



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:40 AM GMT

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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

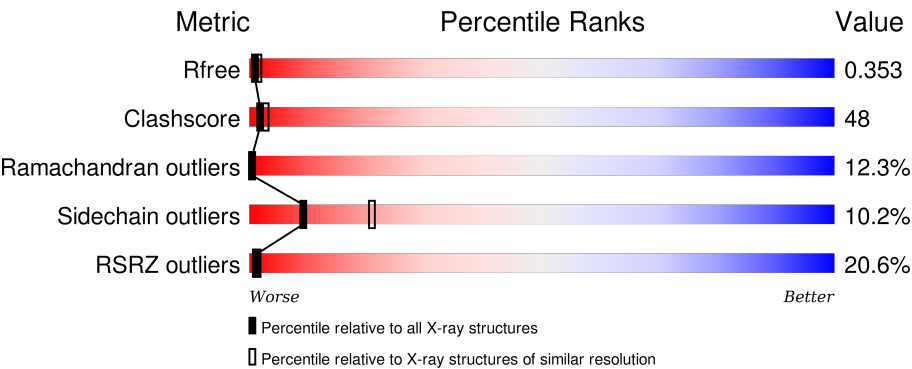
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	<div><div>15%</div><div>35%39%13%•13%</div></div>
1	B	220	<div><div>15%</div><div>27%45%13%•13%</div></div>
1	D	220	<div><div>22%</div><div>29%44%14%13%</div></div>
1	E	220	<div><div>16%</div><div>32%40%14%•13%</div></div>
1	F	220	<div><div>18%</div><div>34%39%12%•13%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	220	<div><div></div><div>21%</div><div>34%</div><div>41%</div><div>12%</div><div>13%</div></div>

2 Entry composition

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
1	A	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			
1	B	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			
1	D	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			
1	E	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			
1	F	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			
1	G	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			

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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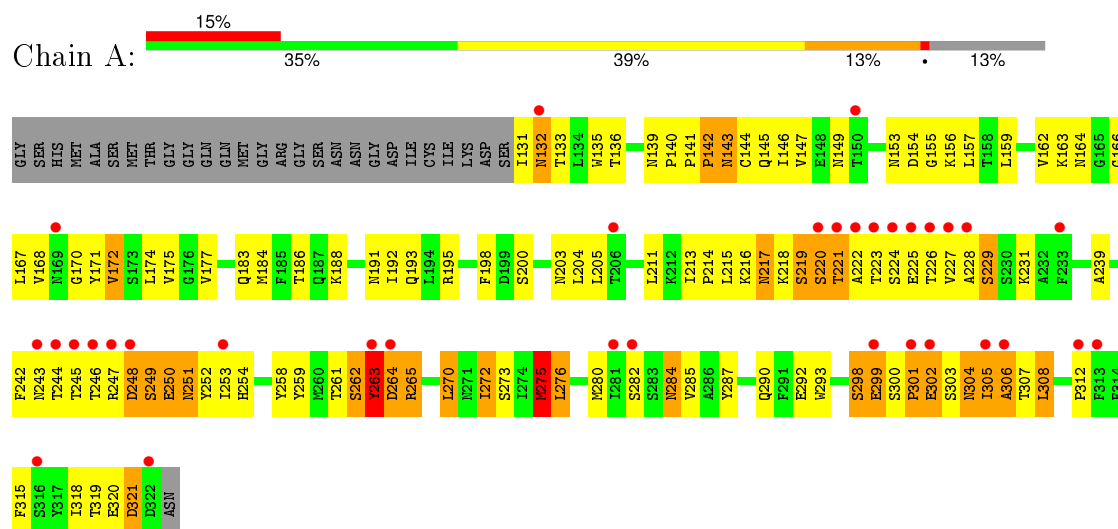
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Chain	Residue	Modelled	Actual	Comment	Reference
G	120	SER	-	EXPRESSION TAG	UNP Q7T925

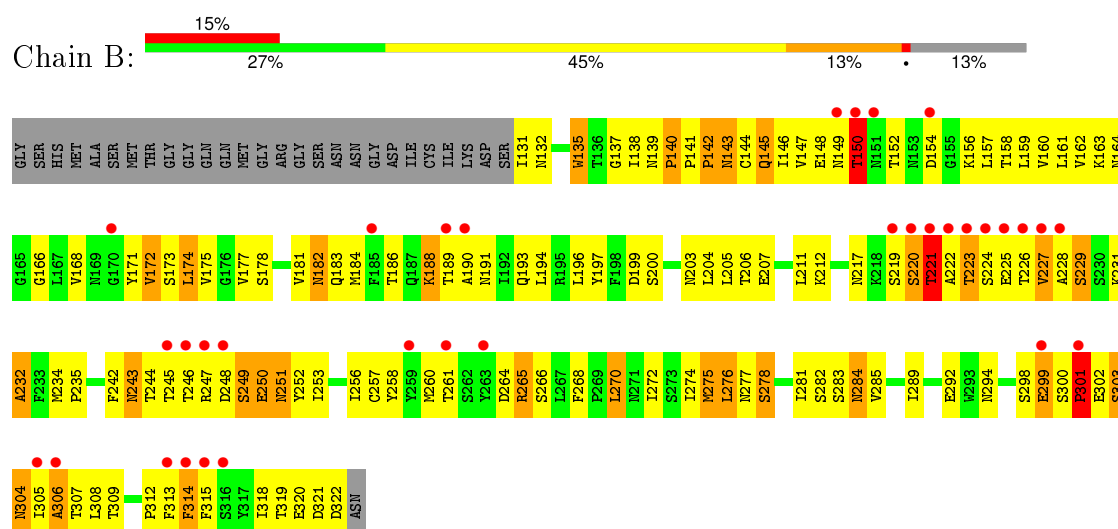
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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

