WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 05:39 AM EDT

PDB ID	:	1XVL
Title	:	The three-dimensional structure of MntC from Synechocystis 6803
Authors	:	Rukhman, V.; Anati, R.; Melamed-Frank, M.; Bhattacharyya-Pakrasi, M.; Pakrasi, H.B.; Adir, N.
Deposited on	:	2004-10-28
Resolution	:	2.90 Å(reported)

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

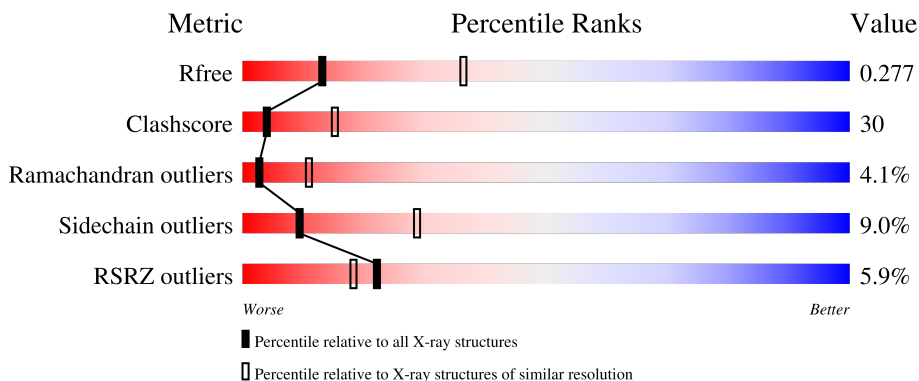|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.90 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		0.277
Clashscore		30
Ramachandran outliers		4.1%
Sidechain outliers		9.0%
RSRZ outliers		5.9%

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	321	2% / 41% / 39% / 6% / 13%
1	B	321	4% / 45% / 33% / 5% · / 16%
1	C	321	7% / 33% / 30% · / 32%

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5996 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 Mn transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total 2177	C 1380	N 358	O 432	S 7	0	0	0
1	B	271	Total 2072	C 1322	N 341	O 402	S 7	0	0	0
1	C	217	Total 1714	C 1095	N 273	O 341	S 5	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	cloning artifact	UNP Q79EF9
A	11	THR	-	cloning artifact	UNP Q79EF9
A	12	SER	-	cloning artifact	UNP Q79EF9
A	13	THR	-	cloning artifact	UNP Q79EF9
A	14	ARG	-	cloning artifact	UNP Q79EF9
A	15	LEU	-	cloning artifact	UNP Q79EF9
A	16	GLN	-	cloning artifact	UNP Q79EF9
A	17	LYS	-	cloning artifact	UNP Q79EF9
A	18	LEU	-	cloning artifact	UNP Q79EF9
A	19	ARG	-	cloning artifact	UNP Q79EF9
A	20	ILE	-	cloning artifact	UNP Q79EF9
A	21	ARG	-	cloning artifact	UNP Q79EF9
A	22	ALA	-	cloning artifact	UNP Q79EF9
A	23	PRO	-	cloning artifact	UNP Q79EF9
A	24	GLY	-	cloning artifact	UNP Q79EF9
A	25	CYS	-	cloning artifact	UNP Q79EF9
B	10	MET	-	cloning artifact	UNP Q79EF9
B	11	THR	-	cloning artifact	UNP Q79EF9
B	12	SER	-	cloning artifact	UNP Q79EF9
B	13	THR	-	cloning artifact	UNP Q79EF9
B	14	ARG	-	cloning artifact	UNP Q79EF9
B	15	LEU	-	cloning artifact	UNP Q79EF9
B	16	GLN	-	cloning artifact	UNP Q79EF9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	17	LYS	-	cloning artifact	UNP Q79EF9
B	18	LEU	-	cloning artifact	UNP Q79EF9
B	19	ARG	-	cloning artifact	UNP Q79EF9
B	20	ILE	-	cloning artifact	UNP Q79EF9
B	21	ARG	-	cloning artifact	UNP Q79EF9
B	22	ALA	-	cloning artifact	UNP Q79EF9
B	23	PRO	-	cloning artifact	UNP Q79EF9
B	24	GLY	-	cloning artifact	UNP Q79EF9
B	25	CYS	-	cloning artifact	UNP Q79EF9
C	10	MET	-	cloning artifact	UNP Q79EF9
C	11	THR	-	cloning artifact	UNP Q79EF9
C	12	SER	-	cloning artifact	UNP Q79EF9
C	13	THR	-	cloning artifact	UNP Q79EF9
C	14	ARG	-	cloning artifact	UNP Q79EF9
C	15	LEU	-	cloning artifact	UNP Q79EF9
C	16	GLN	-	cloning artifact	UNP Q79EF9
C	17	LYS	-	cloning artifact	UNP Q79EF9
C	18	LEU	-	cloning artifact	UNP Q79EF9
C	19	ARG	-	cloning artifact	UNP Q79EF9
C	20	ILE	-	cloning artifact	UNP Q79EF9
C	21	ARG	-	cloning artifact	UNP Q79EF9
C	22	ALA	-	cloning artifact	UNP Q79EF9
C	23	PRO	-	cloning artifact	UNP Q79EF9
C	24	GLY	-	cloning artifact	UNP Q79EF9
C	25	CYS	-	cloning artifact	UNP Q79EF9

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	18	Total 18	O 18	0	0
3	C	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

