Full wwPDB X-ray Structure Validation Report (i)

Oct 27, 2026 – 07:09 pm GMT

PDB ID	:	34FS / pdb_000034fs
Title	:	Pseudo-merohedral twinning crystal form of putative amidase
Authors	:	Bicer, D.; Morth, J.P.
Deposited on	:	2026-09-12
Resolution	:	1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

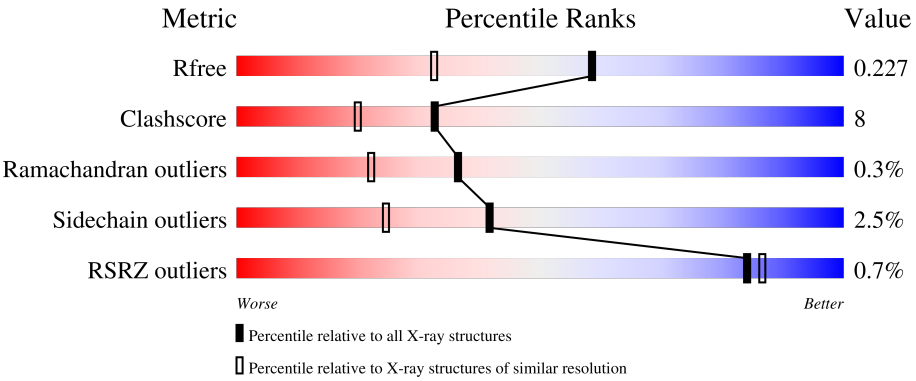
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.70 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.



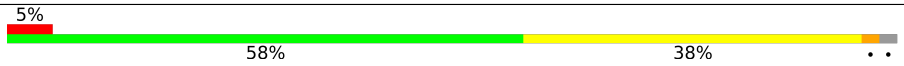
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	433	86% 11%
1	B	433	87% 10%
1	C	433	86% 11%
1	D	433	84% 12%
1	E	433	84% 14%

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Mol	Chain	Length	Quality of chain
1	F	433	
1	G	433	
1	H	433	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 26857 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 Amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3126	1960	573	582	11			
1	B	423	Total	C	N	O	S	0	0	0
			3126	1960	573	582	11			
1	C	423	Total	C	N	O	S	0	0	0
			3126	1960	573	582	11			
1	D	423	Total	C	N	O	S	0	0	0
			3126	1960	573	582	11			
1	E	423	Total	C	N	O	S	0	0	0
			3126	1960	573	582	11			
1	F	423	Total	C	N	O	S	0	0	0
			3126	1960	573	582	11			
1	G	423	Total	C	N	O	S	0	0	0
			3126	1960	573	582	11			
1	H	423	Total	C	N	O	S	0	0	0
			3126	1960	573	582	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	272	Total	O	0	0
			272	272		
2	B	307	Total	O	0	0
			307	307		
2	C	295	Total	O	0	0
			295	295		
2	D	289	Total	O	1	0
			289	289		
2	E	295	Total	O	0	0
			295	295		
2	F	297	Total	O	1	0
			297	297		

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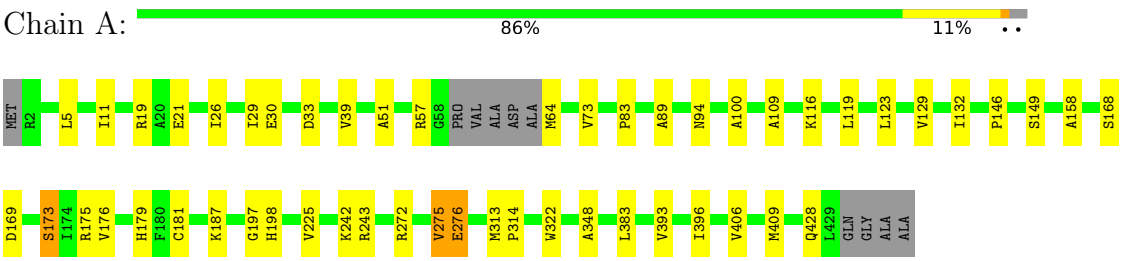
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	70	Total O 70 70	1	0
2	H	24	Total O 24 24	0	0

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.

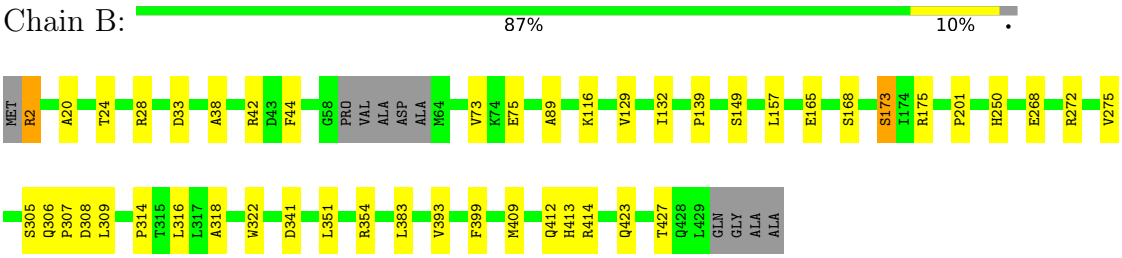
• Molecule 1: Amidase

Chain A:



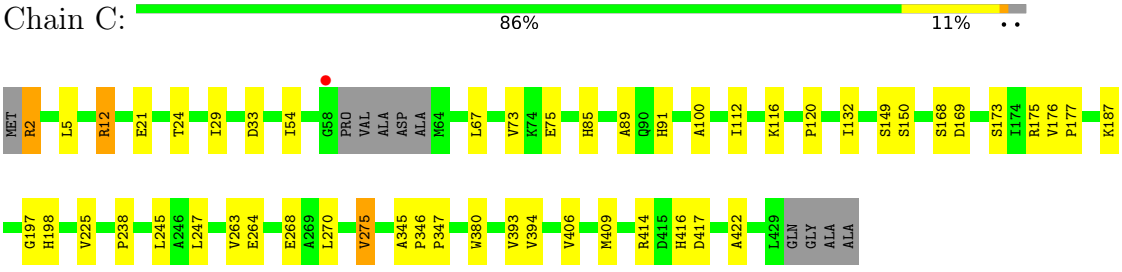
• Molecule 1: Amidase

Chain B:



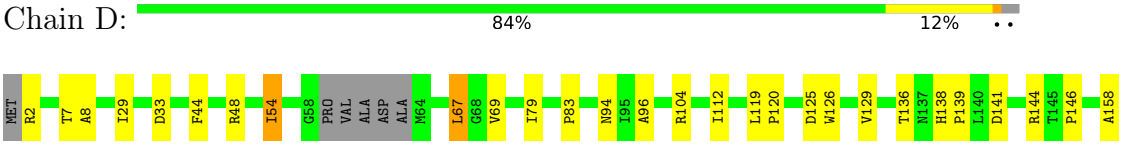
• Molecule 1: Amidase

Chain C:



• Molecule 1: Amidase

Chain D:





• Molecule 1: Amidase

Chain E:

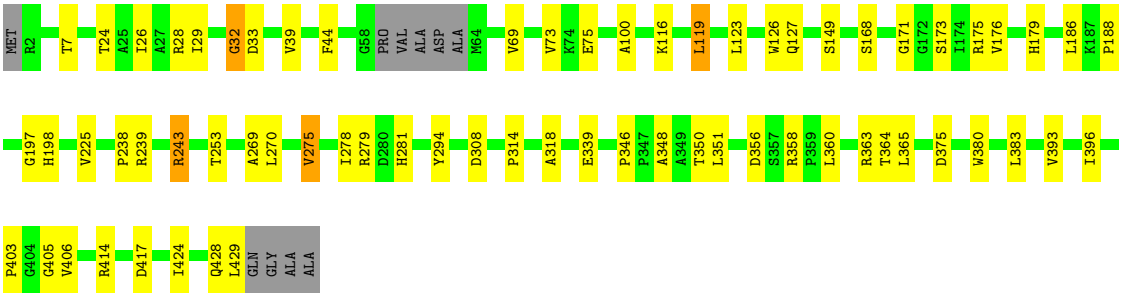




• Molecule 1: Amidase

Chain F:

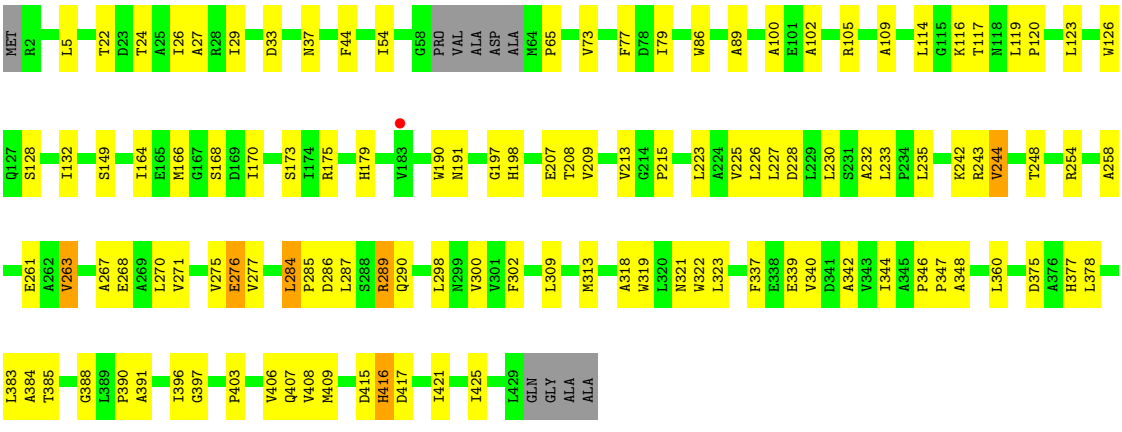




• Molecule 1: Amidase

Chain G:

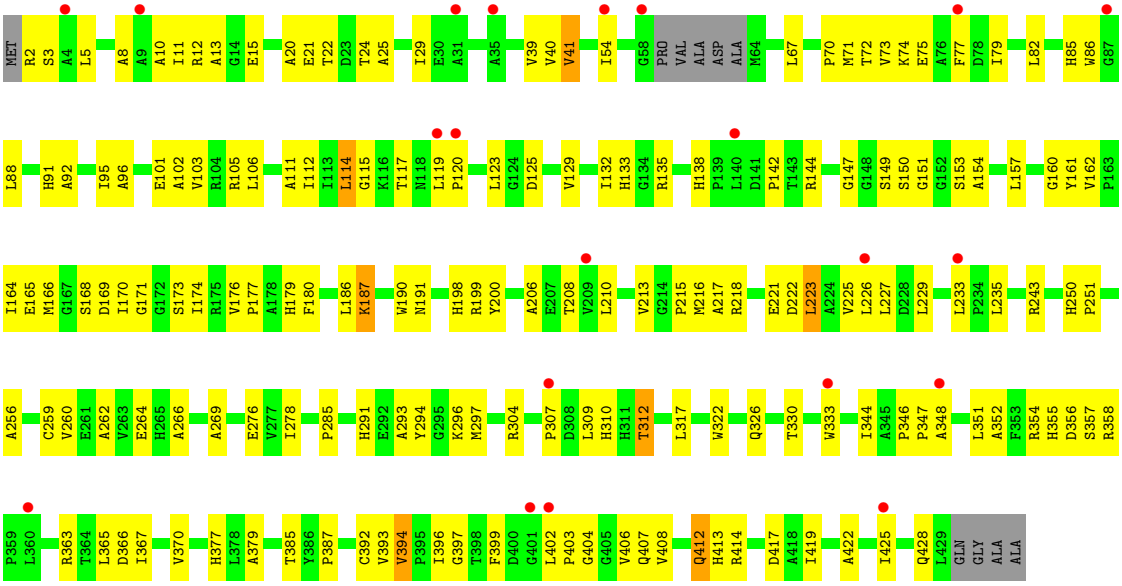




• Molecule 1: Amidase

Chain H:




MET R2 S3 A4 L5 A8 A9 A10 I11 R12 A13 G14 E15 A20 E21 T22 D23 T24 A25 I29 E30 A31 A35 V39 V40 V41 I54 G58 PRO VAL ALA ASP ALA M64 L67 P70 M71 T72 V73 K74 E75 A76 F77 D78 I79 L82 H85 W86 G87
L88 H91 A92 I95 A96 E101 A102 V103 R104 R105 L106 A111 I112 I113 L114 G115 K116 T117 N118 L119 P120 L123 G124 D125 V129 I132 H133 G134 R135 H138 P139 L140 D141 P142 T143 R144 G147 G148 S149 S150 G151 G152 S153 A154 L157 G160 Y161 V162 P163
I164 E165 M166 G167 S168 D169 I170 G171 G172 S173 I174 R175 V176 P177 A178 H179 F180 L186 K187 W190 N191 H198 R199 Y200 A206 E207 T208 V209 L210 V213 G214 P215 M216 A217 R218 E221 D222 L223 A224 V225 L226 L227 D228 L229 L233 P234 L235 R243 H250 P251
A256 C259 V260 E261 A262 V263 E264 H265 A266 A269 E276 V277 I278 P285 H291 E292 A293 Y294 G295 K296 M297 R304 P307 D308 L309 H310 H311 T312 L317 W322 Q326 T330 W333 I344 A345 P346 P347 A348 L351 A352 F353 R354 H355 D356 S357 R358
P359 L360 R363 T364 L365 D366 I367 V370 H377 L378 A379 T385 Y386 P387 C392 V393 V394 P395 I396 G397 T398 F399 D400 G401 L402 P403 G404 G405 V406 Q407 V408 Q412 H413 R414 D417 A418 I419 A422 I425 Q428 L429 GLN GLY ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	111.43Å 193.25Å 436.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 1.70 49.63 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.63-1.70) 98.9 (49.63-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.222 , 0.250 0.212 , 0.227	Depositor DCC
R_{free} test set	25457 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 32.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.477 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.477 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
Reported twinning fraction	0.530 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Depositor
Outliers	1 of 509017 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26857	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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	0.56	0/3197	0.73	0/4371
1	B	0.55	0/3197	0.74	0/4371
1	C	0.56	0/3197	0.74	0/4371
1	D	0.55	0/3197	0.72	1/4371 (0.0%)
1	E	0.55	0/3197	0.74	0/4371
1	F	0.56	0/3197	0.71	0/4371
1	G	0.61	0/3197	0.86	4/4371 (0.1%)
1	H	0.48	0/3197	0.70	0/4371
All	All	0.55	0/25576	0.74	5/34968 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	1
1	H	0	1
All	All	0	8