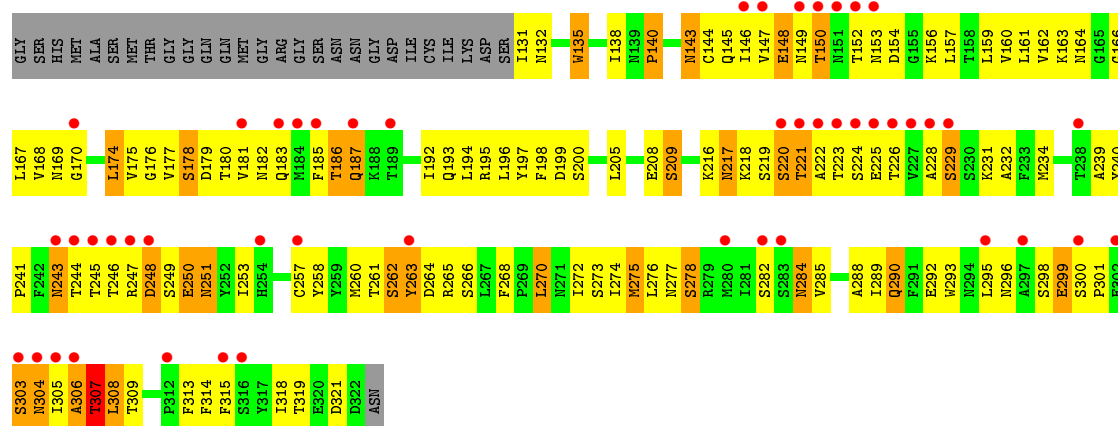


• Molecule 1: Fiber

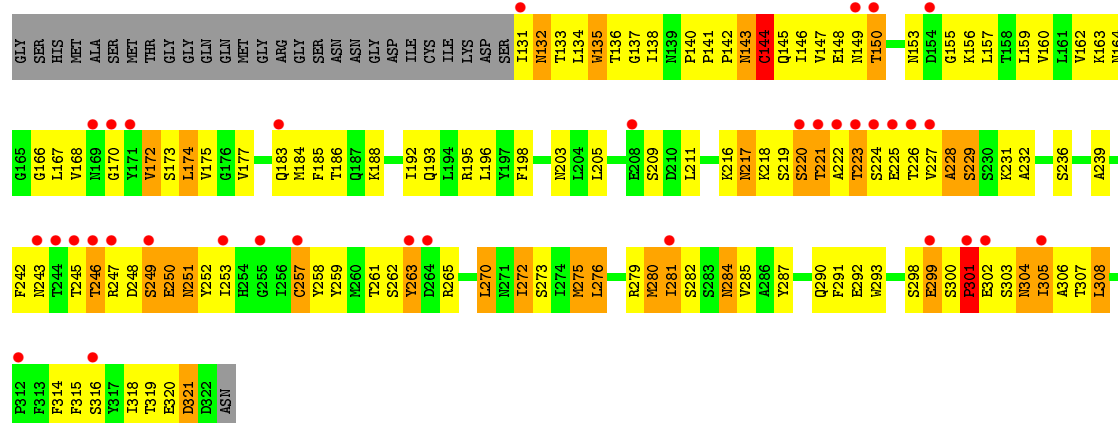


• Molecule 1: Fiber

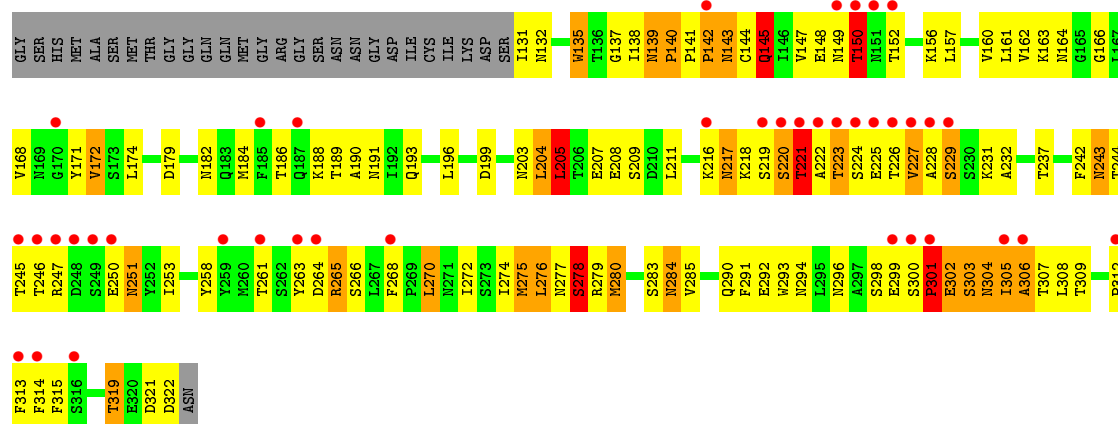




• Molecule 1: Fiber

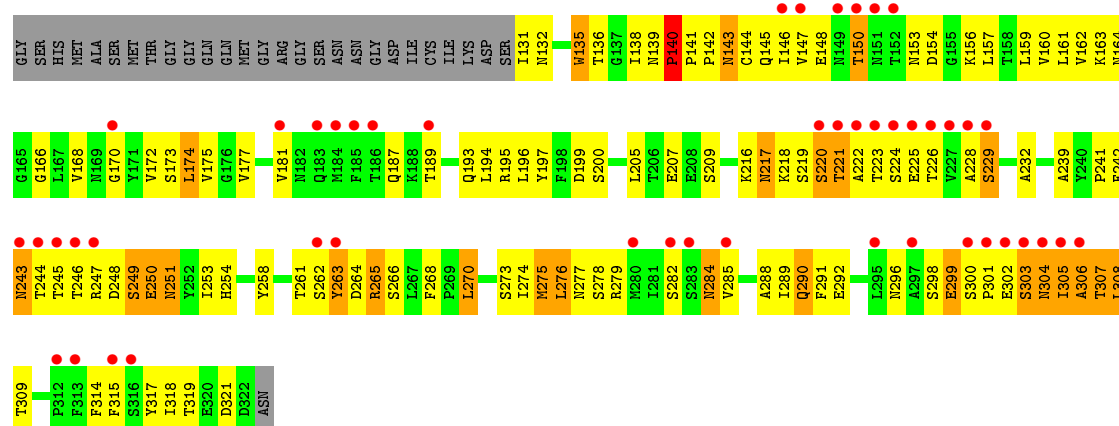


• Molecule 1: Fiber



• Molecule 1: Fiber





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
$\langle I/\sigma(I) \rangle$ 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%)	DCC
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.9	EDS
Estimated twinning fraction	0.468 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57497 reflections	Xtriage
F_o, F_c correlation	0.86	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	Ideal(°)
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:G:172:VAL:HG21	1:G:291:PHE:CE2	2.10	0.87
1:D:174:LEU:HD23	1:D:175:VAL:H	1.39	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:H	1:E:217:ASN:ND2	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:D:140:PRO:O	1:D:156:LYS:HE2	1.77	0.84
1:B:225:GLU:HG3	1:B:226:THR:H	1.41	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:G:217:ASN:H	1:G:217:ASN:HD22	1.24	0.82
1:B:142:PRO:HB3	1:B:177:VAL:HG21	1.60	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:E:245:THR:HG22	1:E:246:THR:H	1.45	0.80
1:A:216:LYS:HB2	1:A:223:THR:HB	1.64	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: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:B:193:GLN:HB3	1:B:292:GLU:HG3	1.62	0.79
1:G:159:LEU:HD13	1:G:172:VAL:HG22	1.65	0.78
1:E:216:LYS:HB2	1:E:223:THR:HB	1.65	0.78
1:G:217:ASN:ND2	1:G:217:ASN:H	1.82	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: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:G:172:VAL:HG23	1:G:315:PHE:HE2	1.48	0.77
1:A:193:GLN:HB3	1:A:292:GLU:HG3	1.66	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:B:268:PHE:CE1	1:B:300:SER:HA	2.18	0.77
1:A:164:ASN:HD21	1:D:164:ASN:HD21	1.32	0.77
1:E:144:CYS:O	1:E:153:ASN:HA	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:SER:O	1:D:299:GLU:HB2	1.85	0.76
1:D:219:SER:HB2	1:D:224:SER:HB2	1.67	0.76
1:E:219:SER:CB	1:E:224:SER:HB2	2.16	0.76
1:D:277:ASN:HA	1:D:288:ALA:HB3	1.67	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:E:259:TYR:HE2	1:E:301:PRO:HG2	1.50	0.75
1:A:250:GLU:HB2	1:D:309:THR:HG21	1.68	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:B:247:ARG:O	1:B:250:GLU:HG2	1.88	0.74
1:A:315:PHE:HA	1:D:314:PHE:CE1	2.23	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:D:217:ASN:HD22	1:D:217:ASN:N	1.85	0.73
1:B:199:ASP:HB3	1:B:205:LEU:HD11	1.71	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:HD12	1:G:131:ILE:C	2.09	0.72
1:F:308:LEU:O	1:F:308:LEU:HD23	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:ND2	1:G:284:ASN:H	1.86	0.72
1:B:143:ASN:HD21	1:B:157:LEU:H	1.33	0.72
1:F:217:ASN:HD22	1:F:217:ASN:C	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:D:217:ASN:H	1:D:217:ASN:ND2	1.87	0.71
1:A:217:ASN:HD21	1:A:224:SER:H	1.38	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:H	1:A:217:ASN:ND2	1.88	0.70
1:E:228:ALA:O	1:E:229:SER:HB3	1.92	0.70
1:D:159:LEU:HG	1:D:161:LEU:HD21	1.73	0.70
1:A:300:SER:OG	1:A:301:PRO:HD2	1.90	0.70
1:A:143:ASN:HD21	1:A:157:LEU:N	1.87	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:A:239:ALA:HB2	1:D:138:ILE:HG23	1.73	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:O	1:D:308:LEU:HD23	1.94	0.68
1:G:217:ASN:HD22	1:G:217:ASN:N	1.86	0.68
1:G:245:THR:HG22	1:G:246:THR:N	2.09	0.68
1:B:251:ASN:C	1:B:251:ASN:HD22	1.96	0.68
1:G:270:LEU:N	1:G:270:LEU:HD23	2.09	0.68
1:D:156:LYS:HB3	1:D:156:LYS:NZ	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:G:284:ASN:HD22	1:G:284:ASN:N	1.91	0.67