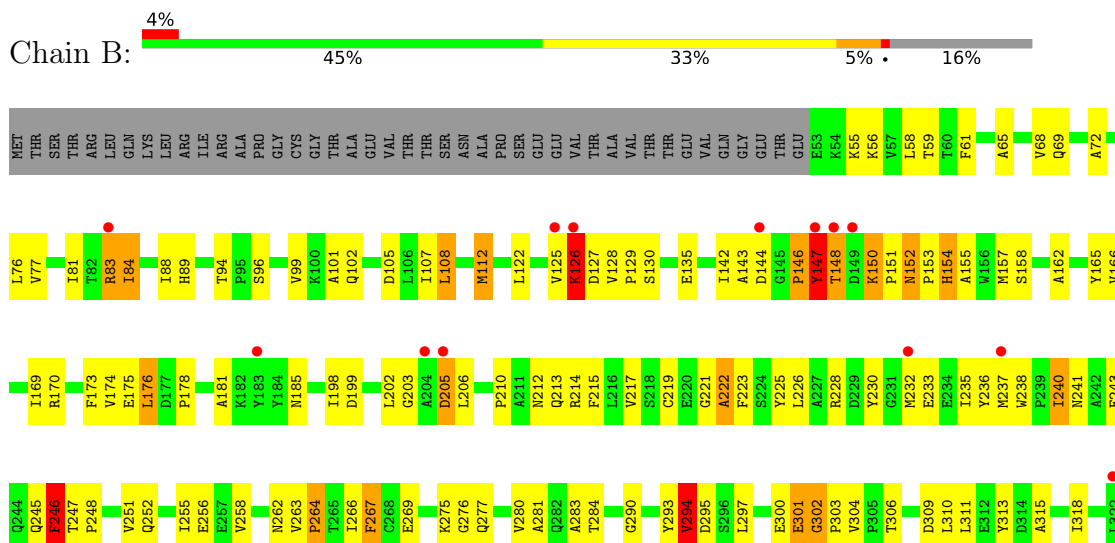These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.
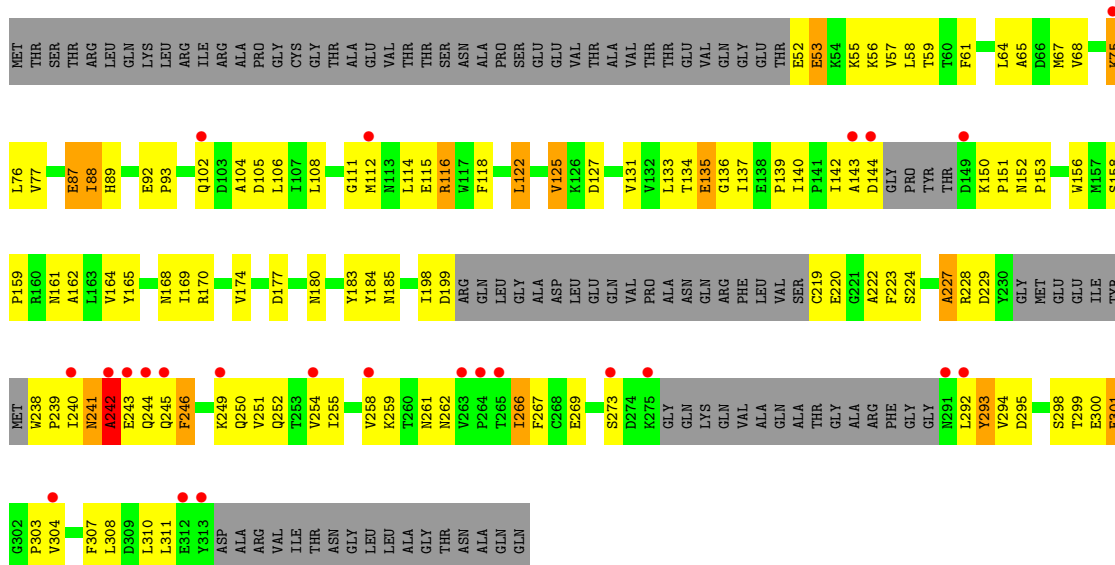
• Molecule 1: Mn transporter
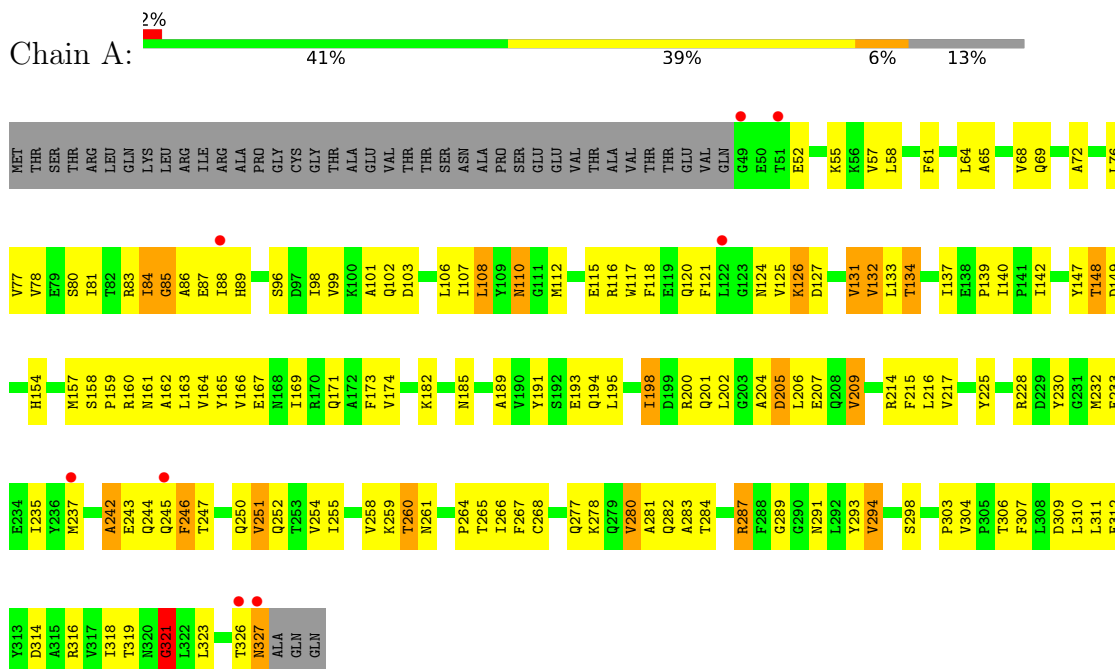
• Molecule 1: Mn transporter

L323 ALA GLY THR ASN ALA GLN GLN

• Molecule 1: Mn transporter

7%

Chain C:　　33%　　30%　•　32%

MET THR SER THR ARG LEU GLN LYS LEU ARG ILE ARG ALA ALA PRO GLY CYS GLY THR ALA GLU VAL VAL THR THR SER ASN ALA PRO SER GLU GLU VAL THR ALA VAL THR THR GLU VAL GLN GLY GLU THR E52 E53 K54 K55 K56 V57 L58 T59 T60 F61 L64 A65 D66 M67 V68 K75