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	385	THR	CA-C-N	6.97	128.42	119.78
1	G	385	THR	C-N-CA	6.97	128.42	119.78
1	G	388	GLY	CA-C-N	6.84	140.87	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	388	GLY	C-N-CA	6.84	140.87	120.69
1	D	205	GLY	N-CA-C	6.14	119.74	111.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	HIS	Peptide
1	C	198	HIS	Peptide
1	D	198	HIS	Peptide
1	E	198	HIS	Peptide
1	F	198	HIS	Peptide
1	F	243	ARG	Sidechain
1	G	198	HIS	Peptide
1	H	198	HIS	Peptide

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	3126	0	3105	31	0
1	B	3126	0	3105	30	0
1	C	3126	0	3105	27	0
1	D	3126	0	3105	30	0
1	E	3126	0	3105	36	0
1	F	3126	0	3105	41	0
1	G	3126	0	3105	87	0
1	H	3126	0	3105	119	0
2	A	272	0	0	2	0
2	B	307	0	0	4	0
2	C	295	0	0	2	0
2	D	289	0	0	1	0
2	E	295	0	0	2	0
2	F	297	0	0	4	0
2	G	70	0	0	9	0
2	H	24	0	0	1	0
All	All	26857	0	24840	395	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 8.

All (395) 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:G:248:THR:HG22	1:G:263:VAL:HG11	1.32	1.08
1:G:286:ASP:HB3	1:G:289:ARG:HG2	1.32	1.06
1:G:383:LEU:HG	1:G:409:MET:HE1	1.54	0.89
1:G:384:ALA:HB2	1:G:409:MET:HE2	1.56	0.87
1:H:285:PRO:HG2	1:H:333:TRP:CE2	2.17	0.80
1:G:286:ASP:HB3	1:G:289:ARG:CG	2.13	0.79
1:B:175:ARG:HA	1:B:393:VAL:HG21	1.65	0.78
1:H:266:ALA:HB2	1:H:396:ILE:HD11	1.64	0.76
1:G:248:THR:HG22	1:G:263:VAL:CG1	2.15	0.76
1:A:383:LEU:HD23	1:A:409:MET:HE1	1.70	0.73
1:G:344:ILE:HG22	1:G:408:VAL:HG22	1.70	0.72
1:H:102:ALA:HB1	1:H:166:MET:HE2	1.71	0.72
1:H:71:MET:HA	1:H:162:VAL:HG21	1.73	0.70
1:H:367:ILE:O	1:H:370:VAL:HG12	1.92	0.69
1:H:169:ASP:HA	1:H:173:SER:HB2	1.73	0.69
1:F:269:ALA:HB1	1:F:428:GLN:HB2	1.73	0.69
1:G:243:ARG:HH21	1:G:339:GLU:HB3	1.57	0.68
1:G:285:PRO:HD3	2:G:511:HOH:O	1.93	0.68
1:F:24:THR:HG23	1:F:28:ARG:HH12	1.58	0.68
1:E:29:ILE:O	1:E:33:ASP:HB2	1.93	0.67
1:H:293:ALA:HA	1:H:296:LYS:HE2	1.77	0.67
1:H:92:ALA:HB2	1:H:132:ILE:HD13	1.76	0.67
1:H:12:ARG:HH21	1:H:67:LEU:HB3	1.59	0.66
1:H:11:ILE:HD11	1:H:21:GLU:HG3	1.77	0.65
1:H:396:ILE:HB	1:H:404:GLY:O	1.96	0.65
1:A:175:ARG:HG2	1:A:393:VAL:CG2	2.27	0.65
1:H:72:THR:HG22	1:H:115:GLY:H	1.61	0.65
1:G:190:TRP:CE3	1:G:191:ASN:HB2	2.32	0.64
1:E:383:LEU:HD23	1:E:409:MET:HE1	1.80	0.64
1:A:313:MET:HE3	1:B:316:LEU:HD23	1.79	0.64
1:H:71:MET:HE3	1:H:111:ALA:CB	2.28	0.64
1:H:351:LEU:HD23	1:H:402:LEU:HB3	1.78	0.64
1:H:157:LEU:HD11	1:H:165:GLU:HB2	1.80	0.63
1:H:154:ALA:HB2	1:H:177:PRO:HB2	1.78	0.63
1:H:358:ARG:HG3	1:H:358:ARG:HH11	1.63	0.62
1:G:263:VAL:HG13	2:G:537:HOH:O	1.99	0.62
1:G:179:HIS:CG	1:G:347:PRO:HG2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:266:ALA:HB1	1:H:425:ILE:HD13	1.81	0.61
1:H:77:PHE:HZ	1:H:213:VAL:HB	1.65	0.61
1:G:289:ARG:CZ	1:G:290:GLN:HB2	2.30	0.61
1:H:250:HIS:ND1	1:H:379:ALA:HB1	2.14	0.61
1:F:238:PRO:HA	1:F:417:ASP:OD1	2.01	0.61
1:E:396:ILE:HG12	1:E:405:GLY:HA2	1.83	0.60
1:G:168:SER:HB3	1:G:213:VAL:HG12	1.83	0.60
1:H:262:ALA:HA	1:H:396:ILE:HG21	1.82	0.60
1:G:168:SER:O	1:G:173:SER:HB2	2.02	0.60
1:F:100:ALA:HA	1:F:197:GLY:HA3	1.84	0.59
1:D:383:LEU:HD23	1:D:409:MET:HE1	1.84	0.59
1:H:75:GLU:HB3	1:H:119:LEU:HD22	1.84	0.59
1:H:397:GLY:O	1:H:403:PRO:HA	2.02	0.59
1:D:94:ASN:OD1	1:D:202:LYS:HD3	2.03	0.59
1:G:235:LEU:HD23	1:H:233:LEU:HD11	1.85	0.58
1:H:344:ILE:HG22	1:H:408:VAL:HG22	1.86	0.58
1:F:358:ARG:NH2	1:F:364:THR:H	2.02	0.58
1:G:126:TRP:CZ3	1:G:375:ASP:HA	2.38	0.58
1:E:73:VAL:O	1:E:116:LYS:HA	2.04	0.58
1:G:267:ALA:HB1	1:G:277:VAL:HG11	1.86	0.58
1:G:417:ASP:O	1:G:421:ILE:HG13	2.03	0.58
1:H:25:ALA:O	1:H:29:ILE:HG13	2.04	0.58
1:E:157:LEU:O	1:E:218:ARG:HD3	2.04	0.57
1:G:244:VAL:HG22	1:G:342:ALA:HB3	1.87	0.57
1:D:387:PRO:HG2	1:D:389:LEU:HG	1.87	0.57
1:F:7:THR:HB	1:F:69:VAL:HG22	1.86	0.57
1:A:176:VAL:HG22	1:A:348:ALA:HB2	1.86	0.57
1:H:176:VAL:HG22	1:H:348:ALA:HB2	1.86	0.57
1:D:139:PRO:HG2	1:D:158:ALA:HB3	1.85	0.56
1:G:227:LEU:HD23	1:G:416:HIS:CE1	2.40	0.56
1:A:175:ARG:HA	1:A:393:VAL:HG21	1.87	0.56
1:B:314:PRO:HB2	1:B:318:ALA:HB3	1.86	0.56
1:E:186:LEU:HD22	1:E:419:ILE:HD11	1.87	0.56
1:F:149:SER:H	1:F:173:SER:HB3	1.71	0.56
1:H:309:LEU:O	1:H:312:THR:HG22	2.05	0.56
1:A:89:ALA:HA	1:A:132:ILE:HD11	1.88	0.56
1:B:20:ALA:O	1:B:24:THR:HG23	2.05	0.55
1:G:318:ALA:HA	1:G:321:ASN:HB2	1.89	0.55
1:G:289:ARG:HG3	1:G:290:GLN:N	2.21	0.55
1:H:174:ILE:HG23	1:H:216:MET:HE3	1.88	0.55
1:H:179:HIS:HB2	1:H:347:PRO:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:VAL:O	1:H:264:GLU:HG2	2.07	0.55
1:A:26:ILE:O	1:A:30:GLU:HG3	2.07	0.55
1:E:351:LEU:HD11	1:E:399:PHE:HB2	1.89	0.54
1:G:22:THR:HG23	1:G:114:LEU:HD11	1.89	0.54
1:H:243:ARG:NH1	1:H:278:ILE:HG21	2.23	0.54
1:G:344:ILE:HG13	2:G:537:HOH:O	2.05	0.54