1:E:227:VAL:C	1:E:229:SER:H	1.97	0.67
1:D:146:ILE:HD12	1:D:181:VAL:HG11	1.75	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:216:LYS:CB	1:A:223:THR:HB	2.24	0.67
1:A:183:GLN:HG2	1:A:186:THR:HG21	1.77	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:N	1:D:161:LEU:HD22	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:HA	1:B:265:ARG:HE	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:304:ASN:C	1:G:306:ALA:H	1.98	0.65
1:G:277:ASN:HA	1:G:288:ALA:HB3	1.79	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:H	1:G:270:LEU:HD23	1.63	0.64
1:E:132:ASN:O	1:E:162:VAL:HA	1.97	0.64
1:D:174:LEU:CD2	1:D:175:VAL:N	2.61	0.64
1:B:172:VAL:HG23	1:B:313:PHE:O	1.98	0.64
1:D:270:LEU:N	1:D:270:LEU:HD23	2.11	0.63
1:E:157:LEU:HD23	1:E:211:LEU:HD22	1.80	0.63
1:D:163:LYS:HE2	1:D:232:ALA:O	1.97	0.63
1:A:303:SER:O	1:A:304:ASN:HB2	1.98	0.63
1:G:274:ILE:HA	1:G:290:GLN:O	1.97	0.63
1:F:150:THR:HB	1:F:152:THR:O	1.98	0.63
1:F:228:ALA:O	1:F:229:SER:HB3	1.98	0.63
1:E:164:ASN:ND2	1:G:164:ASN:HD21	1.94	0.63
1:B:204:LEU:HD22	1:B:211:LEU:HD23	1.81	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:C	1:D:131:ILE:HD12	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:245:THR:HG22	1:B:246:THR:N	2.14	0.62
1:B:138:ILE:HG12	1:D:318:ILE:HG21	1.80	0.62
1:G:303:SER:O	1:G:304:ASN:HB2	1.98	0.62
1:F:225:GLU:CG	1:F:226:THR:H	2.06	0.62
1:D:205:LEU:HD23	1:D:208:GLU:OE1	1.99	0.62
1:A:172:VAL:HG22	1:A:315:PHE:HE2	1.64	0.62
1:E:217:ASN:N	1:E:217:ASN:HD22	1.97	0.62
1:B:207:GLU:HA	1:B:207:GLU:OE2	1.99	0.62
1:A:166:GLY:O	1:A:319:THR:HG22	2.00	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:E:164:ASN:OD1	1:G:162:VAL:HG11	1.99	0.61
1:D:282:SER:HB3	1:D:284:ASN:HD21	1.65	0.61
1:F:278:SER:OG	1:F:279:ARG:N	2.31	0.61
1:F:172:VAL:HG23	1:F:313:PHE:HB3	1.83	0.61
1:D:253:ILE:HG21	1:D:274:ILE:HD12	1.82	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:300:SER:O	1:B:302:GLU:N	2.34	0.60
1:G:163:LYS:NZ	1:G:319:THR:HG21	2.15	0.60
1:B:282:SER:HB3	1:B:284:ASN:ND2	2.15	0.60
1:E:205:LEU:HD21	1:E:284:ASN:O	2.01	0.60
1:G:282:SER:HB3	1:G:284:ASN:ND2	2.16	0.60
1:A:167:LEU:HG	1:D:160:VAL:HG11	1.83	0.60
1:G:306:ALA:C	1:G:308:LEU:H	2.05	0.60
1:D:195:ARG:HH11	1:D:195:ARG:HG3	1.65	0.60
1:A:228:ALA:O	1:A:229:SER:HB3	2.01	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:HD12	1:B:131:ILE:C	2.22	0.60
1:B:143:ASN:HD21	1:B:157:LEU:N	2.00	0.59
1:G:131:ILE:O	1:G:131:ILE:HD12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:ILE:HA	1:D:290:GLN:O	2.02	0.59
1:G:196:LEU:HA	1:G:209:SER:CB	2.33	0.59
1:G:195:ARG:HG2	1:G:290:GLN:NE2	2.17	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:D:268:PHE:HE1	1:D:301:PRO:HD3	1.66	0.59
1:B:227:VAL:O	1:F:227:VAL:HB	2.01	0.59
1:G:163:LYS:HE3	1:G:232:ALA:HB1	1.84	0.59
1:B:141:PRO:O	1:B:143:ASN:N	2.36	0.59
1:E:218:LYS:NZ	1:F:166:GLY:HA2	2.16	0.59
1:D:284:ASN:H	1:D:284:ASN:ND2	2.01	0.59
1:B:157:LEU:HD13	1:B:194:LEU:HD12	1.83	0.59
1:A:251:ASN:H	1:A:251:ASN:HD22	1.50	0.59
1:A:164:ASN:HD21	1:B:164:ASN:HD21	1.49	0.59
1:D:159:LEU:HG	1:D:161:LEU:CD2	2.32	0.59
1:E:245:THR:C	1:E:247:ARG:H	2.06	0.58
1:E:192:ILE:HG12	1:E:293:TRP:HB2	1.85	0.58
1:D:228:ALA:O	1:D:229:SER:HB3	2.01	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:F:300:SER:O	1:F:302:GLU:N	2.36	0.58
1:E:249:SER:O	1:E:251:ASN:N	2.37	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:B:182:ASN:HD22	1:B:307:THR:HA	1.68	0.58
1:B:166:GLY:O	1:B:319:THR:HG22	2.04	0.58
1:A:259:TYR:HE1	1:A:308:LEU: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:E:272:ILE:HD13	1:E:293:TRP:NE1	2.18	0.58