L76 V77 E87 I88 H89 E92 P93 Q102 D103 A104 D105 L106 I107 L108 G111 M112 N113 L114 E115 R116 W117 F118 L122 V125 K126 D127 V131 V132 L133 T134 E135 G136 I137 E138 P139 I140 P141 I142 A143 D144 GLY PRO TYR THR D149 K150 P151 N152 P153 W156 M157 S158

P159 R160 N161 A162 L163 V164 Y165 N168 I169 R170 V174 D177 N180 Y183 Y184 N185 I198 D199 ARG GLN LEU GLY ALA ASP LEU GLU GLN VAL PRO ALA ASN GLN ARG PHE LEU VAL SER C219 E220 G221 A222 F223 S224 A227 R228 D229 Y230 GLY MET GLU GLU ILE TYR

MET W238 P239 I240 N241 A242 E243 Q244 Q245 F246 K249 Q250 V251 Q252 T253 V254 I255 V258 K259 T260 N261 N262 V263 P264 T265 I266 F267 C268 E269 S273 D274 K275 GLY LYS GLN VAL ALA GLN ALA THR GLY ALA ARG PHE GLY GLY N291 L292 Y293 V294 D295 S298 T299 E300 E301

G302 P303 V304 F307 L308 D309 L310 L311 E312 Y313 ASP ALA ARG VAL ILE THR ASN GLY LEU LEU ALA GLY THR ASN ALA GLN GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.55Å 128.55Å 91.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.90 111.33 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.9 (8.00-2.90) 99.6 (111.33-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.289 0.263 , 0.277	Depositor DCC
R_{free} test set	2003 reflections (10.22%)	wwPDB-VP
Wilson B-factor (Å^2)	79.7	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.2	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5996	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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 ⓘ

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	0.36	0/2222	0.66	1/3029 (0.0%)
1	B	0.34	0/2117	0.67	1/2896 (0.0%)
1	C	0.59	2/1749 (0.1%)	0.76	2/2385 (0.1%)
All	All	0.43	2/6088 (0.0%)	0.69	4/8310 (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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	241	ASN	C-N	17.19	1.73	1.34
1	C	242	ALA	C-N	-7.42	1.17	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	242	ALA	O-C-N	-11.61	104.13	122.70
1	C	241	ASN	C-N-CA	-8.91	99.43	121.70
1	A	321	GLY	N-CA-C	-5.47	99.42	113.10
1	B	301	GLU	N-CA-C	-5.07	97.30	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	242	ALA	Mainchain

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	2177	0	2118	127	0
1	B	2072	0	1990	125	0
1	C	1714	0	1652	115	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	8	0	0	1	0
3	B	18	0	0	5	0
3	C	4	0	0	0	0
All	All	5996	0	5760	354	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 30.

