 99	0
All	All	767/846 (90%)	-0.02	11 (1%)	75	70	26, 51, 84, 99	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	GLY	5.6
1	B	26	ALA	5.2
1	B	175	PRO	3.9
1	B	27	GLY	3.1
1	B	129	GLU	2.9
1	B	131	SER	2.8
1	B	61	VAL	2.4
1	A	86	THR	2.3
1	A	129	GLU	2.3
1	A	75	GLN	2.3
1	B	54	LEU	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.