1:A:245:THR:O	1:A:246:THR:OG1	2.21	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:D:264:ASP:OD2	1:D:266:SER:HB2	2.04	0.57
1:A:174:LEU:HD13	1:A:192:ILE:HD12	1.86	0.57
1:G:261:THR:OG1	1:G:266:SER:N	2.37	0.57
1:F:160:VAL:HG21	1:G:318:ILE:HD11	1.86	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:G:159:LEU:CD1	1:G:172:VAL:HG22	2.33	0.57
1:E:225:GLU:CG	1:E:226:THR:H	2.17	0.57
1:A:218:LYS:HZ3	1:B:166:GLY:HA2	1.69	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:D:239:ALA:C	1:D:241:PRO:HD3	2.24	0.57
1:D:170:GLY:HA3	1:D:315:PHE:CE2	2.40	0.57
1:A:155:GLY:HA2	1:A:177:VAL:HG23	1.86	0.57
1:F:172:VAL:O	1:F:312:PRO:HA	2.05	0.57
1:A:275:MET:O	1:A:276:LEU:HB2	2.05	0.57
1:A:192:ILE:HG12	1:A:293:TRP:HB2	1.87	0.57
1:A:131:ILE:C	1:A:131:ILE:HD12	2.24	0.57
1:F:300:SER:OG	1:F:301:PRO:HD2	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:B:217:ASN:HB3	1:B:224:SER:HB3	1.87	0.57
1:F:157:LEU:HD23	1:F:211:LEU:HD13	1.87	0.57
1:E:184:MET:C	1:E:186:THR:H	2.07	0.57
1:G:156:LYS:NZ	1:G:156:LYS:HB3	2.19	0.56
1:G:143:ASN:HD21	1:G:157:LEU:H	1.52	0.56
1:E:216:LYS:CB	1:E:223:THR:HB	2.33	0.56
1:D:253:ILE:O	1:D:273:SER:HA	2.05	0.56
1:A:249:SER:O	1:A:251:ASN:N	2.39	0.56
1:A:164:ASN:ND2	1:D:164:ASN:ND2	2.48	0.56
1:F:268:PHE:CE1	1:F:300:SER:HA	2.34	0.56
1:D:143:ASN:CA	1:D:153:ASN:HD22	2.17	0.56
1:B:308:LEU:HD23	1:B:308:LEU:O	2.06	0.56
1:E:140:PRO:O	1:E:156:LYS:NZ	2.32	0.56
1:B:147:VAL:C	1:B:149:ASN:H	2.08	0.56
1:B:147:VAL:HG12	1:B:149:ASN:H	1.70	0.56
1:G:217:ASN:ND2	1:G:224:SER:HB3	2.20	0.56
1:E:216:LYS:HB2	1:E:223:THR:CB	2.34	0.56
1:A:304:ASN:C	1:A:306:ALA:N	2.58	0.56
1:F:228:ALA:O	1:F:229:SER:CB	2.52	0.56
1:D:251:ASN:H	1:D:251:ASN:HD22	1.54	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:F:261:THR:HG22	1:F:301:PRO:CG	2.36	0.55
1:D:143:ASN:HA	1:D:153:ASN:ND2	2.19	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:A:239:ALA:HB2	1:D:138:ILE:CG2	2.36	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:D:253:ILE:HB	1:D:274:ILE:HB	1.89	0.55
1:B:189:THR:HG22	1:B:190:ALA:N	2.21	0.55
1:E:239:ALA:HB2	1:G:138:ILE:HG23	1.88	0.55
1:G:300:SER:OG	1:G:301:PRO:HD2	2.06	0.55
1:B:166:GLY:C	1:B:319:THR:HG22	2.27	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:E:149:ASN:O	1:E:150:THR:O	2.25	0.55
1:F:237:THR:HG22	1:F:277:ASN:ND2	2.21	0.55
1:E:167:LEU:CD2	1:E:318:ILE:HD12	2.37	0.55
1:E:251:ASN:HD22	1:E:251:ASN:H	1.52	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:B:275:MET:O	1:B:276:LEU:O	2.25	0.55
1:A:280:MET:HA	1:A:285:VAL:HG11	1.89	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:F:298:SER:O	1:F:299:GLU:HB2	2.07	0.54
1:D:179:ASP:HA	1:D:182:ASN:HB2	1.89	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:F:302:GLU:OE1	1:F:303:SER:N	2.40	0.54
1:F:245:THR:C	1:F:247:ARG:H	2.10	0.54
1:D:275:MET:SD	1:D:278:SER:HA	2.47	0.54
1:F:204:LEU:O	1:F:204:LEU:HG	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:ASN:O	1:E:306:ALA:N	2.41	0.54
1:E:135:TRP:CH2	1:E:138:ILE:HG13	2.42	0.54
1:G:244:THR:HG22	1:G:245:THR:O	2.07	0.54
1:E:251:ASN:O	1:E:275:MET:O	2.26	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:E:172:VAL:HG11	1:E:291:PHE:CE2	2.43	0.54
1:B:207:GLU:OE2	1:F:283:SER:HB3	2.07	0.54
1:G:249:SER:C	1:G:251:ASN:H	2.10	0.54
1:G:308:LEU:HD23	1:G:308:LEU:C	2.28	0.54
1:B:154:ASP:HB2	1:B:178:SER:HB3	1.89	0.54
1:G:298:SER:O	1:G:299:GLU:CB	2.56	0.54
1:F:141:PRO:O	1:F:143:ASN:N	2.40	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:F:304:ASN:C	1:F:306:ALA:N	2.60	0.53
1:B:135:TRP:CE2	1:B:137:GLY:HA2	2.44	0.53
1:B:302:GLU:C	1:B:302:GLU:OE1	2.47	0.53
1:G:265:ARG:HA	1:G:265:ARG:HE	1.72	0.53
