Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 09:43 AM EDT

PDB ID	:	4HYD
Title	:	Structure of a presenilin family intramembrane aspartate protease in C2221 space group
Authors	:	Li, X.; Dang, S.; Yan, C.; Wang, J.; Shi, Y.
Deposited on	:	2012-11-13
Resolution	:	3.80 Å(reported)

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

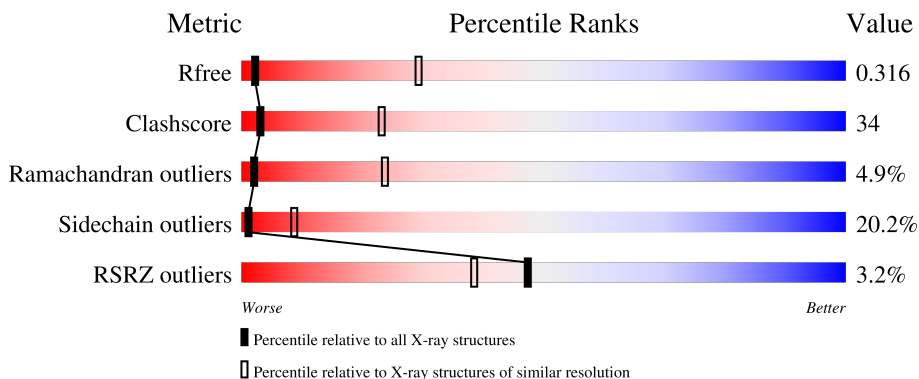|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.316
Clashscore		34
Ramachandran outliers		4.9%
Sidechain outliers		20.2%
RSRZ outliers		3.2%

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))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	301	4% / 34% / 37% / 10% / 18%
1	B	301	% / 36% / 37% / 8% / 18%
1	C	301	3% / 34% / 37% / 11% / 18%
1	D	301	2% / 34% / 38% / 9% / · / 18%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 7199 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 Putative uncharacterized protein.

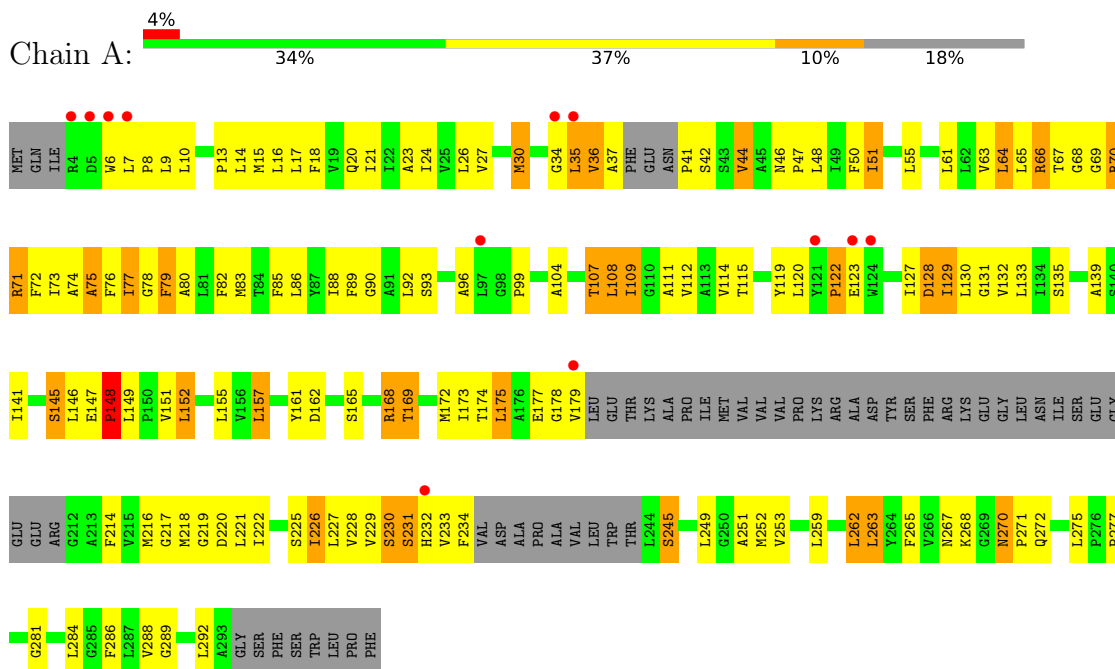| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	B	246	Total	C	N	O	S	0	0	0
			1799	1216	276	296	11			
1	C	246	Total	C	N	O	S	0	0	0
			1799	1216	276	296	11			
1	D	246	Total	C	N	O	S	0	0	0
			1799	1216	276	296	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ASN	ASP	engineered mutation	UNP A3CWV0
A	42	SER	GLU	engineered mutation	UNP A3CWV0
A	147	GLU	ALA	engineered mutation	UNP A3CWV0
A	148	PRO	VAL	engineered mutation	UNP A3CWV0
A	229	VAL	ALA	engineered mutation	UNP A3CWV0
B	40	ASN	ASP	engineered mutation	UNP A3CWV0
B	42	SER	GLU	engineered mutation	UNP A3CWV0
B	147	GLU	ALA	engineered mutation	UNP A3CWV0
B	148	PRO	VAL	engineered mutation	UNP A3CWV0
B	229	VAL	ALA	engineered mutation	UNP A3CWV0
C	40	ASN	ASP	engineered mutation	UNP A3CWV0
C	42	SER	GLU	engineered mutation	UNP A3CWV0
C	147	GLU	ALA	engineered mutation	UNP A3CWV0
C	148	PRO	VAL	engineered mutation	UNP A3CWV0
C	229	VAL	ALA	engineered mutation	UNP A3CWV0
D	40	ASN	ASP	engineered mutation	UNP A3CWV0
D	42	SER	GLU	engineered mutation	UNP A3CWV0
D	147	GLU	ALA	engineered mutation	UNP A3CWV0
D	148	PRO	VAL	engineered mutation	UNP A3CWV0
D	229	VAL	ALA	engineered mutation	UNP A3CWV0

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 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: Putative uncharacterized protein