All (354) 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:C:241:ASN:C	1:C:242:ALA:N	1.73	1.40
1:C:88:ILE:HD13	1:C:88:ILE:H	1.26	0.99
1:B:58:LEU:HD21	1:B:81:ILE:HD11	1.46	0.98
1:A:237:MET:HG3	1:A:254:VAL:HG21	1.50	0.93
1:C:52:GLU:HG3	1:C:53:GLU:H	1.34	0.93
1:A:214:ARG:HG2	1:A:232:MET:HG2	1.50	0.93
1:B:251:VAL:HG13	1:B:280:VAL:HG12	1.52	0.90
1:B:210:PRO:HG2	1:B:213:GLN:HB2	1.52	0.90
1:A:98:ILE:HD12	1:A:124:ASN:HD21	1.33	0.90
1:B:102:GLN:HE22	1:B:126:LYS:HB2	1.38	0.89
1:C:88:ILE:HD11	1:C:295:ASP:HB3	1.55	0.89
1:B:72:ALA:HB1	1:B:76:LEU:HB2	1.53	0.89
1:C:241:ASN:O	1:C:242:ALA:HB2	1.72	0.89
1:A:200:ARG:NH1	1:B:130:SER:H	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:HD23	1:C:133:LEU:HD11	1.57	0.86
1:A:242:ALA:H	1:A:244:GLN:HG3	1.40	0.85
1:C:61:PHE:HB3	1:C:88:ILE:HG21	1.57	0.85
1:C:241:ASN:C	1:C:242:ALA:CA	2.44	0.85
1:A:148:THR:HG23	1:A:149:ASP:H	1.42	0.84
1:A:217:VAL:HG11	1:A:266:ILE:HG22	1.59	0.84
1:A:84:ILE:HG23	1:A:85:GLY:H	1.42	0.83
1:C:304:VAL:HG13	1:C:310:LEU:HB2	1.61	0.82
1:A:112:MET:HE1	1:A:139:PRO:HB3	1.65	0.79
1:B:112:MET:HE3	1:B:153:PRO:HA	1.64	0.78
1:A:200:ARG:HG3	1:C:301:GLU:HG3	1.65	0.78
1:B:59:THR:HG22	1:B:108:LEU:HB2	1.66	0.78
1:A:312:GLU:O	1:A:316:ARG:HB2	1.85	0.77
1:A:112:MET:HG3	1:A:134:THR:HG21	1.66	0.77
1:C:114:LEU:HB2	1:C:153:PRO:HB2	1.66	0.77
1:A:55:LYS:HB2	1:A:76:LEU:HD22	1.65	0.77
1:B:68:VAL:HG12	1:B:169:ILE:HD12	1.67	0.76
1:B:102:GLN:NE2	1:B:126:LYS:HB2	1.99	0.76
1:A:165:TYR:O	1:A:169:ILE:HG13	1.86	0.75
1:C:116:ARG:HH22	1:C:242:ALA:HA	1.52	0.75
1:C:137:ILE:CG1	1:C:164:VAL:HG21	2.16	0.75
1:B:150:LYS:H	1:B:151:PRO:CD	2.00	0.74
1:B:277:GLN:O	1:B:280:VAL:HG22	1.88	0.74
1:A:102:GLN:HG2	1:A:125:VAL:HG12	1.69	0.74
1:C:161:ASN:O	1:C:164:VAL:HG22	1.88	0.73
1:B:150:LYS:H	1:B:151:PRO:HD2	1.52	0.73
1:B:246:PHE:CE1	1:B:276:GLY:HA3	2.24	0.73
1:A:217:VAL:HA	1:A:235:ILE:O	1.89	0.73
1:A:194:GLN:NE2	1:B:135:GLU:HA	2.04	0.72
1:A:98:ILE:HD12	1:A:124:ASN:ND2	2.05	0.72
1:C:135:GLU:HB3	1:C:168:ASN:OD1	1.90	0.71
1:C:165:TYR:O	1:C:169:ILE:HG13	1.91	0.71
1:A:112:MET:CE	1:A:139:PRO:HB3	2.20	0.71
1:A:194:GLN:O	1:A:198:ILE:HG23	1.91	0.71
1:B:219:CYS:HB3	1:B:238:TRP:CH2	2.26	0.70
1:A:185:ASN:HB2	1:B:146:PRO:HB2	1.73	0.70
1:A:194:GLN:HE21	1:B:135:GLU:HA	1.56	0.70
1:C:249:LYS:O	1:C:252:GLN:HB3	1.92	0.70
1:B:102:GLN:HE22	1:B:126:LYS:CB	2.04	0.70
1:C:162:ALA:HA	1:C:165:TYR:HD2	1.56	0.69
1:B:198:ILE:HD13	1:B:311:LEU:HD13	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ARG:NH2	1:C:242:ALA:HA	2.08	0.69
1:B:251:VAL:O	1:B:255:ILE:HG12	1.93	0.68
1:A:147:TYR:HE1	1:A:242:ALA:HB2	1.58	0.68
1:B:215:PHE:HD2	1:B:235:ILE:HD11	1.58	0.67
1:A:112:MET:CG	1:A:134:THR:HG21	2.23	0.67
1:B:56:LYS:HA	1:B:77:VAL:HG22	1.77	0.66
1:B:221:GLY:O	1:B:223:PHE:N	2.28	0.66
1:C:61:PHE:HB3	1:C:88:ILE:CG2	2.27	0.65
1:C:102:GLN:HG2	1:C:125:VAL:HB	1.77	0.65
1:C:137:ILE:HD11	1:C:164:VAL:HG11	1.78	0.65
1:B:214:ARG:HB3	1:B:232:MET:HA	1.78	0.64
1:C:142:ILE:O	1:C:144:ASP:N	2.30	0.64
1:B:283:ALA:HB3	3:B:910:HOH:O	1.98	0.64
1:C:114:LEU:HB2	1:C:153:PRO:CB	2.27	0.64
1:A:201:GLN:NE2	1:A:312:GLU:HG2	2.13	0.63
1:B:215:PHE:CD2	1:B:235:ILE:HD11	2.33	0.63
1:B:142:ILE:HD11	1:B:152:ASN:HA	1.79	0.63
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.63	0.63
1:C:198:ILE:HD12	1:C:199:ASP:N	2.14	0.62
1:C:55:LYS:HB2	1:C:76:LEU:CD2	2.29	0.62
1:B:258:VAL:HG11	3:B:911:HOH:O	1.99	0.62
1:C:251:VAL:O	1:C:255:ILE:HG13	1.99	0.62
1:B:293:TYR:CD1	1:B:304:VAL:HG21	2.34	0.61
1:A:298:SER:HB3	1:A:303:PRO:O	2.00	0.61
1:A:110:ASN:O	1:A:134:THR:HB	2.01	0.61
1:C:112:MET:SD	1:C:153:PRO:HA	2.41	0.61
1:A:102:GLN:CG	1:A:125:VAL:HG12	2.31	0.61
1:A:84:ILE:CG2	1:A:85:GLY:H	2.11	0.61
1:C:159:PRO:HB3	1:C:198:ILE:HD11	1.82	0.60
1:A:326:THR:HG23	1:A:327:ASN:N	2.16	0.60
1:A:84:ILE:O	1:A:86:ALA:N	2.33	0.60
1:A:217:VAL:CG1	1:A:266:ILE:HG22	2.30	0.60
1:B:256:GLU:HA	3:B:907:HOH:O	2.01	0.60