1:H:250:HIS:CE1	1:H:379:ALA:HB1	2.43	0.54
1:H:79:ILE:O	1:H:96:ALA:HB3	2.07	0.54
1:E:171:GLY:HA2	1:E:294:TYR:OH	2.07	0.54
1:H:262:ALA:HB1	1:H:396:ILE:HG13	1.89	0.54
1:H:358:ARG:HB2	1:H:363:ARG:HG2	1.89	0.54
1:H:85:HIS:HE2	1:H:133:HIS:CD2	2.25	0.54
1:C:5:LEU:HD21	1:C:225:VAL:HG21	1.89	0.54
1:G:79:ILE:HD12	1:G:116:LYS:HD3	1.88	0.54
1:G:89:ALA:HA	1:G:132:ILE:HD11	1.89	0.54
1:G:207:GLU:HB3	2:G:540:HOH:O	2.08	0.54
1:E:120:PRO:HD2	1:E:149:SER:HB2	1.88	0.54
1:H:210:LEU:HD22	1:H:385:THR:HG22	1.89	0.54
1:G:270:LEU:HB3	1:G:275:VAL:CG2	2.37	0.53
1:A:119:LEU:HD22	1:A:123:LEU:HD11	1.90	0.53
1:A:175:ARG:HG2	1:A:393:VAL:HG21	1.89	0.53
1:H:106:LEU:HD11	1:H:166:MET:HG3	1.89	0.53
1:B:423:GLN:O	1:B:427:THR:HG23	2.09	0.53
1:E:267:ALA:O	1:E:271:VAL:HG23	2.09	0.53
1:E:279:ARG:HD2	2:E:615:HOH:O	2.07	0.53
1:F:175:ARG:HG2	1:F:393:VAL:HG23	1.90	0.53
1:H:8:ALA:HB1	1:H:12:ARG:NH2	2.24	0.53
1:B:42:ARG:HD3	1:B:44:PHE:CZ	2.44	0.53
1:B:149:SER:H	1:B:173:SER:HB3	1.74	0.53
1:E:5:LEU:HD21	1:E:225:VAL:HG21	1.89	0.53
1:D:54:ILE:HD12	1:D:112:ILE:HD11	1.91	0.52
1:G:287:LEU:HD23	2:G:527:HOH:O	2.09	0.52
1:G:243:ARG:HG2	1:G:340:VAL:HG22	1.91	0.52
1:H:296:LYS:HB3	1:H:322:TRP:CH2	2.45	0.52
1:E:250:HIS:HB2	1:E:380:TRP:CZ2	2.45	0.52
1:A:29:ILE:O	1:A:33:ASP:HB2	2.09	0.52
1:B:73:VAL:O	1:B:116:LYS:HA	2.09	0.52
1:G:313:MET:HE2	1:H:317:LEU:HG	1.91	0.52
1:H:164:ILE:HG22	1:H:217:ALA:HB2	1.91	0.52
1:C:263:VAL:HA	1:C:406:VAL:HG11	1.92	0.52
1:G:384:ALA:CB	1:G:409:MET:HE2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ALA:HA	1:B:132:ILE:HD11	1.91	0.51
1:F:75:GLU:HA	1:F:116:LYS:HB3	1.91	0.51
1:H:180:PHE:HZ	1:H:377:HIS:HE1	1.57	0.51
1:G:164:ILE:HB	1:G:226:LEU:HD11	1.91	0.51
1:H:75:GLU:HB2	1:H:117:THR:O	2.11	0.51
1:E:175:ARG:HG2	1:E:393:VAL:HG23	1.93	0.51
1:G:258:ALA:HA	1:G:261:GLU:HB2	1.92	0.51
1:F:281:HIS:CE1	1:F:339:GLU:HG3	2.46	0.51
1:B:175:ARG:HG2	1:B:393:VAL:CG2	2.40	0.51
1:H:73:VAL:HG12	1:H:166:MET:HB2	1.93	0.51
1:B:268:GLU:O	1:B:272:ARG:HG3	2.10	0.51
1:F:127:GLN:HE22	1:F:356:ASP:HB3	1.76	0.51
1:C:346:PRO:HD2	1:C:380:TRP:CH2	2.47	0.50
1:G:149:SER:H	1:G:173:SER:HB3	1.76	0.50
1:G:289:ARG:HG3	1:G:290:GLN:H	1.76	0.50
1:H:71:MET:HE2	1:H:164:ILE:HD11	1.92	0.50
1:G:215:PRO:HB2	1:G:223:LEU:HD12	1.92	0.50
1:C:238:PRO:HG3	1:C:416:HIS:HB3	1.94	0.50
1:C:264:GLU:O	1:C:268:GLU:HG3	2.12	0.50
1:A:5:LEU:HD21	1:A:225:VAL:HG21	1.94	0.50
1:H:120:PRO:HD2	1:H:149:SER:HA	1.94	0.50
1:B:306:GLN:HB3	1:B:309:LEU:HG	1.93	0.49
1:H:5:LEU:HD11	1:H:225:VAL:HG21	1.95	0.49
1:H:88:LEU:HD23	1:H:91:HIS:ND1	2.27	0.49
1:H:129:VAL:HG23	1:H:135:ARG:HB2	1.93	0.49
1:A:146:PRO:HD2	2:A:549:HOH:O	2.12	0.49
1:D:136:THR:HG22	1:D:146:PRO:HG3	1.95	0.49
1:G:286:ASP:CB	1:G:289:ARG:HG2	2.22	0.49
1:H:147:GLY:O	1:H:151:GLY:HA3	2.13	0.49
1:H:215:PRO:HB2	1:H:226:LEU:HD13	1.94	0.49
1:G:300:VAL:HG11	1:G:319:TRP:CZ3	2.47	0.49
1:B:354:ARG:HD3	2:B:656:HOH:O	2.13	0.49
1:E:383:LEU:HB3	1:E:409:MET:HE1	1.94	0.49
1:B:157:LEU:HD11	1:B:165:GLU:HB2	1.94	0.49
1:B:351:LEU:HD11	1:B:399:PHE:HB2	1.94	0.49
1:B:383:LEU:HB3	1:B:409:MET:HE1	1.94	0.49
1:D:83:PRO:HA	1:D:94:ASN:O	2.13	0.49
1:F:175:ARG:HG2	1:F:393:VAL:CG2	2.43	0.49
1:G:344:ILE:HA	1:G:407:GLN:O	2.13	0.49
1:H:186:LEU:HD22	1:H:419:ILE:HD11	1.95	0.49
1:H:256:ALA:O	1:H:259:CYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ALA:HB1	1:D:67:LEU:HB3	1.95	0.49
1:E:83:PRO:HA	1:E:94:ASN:O	2.13	0.49
1:G:267:ALA:O	1:G:271:VAL:HG23	2.12	0.49
1:F:346:PRO:HD2	1:F:380:TRP:CH2	2.47	0.48
1:H:40:VAL:HB	1:H:133:HIS:HB3	1.95	0.48
1:A:73:VAL:O	1:A:116:LYS:HA	2.13	0.48
1:G:232:ALA:O	1:G:233:LEU:HD23	2.13	0.48
1:H:74:LYS:HE3	1:H:149:SER:O	2.14	0.48
1:H:71:MET:HE3	1:H:111:ALA:HB3	1.96	0.48
1:G:233:LEU:HD11	1:H:413:HIS:CD2	2.49	0.48
1:G:298:LEU:HD22	1:G:302:PHE:CZ	2.49	0.48
1:G:29:ILE:HD12	1:G:114:LEU:HD23	1.96	0.48
1:A:29:ILE:HD13	1:A:39:VAL:HG21	1.95	0.48
1:F:424:ILE:O	1:F:428:GLN:HG2	2.13	0.48
1:H:291:HIS:ND1	1:H:379:ALA:HA	2.29	0.48
1:C:409:MET:HE3	1:C:409:MET:HB2	1.67	0.48
1:D:344:ILE:HA	1:D:407:GLN:O	2.14	0.48
1:G:65:PRO:HG2	1:G:109:ALA:HB1	1.96	0.48
1:B:250:HIS:HD2	1:B:383:LEU:HD11	1.78	0.47
1:E:298:LEU:HG	1:E:302:PHE:CE2	2.49	0.47
1:E:86:TRP:CE3	1:E:123:LEU:HD13	2.49	0.47
1:B:24:THR:O	1:B:28:ARG:HG3	2.15	0.47
1:F:396:ILE:HG13	1:F:406:VAL:HG13	1.95	0.47
1:B:75:GLU:HA	1:B:116:LYS:HB3	1.96	0.47
1:F:243:ARG:NH2	2:F:506:HOH:O	2.47	0.47
1:H:74:LYS:HE2	1:H:119:LEU:HD12	1.97	0.47
1:H:120:PRO:CD	1:H:149:SER:HA	2.45	0.47
1:H:250:HIS:CG	1:H:251:PRO:HD2	2.50	0.47
1:G:179:HIS:HB2	1:G:347:PRO:HG2	1.96	0.47
1:F:179:HIS:CE1	1:F:405:GLY:H	2.33	0.47
1:H:330:THR:HG21	1:H:412:GLN:NE2	2.30	0.47
1:H:40:VAL:HG23	1:H:41:VAL:HG23	1.95	0.47
1:H:365:LEU:HD12	1:H:366:ASP:H	1.79	0.47