1:B:309:THR:HG21	1:D:250:GLU:HB2	1.90	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:A:282:SER:HB2	1:A:285:VAL:HG23	1.91	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:G:282:SER:CB	1:G:284:ASN:ND2	2.72	0.53
1:E:147:VAL:C	1:E:149:ASN:H	2.12	0.53
1:G:306:ALA:C	1:G:308:LEU:N	2.60	0.53
1:G:172:VAL:HG23	1:G:315:PHE:CE2	2.38	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:B:242:PHE:O	1:B:243:ASN:C	2.46	0.53
1:D:268:PHE:CE1	1:D:301:PRO:HD3	2.45	0.52
1:A:261:THR:HB	1:A:301:PRO:HG3	1.90	0.52
1:F:251:ASN:HD22	1:F:251:ASN:C	2.13	0.52
1:E:143:ASN:O	1:E:211:LEU:HD12	2.09	0.52
1:G:282:SER:HB3	1:G:284:ASN:HD21	1.72	0.52
1:E:263:TYR:HD1	1:E:263:TYR:H	1.56	0.52
1:F:216:LYS:HB2	1:F:223:THR:CB	2.39	0.52
1:E:196:LEU:HA	1:E:209:SER:HB3	1.91	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:E:220:SER:HB3	1:E:222:ALA:N	2.21	0.52
1:B:245:THR:C	1:B:247:ARG:H	2.11	0.52
1:B:174:LEU:HD23	1:B:175:VAL:N	2.25	0.52
1:B:251:ASN:C	1:B:251:ASN:ND2	2.61	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:B:253:ILE:HB	1:B:274:ILE:HB	1.91	0.52
1:G:156:LYS:HG3	1:G:177:VAL:HG21	1.91	0.52
1:A:242:PHE:CE2	1:A:280:MET:HG2	2.45	0.52
1:G:242:PHE:HD2	1:G:279:ARG:HA	1.73	0.52
1:D:244:THR:HG22	1:D:245:THR:O	2.10	0.52
1:D:156:LYS:CB	1:D:156:LYS:NZ	2.73	0.52
1:A:198:PHE:HA	1:A:203:ASN:O	2.09	0.52
1:G:163:LYS:HZ3	1:G:319:THR:HG21	1.74	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:A:245:THR:C	1:A:247:ARG:H	2.14	0.52
1:E:132:ASN:O	1:E:162:VAL:HG13	2.10	0.52
1:F:300:SER:O	1:F:301:PRO:C	2.49	0.52
1:F:131:ILE:O	1:F:131:ILE:HD12	2.10	0.52
1:B:314:PHE:CE1	1:D:315:PHE:HA	2.45	0.52
1:F:245:THR:C	1:F:247:ARG:N	2.63	0.51
1:F:309:THR:HG21	1:G:250:GLU:CB	2.38	0.51
1:F:204:LEU:CD2	1:F:211:LEU:HD23	2.38	0.51
1:E:225:GLU:HG3	1:E:226:THR:N	2.25	0.51
1:F:258:TYR:CD1	1:F:258:TYR:N	2.78	0.51
1:A:318:ILE:HG22	1:A:318:ILE:O	2.09	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:D:231:LYS:HA	1:D:234:MET:HG2	1.91	0.51
1:B:150:THR:HB	1:B:152:THR:O	2.09	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:B:272:ILE:HD13	1:B:313:PHE:CD2	2.45	0.51
1:A:227:VAL:C	1:A:229:SER:H	2.12	0.51
1:G:251:ASN:H	1:G:251:ASN:ND2	2.09	0.51
1:F:314:PHE:CE1	1:G:315:PHE:HA	2.46	0.51
1:E:163:LYS:HD3	1:E:232:ALA:O	2.10	0.51
1:F:302:GLU:C	1:F:302:GLU:OE1	2.48	0.51
1:E:227:VAL:O	1:E:229:SER:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:HB	1:B:171:TYR:HB3	1.91	0.51
1:D:284:ASN:H	1:D:284:ASN:HD22	1.59	0.51
1:G:261:THR:O	1:G:264:ASP:O	2.29	0.51
1:A:270:LEU:N	1:A:270:LEU:HD23	2.25	0.51
1:D:146:ILE:O	1:D:146:ILE:HG22	2.10	0.51
1:E:281:ILE:O	1:E:281:ILE:HG13	2.11	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:B:141:PRO:O	1:B:142:PRO:C	2.50	0.51
1:F:304:ASN:O	1:F:306:ALA:N	2.44	0.51
1:F:182:ASN:ND2	1:F:307:THR:HA	2.26	0.51
1:A:284:ASN:N	1:A:284:ASN:HD22	2.09	0.51
1:E:245:THR:O	1:E:247:ARG:N	2.44	0.51
1:D:197:TYR:N	1:D:209:SER:OG	2.39	0.50
1:B:260:MET:HA	1:B:266:SER:O	2.11	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: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:G:131:ILE:CD1	1:G:131:ILE:C	2.77	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:B:219:SER:HB2	1:B:224:SER:HB2	1.93	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:B:244:THR:HG22	1:B:245:THR:N	2.27	0.50
1:A:259:TYR:CE1	1:A:308:LEU:HA	2.46	0.50
1:G:161:LEU:HD12	1:G:168:VAL:HG11	1.93	0.50
1:E:143:ASN:ND2	1:E:157:LEU:H	2.05	0.50
1:D:199:ASP:HB3	1:D:205:LEU:HD11	1.93	0.50
1:B:131:ILE:HD12	1:B:131:ILE:O	2.12	0.50
1:G:249:SER:O	1:G:251:ASN:N	2.45	0.50
1:A:147:VAL:C	1:A:149:ASN:H	2.15	0.50
1:D:263:TYR:CG	1:D:264:ASP:N	2.77	0.50
1:F:242:PHE:O	1:F:243:ASN:C	2.49	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