1:A:108:LEU:HD12	1:A:131:VAL:HG22	1.84	0.60
1:C:88:ILE:HD13	1:C:88:ILE:N	2.08	0.60
1:C:298:SER:HB3	1:C:303:PRO:O	2.00	0.60
1:B:212:ASN:O	1:B:215:PHE:HE1	1.85	0.59
1:B:217:VAL:HG11	1:B:266:ILE:HG22	1.82	0.59
1:A:84:ILE:CG2	1:A:85:GLY:N	2.64	0.59
1:A:215:PHE:CD2	1:A:233:GLU:HB3	2.37	0.59
1:A:87:GLU:OE1	1:A:89:HIS:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:HA	1:A:207:GLU:OE2	2.03	0.59
1:B:68:VAL:HG12	1:B:169:ILE:CD1	2.33	0.58
1:A:101:ALA:HB1	1:A:107:ILE:HD11	1.85	0.58
1:A:140:ILE:HD11	1:A:228:ARG:NH2	2.19	0.58
1:A:84:ILE:HG23	1:A:85:GLY:N	2.17	0.58
1:B:150:LYS:N	1:B:151:PRO:HD2	2.18	0.58
1:A:58:LEU:HD21	1:A:81:ILE:HD11	1.84	0.58
1:A:326:THR:HG23	1:A:327:ASN:H	1.69	0.58
1:A:137:ILE:HG12	1:A:164:VAL:HG21	1.85	0.57
1:A:191:TYR:HA	1:A:194:GLN:OE1	2.04	0.57
1:A:316:ARG:HD2	1:B:175:GLU:OE2	2.04	0.57
1:C:219:CYS:HB3	1:C:238:TRP:CH2	2.40	0.57
1:C:224:SER:O	1:C:227:ALA:HB3	2.04	0.57
1:B:165:TYR:O	1:B:169:ILE:HG12	2.04	0.57
1:A:189:ALA:HB1	1:B:148:THR:HA	1.87	0.57
1:A:293:TYR:CD1	1:A:304:VAL:HG21	2.40	0.57
1:C:250:GLN:O	1:C:254:VAL:HG23	2.05	0.57
1:C:293:TYR:CD1	1:C:304:VAL:HG21	2.40	0.57
1:A:237:MET:O	1:A:250:GLN:HB3	2.04	0.56
1:B:251:VAL:HG13	1:B:280:VAL:CG1	2.32	0.56
1:C:140:ILE:HD11	1:C:228:ARG:HH21	1.70	0.56
1:A:162:ALA:O	1:A:166:VAL:HG13	2.05	0.56
1:A:201:GLN:O	1:A:205:ASP:HB2	2.05	0.56
1:A:161:ASN:O	1:A:164:VAL:HG22	2.06	0.56
1:A:163:LEU:O	1:A:166:VAL:HG22	2.06	0.56
1:C:299:THR:C	1:C:301:GLU:H	2.08	0.56
1:A:140:ILE:HD11	1:A:228:ARG:HH21	1.71	0.55
1:B:72:ALA:HB2	1:B:173:PHE:HE2	1.70	0.55
1:A:148:THR:HG23	1:A:149:ASP:N	2.19	0.55
1:B:84:ILE:HG23	1:B:297:LEU:O	2.05	0.55
1:A:200:ARG:NH2	1:A:200:ARG:HB3	2.22	0.55
1:B:258:VAL:HG11	1:B:284:THR:HG21	1.89	0.55
1:C:137:ILE:HG12	1:C:164:VAL:HG21	1.89	0.55
1:C:304:VAL:CG1	1:C:310:LEU:HB2	2.36	0.55
1:B:55:LYS:HB2	1:B:76:LEU:CD2	2.37	0.55
1:B:178:PRO:HA	1:B:181:ALA:HB2	1.87	0.54
1:B:222:ALA:HB1	1:B:294:VAL:HG11	1.88	0.54
1:C:58:LEU:HD13	1:C:104:ALA:CB	2.37	0.54
1:A:189:ALA:CB	1:B:148:THR:HA	2.38	0.54
1:B:150:LYS:N	1:B:151:PRO:CD	2.68	0.54
1:C:222:ALA:HB1	1:C:294:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TYR:HE1	1:A:242:ALA:CB	2.21	0.54
1:A:244:GLN:C	1:A:246:PHE:H	2.10	0.54
1:C:259:LYS:C	1:C:261:ASN:H	2.10	0.54
1:B:170:ARG:HD2	1:B:185:ASN:OD1	2.08	0.54
1:B:219:CYS:HB2	1:B:269:GLU:OE1	2.08	0.54
1:C:134:THR:CG2	1:C:137:ILE:HB	2.38	0.54
1:A:247:THR:O	1:A:251:VAL:HG13	2.08	0.54
1:B:58:LEU:HD22	1:B:101:ALA:HA	1.90	0.54
1:C:258:VAL:O	1:C:262:ASN:N	2.41	0.54
1:A:65:ALA:HB2	1:A:80:SER:HB2	1.90	0.53
1:C:177:ASP:HB3	1:C:184:TYR:HE2	1.71	0.53
1:C:55:LYS:HB2	1:C:76:LEU:HD22	1.91	0.53
1:C:158:SER:HB3	1:C:161:ASN:HD22	1.73	0.53
1:C:158:SER:CB	1:C:161:ASN:HD22	2.21	0.53
1:A:259:LYS:C	1:A:261:ASN:H	2.12	0.53
1:A:277:GLN:O	1:A:280:VAL:HG13	2.07	0.53
1:C:162:ALA:HA	1:C:165:TYR:CD2	2.42	0.53
1:A:140:ILE:HG12	1:A:225:TYR:CE1	2.44	0.53
1:B:251:VAL:CG1	1:B:280:VAL:HG12	2.31	0.53
1:B:245:GLN:O	1:B:246:PHE:CD2	2.62	0.52
1:A:96:SER:O	1:A:99:VAL:HG12	2.10	0.52
1:B:152:ASN:HD22	1:B:152:ASN:C	2.13	0.52
1:C:180:ASN:HB2	1:C:184:TYR:CE2	2.45	0.52
1:A:251:VAL:O	1:A:255:ILE:HG13	2.09	0.52
1:C:170:ARG:O	1:C:174:VAL:HG13	2.09	0.52
1:C:52:GLU:HG3	1:C:53:GLU:N	2.14	0.52
1:C:241:ASN:O	1:C:242:ALA:CB	2.52	0.52
1:C:134:THR:O	1:C:136:GLY:N	2.43	0.52
1:C:252:GLN:O	1:C:255:ILE:HB	2.10	0.51
1:A:157:MET:SD	1:A:294:VAL:HG12	2.50	0.51
1:B:158:SER:HB2	1:B:225:TYR:HB3	1.93	0.51
1:B:303:PRO:HB2	1:B:313:TYR:CE1	2.45	0.51
1:B:153:PRO:O	1:B:155:ALA:N	2.39	0.51
1:A:108:LEU:CD1	1:A:131:VAL:HG22	2.41	0.51
1:A:278:LYS:O	1:A:281:ALA:HB3	2.10	0.51
1:A:250:GLN:O	1:A:254:VAL:HG23	2.10	0.51
1:C:241:ASN:C	1:C:242:ALA:CB	2.78	0.51
1:A:159:PRO:HG2	1:A:202:LEU:HD22	1.93	0.51
1:C:243:GLU:HG3	1:C:244:GLN:N	2.26	0.51
1:A:264:PRO:HG2	1:A:321:GLY:O	2.11	0.51
1:B:58:LEU:O	1:B:107:ILE:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PHE:CB	1:B:88:ILE:HG21	2.41	0.51
