Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 03:45 PM EST

PDB ID	:	3BQ4
Title	:	Crystal Structure of Ad35 fiber knob
Authors	:	Pache, L.; Venkataraman, S.; Nemerow, G.R.; Reddy, V.S.
Deposited on	:	2007-12-19
Resolution	:	2.70 Å(reported)

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

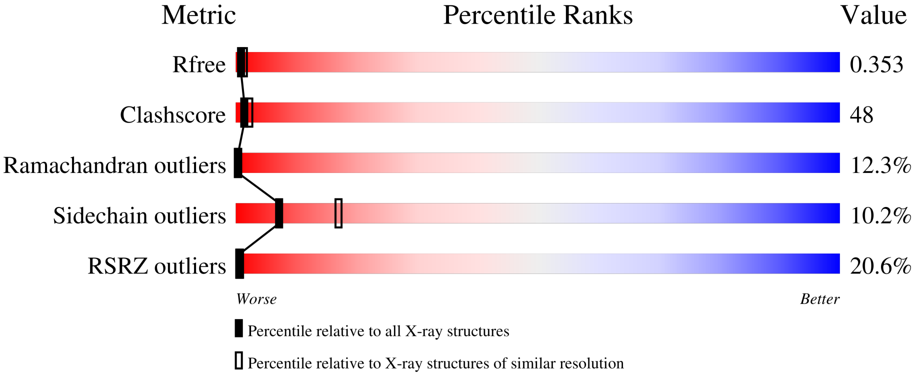
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

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

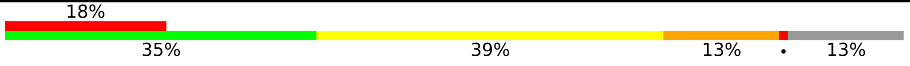
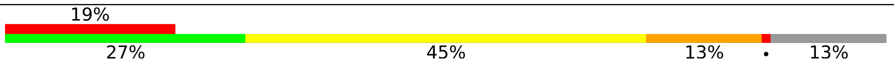
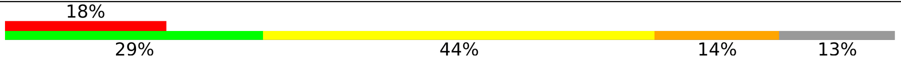
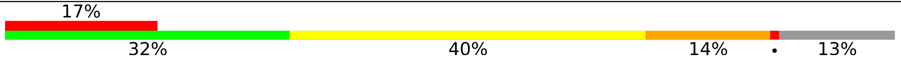
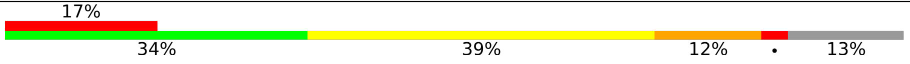
The reported resolution of this entry is 2.70 Å.

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



Metric	**Whole archive (#Entries)**	**Similar resolution (#Entries, resolution range(Å))**
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	**Chain**	**Length**	**Quality of chain**
1	A	220	
1	B	220	
1	D	220	
1	E	220	
1	F	220	

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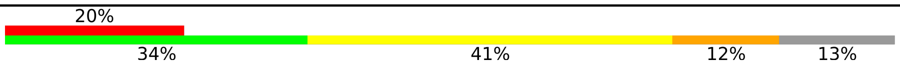
Mol	**Chain**	**Length**	**Quality of chain**
1	G	220	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8976 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 Fiber.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	192	1496	944	240	305	7	0	0	0
1	B	192	1496	944	240	305	7	0	0	0
1	D	192	1496	944	240	305	7	0	0	0
1	E	192	1496	944	240	305	7	0	0	0
1	F	192	1496	944	240	305	7	0	0	0
1	G	192	1496	944	240	305	7	0	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLY	-	expression tag	UNP Q7T925
A	105	SER	-	expression tag	UNP Q7T925
A	106	HIS	-	expression tag	UNP Q7T925
A	107	MET	-	expression tag	UNP Q7T925
A	108	ALA	-	expression tag	UNP Q7T925
A	109	SER	-	expression tag	UNP Q7T925
A	110	MET	-	expression tag	UNP Q7T925
A	111	THR	-	expression tag	UNP Q7T925
A	112	GLY	-	expression tag	UNP Q7T925
A	113	GLY	-	expression tag	UNP Q7T925
A	114	GLN	-	expression tag	UNP Q7T925
A	115	GLN	-	expression tag	UNP Q7T925
A	116	MET	-	expression tag	UNP Q7T925
A	117	GLY	-	expression tag	UNP Q7T925
A	118	ARG	-	expression tag	UNP Q7T925
A	119	GLY	-	expression tag	UNP Q7T925
A	120	SER	-	expression tag	UNP Q7T925

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Chain	Residue	Modelled	Actual	Comment	Reference
B	104	GLY	-	expression tag	UNP Q7T925
B	105	SER	-	expression tag	UNP Q7T925
B	106	HIS	-	expression tag	UNP Q7T925
B	107	MET	-	expression tag	UNP Q7T925
B	108	ALA	-	expression tag	UNP Q7T925
B	109	SER	-	expression tag	UNP Q7T925
B	110	MET	-	expression tag	UNP Q7T925
B	111	THR	-	expression tag	UNP Q7T925
B	112	GLY	-	expression tag	UNP Q7T925
B	113	GLY	-	expression tag	UNP Q7T925
B	114	GLN	-	expression tag	UNP Q7T925
B	115	GLN	-	expression tag	UNP Q7T925
B	116	MET	-	expression tag	UNP Q7T925
B	117	GLY	-	expression tag	UNP Q7T925
B	118	ARG	-	expression tag	UNP Q7T925
B	119	GLY	-	expression tag	UNP Q7T925
B	120	SER	-	expression tag	UNP Q7T925
D	104	GLY	-	expression tag	UNP Q7T925
D	105	SER	-	expression tag	UNP Q7T925
D	106	HIS	-	expression tag	UNP Q7T925
D	107	MET	-	expression tag	UNP Q7T925
D	108	ALA	-	expression tag	UNP Q7T925
D	109	SER	-	expression tag	UNP Q7T925
D	110	MET	-	expression tag	UNP Q7T925
D	111	THR	-	expression tag	UNP Q7T925
D	112	GLY	-	expression tag	UNP Q7T925
D	113	GLY	-	expression tag	UNP Q7T925
D	114	GLN	-	expression tag	UNP Q7T925
D	115	GLN	-	expression tag	UNP Q7T925
D	116	MET	-	expression tag	UNP Q7T925
D	117	GLY	-	expression tag	UNP Q7T925
D	118	ARG	-	expression tag	UNP Q7T925
D	119	GLY	-	expression tag	UNP Q7T925
D	120	SER	-	expression tag	UNP Q7T925
E	104	GLY	-	expression tag	UNP Q7T925
E	105	SER	-	expression tag	UNP Q7T925
E	106	HIS	-	expression tag	UNP Q7T925
E	107	MET	-	expression tag	UNP Q7T925
E	108	ALA	-	expression tag	UNP Q7T925
E	109	SER	-	expression tag	UNP Q7T925
E	110	MET	-	expression tag	UNP Q7T925
E	111	THR	-	expression tag	UNP Q7T925

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Chain	Residue	Modelled	Actual	Comment	Reference
E	112	GLY	-	expression tag	UNP Q7T925
E	113	GLY	-	expression tag	UNP Q7T925
E	114	GLN	-	expression tag	UNP Q7T925
E	115	GLN	-	expression tag	UNP Q7T925
E	116	MET	-	expression tag	UNP Q7T925
E	117	GLY	-	expression tag	UNP Q7T925
E	118	ARG	-	expression tag	UNP Q7T925
E	119	GLY	-	expression tag	UNP Q7T925
E	120	SER	-	expression tag	UNP Q7T925
F	104	GLY	-	expression tag	UNP Q7T925
F	105	SER	-	expression tag	UNP Q7T925
F	106	HIS	-	expression tag	UNP Q7T925
F	107	MET	-	expression tag	UNP Q7T925
F	108	ALA	-	expression tag	UNP Q7T925
F	109	SER	-	expression tag	UNP Q7T925
F	110	MET	-	expression tag	UNP Q7T925
F	111	THR	-	expression tag	UNP Q7T925
F	112	GLY	-	expression tag	UNP Q7T925
F	113	GLY	-	expression tag	UNP Q7T925
F	114	GLN	-	expression tag	UNP Q7T925
F	115	GLN	-	expression tag	UNP Q7T925
F	116	MET	-	expression tag	UNP Q7T925
F	117	GLY	-	expression tag	UNP Q7T925
F	118	ARG	-	expression tag	UNP Q7T925
F	119	GLY	-	expression tag	UNP Q7T925
F	120	SER	-	expression tag	UNP Q7T925
G	104	GLY	-	expression tag	UNP Q7T925
G	105	SER	-	expression tag	UNP Q7T925
G	106	HIS	-	expression tag	UNP Q7T925
G	107	MET	-	expression tag	UNP Q7T925
G	108	ALA	-	expression tag	UNP Q7T925
G	109	SER	-	expression tag	UNP Q7T925
G	110	MET	-	expression tag	UNP Q7T925
G	111	THR	-	expression tag	UNP Q7T925
G	112	GLY	-	expression tag	UNP Q7T925
G	113	GLY	-	expression tag	UNP Q7T925
G	114	GLN	-	expression tag	UNP Q7T925
G	115	GLN	-	expression tag	UNP Q7T925
G	116	MET	-	expression tag	UNP Q7T925
G	117	GLY	-	expression tag	UNP Q7T925
G	118	ARG	-	expression tag	UNP Q7T925
G	119	GLY	-	expression tag	UNP Q7T925

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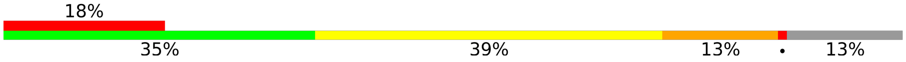
Chain	Residue	Modelled	Actual	Comment	Reference
G	120	SER	-	expression tag	UNP Q7T925

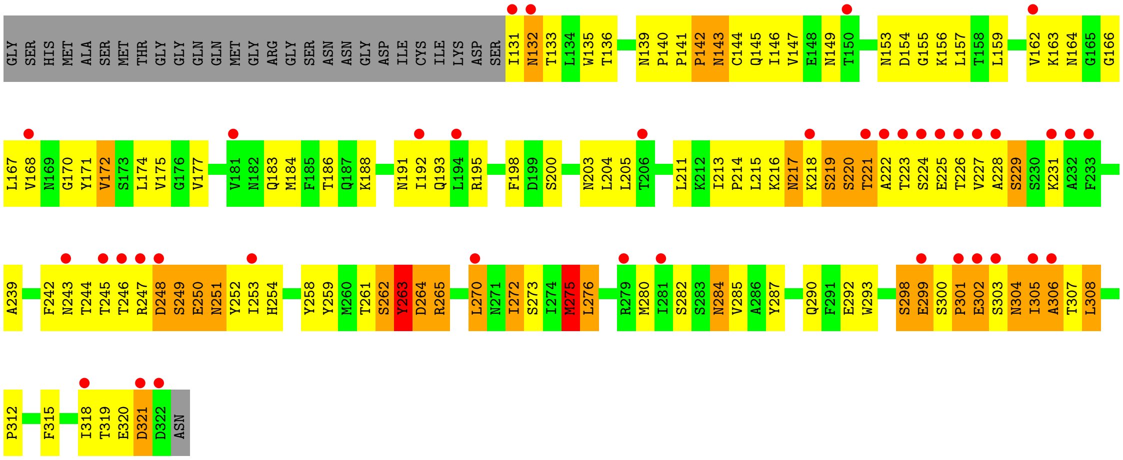
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fiber

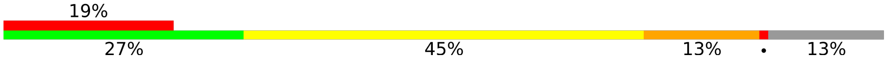
Chain A:

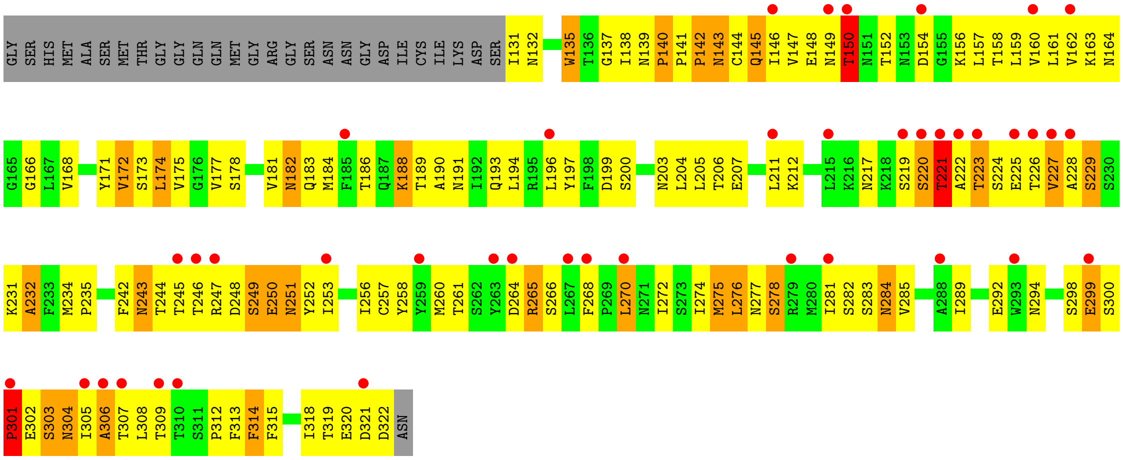




- Molecule 1: Fiber

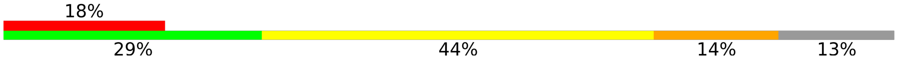
Chain B:

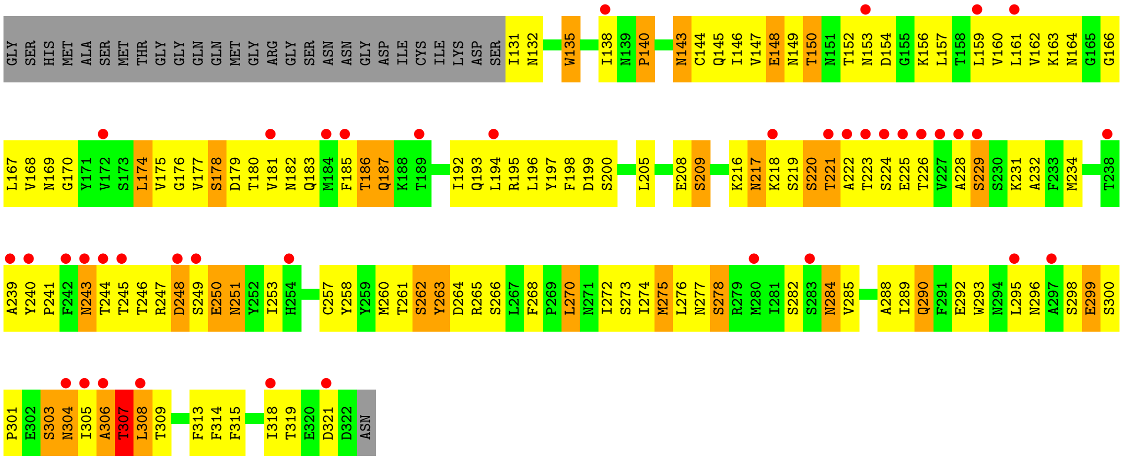




- Molecule 1: Fiber

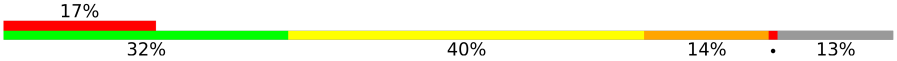
Chain D:

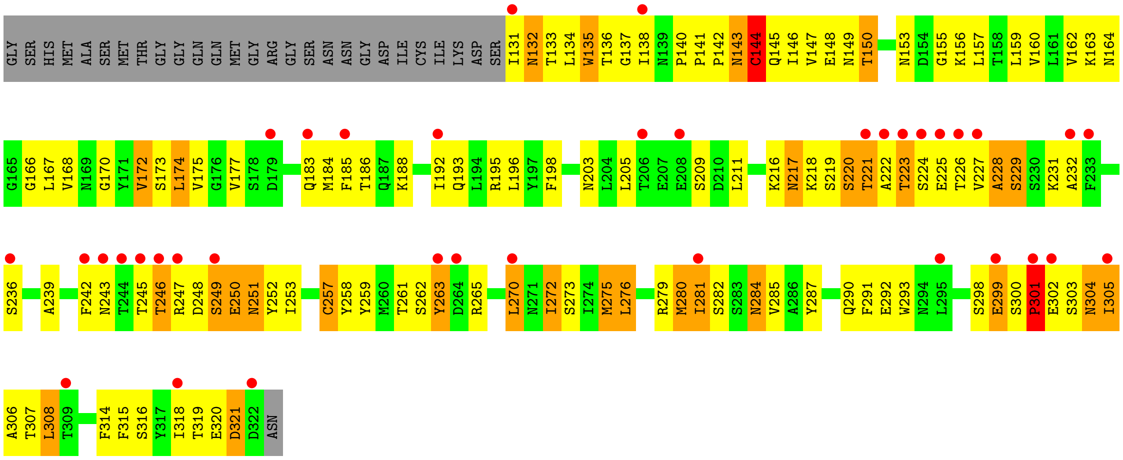




- Molecule 1: Fiber

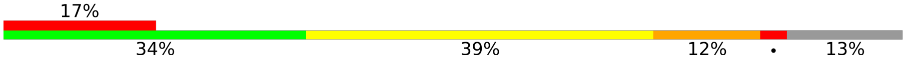
Chain E:

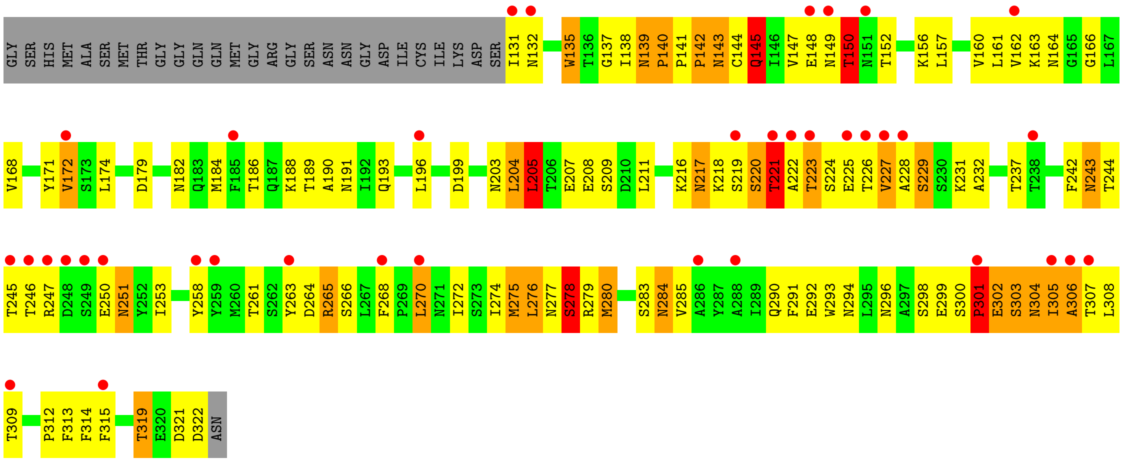




- Molecule 1: Fiber

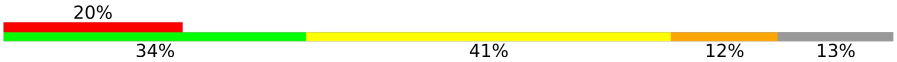
Chain F:

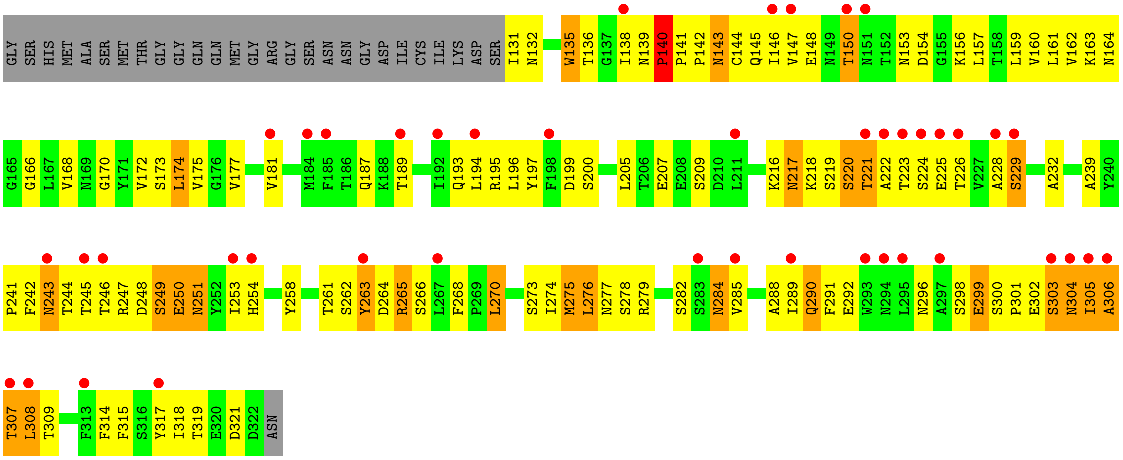




- Molecule 1: Fiber

Chain G:


20%
34%
41%
12%
13%


GLY
SER
HIS
MET
ALA
SER
MET
THR
GLY
GLY
GLN
GLN
MET
GLY
ARG
GLY
SER
ASN
ASN
GLY
ASP
ILE
CYS
ILE
LYS
ASP
SER
I131
N132
W135
T136
G137
I138
N139
P140
P141
P142
N143
C144
Q145
I146
V147
E148
N149
T150
N151
T152
N153
D154
G155
K156
L157
T158
L159
V160
L161
V162
K163
N164
G165
G166
L167
V168
N169
G170
Y171
V172
S173
L174
V175
G176
V177
V181
M184
F185
T186
Q187
K188
T189
I192
Q193
L194
R195
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L205
T206
E207
E208
S209
D210
L211
K216
N217
K218
S219
S220
T221
A222
T223
S224
E225
T226
V227
A228
S229
A232
A239
Y240
P241
F242
N243
T244
T245
T246
R247
D248
S249
E250
N251
Y252
I253
H254
Y258
T261
S262
Y263
D264
R265
S266
L267
F268
P269
L270
S273
I274
M275
L276
N277
S278
R279
S282
S283
N284
V285
A288
I289
Q290
F291
E292
W293
N294
L295
N296
A297
S298
E299
S300
P301
E302
S303
N304
I305
A306
T307
L308
T309
F313
F314
F315
S316
Y317
I318
T319
E320
D321
D322
ASN

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	173.91Å 173.91Å 154.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.03 – 2.70 46.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.5 (46.03-2.70) 91.5 (46.03-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.332 , 0.352 0.332 , 0.353	Depositor DCC
R_{free} test set	2911 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	62.8	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.8	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.49, $< L^2 >$ = 0.32	Xtriage
Estimated twinning fraction	0.468 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	8976	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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	0.50	0/1527	0.80	1/2084 (0.0%)
1	B	0.48	0/1527	0.82	1/2084 (0.0%)
1	D	0.47	0/1527	0.75	1/2084 (0.0%)
1	E	0.50	1/1527 (0.1%)	0.80	1/2084 (0.0%)
1	F	0.49	0/1527	0.82	1/2084 (0.0%)
1	G	0.48	0/1527	0.75	1/2084 (0.0%)
All	All	0.49	1/9162 (0.0%)	0.79	6/12504 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	144	CYS	CB-SG	-6.08	1.72	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	221	THR	N-CA-C	-7.55	90.62	111.00
1	A	221	THR	N-CA-C	-7.17	91.64	111.00
1	G	221	THR	N-CA-C	-6.30	94.00	111.00
1	D	221	THR	N-CA-C	-6.18	94.31	111.00
1	B	221	THR	N-CA-C	-5.64	95.76	111.00
1	F	221	THR	N-CA-C	-5.63	95.78	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1496	0	1453	153	1
1	B	1496	0	1453	154	0
1	D	1496	0	1453	160	0
1	E	1496	0	1453	149	1
1	F	1496	0	1453	133	0
1	G	1496	0	1453	150	0
All	All	8976	0	8718	840	1

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 48.