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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:A:287:TYR:HE2	1:A:320:GLU:OE1	1.95	0.50
1:E:258:TYR:C	1:E:270:LEU:HD21	2.32	0.50
1:E:183:GLN:HG2	1:E:186:THR:CG2	2.41	0.50
1:B:277:ASN:O	1:B:278:SER:O	2.29	0.50
1:D:257:CYS:O	1:D:270:LEU:HD23	2.12	0.49
1:F:217:ASN:ND2	1:F:217:ASN:C	2.64	0.49
1:E:261:THR:HG22	1:E:301:PRO:CG	2.40	0.49
1:A:170:GLY:HA3	1:A:315:PHE:CZ	2.46	0.49
1:E:252:TYR:CE2	1:E:275:MET:HG2	2.47	0.49
1:A:320:GLU:O	1:A:321:ASP:C	2.51	0.49
1:A:171:TYR:CE2	1:B:318:ILE:HD11	2.47	0.49
1:D:275:MET:O	1:D:276:LEU:HB2	2.11	0.49
1:B:168:VAL:HG23	1:B:319:THR:HB	1.95	0.49
1:D:307:THR:HG23	1:D:307:THR:O	2.11	0.49
1:B:132:ASN:HD22	1:B:132:ASN:N	2.10	0.49
1:D:147:VAL:HB	1:D:150:THR:OG1	2.11	0.49
1:A:302:GLU:O	1:A:302:GLU:HG3	2.12	0.49
1:F:225:GLU:HG3	1:F:226:THR:N	2.15	0.49
1:A:219:SER:O	1:A:220:SER:HB2	2.12	0.49
1:D:132:ASN:O	1:D:162:VAL:HG13	2.12	0.49
1:B:261:THR:HG22	1:B:301:PRO:HG3	1.94	0.49
1:D:305:ILE:HG22	1:D:305:ILE:O	2.12	0.49
1:G:226:THR:HG22	1:G:228:ALA:HB2	1.93	0.49
1:E:167:LEU:HG	1:G:160:VAL:HG11	1.95	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:D:270:LEU:N	1:D:270:LEU:CD2	2.76	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: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:A:284:ASN:HD22	1:A:284:ASN:H	1.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ASN:O	1:D:150:THR:O	2.30	0.48
1:A:136:THR:HG23	1:A:159:LEU:HB3	1.94	0.48
1:F:220:SER:HB3	1:F:222:ALA:H	1.78	0.48
1:B:304:ASN:O	1:B:306:ALA:N	2.47	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:D:176:GLY:H	1:D:308:LEU:HD23	1.79	0.48
1:A:258:TYR:HA	1:A:270:LEU:CD2	2.43	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:D:282:SER:CB	1:D:284:ASN:ND2	2.72	0.48
1:B:143:ASN:ND2	1:B:157:LEU:H	2.07	0.48
1:A:304:ASN:O	1:A:305:ILE:C	2.52	0.48
1:F:275:MET:O	1:F:276:LEU:C	2.52	0.48
1:F:231:LYS:HE3	1:F:322:ASP:O	2.14	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:249:SER:CB	1:D:260:MET:HE3	2.44	0.47
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:E:314:PHE:CE1	1:F:315:PHE:HA	2.48	0.47
1:B:281:ILE:O	1:B:281:ILE:HG13	2.13	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:E:219:SER:O	1:E:220:SER:HB2	2.14	0.47
1:B:162:VAL:HG11	1:D:164:ASN:O	2.13	0.47
1:G:268:PHE:CE1	1:G:300:SER:HA	2.39	0.47
1:E:307:THR:O	1:E:308:LEU:HB3	2.15	0.47
1:B:163:LYS:HE3	1:B:232:ALA:HB1	1.95	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:D:185:PHE:O	1:D:187:GLN:N	2.48	0.47
1:A:192:ILE:CG1	1:A:293:TRP:HB2	2.44	0.47
1:F:164:ASN:ND2	1:G:164:ASN:HD21	2.12	0.47
1:E:198:PHE:HB3	1:E:203:ASN:O	2.14	0.47
1:B:164:ASN:ND2	1:D:164:ASN:HD21	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:THR:O	1:A:217:ASN:HA	2.14	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:E:220:SER:CB	1:E:222:ALA:H	2.23	0.47
1:E:185:PHE:O	1:E:300:SER:HB3	2.15	0.47
1:D:251:ASN:N	1:D:251:ASN:HD22	2.11	0.47
1:B:174:LEU:HD23	1:B:175:VAL:H	1.79	0.47
1:E:155:GLY:HA2	1:E:177:VAL:HG23	1.96	0.47
1:B:282:SER:O	1:B:285:VAL:HG23	2.15	0.47
1:B:257:CYS:C	1:B:258:TYR:CD1	2.88	0.47
1:A:217:ASN:HD22	1:A:217:ASN:N	2.12	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:B:220:SER:HB3	1:B:222:ALA:H	1.80	0.46
1:G:170:GLY:HA3	1:G:315:PHE:CE2	2.50	0.46
1:D:143:ASN:C	1:D:143:ASN:HD22	2.18	0.46
1:F:144:CYS:HB3	1:F:145:GLN:H	1.50	0.46
1:A:308:LEU:C	1:A:308:LEU:HD23	2.36	0.46
1:A:200:SER:O	1:A:231:LYS:HD3	2.16	0.46
1:B:189:THR:CG2	1:B:190:ALA:N	2.78	0.46
1:D:150:THR:CG2	1:D:152:THR:O	2.63	0.46
1:A:263:TYR:CG	1:A:264:ASP:N	2.79	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:A:159:LEU:HD23	1:A:215:LEU:HD21	1.98	0.46
1:E:217:ASN:N	1:E:217:ASN:ND2	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:E:195:ARG:HG2	1:E:290:GLN:HG3	1.98	0.46
1:B:199:ASP:CB	1:B:205:LEU:HD11	2.44	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:F:204:LEU:HD11	1:F:209:SER:OG	2.15	0.46
1:D:131:ILE:CD1	1:D:131:ILE:C	2.85	0.46
1:D:156:LYS:HG3	1:D:177:VAL:CG2	2.46	0.46
1:G:225:GLU:CG	1:G:226:THR:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:VAL:HG12	1:B:149:ASN:N	2.31	0.46
1:G:245:THR:C	1:G:247:ARG:N	2.69	0.45
1:F:162:VAL:HG11	1:G:164:ASN:O	2.16	0.45
1:A:191:ASN:ND2	1:A:193:GLN:HE21	2.14	0.45