1:C:134:THR:O	1:C:134:THR:HG22	2.11	0.51
1:C:89:HIS:HA	1:C:114:LEU:O	2.11	0.50
1:B:283:ALA:HB1	3:B:908:HOH:O	2.11	0.50
1:C:137:ILE:HG13	1:C:164:VAL:HG21	1.92	0.50
1:C:259:LYS:C	1:C:261:ASN:N	2.63	0.50
1:C:162:ALA:O	1:C:165:TYR:HB2	2.11	0.50
1:C:310:LEU:HD23	1:C:311:LEU:N	2.26	0.50
1:C:58:LEU:HD13	1:C:104:ALA:HB2	1.93	0.50
1:B:143:ALA:HB3	1:B:236:TYR:OH	2.12	0.50
1:B:181:ALA:O	1:B:185:ASN:ND2	2.44	0.50
1:B:306:THR:HG22	1:B:309:ASP:HB2	1.94	0.49
1:B:226:LEU:HD12	1:B:230:TYR:CE2	2.47	0.49
1:A:306:THR:O	1:A:309:ASP:HB2	2.13	0.49
1:C:223:PHE:N	1:C:223:PHE:CD1	2.80	0.49
1:B:72:ALA:HB2	1:B:173:PHE:CE2	2.48	0.49
1:A:193:GLU:CD	1:B:112:MET:H	2.17	0.49
1:B:128:VAL:CG2	1:B:129:PRO:HD2	2.42	0.48
1:C:242:ALA:O	1:C:243:GLU:C	2.52	0.48
1:B:255:ILE:HD11	1:B:280:VAL:HA	1.95	0.48
1:B:198:ILE:CD1	1:B:311:LEU:HD13	2.40	0.48
1:B:252:GLN:O	1:B:255:ILE:HB	2.13	0.48
1:B:198:ILE:HD12	1:B:199:ASP:N	2.29	0.48
1:A:57:VAL:CG1	1:A:108:LEU:HD22	2.44	0.48
1:A:244:GLN:C	1:A:246:PHE:N	2.67	0.48
1:A:110:ASN:O	1:A:132:VAL:HG23	2.13	0.48
1:A:266:ILE:CD1	1:A:280:VAL:HG22	2.43	0.48
1:A:307:PHE:O	1:A:310:LEU:HB3	2.14	0.48
1:A:133:LEU:HD22	1:A:169:ILE:HG12	1.95	0.48
1:A:319:THR:O	1:A:323:LEU:HD13	2.13	0.48
1:B:55:LYS:HB2	1:B:76:LEU:HD21	1.96	0.48
1:B:267:PHE:CD1	1:B:267:PHE:N	2.82	0.48
1:A:182:LYS:HA	1:B:146:PRO:HB3	1.96	0.47
1:B:61:PHE:HB3	1:B:88:ILE:HG21	1.96	0.47
1:C:137:ILE:HD11	1:C:164:VAL:CG1	2.44	0.47
1:A:206:LEU:O	1:A:209:VAL:HG13	2.15	0.47
1:B:246:PHE:CE1	1:B:276:GLY:CA	2.97	0.47
1:C:115:GLU:CG	1:C:118:PHE:HB2	2.45	0.47
1:A:98:ILE:O	1:A:102:GLN:HG3	2.15	0.47
1:A:147:TYR:CE1	1:A:242:ALA:HB2	2.46	0.47
1:C:293:TYR:OH	1:C:303:PRO:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ILE:HG23	1:C:241:ASN:O	2.14	0.47
1:C:299:THR:C	1:C:301:GLU:N	2.68	0.47
1:C:246:PHE:HE2	1:C:251:VAL:CG1	2.28	0.47
1:B:59:THR:HA	1:B:108:LEU:O	2.15	0.46
1:B:89:HIS:HD1	1:B:240:ILE:HD11	1.81	0.46
1:C:266:ILE:HD13	1:C:266:ILE:H	1.80	0.46
1:B:101:ALA:HB1	1:B:107:ILE:HD11	1.98	0.46
1:A:57:VAL:HG11	1:A:108:LEU:HD22	1.97	0.46
1:A:89:HIS:O	1:A:116:ARG:HB2	2.16	0.46
1:B:306:THR:HG23	1:B:309:ASP:H	1.80	0.46
1:C:59:THR:HG21	1:C:65:ALA:N	2.31	0.46
1:C:170:ARG:HD3	1:C:185:ASN:OD1	2.15	0.46
1:C:75:LYS:HD3	1:C:183:TYR:CD2	2.50	0.46
1:C:134:THR:HG22	1:C:137:ILE:HB	1.98	0.46
1:A:202:LEU:HB3	1:A:230:TYR:CZ	2.50	0.46
1:B:152:ASN:HD21	1:B:154:HIS:HD1	1.62	0.46
1:B:280:VAL:HA	3:B:910:HOH:O	2.15	0.46
1:B:304:VAL:HG12	1:B:304:VAL:O	2.15	0.46
1:A:142:ILE:HB	1:A:148:THR:O	2.14	0.46
1:A:159:PRO:HG3	1:A:311:LEU:HD13	1.98	0.46
1:B:240:ILE:HD13	1:B:241:ASN:N	2.31	0.46
1:C:87:GLU:HG3	1:C:87:GLU:O	2.14	0.46
1:B:198:ILE:HD12	1:B:198:ILE:C	2.37	0.45
1:C:55:LYS:HA	1:C:105:ASP:OD2	2.16	0.45
1:B:263:VAL:HA	1:B:264:PRO:HD2	1.75	0.45
1:C:64:LEU:O	1:C:68:VAL:HG23	2.16	0.45
1:A:200:ARG:HH11	1:B:130:SER:H	1.61	0.45
1:A:217:VAL:HB	1:A:235:ILE:HB	1.98	0.45
1:A:244:GLN:HB3	1:A:245:GLN:H	1.32	0.45
1:B:102:GLN:CD	1:B:126:LYS:HB2	2.36	0.45
1:B:128:VAL:HG22	1:B:129:PRO:HD2	1.98	0.45
1:B:152:ASN:HD22	1:B:153:PRO:N	2.15	0.45
1:B:203:GLY:C	1:B:205:ASP:H	2.20	0.45
1:A:314:ASP:O	1:A:318:ILE:HG13	2.17	0.45
1:B:147:TYR:O	1:B:150:LYS:CB	2.65	0.45
1:C:244:GLN:O	1:C:245:GLN:HB2	2.17	0.45
1:C:246:PHE:HE2	1:C:251:VAL:HG11	1.81	0.45
1:A:304:VAL:HG13	1:A:310:LEU:CB	2.47	0.45
1:B:105:ASP:HB3	1:B:176:LEU:HD11	1.99	0.45
1:A:68:VAL:HG23	1:A:78:VAL:HG11	1.97	0.45
1:A:200:ARG:CG	1:C:301:GLU:HG3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LYS:C	1:C:262:ASN:H	2.21	0.45
1:C:269:GLU:HA	1:C:292:LEU:O	2.17	0.45
1:A:304:VAL:HG13	1:A:310:LEU:HA	1.99	0.45
1:B:147:TYR:CE2	1:B:148:THR:HG22	2.51	0.45
1:B:245:GLN:O	1:B:246:PHE:HD2	1.99	0.44
1:C:116:ARG:NH2	1:C:241:ASN:O	2.51	0.44
1:A:267:PHE:CD2	1:A:289:GLY:HA3	2.51	0.44
1:C:115:GLU:HG3	1:C:118:PHE:HB2	1.99	0.44
1:A:68:VAL:CG2	1:A:78:VAL:HG11	2.48	0.44
