Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 10:47 AM EDT

PDB ID	:	1P8S
Title	:	Structural and Functional Importance of First-Shell Metal Ligands in the Binuclear Manganese Cluster of Arginase I.
Authors	:	Cama, E.; Emig, F.A.; Ash, D.E.; Christianson, D.W.
Deposited on	:	2003-05-07
Resolution	:	3.20 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:

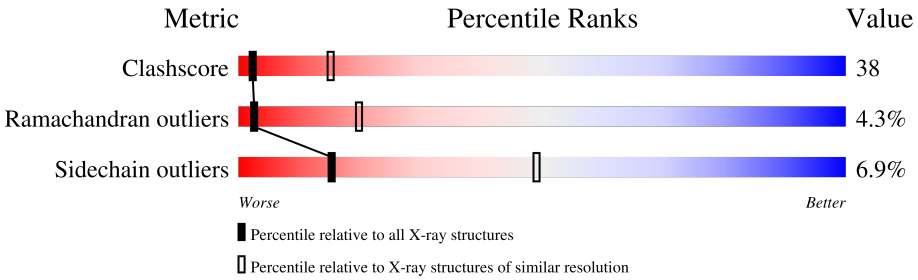
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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	314	50% 43% 7%
1	B	314	42% 50% 8%
1	C	314	46% 47% 6% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7221 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 Arginase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2394	1527	405	454	8			
1	B	314	Total	C	N	O	S	0	0	0
			2394	1527	405	454	8			
1	C	314	Total	C	N	O	S	0	0	0
			2394	1527	405	454	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	CYS	ASP	engineered mutation	UNP P07824
B	232	CYS	ASP	engineered mutation	UNP P07824
C	232	CYS	ASP	engineered mutation	UNP P07824

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	10	Total O 10 10	0	0

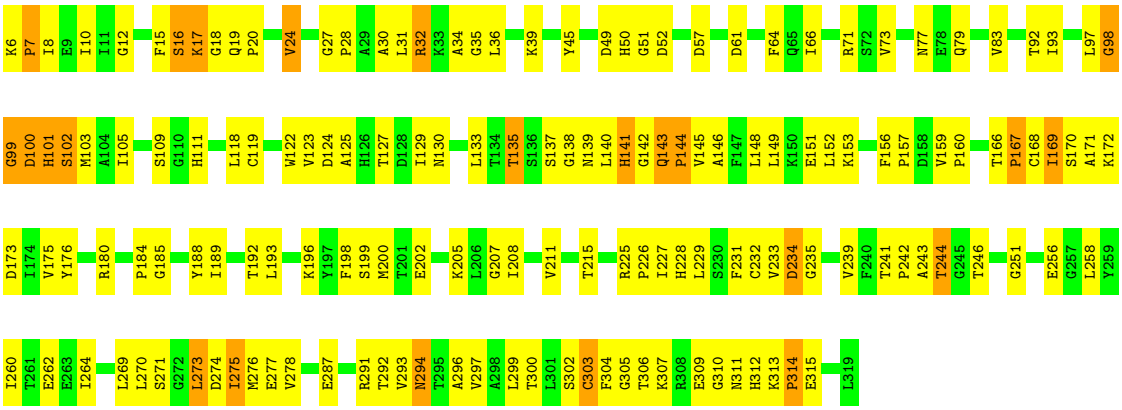
3 Residue-property plots (i)

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. 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.

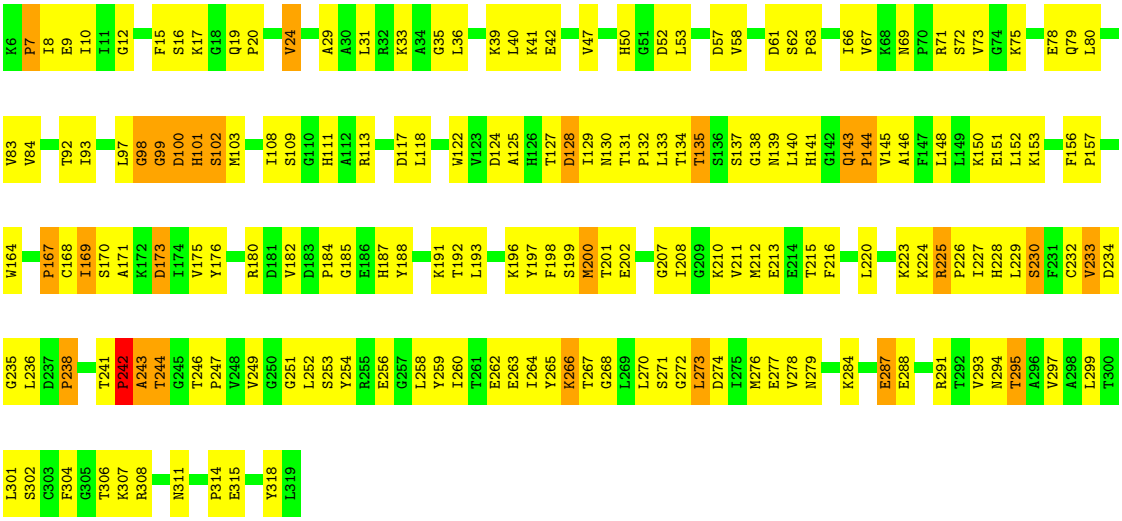
• Molecule 1: Arginase 1

Chain A:



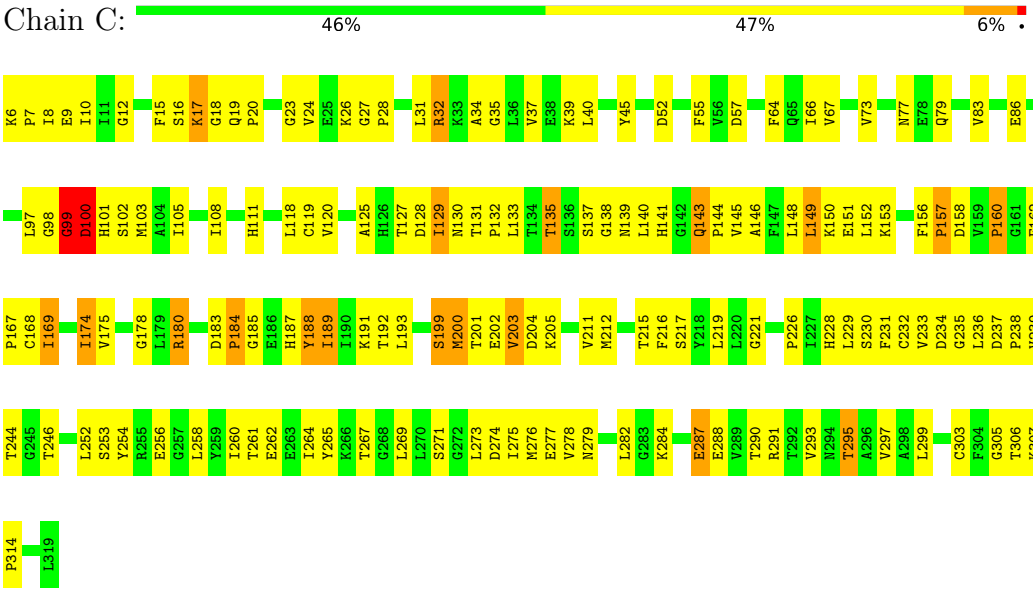
• Molecule 1: Arginase 1

Chain B:



• Molecule 1: Arginase 1

Chain C:


46%
47%
6%
K6 P7 I8 E9 I10 I11 G12 F15 S16 K17 G18 Q19 P20 G23 V24 E25 K26 G27 P28 L31 R32 K33 A34 G35 L36 V37 E38 K39 L40 Y45 D52 F55 V56 D57 F64 Q65 I66 V67 V73 N77 E78 Q79 V83 E86 N90 G91 T92 I93
L97 G98 G99 D100 H101 S102 M103 A104 I105 I108 H111 L118 C119 V120 A125 H126 T127 D128 I129 N130 T131 P132 L133 T134 T135 S136 S137 G138 N139 L140 H141 G142 Q143 P144 V145 A146 F147 L148 L149 K150 E151 L152 K153 F156 P157 D158 V159 P160 G161 F162 S163 W164 V165 T166
P167 C168 I169 I174 V175 G178 L179 R180 D183 P184 G185 E186 H187 Y188 I189 I190 K191 T192 L193 S199 M200 T201 E202 V203 D204 K205 V211 M212 T215 F216 S217 Y218 L219 L220 G221 P226 I227 H228 L229 S230 F231 C232 V233 D234 G235 L236 D237 P238 V239 F240 T241 P242 A243
T244 G245 T246 L252 S253 Y254 R255 E256 G257 L258 Y259 I260 T261 E262 E263 I264 Y265 K266 T267 G268 L269 L270 S271 G272 L273 D274 I275 M276 E277 V278 N279 L282 G283 K284 E287 E288 V289 T290 R291 T292 V293 N294 T295 A296 V297 A298 L299 C303 F304 G305 T306 K307 N311 H312 K313
P314 L319

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	90.94Å 90.94Å 105.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.77 – 3.20	Depositor
% Data completeness (in resolution range)	92.9 (29.77-3.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.286 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7221	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.49	0/2447	0.77	1/3322 (0.0%)
1	B	0.51	0/2447	0.80	2/3322 (0.1%)
1	C	0.53	0/2447	0.81	1/3322 (0.0%)
All	All	0.51	0/7341	0.79	4/9966 (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	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	GLY	N-CA-C	10.12	138.39	113.10
1	B	99	GLY	N-CA-C	8.88	135.29	113.10
1	C	99	GLY	N-CA-C	8.43	134.16	113.10
1	B	242	PRO	CA-N-CD	-5.05	104.43	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	GLY	Peptide
1	B	98	GLY	Peptide
1	C	98	GLY	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	2394	0	2421	186	0
1	B	2394	0	2421	194	0
1	C	2394	0	2421	192	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	11	0	0	0	0
3	B	12	0	0	0	0
3	C	10	0	0	5	0
All	All	7221	0	7263	556	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 38.

