W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 09:19 AM EDT

PDB ID	:	1XFH
Title	:	Structure of glutamate transporter homolog from Pyrococcus horikoshii
Authors	:	Yernool, D.; Boudker, O.; Jin, Y.; Gouaux, E.
Deposited on	:	2004-09-14
Resolution	:	3.50 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 following versions of software and data (see references (i)) were used in the production of this report:

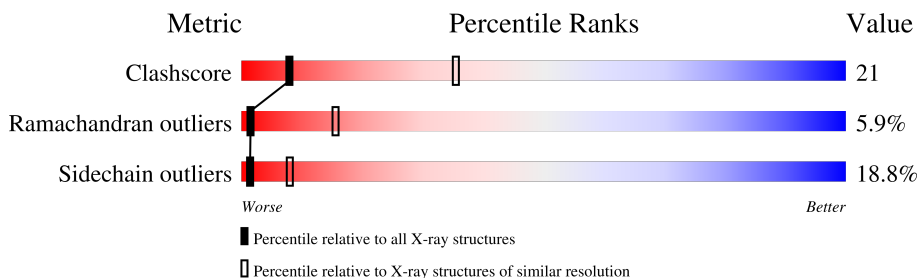|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.50 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	Percentile Ranks	Value
Clashscore		21
Ramachandran outliers		5.9%
Sidechain outliers		18.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	422	49% 36% 10% • •
1	B	422	48% 40% 8% •
1	C	422	54% 34% 9% •

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 8652 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 proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	1
			2884	1895	464	508	17			
1	B	406	Total	C	N	O	S	0	0	1
			2884	1895	464	508	17			
1	C	406	Total	C	N	O	S	0	0	1
			2884	1895	464	508	17			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	418	THR	-	cloning artifact	UNP O59010
A	419	LEU	-	cloning artifact	UNP O59010
A	420	VAL	-	cloning artifact	UNP O59010
A	421	PRO	-	cloning artifact	UNP O59010
A	422	ARG	-	cloning artifact	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	418	THR	-	cloning artifact	UNP O59010
B	419	LEU	-	cloning artifact	UNP O59010
B	420	VAL	-	cloning artifact	UNP O59010
B	421	PRO	-	cloning artifact	UNP O59010

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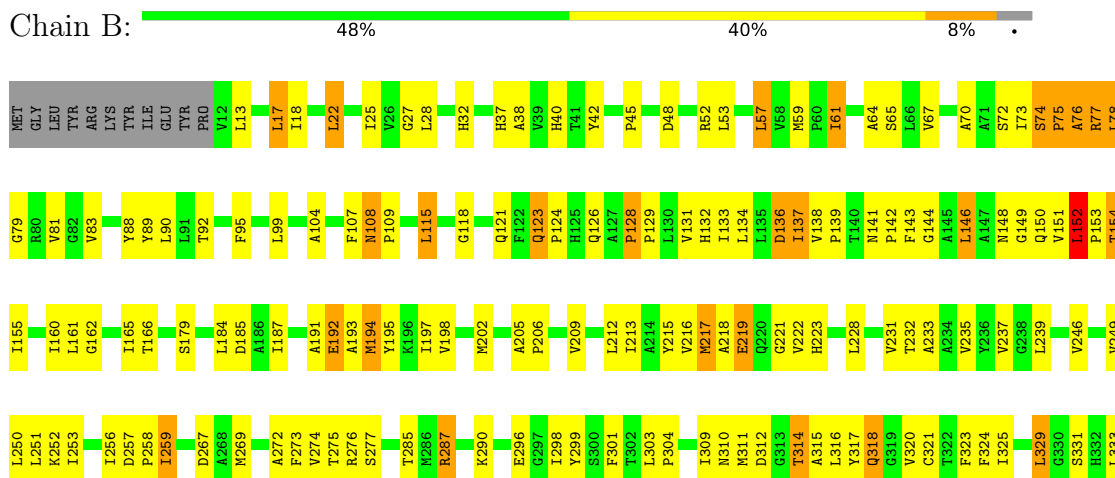| Chain	Residue	Modelled	Actual	Comment	Reference
B	422	ARG	-	cloning artifact	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	418	THR	-	cloning artifact	UNP O59010
C	419	LEU	-	cloning artifact	UNP O59010
C	420	VAL	-	cloning artifact	UNP O59010
C	421	PRO	-	cloning artifact	UNP O59010
C	422	ARG	-	cloning artifact	UNP O59010

3 Residue-property plots ⓘ

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. 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. 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.
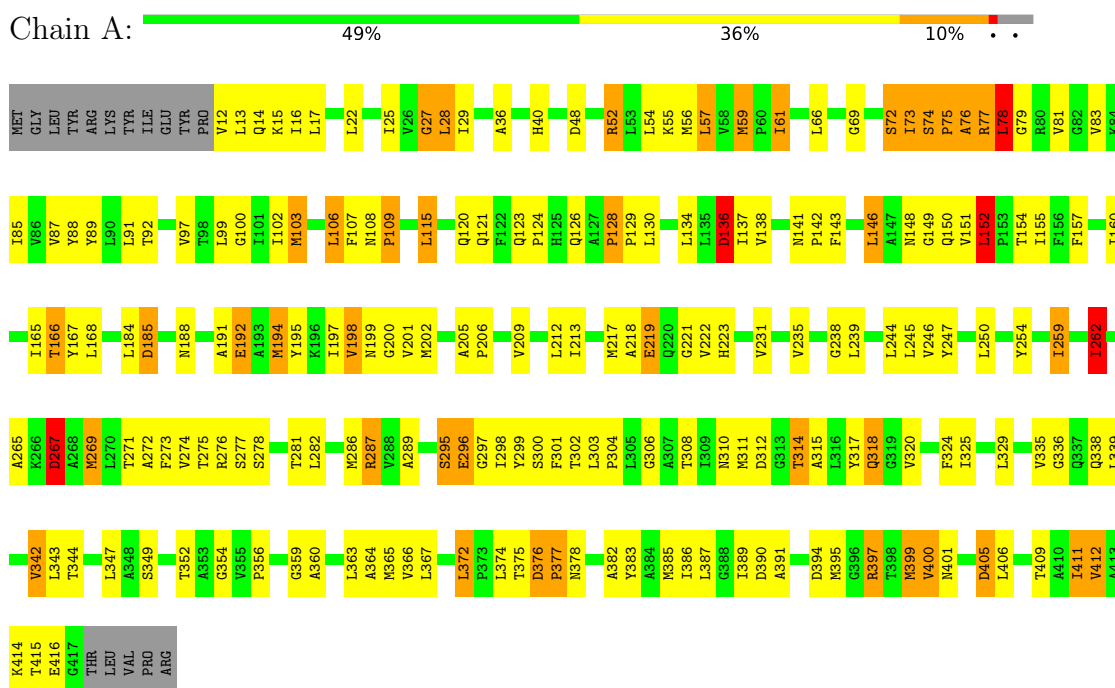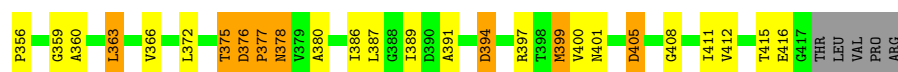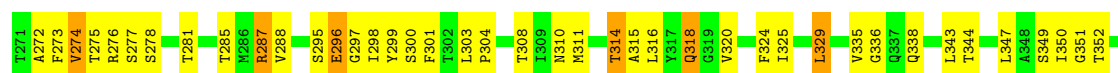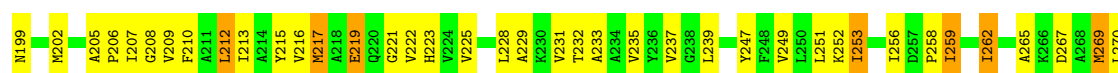
• Molecule 1: proton glutamate symport protein