• Molecule 1: Putative uncharacterized protein

G285 F286 L287 V288 A293 GLY SER PHE SER TRP LEU PRO PHE
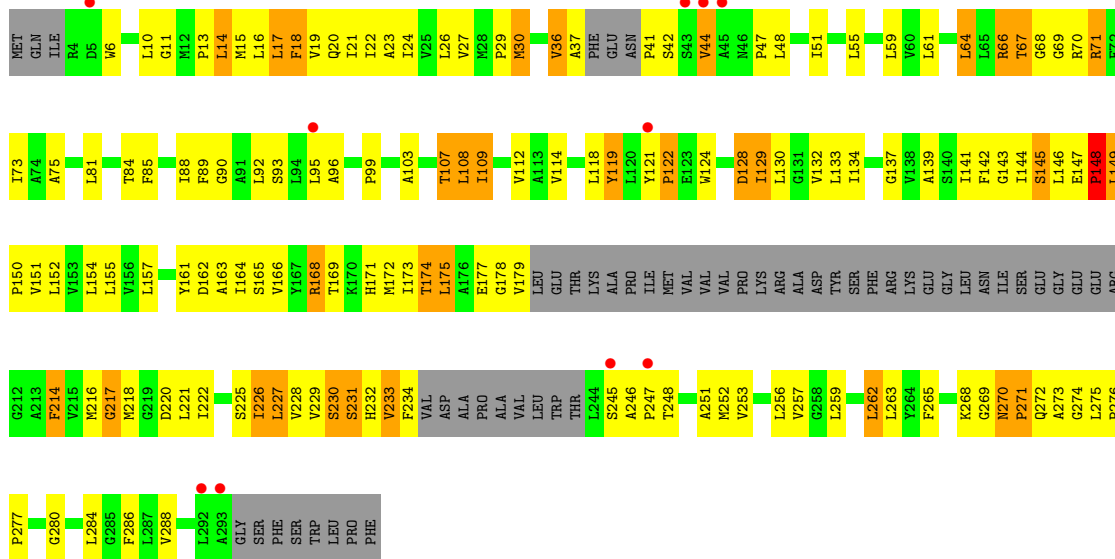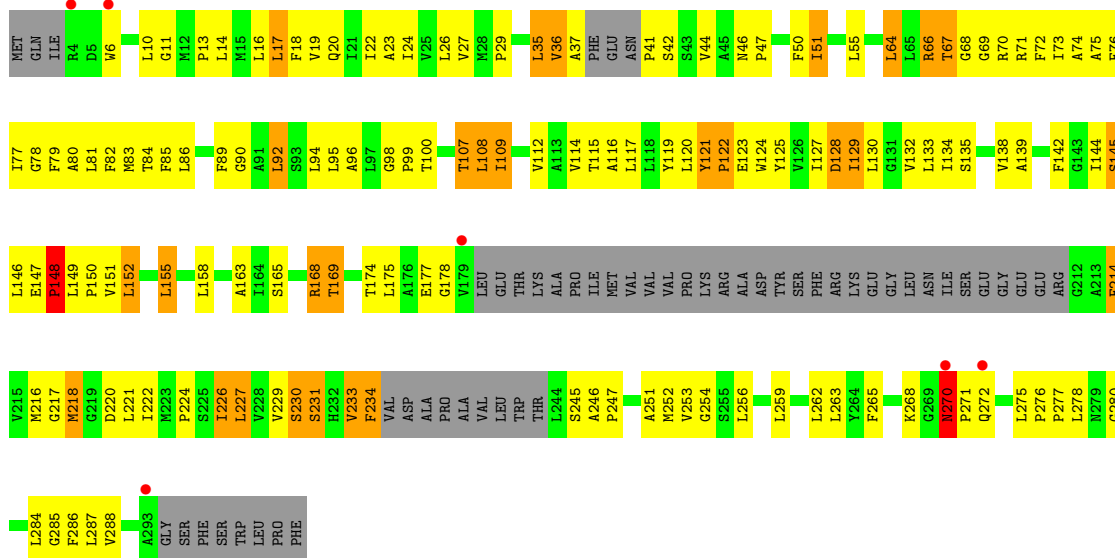
• Molecule 1: Putative uncharacterized protein

Chain C:

3%

34% 37% 11% 18%

MET GLN ILE R4 D5 W6 L10 G11 M12 P13 L14 M15 L16 L17 F18 V19 Q20 I21 I22 A23 I24 V25 L26 V27 M28 P29 M30 V36 A37 PHE GLU ASN P41 S42 S43 V44 A45 N46 P47 L48 I51 L55 L59 V60 L61 L64 L65 R66 T67 G68 G69 R70 R71 F72

I73 A74 A75 L81 T84 F85 I88 F89 G90 A91 L92 S93 L94 L95 A96 P99 A103 T107 L108 I109 V112 A113 V114 L118 Y119 L120 Y121 P122 E123 W124 D128 I129 L130 G131 V132 L133 I134 G137 V138 A139 S140 I141 F142 G143 I144 S145 L146 E147 P148 L149

P150 V151 L152 V153 L154 L155 V156 L157 Y161 D162 A163 I164 S165 V166 Y167 R168 T169 K170 H171 M172 I173 T174 L175 A176 E177 G178 V179 LEU GLU THR LYS ALA PRO ILE MET VAL VAL PRO LYS ARG ASP ALA TYR SER PHE ARG LYS GLU GLY LEU LEU ASN ILE SER GLU GLY GLU GLU ARG

G212 A213 F214 V215 M216 G217 M218 G219 D220 L221 I222 S225 I226 L227 V228 V229 S230 S231 H232 V233 F234 VAL ASP ALA PRO ALA VAL LEU TRP THR L244 S245 A246 P247 T248 A251 M252 V253 L256 V257 G258 L259 L262 L263 Y264 F265 K268 G269 N270 P271 Q272 A273 C274 L275 P276

P277 G280 L284 G285 F286 L287 V288 L292 A293 GLY SER PHE SER TRP LEU PRO PHE

• Molecule 1: Putative uncharacterized protein

Chain D:

2%

34% 38% 9% • 18%

MET GLN ILE R4 D5 W6 L10 G11 M12 P13 L14 M15 L16 L17 F18 V19 Q20 I21 I22 A23 I24 V25 L26 V27 M28 P29 L35 V36 A37 PHE GLU ASN P41 S42 S43 V44 A45 N46 P47 F50 I51 L55 L64 L65 R66 T67 G68 G69 R70 R71 F72 I73 A74 A75 F76

I77 G78 F79 A80 L81 F82 M83 T84 F85 L86 F89 G90 A91 L92 S93 L94 L95 A96 L97 G98 P99 T100 T107 L108 I109 V112 A113 V114 T115 A116 L117 L118 Y119 L120 Y121 P122 E123 W124 V125 V126 I127 D128 I129 L130 G131 V132 L133 I134 S135 V138 A139 F142 G143 I144 S145

L146 E147 P148 L149 P150 V151 L152 L155 L158 A163 I164 S165 R168 T169 T174 L175 A176 E177 G178 V179 LEU GLU THR LYS ALA PRO ILE MET VAL VAL PRO LYS ARG ASP ALA TYR SER PHE ARG LYS GLU GLY LEU LEU ASN ILE SER GLU GLY GLU GLU ARG G212 A213 F214

V215 M216 G217 M218 G219 D220 L221 I222 M223 P224 S225 I226 L227 V228 V229 S230 S231 H232 V233 F234 VAL ASP ALA PRO ALA VAL LEU TRP THR L244 S245 A246 P247 A251 M252 V253 G254 S255 L256 L259 L262 L263 Y264 F265 K268 G269 N270 P271 Q272 L275 P276 P277 L278 N279 G280

L284 G285 F286 L287 V288 A293 GLY SER PHE SER TRP LEU PRO PHE

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	114.08Å 170.03Å 181.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.58 – 3.80 31.58 – 3.79	Depositor EDS
% Data completeness (in resolution range)	84.7 (31.58-3.80) 83.9 (31.58-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.307 , 0.308 0.309 , 0.316	Depositor DCC
R_{free} test set	650 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å^2)	122.8	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 102.7	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7199	wwPDB-VP
Average B, all atoms (Å^2)	184.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.49	0/1839	0.77	0/2511
1	B	0.47	0/1836	0.76	0/2507
1	C	0.44	0/1836	0.74	0/2507
1	D	0.51	0/1836	0.79	0/2507
All	All	0.48	0/7347	0.77	0/10032