1:A:318:ILE:N	1:A:318:ILE:HD12	2.31	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:E:162:VAL:HG11	1:F:164:ASN:OD1	2.16	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:G:143:ASN:HD22	1:G:143:ASN:C	2.19	0.45
1:A:304:ASN:C	1:A:306:ALA:H	2.19	0.45
1:A:154:ASP:C	1:A:177:VAL:HB	2.36	0.45
1:F:253:ILE:HB	1:F:274:ILE:HB	1.98	0.45
1:F:245:THR:CG2	1:F:246:THR:H	2.22	0.45
1:A:172:VAL:O	1:A:312:PRO:HA	2.17	0.45
1:E:251:ASN:ND2	1:E:251:ASN:H	2.15	0.45
1:F:272:ILE:HA	1:F:292:GLU:O	2.17	0.45
1:D:304:ASN:O	1:D:306:ALA:N	2.48	0.45
1:A:303:SER:O	1:A:304:ASN:CB	2.65	0.45
1:A:143:ASN:HD22	1:A:143:ASN:C	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: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:249:SER:HB3	1:E:252:TYR:CE1	2.52	0.45
1:E:218:LYS:HZ2	1:F:166:GLY:HA2	1.79	0.45
1:D:150:THR:HG22	1:D:152:THR:H	1.82	0.45
1:G:197:TYR:H	1:G:209:SER:CB	2.20	0.45
1:D:307:THR:O	1:D:308:LEU:O	2.34	0.45
1:D:178:SER:O	1:D:181:VAL:N	2.50	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:251:ASN:N	1:A:251:ASN:HD22	2.10	0.45
1:A:174:LEU:CD1	1:A:192:ILE:HD12	2.47	0.45
1:E:146:ILE:HD11	1:E:174:LEU:HD21	1.98	0.45
1:E:275:MET:HB2	1:E:290:GLN:HB3	1.98	0.45
1:E:196:LEU:HA	1:E:209:SER:CB	2.47	0.45
1:A:143:ASN:HA	1:A:153:ASN:ND2	2.32	0.45
1:F:305:ILE:O	1:F:307:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PRO:O	1:A:156:LYS:HE2	2.16	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:F:304:ASN:O	1:F:305:ILE:C	2.55	0.44
1:E:245:THR:C	1:E:247:ARG:N	2.71	0.44
1:B:304:ASN:O	1:B:305:ILE:C	2.56	0.44
1:D:196:LEU:HB2	1:D:289:ILE:O	2.18	0.44
1:A:131:ILE:O	1:A:133:THR:N	2.51	0.44
1:B:199:ASP:OD1	1:B:203:ASN:HB2	2.17	0.44
1:E:225:GLU:CG	1:E:226:THR:N	2.80	0.44
1:B:284:ASN:N	1:B:284:ASN:ND2	2.65	0.44
1:A:227:VAL:C	1:A:229:SER:N	2.71	0.44
1:A:141:PRO:O	1:A:142:PRO:C	2.55	0.44
1:D:185:PHE:O	1:D:300:SER:OG	2.35	0.44
1:B:225:GLU:HG3	1:B:226:THR:N	2.21	0.44
1:E:251:ASN:HD22	1:E:251:ASN:N	2.12	0.44
1:E:218:LYS:HZ3	1:F:166:GLY:HA2	1.83	0.44
1:E:142:PRO:HA	1:E:155:GLY:O	2.17	0.44
1:B:164:ASN:ND2	1:D:164:ASN:OD1	2.50	0.44
1:F:307:THR:HG22	1:F:307:THR:O	2.17	0.44
1:A:244:THR:HG22	1:A:245:THR:N	2.33	0.44
1:E:135:TRP:HB2	1:E:160:VAL:HG22	1.99	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:G:217:ASN:HD21	1:G:224:SER:HB3	1.82	0.44
1:A:184:MET:C	1:A:186:THR:H	2.21	0.44
1:A:146:ILE:HB	1:A:154:ASP:OD1	2.18	0.44
1:F:261:THR:O	1:F:264:ASP:O	2.36	0.44
1:E:257:CYS:SG	1:E:293:TRP:HD1	2.41	0.44
1:D:156:LYS:HG3	1:D:177:VAL:HG21	1.99	0.44
1:B:140:PRO:HB2	1:B:141:PRO:HD2	2.00	0.44
1:A:163:LYS:HE2	1:A:319:THR:HG21	1.99	0.44
1:B:188:LYS:N	1:B:188:LYS:HD3	2.33	0.44
1:G:141:PRO:O	1:G:142:PRO:C	2.55	0.44
1:G:282:SER:CB	1:G:284:ASN:HD21	2.29	0.43
1:F:196:LEU:HD11	1:F:211:LEU:HB2	1.98	0.43
1:E:198:PHE:HA	1:E:203:ASN:O	2.17	0.43
1:G:305:ILE:O	1:G:307:THR:N	2.47	0.43
1:G:161:LEU:N	1:G:161:LEU:HD22	2.33	0.43
1:G:144:CYS:O	1:G:153:ASN:HA	2.18	0.43
1:E:149:ASN:O	1:E:150:THR:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:PRO:O	1:E:142:PRO:C	2.57	0.43
1:F:219:SER:CB	1:F:224:SER:HB2	2.41	0.43
1:E:185:PHE:CE2	1:E:308:LEU:HG	2.53	0.43
1:E:135:TRP:CE2	1:E:137:GLY:HA2	2.53	0.43
1:F:303:SER:O	1:F:304:ASN:HB2	2.18	0.43
1:E:155:GLY:CA	1:E:177:VAL:HG23	2.48	0.43
1:G:305:ILE:HG22	1:G:305:ILE:O	2.19	0.43
1:D:260:MET:HA	1:D:266:SER:O	2.19	0.43
1:A:143:ASN:HA	1:A:153:ASN:HD22	1.81	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:F:245:THR:CG2	1:F:246:THR:N	2.81	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:A:300:SER:OG	1:A:301:PRO:CD	2.62	0.43
1:F:284:ASN:H	1:F:284:ASN:HD22	1.65	0.43
1:F:225:GLU:CG	1:F:226:THR:N	2.76	0.43
1:D:284:ASN:HD22	1:D:284:ASN:N	2.15	0.43
1:G:199:ASP:C	1:G:199:ASP:OD1	2.57	0.43
1:F:199:ASP:OD1	1:F:203:ASN:N	2.49	0.43
1:G:302:GLU:C	1:G:302:GLU:OE1	2.57	0.43
1:F:296:ASN:OD1	1:F:296:ASN:O	2.36	0.43
1:D:264:ASP:OD2	1:D:266:SER:CB	2.66	0.43
1:A:284:ASN:N	1:A:284:ASN:ND2	2.56	0.43
1:F:191:ASN:OD1	1:F:294:ASN:OD1	2.37	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:140:PRO:O	1:A:156:LYS:NZ	2.47	0.43
1:D:277:ASN:O	1:D:278:SER:C	2.57	0.43
1:A:225:GLU:O	1:A:226:THR:HB	2.19	0.43
1:G:277:ASN:O	1:G:278:SER:C	2.57	0.43
1:B:219:SER:O	1:B:220:SER:HB2	2.19	0.43
1:D:149:ASN:O	1:D:150:THR:C	2.57	0.43
1:B:258:TYR:N	1:B:258:TYR:CD1	2.86	0.43
1:B:283:SER:HB3	1:F:207:GLU:OE2	2.18	0.43
1:B:181:VAL:C	1:B:183:GLN:H	2.22	0.43