All (840) 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:E:217:ASN:ND2	1:E:224:SER:H	1.57	1.00
1:D:261:THR:HG22	1:D:301:PRO:HG3	1.45	0.98
1:A:143:ASN:HD21	1:A:157:LEU:H	1.09	0.96
1:B:268:PHE:HE1	1:B:300:SER:HA	1.27	0.96
1:F:242:PHE:CE1	1:F:277:ASN:ND2	2.38	0.92
1:F:225:GLU:HG3	1:F:226:THR:H	1.33	0.91
1:D:196:LEU:HA	1:D:209:SER:HB3	1.50	0.90
1:A:164:ASN:ND2	1:B:164:ASN:HD21	1.69	0.89
1:D:245:THR:HG22	1:D:246:THR:H	1.35	0.88
1:G:219:SER:HB2	1:G:224:SER:HB2	1.52	0.88
1:G:245:THR:HG22	1:G:246:THR:H	1.39	0.87
1:G:140:PRO:O	1:G:156:LYS:HE2	1.75	0.87
1:A:174:LEU:HD23	1:A:175:VAL:N	1.90	0.87
1:D:174:LEU:HD23	1:D:175:VAL:H	1.39	0.87
1:G:172:VAL:HG21	1:G:291:PHE:CE2	2.10	0.87
1:D:217:ASN:H	1:D:217:ASN:HD22	1.23	0.86
1:E:164:ASN:ND2	1:F:164:ASN:HD21	1.74	0.86
1:E:217:ASN:ND2	1:E:217:ASN:H	1.72	0.85
1:G:197:TYR:H	1:G:209:SER:HB3	1.41	0.85
1:D:217:ASN:ND2	1:D:224:SER:HB3	1.90	0.85
1:E:163:LYS:HE2	1:E:319:THR:HG21	1.59	0.85
1:D:270:LEU:HD23	1:D:270:LEU:H	1.39	0.85
1:D:174:LEU:HD23	1:D:175:VAL:N	1.91	0.85
1:A:164:ASN:HD21	1:D:164:ASN:ND2	1.75	0.84
1:B:225:GLU:HG3	1:B:226:THR:H	1.41	0.84
1:D:140:PRO:O	1:D:156:LYS:HE2	1.77	0.84
1:A:217:ASN:ND2	1:A:224:SER:H	1.77	0.83
1:D:282:SER:HB3	1:D:284:ASN:ND2	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:GLY:O	1:G:319:THR:HG22	1.77	0.83
1:E:219:SER:HB2	1:E:224:SER:HB2	1.61	0.83
1:E:193:GLN:HB3	1:E:292:GLU:HG3	1.59	0.82
1:B:142:PRO:HB3	1:B:177:VAL:HG21	1.60	0.82
1:G:217:ASN:H	1:G:217:ASN:HD22	1.24	0.82
1:F:217:ASN:HD21	1:F:224:SER:HB3	1.45	0.82
1:B:245:THR:HG22	1:B:246:THR:H	1.42	0.82
1:G:163:LYS:HE2	1:G:232:ALA:O	1.81	0.81
1:E:220:SER:HB3	1:E:222:ALA:H	1.46	0.81
1:F:268:PHE:HE1	1:F:300:SER:HA	1.44	0.81
1:G:225:GLU:HG3	1:G:226:THR:H	1.46	0.81
1:F:242:PHE:HE1	1:F:277:ASN:ND2	1.80	0.80
1:F:245:THR:HG22	1:F:246:THR:H	1.45	0.80
1:A:216:LYS:HB2	1:A:223:THR:HB	1.64	0.80
1:E:245:THR:HG22	1:E:246:THR:H	1.45	0.80
1:D:225:GLU:HG3	1:D:226:THR:H	1.46	0.80
1:A:219:SER:HB2	1:A:224:SER:HB2	1.64	0.79
1:A:220:SER:HB3	1:A:222:ALA:H	1.48	0.79
1:G:261:THR:HG22	1:G:301:PRO:HG3	1.63	0.79
1:B:193:GLN:HB3	1:B:292:GLU:HG3	1.62	0.79
1:D:261:THR:HG22	1:D:301:PRO:CG	2.11	0.79
1:F:219:SER:HB2	1:F:224:SER:HB2	1.65	0.79
1:E:216:LYS:HB2	1:E:223:THR:HB	1.65	0.78
1:G:159:LEU:HD13	1:G:172:VAL:HG22	1.65	0.78
1:E:164:ASN:HD22	1:F:164:ASN:HD21	1.26	0.78
1:G:146:ILE:HD12	1:G:181:VAL:HG11	1.65	0.78
1:G:217:ASN:H	1:G:217:ASN:ND2	1.82	0.78
1:B:272:ILE:HA	1:B:292:GLU:O	1.84	0.78
1:E:143:ASN:HD21	1:E:157:LEU:H	1.30	0.78
1:A:219:SER:CB	1:A:224:SER:HB2	2.13	0.78
1:G:284:ASN:HD22	1:G:284:ASN:H	1.32	0.78
1:D:143:ASN:HA	1:D:153:ASN:HD22	1.49	0.77
1:A:193:GLN:HB3	1:A:292:GLU:HG3	1.66	0.77
1:G:172:VAL:HG23	1:G:315:PHE:HE2	1.48	0.77
1:E:217:ASN:HD21	1:E:224:SER:H	1.31	0.77
1:G:264:ASP:OD2	1:G:266:SER:HB2	1.84	0.77
1:B:306:ALA:C	1:B:308:LEU:H	1.87	0.77
1:G:268:PHE:HE1	1:G:300:SER:HA	1.49	0.77
1:A:164:ASN:HD21	1:D:164:ASN:HD21	1.32	0.77
1:B:268:PHE:CE1	1:B:300:SER:HA	2.18	0.77
1:D:298:SER:O	1:D:299:GLU:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:CYS:O	1:E:153:ASN:HA	1.85	0.76
1:D:219:SER:HB2	1:D:224:SER:HB2	1.67	0.76
1:D:277:ASN:HA	1:D:288:ALA:HB3	1.67	0.76
1:E:219:SER:CB	1:E:224:SER:HB2	2.16	0.76
1:E:298:SER:O	1:E:299:GLU:HB2	1.86	0.76
1:E:300:SER:OG	1:E:301:PRO:HD2	1.86	0.75
1:E:174:LEU:HD13	1:E:192:ILE:HD12	1.66	0.75
1:A:250:GLU:HB2	1:D:309:THR:HG21	1.68	0.75
1:E:259:TYR:HE2	1:E:301:PRO:HG2	1.50	0.75
1:E:143:ASN:C	1:E:143:ASN:HD22	1.90	0.74
1:G:298:SER:O	1:G:299:GLU:HB2	1.87	0.74
1:G:196:LEU:HA	1:G:209:SER:HB2	1.70	0.74
1:A:315:PHE:HA	1:D:314:PHE:CE1	2.23	0.74
1:B:247:ARG:O	1:B:250:GLU:HG2	1.88	0.74
1:D:166:GLY:O	1:D:319:THR:HG22	1.87	0.74
1:F:309:THR:HG21	1:G:250:GLU:HB2	1.67	0.74
1:A:205:LEU:HD21	1:A:284:ASN:O	1.87	0.74
1:B:264:ASP:OD2	1:B:266:SER:HB2	1.88	0.73
1:E:275:MET:O	1:E:276:LEU:HB2	1.87	0.73
1:E:315:PHE:HA	1:G:314:PHE:CE1	2.23	0.73
1:F:204:LEU:HD22	1:F:211:LEU:HD23	1.69	0.73
1:A:218:LYS:NZ	1:B:166:GLY:HA2	2.02	0.73
1:D:217:ASN:HD21	1:D:224:SER:HB3	1.51	0.73
1:F:264:ASP:OD2	1:F:266:SER:HB2	1.88	0.73
1:B:199:ASP:HB3	1:B:205:LEU:HD11	1.71	0.73
1:D:217:ASN:HD22	1:D:217:ASN:N	1.85	0.73
1:G:197:TYR:N	1:G:209:SER:HB3	2.04	0.73
1:G:228:ALA:O	1:G:229:SER:HB3	1.88	0.73
1:D:245:THR:HG22	1:D:246:THR:N	2.04	0.72
1:G:131:ILE:C	1:G:131:ILE:HD12	2.09	0.72
1:F:308:LEU:HD23	1:F:308:LEU:O	1.89	0.72
1:E:164:ASN:HD21	1:G:164:ASN:HD21	1.36	0.72
1:F:244:THR:HG22	1:F:245:THR:O	1.89	0.72
1:G:284:ASN:H	1:G:284:ASN:ND2	1.86	0.72
1:B:143:ASN:HD21	1:B:157:LEU:H	1.33	0.72
1:F:217:ASN:C	1:F:217:ASN:HD22	1.91	0.72
1:F:193:GLN:HB3	1:F:292:GLU:HG3	1.72	0.72
1:G:144:CYS:SG	1:G:157:LEU:HB2	2.29	0.72
1:A:217:ASN:HD21	1:A:224:SER:H	1.38	0.71
1:D:217:ASN:H	1:D:217:ASN:ND2	1.87	0.71
1:B:182:ASN:ND2	1:B:307:THR:HA	2.05	0.71