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
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	SER	Peptide
1	B	145	SER	Peptide
1	C	145	SER	Peptide
1	D	145	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1802	0	1949	128	3
1	B	1799	0	1940	136	0
1	C	1799	0	1940	140	0
1	D	1799	0	1940	119	0
All	All	7199	0	7769	503	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (503) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:VAL:CG2	1:B:144:ILE:HG22	1.65	1.25
1:C:36:VAL:CG2	1:C:144:ILE:HG22	1.68	1.21
1:C:36:VAL:HG12	1:C:37:ALA:H	1.01	1.17
1:B:36:VAL:HG22	1:B:144:ILE:HG22	1.18	1.15
1:C:36:VAL:HG13	1:C:145:SER:HA	1.15	1.13
1:B:36:VAL:HG12	1:B:37:ALA:N	1.59	1.12
1:B:36:VAL:CG1	1:B:37:ALA:H	1.61	1.12
1:A:36:VAL:CG1	1:A:37:ALA:H	1.63	1.10
1:D:36:VAL:CG1	1:D:37:ALA:H	1.62	1.10
1:A:36:VAL:HG12	1:A:37:ALA:H	0.97	1.09
1:B:36:VAL:HG13	1:B:145:SER:HA	1.31	1.09
1:A:36:VAL:HG12	1:A:37:ALA:N	1.61	1.08
1:D:36:VAL:HG12	1:D:37:ALA:N	1.60	1.08
1:B:36:VAL:CG2	1:B:144:ILE:CG2	2.32	1.07
1:C:36:VAL:HG12	1:C:37:ALA:N	1.66	1.06
1:C:36:VAL:HG22	1:C:144:ILE:CG2	1.84	1.06
1:D:36:VAL:HG12	1:D:37:ALA:H	0.90	1.04
1:B:36:VAL:HG12	1:B:37:ALA:H	0.88	1.04
1:C:36:VAL:CG1	1:C:37:ALA:H	1.71	1.04
1:C:36:VAL:HG22	1:C:144:ILE:HG22	1.02	1.02
1:A:64:LEU:HD21	1:A:73:ILE:HA	1.42	1.01
1:C:36:VAL:CG2	1:C:144:ILE:CG2	2.37	1.00
1:B:36:VAL:HG22	1:B:144:ILE:CG2	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:CG1	1:A:146:LEU:HD23	1.99	0.91
1:A:161:TYR:OH	1:D:71:ARG:NH1	2.05	0.89
1:B:36:VAL:HG23	1:B:144:ILE:HG22	1.53	0.89
1:C:36:VAL:CG1	1:C:145:SER:HA	2.04	0.86
1:A:36:VAL:HG13	1:A:146:LEU:HD23	1.55	0.85
1:A:70:ARG:HH12	1:B:168:ARG:HH12	1.24	0.84
1:D:36:VAL:HG13	1:D:145:SER:HA	1.59	0.84
1:A:86:LEU:HD21	1:A:108:LEU:HA	1.57	0.83
1:C:30:MET:HE1	1:C:141:ILE:HA	1.59	0.82
1:C:36:VAL:HG13	1:C:145:SER:CA	2.05	0.81
1:B:36:VAL:HG23	1:B:144:ILE:CG2	2.09	0.80
1:A:262:LEU:HD23	1:A:277:PRO:HG2	1.62	0.80
1:B:30:MET:HE1	1:B:141:ILE:HA	1.62	0.80
1:B:42:SER:HA	1:B:146:LEU:HB3	1.64	0.80
1:C:64:LEU:HD21	1:C:73:ILE:HA	1.63	0.79
1:B:128:ASP:N	1:B:128:ASP:OD2	2.15	0.79
1:B:220:ASP:HB2	1:B:275:LEU:HD21	1.66	0.78
1:D:262:LEU:HD23	1:D:277:PRO:HG2	1.66	0.77
1:B:253:VAL:HA	1:B:256:LEU:HD12	1.66	0.77
1:D:121:TYR:HD1	1:D:124:TRP:HZ2	1.31	0.76
1:B:80:ALA:HA	1:B:83:MET:HE2	1.68	0.76
1:C:139:ALA:HA	1:C:226:ILE:HD12	1.68	0.76
1:D:124:TRP:HA	1:D:127:ILE:HG12	1.67	0.76
1:A:36:VAL:HA	1:A:145:SER:HA	1.68	0.75
1:B:41:PRO:C	1:B:146:LEU:HG	2.06	0.75
1:C:30:MET:HE2	1:C:144:ILE:HD12	1.67	0.75
1:D:148:PRO:O	1:D:151:VAL:N	2.20	0.75
1:B:71:ARG:O	1:B:75:ALA:N	2.20	0.74
1:D:86:LEU:HD21	1:D:108:LEU:HA	1.70	0.74
1:B:70:ARG:HH12	1:C:169:THR:HG21	1.50	0.74
1:D:253:VAL:HA	1:D:256:LEU:HD12	1.69	0.73
1:D:151:VAL:HG11	1:D:227:LEU:HB2	1.71	0.72
1:B:16:LEU:HD23	1:B:256:LEU:HD23	1.71	0.72
1:C:118:LEU:HD12	1:C:130:LEU:HD12	1.70	0.71
1:D:135:SER:HA	1:D:222:ILE:HD11	1.72	0.71
1:C:36:VAL:CG1	1:C:146:LEU:HD22	2.20	0.71
1:D:64:LEU:HD11	1:D:73:ILE:HG23	1.73	0.70
1:A:36:VAL:HG11	1:A:146:LEU:HD23	1.73	0.69
1:A:148:PRO:O	1:A:151:VAL:N	2.24	0.69
1:C:144:ILE:HA	1:C:233:VAL:HG21	1.75	0.69
1:A:36:VAL:HG11	1:A:41:PRO:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:VAL:CG1	1:C:37:ALA:N	2.37	0.68
1:D:165:SER:OG	1:D:168:ARG:NH2	2.26	0.68
1:D:128:ASP:OD2	1:D:128:ASP:N	2.27	0.67
1:A:139:ALA:HA	1:A:226:ILE:HD12	1.77	0.66
1:A:36:VAL:CG1	1:A:41:PRO:HD2	2.25	0.66
1:D:155:LEU:HD11	1:D:224:PRO:HA	1.76	0.66
1:C:165:SER:O	1:C:169:THR:HG23	1.96	0.66
1:A:129:ILE:HG22	1:A:130:LEU:HD23	1.78	0.65
1:D:138:VAL:HB	1:D:222:ILE:HD13	1.77	0.65
1:D:41:PRO:C	1:D:146:LEU:HG	2.17	0.65
1:D:90:GLY:O	1:D:94:LEU:HB2	1.97	0.65
1:C:142:PHE:HB2	1:C:226:ILE:HD11	1.79	0.65
1:B:118:LEU:HD12	1:B:130:LEU:HD12	1.80	0.64
1:C:71:ARG:HG2	1:D:168:ARG:HH22	1.62	0.64
1:D:268:LYS:HE2	1:D:272:GLN:HE22	1.62	0.64
1:D:24:ILE:HD13	1:D:229:VAL:HG22	1.80	0.64
1:A:220:ASP:HB2	1:A:275:LEU:HD21	1.79	0.64
1:C:89:PHE:HD1	1:C:92:LEU:HD12	1.63	0.64
1:B:19:VAL:HG22	1:B:132:VAL:HA	1.81	0.63
1:C:121:TYR:HA	1:C:124:TRP:CZ2	2.33	0.63
1:C:129:ILE:HG22	1:C:130:LEU:HD23	1.80	0.63
1:D:246:ALA:HB1	1:D:247:PRO:HD2	1.81	0.63
1:B:17:LEU:HD23	1:B:256:LEU:HD11	1.80	0.63
1:D:218:MET:HA	1:D:221:LEU:HB3	1.81	0.63
1:B:20:GLN:NE2	1:B:252:MET:HG2	2.13	0.63
1:A:63:VAL:O	1:A:67:THR:OG1	2.12	0.63
1:D:142:PHE:HB2	1:D:226:ILE:HD11	1.81	0.63
1:B:85:PHE:HE1	1:B:133:LEU:HD23	1.62	0.62
1:A:13:PRO:HB3	1:A:259:LEU:HD22	1.81	0.62
1:B:142:PHE:HB2	1:B:226:ILE:HD11	1.79	0.62
1:B:13:PRO:HB3	1:B:259:LEU:HD22	1.81	0.62
1:B:265:PHE:O	1:B:268:LYS:HG2	1.99	0.62
1:B:36:VAL:HG22	1:B:144:ILE:C	2.19	0.62
1:D:254:GLY:HA3	1:D:285:GLY:HA3	1.82	0.62
1:A:265:PHE:HB3	1:A:272:GLN:OE1	1.99	0.61
1:D:42:SER:HA	1:D:146:LEU:HB3	1.82	0.61
1:C:21:ILE:HG22	1:C:22:ILE:HD13	1.82	0.61
1:C:108:LEU:O	1:C:112:VAL:HG23	2.00	0.61
1:D:29:PRO:HA	1:D:95:LEU:HD22	1.82	0.61
1:B:135:SER:HA	1:B:222:ILE:HD11	1.82	0.61
1:A:64:LEU:HD11	1:A:73:ILE:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:HD1	1:A:92:LEU:HD12	1.65	0.61
1:C:231:SER:HB2	1:C:248:THR:HG21	1.82	0.61
1:B:122:PRO:HD2	1:B:124:TRP:CE2	2.35	0.60
1:C:147:GLU:HB3	1:C:148:PRO:HD2	1.83	0.60
1:C:36:VAL:HG23	1:C:144:ILE:HG22	1.76	0.60
1:A:68:GLY:HA3	1:A:73:ILE:HD11	1.83	0.60
1:A:108:LEU:O	1:A:112:VAL:HG23	2.02	0.60
1:B:116:ALA:HA	1:C:164:ILE:HD11	1.82	0.60
1:C:16:LEU:HA	1:C:221:LEU:HD11	1.82	0.60
1:D:68:GLY:HA3	1:D:73:ILE:HD11	1.84	0.60
1:B:36:VAL:CG2	1:B:144:ILE:HG23	2.30	0.60
1:A:251:ALA:HB2	1:A:286:PHE:HB2	1.83	0.60
1:C:253:VAL:HA	1:C:256:LEU:HD12	1.83	0.59