• Molecule 1: proton glutamate symport protein

T334 V335 G336 Q337 Q338 L339 T344 A345 V346 L347 A348 S349 I350 G351 T352 A353 G354 V355 P356 A360 I361 M362 L363 A364 M365 V366 L367 G371 L372 P373 L374 T375 D376 P377 N378 V379 A380 Y383 A384 M385 I386 L387 G388 I389 D390 A391 I392 L393 D394 M399 V400 N401 V402 T407

G408 I411 V412 A413 K414 T415 E416 G417 THR LEU VAL PRO ARG

● Molecule 1: proton glutamate symport protein

Chain C:

54%　　　　34%　　　　9%　　　•

MET GLY LEU TYR ARG LYS TYR ILE GLU TYR PRO V12 L17 L22 G23 A24 I25 L28 H37 V51 R52 M56 L57 V58 M59 P60 I61 V62 L66 V67 A70 A71 S72 I73 S74 P75 A76 R77 L78 G79 R80 V81 G82 V83 K84 I85 Y88 Y89 T92

L99 F107 N108 P109 L115 A116 Q120 Q121 Q126 A127 P128 P129 L130 I133 D136 I137 V138 P139 T140 N141 P142 F143 L146 A147 N148 G149 Q150 V151 L152 P153 T154 I155 F156 G162 I165 T166 Y167 L168 L184 D185 A186 I187 E192 A193 M194 Y195 K196 I197 V198

N199 M202 A205 P206 I207 G208 V209 F210 A211 L212 I213 A214 Y215 V216 M217 A218 E219 Q220 G221 V222 H223 V224 V225 L228 A229 K230 V231 T232 A233 A234 V235 Y236 V237 G238 L239 Y247 F248 V249 L250 L251 K252 I253 I256 D257 P258 I259 I262 A265 K266 D267 A268 M269 L270

T271 A272 F273 V274 T275 R276 S277 S278 T281 T285 M286 R287 V288 S295 E296 G297 I298 Y299 S300 F301 L303 P304 T308 I309 N310 M311 T314 A315 L316 Y317 Q318 G319 V320 F324 I325 L329 V335 G336 Q337 Q338 L343 T344 L347 A348 S349 I350 G351 T352

P356 G359 A360 L363 V366 L372 T375 D376 P377 N378 V379 A380 I386 L387 G388 I389 D390 A391 D394 R397 T398 M399 V400 N401 D405 G408 I411 V412 T415 E416 G417 THR LEU VAL PRO ARG

4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	116.00Å 116.00Å 322.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.50	Depositor
% Data completeness (in resolution range)	97.1 (10.00-3.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.290 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8652	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

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	0.61	1/2937 (0.0%)	0.85	8/4019 (0.2%)
1	B	0.51	1/2937 (0.0%)	0.75	3/4019 (0.1%)
1	C	0.51	1/2937 (0.0%)	0.77	3/4019 (0.1%)
All	All	0.54	3/8811 (0.0%)	0.79	14/12057 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	416	GLU	C-N	-5.61	1.23	1.33
1	B	416	GLU	C-N	-5.29	1.23	1.33
1	C	416	GLU	C-N	-5.25	1.23	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	394	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	136	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	394	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	149	GLY	N-CA-C	-5.91	98.31	113.10
1	A	390	ASP	CB-CG-OD2	5.76	123.49	118.30
1	B	394	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	149	GLY	N-CA-C	-5.67	98.92	113.10
1	A	48	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	267	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	185	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	405	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	257	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	390	ASP	CB-CG-OD2	5.08	122.88	118.30
1	C	405	ASP	CB-CG-OD2	5.02	122.82	118.30

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	2884	0	2927	135	0
1	B	2884	0	2927	137	0
1	C	2884	0	2927	116	0
All	All	8652	0	8781	374	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 21.