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:D:306:ALA:C	1:D:308:LEU:H	1.91	0.71
1:A:298:SER:O	1:A:299:GLU:HB2	1.89	0.71
1:D:216:LYS:HB2	1:D:223:THR:HA	1.73	0.70
1:B:244:THR:HG22	1:B:245:THR:O	1.91	0.70
1:A:217:ASN:ND2	1:A:217:ASN:H	1.88	0.70
1:E:228:ALA:O	1:E:229:SER:HB3	1.92	0.70
1:A:300:SER:OG	1:A:301:PRO:HD2	1.90	0.70
1:D:159:LEU:HG	1:D:161:LEU:HD21	1.73	0.70
1:A:143:ASN:HD21	1:A:157:LEU:N	1.87	0.70
1:A:239:ALA:HB2	1:D:138:ILE:HG23	1.73	0.70
1:E:164:ASN:HD21	1:G:164:ASN:ND2	1.90	0.70
1:F:306:ALA:C	1:F:308:LEU:H	1.95	0.70
1:D:304:ASN:C	1:D:306:ALA:H	1.95	0.69
1:A:225:GLU:HG3	1:A:226:THR:H	1.57	0.69
1:G:216:LYS:HB2	1:G:223:THR:HA	1.73	0.69
1:A:164:ASN:ND2	1:D:164:ASN:HD21	1.90	0.69
1:E:172:VAL:HG22	1:E:315:PHE:HE2	1.58	0.69
1:G:261:THR:HG22	1:G:301:PRO:CG	2.22	0.69
1:G:219:SER:CB	1:G:224:SER:HB2	2.23	0.69
1:B:298:SER:O	1:B:299:GLU:HB2	1.93	0.69
1:E:183:GLN:HG2	1:E:186:THR:HG21	1.75	0.68
1:D:308:LEU:HD23	1:D:308:LEU:O	1.94	0.68
1:G:217:ASN:HD22	1:G:217:ASN:N	1.86	0.68
1:B:251:ASN:C	1:B:251:ASN:HD22	1.96	0.68
1:G:245:THR:HG22	1:G:246:THR:N	2.09	0.68
1:G:270:LEU:N	1:G:270:LEU:HD23	2.09	0.68
1:D:156:LYS:NZ	1:D:156:LYS:HB3	2.08	0.68
1:A:143:ASN:ND2	1:A:157:LEU:H	1.88	0.68
1:A:143:ASN:O	1:A:211:LEU:HD12	1.94	0.67
1:D:146:ILE:HD12	1:D:181:VAL:HG11	1.75	0.67
1:E:227:VAL:C	1:E:229:SER:H	1.97	0.67
1:G:284:ASN:HD22	1:G:284:ASN:N	1.91	0.67
1:E:174:LEU:CD1	1:E:192:ILE:HD12	2.23	0.67
1:F:199:ASP:OD1	1:F:203:ASN:HB2	1.94	0.67
1:D:306:ALA:O	1:D:308:LEU:N	2.27	0.67
1:A:258:TYR:C	1:A:270:LEU:HD21	2.15	0.67
1:E:225:GLU:HG3	1:E:226:THR:H	1.58	0.67
1:B:251:ASN:O	1:B:251:ASN:ND2	2.27	0.67
1:E:172:VAL:HG11	1:E:291:PHE:CD2	2.30	0.67
1:A:183:GLN:HG2	1:A:186:THR:HG21	1.77	0.67
1:A:216:LYS:CB	1:A:223:THR:HB	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:ASN:HD21	1:F:157:LEU:H	1.41	0.67
1:D:304:ASN:C	1:D:306:ALA:N	2.46	0.67
1:E:250:GLU:HB2	1:G:309:THR:HG21	1.76	0.67
1:D:239:ALA:O	1:D:241:PRO:HD3	1.95	0.66
1:D:144:CYS:SG	1:D:157:LEU:HB2	2.35	0.66
1:D:261:THR:OG1	1:D:266:SER:N	2.28	0.66
1:D:161:LEU:HD22	1:D:161:LEU:N	2.11	0.66
1:A:144:CYS:O	1:A:153:ASN:HA	1.96	0.66
1:G:304:ASN:C	1:G:306:ALA:N	2.48	0.66
1:A:284:ASN:ND2	1:A:284:ASN:H	1.93	0.66
1:B:265:ARG:HE	1:B:265:ARG:HA	1.60	0.66
1:A:132:ASN:O	1:A:162:VAL:HA	1.96	0.65
1:A:195:ARG:HG2	1:A:290:GLN:HG3	1.77	0.65
1:E:253:ILE:HD13	1:G:314:PHE:HZ	1.61	0.65
1:G:277:ASN:HA	1:G:288:ALA:HB3	1.79	0.65
1:G:304:ASN:C	1:G:306:ALA:H	1.98	0.65
1:F:245:THR:HG22	1:F:246:THR:N	2.11	0.65
1:G:147:VAL:HB	1:G:150:THR:HG23	1.78	0.65
1:E:287:TYR:HE2	1:E:320:GLU:OE1	1.78	0.65
1:E:192:ILE:HG13	1:E:293:TRP:HE3	1.62	0.65
1:E:136:THR:HG23	1:E:159:LEU:HB3	1.79	0.64
1:F:147:VAL:HG12	1:F:149:ASN:H	1.61	0.64
1:B:306:ALA:C	1:B:308:LEU:N	2.50	0.64
1:G:275:MET:SD	1:G:278:SER:HA	2.37	0.64
1:B:305:ILE:O	1:B:307:THR:N	2.30	0.64
1:G:239:ALA:O	1:G:241:PRO:HD3	1.98	0.64
1:E:217:ASN:H	1:E:217:ASN:HD22	1.46	0.64
1:G:270:LEU:HD23	1:G:270:LEU:H	1.63	0.64
1:E:132:ASN:O	1:E:162:VAL:HA	1.97	0.64
1:B:172:VAL:HG23	1:B:313:PHE:O	1.98	0.64
1:D:174:LEU:CD2	1:D:175:VAL:N	2.61	0.64
1:D:163:LYS:HE2	1:D:232:ALA:O	1.97	0.63
1:D:270:LEU:HD23	1:D:270:LEU:N	2.11	0.63
1:E:157:LEU:HD23	1:E:211:LEU:HD22	1.80	0.63
1:A:303:SER:O	1:A:304:ASN:HB2	1.98	0.63
1:F:150:THR:HB	1:F:152:THR:O	1.98	0.63
1:G:274:ILE:HA	1:G:290:GLN:O	1.97	0.63
1:B:204:LEU:HD22	1:B:211:LEU:HD23	1.81	0.63
1:E:164:ASN:ND2	1:G:164:ASN:HD21	1.94	0.63
1:F:228:ALA:O	1:F:229:SER:HB3	1.98	0.63
1:B:304:ASN:C	1:B:306:ALA:N	2.49	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ILE:HD12	1:D:131:ILE:C	2.19	0.63
1:B:172:VAL:HG22	1:B:315:PHE:HE2	1.63	0.62
1:E:172:VAL:HG22	1:E:315:PHE:CE2	2.34	0.62
1:A:304:ASN:O	1:A:306:ALA:N	2.31	0.62
1:B:138:ILE:HG12	1:D:318:ILE:HG21	1.80	0.62
1:B:245:THR:HG22	1:B:246:THR:N	2.14	0.62
1:G:303:SER:O	1:G:304:ASN:HB2	1.98	0.62
1:D:205:LEU:HD23	1:D:208:GLU:OE1	1.99	0.62
1:F:225:GLU:CG	1:F:226:THR:H	2.06	0.62
1:A:172:VAL:HG22	1:A:315:PHE:HE2	1.64	0.62
1:A:166:GLY:O	1:A:319:THR:HG22	2.00	0.62
1:B:207:GLU:OE2	1:B:207:GLU:HA	1.99	0.62
1:E:217:ASN:HD22	1:E:217:ASN:N	1.97	0.62
1:A:305:ILE:O	1:A:307:THR:N	2.33	0.61
1:D:306:ALA:C	1:D:308:LEU:N	2.53	0.61
1:D:154:ASP:HB2	1:D:178:SER:HB3	1.81	0.61
1:D:282:SER:HB3	1:D:284:ASN:HD21	1.65	0.61
1:E:164:ASN:OD1	1:G:162:VAL:HG11	1.99	0.61
1:D:253:ILE:HG21	1:D:274:ILE:HD12	1.82	0.61
1:F:172:VAL:HG23	1:F:313:PHE:HB3	1.83	0.61
1:F:278:SER:OG	1:F:279:ARG:N	2.31	0.61
1:E:170:GLY:HA3	1:E:315:PHE:CZ	2.36	0.61
1:E:229:SER:OG	1:E:231:LYS:HG3	2.01	0.61
1:F:172:VAL:HG11	1:F:291:PHE:CE2	2.36	0.61
1:B:225:GLU:CG	1:B:226:THR:H	2.11	0.61
1:B:282:SER:HB3	1:B:284:ASN:ND2	2.15	0.60
1:B:300:SER:O	1:B:302:GLU:N	2.34	0.60
1:E:205:LEU:HD21	1:E:284:ASN:O	2.01	0.60
1:G:163:LYS:NZ	1:G:319:THR:HG21	2.15	0.60
1:A:167:LEU:HG	1:D:160:VAL:HG11	1.83	0.60
1:G:282:SER:HB3	1:G:284:ASN:ND2	2.16	0.60
1:A:228:ALA:O	1:A:229:SER:HB3	2.01	0.60
1:D:195:ARG:HG3	1:D:195:ARG:HH11	1.65	0.60
1:G:306:ALA:C	1:G:308:LEU:H	2.05	0.60
1:D:193:GLN:O	1:D:194:LEU:HD23	2.01	0.60
1:A:172:VAL:HG22	1:A:315:PHE:CE2	2.36	0.60
1:E:131:ILE:C	1:E:131:ILE:HD12	2.22	0.60
1:G:282:SER:HB2	1:G:285:VAL:HG23	1.84	0.60
1:B:131:ILE:C	1:B:131:ILE:HD12	2.22	0.60
1:B:143:ASN:HD21	1:B:157:LEU:N	2.00	0.59
1:D:274:ILE:HA	1:D:290:GLN:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:ILE:HD12	1:G:131:ILE:O	2.01	0.59
1:G:195:ARG:HG2	1:G:290:GLN:NE2	2.17	0.59
1:G:196:LEU:HA	1:G:209:SER:CB	2.33	0.59
1:A:164:ASN:HD22	1:B:164:ASN:HD21	1.49	0.59
1:E:302:GLU:O	1:E:302:GLU:HG3	2.01	0.59
1:B:141:PRO:O	1:B:143:ASN:N	2.36	0.59
1:B:227:VAL:O	1:F:227:VAL:HB	2.01	0.59
1:D:268:PHE:HE1	1:D:301:PRO:HD3	1.66	0.59
1:E:218:LYS:NZ	1:F:166:GLY:HA2	2.16	0.59
1:G:163:LYS:HE3	1:G:232:ALA:HB1	1.84	0.59
1:B:157:LEU:HD13	1:B:194:LEU:HD12	1.83	0.59
1:D:284:ASN:ND2	1:D:284:ASN:H	2.01	0.59
1:A:164:ASN:HD21	1:B:164:ASN:HD21	1.49	0.59
1:A:251:ASN:H	1:A:251:ASN:HD22	1.50	0.59
1:D:159:LEU:HG	1:D:161:LEU:CD2	2.32	0.59
1:D:228:ALA:O	1:D:229:SER:HB3	2.01	0.58
1:E:192:ILE:HG12	1:E:293:TRP:HB2	1.85	0.58
1:E:245:THR:C	1:E:247:ARG:H	2.06	0.58
1:D:282:SER:HB2	1:D:285:VAL:HG23	1.84	0.58
1:A:218:LYS:HZ2	1:B:166:GLY:HA2	1.66	0.58
1:G:304:ASN:O	1:G:306:ALA:N	2.36	0.58
1:E:249:SER:O	1:E:251:ASN:N	2.37	0.58
1:F:300:SER:O	1:F:302:GLU:N	2.36	0.58
1:G:253:ILE:O	1:G:273:SER:HA	2.03	0.58
1:F:270:LEU:HD12	1:F:293:TRP:HD1	1.67	0.58
1:A:259:TYR:HE1	1:A:308:LEU:HA	1.68	0.58
1:B:166:GLY:O	1:B:319:THR:HG22	2.04	0.58
1:B:182:ASN:HD22	1:B:307:THR:HA	1.68	0.58
1:F:275:MET:O	1:F:276:LEU:O	2.21	0.58
1:A:249:SER:C	1:A:251:ASN:H	2.07	0.58
1:B:227:VAL:HB	1:F:227:VAL:O	2.03	0.58
1:D:193:GLN:HB3	1:D:292:GLU:HG3	1.85	0.58
1:G:251:ASN:HD22	1:G:251:ASN:H	1.51	0.58
1:A:245:THR:O	1:A:246:THR:OG1	2.21	0.58
1:E:272:ILE:HD13	1:E:293:TRP:NE1	2.18	0.58
1:E:242:PHE:HD2	1:E:279:ARG:HA	1.69	0.57
1:F:131:ILE:HD12	1:F:131:ILE:C	2.24	0.57
1:A:174:LEU:HD13	1:A:192:ILE:HD12	1.86	0.57
1:D:264:ASP:OD2	1:D:266:SER:HB2	2.04	0.57
1:F:160:VAL:HG21	1:G:318:ILE:HD11	1.86	0.57
1:G:261:THR:OG1	1:G:266:SER:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:ASN:O	1:G:162:VAL:HG13	2.04	0.57
1:E:225:GLU:CG	1:E:226:THR:H	2.17	0.57
1:G:159:LEU:CD1	1:G:172:VAL:HG22	2.33	0.57
1:A:218:LYS:HZ3	1:B:166:GLY:HA2	1.69	0.57
1:A:155:GLY:HA2	1:A:177:VAL:HG23	1.86	0.57
1:D:170:GLY:HA3	1:D:315:PHE:CE2	2.40	0.57
1:D:239:ALA:C	1:D:241:PRO:HD3	2.24	0.57
1:G:136:THR:CG2	1:G:159:LEU:HB3	2.34	0.57
1:G:168:VAL:HG23	1:G:319:THR:HB	1.87	0.57
1:G:261:THR:HA	1:G:301:PRO:HG2	1.86	0.57
1:F:172:VAL:O	1:F:312:PRO:HA	2.05	0.57
1:A:131:ILE:HD12	1:A:131:ILE:C	2.24	0.57
1:A:192:ILE:HG12	1:A:293:TRP:HB2	1.87	0.57
1:A:275:MET:O	1:A:276:LEU:HB2	2.05	0.57
1:E:249:SER:C	1:E:251:ASN:H	2.08	0.57
1:F:163:LYS:HE3	1:F:232:ALA:HB1	1.87	0.57
1:F:300:SER:OG	1:F:301:PRO:HD2	2.05	0.57
1:B:217:ASN:HB3	1:B:224:SER:HB3	1.87	0.57
1:E:184:MET:C	1:E:186:THR:H	2.07	0.57
1:F:157:LEU:HD23	1:F:211:LEU:HD13	1.87	0.57
1:G:143:ASN:HD21	1:G:157:LEU:H	1.52	0.56
1:G:156:LYS:NZ	1:G:156:LYS:HB3	2.19	0.56
1:D:253:ILE:O	1:D:273:SER:HA	2.05	0.56
1:E:216:LYS:CB	1:E:223:THR:HB	2.33	0.56
1:A:164:ASN:ND2	1:D:164:ASN:ND2	2.48	0.56
1:A:249:SER:O	1:A:251:ASN:N	2.39	0.56
1:B:147:VAL:C	1:B:149:ASN:H	2.08	0.56
1:B:308:LEU:HD23	1:B:308:LEU:O	2.06	0.56
1:D:143:ASN:CA	1:D:153:ASN:HD22	2.17	0.56
1:E:140:PRO:O	1:E:156:LYS:NZ	2.32	0.56
1:F:268:PHE:CE1	1:F:300:SER:HA	2.34	0.56
1:B:147:VAL:HG12	1:B:149:ASN:H	1.70	0.56
1:A:304:ASN:C	1:A:306:ALA:N	2.58	0.56
1:E:216:LYS:HB2	1:E:223:THR:CB	2.34	0.56
1:G:217:ASN:ND2	1:G:224:SER:HB3	2.20	0.56
1:D:251:ASN:HD22	1:D:251:ASN:H	1.54	0.56
1:F:228:ALA:O	1:F:229:SER:CB	2.52	0.56
1:E:168:VAL:O	1:E:316:SER:HA	2.05	0.56
1:F:217:ASN:ND2	1:F:224:SER:HB3	2.18	0.56
1:E:167:LEU:HD23	1:E:318:ILE:HD12	1.87	0.56
1:D:300:SER:OG	1:D:301:PRO:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:ALA:C	1:F:308:LEU:N	2.58	0.56
1:D:245:THR:CG2	1:D:246:THR:H	2.14	0.56
1:E:261:THR:HG22	1:E:301:PRO:HG3	1.87	0.56
1:G:150:THR:HG21	1:G:154:ASP:OD2	2.06	0.56
1:B:196:LEU:HB2	1:B:289:ILE:O	2.06	0.55
1:A:164:ASN:OD1	1:D:162:VAL:HG11	2.05	0.55
1:D:143:ASN:HA	1:D:153:ASN:ND2	2.19	0.55
1:F:261:THR:HG22	1:F:301:PRO:CG	2.36	0.55
1:A:239:ALA:HB2	1:D:138:ILE:CG2	2.36	0.55
1:B:228:ALA:O	1:B:229:SER:HB3	2.05	0.55
1:E:298:SER:O	1:E:299:GLU:CB	2.55	0.55
1:F:138:ILE:HG12	1:G:318:ILE:HG21	1.89	0.55
1:A:259:TYR:HE2	1:A:301:PRO:HG2	1.69	0.55
1:B:189:THR:HG22	1:B:190:ALA:N	2.21	0.55
1:D:253:ILE:HB	1:D:274:ILE:HB	1.89	0.55
1:E:239:ALA:HB2	1:G:138:ILE:HG23	1.88	0.55
1:B:166:GLY:C	1:B:319:THR:HG22	2.27	0.55
1:E:149:ASN:O	1:E:150:THR:O	2.25	0.55
1:E:304:ASN:C	1:E:306:ALA:N	2.57	0.55
1:F:135:TRP:CE2	1:F:137:GLY:HA2	2.40	0.55
1:G:300:SER:OG	1:G:301:PRO:HD2	2.06	0.55
1:E:167:LEU:CD2	1:E:318:ILE:HD12	2.37	0.55
1:F:237:THR:HG22	1:F:277:ASN:ND2	2.21	0.55
1:A:307:THR:O	1:A:308:LEU:HB3	2.05	0.55
1:B:284:ASN:ND2	1:B:284:ASN:H	2.04	0.55
1:D:150:THR:HG22	1:D:152:THR:O	2.06	0.55
1:E:251:ASN:H	1:E:251:ASN:HD22	1.52	0.55
1:A:280:MET:HA	1:A:285:VAL:HG11	1.89	0.55
1:B:275:MET:O	1:B:276:LEU:O	2.25	0.55
1:B:158:THR:HB	1:B:173:SER:OG	2.07	0.55
1:D:168:VAL:HG23	1:D:319:THR:HB	1.88	0.55
1:E:227:VAL:C	1:E:229:SER:N	2.61	0.55
1:G:193:GLN:HB3	1:G:292:GLU:HG3	1.87	0.55
1:D:179:ASP:HA	1:D:182:ASN:HB2	1.89	0.54
1:F:298:SER:O	1:F:299:GLU:HB2	2.07	0.54
1:A:280:MET:HB3	1:A:285:VAL:HB	1.88	0.54
1:B:159:LEU:HD12	1:B:171:TYR:O	2.06	0.54
1:D:275:MET:SD	1:D:278:SER:HA	2.47	0.54
1:E:135:TRP:CH2	1:E:138:ILE:HG13	2.42	0.54
1:E:304:ASN:O	1:E:306:ALA:N	2.41	0.54
1:F:204:LEU:HG	1:F:204:LEU:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:THR:C	1:F:247:ARG:H	2.10	0.54
1:F:302:GLU:OE1	1:F:303:SER:N	2.40	0.54
1:E:251:ASN:O	1:E:275:MET:O	2.26	0.54
1:G:244:THR:HG22	1:G:245:THR:O	2.07	0.54
1:G:254:HIS:ND1	1:G:273:SER:HB3	2.23	0.54
1:E:174:LEU:HD12	1:E:293:TRP:CZ3	2.42	0.54
1:F:251:ASN:HD21	1:F:275:MET:CE	2.20	0.54
1:B:207:GLU:OE2	1:F:283:SER:HB3	2.07	0.54
1:E:172:VAL:HG11	1:E:291:PHE:CE2	2.43	0.54
1:G:249:SER:C	1:G:251:ASN:H	2.10	0.54
1:B:154:ASP:HB2	1:B:178:SER:HB3	1.89	0.54
1:G:308:LEU:C	1:G:308:LEU:HD23	2.28	0.54
1:F:141:PRO:O	1:F:143:ASN:N	2.40	0.54
1:G:298:SER:O	1:G:299:GLU:CB	2.56	0.54
1:B:140:PRO:O	1:B:156:LYS:NZ	2.39	0.53
1:D:305:ILE:O	1:D:307:THR:N	2.37	0.53
1:B:135:TRP:CE2	1:B:137:GLY:HA2	2.44	0.53
1:F:304:ASN:C	1:F:306:ALA:N	2.60	0.53
1:B:302:GLU:OE1	1:B:302:GLU:C	2.47	0.53
1:B:309:THR:HG21	1:D:250:GLU:HB2	1.90	0.53
1:G:265:ARG:HE	1:G:265:ARG:HA	1.72	0.53
1:A:282:SER:HB2	1:A:285:VAL:HG23	1.91	0.53
1:F:147:VAL:C	1:F:149:ASN:H	2.12	0.53
1:G:239:ALA:C	1:G:241:PRO:HD3	2.28	0.53
1:B:251:ASN:O	1:B:275:MET:O	2.26	0.53
1:D:219:SER:CB	1:D:224:SER:HB2	2.34	0.53
1:E:147:VAL:C	1:E:149:ASN:H	2.12	0.53
1:G:282:SER:CB	1:G:284:ASN:ND2	2.72	0.53
1:G:306:ALA:C	1:G:308:LEU:N	2.60	0.53
1:B:242:PHE:O	1:B:243:ASN:C	2.46	0.53
1:B:303:SER:OG	1:B:304:ASN:N	2.40	0.53
1:F:216:LYS:HB2	1:F:223:THR:HB	1.90	0.53
1:G:172:VAL:HG23	1:G:315:PHE:CE2	2.38	0.53
1:A:261:THR:HB	1:A:301:PRO:HG3	1.90	0.52
1:D:268:PHE:CE1	1:D:301:PRO:HD3	2.45	0.52
1:F:251:ASN:C	1:F:251:ASN:HD22	2.13	0.52
1:E:143:ASN:O	1:E:211:LEU:HD12	2.09	0.52
1:E:263:TYR:H	1:E:263:TYR:HD1	1.56	0.52
1:G:282:SER:HB3	1:G:284:ASN:HD21	1.72	0.52
1:E:196:LEU:HA	1:E:209:SER:HB3	1.91	0.52
1:F:216:LYS:HB2	1:F:223:THR:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:VAL:O	1:B:312:PRO:HA	2.09	0.52
1:B:174:LEU:HD23	1:B:175:VAL:N	2.25	0.52
1:B:245:THR:C	1:B:247:ARG:H	2.11	0.52
1:E:220:SER:HB3	1:E:222:ALA:N	2.21	0.52
1:B:251:ASN:C	1:B:251:ASN:ND2	2.61	0.52
1:B:253:ILE:HB	1:B:274:ILE:HB	1.91	0.52
1:E:320:GLU:O	1:E:321:ASP:C	2.46	0.52
1:F:160:VAL:HB	1:F:171:TYR:HB3	1.91	0.52
1:A:242:PHE:CE2	1:A:280:MET:HG2	2.45	0.52
1:G:156:LYS:HG3	1:G:177:VAL:HG21	1.91	0.52
1:G:242:PHE:HD2	1:G:279:ARG:HA	1.73	0.52
1:A:198:PHE:HA	1:A:203:ASN:O	2.09	0.52
1:D:156:LYS:NZ	1:D:156:LYS:CB	2.73	0.52
1:D:244:THR:HG22	1:D:245:THR:O	2.10	0.52
1:A:245:THR:C	1:A:247:ARG:H	2.14	0.52
1:B:249:SER:O	1:B:251:ASN:N	2.42	0.52
1:D:225:GLU:CG	1:D:226:THR:H	2.19	0.52
1:G:163:LYS:HZ3	1:G:319:THR:HG21	1.74	0.52
1:B:314:PHE:CE1	1:D:315:PHE:HA	2.45	0.52