All (556) 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:227:ILE:HG13	1:A:270:LEU:HA	1.33	1.08
1:A:311:ASN:O	1:B:184:PRO:HA	1.53	1.05
1:B:238:PRO:O	1:B:242:PRO:HD3	1.56	1.05
1:C:211:VAL:O	1:C:215:THR:HG23	1.63	0.99
1:C:143:GLN:H	1:C:144:PRO:HD3	1.29	0.97
1:A:143:GLN:H	1:A:144:PRO:CD	1.77	0.96
1:A:12:GLY:HA3	1:A:52:ASP:OD1	1.67	0.94
1:B:16:SER:HB3	1:B:24:VAL:HG23	1.52	0.92
1:B:258:LEU:O	1:B:262:GLU:HG3	1.71	0.90
1:A:307:LYS:H	1:A:311:ASN:HD21	1.21	0.87
1:B:243:ALA:HB1	1:B:279:ASN:O	1.74	0.87
1:A:227:ILE:CG1	1:A:270:LEU:HA	2.03	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:GLY:HA3	1:B:52:ASP:OD1	1.74	0.85
1:A:153:LYS:HD2	1:A:167:PRO:HG2	1.57	0.85
1:B:102:SER:HA	1:B:144:PRO:HG3	1.58	0.85
1:B:103:MET:HB2	1:B:276:MET:CE	2.07	0.85
1:C:135:THR:HB	1:C:137:SER:O	1.77	0.84
1:C:32:ARG:HH11	1:C:32:ARG:HG3	1.43	0.84
1:B:143:GLN:H	1:B:144:PRO:HD3	1.40	0.83
1:C:256:GLU:O	1:C:260:ILE:HG13	1.76	0.83
1:A:100:ASP:HA	1:A:277:GLU:HG2	1.60	0.82
1:A:258:LEU:O	1:A:262:GLU:HG3	1.78	0.82
1:B:256:GLU:O	1:B:260:ILE:HG13	1.80	0.82
1:A:16:SER:HB3	1:A:24:VAL:HG23	1.60	0.81
1:A:233:VAL:HG13	1:A:241:THR:HB	1.59	0.81
1:A:143:GLN:H	1:A:144:PRO:HD3	1.44	0.80
1:C:103:MET:HB2	1:C:276:MET:CE	2.12	0.80
1:A:300:THR:HA	1:A:303:CYS:SG	2.22	0.80
1:B:100:ASP:HA	1:B:277:GLU:CD	2.02	0.80
1:B:173:ASP:HB3	1:B:225:ARG:HH22	1.45	0.80
1:A:102:SER:HA	1:A:144:PRO:HG3	1.64	0.79
1:B:93:ILE:HG23	1:B:271:SER:O	1.83	0.78
1:C:143:GLN:H	1:C:144:PRO:CD	1.97	0.78
1:C:100:ASP:HA	1:C:277:GLU:CD	2.04	0.78
1:B:71:ARG:O	1:B:75:LYS:HG3	1.84	0.78
1:C:148:LEU:HD22	1:C:168:CYS:SG	2.23	0.77
1:A:36:LEU:HD13	1:A:297:VAL:HG22	1.64	0.77
1:A:50:HIS:O	1:A:50:HIS:ND1	2.17	0.77
1:C:143:GLN:N	1:C:144:PRO:CD	2.46	0.77
1:A:103:MET:HB2	1:A:276:MET:CE	2.15	0.77
1:C:67:VAL:CG1	1:C:140:LEU:HD21	2.15	0.77
1:A:227:ILE:HG12	1:A:269:LEU:C	2.05	0.77
1:C:129:ILE:HG13	1:C:145:VAL:HB	1.67	0.77
1:A:229:LEU:HD22	1:A:264:ILE:CD1	2.16	0.76
1:B:118:LEU:HD12	1:B:118:LEU:C	2.06	0.76
1:A:8:ILE:HD13	1:A:93:ILE:HB	1.67	0.76
1:B:175:VAL:HG22	1:B:196:LYS:HB3	1.68	0.75
1:A:135:THR:HB	1:A:137:SER:O	1.86	0.75
1:C:143:GLN:N	1:C:144:PRO:HD3	2.01	0.75
1:C:291:ARG:O	1:C:295:THR:HG23	1.84	0.75
1:A:133:LEU:HD11	1:A:156:PHE:HA	1.68	0.75
1:A:119:CYS:SG	1:A:227:ILE:HG22	2.27	0.75
1:A:175:VAL:HG13	1:A:196:LYS:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLY:O	1:B:211:VAL:HG23	1.87	0.74
1:C:119:CYS:SG	1:C:219:LEU:HD13	2.27	0.74
1:C:32:ARG:HG3	1:C:32:ARG:NH1	1.99	0.74
1:C:16:SER:HB3	1:C:24:VAL:HG23	1.70	0.74
1:B:117:ASP:O	1:B:225:ARG:NH1	2.22	0.73
1:B:211:VAL:O	1:B:215:THR:HG23	1.89	0.73
1:B:227:ILE:HB	1:B:270:LEU:HA	1.71	0.73
1:C:203:VAL:HG12	1:C:203:VAL:O	1.87	0.73
1:A:275:ILE:O	1:A:275:ILE:CG2	2.36	0.73
1:B:314:PRO:O	1:B:315:GLU:HB2	1.88	0.73
1:C:288:GLU:HG2	1:C:291:ARG:NH2	2.04	0.73
1:C:19:GLN:HB2	1:C:20:PRO:HD2	1.72	0.72
1:C:130:ASN:O	1:C:146:ALA:HB2	1.90	0.72
1:C:307:LYS:H	1:C:311:ASN:HD21	1.38	0.72
1:B:124:ASP:OD2	1:B:125:ALA:N	2.21	0.72
1:B:66:ILE:HG22	1:B:138:GLY:HA2	1.72	0.72
1:B:232:CYS:O	1:B:235:GLY:N	2.20	0.72
1:A:227:ILE:HD12	1:A:264:ILE:CG2	2.20	0.72
1:B:103:MET:HB2	1:B:276:MET:HE3	1.71	0.72
1:A:103:MET:HB2	1:A:276:MET:HE3	1.71	0.71
1:B:143:GLN:H	1:B:144:PRO:CD	2.03	0.71
1:B:101:HIS:HD2	1:B:276:MET:HG3	1.55	0.71
1:A:19:GLN:HB2	1:A:20:PRO:HD2	1.71	0.71
1:B:173:ASP:CB	1:B:225:ARG:HH22	2.04	0.71
1:A:275:ILE:HD11	1:A:296:ALA:O	1.90	0.71
1:B:233:VAL:HG21	1:B:278:VAL:HG22	1.73	0.71
1:C:79:GLN:O	1:C:83:VAL:HG23	1.88	0.71
1:A:198:PHE:CD2	1:A:211:VAL:HG13	2.26	0.71
1:B:103:MET:HB2	1:B:276:MET:HE1	1.72	0.70
1:A:135:THR:HG21	1:A:143:GLN:HE21	1.56	0.70
1:C:15:PHE:CZ	1:C:17:LYS:HB2	2.26	0.70
1:C:129:ILE:CG1	1:C:145:VAL:HB	2.22	0.70
1:A:198:PHE:CE1	1:A:215:THR:HG22	2.27	0.70
1:A:135:THR:CG2	1:A:143:GLN:HE21	2.05	0.70
1:B:308:ARG:NH1	1:C:200:MET:HB3	2.06	0.70
1:B:232:CYS:SG	1:B:234:ASP:CG	2.70	0.69
1:B:236:LEU:HB3	1:B:252:LEU:O	1.92	0.69
1:A:229:LEU:HD22	1:A:264:ILE:HD12	1.74	0.69
1:B:232:CYS:SG	1:B:234:ASP:OD2	2.51	0.69
1:A:143:GLN:N	1:A:144:PRO:CD	2.51	0.69
1:B:295:THR:O	1:B:299:LEU:HG	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLY:HA3	1:C:52:ASP:OD1	1.92	0.68
1:A:227:ILE:HD12	1:A:264:ILE:HG23	1.73	0.68
1:B:233:VAL:HG13	1:B:241:THR:HB	1.74	0.68
1:C:103:MET:HB2	1:C:276:MET:HE3	1.74	0.68
1:C:8:ILE:HD13	1:C:93:ILE:HB	1.74	0.68
1:C:100:ASP:HA	1:C:277:GLU:OE1	1.93	0.68
1:C:129:ILE:HB	1:C:145:VAL:HB	1.75	0.68
1:A:180:ARG:NH2	1:A:235:GLY:O	2.27	0.68
1:B:175:VAL:HA	1:B:196:LYS:O	1.93	0.68
1:C:287:GLU:HG3	1:C:288:GLU:N	2.08	0.68
1:A:256:GLU:O	1:A:260:ILE:HG13	1.94	0.68
1:C:153:LYS:HD2	1:C:167:PRO:HG2	1.76	0.68
1:A:242:PRO:HD2	1:A:292:THR:OG1	1.94	0.67
1:B:19:GLN:HB2	1:B:20:PRO:HD2	1.77	0.67
1:A:127:THR:OG1	1:A:129:ILE:HG22	1.94	0.67
1:A:260:ILE:O	1:A:264:ILE:HG13	1.94	0.67
1:A:118:LEU:C	1:A:118:LEU:HD12	2.15	0.67
1:A:227:ILE:HG12	1:A:269:LEU:O	1.94	0.67
1:A:105:ILE:HD11	1:A:144:PRO:HA	1.76	0.67
1:C:200:MET:HE1	1:C:252:LEU:HD21	1.76	0.67
1:B:16:SER:CB	1:B:24:VAL:HG23	2.24	0.66
1:C:67:VAL:HG13	1:C:140:LEU:HD21	1.77	0.66
1:C:230:SER:HA	1:C:274:ASP:HB2	1.78	0.66
1:A:111:HIS:CE1	1:A:271:SER:HB3	2.31	0.66
1:B:108:ILE:HG12	1:B:228:HIS:NE2	2.11	0.66
1:B:318:TYR:HB2	1:C:188:TYR:CD2	2.31	0.66
1:B:227:ILE:O	1:B:270:LEU:HD12	1.96	0.66
1:C:103:MET:HB2	1:C:276:MET:HE1	1.76	0.66
1:B:180:ARG:NH2	1:B:235:GLY:O	2.29	0.66
1:B:288:GLU:HG2	1:B:291:ARG:NH2	2.09	0.66
1:C:129:ILE:HG12	1:C:129:ILE:O	1.95	0.65
1:A:233:VAL:HG13	1:A:241:THR:CB	2.27	0.65
1:A:20:PRO:HD3	1:A:139:ASN:OD1	1.97	0.64
1:A:275:ILE:CD1	1:A:296:ALA:O	2.45	0.64
1:B:127:THR:OG1	1:B:129:ILE:HG22	1.97	0.64
1:C:200:MET:CE	1:C:252:LEU:HD21	2.27	0.64
1:A:139:ASN:HB3	1:A:141:HIS:CD2	2.32	0.64
1:B:111:HIS:CE1	1:B:271:SER:HB3	2.33	0.64
1:A:275:ILE:O	1:A:275:ILE:HG22	1.98	0.64
1:C:67:VAL:HG11	1:C:140:LEU:HD21	1.79	0.64
1:B:238:PRO:O	1:B:242:PRO:CD	2.41	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:CZ	1:A:251:GLY:HA2	2.27	0.64
1:C:200:MET:HE2	1:C:252:LEU:HD23	1.79	0.64
1:B:101:HIS:CD2	1:B:276:MET:HG3	2.32	0.63