1:D:64:LEU:HD21	1:D:73:ILE:HA	1.84	0.59
1:D:69:GLY:HA2	1:D:72:PHE:HB3	1.84	0.59
1:B:170:LYS:HZ1	1:B:271:PRO:C	2.06	0.59
1:A:229:VAL:O	1:A:231:SER:N	2.35	0.59
1:B:171:HIS:HA	1:B:174:THR:HG23	1.85	0.59
1:D:149:LEU:HB3	1:D:150:PRO:HD3	1.85	0.59
1:A:42:SER:HA	1:A:146:LEU:HB3	1.84	0.59
1:A:120:LEU:HD21	1:B:164:ILE:HG12	1.84	0.59
1:A:23:ALA:O	1:A:27:VAL:HG23	2.02	0.58
1:A:72:PHE:CE2	1:B:59:LEU:HD23	2.38	0.58
1:D:16:LEU:HD23	1:D:256:LEU:HD23	1.85	0.58
1:D:151:VAL:CG1	1:D:227:LEU:HB2	2.33	0.58
1:D:24:ILE:O	1:D:27:VAL:N	2.36	0.58
1:B:41:PRO:O	1:B:146:LEU:HG	2.04	0.58
1:B:122:PRO:HD2	1:B:124:TRP:CZ2	2.39	0.58
1:C:15:MET:SD	1:C:128:ASP:HB3	2.45	0.57
1:C:41:PRO:C	1:C:146:LEU:HG	2.24	0.57
1:A:24:ILE:HD13	1:A:229:VAL:HG22	1.86	0.57
1:A:30:MET:HE1	1:A:141:ILE:HA	1.86	0.57
1:B:262:LEU:HD21	1:B:274:GLY:HA2	1.85	0.57
1:D:75:ALA:O	1:D:78:GLY:N	2.38	0.57
1:B:138:VAL:HB	1:B:222:ILE:HD13	1.87	0.56
1:C:36:VAL:HG23	1:C:144:ILE:CG2	2.32	0.56
1:C:121:TYR:HA	1:C:124:TRP:HZ2	1.68	0.56
1:D:108:LEU:O	1:D:112:VAL:HG23	2.06	0.56
1:D:220:ASP:HB2	1:D:275:LEU:HD21	1.87	0.56
1:C:20:GLN:CD	1:C:252:MET:HG2	2.26	0.56
1:D:139:ALA:HA	1:D:226:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:HA	1:A:222:ILE:HD11	1.87	0.56
1:C:90:GLY:HA2	1:C:107:THR:HG21	1.88	0.56
1:B:165:SER:O	1:B:169:THR:HG23	2.06	0.56
1:D:47:PRO:O	1:D:50:PHE:HB3	2.05	0.56
1:A:89:PHE:HZ	1:A:114:VAL:HG21	1.70	0.55
1:A:165:SER:O	1:A:169:THR:HG23	2.07	0.55
1:B:36:VAL:CG1	1:B:37:ALA:N	2.32	0.55
1:A:85:PHE:HE1	1:A:133:LEU:HD23	1.70	0.55
1:A:128:ASP:OD2	1:A:128:ASP:N	2.40	0.55
1:B:89:PHE:HA	1:B:92:LEU:HB2	1.88	0.55
1:B:121:TYR:HA	1:B:124:TRP:CZ2	2.41	0.55
1:C:85:PHE:HE1	1:C:133:LEU:HD23	1.71	0.55
1:C:225:SER:HA	1:C:228:VAL:HB	1.89	0.55
1:B:69:GLY:HA2	1:B:72:PHE:HB3	1.89	0.55
1:A:70:ARG:HH22	1:B:168:ARG:CZ	2.20	0.55
1:C:24:ILE:O	1:C:27:VAL:HB	2.07	0.55
1:B:81:LEU:O	1:B:84:THR:OG1	2.18	0.55
1:B:149:LEU:HB3	1:B:150:PRO:HD3	1.87	0.55
1:D:163:ALA:HB2	1:D:276:PRO:HG2	1.88	0.55
1:B:220:ASP:O	1:B:224:PRO:HD3	2.08	0.55
1:B:259:LEU:HB2	1:B:278:LEU:HD11	1.89	0.55
1:D:42:SER:HB2	1:D:146:LEU:HD12	1.87	0.54
1:B:35:LEU:HD23	1:B:141:ILE:HG12	1.89	0.54
1:B:42:SER:OG	1:B:147:GLU:HB2	2.07	0.54
1:C:6:TRP:O	1:C:10:LEU:HB2	2.08	0.54
1:D:129:ILE:HG22	1:D:130:LEU:HD23	1.88	0.54
1:B:147:GLU:HB3	1:B:148:PRO:HD2	1.90	0.54
1:D:13:PRO:HB3	1:D:259:LEU:HD22	1.90	0.54
1:B:89:PHE:HD1	1:B:92:LEU:HD12	1.73	0.54
1:C:147:GLU:O	1:C:150:PRO:HD2	2.08	0.54
1:B:97:LEU:HB2	1:B:103:ALA:HB2	1.89	0.54
1:C:226:ILE:O	1:C:230:SER:N	2.33	0.54
1:C:231:SER:HA	1:C:234:PHE:HB3	1.88	0.54
1:C:84:THR:O	1:C:88:ILE:HG13	2.08	0.54
1:A:48:LEU:HD23	1:D:83:MET:HG2	1.88	0.54
1:D:85:PHE:HE1	1:D:133:LEU:HD23	1.73	0.54
1:A:168:ARG:HH12	1:A:169:THR:HG22	1.73	0.54
1:B:148:PRO:O	1:B:151:VAL:N	2.41	0.53
1:D:24:ILE:HA	1:D:27:VAL:HG23	1.90	0.53
1:D:280:GLY:O	1:D:284:LEU:HG	2.08	0.53
1:A:70:ARG:O	1:A:70:ARG:NE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HD12	1:A:147:GLU:HG2	1.90	0.53
1:C:44:VAL:HG12	1:C:150:PRO:HA	1.89	0.53
1:D:146:LEU:HD12	1:D:147:GLU:HG2	1.90	0.53
1:C:13:PRO:HB3	1:C:259:LEU:HD22	1.89	0.53
1:B:71:ARG:NH1	1:C:161:TYR:OH	2.35	0.53
1:C:27:VAL:HG22	1:C:229:VAL:HG13	1.91	0.53
1:A:128:ASP:O	1:A:132:VAL:HG23	2.09	0.53
1:D:122:PRO:HG3	1:D:127:ILE:HD11	1.90	0.53
1:A:169:THR:HA	1:A:172:MET:HB2	1.91	0.53
1:C:42:SER:HA	1:C:146:LEU:HB3	1.91	0.53
1:A:157:LEU:HD21	1:D:82:PHE:CE2	2.44	0.52
1:B:86:LEU:HD21	1:B:108:LEU:HA	1.91	0.52
1:C:20:GLN:O	1:C:24:ILE:HG12	2.09	0.52
1:A:15:MET:SD	1:A:128:ASP:HB3	2.50	0.52
1:B:36:VAL:HG22	1:B:144:ILE:O	2.08	0.52
1:C:68:GLY:HA3	1:C:73:ILE:HD11	1.90	0.52
1:D:69:GLY:HA3	1:D:73:ILE:HG13	1.91	0.52
1:D:122:PRO:HD2	1:D:124:TRP:CE2	2.45	0.52
1:A:265:PHE:O	1:A:268:LYS:HG2	2.09	0.52
1:B:75:ALA:O	1:B:78:GLY:N	2.43	0.52
1:C:128:ASP:OD2	1:C:128:ASP:N	2.39	0.52
1:C:142:PHE:HA	1:C:145:SER:HB3	1.92	0.52
1:B:90:GLY:HA2	1:B:107:THR:HG21	1.92	0.52
1:C:11:GLY:HA2	1:C:14:LEU:HB3	1.91	0.52
1:C:18:PHE:O	1:C:22:ILE:HG12	2.10	0.52
1:C:24:ILE:HA	1:C:27:VAL:HG23	1.92	0.51
1:D:51:ILE:HD11	1:D:158:LEU:HD21	1.92	0.51
1:A:148:PRO:HD3	1:A:230:SER:OG	2.10	0.51
1:C:151:VAL:HG11	1:C:227:LEU:HB2	1.91	0.51
1:A:82:PHE:HE1	1:A:112:VAL:HA	1.75	0.51
1:A:89:PHE:CZ	1:A:114:VAL:HG21	2.45	0.51
1:C:93:SER:HB2	1:C:103:ALA:HB1	1.92	0.51
1:C:128:ASP:O	1:C:132:VAL:HG23	2.09	0.51
1:B:218:MET:HA	1:B:221:LEU:HB3	1.91	0.51
1:D:36:VAL:CG1	1:D:37:ALA:N	2.32	0.51
1:A:36:VAL:HA	1:A:145:SER:CA	2.38	0.51
1:C:143:GLY:HA2	1:C:230:SER:HB2	1.92	0.51
1:C:265:PHE:HB3	1:C:272:GLN:CD	2.31	0.51
1:D:71:ARG:O	1:D:75:ALA:N	2.38	0.51
1:A:36:VAL:CG1	1:A:37:ALA:N	2.31	0.51
1:A:24:ILE:HA	1:A:27:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:VAL:HG21	1:D:221:LEU:HD21	1.93	0.50
1:D:42:SER:N	1:D:146:LEU:HG	2.26	0.50
1:A:225:SER:HA	1:A:228:VAL:HB	1.93	0.50
1:D:26:LEU:C	1:D:29:PRO:HD2	2.31	0.50
1:D:44:VAL:O	1:D:47:PRO:HD2	2.11	0.50
1:C:44:VAL:O	1:C:47:PRO:HD2	2.10	0.50
1:B:70:ARG:NH1	1:C:169:THR:HG21	2.23	0.50
1:D:275:LEU:O	1:D:278:LEU:N	2.44	0.50
1:D:168:ARG:HH12	1:D:169:THR:HG22	1.77	0.50
1:A:16:LEU:HA	1:A:221:LEU:HD11	1.92	0.50
1:B:35:LEU:HD23	1:B:141:ILE:HG23	1.93	0.50
1:A:245:SER:H	1:A:249:LEU:HD11	1.77	0.50
1:B:20:GLN:O	1:B:24:ILE:HG12	2.12	0.50
1:B:26:LEU:C	1:B:29:PRO:HD2	2.32	0.50
1:A:107:THR:OG1	1:A:108:LEU:N	2.45	0.50
1:C:14:LEU:O	1:C:18:PHE:HB2	2.12	0.50
1:C:36:VAL:HG22	1:C:144:ILE:C	2.31	0.50
1:A:44:VAL:O	1:A:47:PRO:HD2	2.12	0.49
1:A:61:LEU:O	1:A:64:LEU:HB3	2.11	0.49
1:A:66:ARG:CZ	1:B:66:ARG:HE	2.26	0.49
1:C:139:ALA:HB2	1:C:222:ILE:HG23	1.95	0.49