1:G:390:PRO:HB3	1:G:415:ASP:OD2	2.15	0.46
1:H:71:MET:HA	1:H:162:VAL:CG2	2.42	0.46
1:H:164:ILE:HG22	1:H:217:ALA:CB	2.45	0.46
1:A:83:PRO:HA	1:A:94:ASN:O	2.15	0.46
1:D:120:PRO:HA	1:D:129:VAL:O	2.15	0.46
1:D:250:HIS:ND1	1:D:252:GLU:HB2	2.31	0.46
1:H:190:TRP:CE3	1:H:191:ASN:HB2	2.51	0.46
1:A:179:HIS:CD2	1:A:348:ALA:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:THR:HG21	2:B:752:HOH:O	2.14	0.46
1:G:102:ALA:HB1	1:G:166:MET:HE2	1.97	0.46
1:H:2:ARG:NH2	1:H:10:ALA:HB2	2.29	0.46
1:H:180:PHE:HB3	1:H:352:ALA:HB2	1.96	0.46
1:G:318:ALA:O	1:G:322:TRP:CD1	2.69	0.46
1:G:347:PRO:HD3	1:G:406:VAL:HA	1.97	0.46
1:H:187:LYS:HB3	1:H:187:LYS:HE3	1.69	0.46
1:H:394:VAL:HB	1:H:422:ALA:HB1	1.97	0.46
1:B:341:ASP:HA	2:B:699:HOH:O	2.16	0.46
1:C:345:ALA:HB1	1:C:380:TRP:CZ3	2.50	0.46
1:C:414:ARG:HD2	1:C:417:ASP:OD2	2.16	0.46
1:F:73:VAL:O	1:F:116:LYS:HA	2.16	0.46
1:E:75:GLU:HA	1:E:116:LYS:HB3	1.98	0.46
1:E:270:LEU:HB3	1:E:275:VAL:CG2	2.45	0.46
1:F:239:ARG:HH21	1:F:414:ARG:HG3	1.81	0.46
1:C:73:VAL:O	1:C:116:LYS:HA	2.16	0.46
1:E:270:LEU:HB3	1:E:275:VAL:HG22	1.97	0.46
1:F:314:PRO:HB2	1:F:318:ALA:HB3	1.96	0.46
1:F:346:PRO:HD2	1:F:380:TRP:CZ3	2.51	0.46
1:H:235:LEU:HD22	1:H:413:HIS:HD2	1.81	0.45
1:C:75:GLU:HA	1:C:116:LYS:HE3	1.99	0.45
1:H:101:GLU:C	1:H:103:VAL:H	2.25	0.45
1:F:171:GLY:HA2	1:F:294:TYR:OH	2.17	0.45
1:G:323:LEU:O	1:H:206:ALA:HB2	2.16	0.45
1:G:29:ILE:O	1:G:33:ASP:HB2	2.16	0.45
1:E:409:MET:HE3	1:E:409:MET:HB2	1.71	0.45
1:A:149:SER:H	1:A:173:SER:HB3	1.81	0.45
1:B:412:GLN:HG2	1:B:413:HIS:CD2	2.52	0.45
1:H:120:PRO:HG3	1:H:125:ASP:O	2.17	0.45
1:B:2:ARG:HB2	2:B:745:HOH:O	2.15	0.45
1:E:246:ALA:HA	1:E:344:ILE:HG12	1.99	0.45
1:F:26:ILE:HG23	1:F:44:PHE:CE2	2.51	0.45
1:G:270:LEU:HB3	1:G:275:VAL:HG22	1.97	0.45
1:H:20:ALA:O	1:H:24:THR:HG23	2.16	0.45
1:H:333:TRP:NE1	1:H:387:PRO:HG3	2.32	0.45
1:E:85:HIS:HB3	1:E:91:HIS:O	2.16	0.45
1:E:169:ASP:HA	1:E:173:SER:HB2	1.97	0.45
1:G:100:ALA:HA	1:G:197:GLY:HA3	1.98	0.45
1:G:228:ASP:OD1	1:G:416:HIS:NE2	2.42	0.45
1:G:86:TRP:CE3	1:G:123:LEU:HD13	2.52	0.45
1:A:242:LYS:HA	1:A:275:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:VAL:HB	1:E:422:ALA:HB1	1.99	0.45
1:D:29:ILE:O	1:D:33:ASP:HB2	2.18	0.44
1:F:168:SER:O	1:F:173:SER:HB2	2.17	0.44
1:G:24:THR:O	1:G:27:ALA:HB3	2.17	0.44
1:G:243:ARG:HD2	1:G:276:GLU:OE1	2.16	0.44
1:H:5:LEU:HD21	1:H:225:VAL:HG11	1.99	0.44
1:H:29:ILE:HG12	1:H:161:TYR:HB3	2.00	0.44
1:H:269:ALA:O	1:H:428:GLN:HG3	2.17	0.44
1:C:85:HIS:HB3	1:C:91:HIS:O	2.18	0.44
1:D:344:ILE:HG22	1:D:408:VAL:HG22	2.00	0.44
1:F:119:LEU:HD22	1:F:123:LEU:HD11	1.98	0.44
1:H:160:GLY:HA3	2:H:508:HOH:O	2.18	0.44
1:G:102:ALA:CB	1:G:166:MET:HE2	2.48	0.44
1:D:175:ARG:HG2	1:D:393:VAL:HG23	1.98	0.44
1:G:175:ARG:NH1	2:G:501:HOH:O	2.41	0.44
1:C:168:SER:O	1:C:173:SER:HB2	2.18	0.44
1:E:21:GLU:HA	1:E:24:THR:HG22	1.99	0.44
1:E:179:HIS:CE1	1:E:405:GLY:H	2.36	0.44
1:H:106:LEU:HD23	1:H:229:LEU:HD11	2.00	0.44
1:D:79:ILE:O	1:D:96:ALA:HB3	2.17	0.44
1:E:29:ILE:HG12	1:E:39:VAL:HG21	2.00	0.44
1:H:144:ARG:HA	1:H:354:ARG:HA	2.00	0.44
1:D:104:ARG:HG3	2:D:776:HOH:O	2.18	0.44
1:G:73:VAL:O	1:G:116:LYS:HA	2.17	0.44
1:A:64:MET:N	2:A:502:HOH:O	2.50	0.44
1:G:263:VAL:HA	1:G:406:VAL:HG11	2.00	0.44
1:C:54:ILE:HD12	1:C:112:ILE:HD11	1.99	0.43
1:C:245:LEU:HD21	1:C:247:LEU:HD21	2.00	0.43
1:G:105:ARG:HD3	1:G:230:LEU:HA	2.00	0.43
1:G:391:ALA:CB	2:G:501:HOH:O	2.65	0.43
1:H:297:MET:HE1	1:H:326:GLN:CD	2.43	0.43
1:D:44:PHE:O	1:D:48:ARG:HG3	2.17	0.43
1:H:74:LYS:HE2	1:H:119:LEU:CD1	2.47	0.43
1:F:429:LEU:HD23	1:F:429:LEU:HA	1.84	0.43
1:H:54:ILE:HD13	1:H:54:ILE:HA	1.79	0.43
1:H:171:GLY:HA2	1:H:294:TYR:OH	2.19	0.43
1:H:285:PRO:HG2	1:H:333:TRP:CD2	2.52	0.43
1:A:169:ASP:HB3	1:A:187:LYS:HG2	2.00	0.43
1:C:21:GLU:HA	1:C:24:THR:HG22	1.99	0.43
1:D:250:HIS:CE1	1:D:252:GLU:HB2	2.54	0.43
1:H:396:ILE:HG22	1:H:399:PHE:HZ	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:ALA:HB3	1:H:15:GLU:HG3	1.99	0.43
1:H:356:ASP:OD2	1:H:358:ARG:HD2	2.18	0.43
1:E:176:VAL:O	1:E:179:HIS:HB3	2.18	0.43
1:F:75:GLU:HA	1:F:116:LYS:HD2	2.01	0.43
1:G:77:PHE:HZ	1:G:213:VAL:HB	1.83	0.43
1:H:165:GLU:HB2	1:H:216:MET:HB2	1.99	0.43
1:H:392:CYS:O	1:H:407:GLN:HA	2.18	0.43
1:A:100:ALA:HA	1:A:197:GLY:HA3	2.00	0.43
1:B:33:ASP:OD1	1:B:38:ALA:N	2.43	0.43
1:C:12:ARG:HD2	2:C:677:HOH:O	2.18	0.43
1:H:307:PRO:HA	1:H:310:HIS:CG	2.54	0.43
1:D:171:GLY:HA2	1:D:294:TYR:OH	2.19	0.43
1:D:190:TRP:CE3	1:D:191:ASN:HB2	2.53	0.43
1:D:7:THR:HB	1:D:69:VAL:HG22	2.00	0.43
1:D:138:HIS:HB3	1:D:141:ASP:O	2.19	0.43
1:D:289:ARG:HA	1:D:289:ARG:HD3	1.75	0.43
1:D:313:MET:HE2	1:E:317:LEU:HG	2.01	0.43
1:F:239:ARG:NH2	1:F:414:ARG:HG3	2.34	0.43
1:H:221:GLU:OE2	1:H:221:GLU:N	2.52	0.43