1:B:174:VAL:HG12	1:B:181:ALA:HA	1.99	0.44
1:C:102:GLN:HE21	1:C:125:VAL:HA	1.83	0.44
1:A:243:GLU:CG	1:A:244:GLN:N	2.81	0.44
1:B:162:ALA:O	1:B:166:VAL:HG23	2.18	0.44
1:B:202:LEU:HG	1:B:315:ALA:HB2	1.99	0.44
1:C:137:ILE:O	1:C:139:PRO:HD3	2.18	0.44
1:A:304:VAL:HG13	1:A:310:LEU:HB2	2.00	0.43
1:B:102:GLN:HA	1:B:125:VAL:HG13	1.98	0.43
1:C:245:GLN:O	1:C:246:PHE:O	2.36	0.43
1:A:98:ILE:HD13	1:A:121:PHE:CD1	2.53	0.43
1:A:115:GLU:CG	1:A:118:PHE:HB2	2.49	0.43
1:C:89:HIS:CG	1:C:241:ASN:HB2	2.52	0.43
1:C:106:LEU:HD11	1:C:131:VAL:HG13	2.00	0.43
1:A:198:ILE:HD11	1:A:311:LEU:HD13	2.00	0.43
1:B:300:GLU:O	1:B:301:GLU:CB	2.67	0.43
1:B:304:VAL:HG13	1:B:310:LEU:CA	2.48	0.43
1:A:86:ALA:O	1:A:88:ILE:HG23	2.18	0.43
1:A:106:LEU:HG	1:A:108:LEU:HD13	2.01	0.43
1:B:102:GLN:OE1	1:B:126:LYS:HB2	2.18	0.43
1:B:301:GLU:O	1:B:302:GLY:O	2.36	0.43
1:A:68:VAL:HG23	1:A:69:GLN:N	2.33	0.43
1:C:118:PHE:CZ	1:C:122:LEU:HD23	2.53	0.43
1:C:111:GLY:O	1:C:112:MET:HB2	2.19	0.43
1:C:114:LEU:HD22	1:C:156:TRP:HZ3	1.83	0.43
1:B:157:MET:HG3	1:B:294:VAL:CG1	2.48	0.42
1:B:94:THR:OG1	1:B:96:SER:HB3	2.18	0.42
1:B:304:VAL:HG13	1:B:310:LEU:HA	2.02	0.42
1:A:158:SER:O	1:A:161:ASN:N	2.53	0.42
1:A:304:VAL:HG13	1:A:310:LEU:CA	2.50	0.42
1:B:147:TYR:CE1	1:B:148:THR:O	2.72	0.42
1:A:115:GLU:HB2	1:A:117:TRP:CE2	2.55	0.42
1:A:182:LYS:HA	1:B:146:PRO:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:VAL:HG12	1:A:304:VAL:O	2.19	0.42
1:C:87:GLU:OE1	1:C:89:HIS:HB2	2.19	0.42
1:C:228:ARG:HD2	1:C:229:ASP:OD1	2.19	0.42
1:C:254:VAL:O	1:C:258:VAL:HG12	2.19	0.42
1:C:293:TYR:CD1	1:C:293:TYR:N	2.87	0.42
1:A:61:PHE:CE2	1:A:64:LEU:HG	2.55	0.42
1:A:255:ILE:O	1:A:258:VAL:HG12	2.20	0.42
1:B:61:PHE:HB3	1:B:88:ILE:CG2	2.50	0.42
1:C:241:ASN:C	1:C:242:ALA:HB2	2.34	0.42
1:C:246:PHE:CE2	1:C:251:VAL:CG1	3.02	0.42
1:A:126:LYS:HB3	1:A:127:ASP:H	1.73	0.42
1:A:258:VAL:HG13	1:A:259:LYS:N	2.35	0.42
1:B:206:LEU:HD22	1:B:232:MET:HE1	2.02	0.42
1:B:267:PHE:CZ	1:B:318:ILE:HA	2.54	0.42
1:A:72:ALA:HB2	1:A:173:PHE:HE2	1.85	0.42
1:A:243:GLU:HB3	3:A:903:HOH:O	2.20	0.42
1:A:160:ARG:HG2	1:A:160:ARG:HH21	1.84	0.41
1:B:146:PRO:HG2	1:B:147:TYR:H	1.84	0.41
1:B:142:ILE:HG22	1:B:144:ASP:H	1.85	0.41
1:C:56:LYS:HA	1:C:77:VAL:HG13	2.02	0.41
1:C:246:PHE:CE2	1:C:251:VAL:HG12	2.56	0.41
1:A:101:ALA:CB	1:A:107:ILE:HD11	2.50	0.41
1:B:217:VAL:HG13	1:B:266:ILE:HA	2.02	0.41
1:A:243:GLU:HG2	1:A:244:GLN:H	1.85	0.41
1:C:159:PRO:HB3	1:C:198:ILE:CD1	2.47	0.41
1:C:220:GLU:C	1:C:222:ALA:H	2.23	0.41
1:C:241:ASN:CA	1:C:242:ALA:N	2.72	0.41
1:C:255:ILE:O	1:C:258:VAL:HG12	2.20	0.41
1:B:125:VAL:O	1:B:126:LYS:C	2.58	0.41
1:C:67:MET:HG2	1:C:307:PHE:CD2	2.56	0.41
1:B:247:THR:HA	1:B:248:PRO:HD3	1.91	0.41
1:A:167:GLU:HG3	1:A:171:GLN:HE21	1.86	0.41
1:A:171:GLN:O	1:A:174:VAL:HG22	2.21	0.41
1:B:226:LEU:HD12	1:B:230:TYR:HE2	1.83	0.41
1:B:246:PHE:O	1:B:246:PHE:CG	2.74	0.41
1:B:266:ILE:HD11	1:B:281:ALA:HB2	2.03	0.41
1:C:150:LYS:HA	1:C:151:PRO:HD2	1.85	0.41
1:C:177:ASP:HB3	1:C:184:TYR:CE2	2.52	0.41
1:C:304:VAL:O	1:C:304:VAL:HG12	2.21	0.41
1:A:268:CYS:O	1:A:291:ASN:HA	2.21	0.40
1:B:65:ALA:O	1:B:69:GLN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ALA:N	1:C:244:GLN:HG2	2.35	0.40
1:A:252:GLN:O	1:A:255:ILE:HB	2.21	0.40
1:C:92:GLU:HA	1:C:93:PRO:HD2	1.93	0.40
1:C:152:ASN:HA	1:C:153:PRO:HD2	1.81	0.40
1:A:133:LEU:CD2	1:A:169:ILE:HG12	2.51	0.40
1:B:246:PHE:HE1	1:B:276:GLY:HA3	1.79	0.40
1:B:94:THR:C	1:B:96:SER:N	2.75	0.40
1:B:206:LEU:HD22	1:B:232:MET:CE	2.51	0.40
1:C:142:ILE:HD12	1:C:142:ILE:HA	1.98	0.40
1:A:265:THR:HA	1:A:287:ARG:O	2.22	0.40
1:B:154:HIS:HD2	1:B:295:ASP:OD1	2.04	0.40
1:B:304:VAL:CG1	1:B:310:LEU:HB2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/321 (86%)	229 (83%)	38 (14%)	10 (4%)	3	14
1	B	269/321 (84%)	224 (83%)	32 (12%)	13 (5%)	2	8
1	C	207/321 (64%)	161 (78%)	38 (18%)	8 (4%)	3	12
All	All	753/963 (78%)	614 (82%)	108 (14%)	31 (4%)	3	11