1:B:230:SER:HA	1:B:274:ASP:HB2	1.78	0.63
1:C:233:VAL:HG21	1:C:278:VAL:HG22	1.80	0.63
1:C:129:ILE:CB	1:C:145:VAL:HB	2.29	0.63
1:B:143:GLN:N	1:B:144:PRO:CD	2.60	0.63
1:B:187:HIS:O	1:B:191:LYS:HG2	1.99	0.63
1:C:100:ASP:OD1	1:C:102:SER:N	2.31	0.63
1:A:233:VAL:CG1	1:A:241:THR:HB	2.28	0.63
1:C:7:PRO:HB2	1:C:92:THR:HG22	1.80	0.63
1:C:135:THR:HG21	1:C:143:GLN:NE2	2.13	0.63
1:A:211:VAL:O	1:A:215:THR:HG23	1.99	0.63
1:B:223:LYS:CE	1:B:225:ARG:HD2	2.29	0.63
1:B:233:VAL:HG21	1:B:278:VAL:CG2	2.29	0.63
1:C:200:MET:HE2	1:C:252:LEU:CD2	2.28	0.62
1:B:66:ILE:HG22	1:B:138:GLY:CA	2.28	0.62
1:C:135:THR:HG21	1:C:143:GLN:HE21	1.63	0.62
1:C:129:ILE:HD12	1:C:145:VAL:HG11	1.81	0.62
1:A:139:ASN:HB3	1:A:141:HIS:HD2	1.64	0.62
1:A:8:ILE:HD11	1:A:93:ILE:HD12	1.81	0.62
1:C:102:SER:HA	1:C:144:PRO:HG3	1.80	0.62
1:A:123:VAL:HG11	1:A:231:PHE:CE2	2.35	0.62
1:C:19:GLN:HB3	1:C:141:HIS:CD2	2.34	0.62
1:C:233:VAL:CG1	1:C:241:THR:HB	2.30	0.62
1:B:254:TYR:CE1	1:B:295:THR:HB	2.35	0.61
1:C:83:VAL:O	1:C:86:GLU:HB3	1.98	0.61
1:B:150:LYS:HG3	1:B:169:ILE:O	2.00	0.61
1:C:265:TYR:HD1	3:C:802:HOH:O	1.84	0.61
1:B:111:HIS:HE1	1:B:271:SER:HB3	1.66	0.61
1:A:305:GLY:O	1:A:306:THR:C	2.38	0.61
1:C:180:ARG:NH2	1:C:235:GLY:O	2.33	0.61
1:B:79:GLN:O	1:B:83:VAL:HG23	2.01	0.61
1:C:131:THR:C	1:C:133:LEU:H	2.03	0.61
1:B:273:LEU:HD22	1:B:274:ASP:N	2.17	0.60
1:C:234:ASP:HB3	1:C:244:THR:HG21	1.82	0.60
1:C:148:LEU:O	1:C:167:PRO:HA	2.01	0.60
1:C:187:HIS:O	1:C:191:LYS:HG2	2.00	0.60
1:A:275:ILE:HD11	1:A:300:THR:OG1	2.01	0.60
1:B:130:ASN:HB3	1:B:135:THR:HG23	1.82	0.60
1:A:31:LEU:HD13	1:A:97:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:MET:HB2	1:A:276:MET:HE1	1.84	0.60
1:C:233:VAL:HG13	1:C:241:THR:HB	1.83	0.60
1:A:100:ASP:HA	1:A:277:GLU:CG	2.30	0.60
1:B:199:SER:O	1:B:202:GLU:N	2.32	0.60
1:C:232:CYS:SG	1:C:234:ASP:CG	2.81	0.60
1:A:228:HIS:HE1	1:A:274:ASP:OD2	1.85	0.59
1:C:288:GLU:HG2	1:C:291:ARG:HH21	1.66	0.59
1:A:227:ILE:CG1	1:A:270:LEU:CA	2.79	0.59
1:B:101:HIS:O	1:B:103:MET:N	2.35	0.59
1:C:118:LEU:C	1:C:118:LEU:HD12	2.23	0.59
1:A:135:THR:OG1	1:A:143:GLN:NE2	2.33	0.59
1:C:127:THR:CB	1:C:129:ILE:HG22	2.33	0.59
1:B:233:VAL:C	1:B:235:GLY:H	2.04	0.59
1:B:307:LYS:H	1:B:311:ASN:HD21	1.49	0.59
1:C:217:SER:O	1:C:221:GLY:HA3	2.03	0.58
1:C:297:VAL:CG1	3:C:804:HOH:O	2.51	0.58
1:C:7:PRO:CB	1:C:92:THR:HG22	2.34	0.58
1:C:226:PRO:HB3	1:C:271:SER:HB2	1.85	0.58
1:A:198:PHE:HA	1:A:202:GLU:HG2	1.85	0.58
1:A:149:LEU:HD12	1:A:152:LEU:HD13	1.86	0.58
1:A:185:GLY:O	1:A:188:TYR:HB3	2.04	0.58
1:C:130:ASN:O	1:C:146:ALA:CB	2.51	0.58
1:B:20:PRO:HD3	1:B:139:ASN:OD1	2.04	0.58
1:B:146:ALA:HA	1:B:152:LEU:CD2	2.34	0.57
1:B:173:ASP:HB3	1:B:225:ARG:NH2	2.18	0.57
1:C:139:ASN:HB3	1:C:141:HIS:CD2	2.39	0.57
1:C:212:MET:HE2	1:C:260:ILE:HA	1.86	0.57
1:C:261:THR:HG22	1:C:303:CYS:SG	2.44	0.57
1:A:229:LEU:HD22	1:A:264:ILE:HD13	1.86	0.57
1:C:139:ASN:HB3	1:C:141:HIS:HD2	1.68	0.57
1:A:16:SER:CB	1:A:24:VAL:HG23	2.34	0.57
1:B:263:GLU:OE2	1:B:266:LYS:HD3	2.04	0.57
1:A:135:THR:CG2	1:A:143:GLN:NE2	2.68	0.57
1:B:223:LYS:HE3	1:B:225:ARG:HD2	1.86	0.57
1:B:308:ARG:HH11	1:C:200:MET:HB3	1.67	0.56
1:B:129:ILE:HG23	1:B:129:ILE:O	2.05	0.56
1:B:262:GLU:OE1	1:C:201:THR:HG22	2.05	0.56
1:A:7:PRO:HB2	1:A:92:THR:HA	1.86	0.56
1:A:312:HIS:HB3	1:B:184:PRO:O	2.05	0.56
1:C:125:ALA:HA	1:C:178:GLY:O	2.06	0.56
1:B:131:THR:H	1:B:134:THR:HG1	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ILE:HG13	1:A:145:VAL:HB	1.87	0.56
1:B:100:ASP:HA	1:B:277:GLU:OE1	2.06	0.56
1:B:156:PHE:HB2	1:B:157:PRO:HD2	1.86	0.56
1:A:35:GLY:O	1:A:39:LYS:HG3	2.06	0.56
1:A:140:LEU:O	1:A:144:PRO:HD3	2.06	0.55
1:A:310:GLY:HA3	1:B:182:VAL:HB	1.88	0.55
1:A:184:PRO:HA	1:C:311:ASN:O	2.06	0.55
1:A:77:ASN:OD1	1:A:103:MET:HA	2.05	0.55
1:A:229:LEU:CD2	1:A:264:ILE:HD12	2.34	0.55
1:A:143:GLN:H	1:A:144:PRO:HD2	1.65	0.55
1:B:131:THR:O	1:B:133:LEU:N	2.39	0.55
1:B:185:GLY:O	1:B:188:TYR:HB3	2.06	0.55
1:B:293:VAL:HG12	1:B:294:ASN:N	2.22	0.55
1:B:284:LYS:HB2	1:B:288:GLU:OE1	2.07	0.55
1:A:10:ILE:HD12	1:A:10:ILE:N	2.21	0.55
1:B:131:THR:C	1:B:133:LEU:H	2.10	0.55
1:A:8:ILE:CD1	1:A:93:ILE:HD12	2.36	0.55
1:A:36:LEU:HD21	1:A:97:LEU:HD21	1.89	0.55
1:B:192:THR:HG22	1:B:193:LEU:HD12	1.88	0.55
1:C:200:MET:CE	1:C:252:LEU:CD2	2.85	0.55
1:A:199:SER:O	1:A:202:GLU:HB2	2.07	0.54
1:B:151:GLU:OE1	1:B:151:GLU:N	2.40	0.54
1:A:123:VAL:HG11	1:A:231:PHE:CZ	2.43	0.54
1:C:32:ARG:HH11	1:C:32:ARG:CG	2.15	0.54
1:A:314:PRO:O	1:A:315:GLU:HB2	2.07	0.54
1:B:254:TYR:HE1	1:B:295:THR:HB	1.73	0.54
1:C:200:MET:CE	1:C:200:MET:HA	2.38	0.54
1:B:39:LYS:HD3	1:B:301:LEU:HD11	1.90	0.54
1:C:260:ILE:O	1:C:264:ILE:HG13	2.08	0.54
1:C:297:VAL:HG12	3:C:804:HOH:O	2.07	0.54
1:A:15:PHE:CZ	1:A:73:VAL:HA	2.42	0.53
1:A:124:ASP:OD1	1:A:232:CYS:HB2	2.07	0.53
1:A:299:LEU:O	1:A:302:SER:HB3	2.08	0.53
1:B:39:LYS:O	1:B:42:GLU:HB2	2.09	0.53
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.44	0.53
1:B:137:SER:HB2	1:B:139:ASN:ND2	2.23	0.53
1:C:127:THR:OG1	1:C:129:ILE:HG22	2.08	0.53
1:C:242:PRO:CG	1:C:288:GLU:HB3	2.38	0.53
1:A:64:PHE:CD2	1:A:159:VAL:HG22	2.43	0.53
1:B:8:ILE:HD13	1:B:93:ILE:HB	1.91	0.53
1:B:131:THR:C	1:B:133:LEU:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.44	0.53
1:A:244:THR:HG23	1:A:277:GLU:O	2.08	0.53
1:A:192:THR:HG22	1:A:193:LEU:HD12	1.90	0.53
1:B:124:ASP:CG	1:B:232:CYS:HB3	2.29	0.53
1:A:105:ILE:O	1:A:109:SER:HB2	2.09	0.53
1:C:233:VAL:HG21	1:C:278:VAL:CG2	2.38	0.53
1:C:174:ILE:HG12	1:C:175:VAL:N	2.24	0.52
1:A:79:GLN:O	1:A:83:VAL:HG23	2.09	0.52
1:B:135:THR:HB	1:B:137:SER:O	2.09	0.52
1:C:120:VAL:HG22	1:C:228:HIS:HB3	1.92	0.52
1:A:6:LYS:O	1:A:45:TYR:HD2	1.93	0.52
1:A:31:LEU:CD1	1:A:97:LEU:HD22	2.39	0.52
1:B:223:LYS:HE2	1:B:225:ARG:HD2	1.91	0.52
1:A:258:LEU:HD23	1:A:299:LEU:HD23	1.91	0.52
1:B:137:SER:C	1:B:139:ASN:H	2.13	0.52
1:C:105:ILE:HD11	1:C:144:PRO:HA	1.89	0.52
1:C:307:LYS:H	1:C:311:ASN:ND2	2.05	0.52
1:A:98:GLY:HA3	1:A:276:MET:SD	2.49	0.52
1:A:133:LEU:CD1	1:A:156:PHE:HA	2.39	0.52
1:B:12:GLY:CA	1:B:52:ASP:OD1	2.54	0.52