1:D:168:ARG:HB3	1:D:168:ARG:NH1	2.28	0.49
1:B:274:GLY:O	1:B:277:PRO:HD2	2.13	0.49
1:A:47:PRO:O	1:A:50:PHE:HB3	2.13	0.49
1:A:89:PHE:HD2	1:A:111:ALA:N	2.10	0.49
1:C:89:PHE:HZ	1:C:114:VAL:HG21	1.76	0.49
1:C:93:SER:CB	1:C:103:ALA:HB1	2.43	0.49
1:C:218:MET:O	1:C:222:ILE:HG13	2.12	0.49
1:A:74:ALA:HA	1:A:77:ILE:HD11	1.94	0.49
1:B:16:LEU:HD23	1:B:256:LEU:CD2	2.42	0.49
1:B:31:GLN:OE1	1:B:31:GLN:N	2.40	0.49
1:D:74:ALA:HA	1:D:77:ILE:HD11	1.95	0.49
1:A:36:VAL:HG11	1:A:41:PRO:CD	2.43	0.48
1:A:72:PHE:CZ	1:B:59:LEU:HD23	2.48	0.48
1:B:42:SER:HA	1:B:146:LEU:CB	2.39	0.48
1:B:128:ASP:O	1:B:132:VAL:HG23	2.13	0.48
1:A:36:VAL:HG13	1:A:146:LEU:CD2	2.35	0.48
1:B:129:ILE:HG22	1:B:130:LEU:HD23	1.95	0.48
1:B:170:LYS:HZ2	1:B:271:PRO:HG2	1.78	0.48
1:C:36:VAL:CG1	1:C:146:LEU:CD2	2.89	0.48
1:C:47:PRO:HG3	1:C:154:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HD13	1:A:65:LEU:HG	1.96	0.48
1:A:162:ASP:HB2	1:A:275:LEU:HD12	1.96	0.48
1:C:162:ASP:HB2	1:C:275:LEU:HD12	1.94	0.48
1:D:66:ARG:NH1	1:D:67:THR:OG1	2.46	0.48
1:D:230:SER:HA	1:D:233:VAL:HG12	1.95	0.48
1:C:66:ARG:HH12	1:C:67:THR:HG23	1.79	0.48
1:C:262:LEU:HD21	1:C:274:GLY:HA2	1.95	0.48
1:A:70:ARG:HH12	1:B:169:THR:HG22	1.78	0.48
1:A:245:SER:HB2	1:A:249:LEU:HD21	1.96	0.48
1:A:268:LYS:HE2	1:A:272:GLN:HE22	1.79	0.48
1:A:24:ILE:O	1:A:27:VAL:N	2.46	0.47
1:B:24:ILE:O	1:B:27:VAL:HB	2.13	0.47
1:B:47:PRO:O	1:B:50:PHE:HB3	2.13	0.47
1:D:148:PRO:HD3	1:D:230:SER:O	2.14	0.47
1:D:165:SER:O	1:D:169:THR:HG23	2.14	0.47
1:D:231:SER:HA	1:D:234:PHE:HB3	1.96	0.47
1:B:114:VAL:O	1:B:117:LEU:HB3	2.14	0.47
1:C:71:ARG:O	1:C:75:ALA:N	2.44	0.47
1:C:168:ARG:HH12	1:C:169:THR:HG22	1.79	0.47
1:D:20:GLN:O	1:D:24:ILE:HG12	2.14	0.47
1:C:88:ILE:O	1:C:92:LEU:HG	2.13	0.47
1:B:64:LEU:HD21	1:B:73:ILE:HA	1.96	0.47
1:C:231:SER:OG	1:C:232:HIS:N	2.47	0.47
1:D:80:ALA:O	1:D:84:THR:HG23	2.15	0.47
1:B:170:LYS:NZ	1:B:271:PRO:HG2	2.30	0.47
1:C:19:VAL:HG22	1:C:132:VAL:HG13	1.97	0.47
1:C:61:LEU:O	1:C:64:LEU:HB3	2.14	0.47
1:C:163:ALA:HB2	1:C:276:PRO:HG2	1.97	0.47
1:C:227:LEU:O	1:C:231:SER:HB3	2.15	0.47
1:D:24:ILE:O	1:D:27:VAL:HB	2.15	0.47
1:A:20:GLN:CD	1:A:252:MET:HG2	2.35	0.47
1:A:64:LEU:HD23	1:A:72:PHE:CE2	2.50	0.47
1:B:36:VAL:CG1	1:B:146:LEU:HD22	2.44	0.47
1:B:124:TRP:HA	1:B:127:ILE:HG12	1.97	0.47
1:C:217:GLY:O	1:C:220:ASP:OD2	2.33	0.47
1:B:24:ILE:HA	1:B:27:VAL:HG23	1.97	0.47
1:B:20:GLN:CD	1:B:252:MET:HG2	2.36	0.46
1:C:129:ILE:HD13	1:C:129:ILE:HA	1.76	0.46
1:A:68:GLY:HA2	1:A:69:GLY:HA3	1.61	0.46
1:A:131:GLY:O	1:A:135:SER:OG	2.17	0.46
1:C:36:VAL:HG11	1:C:146:LEU:HD22	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:CG1	1:A:146:LEU:CD2	2.83	0.46
1:C:109:ILE:HA	1:C:109:ILE:HD13	1.67	0.46
1:B:115:THR:O	1:B:119:TYR:HB2	2.16	0.46
1:B:251:ALA:HA	1:B:285:GLY:HA3	1.97	0.46
1:C:166:VAL:HG11	1:C:273:ALA:HA	1.98	0.46
1:D:42:SER:HA	1:D:146:LEU:CB	2.43	0.46
1:D:148:PRO:O	1:D:149:LEU:C	2.54	0.46
1:A:35:LEU:HB3	1:A:36:VAL:H	1.48	0.46
1:A:175:LEU:HD22	1:A:179:VAL:HB	1.98	0.46
1:B:162:ASP:HB2	1:B:275:LEU:HD12	1.98	0.46
1:C:85:PHE:CE1	1:C:133:LEU:HD23	2.49	0.46
1:D:151:VAL:HG11	1:D:227:LEU:CB	2.42	0.46
1:A:30:MET:HB3	1:A:30:MET:HE3	1.58	0.46
1:C:24:ILE:HD13	1:C:229:VAL:HG22	1.97	0.46
1:D:148:PRO:HA	1:D:151:VAL:HB	1.98	0.46
1:A:93:SER:HB3	1:A:107:THR:HG22	1.97	0.45
1:A:289:GLY:HA2	1:A:292:LEU:HD12	1.97	0.45
1:B:30:MET:HE2	1:B:144:ILE:HD12	1.98	0.45
1:C:20:GLN:HE22	1:C:252:MET:HA	1.82	0.45
1:C:23:ALA:HB1	1:C:229:VAL:HG21	1.97	0.45
1:D:134:ILE:O	1:D:138:VAL:HG23	2.15	0.45
1:A:13:PRO:HD3	1:A:259:LEU:HD21	1.97	0.45
1:D:116:ALA:O	1:D:120:LEU:HG	2.16	0.45
1:A:80:ALA:HA	1:A:83:MET:HE2	1.97	0.45
1:B:13:PRO:HD3	1:B:259:LEU:HD21	1.98	0.45
1:B:29:PRO:HB2	1:B:91:ALA:O	2.16	0.45
1:B:173:ILE:HD12	1:B:173:ILE:HA	1.72	0.45
1:D:23:ALA:O	1:D:27:VAL:HG23	2.17	0.45
1:A:75:ALA:O	1:A:78:GLY:N	2.49	0.45
1:D:89:PHE:HZ	1:D:114:VAL:HG21	1.81	0.45
1:D:44:VAL:C	1:D:47:PRO:HD2	2.36	0.45
1:D:109:ILE:HD13	1:D:109:ILE:HA	1.70	0.45
1:A:26:LEU:O	1:A:30:MET:HG3	2.17	0.45
1:A:90:GLY:HA2	1:A:107:THR:HG21	1.99	0.45
1:B:275:LEU:HB2	1:B:276:PRO:HD3	1.98	0.45
1:C:148:PRO:O	1:C:151:VAL:N	2.50	0.45
1:A:79:PHE:CD1	1:A:80:ALA:N	2.85	0.45
1:A:85:PHE:HD2	1:A:115:THR:HG1	1.63	0.45
1:C:36:VAL:CG2	1:C:144:ILE:HG23	2.40	0.45
1:C:64:LEU:HD11	1:C:73:ILE:HG23	1.99	0.45
1:C:122:PRO:HD2	1:C:124:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LYS:HG3	1:C:269:GLY:O	2.17	0.45
1:A:72:PHE:CZ	1:B:59:LEU:HB2	2.52	0.44
1:A:218:MET:HA	1:A:221:LEU:HB3	1.98	0.44
1:C:27:VAL:CG2	1:C:229:VAL:HG13	2.47	0.44
1:C:246:ALA:HB1	1:C:247:PRO:HD2	1.99	0.44
1:D:89:PHE:HB2	1:D:107:THR:HB	1.98	0.44
1:A:76:PHE:O	1:A:79:PHE:HB3	2.16	0.44
1:C:232:HIS:HA	1:C:246:ALA:HB2	1.99	0.44
1:B:280:GLY:O	1:B:284:LEU:HG	2.17	0.44
1:B:70:ARG:HH22	1:C:169:THR:HG22	1.83	0.44
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.76	0.44
1:A:72:PHE:O	1:A:75:ALA:HB3	2.18	0.44
1:B:88:ILE:HD12	1:B:133:LEU:HG	2.00	0.44
1:B:246:ALA:O	1:B:249:LEU:HG	2.18	0.44
1:C:118:LEU:HD23	1:C:119:TYR:HD1	1.83	0.44
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.74	0.44
1:B:123:GLU:O	1:B:125:TYR:N	2.51	0.44
1:D:125:TYR:HA	1:D:128:ASP:OD2	2.18	0.44
1:D:251:ALA:HB2	1:D:286:PHE:HB2	1.99	0.44
1:B:138:VAL:HA	1:B:141:ILE:HD12	2.00	0.44
1:C:284:LEU:HD23	1:C:284:LEU:HA	1.83	0.44
1:D:82:PHE:HE1	1:D:112:VAL:HA	1.82	0.44
1:A:263:LEU:O	1:A:267:ASN:HB2	2.18	0.44
1:A:270:ASN:HA	1:A:271:PRO:HD2	1.65	0.44
1:B:89:PHE:O	1:B:107:THR:HG22	2.18	0.44
1:B:118:LEU:HA	1:B:122:PRO:HG3	2.00	0.44
1:B:118:LEU:CD1	1:B:130:LEU:HD12	2.45	0.44