All (374) 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:155:ILE:HD11	1:A:304:PRO:HB2	1.40	1.02
1:C:81:VAL:HG21	1:C:298:ILE:HD12	1.42	1.01
1:A:81:VAL:HG21	1:A:298:ILE:HD12	1.46	0.96
1:A:109:PRO:HB3	1:A:324:PHE:HA	1.48	0.92
1:A:138:VAL:O	1:C:52:ARG:NH1	2.03	0.92
1:A:235:VAL:HG22	1:A:320:VAL:HG11	1.53	0.91
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.53	0.88
1:A:376:ASP:O	1:A:378:ASN:N	2.10	0.84
1:A:375:THR:O	1:A:377:PRO:HD3	1.77	0.83
1:A:197:ILE:HD13	1:B:160:ILE:HG22	1.62	0.82
1:B:142:PRO:O	1:B:146:LEU:HB2	1.81	0.81
1:C:109:PRO:HB3	1:C:324:PHE:HA	1.62	0.81
1:B:311:MET:HG2	1:B:401:ASN:ND2	1.97	0.78
1:A:115:LEU:HD12	1:A:115:LEU:H	1.49	0.77
1:B:52:ARG:NH1	1:C:138:VAL:O	2.18	0.77
1:B:249:VAL:O	1:B:253:ILE:HG22	1.85	0.77
1:A:198:VAL:O	1:A:202:MET:HB2	1.84	0.76
1:C:311:MET:HG2	1:C:401:ASN:ND2	2.00	0.74
1:A:265:ALA:O	1:A:269:MET:HB2	1.88	0.74
1:C:267:ASP:OD2	1:C:287:ARG:NH2	2.21	0.73
1:B:285:THR:HG22	1:B:303:LEU:HD13	1.71	0.73
1:C:273:PHE:HB2	1:C:399:MET:HG3	1.69	0.72
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.71	0.72
1:B:273:PHE:HB2	1:B:399:MET:HG3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ILE:O	1:C:258:PRO:HD3	1.89	0.71
1:B:235:VAL:HG22	1:B:320:VAL:HG11	1.71	0.71
1:C:262:ILE:HG22	1:C:262:ILE:O	1.88	0.71
1:A:81:VAL:HG23	1:A:412:VAL:HG12	1.71	0.71
1:A:157:PHE:HD1	1:C:56:MET:HE2	1.56	0.71
1:C:310:ASN:HB3	1:C:405:ASP:OD1	1.91	0.70
1:A:61:ILE:HG13	1:A:194:MET:HB3	1.72	0.70
1:A:12:VAL:O	1:A:14:GLN:N	2.25	0.70
1:A:239:LEU:HB3	1:A:400:VAL:HG21	1.73	0.69
1:A:296:GLU:HA	1:A:299:TYR:CE1	2.27	0.69
1:A:83:VAL:O	1:A:87:VAL:HG23	1.93	0.69
1:C:142:PRO:O	1:C:146:LEU:HB2	1.93	0.68
1:B:325:ILE:O	1:B:329:LEU:HB2	1.93	0.68
1:C:205:ALA:O	1:C:209:VAL:HG23	1.94	0.68
1:B:317:TYR:HE1	1:B:393:LEU:HD13	1.58	0.68
1:A:76:ALA:O	1:A:77:ARG:C	2.32	0.67
1:A:136:ASP:HA	1:C:52:ARG:HH22	1.59	0.67
1:B:296:GLU:HA	1:B:299:TYR:CE1	2.28	0.67
1:A:311:MET:HG2	1:A:401:ASN:ND2	2.09	0.66
1:A:363:LEU:O	1:A:366:VAL:HG12	1.95	0.66
1:C:215:TYR:CE1	1:C:219:GLU:HG3	2.30	0.66
1:A:199:ASN:OD1	1:A:287:ARG:NH1	2.28	0.66
1:B:81:VAL:HG21	1:B:298:ILE:HD12	1.77	0.66
1:B:212:LEU:HB3	1:B:274:VAL:HG12	1.78	0.66
1:B:256:ILE:O	1:B:258:PRO:HD3	1.96	0.66
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.30	0.65
1:A:160:ILE:HG22	1:C:197:ILE:HD13	1.79	0.64
1:B:272:ALA:CB	1:B:402:VAL:HG21	2.28	0.64
1:B:61:ILE:HG13	1:B:194:MET:HB3	1.80	0.64
1:A:197:ILE:HD13	1:B:160:ILE:CG2	2.28	0.64
1:C:233:ALA:O	1:C:237:VAL:HG12	1.98	0.63
1:A:246:VAL:O	1:A:250:LEU:HB2	1.98	0.63
1:B:88:TYR:CE2	1:B:408:GLY:HA3	2.34	0.63
1:C:325:ILE:O	1:C:329:LEU:HB2	1.98	0.63
1:A:262:ILE:CG2	1:A:262:ILE:O	2.47	0.62
1:A:315:ALA:HB2	1:A:349:SER:OG	1.98	0.62
1:A:78:LEU:O	1:A:81:VAL:HG12	1.99	0.62
1:A:12:VAL:O	1:A:15:LYS:N	2.32	0.62
1:B:198:VAL:O	1:B:202:MET:HB2	2.00	0.62
1:B:344:THR:HB	1:B:366:VAL:HG23	1.80	0.62
1:A:52:ARG:NH1	1:B:138:VAL:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:SER:HB3	1:A:75:PRO:HD3	1.82	0.62
1:A:136:ASP:HA	1:C:52:ARG:NH2	2.14	0.62
1:B:362:MET:CE	1:B:362:MET:HA	2.30	0.61
1:B:195:TYR:O	1:B:198:VAL:HG12	2.00	0.61
1:C:139:PRO:HG3	1:C:153:PRO:HB3	1.82	0.61
1:B:76:ALA:O	1:B:77:ARG:C	2.37	0.61
1:C:76:ALA:O	1:C:77:ARG:C	2.38	0.61
1:C:296:GLU:HA	1:C:299:TYR:CE1	2.35	0.61
1:B:363:LEU:O	1:B:366:VAL:HG12	2.01	0.61
1:C:89:TYR:CD2	1:C:310:ASN:HB2	2.34	0.61
1:C:265:ALA:O	1:C:269:MET:HB2	2.00	0.61
1:B:81:VAL:HG21	1:B:298:ILE:HG23	1.83	0.61
1:A:399:MET:C	1:A:401:ASN:H	2.04	0.60
1:C:198:VAL:O	1:C:202:MET:HB2	2.01	0.60
1:C:336:GLY:H	1:C:338:GLN:HE21	1.46	0.60
1:B:205:ALA:O	1:B:209:VAL:HG23	2.02	0.60
1:C:249:VAL:O	1:C:253:ILE:HG22	2.02	0.60
1:A:311:MET:CE	1:A:352:THR:O	2.50	0.60
1:A:399:MET:O	1:A:401:ASN:N	2.35	0.60
1:B:104:ALA:O	1:B:109:PRO:HD3	2.01	0.60
1:B:325:ILE:HG21	1:B:379:VAL:HG13	1.84	0.59
1:A:275:THR:HG22	1:A:277:SER:H	1.66	0.59
1:A:352:THR:CG2	1:A:359:GLY:HA2	2.33	0.59
1:A:336:GLY:H	1:A:338:GLN:HE21	1.50	0.59
1:B:52:ARG:NH2	1:C:136:ASP:HA	2.17	0.59
1:C:376:ASP:O	1:C:378:ASN:N	2.33	0.59
1:C:141:ASN:OD1	1:C:143:PHE:HB2	2.03	0.59
1:A:102:ILE:HG22	1:A:106:LEU:HD11	1.85	0.58