1:G:168:SER:HA	1:G:213:VAL:HA	2.01	0.42
1:G:170:ILE:HG12	1:G:298:LEU:HD21	2.01	0.42
1:G:289:ARG:NH2	1:G:290:GLN:HB2	2.34	0.42
1:A:314:PRO:HG3	1:A:322:TRP:CH2	2.55	0.42
1:B:305:SER:O	1:B:307:PRO:HD3	2.18	0.42
1:G:270:LEU:HD11	1:G:425:ILE:HD11	2.00	0.42
1:H:293:ALA:HA	1:H:296:LYS:CE	2.47	0.42
1:H:304:ARG:O	1:H:310:HIS:HE1	2.02	0.42
1:F:270:LEU:HD22	1:F:275:VAL:HG11	2.00	0.42
1:G:179:HIS:ND1	1:G:347:PRO:HG2	2.33	0.42
1:H:179:HIS:HE2	1:H:351:LEU:HD12	1.84	0.42
1:B:308:ASP:O	1:B:309:LEU:HD23	2.19	0.42
1:E:384:ALA:HB2	1:E:409:MET:HE2	2.00	0.42
1:G:378:LEU:HD23	1:G:378:LEU:HA	1.77	0.42
1:H:22:THR:HG23	1:H:114:LEU:HD21	2.01	0.42
1:H:160:GLY:HA2	1:H:218:ARG:NH1	2.35	0.42
1:D:346:PRO:HA	1:D:347:PRO:HD3	1.92	0.42
1:G:120:PRO:HD3	1:G:128:SER:HA	2.02	0.42
1:G:384:ALA:HB3	2:G:501:HOH:O	2.18	0.42
1:H:358:ARG:HG3	1:H:358:ARG:NH1	2.33	0.42
1:A:168:SER:O	1:A:173:SER:HB2	2.19	0.42
1:B:250:HIS:CD2	1:B:383:LEU:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ALA:HA	1:C:197:GLY:HA3	2.02	0.42
1:D:125:ASP:OD1	1:D:126:TRP:N	2.53	0.42
1:D:144:ARG:HD2	1:D:402:LEU:HD21	2.02	0.42
1:F:350:THR:CG2	1:F:365:LEU:HD21	2.49	0.42
1:F:358:ARG:HH22	1:F:364:THR:H	1.66	0.42
1:G:397:GLY:O	1:G:403:PRO:HA	2.20	0.42
1:C:176:VAL:HB	1:C:177:PRO:HD3	2.01	0.42
1:H:79:ILE:HB	1:H:82:LEU:HD12	2.01	0.42
1:A:396:ILE:HD11	1:A:406:VAL:HG22	2.00	0.42
1:B:314:PRO:HG3	1:B:322:TRP:CH2	2.54	0.42
1:C:2:ARG:HB3	2:C:714:HOH:O	2.18	0.42
1:G:126:TRP:CZ2	1:G:378:LEU:HG	2.55	0.42
1:H:333:TRP:CD1	1:H:387:PRO:HG3	2.54	0.42
1:A:158:ALA:HB2	1:A:181:CYS:HB3	2.01	0.41
1:G:396:ILE:HD11	1:G:406:VAL:HG22	2.02	0.41
1:C:120:PRO:HD2	1:C:149:SER:HB2	2.02	0.41
1:H:414:ARG:HD2	1:H:417:ASP:OD1	2.20	0.41
1:F:360:LEU:HA	1:F:363:ARG:HG3	2.01	0.41
1:H:86:TRP:CE3	1:H:123:LEU:HD13	2.54	0.41
1:H:179:HIS:NE2	1:H:351:LEU:HD12	2.35	0.41
1:H:199:ARG:HG2	1:H:200:TYR:O	2.19	0.41
1:F:32:GLY:HA2	2:F:646:HOH:O	2.19	0.41
1:H:180:PHE:HZ	1:H:377:HIS:CE1	2.37	0.41
1:C:29:ILE:O	1:C:33:ASP:HB2	2.20	0.41
1:C:89:ALA:HA	1:C:132:ILE:HD11	2.03	0.41
1:E:175:ARG:HA	1:E:393:VAL:HG21	2.03	0.41
1:A:11:ILE:HD11	1:A:21:GLU:HG3	2.01	0.41
1:A:19:ARG:HA	1:A:51:ALA:HB1	2.02	0.41
1:D:309:LEU:HD22	1:D:309:LEU:HA	1.91	0.41
1:F:29:ILE:HD13	1:F:39:VAL:HG11	2.01	0.41
1:F:176:VAL:HG22	1:F:348:ALA:HB2	2.03	0.41
1:F:351:LEU:HD22	1:F:403:PRO:O	2.21	0.41
1:G:268:GLU:HB2	2:G:505:HOH:O	2.20	0.41
1:A:272:ARG:HG2	1:A:428:GLN:OE1	2.21	0.41
1:F:126:TRP:CZ3	1:F:375:ASP:HA	2.56	0.41
1:G:284:LEU:HA	1:G:285:PRO:HD3	1.95	0.41
1:D:269:ALA:O	1:D:428:GLN:HG3	2.21	0.41
1:E:360:LEU:HD13	1:E:360:LEU:O	2.21	0.41
1:F:186:LEU:O	1:F:188:PRO:HD3	2.21	0.41
1:F:278:ILE:HD13	2:F:506:HOH:O	2.20	0.41
1:F:403:PRO:HD2	2:F:543:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:LYS:HE3	1:G:242:LYS:HB3	1.96	0.41
1:H:210:LEU:HA	1:H:210:LEU:HD23	1.76	0.41
1:H:243:ARG:HD2	1:H:276:GLU:OE2	2.21	0.41
1:C:169:ASP:HB3	1:C:187:LYS:HG2	2.03	0.41
1:H:346:PRO:HA	1:H:347:PRO:HD3	1.89	0.41
1:A:169:ASP:HA	1:A:173:SER:HB2	2.02	0.40
1:A:243:ARG:HG3	1:A:276:GLU:HG2	2.03	0.40
1:B:168:SER:O	1:B:173:SER:HB2	2.22	0.40
1:G:26:ILE:HG23	1:G:44:PHE:CE2	2.56	0.40
1:H:138:HIS:HB2	1:H:144:ARG:O	2.21	0.40
1:C:175:ARG:HG2	1:C:393:VAL:HG23	2.03	0.40
1:H:223:LEU:HA	1:H:226:LEU:HD12	2.03	0.40
1:C:270:LEU:HB3	1:C:275:VAL:HG22	2.03	0.40
1:F:279:ARG:HA	1:F:279:ARG:HD3	1.92	0.40
1:G:346:PRO:O	1:G:407:GLN:NE2	2.54	0.40
1:H:70:PRO:HA	1:H:112:ILE:HB	2.04	0.40
1:H:142:PRO:O	1:H:355:HIS:HE1	2.05	0.40
1:H:173:SER:O	1:H:177:PRO:HG3	2.21	0.40
1:C:347:PRO:HD3	1:C:406:VAL:HA	2.03	0.40
1:E:48:ARG:HD2	2:E:553:HOH:O	2.20	0.40
1:G:179:HIS:CD2	1:G:348:ALA:HB3	2.56	0.40
1:A:64:MET:HB3	1:A:109:ALA:O	2.22	0.40
1:B:414:ARG:HD3	1:B:414:ARG:HA	1.81	0.40
1:C:394:VAL:HB	1:C:422:ALA:HB1	2.04	0.40
1:D:284:LEU:HD12	1:D:285:PRO:HD2	2.04	0.40
1:E:264:GLU:O	1:E:268:GLU:HG3	2.21	0.40
1:G:5:LEU:HD21	1:G:225:VAL:HG21	2.04	0.40
1:G:208:THR:HG22	1:G:209:VAL:O	2.21	0.40
1:G:337:PHE:HD1	1:G:340:VAL:O	2.04	0.40
1:H:150:SER:HB2	1:H:173:SER:O	2.21	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	419/433 (97%)	407 (97%)	11 (3%)	1 (0%)	43 28
1	B	419/433 (97%)	400 (96%)	19 (4%)	0	100 100
1	C	419/433 (97%)	404 (96%)	14 (3%)	1 (0%)	43 28
1	D	419/433 (97%)	404 (96%)	14 (3%)	1 (0%)	43 28
1	E	419/433 (97%)	401 (96%)	18 (4%)	0	100 100
1	F	419/433 (97%)	398 (95%)	20 (5%)	1 (0%)	43 28
1	G	419/433 (97%)	396 (94%)	22 (5%)	1 (0%)	43 28
1	H	419/433 (97%)	379 (90%)	35 (8%)	5 (1%)	10 2
All	All	3352/3464 (97%)	3189 (95%)	153 (5%)	10 (0%)	36 22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	LEU
1	H	223	LEU
1	A	57	ARG
1	D	67	LEU
1	H	3	SER
1	H	114	LEU
1	H	222	ASP
1	G	37	ASN
1	F	32	GLY
1	H	170	ILE