1:C:88:ILE:HD11	1:C:134:ILE:HD13	1.99	0.43
1:A:71:ARG:O	1:A:75:ALA:N	2.51	0.43
1:C:103:ALA:O	1:C:107:THR:HG23	2.18	0.43
1:C:149:LEU:HB3	1:C:150:PRO:HD3	2.00	0.43
1:A:42:SER:CA	1:A:146:LEU:HB3	2.48	0.43
1:B:134:ILE:O	1:B:138:VAL:HG23	2.18	0.43
1:C:175:LEU:HD22	1:C:179:VAL:HB	1.99	0.43
1:A:64:LEU:HD22	1:A:64:LEU:O	2.18	0.43
1:B:171:HIS:HA	1:B:174:THR:CG2	2.47	0.43
1:C:64:LEU:HD22	1:C:64:LEU:O	2.19	0.43
1:A:70:ARG:HB3	1:A:71:ARG:HE	1.84	0.43
1:B:121:TYR:HA	1:B:124:TRP:HZ2	1.84	0.43
1:B:270:ASN:HA	1:B:271:PRO:HD2	1.81	0.43
1:A:14:LEU:HA	1:A:14:LEU:HD22	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:HD13	1:A:127:ILE:HA	1.85	0.43
1:B:83:MET:HG2	1:C:48:LEU:HD21	2.00	0.43
1:C:231:SER:H	1:C:233:VAL:H	1.66	0.43
1:D:35:LEU:HB3	1:D:36:VAL:H	1.67	0.43
1:D:122:PRO:HG2	1:D:124:TRP:CG	2.54	0.43
1:B:36:VAL:HG13	1:B:146:LEU:HD22	2.00	0.43
1:A:44:VAL:C	1:A:47:PRO:HD2	2.38	0.43
1:B:274:GLY:C	1:B:277:PRO:HD2	2.39	0.43
1:B:275:LEU:O	1:B:278:LEU:N	2.49	0.43
1:C:275:LEU:HB2	1:C:276:PRO:HD3	2.01	0.43
1:C:280:GLY:O	1:C:284:LEU:HG	2.19	0.43
1:A:122:PRO:HB2	1:A:123:GLU:H	1.69	0.43
1:B:93:SER:O	1:B:97:LEU:N	2.52	0.43
1:B:220:ASP:C	1:B:220:ASP:OD2	2.58	0.43
1:D:92:LEU:HA	1:D:92:LEU:HD23	1.67	0.43
1:D:128:ASP:O	1:D:132:VAL:HG23	2.19	0.43
1:A:219:GLY:O	1:A:222:ILE:HB	2.18	0.43
1:C:217:GLY:O	1:C:220:ASP:N	2.52	0.43
1:D:6:TRP:O	1:D:10:LEU:HB2	2.18	0.43
1:B:42:SER:HB2	1:B:147:GLU:HG2	2.00	0.42
1:C:89:PHE:HA	1:C:92:LEU:HB2	2.01	0.42
1:C:270:ASN:HA	1:C:271:PRO:HD2	1.67	0.42
1:A:104:ALA:HA	1:A:107:THR:HG23	2.00	0.42
1:A:152:LEU:HD22	1:A:152:LEU:HA	1.76	0.42
1:C:169:THR:HA	1:C:172:MET:HB2	2.00	0.42
1:D:68:GLY:HA2	1:D:69:GLY:HA3	1.81	0.42
1:A:6:TRP:O	1:A:10:LEU:HB2	2.19	0.42
1:A:9:LEU:O	1:A:263:LEU:HD12	2.19	0.42
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.75	0.42
1:C:26:LEU:HD23	1:C:26:LEU:HA	1.79	0.42
1:D:90:GLY:HA2	1:D:107:THR:HG21	1.99	0.42
1:A:24:ILE:O	1:A:27:VAL:HB	2.19	0.42
1:A:34:GLY:O	1:A:35:LEU:HB2	2.19	0.42
1:A:168:ARG:NH1	1:A:169:THR:HG22	2.35	0.42
1:C:68:GLY:HA2	1:C:69:GLY:HA3	1.50	0.42
1:C:81:LEU:O	1:C:84:THR:OG1	2.24	0.42
1:D:51:ILE:HD11	1:D:158:LEU:CD2	2.50	0.42
1:D:76:PHE:C	1:D:76:PHE:CD2	2.93	0.42
1:D:270:ASN:HA	1:D:271:PRO:HD2	1.81	0.42
1:D:278:LEU:HA	1:D:278:LEU:HD13	1.82	0.42
1:A:263:LEU:HD22	1:A:263:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:CZ	1:B:71:ARG:HG3	2.49	0.42
1:C:29:PRO:HB3	1:C:95:LEU:HD22	2.02	0.42
1:C:89:PHE:CZ	1:C:114:VAL:HG21	2.55	0.42
1:D:17:LEU:HD22	1:D:17:LEU:HA	1.81	0.42
1:D:11:GLY:O	1:D:14:LEU:HB3	2.19	0.42
1:D:129:ILE:HD13	1:D:129:ILE:HA	1.83	0.42
1:A:88:ILE:O	1:A:92:LEU:HG	2.18	0.42
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.76	0.42
1:C:143:GLY:HA3	1:C:229:VAL:CG1	2.50	0.42
1:D:98:GLY:O	1:D:100:THR:N	2.53	0.42
1:D:123:GLU:HB3	1:D:125:TYR:CE2	2.55	0.42
1:B:63:VAL:O	1:B:67:THR:OG1	2.22	0.41
1:B:165:SER:OG	1:B:168:ARG:NH2	2.52	0.41
1:B:281:GLY:O	1:B:284:LEU:HB2	2.20	0.41
1:C:214:PHE:CD2	1:C:218:MET:HG2	2.55	0.41
1:D:121:TYR:HA	1:D:122:PRO:HD2	1.89	0.41
1:D:122:PRO:HB2	1:D:123:GLU:H	1.67	0.41
1:C:229:VAL:O	1:C:231:SER:N	2.50	0.41
1:D:152:LEU:HD22	1:D:152:LEU:HA	1.82	0.41
1:A:281:GLY:O	1:A:284:LEU:HB2	2.20	0.41
1:B:79:PHE:CD1	1:B:80:ALA:N	2.88	0.41
1:B:117:LEU:HD13	1:B:118:LEU:N	2.36	0.41
1:D:246:ALA:HB1	1:D:247:PRO:CD	2.49	0.41
1:B:10:LEU:HD23	1:B:10:LEU:HA	1.71	0.41
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.86	0.41
1:B:59:LEU:HD13	1:B:59:LEU:O	2.21	0.41
1:C:134:ILE:O	1:C:137:GLY:N	2.53	0.41
1:D:13:PRO:HB3	1:D:259:LEU:CD2	2.51	0.41
1:D:36:VAL:HG22	1:D:144:ILE:HG22	2.02	0.41
1:D:287:LEU:HD23	1:D:287:LEU:HA	1.88	0.41
1:A:70:ARG:HE	1:A:70:ARG:C	2.23	0.41
1:B:36:VAL:CG1	1:B:146:LEU:CD2	2.98	0.41
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.78	0.41
1:B:163:ALA:HB2	1:B:276:PRO:HG2	2.03	0.41
1:C:20:GLN:NE2	1:C:252:MET:HA	2.35	0.41
1:C:122:PRO:HD2	1:C:124:TRP:CZ2	2.55	0.41
1:A:114:VAL:HG13	1:A:130:LEU:HD13	2.02	0.41
1:A:147:GLU:HB3	1:A:148:PRO:HD2	2.03	0.41
1:C:251:ALA:HB2	1:C:286:PHE:HB2	2.03	0.41
1:A:51:ILE:HG22	1:D:79:PHE:HD2	1.86	0.41
1:A:70:ARG:HH22	1:B:168:ARG:NH1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:HD2	1:A:115:THR:OG1	2.04	0.41
1:B:68:GLY:HA2	1:B:69:GLY:HA3	1.71	0.41
1:B:122:PRO:HB2	1:B:123:GLU:H	1.69	0.41
1:C:17:LEU:O	1:C:21:ILE:HD13	2.21	0.41
1:C:171:HIS:HA	1:C:174:THR:HG23	2.03	0.41
1:D:114:VAL:O	1:D:117:LEU:HB3	2.20	0.41
1:A:64:LEU:HD22	1:A:64:LEU:C	2.41	0.41
1:A:86:LEU:HA	1:A:86:LEU:HD23	1.81	0.41
1:C:121:TYR:HD1	1:C:124:TRP:CZ2	2.39	0.41
1:C:274:GLY:O	1:C:277:PRO:HD2	2.21	0.41
1:C:30:MET:HE3	1:C:30:MET:HB3	1.91	0.40
1:C:143:GLY:N	1:C:226:ILE:HG13	2.36	0.40
1:D:22:ILE:O	1:D:26:LEU:HB2	2.21	0.40
1:A:7:LEU:HB2	1:A:8:PRO:HD3	2.03	0.40
1:A:146:LEU:HD13	1:A:147:GLU:OE2	2.20	0.40
1:B:35:LEU:O	1:B:36:VAL:HB	2.22	0.40
1:C:88:ILE:HD13	1:C:133:LEU:HG	2.03	0.40
1:D:168:ARG:HB3	1:D:168:ARG:CZ	2.52	0.40
1:A:36:VAL:HA	1:A:145:SER:CB	2.50	0.40
1:A:109:ILE:HD13	1:A:109:ILE:HA	1.74	0.40
1:B:30:MET:HE3	1:B:30:MET:HB3	1.73	0.40
1:C:64:LEU:CD2	1:C:73:ILE:HA	2.44	0.40
1:D:10:LEU:HA	1:D:10:LEU:HD23	1.79	0.40
1:D:20:GLN:CD	1:D:252:MET:HG2	2.41	0.40
1:D:81:LEU:HD13	1:D:115:THR:HG23	2.03	0.40
1:D:214:PHE:O	1:D:218:MET:HG3	2.21	0.40
1:A:41:PRO:N	1:A:146:LEU:HG	2.37	0.40
1:B:13:PRO:O	1:B:16:LEU:HB3	2.21	0.40
1:D:265:PHE:HB3	1:D:272:GLN:OE1	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:CD2	1:A:292:LEU:CD2[3_654]	1.64	0.56
1:A:292:LEU:CD1	1:A:292:LEU:CD2[3_654]	1.90	0.30
1:A:292:LEU:CG	1:A:292:LEU:CD2[3_654]	2.00	0.20