1:B:74:SER:HB3	1:B:75:PRO:HD3	1.84	0.58
1:B:233:ALA:O	1:B:237:VAL:HG12	2.04	0.58
1:A:198:VAL:HG13	1:A:287:ARG:HD3	1.84	0.58
1:A:142:PRO:O	1:A:146:LEU:HB2	2.04	0.58
1:B:407:THR:O	1:B:411:ILE:HG12	2.03	0.58
1:C:318:GLN:HG2	1:C:366:VAL:HG11	1.85	0.57
1:A:399:MET:C	1:A:401:ASN:N	2.57	0.57
1:B:192:GLU:HB3	1:C:168:LEU:HD11	1.86	0.57
1:A:89:TYR:CG	1:A:310:ASN:HB2	2.39	0.57
1:C:231:VAL:HG21	1:C:324:PHE:CD1	2.38	0.57
1:B:209:VAL:HG13	1:B:274:VAL:HG21	1.87	0.57
1:A:195:TYR:O	1:A:198:VAL:HG12	2.04	0.57
1:A:352:THR:HG23	1:A:359:GLY:HA2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:VAL:O	1:B:235:VAL:HG23	2.05	0.56
1:A:235:VAL:HG22	1:A:320:VAL:CG1	2.33	0.56
1:A:304:PRO:C	1:A:306:GLY:H	2.07	0.56
1:B:273:PHE:HB2	1:B:399:MET:CG	2.35	0.56
1:C:139:PRO:HG3	1:C:153:PRO:CB	2.35	0.56
1:C:195:TYR:O	1:C:198:VAL:HG12	2.06	0.56
1:C:295:SER:C	1:C:297:GLY:H	2.08	0.56
1:C:61:ILE:HG13	1:C:194:MET:HB3	1.85	0.56
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.41	0.56
1:B:162:GLY:O	1:B:165:ILE:N	2.39	0.56
1:B:317:TYR:CE1	1:B:393:LEU:HD13	2.38	0.56
1:C:221:GLY:O	1:C:223:HIS:N	2.32	0.56
1:B:52:ARG:HH22	1:C:136:ASP:HA	1.71	0.55
1:A:52:ARG:NH2	1:B:136:ASP:HA	2.21	0.55
1:A:318:GLN:HG2	1:A:366:VAL:HG11	1.86	0.55
1:C:78:LEU:O	1:C:81:VAL:HG12	2.06	0.55
1:B:251:LEU:O	1:B:256:ILE:HG22	2.05	0.55
1:B:408:GLY:O	1:B:412:VAL:HG23	2.06	0.55
1:A:221:GLY:C	1:A:223:HIS:H	2.10	0.55
1:B:272:ALA:HB2	1:B:402:VAL:HG21	1.89	0.55
1:C:221:GLY:C	1:C:223:HIS:H	2.10	0.55
1:B:275:THR:O	1:B:276:ARG:HB2	2.07	0.55
1:B:139:PRO:HG3	1:B:153:PRO:HB3	1.90	0.54
1:C:262:ILE:O	1:C:262:ILE:CG2	2.56	0.54
1:C:107:PHE:HD1	1:C:237:VAL:HG11	1.73	0.54
1:C:199:ASN:OD1	1:C:287:ARG:NH1	2.41	0.54
1:C:275:THR:O	1:C:276:ARG:HB2	2.08	0.54
1:B:139:PRO:HG3	1:B:153:PRO:CB	2.38	0.54
1:B:134:LEU:O	1:B:137:ILE:HB	2.07	0.54
1:C:81:VAL:HG23	1:C:412:VAL:HG12	1.90	0.54
1:A:363:LEU:O	1:A:366:VAL:CG1	2.55	0.54
1:C:155:ILE:HG22	1:C:156:PHE:N	2.23	0.54
1:A:310:ASN:HB3	1:A:405:ASP:OD1	2.08	0.54
1:A:301:PHE:CG	1:A:301:PHE:O	2.61	0.53
1:A:336:GLY:H	1:A:338:GLN:NE2	2.05	0.53
1:C:311:MET:HB3	1:C:314:THR:HB	1.90	0.53
1:B:323:PHE:HZ	1:B:338:GLN:OE1	1.91	0.53
1:A:81:VAL:HG23	1:A:412:VAL:CG1	2.38	0.53
1:B:141:ASN:OD1	1:B:143:PHE:HB2	2.09	0.53
1:A:267:ASP:OD2	1:A:287:ARG:NH2	2.38	0.53
1:B:272:ALA:HB1	1:B:402:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:THR:HG22	1:B:277:SER:H	1.74	0.53
1:C:205:ALA:N	1:C:206:PRO:HD2	2.24	0.52
1:C:228:LEU:HD22	1:C:389:ILE:HG12	1.91	0.52
1:A:360:ALA:O	1:A:363:LEU:HB3	2.09	0.52
1:B:92:THR:HB	1:B:312:ASP:OD2	2.09	0.52
1:A:205:ALA:O	1:A:209:VAL:HG23	2.10	0.52
1:B:74:SER:CB	1:B:75:PRO:HD3	2.39	0.52
1:B:76:ALA:O	1:B:79:GLY:N	2.42	0.52
1:C:76:ALA:O	1:C:80:ARG:N	2.36	0.52
1:C:109:PRO:HB3	1:C:324:PHE:CA	2.36	0.52
1:C:231:VAL:O	1:C:235:VAL:HG23	2.09	0.52
1:B:194:MET:HE3	1:B:197:ILE:HD12	1.92	0.51
1:C:73:ILE:O	1:C:77:ARG:HB2	2.10	0.51
1:C:235:VAL:HG22	1:C:320:VAL:HG11	1.91	0.51
1:A:235:VAL:O	1:A:239:LEU:HG	2.10	0.51
1:A:76:ALA:O	1:A:78:LEU:N	2.43	0.51
1:C:23:GLY:HA2	1:C:210:PHE:CD2	2.45	0.51
1:A:74:SER:CB	1:A:75:PRO:HD3	2.40	0.51
1:B:275:THR:HG22	1:B:277:SER:HB3	1.93	0.51
1:B:311:MET:CE	1:B:352:THR:O	2.59	0.51
1:C:165:ILE:HG21	1:C:184:LEU:HB2	1.93	0.51
1:B:309:ILE:HG23	1:B:350:ILE:HG23	1.93	0.51
1:C:247:TYR:O	1:C:251:LEU:HG	2.11	0.51
1:A:40:HIS:ND1	1:A:40:HIS:O	2.44	0.51
1:B:79:GLY:O	1:B:83:VAL:HG23	2.10	0.51
1:B:77:ARG:O	1:B:81:VAL:HG12	2.11	0.51
1:C:59:MET:HE3	1:C:154:THR:HG21	1.93	0.51
1:C:225:VAL:HA	1:C:229:ALA:HB2	1.92	0.50
1:B:88:TYR:O	1:B:92:THR:HG23	2.10	0.50
1:A:231:VAL:O	1:A:235:VAL:HG23	2.11	0.50
1:B:275:THR:CG2	1:B:277:SER:HB3	2.42	0.50
1:B:345:ALA:O	1:B:349:SER:OG	2.26	0.50
1:A:89:TYR:CD2	1:A:310:ASN:HB2	2.46	0.50
1:B:371:GLY:O	1:B:373:PRO:HD3	2.12	0.50
1:A:99:LEU:O	1:A:103:MET:HB2	2.11	0.50
1:A:36:ALA:HB1	1:A:219:GLU:HG2	1.93	0.50
1:A:109:PRO:CB	1:A:324:PHE:HA	2.31	0.50
1:A:28:LEU:HD13	1:A:217:MET:HG3	1.94	0.49
1:C:360:ALA:O	1:C:363:LEU:HB3	2.12	0.49
1:B:194:MET:CE	1:B:197:ILE:HD12	2.42	0.49