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	311/316 (98%)	307 (99%)	4 (1%)	61 48
1	B	311/316 (98%)	305 (98%)	6 (2%)	50 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	311/316 (98%)	307 (99%)	4 (1%)	61 48
1	D	311/316 (98%)	304 (98%)	7 (2%)	44 27
1	E	311/316 (98%)	305 (98%)	6 (2%)	50 34
1	F	311/316 (98%)	304 (98%)	7 (2%)	44 27
1	G	311/316 (98%)	298 (96%)	13 (4%)	26 11
1	H	311/316 (98%)	296 (95%)	15 (5%)	23 8
All	All	2488/2528 (98%)	2426 (98%)	62 (2%)	42 24

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	VAL
1	A	173	SER
1	A	275	VAL
1	A	276	GLU
1	B	2	ARG
1	B	129	VAL
1	B	139	PRO
1	B	173	SER
1	B	201	PRO
1	B	275	VAL
1	C	2	ARG
1	C	12	ARG
1	C	150	SER
1	C	275	VAL
1	D	2	ARG
1	D	54	ILE
1	D	119	LEU
1	D	275	VAL
1	D	289	ARG
1	D	309	LEU
1	D	357	SER
1	E	22	THR
1	E	129	VAL
1	E	201	PRO
1	E	254	ARG
1	E	275	VAL
1	E	307	PRO
1	F	33	ASP
1	F	119	LEU