1:E:132:ASN:O	1:E:162:VAL:HG13	2.10	0.52
1:F:131:ILE:HD12	1:F:131:ILE:O	2.10	0.52
1:F:300:SER:O	1:F:301:PRO:C	2.49	0.52
1:A:318:ILE:O	1:A:318:ILE:HG22	2.09	0.51
1:E:225:GLU:HG3	1:E:226:THR:N	2.25	0.51
1:F:204:LEU:CD2	1:F:211:LEU:HD23	2.38	0.51
1:F:245:THR:C	1:F:247:ARG:N	2.63	0.51
1:F:258:TYR:N	1:F:258:TYR:CD1	2.78	0.51
1:F:309:THR:HG21	1:G:250:GLU:CB	2.38	0.51
1:B:163:LYS:CE	1:B:232:ALA:HB1	2.40	0.51
1:A:272:ILE:HG13	1:A:273:SER:N	2.24	0.51
1:B:150:THR:HB	1:B:152:THR:O	2.09	0.51
1:D:231:LYS:HA	1:D:234:MET:HG2	1.91	0.51
1:A:139:ASN:HD21	1:B:247:ARG:NH2	2.07	0.51
1:A:143:ASN:CA	1:A:153:ASN:HD22	2.23	0.51
1:A:227:VAL:C	1:A:229:SER:H	2.12	0.51
1:B:272:ILE:HD13	1:B:313:PHE:CD2	2.45	0.51
1:G:251:ASN:H	1:G:251:ASN:ND2	2.09	0.51
1:B:160:VAL:HB	1:B:171:TYR:HB3	1.91	0.51
1:E:163:LYS:HD3	1:E:232:ALA:O	2.10	0.51
1:E:227:VAL:O	1:E:229:SER:N	2.42	0.51
1:F:302:GLU:OE1	1:F:302:GLU:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:314:PHE:CE1	1:G:315:PHE:HA	2.46	0.51
1:A:270:LEU:HD23	1:A:270:LEU:N	2.25	0.51
1:D:146:ILE:HG22	1:D:146:ILE:O	2.10	0.51
1:D:284:ASN:H	1:D:284:ASN:HD22	1.59	0.51
1:E:281:ILE:O	1:E:281:ILE:HG13	2.11	0.51
1:G:261:THR:O	1:G:264:ASP:O	2.29	0.51
1:A:191:ASN:HD21	1:A:193:GLN:HE21	1.59	0.51
1:D:303:SER:O	1:D:304:ASN:HB2	2.10	0.51
1:G:189:THR:OG1	1:G:296:ASN:HA	2.10	0.51
1:A:284:ASN:N	1:A:284:ASN:HD22	2.09	0.51
1:B:141:PRO:O	1:B:142:PRO:C	2.50	0.51
1:F:182:ASN:ND2	1:F:307:THR:HA	2.26	0.51
1:F:304:ASN:O	1:F:306:ALA:N	2.44	0.51
1:E:245:THR:O	1:E:247:ARG:N	2.44	0.51
1:B:260:MET:HA	1:B:266:SER:O	2.11	0.50
1:D:197:TYR:N	1:D:209:SER:OG	2.39	0.50
1:E:304:ASN:O	1:E:305:ILE:C	2.50	0.50
1:F:226:THR:HG22	1:F:228:ALA:HB2	1.93	0.50
1:G:131:ILE:C	1:G:131:ILE:CD1	2.77	0.50
1:G:217:ASN:ND2	1:G:217:ASN:N	2.47	0.50
1:G:245:THR:CG2	1:G:246:THR:H	2.19	0.50
1:B:219:SER:HB2	1:B:224:SER:HB2	1.93	0.50
1:B:226:THR:HG22	1:B:228:ALA:HB2	1.93	0.50
1:D:170:GLY:HA3	1:D:315:PHE:CZ	2.47	0.50
1:F:135:TRP:CH2	1:F:218:LYS:HD2	2.47	0.50
1:F:284:ASN:ND2	1:F:284:ASN:H	2.09	0.50
1:B:193:GLN:NE2	1:B:292:GLU:OE2	2.45	0.50
1:E:284:ASN:H	1:E:284:ASN:ND2	2.10	0.50
1:F:184:MET:C	1:F:186:THR:H	2.14	0.50
1:A:259:TYR:CE1	1:A:308:LEU:HA	2.46	0.50
1:B:244:THR:HG22	1:B:245:THR:N	2.27	0.50
1:A:147:VAL:C	1:A:149:ASN:H	2.15	0.50
1:B:131:ILE:HD12	1:B:131:ILE:O	2.12	0.50
1:D:199:ASP:HB3	1:D:205:LEU:HD11	1.93	0.50
1:E:143:ASN:ND2	1:E:157:LEU:H	2.05	0.50
1:G:161:LEU:HD12	1:G:168:VAL:HG11	1.93	0.50
1:G:249:SER:O	1:G:251:ASN:N	2.45	0.50
1:A:287:TYR:HE2	1:A:320:GLU:OE1	1.95	0.50
1:B:245:THR:C	1:B:247:ARG:N	2.65	0.50
1:B:304:ASN:C	1:B:306:ALA:H	2.15	0.50
1:D:263:TYR:CG	1:D:264:ASP:N	2.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:SER:C	1:E:251:ASN:N	2.65	0.50
1:E:258:TYR:C	1:E:270:LEU:HD21	2.32	0.50
1:F:242:PHE:O	1:F:243:ASN:C	2.49	0.50
1:B:277:ASN:O	1:B:278:SER:O	2.29	0.50
1:E:183:GLN:HG2	1:E:186:THR:CG2	2.41	0.50
1:A:170:GLY:HA3	1:A:315:PHE:CZ	2.46	0.49
1:A:171:TYR:CE2	1:B:318:ILE:HD11	2.47	0.49
1:A:320:GLU:O	1:A:321:ASP:C	2.51	0.49
1:D:257:CYS:O	1:D:270:LEU:HD23	2.12	0.49
1:E:252:TYR:CE2	1:E:275:MET:HG2	2.47	0.49
1:E:261:THR:HG22	1:E:301:PRO:CG	2.40	0.49
1:F:217:ASN:C	1:F:217:ASN:ND2	2.64	0.49
1:A:302:GLU:HG3	1:A:302:GLU:O	2.12	0.49
1:B:132:ASN:N	1:B:132:ASN:HD22	2.10	0.49
1:B:168:VAL:HG23	1:B:319:THR:HB	1.95	0.49
1:D:147:VAL:HB	1:D:150:THR:OG1	2.11	0.49
1:D:275:MET:O	1:D:276:LEU:HB2	2.11	0.49
1:D:307:THR:HG23	1:D:307:THR:O	2.11	0.49
1:A:219:SER:O	1:A:220:SER:HB2	2.12	0.49
1:F:225:GLU:HG3	1:F:226:THR:N	2.15	0.49
1:B:261:THR:HG22	1:B:301:PRO:HG3	1.94	0.49
1:D:132:ASN:O	1:D:162:VAL:HG13	2.12	0.49
1:D:305:ILE:O	1:D:305:ILE:HG22	2.12	0.49
1:E:167:LEU:HG	1:G:160:VAL:HG11	1.95	0.49
1:G:226:THR:HG22	1:G:228:ALA:HB2	1.93	0.49
1:A:198:PHE:CE2	1:A:204:LEU:HD13	2.47	0.49
1:D:220:SER:HB3	1:D:222:ALA:H	1.77	0.49
1:D:156:LYS:HB3	1:D:156:LYS:HZ3	1.74	0.49
1:G:270:LEU:N	1:G:270:LEU:CD2	2.75	0.49
1:B:144:CYS:SG	1:B:157:LEU:HB2	2.53	0.49
1:B:157:LEU:HD13	1:B:194:LEU:CD1	2.43	0.49
1:D:270:LEU:N	1:D:270:LEU:CD2	2.76	0.49
1:A:284:ASN:H	1:A:284:ASN:HD22	1.59	0.49
1:B:225:GLU:O	1:B:226:THR:HB	2.12	0.49
1:B:227:VAL:C	1:B:229:SER:H	2.16	0.49
1:G:306:ALA:O	1:G:308:LEU:N	2.45	0.49
1:D:240:TYR:OH	1:D:318:ILE:N	2.42	0.49
1:A:225:GLU:CG	1:A:226:THR:H	2.25	0.48
1:E:282:SER:HB2	1:E:285:VAL:HG23	1.94	0.48
1:A:136:THR:HG23	1:A:159:LEU:HB3	1.94	0.48
1:D:149:ASN:O	1:D:150:THR:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:ASN:ND2	1:F:164:ASN:ND2	2.55	0.48
1:F:147:VAL:HG12	1:F:149:ASN:N	2.27	0.48
1:B:304:ASN:O	1:B:306:ALA:N	2.47	0.48
1:F:220:SER:HB3	1:F:222:ALA:H	1.78	0.48
1:A:216:LYS:HB2	1:A:223:THR:CB	2.41	0.48
1:G:302:GLU:OE1	1:G:303:SER:N	2.47	0.48
1:A:258:TYR:HA	1:A:270:LEU:CD2	2.43	0.48
1:D:176:GLY:H	1:D:308:LEU:HD23	1.79	0.48
1:G:193:GLN:O	1:G:194:LEU:HD23	2.14	0.48
1:A:174:LEU:HD13	1:A:192:ILE:CD1	2.44	0.48
1:A:304:ASN:O	1:A:305:ILE:C	2.52	0.48
1:B:143:ASN:ND2	1:B:157:LEU:H	2.07	0.48
1:D:282:SER:CB	1:D:284:ASN:ND2	2.72	0.48
1:F:231:LYS:HE3	1:F:322:ASP:O	2.14	0.48
1:F:275:MET:O	1:F:276:LEU:C	2.52	0.48
1:F:141:PRO:O	1:F:142:PRO:C	2.50	0.48
1:G:195:ARG:HG3	1:G:195:ARG:HH11	1.78	0.48
1:G:251:ASN:HD22	1:G:251:ASN:N	2.09	0.48
1:A:131:ILE:C	1:A:133:THR:H	2.16	0.47
1:A:229:SER:OG	1:A:231:LYS:HG3	2.14	0.47
1:A:249:SER:CB	1:D:260:MET:HE3	2.44	0.47
1:B:281:ILE:HG13	1:B:281:ILE:O	2.13	0.47
1:E:314:PHE:CE1	1:F:315:PHE:HA	2.48	0.47
1:D:144:CYS:O	1:D:153:ASN:HA	2.13	0.47
1:F:265:ARG:HE	1:F:265:ARG:HA	1.79	0.47
1:B:162:VAL:HG11	1:D:164:ASN:O	2.13	0.47
1:B:163:LYS:HE3	1:B:232:ALA:HB1	1.95	0.47
1:E:219:SER:O	1:E:220:SER:HB2	2.14	0.47
1:E:307:THR:O	1:E:308:LEU:HB3	2.15	0.47
1:G:268:PHE:CE1	1:G:300:SER:HA	2.39	0.47
1:A:275:MET:HB2	1:A:290:GLN:HB3	1.96	0.47
1:B:303:SER:O	1:B:304:ASN:HB2	2.15	0.47
1:E:236:SER:HB2	1:E:318:ILE:HG22	1.96	0.47
1:F:189:THR:HG22	1:F:190:ALA:N	2.29	0.47
1:A:174:LEU:HD23	1:A:175:VAL:H	1.76	0.47
1:D:163:LYS:HE3	1:D:232:ALA:HB1	1.96	0.47
1:A:192:ILE:CG1	1:A:293:TRP:HB2	2.44	0.47
1:D:185:PHE:O	1:D:187:GLN:N	2.48	0.47
1:E:198:PHE:HB3	1:E:203:ASN:O	2.14	0.47
1:F:164:ASN:ND2	1:G:164:ASN:HD21	2.12	0.47
1:A:133:THR:O	1:A:217:ASN:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASN:ND2	1:D:164:ASN:HD21	2.13	0.47
1:D:161:LEU:N	1:D:161:LEU:CD2	2.77	0.47
1:D:272:ILE:HD13	1:D:313:PHE:CD2	2.50	0.47
1:F:274:ILE:HA	1:F:290:GLN:O	2.14	0.47
1:A:251:ASN:O	1:A:275:MET:O	2.32	0.47
1:F:245:THR:O	1:F:247:ARG:N	2.48	0.47
1:B:174:LEU:HD23	1:B:175:VAL:H	1.79	0.47
1:D:251:ASN:HD22	1:D:251:ASN:N	2.11	0.47
1:E:155:GLY:HA2	1:E:177:VAL:HG23	1.96	0.47
1:E:185:PHE:O	1:E:300:SER:HB3	2.15	0.47
1:E:220:SER:CB	1:E:222:ALA:H	2.23	0.47
1:B:257:CYS:C	1:B:258:TYR:CD1	2.88	0.47
1:B:282:SER:O	1:B:285:VAL:HG23	2.15	0.47
1:A:217:ASN:N	1:A:217:ASN:HD22	2.12	0.46
1:B:220:SER:HB3	1:B:222:ALA:H	1.80	0.46
1:B:261:THR:O	1:B:264:ASP:O	2.33	0.46
1:F:138:ILE:O	1:F:139:ASN:O	2.33	0.46
1:A:200:SER:O	1:A:231:LYS:HD3	2.16	0.46
1:A:263:TYR:CG	1:A:264:ASP:N	2.79	0.46
1:A:308:LEU:HD23	1:A:308:LEU:C	2.36	0.46
1:B:189:THR:CG2	1:B:190:ALA:N	2.78	0.46
1:D:143:ASN:C	1:D:143:ASN:HD22	2.18	0.46
1:D:150:THR:CG2	1:D:152:THR:O	2.63	0.46
1:F:144:CYS:HB3	1:F:145:GLN:H	1.50	0.46
1:G:170:GLY:HA3	1:G:315:PHE:CE2	2.50	0.46
1:A:159:LEU:HD23	1:A:215:LEU:HD21	1.98	0.46
1:D:258:TYR:HA	1:D:270:LEU:CD2	2.45	0.46
1:G:242:PHE:O	1:G:243:ASN:C	2.54	0.46
1:E:217:ASN:ND2	1:E:217:ASN:N	2.41	0.46
1:F:219:SER:O	1:F:220:SER:HB2	2.16	0.46
1:G:258:TYR:HA	1:G:270:LEU:CD2	2.45	0.46
1:B:199:ASP:CB	1:B:205:LEU:HD11	2.44	0.46
1:E:195:ARG:HG2	1:E:290:GLN:HG3	1.98	0.46
1:E:166:GLY:O	1:E:319:THR:HG22	2.16	0.46
1:E:174:LEU:HD23	1:E:175:VAL:H	1.81	0.46
1:G:263:TYR:CG	1:G:264:ASP:N	2.84	0.46
1:A:252:TYR:CE2	1:A:275:MET:HG2	2.51	0.46
1:D:131:ILE:C	1:D:131:ILE:CD1	2.85	0.46
1:F:204:LEU:HD11	1:F:209:SER:OG	2.15	0.46
1:B:147:VAL:HG12	1:B:149:ASN:N	2.31	0.46
1:D:156:LYS:HG3	1:D:177:VAL:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:225:GLU:CG	1:G:226:THR:H	2.18	0.46
1:A:191:ASN:ND2	1:A:193:GLN:HE21	2.14	0.45
1:A:318:ILE:HD12	1:A:318:ILE:N	2.31	0.45
1:F:162:VAL:HG11	1:G:164:ASN:O	2.16	0.45
1:G:245:THR:C	1:G:247:ARG:N	2.69	0.45
1:D:154:ASP:CB	1:D:178:SER:HB3	2.46	0.45
1:F:270:LEU:HD12	1:F:293:TRP:CD1	2.50	0.45
1:A:154:ASP:C	1:A:177:VAL:HB	2.36	0.45
1:A:304:ASN:C	1:A:306:ALA:H	2.19	0.45
1:B:135:TRP:CZ3	1:B:138:ILE:HG13	2.52	0.45
1:B:261:THR:OG1	1:B:264:ASP:O	2.33	0.45
1:E:162:VAL:HG11	1:F:164:ASN:OD1	2.16	0.45
1:F:253:ILE:HB	1:F:274:ILE:HB	1.98	0.45
1:G:143:ASN:C	1:G:143:ASN:HD22	2.19	0.45
1:A:172:VAL:O	1:A:312:PRO:HA	2.17	0.45
1:A:303:SER:O	1:A:304:ASN:CB	2.65	0.45
1:D:304:ASN:O	1:D:306:ALA:N	2.48	0.45
1:E:251:ASN:H	1:E:251:ASN:ND2	2.15	0.45
1:F:245:THR:CG2	1:F:246:THR:H	2.22	0.45
1:F:272:ILE:HA	1:F:292:GLU:O	2.17	0.45
1:A:143:ASN:C	1:A:143:ASN:HD22	2.20	0.45
1:A:315:PHE:HA	1:D:314:PHE:CD1	2.50	0.45
1:E:280:MET:HA	1:E:285:VAL:HG11	1.99	0.45
1:D:150:THR:HG22	1:D:152:THR:H	1.82	0.45
1:D:300:SER:OG	1:D:301:PRO:CD	2.65	0.45
1:E:170:GLY:HA3	1:E:315:PHE:CE1	2.52	0.45
1:E:218:LYS:HZ2	1:F:166:GLY:HA2	1.79	0.45
1:E:249:SER:HB3	1:E:252:TYR:CE1	2.52	0.45
1:D:178:SER:O	1:D:181:VAL:N	2.50	0.45
1:D:307:THR:O	1:D:308:LEU:O	2.34	0.45
1:G:197:TYR:H	1:G:209:SER:CB	2.20	0.45
1:G:289:ILE:HD11	1:G:317:TYR:OH	2.17	0.45
1:F:242:PHE:CD2	1:F:280:MET:HG2	2.51	0.45
1:G:131:ILE:O	1:G:131:ILE:CD1	2.65	0.45
1:A:174:LEU:CD1	1:A:192:ILE:HD12	2.47	0.45
1:A:251:ASN:HD22	1:A:251:ASN:N	2.10	0.45
1:E:146:ILE:HD11	1:E:174:LEU:HD21	1.98	0.45
1:E:196:LEU:HA	1:E:209:SER:CB	2.47	0.45
1:E:275:MET:HB2	1:E:290:GLN:HB3	1.98	0.45
1:A:140:PRO:O	1:A:156:LYS:HE2	2.16	0.45
1:A:143:ASN:HA	1:A:153:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:ILE:O	1:F:307:THR:N	2.50	0.45
1:A:225:GLU:HG3	1:A:226:THR:N	2.30	0.44
1:A:249:SER:C	1:A:251:ASN:N	2.70	0.44
1:B:304:ASN:O	1:B:305:ILE:C	2.56	0.44
1:E:245:THR:C	1:E:247:ARG:N	2.71	0.44
1:F:304:ASN:O	1:F:305:ILE:C	2.55	0.44
1:A:131:ILE:O	1:A:133:THR:N	2.51	0.44
1:A:141:PRO:O	1:A:142:PRO:C	2.55	0.44
1:A:227:VAL:C	1:A:229:SER:N	2.71	0.44
1:B:199:ASP:OD1	1:B:203:ASN:HB2	2.17	0.44
1:B:284:ASN:ND2	1:B:284:ASN:N	2.65	0.44
1:D:196:LEU:HB2	1:D:289:ILE:O	2.18	0.44
1:E:225:GLU:CG	1:E:226:THR:N	2.80	0.44
1:B:225:GLU:HG3	1:B:226:THR:N	2.21	0.44
1:D:185:PHE:O	1:D:300:SER:OG	2.35	0.44
1:E:142:PRO:HA	1:E:155:GLY:O	2.17	0.44
1:E:218:LYS:HZ3	1:F:166:GLY:HA2	1.83	0.44
1:E:251:ASN:N	1:E:251:ASN:HD22	2.12	0.44
1:A:244:THR:HG22	1:A:245:THR:N	2.33	0.44
1:B:164:ASN:ND2	1:D:164:ASN:OD1	2.50	0.44
1:E:135:TRP:HB2	1:E:160:VAL:HG22	1.99	0.44
1:F:307:THR:O	1:F:307:THR:HG22	2.17	0.44
1:B:164:ASN:HD21	1:D:164:ASN:HD21	1.65	0.44
1:E:245:THR:HG22	1:E:246:THR:N	2.22	0.44
1:A:146:ILE:HB	1:A:154:ASP:OD1	2.18	0.44
1:A:184:MET:C	1:A:186:THR:H	2.21	0.44
1:G:217:ASN:HD21	1:G:224:SER:HB3	1.82	0.44
1:E:257:CYS:SG	1:E:293:TRP:HD1	2.41	0.44
1:F:261:THR:O	1:F:264:ASP:O	2.36	0.44
1:A:163:LYS:HE2	1:A:319:THR:HG21	1.99	0.44
1:B:140:PRO:HB2	1:B:141:PRO:HD2	2.00	0.44
1:B:188:LYS:HD3	1:B:188:LYS:N	2.33	0.44
1:D:156:LYS:HG3	1:D:177:VAL:HG21	1.99	0.44
1:G:141:PRO:O	1:G:142:PRO:C	2.55	0.44
1:E:198:PHE:HA	1:E:203:ASN:O	2.17	0.43
1:F:196:LEU:HD11	1:F:211:LEU:HB2	1.98	0.43
1:G:282:SER:CB	1:G:284:ASN:HD21	2.29	0.43
1:G:305:ILE:O	1:G:307:THR:N	2.47	0.43
1:E:141:PRO:O	1:E:142:PRO:C	2.57	0.43
1:E:149:ASN:O	1:E:150:THR:C	2.55	0.43
1:G:144:CYS:O	1:G:153:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:LEU:N	1:G:161:LEU:HD22	2.33	0.43
1:E:135:TRP:CE2	1:E:137:GLY:HA2	2.53	0.43
1:E:185:PHE:CE2	1:E:308:LEU:HG	2.53	0.43
1:F:219:SER:CB	1:F:224:SER:HB2	2.41	0.43
1:E:155:GLY:CA	1:E:177:VAL:HG23	2.48	0.43
1:F:303:SER:O	1:F:304:ASN:HB2	2.18	0.43
1:G:305:ILE:O	1:G:305:ILE:HG22	2.19	0.43
1:A:143:ASN:HA	1:A:153:ASN:HD22	1.81	0.43
1:A:300:SER:OG	1:A:301:PRO:CD	2.62	0.43
1:D:260:MET:HA	1:D:266:SER:O	2.19	0.43
1:E:192:ILE:HG13	1:E:293:TRP:CE3	2.49	0.43
1:F:144:CYS:SG	1:F:157:LEU:HB2	2.58	0.43
1:F:245:THR:CG2	1:F:246:THR:N	2.81	0.43
1:F:284:ASN:H	1:F:284:ASN:HD22	1.65	0.43
1:G:156:LYS:HG3	1:G:177:VAL:CG2	2.47	0.43
1:G:172:VAL:HG21	1:G:291:PHE:CZ	2.51	0.43
1:D:284:ASN:HD22	1:D:284:ASN:N	2.15	0.43
1:F:199:ASP:OD1	1:F:203:ASN:N	2.49	0.43
1:F:225:GLU:CG	1:F:226:THR:N	2.76	0.43
1:F:296:ASN:OD1	1:F:296:ASN:O	2.36	0.43
1:G:199:ASP:OD1	1:G:199:ASP:C	2.57	0.43
1:G:302:GLU:OE1	1:G:302:GLU:C	2.57	0.43
1:A:284:ASN:ND2	1:A:284:ASN:N	2.56	0.43
1:D:264:ASP:OD2	1:D:266:SER:CB	2.66	0.43
1:F:191:ASN:OD1	1:F:294:ASN:OD1	2.37	0.43
1:A:140:PRO:O	1:A:156:LYS:NZ	2.47	0.43
1:A:248:ASP:O	1:A:249:SER:HB2	2.19	0.43
1:B:314:PHE:N	1:B:314:PHE:CD2	2.81	0.43
1:A:225:GLU:O	1:A:226:THR:HB	2.19	0.43
1:B:181:VAL:C	1:B:183:GLN:H	2.22	0.43
1:B:219:SER:O	1:B:220:SER:HB2	2.19	0.43
1:B:258:TYR:CD1	1:B:258:TYR:N	2.86	0.43
1:B:283:SER:HB3	1:F:207:GLU:OE2	2.18	0.43
1:D:149:ASN:O	1:D:150:THR:C	2.57	0.43
1:D:192:ILE:HG13	1:D:293:TRP:HB2	2.00	0.43
1:D:277:ASN:O	1:D:278:SER:C	2.57	0.43
1:G:277:ASN:O	1:G:278:SER:C	2.57	0.43
1:B:174:LEU:CD2	1:B:175:VAL:N	2.82	0.43
1:B:219:SER:CB	1:B:224:SER:HB2	2.48	0.43
1:B:249:SER:HB2	1:B:250:GLU:H	1.66	0.43
1:D:245:THR:O	1:D:247:ARG:N	2.52	0.43