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	A	85	GLY
1	A	148	THR
1	A	246	PHE
1	B	126	LYS

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Mol	Chain	Res	Type
1	B	154	HIS
1	B	222	ALA
1	B	246	PHE
1	C	135	GLU
1	C	143	ALA
1	C	242	ALA
1	C	246	PHE
1	A	126	LYS
1	A	283	ALA
1	B	84	ILE
1	B	127	ASP
1	B	146	PRO
1	B	150	LYS
1	B	302	GLY
1	C	127	ASP
1	C	227	ALA
1	B	147	TYR
1	C	239	PRO
1	A	154	HIS
1	A	321	GLY
1	C	116	ARG
1	A	260	THR
1	B	290	GLY
1	B	294	VAL
1	A	242	ALA
1	B	264	PRO

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	236/272 (87%)	213 (90%)	23 (10%)	8	25
1	B	218/272 (80%)	197 (90%)	21 (10%)	8	25
1	C	190/272 (70%)	176 (93%)	14 (7%)	13	38
All	All	644/816 (79%)	586 (91%)	58 (9%)	9	29

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	77	VAL
1	A	83	ARG
1	A	103	ASP
1	A	108	LEU
1	A	110	ASN
1	A	120	GLN
1	A	131	VAL
1	A	132	VAL
1	A	134	THR
1	A	195	LEU
1	A	198	ILE
1	A	205	ASP
1	A	209	VAL
1	A	216	LEU
1	A	251	VAL
1	A	260	THR
1	A	280	VAL
1	A	282	GLN
1	A	284	THR
1	A	287	ARG
1	A	294	VAL
1	A	327	ASN
1	B	83	ARG
1	B	99	VAL
1	B	108	LEU
1	B	112	MET
1	B	122	LEU
1	B	126	LYS
1	B	147	TYR
1	B	148	THR
1	B	152	ASN
1	B	176	LEU
1	B	205	ASP
1	B	228	ARG
1	B	233	GLU
1	B	237	MET
1	B	240	ILE
1	B	243	GLU
1	B	246	PHE
1	B	262	ASN
1	B	267	PHE

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Mol	Chain	Res	Type
1	B	275	LYS
1	B	294	VAL
1	C	53	GLU
1	C	57	VAL
1	C	75	LYS
1	C	87	GLU
1	C	88	ILE
1	C	122	LEU
1	C	125	VAL
1	C	266	ILE
1	C	267	PHE
1	C	273	SER
1	C	293	TYR
1	C	300	GLU
1	C	301	GLU
1	C	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	161	ASN
1	A	171	GLN
1	A	201	GLN
1	A	213	GLN
1	A	282	GLN
1	B	110	ASN
1	B	120	GLN
1	B	152	ASN
1	B	201	GLN
1	B	277	GLN
1	C	124	ASN
1	C	180	ASN
1	C	187	ASN
1	C	291	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 3 ligands modelled in this entry, 3 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	241:ASN	C	242:ALA	N	1.73
1	C	242:ALA	C	243:GLU	N	1.17

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	279/321 (86%)	0.29	8 (2%)	51	47	39, 58, 75, 100	0
1	B	271/321 (84%)	0.24	13 (4%)	30	27	32, 58, 84, 90	0
1	C	217/321 (67%)	0.63	24 (11%)	5	4	46, 72, 127, 139	0
All	All	767/963 (79%)	0.37	45 (5%)	22	18	32, 61, 98, 139	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	263	VAL	9.5
1	B	148	THR	7.5
1	A	237	MET	6.4
1	C	243	GLU	5.5
1	A	327	ASN	5.3
1	C	244	GLN	4.3
1	A	326	THR	4.3
1	B	147	TYR	4.1
1	C	149	ASP	4.1
1	C	275	LYS	3.9
1	A	51	THR	3.9
1	B	149	ASP	3.7
1	C	265	THR	3.7
1	C	313	TYR	3.5
1	A	245	GLN	3.3
1	C	312	GLU	3.2
1	C	144	ASP	3.2
1	B	322	LEU	3.1
1	B	144	ASP	3.1
1	C	112	MET	3.0
1	C	273	SER	3.0
1	A	49	GLY	3.0
1	C	240	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	249	LYS	2.9
1	C	264	PRO	2.9
1	B	232	MET	2.9
1	C	143	ALA	2.8
1	B	204	ALA	2.8
1	C	254	VAL	2.7
1	C	292	LEU	2.6
1	A	88	ILE	2.5
1	C	245	GLN	2.5
1	B	237	MET	2.4
1	B	183	TYR	2.4
1	C	258	VAL	2.4
1	B	126	LYS	2.3
1	B	205	ASP	2.3
1	A	122	LEU	2.2
1	C	291	ASN	2.2
1	C	242	ALA	2.2
1	C	75	LYS	2.1
1	B	125	VAL	2.1
1	C	102	GLN	2.1
1	B	83	ARG	2.1
1	C	304	VAL	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	B	900	1/1	0.88	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	C	900	1/1	0.94	0.09	69,69,69,69	0
2	MN	A	900	1/1	0.97	0.16	39,39,39,39	0

6.5　Other polymers ⓘ

There are no such residues in this entry.