1:B:229:LEU:HD22	1:B:264:ILE:HD12	1.92	0.52
1:C:133:LEU:HD11	1:C:156:PHE:HA	1.91	0.52
1:B:265:TYR:O	1:B:268:GLY:N	2.40	0.51
1:B:233:VAL:C	1:B:235:GLY:N	2.63	0.51
1:A:101:HIS:O	1:A:103:MET:N	2.43	0.51
1:C:199:SER:O	1:C:200:MET:C	2.45	0.51
1:C:258:LEU:HD23	1:C:299:LEU:HD23	1.93	0.51
1:B:129:ILE:HG13	1:B:145:VAL:HB	1.93	0.51
1:C:232:CYS:HG	1:C:234:ASP:CG	2.14	0.51
1:C:131:THR:O	1:C:133:LEU:N	2.44	0.51
1:A:130:ASN:O	1:A:146:ALA:HB2	2.11	0.51
1:A:234:ASP:HB3	1:A:244:THR:HG21	1.93	0.51
1:C:240:PHE:CD1	1:C:254:TYR:HB2	2.46	0.51
1:A:100:ASP:OD1	1:A:102:SER:N	2.43	0.51
1:A:311:ASN:O	1:B:184:PRO:CA	2.44	0.51
1:C:233:VAL:HG13	1:C:241:THR:CB	2.41	0.50
1:A:16:SER:O	1:A:18:GLY:N	2.44	0.50
1:B:198:PHE:CD2	1:B:211:VAL:HG13	2.45	0.50
1:C:77:ASN:OD1	1:C:103:MET:HA	2.11	0.50
1:C:233:VAL:HG13	1:C:241:THR:CG2	2.42	0.50
1:B:199:SER:O	1:B:200:MET:C	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD23	1:B:143:GLN:NE2	2.26	0.50
1:A:124:ASP:OD1	1:A:232:CYS:CB	2.60	0.50
1:B:212:MET:O	1:B:216:PHE:CD2	2.64	0.50
1:B:210:LYS:O	1:B:213:GLU:HB3	2.12	0.50
1:A:156:PHE:HB2	1:A:157:PRO:HD2	1.94	0.50
1:B:15:PHE:CZ	1:B:73:VAL:HA	2.47	0.50
1:C:185:GLY:O	1:C:188:TYR:HB3	2.11	0.50
1:B:148:LEU:HB3	1:B:169:ILE:CD1	2.42	0.50
1:C:212:MET:O	1:C:216:PHE:CD2	2.65	0.50
1:C:239:VAL:HG12	1:C:239:VAL:O	2.12	0.50
1:C:203:VAL:O	1:C:203:VAL:CG1	2.59	0.49
1:A:8:ILE:CD1	1:A:93:ILE:HB	2.39	0.49
1:A:307:LYS:N	1:A:311:ASN:HD21	1.99	0.49
1:B:131:THR:N	1:B:134:THR:OG1	2.35	0.49
1:C:31:LEU:HD13	1:C:97:LEU:HD22	1.94	0.49
1:C:237:ASP:CG	1:C:238:PRO:HD2	2.33	0.49
1:C:258:LEU:HA	1:C:261:THR:OG1	2.12	0.49
1:A:153:LYS:HD2	1:A:167:PRO:CG	2.37	0.49
1:B:226:PRO:HB3	1:B:271:SER:HB2	1.94	0.49
1:C:32:ARG:HD3	1:C:37:VAL:HG21	1.95	0.49
1:C:131:THR:C	1:C:133:LEU:N	2.66	0.49
1:A:19:GLN:HB3	1:A:141:HIS:CD2	2.48	0.49
1:B:66:ILE:O	1:B:138:GLY:HA3	2.12	0.49
1:B:67:VAL:HG13	1:B:140:LEU:HD21	1.95	0.49
1:A:207:GLY:O	1:A:211:VAL:HG23	2.13	0.49
1:B:7:PRO:CB	1:B:92:THR:HG22	2.42	0.49
1:B:19:GLN:CB	1:B:20:PRO:HD2	2.41	0.49
1:A:124:ASP:OD2	1:A:125:ALA:N	2.45	0.49
1:A:135:THR:HG21	1:A:143:GLN:NE2	2.24	0.48
1:A:229:LEU:O	1:A:273:LEU:HD23	2.13	0.48
1:C:200:MET:O	1:C:201:THR:C	2.50	0.48
1:C:229:LEU:HD22	1:C:264:ILE:HD12	1.94	0.48
1:A:293:VAL:HG12	1:A:294:ASN:N	2.29	0.48
1:C:200:MET:HA	1:C:200:MET:HE3	1.94	0.48
1:A:18:GLY:HA3	1:A:100:ASP:CG	2.34	0.48
1:B:10:ILE:N	1:B:10:ILE:HD12	2.28	0.48
1:B:146:ALA:HA	1:B:152:LEU:HD23	1.94	0.48
1:C:16:SER:O	1:C:18:GLY:N	2.47	0.48
1:C:73:VAL:HG12	1:C:162:PHE:HZ	1.78	0.48
1:B:197:TYR:C	1:B:198:PHE:CD1	2.87	0.48
1:B:168:CYS:SG	1:B:169:ILE:HG23	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:THR:O	1:B:247:PRO:HD3	2.14	0.48
1:B:180:ARG:NH2	1:B:251:GLY:CA	2.77	0.48
1:B:199:SER:O	1:B:201:THR:N	2.46	0.48
1:C:232:CYS:SG	1:C:234:ASP:OD2	2.72	0.48
1:C:149:LEU:HD12	1:C:152:LEU:HD13	1.95	0.47
1:C:16:SER:C	1:C:18:GLY:H	2.15	0.47
1:C:192:THR:HG22	1:C:193:LEU:HD12	1.95	0.47
1:B:143:GLN:O	1:B:144:PRO:C	2.53	0.47
1:A:16:SER:C	1:A:18:GLY:H	2.16	0.47
1:A:275:ILE:CD1	1:A:300:THR:OG1	2.62	0.47
1:B:229:LEU:HD22	1:B:264:ILE:CD1	2.44	0.47
1:A:36:LEU:CD2	1:A:97:LEU:HD21	2.45	0.47
1:A:173:ASP:CB	1:A:225:ARG:HH22	2.26	0.47
1:B:180:ARG:NH2	1:B:251:GLY:HA2	2.30	0.47
1:B:198:PHE:CE1	1:B:215:THR:HG22	2.50	0.47
1:C:86:GLU:O	1:C:86:GLU:HG3	2.12	0.47
1:C:188:TYR:O	1:C:189:ILE:C	2.53	0.47
1:A:27:GLY:O	1:A:30:ALA:HB3	2.14	0.47
1:A:64:PHE:CE2	1:A:159:VAL:HG22	2.49	0.47
1:B:7:PRO:HB2	1:B:92:THR:HG22	1.95	0.47
1:B:232:CYS:SG	1:B:234:ASP:OD1	2.72	0.47
1:A:234:ASP:C	1:A:234:ASP:OD1	2.52	0.47
1:B:143:GLN:O	1:B:145:VAL:N	2.48	0.47
1:B:308:ARG:NH2	1:C:204:ASP:OD2	2.44	0.47
1:A:205:LYS:O	1:A:205:LYS:HG2	2.15	0.47
1:B:53:LEU:HD22	1:B:83:VAL:HG21	1.97	0.47
1:C:148:LEU:HA	1:C:148:LEU:HD23	1.59	0.47
1:C:237:ASP:CG	1:C:238:PRO:CD	2.83	0.47
1:A:180:ARG:HB3	1:A:200:MET:HG2	1.97	0.46
1:A:307:LYS:H	1:A:311:ASN:ND2	2.00	0.46
1:B:287:GLU:HG3	1:B:288:GLU:N	2.31	0.46
1:C:7:PRO:HB2	1:C:92:THR:CB	2.45	0.46
1:A:32:ARG:NE	1:A:49:ASP:OD2	2.34	0.46
1:C:111:HIS:CE1	1:C:271:SER:HB3	2.51	0.46
1:A:300:THR:C	1:A:302:SER:H	2.17	0.46
1:B:122:TRP:HB3	1:B:176:TYR:CD1	2.50	0.46
1:C:201:THR:OG1	1:C:202:GLU:N	2.49	0.46
1:C:212:MET:CE	1:C:260:ILE:HG23	2.45	0.46
1:C:258:LEU:O	1:C:262:GLU:N	2.47	0.46
1:A:15:PHE:CD2	1:A:103:MET:SD	3.08	0.46
1:A:61:ASP:OD1	1:A:71:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:HD22	1:A:274:ASP:N	2.29	0.46
1:C:7:PRO:HB2	1:C:92:THR:CG2	2.45	0.46
1:C:8:ILE:CD1	1:C:93:ILE:HB	2.42	0.46
1:B:124:ASP:OD1	1:B:232:CYS:HB2	2.16	0.46
1:C:243:ALA:HB1	1:C:279:ASN:O	2.16	0.46
1:B:98:GLY:HA3	1:B:276:MET:SD	2.56	0.46
1:C:108:ILE:HG22	1:C:108:ILE:O	2.16	0.46
1:C:233:VAL:HG13	1:C:241:THR:HG21	1.98	0.46
1:B:124:ASP:CG	1:B:232:CYS:CB	2.84	0.46
1:B:58:VAL:HG21	1:B:75:LYS:HE3	1.98	0.45
1:C:108:ILE:HG12	1:C:228:HIS:CD2	2.51	0.45
1:C:287:GLU:O	1:C:291:ARG:N	2.40	0.45
1:A:101:HIS:C	1:A:103:MET:N	2.69	0.45
1:C:103:MET:CB	1:C:276:MET:HE1	2.45	0.45
1:A:16:SER:C	1:A:18:GLY:N	2.69	0.45
1:B:101:HIS:C	1:B:103:MET:N	2.68	0.45
1:B:108:ILE:HG12	1:B:228:HIS:CD2	2.51	0.45
1:B:109:SER:O	1:B:113:ARG:HG3	2.16	0.45
1:C:16:SER:C	1:C:18:GLY:N	2.70	0.45
1:C:67:VAL:HG13	1:C:140:LEU:CD2	2.45	0.45
1:C:265:TYR:CD1	3:C:802:HOH:O	2.56	0.45
1:B:41:LYS:HG2	1:B:47:VAL:HB	1.97	0.45
1:C:129:ILE:HD12	1:C:145:VAL:CG1	2.45	0.45
1:B:139:ASN:O	1:B:143:GLN:NE2	2.42	0.45
1:B:200:MET:CE	1:B:252:LEU:HD23	2.46	0.45
1:B:291:ARG:O	1:B:295:THR:HG23	2.17	0.45
1:C:133:LEU:HD21	1:C:157:PRO:CD	2.47	0.45
1:C:313:LYS:HE3	1:C:313:LYS:HB2	1.78	0.45
1:A:100:ASP:OD1	1:A:102:SER:CB	2.65	0.45
1:A:111:HIS:HE1	1:A:271:SER:HB3	1.77	0.45
1:B:122:TRP:HB3	1:B:176:TYR:HD1	1.81	0.45
1:B:216:PHE:O	1:B:220:LEU:N	2.46	0.45
1:A:142:GLY:O	1:A:143:GLN:HG2	2.17	0.45
1:A:300:THR:C	1:A:302:SER:N	2.70	0.45
1:B:35:GLY:O	1:B:39:LYS:HG3	2.17	0.45
1:B:152:LEU:CD1	1:B:193:LEU:HD21	2.46	0.45
1:C:137:SER:HB2	1:C:139:ASN:ND2	2.31	0.45
1:A:32:ARG:NH1	1:A:32:ARG:HG3	2.32	0.45
1:B:78:GLU:HB2	1:B:164:TRP:NE1	2.31	0.45
1:C:168:CYS:SG	1:C:169:ILE:HG23	2.57	0.45