1:C:109:PRO:HA	1:C:231:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ALA:O	1:C:197:ILE:HG13	2.13	0.49
1:B:221:GLY:C	1:B:223:HIS:H	2.16	0.49
1:A:271:THR:HG22	1:A:281:THR:HG23	1.93	0.49
1:A:271:THR:CG2	1:A:281:THR:HG23	2.43	0.49
1:A:254:TYR:CD2	1:A:411:ILE:HG23	2.48	0.49
1:A:200:GLY:C	1:A:202:MET:H	2.16	0.49
1:B:165:ILE:HG21	1:B:184:LEU:HB2	1.93	0.48
1:C:209:VAL:HG22	1:C:274:VAL:HG21	1.94	0.48
1:C:79:GLY:O	1:C:83:VAL:HG23	2.13	0.48
1:A:59:MET:HE3	1:A:154:THR:HG21	1.94	0.48
1:A:191:ALA:O	1:A:195:TYR:HD1	1.96	0.48
1:C:61:ILE:CG2	1:C:62:VAL:N	2.76	0.48
1:B:149:GLY:O	1:B:150:GLN:HB2	2.12	0.48
1:B:360:ALA:O	1:B:363:LEU:HB3	2.14	0.48
1:C:239:LEU:HD22	1:C:400:VAL:HG21	1.95	0.48
1:B:81:VAL:HG23	1:B:412:VAL:CG1	2.43	0.48
1:B:269:MET:HG2	1:B:399:MET:SD	2.54	0.48
1:A:184:LEU:O	1:A:184:LEU:HG	2.12	0.48
1:C:109:PRO:CB	1:C:324:PHE:HA	2.37	0.48
1:C:301:PHE:CG	1:C:301:PHE:O	2.67	0.48
1:B:311:MET:HE3	1:B:352:THR:O	2.14	0.47
1:B:318:GLN:HG2	1:B:366:VAL:HG11	1.94	0.47
1:B:18:ILE:O	1:B:22:LEU:HB3	2.14	0.47
1:A:97:VAL:O	1:A:100:GLY:N	2.43	0.47
1:B:108:ASN:HA	1:B:109:PRO:HD3	1.79	0.47
1:A:200:GLY:O	1:A:202:MET:N	2.48	0.47
1:A:259:ILE:H	1:A:259:ILE:HG13	1.39	0.47
1:A:275:THR:O	1:A:276:ARG:HB2	2.15	0.47
1:B:70:ALA:HB3	1:B:162:GLY:HA3	1.97	0.47
1:B:228:LEU:O	1:B:232:THR:N	2.30	0.47
1:C:216:VAL:HG13	1:C:391:ALA:HB1	1.97	0.47
1:C:377:PRO:HA	1:C:380:ALA:HB3	1.95	0.47
1:B:198:VAL:HG13	1:B:287:ARG:HD3	1.97	0.47
1:B:205:ALA:N	1:B:206:PRO:HD2	2.30	0.47
1:B:376:ASP:O	1:B:378:ASN:N	2.48	0.47
1:C:74:SER:HB3	1:C:75:PRO:HD3	1.97	0.46
1:C:194:MET:CE	1:C:197:ILE:HD12	2.45	0.46
1:C:315:ALA:HB2	1:C:349:SER:OG	2.15	0.46
1:B:78:LEU:HD22	1:B:78:LEU:HA	1.71	0.46
1:C:259:ILE:H	1:C:259:ILE:HG13	1.53	0.46
1:C:151:VAL:HA	1:C:154:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG23	1:A:286:MET:CE	2.45	0.46
1:A:272:ALA:HB2	1:A:281:THR:HG21	1.97	0.46
1:B:78:LEU:HA	1:B:81:VAL:HG12	1.96	0.46
1:C:275:THR:HG22	1:C:277:SER:H	1.79	0.46
1:B:27:GLY:O	1:B:218:ALA:HB2	2.15	0.46
1:B:95:PHE:HE2	1:B:99:LEU:HD22	1.80	0.46
1:C:386:ILE:HD13	1:C:386:ILE:HA	1.82	0.46
1:A:197:ILE:O	1:A:199:ASN:N	2.49	0.46
1:A:406:LEU:O	1:A:409:THR:N	2.49	0.46
1:B:315:ALA:HB2	1:B:349:SER:OG	2.16	0.46
1:C:127:ALA:HA	1:C:128:PRO:HD2	1.84	0.46
1:A:295:SER:C	1:A:297:GLY:H	2.19	0.46
1:B:386:ILE:O	1:B:389:ILE:HG13	2.15	0.46
1:C:151:VAL:HA	1:C:154:THR:CG2	2.46	0.46
1:C:76:ALA:O	1:C:79:GLY:N	2.49	0.46
1:B:128:PRO:HA	1:B:129:PRO:HD3	1.83	0.45
1:B:361:ILE:C	1:B:363:LEU:H	2.20	0.45
1:A:197:ILE:O	1:A:200:GLY:N	2.49	0.45
1:C:81:VAL:HG23	1:C:412:VAL:CG1	2.47	0.45
1:A:262:ILE:O	1:A:262:ILE:HG22	2.14	0.45
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.81	0.45
1:C:23:GLY:CA	1:C:210:PHE:HD2	2.30	0.45
1:B:314:THR:O	1:B:318:GLN:N	2.50	0.45
1:C:74:SER:CB	1:C:75:PRO:HD3	2.46	0.45
1:A:273:PHE:HB2	1:A:399:MET:HG3	1.98	0.45
1:B:131:VAL:C	1:B:133:ILE:H	2.20	0.45
1:A:73:ILE:O	1:A:77:ARG:HB2	2.17	0.45
1:A:130:LEU:O	1:A:134:LEU:HG	2.17	0.45
1:A:205:ALA:N	1:A:206:PRO:HD2	2.31	0.45
1:C:17:LEU:HD22	1:C:270:LEU:HD11	1.99	0.45
1:A:195:TYR:O	1:A:199:ASN:ND2	2.50	0.45
1:B:246:VAL:O	1:B:250:LEU:HB2	2.16	0.45
1:B:239:LEU:HD23	1:B:316:LEU:HD22	1.98	0.44
1:B:336:GLY:H	1:B:338:GLN:HE21	1.65	0.44
1:C:85:ILE:HA	1:C:88:TYR:HB3	1.98	0.44
1:A:141:ASN:OD1	1:A:143:PHE:HB2	2.16	0.44
1:A:166:THR:HG22	1:A:167:TYR:HD1	1.82	0.44
1:B:375:THR:O	1:B:377:PRO:HD3	2.17	0.44
1:A:88:TYR:O	1:A:92:THR:HG23	2.16	0.44
1:A:188:ASN:O	1:A:192:GLU:HB2	2.17	0.44
1:A:391:ALA:O	1:A:395:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:SER:O	1:C:297:GLY:N	2.50	0.44
1:B:40:HIS:HB2	1:B:215:TYR:HE1	1.81	0.44
1:B:67:VAL:HB	1:B:187:ILE:HG21	1.99	0.44
1:C:394:ASP:O	1:C:397:ARG:HG3	2.17	0.44
1:C:285:THR:HG22	1:C:303:LEU:HD13	1.98	0.44
1:A:311:MET:HB3	1:A:314:THR:HB	2.00	0.44
1:B:377:PRO:HA	1:B:380:ALA:HB3	2.00	0.44
1:C:85:ILE:HB	1:C:412:VAL:HG21	2.00	0.44
1:B:152:LEU:CB	1:B:153:PRO:HD3	2.48	0.44
1:A:363:LEU:HD12	1:A:366:VAL:CG1	2.48	0.43
1:A:314:THR:HG22	1:A:315:ALA:N	2.33	0.43
1:B:57:LEU:O	1:B:61:ILE:HB	2.18	0.43
1:C:66:LEU:HD13	1:C:300:SER:CB	2.48	0.43
1:A:78:LEU:HD22	1:A:78:LEU:HA	1.82	0.43