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	238/301 (79%)	196 (82%)	30 (13%)	12 (5%)	2	23
1	B	238/301 (79%)	198 (83%)	29 (12%)	11 (5%)	2	24
1	C	238/301 (79%)	196 (82%)	31 (13%)	11 (5%)	2	24
1	D	238/301 (79%)	198 (83%)	27 (11%)	13 (6%)	2	22
All	All	952/1204 (79%)	788 (83%)	117 (12%)	47 (5%)	2	24

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	96	ALA
1	B	36	VAL
1	C	36	VAL
1	D	36	VAL
1	A	230	SER
1	B	96	ALA
1	B	231	SER
1	C	96	ALA
1	C	122	PRO
1	C	230	SER
1	C	231	SER
1	D	96	ALA
1	D	217	GLY
1	D	231	SER
1	A	35	LEU
1	A	122	PRO
1	A	148	PRO
1	A	217	GLY
1	A	231	SER
1	B	35	LEU
1	B	122	PRO

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Mol	Chain	Res	Type
1	B	148	PRO
1	B	217	GLY
1	C	99	PRO
1	C	148	PRO
1	D	122	PRO
1	D	148	PRO
1	D	230	SER
1	A	99	PRO
1	A	178	GLY
1	B	178	GLY
1	B	230	SER
1	C	178	GLY
1	C	217	GLY
1	D	35	LEU
1	D	92	LEU
1	D	99	PRO
1	D	178	GLY
1	A	75	ALA
1	B	42	SER
1	B	124	TRP
1	A	270	ASN
1	C	270	ASN
1	D	270	ASN
1	C	271	PRO
1	D	121	TYR