1:A:100:ASP:HB2	1:A:277:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD23	1:A:304:PHE:CE1	2.52	0.45
1:B:9:GLU:OE2	1:B:50:HIS:HD2	1.99	0.44
1:C:34:ALA:HB2	1:C:293:VAL:HG11	1.99	0.44
1:C:275:ILE:HG22	1:C:275:ILE:O	2.17	0.44
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.85	0.44
1:B:101:HIS:C	1:B:103:MET:H	2.20	0.44
1:B:130:ASN:CB	1:B:135:THR:HG23	2.47	0.44
1:A:100:ASP:CA	1:A:277:GLU:HG2	2.41	0.44
1:B:129:ILE:HD12	1:B:145:VAL:HG11	1.99	0.44
1:B:263:GLU:O	1:B:267:THR:HG23	2.17	0.44
1:A:28:PRO:C	1:A:30:ALA:H	2.21	0.44
1:A:273:LEU:HD11	1:A:303:CYS:SG	2.58	0.44
1:C:10:ILE:HD12	1:C:10:ILE:N	2.33	0.44
1:C:64:PHE:CZ	1:C:158:ASP:O	2.71	0.44
1:C:127:THR:HB	1:C:129:ILE:CG2	2.47	0.44
1:A:97:LEU:HA	1:A:275:ILE:HG22	2.00	0.44
1:A:101:HIS:C	1:A:103:MET:H	2.22	0.44
1:A:105:ILE:O	1:A:109:SER:CB	2.65	0.44
1:B:234:ASP:OD1	1:B:234:ASP:C	2.56	0.44
1:A:7:PRO:CB	1:A:92:THR:HG22	2.48	0.44
1:B:53:LEU:CD2	1:B:83:VAL:HG21	2.48	0.44
1:B:233:VAL:HG12	1:B:244:THR:CG2	2.48	0.44
1:A:27:GLY:O	1:A:30:ALA:N	2.45	0.43
1:A:275:ILE:O	1:A:275:ILE:HG23	2.15	0.43
1:A:111:HIS:ND1	1:A:118:LEU:HD22	2.33	0.43
1:A:122:TRP:HB3	1:A:176:TYR:CD1	2.54	0.43
1:B:102:SER:HB3	1:B:141:HIS:HA	1.99	0.43
1:C:55:PHE:CZ	1:C:103:MET:CE	3.02	0.43
1:C:73:VAL:HG12	1:C:162:PHE:CZ	2.52	0.43
1:C:111:HIS:ND1	1:C:228:HIS:ND1	2.62	0.43
1:C:287:GLU:O	1:C:290:THR:N	2.52	0.43
1:A:239:VAL:O	1:A:239:VAL:HG12	2.18	0.43
1:C:23:GLY:O	1:C:26:LYS:HB2	2.17	0.43
1:A:229:LEU:CD2	1:A:264:ILE:CD1	2.92	0.43
1:B:131:THR:O	1:B:134:THR:N	2.43	0.43
1:B:262:GLU:O	1:B:265:TYR:HB3	2.18	0.43
1:C:284:LYS:HB2	1:C:288:GLU:OE1	2.17	0.43
1:C:267:THR:OG1	1:C:269:LEU:HB2	2.19	0.43
1:A:152:LEU:CD1	1:A:193:LEU:HD21	2.49	0.43
1:C:24:VAL:HB	1:C:99:GLY:HA2	2.00	0.43
1:C:151:GLU:OE1	1:C:151:GLU:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:HB2	1:A:293:VAL:HG11	2.01	0.43
1:A:118:LEU:C	1:A:118:LEU:CD1	2.87	0.43
1:A:143:GLN:O	1:A:146:ALA:N	2.48	0.43
1:A:262:GLU:OE1	1:B:201:THR:CG2	2.67	0.43
1:B:148:LEU:O	1:B:167:PRO:HA	2.19	0.43
1:B:302:SER:C	1:B:304:PHE:N	2.72	0.43
1:B:150:LYS:HD2	1:B:170:SER:HB3	2.01	0.42
1:A:143:GLN:N	1:A:144:PRO:HD2	2.29	0.42
1:A:151:GLU:OE1	1:A:151:GLU:N	2.47	0.42
1:B:58:VAL:HG23	1:B:72:SER:HA	1.99	0.42
1:B:61:ASP:OD2	1:B:69:ASN:HA	2.19	0.42
1:B:124:ASP:OD1	1:B:232:CYS:CB	2.67	0.42
1:B:127:THR:O	1:B:128:ASP:C	2.58	0.42
1:B:241:THR:N	1:B:242:PRO:CD	2.81	0.42
1:C:32:ARG:HD3	1:C:37:VAL:CG2	2.49	0.42
1:A:66:ILE:HG22	1:A:138:GLY:HA2	2.01	0.42
1:A:312:HIS:HA	1:B:184:PRO:HB3	2.01	0.42
1:B:31:LEU:HD13	1:B:97:LEU:HD22	2.00	0.42
1:B:153:LYS:HD2	1:B:167:PRO:HG2	2.00	0.42
1:B:233:VAL:HG12	1:B:244:THR:HG21	2.01	0.42
1:B:233:VAL:O	1:B:235:GLY:N	2.53	0.42
1:A:313:LYS:HE3	1:A:313:LYS:HB2	1.84	0.42
1:B:259:TYR:CE1	1:C:205:LYS:HB2	2.54	0.42
1:C:6:LYS:O	1:C:45:TYR:HD2	2.03	0.42
1:A:148:LEU:O	1:A:167:PRO:HA	2.20	0.42
1:B:40:LEU:CD2	1:B:301:LEU:HD23	2.50	0.42
1:C:27:GLY:O	1:C:28:PRO:C	2.57	0.42
1:C:31:LEU:CD1	1:C:97:LEU:HD22	2.50	0.42
1:C:149:LEU:HD23	1:C:149:LEU:HA	1.80	0.42
1:B:262:GLU:OE1	1:C:201:THR:CG2	2.67	0.42
1:B:306:THR:HA	1:B:311:ASN:HD21	1.84	0.42
1:A:50:HIS:O	1:A:50:HIS:CG	2.72	0.42
1:B:273:LEU:CD2	1:B:274:ASP:N	2.83	0.42
1:B:311:ASN:O	1:C:184:PRO:HA	2.20	0.42
1:C:19:GLN:CB	1:C:20:PRO:HD2	2.45	0.42
1:C:128:ASP:O	1:C:144:PRO:HD2	2.20	0.42
1:A:208:ILE:HD12	1:A:208:ILE:HA	1.88	0.41
1:B:307:LYS:N	1:B:311:ASN:HD21	2.18	0.41
1:A:309:GLU:O	1:B:182:VAL:HG21	2.20	0.41
1:C:232:CYS:O	1:C:235:GLY:N	2.45	0.41
1:A:19:GLN:HB2	1:A:20:PRO:CD	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ALA:O	1:B:33:LYS:HB2	2.19	0.41
1:B:139:ASN:HB3	1:B:141:HIS:CD2	2.55	0.41
1:A:143:GLN:O	1:A:144:PRO:C	2.59	0.41
1:B:62:SER:HA	1:B:63:PRO:HD3	1.87	0.41
1:B:175:VAL:HG13	1:B:196:LYS:O	2.20	0.41
1:B:258:LEU:HD23	1:B:258:LEU:HA	1.85	0.41
1:C:164:TRP:CZ2	1:C:165:VAL:HG22	2.55	0.41
1:C:279:ASN:ND2	1:C:282:LEU:HD12	2.35	0.41
1:A:100:ASP:HA	1:A:277:GLU:CD	2.41	0.41
1:A:227:ILE:HG12	1:A:270:LEU:N	2.35	0.41
1:C:150:LYS:HA	1:C:167:PRO:HB3	2.03	0.41
1:B:208:ILE:HD12	1:B:208:ILE:HA	1.85	0.41
1:C:19:GLN:HB2	1:C:20:PRO:CD	2.47	0.41
1:C:100:ASP:OD1	1:C:102:SER:CB	2.67	0.41
1:C:203:VAL:HG22	1:C:211:VAL:HG21	2.02	0.41
1:A:275:ILE:HD13	1:A:296:ALA:O	2.21	0.41
1:C:6:LYS:HA	1:C:7:PRO:HD3	1.79	0.41
1:C:129:ILE:O	1:C:129:ILE:HG23	2.21	0.41
1:C:183:ASP:O	1:C:184:PRO:C	2.56	0.41
1:C:305:GLY:O	1:C:307:LYS:HG3	2.21	0.41
1:A:10:ILE:HD12	1:A:10:ILE:H	1.85	0.41
1:A:73:VAL:HG21	1:A:140:LEU:HD12	2.03	0.41
1:A:122:TRP:N	1:A:175:VAL:O	2.44	0.41
1:A:166:THR:O	1:A:167:PRO:C	2.59	0.41
1:A:168:CYS:SG	1:A:169:ILE:HG23	2.61	0.41
1:C:306:THR:HA	1:C:311:ASN:ND2	2.36	0.41
1:A:170:SER:O	1:A:172:LYS:N	2.54	0.41
1:A:208:ILE:HB	1:A:256:GLU:HG2	2.02	0.41
1:B:36:LEU:HD13	1:B:297:VAL:HG22	2.02	0.41
1:B:229:LEU:O	1:B:273:LEU:HD23	2.21	0.41
1:C:66:ILE:O	1:C:138:GLY:HA3	2.21	0.41
1:A:232:CYS:SG	1:A:234:ASP:CG	2.99	0.40
1:B:80:LEU:HD23	1:B:103:MET:O	2.21	0.40
1:C:40:LEU:HD23	1:C:40:LEU:HA	1.86	0.40
1:C:231:PHE:HZ	1:C:236:LEU:HD21	1.86	0.40
1:B:80:LEU:O	1:B:84:VAL:HG23	2.21	0.40
1:B:253:SER:OG	1:B:256:GLU:HG3	2.21	0.40
1:C:6:LYS:HG2	3:C:806:HOH:O	2.22	0.40
1:C:66:ILE:HG22	1:C:138:GLY:HA2	2.03	0.40
1:C:118:LEU:HD12	1:C:118:LEU:O	2.21	0.40
1:A:198:PHE:CZ	1:A:215:THR:CG2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LEU:CD1	1:C:193:LEU:HD21	2.51	0.40
1:B:229:LEU:N	1:B:272:GLY:O	2.41	0.40
1:C:35:GLY:O	1:C:39:LYS:HG3	2.22	0.40
1:C:86:GLU:O	1:C:90:ASN:ND2	2.54	0.40
1:C:129:ILE:HG13	1:C:145:VAL:CB	2.44	0.40
1:A:233:VAL:HG21	1:A:278:VAL:HG22	2.02	0.40
1:A:242:PRO:O	1:A:244:THR:N	2.53	0.40
1:B:236:LEU:HD23	1:B:252:LEU:HB2	2.04	0.40
1:C:73:VAL:HG21	1:C:140:LEU:HD12	2.02	0.40
1:C:127:THR:O	1:C:128:ASP:C	2.60	0.40
1:C:175:VAL:HG23	1:C:219:LEU:HD21	2.03	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	312/314 (99%)	261 (84%)	38 (12%)	13 (4%)	3 20
1	B	312/314 (99%)	270 (86%)	29 (9%)	13 (4%)	3 20
1	C	312/314 (99%)	266 (85%)	32 (10%)	14 (4%)	2 18
All	All	936/942 (99%)	797 (85%)	99 (11%)	40 (4%)	2 20