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:E:184:MET:C	1:E:186:THR:N	2.71	0.43
1:B:225:GLU:CG	1:B:226:THR:N	2.80	0.42
1:D:146:ILE:CD1	1:D:181:VAL:HG11	2.47	0.42
1:D:164:ASN:HD22	1:D:169:ASN:ND2	2.17	0.42
1:D:284:ASN:ND2	1:D:284:ASN:N	2.64	0.42
1:E:147:VAL:O	1:E:149:ASN:N	2.52	0.42
1:E:272:ILE:HG13	1:E:273:SER:N	2.33	0.42
1:F:143:ASN:H	1:F:143:ASN:ND2	2.17	0.42
1:F:207:GLU:HB3	1:F:208:GLU:OE1	2.20	0.42
1:E:253:ILE:O	1:E:273:SER:HA	2.17	0.42
1:D:295:LEU:HD12	1:D:296:ASN:H	1.84	0.42
1:E:143:ASN:C	1:E:143:ASN:ND2	2.64	0.42
1:F:140:PRO:HB2	1:F:141:PRO:HD2	2.01	0.42
1:A:252:TYR:HB3	1:A:254:HIS:CE1	2.55	0.42
1:E:164:ASN:OD1	1:G:162:VAL:CG1	2.65	0.42
1:A:168:VAL:CG2	1:A:319:THR:HB	2.50	0.42
1:B:231:LYS:HB3	1:B:231:LYS:HE3	1.81	0.42
1:B:234:MET:O	1:B:320:GLU:N	2.46	0.42
1:B:256:ILE:HG23	1:B:270:LEU:O	2.19	0.42
1:B:306:ALA:O	1:B:308:LEU:N	2.52	0.42
1:F:263:TYR:CG	1:F:264:ASP:N	2.88	0.42
1:B:156:LYS:HG3	1:B:177:VAL:CG2	2.49	0.42
1:E:168:VAL:HG23	1:E:319:THR:HB	2.01	0.42
1:G:156:LYS:NZ	1:G:156:LYS:CB	2.82	0.42
1:G:220:SER:HB3	1:G:222:ALA:H	1.84	0.42
1:A:261:THR:HG22	1:A:301:PRO:CG	2.49	0.42
1:B:244:THR:CG2	1:B:245:THR:N	2.82	0.42
1:E:141:PRO:HB2	1:E:142:PRO:HD2	2.01	0.42
1:G:228:ALA:O	1:G:229:SER:CB	2.62	0.42
1:A:253:ILE:O	1:A:273:SER:HA	2.20	0.42
1:B:131:ILE:HD12	1:B:132:ASN:HD22	1.85	0.42
1:B:184:MET:C	1:B:186:THR:H	2.21	0.42
1:G:156:LYS:HB3	1:G:156:LYS:HZ3	1.84	0.42
1:A:167:LEU:HG	1:D:160:VAL:CG1	2.49	0.42
1:A:280:MET:C	1:A:282:SER:H	2.24	0.42
1:B:245:THR:CG2	1:B:246:THR:H	2.23	0.42
1:B:284:ASN:H	1:B:284:ASN:HD22	1.68	0.42
1:F:132:ASN:N	1:F:132:ASN:HD22	2.17	0.42
1:A:258:TYR:HA	1:A:270:LEU:HD23	2.02	0.42
1:A:275:MET:O	1:A:276:LEU:CB	2.67	0.42
1:B:135:TRP:CH2	1:B:138:ILE:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ARG:HG3	1:D:195:ARG:NH1	2.33	0.42
1:D:240:TYR:CD1	1:D:276:LEU:HD13	2.54	0.42
1:G:303:SER:O	1:G:304:ASN:CB	2.66	0.42
1:A:205:LEU:HD12	1:A:205:LEU:N	2.35	0.41
1:B:132:ASN:N	1:B:132:ASN:ND2	2.68	0.41
1:B:217:ASN:O	1:B:223:THR:HA	2.20	0.41
1:B:302:GLU:O	1:B:302:GLU:HG3	2.20	0.41
1:D:135:TRP:CD1	1:D:135:TRP:C	2.93	0.41
1:D:176:GLY:H	1:D:308:LEU:CD2	2.33	0.41
1:D:303:SER:OG	1:D:304:ASN:N	2.53	0.41
1:F:251:ASN:O	1:F:251:ASN:ND2	2.53	0.41
1:F:258:TYR:C	1:F:270:LEU:HD21	2.40	0.41
1:G:275:MET:O	1:G:276:LEU:HB2	2.20	0.41
1:F:135:TRP:CD1	1:F:135:TRP:C	2.92	0.41
1:F:140:PRO:O	1:F:156:LYS:HE2	2.20	0.41
1:F:221:THR:O	1:F:221:THR:HG22	2.20	0.41
1:G:170:GLY:HA3	1:G:315:PHE:CZ	2.56	0.41
1:G:174:LEU:HD23	1:G:175:VAL:H	1.84	0.41
1:B:282:SER:HB3	1:B:284:ASN:HD21	1.82	0.41
1:D:198:PHE:C	1:D:205:LEU:HD13	2.41	0.41
1:A:213:ILE:HA	1:A:214:PRO:HD3	1.95	0.41
1:A:306:ALA:C	1:A:308:LEU:N	2.73	0.41
1:B:223:THR:OG1	1:B:224:SER:N	2.53	0.41
1:D:261:THR:O	1:D:264:ASP:O	2.39	0.41
1:F:277:ASN:O	1:F:278:SER:O	2.38	0.41
1:G:205:LEU:HD21	1:G:284:ASN:O	2.20	0.41
1:A:265:ARG:NH1	1:B:249:SER:OG	2.53	0.41
1:B:197:TYR:HB3	1:B:285:VAL:HG13	2.02	0.41
1:D:248:ASP:O	1:D:250:GLU:HG2	2.21	0.41
1:E:133:THR:HB	1:E:218:LYS:HB3	2.03	0.41
1:E:157:LEU:CD2	1:E:211:LEU:HD22	2.48	0.41
1:G:207:GLU:OE2	1:G:207:GLU:HA	2.21	0.41
1:A:168:VAL:HG23	1:A:319:THR:HB	2.03	0.41
1:A:231:LYS:HD2	1:A:287:TYR:OH	2.21	0.41
1:D:147:VAL:HG12	1:D:148:GLU:N	2.36	0.41
1:D:228:ALA:O	1:D:229:SER:CB	2.68	0.41
1:E:172:VAL:CG1	1:E:291:PHE:CE2	3.04	0.41
1:A:155:GLY:CA	1:A:177:VAL:HG23	2.51	0.41
1:A:259:TYR:N	1:A:270:LEU:HD21	2.35	0.41
1:B:172:VAL:HG22	1:B:315:PHE:CE2	2.48	0.41
1:B:206:THR:HG22	1:B:212:LYS:HA	2.03	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:B:231:LYS:HE3	1:B:322:ASP:O	2.20	0.41
1:D:183:GLN:O	1:D:186:THR:HG22	2.21	0.41
1:D:231:LYS:HA	1:D:234:MET:CG	2.51	0.41
1:E:219:SER:OG	1:E:224:SER:HB2	2.20	0.41
1:F:205:LEU:HA	1:F:205:LEU:HD12	1.74	0.41
1:G:174:LEU:CD2	1:G:175:VAL:N	2.84	0.41
1:G:245:THR:CG2	1:G:246:THR:N	2.80	0.41
1:A:143:ASN:C	1:A:153:ASN:HD22	2.24	0.41
1:A:198:PHE:HA	1:A:205:LEU:HD13	2.03	0.41
1:A:249:SER:HB2	1:D:260:MET:CE	2.51	0.41
1:A:261:THR:CB	1:A:301:PRO:HG3	2.50	0.41
1:G:199:ASP:HB3	1:G:205:LEU:HD11	2.03	0.41
1:G:216:LYS:HB3	1:G:223:THR:HB	2.03	0.41
1:G:300:SER:OG	1:G:301:PRO:CD	2.68	0.41
1:E:203:ASN:N	1:E:203:ASN:HD22	2.19	0.40
1:E:257:CYS:SG	1:E:293:TRP:CD1	3.14	0.40
1:F:242:PHE:HD2	1:F:279:ARG:HA	1.86	0.40
1:F:280:MET:HB3	1:F:285:VAL:HB	2.02	0.40
1:G:143:ASN:HD22	1:G:144:CYS:N	2.19	0.40
1:B:282:SER:HB2	1:B:285:VAL:HG23	2.03	0.40
1:A:263:TYR:C	1:A:264:ASP:O	2.59	0.40
1:D:243:ASN:OD1	1:D:243:ASN:O	2.38	0.40
1:F:168:VAL:HG23	1:F:319:THR:HB	2.03	0.40
1:G:249:SER:C	1:G:251:ASN:N	2.73	0.40
1:B:252:TYR:CE2	1:B:275:MET:HG3	2.56	0.40
1:D:216:LYS:HD3	1:D:223:THR:HB	2.03	0.40
1:D:257:CYS:SG	1:D:270:LEU:HG	2.61	0.40
1:E:134:LEU:HA	1:E:134:LEU:HD12	1.87	0.40
1:E:217:ASN:HD21	1:E:224:SER:N	2.07	0.40
1:F:143:ASN:HD22	1:F:143:ASN:C	2.25	0.40
1:G:135:TRP:HB2	1:G:136:THR:H	1.67	0.40
1:B:191:ASN:OD1	1:B:294:ASN:OD1	2.40	0.40
1:B:235:PRO:HG2	1:B:277:ASN:OD1	2.21	0.40