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Mol	Chain	Res	Type
1	F	225	VAL
1	F	253	THR
1	F	275	VAL
1	F	308	ASP
1	F	383	LEU
1	G	54	ILE
1	G	117	THR
1	G	119	LEU
1	G	244	VAL
1	G	254	ARG
1	G	263	VAL
1	G	276	GLU
1	G	284	LEU
1	G	289	ARG
1	G	309	LEU
1	G	360	LEU
1	G	377	HIS
1	G	416	HIS
1	H	39	VAL
1	H	41	VAL
1	H	95	ILE
1	H	105	ARG
1	H	153	SER
1	H	168	SER
1	H	187	LYS
1	H	208	THR
1	H	227	LEU
1	H	312	THR
1	H	357	SER
1	H	393	VAL
1	H	394	VAL
1	H	406	VAL
1	H	412	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	HIS
1	B	306	GLN
1	B	310	HIS
1	B	412	GLN
1	B	413	HIS

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Mol	Chain	Res	Type
1	C	91	HIS
1	D	306	GLN
1	F	413	HIS
1	H	249	GLN
1	H	281	HIS
1	H	310	HIS
1	H	311	HIS
1	H	413	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides 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	423/433 (97%)	-0.51	0 100 100	14, 20, 31, 49	0
1	B	423/433 (97%)	-0.44	0 100 100	15, 21, 33, 45	0
1	C	423/433 (97%)	-0.44	1 (0%) 91 92	15, 22, 32, 52	0
1	D	423/433 (97%)	-0.36	0 100 100	16, 24, 34, 47	0
1	E	423/433 (97%)	-0.45	0 100 100	15, 22, 32, 47	0
1	F	423/433 (97%)	-0.41	0 100 100	14, 22, 33, 47	0
1	G	423/433 (97%)	0.06	1 (0%) 91 92	20, 29, 39, 70	0
1	H	423/433 (97%)	0.65	21 (4%) 34 38	23, 56, 93, 110	0
All	All	3384/3464 (97%)	-0.24	23 (0%) 84 86	14, 24, 64, 110	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	140	LEU	3.5
1	H	35	ALA	3.4
1	H	333	TRP	3.4
1	H	233	LEU	3.2
1	H	360	LEU	2.9
1	H	58	GLY	2.8
1	H	54	ILE	2.6
1	H	425	ILE	2.5
1	H	119	LEU	2.4
1	H	4	ALA	2.4
1	H	120	PRO	2.3
1	H	226	LEU	2.3
1	C	58	GLY	2.3
1	H	31	ALA	2.2
1	H	307	PRO	2.2
1	H	348	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	401	GLY	2.2
1	H	209	VAL	2.2
1	H	9	ALA	2.1
1	G	183	VAL	2.1
1	H	77	PHE	2.1
1	H	402	LEU	2.0
1	H	87	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.