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLY
1	A	143	GLN
1	B	99	GLY
1	C	99	GLY
1	A	171	ALA
1	A	189	ILE

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Mol	Chain	Res	Type
1	B	102	SER
1	B	143	GLN
1	B	266	LYS
1	C	149	LEU
1	A	102	SER
1	A	243	ALA
1	A	291	ARG
1	B	243	ALA
1	C	17	LYS
1	C	199	SER
1	A	17	LYS
1	B	200	MET
1	B	249	VAL
1	C	100	ASP
1	C	143	GLN
1	A	294	ASN
1	B	128	ASP
1	B	144	PRO
1	B	171	ALA
1	C	157	PRO
1	C	188	TYR
1	C	189	ILE
1	C	203	VAL
1	A	16	SER
1	A	51	GLY
1	C	132	PRO
1	C	180	ARG
1	B	132	PRO
1	A	167	PRO
1	A	144	PRO
1	B	167	PRO
1	C	129	ILE
1	C	160	PRO
1	B	242	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	264/264 (100%)	246 (93%)	18 (7%)	16 49
1	B	264/264 (100%)	245 (93%)	19 (7%)	14 47
1	C	264/264 (100%)	246 (93%)	18 (7%)	16 49
All	All	792/792 (100%)	737 (93%)	55 (7%)	15 49