1:B:88:TYR:CZ	1:B:92:THR:HG21	2.53	0.43
1:B:152:LEU:HB3	1:B:153:PRO:HD3	2.00	0.43
1:C:108:ASN:HA	1:C:109:PRO:HD3	1.85	0.43
1:C:89:TYR:CD2	1:C:310:ASN:CB	3.02	0.43
1:B:45:PRO:HA	1:B:48:ASP:HB2	2.00	0.43
1:C:59:MET:CE	1:C:154:THR:HG21	2.49	0.43
1:A:374:LEU:HD11	1:A:383:TYR:CG	2.53	0.43
1:B:301:PHE:O	1:B:301:PHE:CG	2.72	0.43
1:B:161:LEU:O	1:B:165:ILE:HG13	2.19	0.43
1:B:231:VAL:HG21	1:B:324:PHE:CD1	2.53	0.43
1:B:57:LEU:H	1:B:57:LEU:HG	1.58	0.43
1:B:77:ARG:O	1:B:81:VAL:N	2.41	0.43
1:B:38:ALA:O	1:B:42:TYR:HB2	2.19	0.43
1:C:99:LEU:HD12	1:C:99:LEU:O	2.19	0.43
1:A:289:ALA:HB2	1:A:303:LEU:HD11	2.01	0.42
1:A:314:THR:HA	1:A:397:ARG:HD3	2.01	0.42
1:A:325:ILE:HG12	1:A:382:ALA:HB3	2.01	0.42
1:A:85:ILE:HD13	1:A:302:THR:HB	2.01	0.42
1:A:386:ILE:HD13	1:A:386:ILE:HA	1.72	0.42
1:C:81:VAL:CG2	1:C:298:ILE:HD12	2.30	0.42
1:A:352:THR:HG21	1:A:359:GLY:HA2	2.01	0.42
1:C:23:GLY:HA2	1:C:210:PHE:HD2	1.84	0.42
1:B:89:TYR:CD2	1:B:310:ASN:HB2	2.54	0.42
1:B:372:LEU:HA	1:B:373:PRO:HD3	1.82	0.42
1:A:54:LEU:C	1:A:56:MET:N	2.73	0.42
1:B:141:ASN:O	1:B:144:GLY:N	2.52	0.42
1:B:331:SER:C	1:B:333:LEU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:THR:CG2	1:B:155:ILE:N	2.82	0.42
1:B:64:ALA:HB1	1:B:191:ALA:HB2	2.02	0.42
1:B:217:MET:C	1:B:219:GLU:H	2.23	0.42
1:A:108:ASN:HA	1:A:109:PRO:HD3	1.88	0.42
1:A:150:GLN:C	1:A:152:LEU:H	2.23	0.42
1:B:141:ASN:O	1:B:142:PRO:C	2.58	0.42
1:B:374:LEU:HD11	1:B:383:TYR:CG	2.55	0.42
1:A:57:LEU:H	1:A:57:LEU:HG	1.61	0.41
1:B:40:HIS:HB2	1:B:215:TYR:CE1	2.55	0.41
1:B:216:VAL:HG13	1:B:391:ALA:HB1	2.01	0.41
1:A:74:SER:CB	1:A:75:PRO:CD	2.97	0.41
1:B:152:LEU:O	1:B:155:ILE:HB	2.21	0.41
1:B:193:ALA:O	1:B:197:ILE:HG13	2.19	0.41
1:C:194:MET:HE3	1:C:197:ILE:HD12	2.02	0.41
1:A:76:ALA:O	1:A:79:GLY:N	2.53	0.41
1:A:191:ALA:O	1:A:195:TYR:CD1	2.73	0.41
1:A:339:LEU:HA	1:A:342:VAL:HB	2.03	0.41
1:B:353:ALA:O	1:B:355:VAL:N	2.49	0.41
1:B:362:MET:HA	1:B:362:MET:HE2	2.02	0.41
1:C:51:VAL:HG13	1:C:275:THR:HG23	2.02	0.41
1:C:375:THR:O	1:C:377:PRO:HD3	2.20	0.41
1:A:344:THR:HG21	1:A:366:VAL:HA	2.03	0.41
1:A:364:ALA:O	1:A:367:LEU:HB2	2.20	0.41
1:B:138:VAL:HA	1:B:139:PRO:HD3	1.90	0.41
1:C:67:VAL:HB	1:C:187:ILE:HG21	2.01	0.41
1:C:231:VAL:O	1:C:232:THR:C	2.59	0.41
1:A:52:ARG:HH22	1:B:136:ASP:HA	1.85	0.41
1:A:123:GLN:HA	1:A:124:PRO:HD3	1.81	0.41
1:A:128:PRO:HA	1:A:129:PRO:HD3	1.70	0.41
1:A:247:TYR:OH	1:A:312:ASP:OD2	2.35	0.41
1:A:296:GLU:HG3	1:A:299:TYR:OH	2.21	0.41
1:A:304:PRO:O	1:A:306:GLY:N	2.53	0.41
1:A:311:MET:HE1	1:A:352:THR:O	2.19	0.41
1:B:123:GLN:HA	1:B:124:PRO:HD3	1.74	0.41
1:C:351:GLY:O	1:C:352:THR:C	2.59	0.41
1:A:103:MET:HG2	1:A:238:GLY:CA	2.50	0.41
1:A:165:ILE:O	1:A:168:LEU:HB2	2.21	0.41
1:B:70:ALA:CB	1:B:162:GLY:HA3	2.51	0.41
1:B:347:LEU:HA	1:B:350:ILE:HD12	2.01	0.41
1:B:53:LEU:HD23	1:B:53:LEU:HA	1.88	0.41
1:B:259:ILE:H	1:B:259:ILE:HG13	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LEU:HA	1:C:133:ILE:HD12	2.02	0.41
1:C:217:MET:C	1:C:219:GLU:H	2.23	0.41
1:A:221:GLY:O	1:A:223:HIS:N	2.48	0.41
1:C:272:ALA:HB2	1:C:281:THR:HG21	2.01	0.41
1:C:316:LEU:O	1:C:320:VAL:HG12	2.21	0.41
1:A:66:LEU:HD13	1:A:300:SER:CB	2.50	0.41
1:A:372:LEU:H	1:A:372:LEU:HG	1.72	0.41
1:B:364:ALA:HA	1:B:367:LEU:HB2	2.03	0.41
1:C:208:GLY:O	1:C:212:LEU:HB2	2.21	0.41
1:A:27:GLY:O	1:A:29:ILE:N	2.54	0.41
1:A:57:LEU:O	1:A:61:ILE:HB	2.21	0.40
1:B:239:LEU:HD22	1:B:400:VAL:HG21	2.02	0.40
1:C:70:ALA:HB3	1:C:162:GLY:HA3	2.04	0.40
1:C:295:SER:C	1:C:297:GLY:N	2.73	0.40
1:B:13:LEU:O	1:B:17:LEU:HB2	2.21	0.40
1:C:352:THR:HG23	1:C:359:GLY:HA2	2.02	0.40
1:C:399:MET:HE3	1:C:399:MET:HB3	2.02	0.40
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.81	0.40
1:A:298:ILE:C	1:A:300:SER:H	2.25	0.40
1:B:81:VAL:HG23	1:B:412:VAL:HG12	2.04	0.40
1:C:57:LEU:O	1:C:60:PRO:HD2	2.20	0.40
1:C:88:TYR:CE2	1:C:408:GLY:HA3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/422 (96%)	301 (74%)	69 (17%)	34 (8%)	1	9
1	B	404/422 (96%)	316 (78%)	70 (17%)	18 (4%)	2	21
1	C	404/422 (96%)	311 (77%)	74 (18%)	19 (5%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1212/1266 (96%)	928 (77%)	213 (18%)	71 (6%)	1 15