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	188/236 (80%)	145 (77%)	43 (23%)	1	6
1	B	187/236 (79%)	152 (81%)	35 (19%)	1	11
1	C	187/236 (79%)	148 (79%)	39 (21%)	1	8
1	D	187/236 (79%)	153 (82%)	34 (18%)	1	11
All	All	749/944 (79%)	598 (80%)	151 (20%)	1	9

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	18	PHE
1	A	21	ILE
1	A	30	MET
1	A	44	VAL
1	A	46	ASN
1	A	51	ILE
1	A	55	LEU
1	A	64	LEU
1	A	66	ARG
1	A	70	ARG
1	A	71	ARG
1	A	77	ILE
1	A	79	PHE
1	A	107	THR
1	A	108	LEU
1	A	109	ILE
1	A	119	TYR
1	A	128	ASP
1	A	129	ILE
1	A	148	PRO
1	A	149	LEU
1	A	152	LEU
1	A	155	LEU
1	A	157	LEU
1	A	168	ARG
1	A	169	THR
1	A	173	ILE
1	A	174	THR
1	A	175	LEU
1	A	177	GLU
1	A	214	PHE
1	A	216	MET
1	A	226	ILE
1	A	227	LEU
1	A	232	HIS
1	A	233	VAL
1	A	234	PHE
1	A	245	SER
1	A	253	VAL
1	A	262	LEU
1	A	263	LEU

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Mol	Chain	Res	Type
1	A	288	VAL
1	B	17	LEU
1	B	18	PHE
1	B	30	MET
1	B	44	VAL
1	B	55	LEU
1	B	64	LEU
1	B	66	ARG
1	B	67	THR
1	B	70	ARG
1	B	71	ARG
1	B	79	PHE
1	B	108	LEU
1	B	109	ILE
1	B	119	TYR
1	B	128	ASP
1	B	129	ILE
1	B	148	PRO
1	B	149	LEU
1	B	152	LEU
1	B	155	LEU
1	B	157	LEU
1	B	173	ILE
1	B	174	THR
1	B	175	LEU
1	B	177	GLU
1	B	214	PHE
1	B	216	MET
1	B	218	MET
1	B	226	ILE
1	B	227	LEU
1	B	233	VAL
1	B	245	SER
1	B	262	LEU
1	B	263	LEU
1	B	288	VAL
1	C	14	LEU
1	C	17	LEU
1	C	18	PHE
1	C	30	MET
1	C	44	VAL
1	C	51	ILE

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Mol	Chain	Res	Type
1	C	55	LEU
1	C	59	LEU
1	C	64	LEU
1	C	66	ARG
1	C	67	THR
1	C	70	ARG
1	C	71	ARG
1	C	107	THR
1	C	108	LEU
1	C	109	ILE
1	C	119	TYR
1	C	128	ASP
1	C	129	ILE
1	C	148	PRO
1	C	149	LEU
1	C	152	LEU
1	C	155	LEU
1	C	157	LEU
1	C	168	ARG
1	C	173	ILE
1	C	174	THR
1	C	175	LEU
1	C	177	GLU
1	C	214	PHE
1	C	216	MET
1	C	226	ILE
1	C	227	LEU
1	C	233	VAL
1	C	245	SER
1	C	257	VAL
1	C	262	LEU
1	C	263	LEU
1	C	288	VAL
1	D	17	LEU
1	D	18	PHE
1	D	46	ASN
1	D	51	ILE
1	D	55	LEU
1	D	64	LEU
1	D	66	ARG
1	D	67	THR
1	D	70	ARG

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Mol	Chain	Res	Type
1	D	107	THR
1	D	108	LEU
1	D	109	ILE
1	D	119	TYR
1	D	128	ASP
1	D	129	ILE
1	D	148	PRO
1	D	152	LEU
1	D	155	LEU
1	D	168	ARG
1	D	169	THR
1	D	174	THR
1	D	175	LEU
1	D	177	GLU
1	D	214	PHE
1	D	216	MET
1	D	218	MET
1	D	226	ILE
1	D	227	LEU
1	D	233	VAL
1	D	234	PHE
1	D	245	SER
1	D	263	LEU
1	D	270	ASN
1	D	288	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	GLN

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 ⓘ

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, 95th 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	246/301 (81%)	-0.45	12 (4%)	29	25	102, 158, 255, 434	0
1	B	246/301 (81%)	-0.40	3 (1%)	79	72	144, 184, 265, 350	0
1	C	246/301 (81%)	-0.39	10 (4%)	37	31	147, 196, 279, 349	0
1	D	246/301 (81%)	-0.52	6 (2%)	59	50	97, 154, 257, 361	0
All	All	984/1204 (81%)	-0.44	31 (3%)	47	38	97, 176, 268, 434	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	293	ALA	5.6
1	A	123	GLU	5.6
1	A	6	TRP	5.0
1	B	234	PHE	3.9
1	D	293	ALA	3.8
1	A	232	HIS	3.8
1	A	34	GLY	3.5
1	A	35	LEU	3.3
1	C	44	VAL	3.1
1	A	7	LEU	2.8
1	C	43	SER	2.8
1	A	124	TRP	2.6
1	D	179	VAL	2.6
1	C	245	SER	2.6
1	A	97	LEU	2.5
1	C	45	ALA	2.5
1	B	179	VAL	2.4
1	D	4	ARG	2.4
1	C	95	LEU	2.4
1	D	272	GLN	2.3
1	C	121	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	121	TYR	2.2
1	B	228	VAL	2.2
1	D	270	ASN	2.2
1	C	247	PRO	2.2
1	C	292	LEU	2.1
1	A	5	ASP	2.1
1	A	179	VAL	2.1
1	A	4	ARG	2.1
1	D	6	TRP	2.1
1	C	5	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.