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	24	VAL
1	A	32	ARG
1	A	57	ASP
1	A	100	ASP
1	A	101	HIS
1	A	135	THR
1	A	141	HIS
1	A	169	ILE
1	A	226	PRO
1	A	234	ASP
1	A	244	THR
1	A	246	THR
1	A	273	LEU
1	A	275	ILE
1	A	287	GLU
1	A	303	CYS
1	A	314	PRO
1	B	7	PRO
1	B	24	VAL
1	B	57	ASP
1	B	100	ASP
1	B	101	HIS
1	B	135	THR
1	B	169	ILE
1	B	173	ASP
1	B	224	LYS
1	B	225	ARG
1	B	230	SER
1	B	233	VAL
1	B	238	PRO
1	B	242	PRO
1	B	244	THR
1	B	246	THR

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Mol	Chain	Res	Type
1	B	273	LEU
1	B	287	GLU
1	B	295	THR
1	C	9	GLU
1	C	32	ARG
1	C	57	ASP
1	C	100	ASP
1	C	101	HIS
1	C	135	THR
1	C	160	PRO
1	C	169	ILE
1	C	174	ILE
1	C	184	PRO
1	C	200	MET
1	C	246	THR
1	C	253	SER
1	C	273	LEU
1	C	287	GLU
1	C	295	THR
1	C	313	LYS
1	C	314	PRO

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	79	GLN
1	A	115	HIS
1	A	141	HIS
1	A	143	GLN
1	A	228	HIS
1	A	311	ASN
1	B	50	HIS
1	B	79	GLN
1	B	90	ASN
1	B	141	HIS
1	B	311	ASN
1	C	79	GLN
1	C	90	ASN
1	C	141	HIS
1	C	143	GLN
1	C	311	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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.