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	75	PRO
1	A	76	ALA
1	A	77	ARG
1	A	356	PRO
1	A	377	PRO
1	B	77	ARG
1	C	77	ARG
1	C	116	ALA
1	C	222	VAL
1	C	296	GLU
1	C	377	PRO
1	A	28	LEU
1	A	151	VAL
1	A	201	VAL
1	A	218	ALA
1	A	222	VAL
1	A	354	GLY
1	A	415	THR
1	B	76	ALA
1	B	115	LEU
1	B	118	GLY
1	B	151	VAL
1	B	222	VAL
1	B	377	PRO
1	B	415	THR
1	C	109	PRO
1	C	115	LEU
1	C	262	ILE
1	C	356	PRO
1	C	415	THR
1	A	72	SER
1	A	73	ILE
1	A	109	PRO
1	A	128	PRO
1	A	152	LEU
1	A	245	LEU

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Mol	Chain	Res	Type
1	B	75	PRO
1	B	132	HIS
1	B	152	LEU
1	B	356	PRO
1	C	151	VAL
1	A	55	LYS
1	A	74	SER
1	A	78	LEU
1	A	244	LEU
1	B	128	PRO
1	B	335	VAL
1	B	350	ILE
1	C	74	SER
1	C	120	GLN
1	C	152	LEU
1	A	198	VAL
1	A	296	GLU
1	A	400	VAL
1	B	73	ILE
1	B	74	SER
1	B	354	GLY
1	C	75	PRO
1	C	128	PRO
1	C	376	ASP
1	A	120	GLN
1	A	335	VAL
1	C	350	ILE
1	A	69	GLY
1	A	262	ILE
1	A	376	ASP
1	A	412	VAL
1	A	389	ILE
1	A	27	GLY
1	C	335	VAL