All (1) 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:186:THR:O	1:E:302:GLU:OE1[7_444]	2.08	0.12

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	190/220 (86%)	139 (73%)	29 (15%)	22 (12%)	0	0
1	B	190/220 (86%)	132 (70%)	31 (16%)	27 (14%)	0	0
1	D	190/220 (86%)	139 (73%)	30 (16%)	21 (11%)	0	0
1	E	190/220 (86%)	135 (71%)	32 (17%)	23 (12%)	0	0
1	F	190/220 (86%)	139 (73%)	28 (15%)	23 (12%)	0	0
1	G	190/220 (86%)	136 (72%)	30 (16%)	24 (13%)	0	0
All	All	1140/1320 (86%)	820 (72%)	180 (16%)	140 (12%)	0	0

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	SER
1	A	221	THR
1	A	248	ASP
1	A	250	GLU
1	A	304	ASN
1	A	306	ALA
1	B	145	GLN
1	B	220	SER
1	B	221	THR
1	B	223	THR
1	B	250	GLU
1	B	276	LEU
1	B	278	SER
1	B	301	PRO
1	B	304	ASN
1	B	306	ALA
1	D	150	THR
1	D	221	THR
1	D	243	ASN
1	D	262	SER

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Mol	Chain	Res	Type
1	D	299	GLU
1	D	304	ASN
1	D	306	ALA
1	D	308	LEU
1	E	150	THR
1	E	220	SER
1	E	221	THR
1	E	248	ASP
1	E	250	GLU
1	E	299	GLU
1	E	301	PRO
1	E	303	SER
1	F	145	GLN
1	F	220	SER
1	F	221	THR
1	F	223	THR
1	F	229	SER
1	F	250	GLU
1	F	276	LEU
1	F	278	SER
1	F	301	PRO
1	F	303	SER
1	F	304	ASN
1	F	306	ALA
1	G	150	THR
1	G	187	GLN
1	G	221	THR
1	G	243	ASN
1	G	250	GLU
1	G	299	GLU
1	G	303	SER
1	G	304	ASN
1	G	321	ASP
1	A	132	ASN
1	A	243	ASN
1	A	275	MET
1	A	301	PRO
1	A	305	ILE
1	A	321	ASP
1	B	150	THR
1	B	243	ASN
1	B	321	ASP

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Mol	Chain	Res	Type
1	D	186	THR
1	D	218	LYS
1	D	220	SER
1	D	248	ASP
1	D	249	SER
1	D	278	SER
1	D	303	SER
1	D	307	THR
1	D	321	ASP
1	E	132	ASN
1	E	148	GLU
1	E	223	THR
1	E	228	ALA
1	E	243	ASN
1	E	304	ASN
1	E	321	ASP
1	G	218	LYS
1	G	220	SER
1	G	248	ASP
1	G	308	LEU
1	A	219	SER
1	A	249	SER
1	A	262	SER
1	A	264	ASP
1	A	276	LEU
1	B	142	PRO
1	B	148	GLU
1	B	182	ASN
1	B	229	SER
1	B	232	ALA
1	B	303	SER
1	D	250	GLU
1	E	246	THR
1	E	281	ILE
1	F	142	PRO
1	F	150	THR
1	F	205	LEU
1	F	243	ASN
1	G	145	GLN
1	G	229	SER
1	G	262	SER
1	G	306	ALA