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/330 (84%)	226 (81%)	53 (19%)	1	8
1	B	279/330 (84%)	225 (81%)	54 (19%)	1	7
1	C	279/330 (84%)	229 (82%)	50 (18%)	2	9
All	All	837/990 (84%)	680 (81%)	157 (19%)	1	8

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	17	LEU
1	A	22	LEU
1	A	25	ILE
1	A	52	ARG
1	A	57	LEU
1	A	59	MET
1	A	61	ILE
1	A	72	SER
1	A	78	LEU
1	A	91	LEU
1	A	103	MET
1	A	106	LEU
1	A	107	PHE
1	A	115	LEU
1	A	121	GLN
1	A	126	GLN
1	A	136	ASP
1	A	137	ILE
1	A	146	LEU
1	A	148	ASN
1	A	152	LEU
1	A	166	THR
1	A	185	ASP
1	A	192	GLU
1	A	194	MET
1	A	212	LEU
1	A	213	ILE
1	A	219	GLU
1	A	259	ILE
1	A	262	ILE
1	A	267	ASP
1	A	269	MET
1	A	274	VAL

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Mol	Chain	Res	Type
1	A	278	SER
1	A	287	ARG
1	A	295	SER
1	A	308	THR
1	A	314	THR
1	A	317	TYR
1	A	318	GLN
1	A	329	LEU
1	A	342	VAL
1	A	343	LEU
1	A	347	LEU
1	A	365	MET
1	A	372	LEU
1	A	385	MET
1	A	387	LEU
1	A	397	ARG
1	A	399	MET
1	A	411	ILE
1	A	414	LYS
1	B	17	LEU
1	B	22	LEU
1	B	25	ILE
1	B	28	LEU
1	B	32	HIS
1	B	37	HIS
1	B	57	LEU
1	B	59	MET
1	B	61	ILE
1	B	65	SER
1	B	72	SER
1	B	78	LEU
1	B	90	LEU
1	B	107	PHE
1	B	108	ASN
1	B	115	LEU
1	B	121	GLN
1	B	123	GLN
1	B	126	GLN
1	B	136	ASP
1	B	137	ILE
1	B	146	LEU
1	B	148	ASN

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Mol	Chain	Res	Type
1	B	152	LEU
1	B	154	THR
1	B	166	THR
1	B	179	SER
1	B	185	ASP
1	B	192	GLU
1	B	194	MET
1	B	213	ILE
1	B	217	MET
1	B	219	GLU
1	B	252	LYS
1	B	259	ILE
1	B	267	ASP
1	B	287	ARG
1	B	290	LYS
1	B	314	THR
1	B	318	GLN
1	B	321	CYS
1	B	329	LEU
1	B	334	THR
1	B	339	LEU
1	B	347	LEU
1	B	362	MET
1	B	372	LEU
1	B	375	THR
1	B	385	MET
1	B	386	ILE
1	B	387	LEU
1	B	389	ILE
1	B	399	MET
1	B	414	LYS
1	C	17	LEU
1	C	22	LEU
1	C	25	ILE
1	C	28	LEU
1	C	37	HIS
1	C	57	LEU
1	C	61	ILE
1	C	72	SER
1	C	78	LEU
1	C	107	PHE
1	C	115	LEU

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Mol	Chain	Res	Type
1	C	120	GLN
1	C	121	GLN
1	C	126	GLN
1	C	136	ASP
1	C	137	ILE
1	C	146	LEU
1	C	148	ASN
1	C	152	LEU
1	C	166	THR
1	C	185	ASP
1	C	192	GLU
1	C	194	MET
1	C	207	ILE
1	C	212	LEU
1	C	213	ILE
1	C	217	MET
1	C	219	GLU
1	C	252	LYS
1	C	253	ILE
1	C	259	ILE
1	C	269	MET
1	C	274	VAL
1	C	278	SER
1	C	287	ARG
1	C	288	VAL
1	C	308	THR
1	C	314	THR
1	C	318	GLN
1	C	329	LEU
1	C	343	LEU
1	C	344	THR
1	C	347	LEU
1	C	363	LEU
1	C	372	LEU
1	C	375	THR
1	C	378	ASN
1	C	387	LEU
1	C	399	MET
1	C	411	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	223	HIS
1	A	310	ASN
1	A	327	ASN
1	A	338	GLN
1	A	378	ASN
1	B	108	ASN
1	B	148	ASN
1	B	310	ASN
1	B	327	ASN
1	B	338	GLN
1	B	378	ASN
1	C	148	ASN
1	C	150	GLN
1	C	327	ASN
1	C	378	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3   Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4   Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5   Other polymers ⓘ

EDS was not executed - this section is therefore empty.