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Mol	Chain	Res	Type
1	A	263	TYR
1	A	299	GLU
1	A	308	LEU
1	B	139	ASN
1	B	140	PRO
1	B	200	SER
1	B	227	VAL
1	B	248	ASP
1	D	187	GLN
1	D	229	SER
1	D	263	TYR
1	E	229	SER
1	E	262	SER
1	E	276	LEU
1	E	308	LEU
1	F	140	PRO
1	F	227	VAL
1	G	249	SER
1	G	307	THR
1	A	229	SER
1	B	249	SER
1	B	299	GLU
1	E	249	SER
1	F	139	ASN
1	F	321	ASP
1	G	276	LEU
1	F	148	GLU
1	F	204	LEU
1	G	263	TYR
1	A	142	PRO
1	E	305	ILE
1	F	305	ILE
1	G	139	ASN
1	G	305	ILE
1	B	146	ILE
1	G	140	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	175/196 (89%)	159 (91%)	16 (9%)	9	21
1	B	175/196 (89%)	159 (91%)	16 (9%)	9	21
1	D	175/196 (89%)	155 (89%)	20 (11%)	5	13
1	E	175/196 (89%)	156 (89%)	19 (11%)	6	14
1	F	175/196 (89%)	153 (87%)	22 (13%)	4	10
1	G	175/196 (89%)	161 (92%)	14 (8%)	12	27
All	All	1050/1176 (89%)	943 (90%)	107 (10%)	7	17

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	TRP
1	A	143	ASN
1	A	145	GLN
1	A	172	VAL
1	A	188	LYS
1	A	217	ASN
1	A	251	ASN
1	A	262	SER
1	A	263	TYR
1	A	265	ARG
1	A	270	LEU
1	A	272	ILE
1	A	275	MET
1	A	284	ASN
1	A	298	SER
1	A	302	GLU
1	B	135	TRP
1	B	143	ASN
1	B	145	GLN
1	B	150	THR
1	B	161	LEU
1	B	172	VAL
1	B	174	LEU
1	B	188	LYS
1	B	221	THR
1	B	251	ASN
1	B	265	ARG

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Mol	Chain	Res	Type
1	B	270	LEU
1	B	275	MET
1	B	284	ASN
1	B	301	PRO
1	B	314	PHE
1	D	135	TRP
1	D	140	PRO
1	D	143	ASN
1	D	145	GLN
1	D	148	GLU
1	D	167	LEU
1	D	174	LEU
1	D	178	SER
1	D	180	THR
1	D	200	SER
1	D	209	SER
1	D	217	ASN
1	D	251	ASN
1	D	262	SER
1	D	265	ARG
1	D	270	LEU
1	D	275	MET
1	D	284	ASN
1	D	290	GLN
1	D	307	THR
1	E	135	TRP
1	E	143	ASN
1	E	144	CYS
1	E	145	GLN
1	E	172	VAL
1	E	173	SER
1	E	174	LEU
1	E	188	LYS
1	E	217	ASN
1	E	251	ASN
1	E	257	CYS
1	E	263	TYR
1	E	265	ARG
1	E	270	LEU
1	E	272	ILE
1	E	275	MET
1	E	280	MET

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Mol	Chain	Res	Type
1	E	284	ASN
1	E	301	PRO
1	F	135	TRP
1	F	143	ASN
1	F	145	GLN
1	F	150	THR
1	F	161	LEU
1	F	172	VAL
1	F	174	LEU
1	F	179	ASP
1	F	188	LYS
1	F	205	LEU
1	F	217	ASN
1	F	221	THR
1	F	251	ASN
1	F	265	ARG
1	F	270	LEU
1	F	275	MET
1	F	278	SER
1	F	280	MET
1	F	284	ASN
1	F	301	PRO
1	F	302	GLU
1	F	319	THR
1	G	135	TRP
1	G	140	PRO
1	G	143	ASN
1	G	148	GLU
1	G	173	SER
1	G	174	LEU
1	G	200	SER
1	G	217	ASN
1	G	251	ASN
1	G	265	ARG
1	G	270	LEU
1	G	275	MET
1	G	284	ASN
1	G	290	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	139	ASN
1	A	143	ASN
1	A	145	GLN
1	A	153	ASN
1	A	169	ASN
1	A	187	GLN
1	A	191	ASN
1	A	203	ASN
1	A	217	ASN
1	A	251	ASN
1	A	284	ASN
1	A	290	GLN
1	B	132	ASN
1	B	143	ASN
1	B	164	ASN
1	B	191	ASN
1	B	193	GLN
1	B	217	ASN
1	B	251	ASN
1	B	284	ASN
1	B	290	GLN
1	D	132	ASN
1	D	143	ASN
1	D	153	ASN
1	D	164	ASN
1	D	203	ASN
1	D	217	ASN
1	D	243	ASN
1	D	251	ASN
1	D	284	ASN
1	D	290	GLN
1	E	132	ASN
1	E	139	ASN
1	E	143	ASN
1	E	145	GLN
1	E	164	ASN
1	E	187	GLN
1	E	193	GLN
1	E	203	ASN
1	E	217	ASN
1	E	251	ASN
1	E	284	ASN

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Mol	Chain	Res	Type
1	E	290	GLN
1	F	132	ASN
1	F	143	ASN
1	F	193	GLN
1	F	217	ASN
1	F	251	ASN
1	F	284	ASN
1	F	290	GLN
1	F	296	ASN
1	G	132	ASN
1	G	143	ASN
1	G	164	ASN
1	G	203	ASN
1	G	217	ASN
1	G	243	ASN
1	G	251	ASN
1	G	284	ASN
1	G	290	GLN
1	G	296	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	192/220 (87%)	1.54	39 (20%)	1	0	34, 79, 108, 113	72 (37%)
1	B	192/220 (87%)	1.46	41 (21%)	0	0	41, 83, 108, 113	77 (40%)
1	D	192/220 (87%)	1.45	40 (20%)	1	0	51, 90, 108, 113	62 (32%)
1	E	192/220 (87%)	1.49	37 (19%)	1	0	42, 79, 108, 113	70 (36%)
1	F	192/220 (87%)	1.54	37 (19%)	1	0	42, 80, 108, 113	69 (35%)
1	G	192/220 (87%)	1.29	43 (22%)	0	0	55, 89, 108, 113	69 (35%)
All	All	1152/1320 (87%)	1.46	237 (20%)	1	0	34, 83, 108, 113	419 (36%)

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	246	THR	29.7
1	A	225	GLU	20.3
1	D	223	THR	17.1
1	E	225	GLU	16.4
1	A	224	SER	16.0
1	F	223	THR	14.3
1	D	245	THR	14.2
1	B	245	THR	13.7
1	E	224	SER	13.0
1	A	223	THR	11.4
1	B	246	THR	11.4
1	A	227	VAL	10.8
1	F	227	VAL	10.5
1	A	245	THR	10.3
1	A	246	THR	10.1
1	F	247	ARG	9.7
1	G	224	SER	9.6
1	G	228	ALA	9.4
1	D	226	THR	8.8

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Mol	Chain	Res	Type	RSRZ
1	D	222	ALA	8.6
1	D	305	ILE	8.3
1	D	224	SER	8.3
1	D	228	ALA	8.2
1	E	243	ASN	7.8
1	B	247	ARG	7.6
1	E	246	THR	7.4
1	F	222	ALA	7.0
1	E	223	THR	6.7
1	E	131	ILE	6.7
1	D	225	GLU	6.6
1	B	219	SER	6.4
1	G	223	THR	6.4
1	F	221	THR	6.1
1	F	248	ASP	6.0
1	E	247	ARG	5.9
1	A	305	ILE	5.9
1	F	245	THR	5.9
1	G	150	THR	5.7
1	E	245	THR	5.2
1	B	221	THR	5.2
1	E	305	ILE	5.1
1	G	305	ILE	5.1
1	G	226	THR	5.0
1	A	306	ALA	4.9
1	A	226	THR	4.8
1	G	245	THR	4.8
1	F	305	ILE	4.8
1	E	221	THR	4.7
1	B	149	ASN	4.7
1	G	297	ALA	4.6
1	G	263	TYR	4.6
1	E	232	ALA	4.6
1	F	226	THR	4.5
1	B	306	ALA	4.5
1	D	297	ALA	4.5
1	D	221	THR	4.4
1	E	222	ALA	4.4
1	F	172	VAL	4.4
1	B	222	ALA	4.4
1	B	185	PHE	4.3
1	A	247	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	228	ALA	4.2
1	B	259	TYR	4.2
1	F	270	LEU	4.2
1	D	218	LYS	4.1
1	B	227	VAL	4.1
1	G	222	ALA	4.1
1	B	225	GLU	4.1
1	E	244	THR	4.1
1	A	206	THR	4.1
1	G	225	GLU	4.0
1	G	185	PHE	4.0
1	D	254	HIS	4.0
1	D	181	VAL	4.0
1	D	185	PHE	4.0
1	A	243	ASN	3.9
1	E	226	THR	3.9
1	G	221	THR	3.9
1	F	225	GLU	3.8
1	F	219	SER	3.8
1	G	147	VAL	3.8
1	D	238	THR	3.8
1	B	299	GLU	3.7
1	B	305	ILE	3.7
1	G	254	HIS	3.7
1	G	146	ILE	3.7
1	B	263	TYR	3.7
1	D	227	VAL	3.7
1	D	249	SER	3.7
1	B	268	PHE	3.7
1	E	138	ILE	3.7
1	F	306	ALA	3.6
1	A	131	ILE	3.6
1	B	270	LEU	3.6
1	B	301	PRO	3.5
1	B	154	ASP	3.5
1	A	318	ILE	3.5
1	F	185	PHE	3.5
1	B	321	ASP	3.4
1	E	281	ILE	3.4
1	A	233	PHE	3.4
1	B	228	ALA	3.4
1	F	151	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	194	LEU	3.4
1	A	232	ALA	3.3
1	F	259	TYR	3.2
1	B	288	ALA	3.2
1	F	307	THR	3.2
1	B	310	THR	3.2
1	D	244	THR	3.2
1	E	270	LEU	3.2
1	G	285	VAL	3.2
1	F	301	PRO	3.1
1	A	132	ASN	3.1
1	D	172	VAL	3.1
1	E	183	GLN	3.1
1	B	160	VAL	3.1
1	B	309	THR	3.1
1	D	159	LEU	3.1
1	D	295	LEU	3.1
1	B	220	SER	3.0
1	B	215	LEU	3.0
1	F	268	PHE	3.0
1	F	288	ALA	3.0
1	B	162	VAL	3.0
1	A	248	ASP	3.0
1	E	322	ASP	2.9
1	D	306	ALA	2.9
1	F	131	ILE	2.9
1	G	138	ILE	2.9
1	E	302	GLU	2.9
1	G	151	ASN	2.9
1	D	248	ASP	2.9
1	F	263	TYR	2.9
1	A	281	ILE	2.9
1	E	233	PHE	2.9
1	G	283	SER	2.9
1	F	250	GLU	2.9
1	G	229	SER	2.8
1	F	196	LEU	2.8
1	A	270	LEU	2.8
1	D	318	ILE	2.8
1	D	243	ASN	2.8
1	E	249	SER	2.8
1	F	149	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	192	ILE	2.7
1	B	226	THR	2.7
1	A	322	ASP	2.7
1	B	223	THR	2.7
1	G	246	THR	2.7
1	B	279	ARG	2.7
1	A	221	THR	2.7
1	G	293	TRP	2.7
1	G	308	LEU	2.7
1	D	239	ALA	2.7
1	D	280	MET	2.6
1	G	211	LEU	2.6
1	E	242	PHE	2.6
1	D	240	TYR	2.6
1	A	301	PRO	2.6
1	A	321	ASP	2.6
1	A	192	ILE	2.6
1	B	264	ASP	2.6
1	G	198	PHE	2.6
1	A	218	LYS	2.5
1	G	192	ILE	2.5
1	A	228	ALA	2.5
1	F	148	GLU	2.5
1	B	253	ILE	2.5
1	E	185	PHE	2.5
1	F	249	SER	2.5
1	D	189	THR	2.5
1	E	227	VAL	2.5
1	G	295	LEU	2.5
1	A	162	VAL	2.5
1	B	211	LEU	2.5
1	G	181	VAL	2.5
1	B	267	LEU	2.5
1	A	279	ARG	2.5
1	A	253	ILE	2.4
1	G	304	ASN	2.4
1	D	184	MET	2.4
1	A	303	SER	2.4
1	B	196	LEU	2.4
1	A	299	GLU	2.4
1	E	263	TYR	2.4
1	A	302	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	231	LYS	2.4
1	D	194	LEU	2.4
1	G	306	ALA	2.4
1	E	299	GLU	2.4
1	G	184	MET	2.4
1	E	295	LEU	2.4
1	F	238	THR	2.3
1	E	208	GLU	2.3
1	E	301	PRO	2.3
1	F	132	ASN	2.3
1	E	206	THR	2.3
1	F	309	THR	2.3
1	D	308	LEU	2.3
1	D	138	ILE	2.3
1	G	289	ILE	2.3
1	G	243	ASN	2.2
1	G	267	LEU	2.2
1	D	229	SER	2.2
1	B	307	THR	2.2
1	E	179	ASP	2.2
1	A	168	VAL	2.2
1	D	304	ASN	2.2
1	E	264	ASP	2.2
1	G	313	PHE	2.2
1	A	222	ALA	2.2
1	G	253	ILE	2.2
1	G	303	SER	2.2
1	F	286	ALA	2.2
1	A	150	THR	2.2
1	B	150	THR	2.2
1	E	318	ILE	2.1
1	A	181	VAL	2.1
1	E	309	THR	2.1
1	B	281	ILE	2.1
1	B	293	TRP	2.1
1	G	307	THR	2.1
1	G	317	TYR	2.1
1	G	294	ASN	2.1
1	D	242	PHE	2.1
1	D	153	ASN	2.1
1	D	161	LEU	2.0
1	F	162	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	146	ILE	2.0
1	D	283	SER	2.0
1	G	189	THR	2.0
1	F	315	PHE	2.0
1	F	258	TYR	2.0
1	E	236	SER	2.0
1	D	321	ASP	2.0
1	G	194	LEU	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.