1:D:192:ILE:HG13	1:D:293:TRP:HB2	2.00	0.43
1:D:245:THR:O	1:D:247:ARG:N	2.52	0.43
1:B:249:SER:HB2	1:B:250:GLU:H	1.66	0.43
1:E:184:MET:C	1:E:186:THR:N	2.71	0.43
1:B:219:SER:CB	1:B:224:SER:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:CD2	1:B:175:VAL:N	2.82	0.43
1:D:164:ASN:HD22	1:D:169:ASN:ND2	2.17	0.42
1:B:225:GLU:CG	1:B:226:THR:N	2.80	0.42
1:D:284:ASN:ND2	1:D:284:ASN:N	2.64	0.42
1:E:272:ILE:HG13	1:E:273:SER:N	2.33	0.42
1:F:143:ASN:ND2	1:F:143:ASN:H	2.17	0.42
1:D:146:ILE:CD1	1:D:181:VAL:HG11	2.47	0.42
1:E:147:VAL:O	1:E:149:ASN:N	2.52	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: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:D:295:LEU:HD12	1:D:296:ASN:H	1.84	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:F:263:TYR:CG	1:F:264:ASP:N	2.88	0.42
1:B:306:ALA:O	1:B:308:LEU:N	2.52	0.42
1:A:168:VAL:CG2	1:A:319:THR:HB	2.50	0.42
1:B:256:ILE:HG23	1:B:270:LEU:O	2.19	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:G:156:LYS:NZ	1:G:156:LYS:CB	2.82	0.42
1:E:168:VAL:HG23	1:E:319:THR:HB	2.01	0.42
1:B:156:LYS:HG3	1:B:177:VAL:CG2	2.49	0.42
1:G:220:SER:HB3	1:G:222:ALA:H	1.84	0.42
1:B:244:THR:CG2	1:B:245:THR:N	2.82	0.42
1:G:228:ALA:O	1:G:229:SER:CB	2.62	0.42
1:A:261:THR:HG22	1:A:301:PRO:CG	2.49	0.42
1:E:141:PRO:HB2	1:E:142:PRO:HD2	2.01	0.42
1:G:156:LYS:HZ3	1:G:156:LYS:HB3	1.84	0.42
1:B:131:ILE:HD12	1:B:132:ASN:HD22	1.85	0.42
1:A:253:ILE:O	1:A:273:SER:HA	2.20	0.42
1:B:184:MET:C	1:B:186:THR:H	2.21	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: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:F:132:ASN:HD22	1:F:132:ASN:N	2.17	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
1:D:240:TYR:CD1	1:D:276:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:TYR:HA	1:A:270:LEU:HD23	2.02	0.42
1:G:303:SER:O	1:G:304:ASN:CB	2.66	0.42
1:D:195:ARG:NH1	1:D:195:ARG:HG3	2.33	0.42
1:B:302:GLU:O	1:B:302:GLU:HG3	2.20	0.41
1:A:205:LEU:N	1:A:205:LEU:HD12	2.35	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:G:275:MET:O	1:G:276:LEU:HB2	2.20	0.41
1:B:132:ASN:N	1:B:132:ASN:ND2	2.68	0.41
1:F:258:TYR:C	1:F:270:LEU:HD21	2.40	0.41
1:F:251:ASN:ND2	1:F:251:ASN:O	2.53	0.41
1:B:217:ASN:O	1:B:223:THR:HA	2.20	0.41
1:D:135:TRP:C	1:D:135:TRP:CD1	2.93	0.41
1:G:170:GLY:HA3	1:G:315:PHE:CZ	2.56	0.41
1:F:140:PRO:O	1:F:156:LYS:HE2	2.20	0.41
1:F:135:TRP:CD1	1:F:135:TRP:C	2.92	0.41
1:F:221:THR:O	1:F:221:THR:HG22	2.20	0.41
1:G:174:LEU:HD23	1:G:175:VAL:H	1.84	0.41
1:D:198:PHE:C	1:D:205:LEU:HD13	2.41	0.41
1:B:282:SER:HB3	1:B:284:ASN:HD21	1.82	0.41
1:A:213:ILE:HA	1:A:214:PRO:HD3	1.95	0.41
1:D:261:THR:O	1:D:264:ASP:O	2.39	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: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:E:157:LEU:CD2	1:E:211:LEU:HD22	2.48	0.41
1:B:197:TYR:HB3	1:B:285:VAL:HG13	2.02	0.41
1:E:133:THR:HB	1:E:218:LYS:HB3	2.03	0.41
1:D:248:ASP:O	1:D:250:GLU:HG2	2.21	0.41
1:G:207:GLU:OE2	1:G:207:GLU:HA	2.21	0.41
1:E:172:VAL:CG1	1:E:291:PHE:CE2	3.04	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:228:ALA:O	1:D:229:SER:CB	2.68	0.41
1:D:147:VAL:HG12	1:D:148:GLU:N	2.36	0.41
1:E:219:SER:OG	1:E:224:SER:HB2	2.20	0.41
1:G:245:THR:CG2	1:G:246:THR:N	2.80	0.41
1:B:172:VAL:HG22	1:B:315:PHE:CE2	2.48	0.41
1:A:259:TYR:N	1:A:270:LEU:HD21	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLY:CA	1:A:177:VAL:HG23	2.51	0.41
1:D:231:LYS:HA	1:D:234:MET:CG	2.51	0.41
1:B:231:LYS:HE3	1:B:322:ASP:O	2.20	0.41
1:G:174:LEU:CD2	1:G:175:VAL:N	2.84	0.41
1:D:183:GLN:O	1:D:186:THR:HG22	2.21	0.41
1:F:205:LEU:HA	1:F:205:LEU:HD12	1.74	0.41
1:B:206:THR:HG22	1:B:212:LYS:HA	2.03	0.41
1:A:249:SER:HB2	1:D:260:MET:CE	2.51	0.41
1:A:143:ASN:C	1:A:153:ASN:HD22	2.24	0.41
1:G:300:SER:OG	1:G:301:PRO:CD	2.68	0.41
1:G:199:ASP:HB3	1:G:205:LEU:HD11	2.03	0.41
1:A:198:PHE:HA	1:A:205:LEU:HD13	2.03	0.41
1:A:261:THR:CB	1:A:301:PRO:HG3	2.50	0.41
1:G:216:LYS:HB3	1:G:223:THR:HB	2.03	0.41
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:E:257:CYS:SG	1:E:293:TRP:CD1	3.14	0.40
1:G:143:ASN:HD22	1:G:144:CYS:N	2.19	0.40
1:E:203:ASN:HD22	1:E:203:ASN:N	2.19	0.40
1:B:282:SER:HB2	1:B:285:VAL:HG23	2.03	0.40
1:G:249:SER:C	1:G:251:ASN:N	2.73	0.40
1:A:263:TYR:C	1:A:264:ASP:O	2.59	0.40
1:D:243:ASN:O	1:D:243:ASN:OD1	2.38	0.40
1:F:168:VAL:HG23	1:F:319:THR:HB	2.03	0.40
1:E:217:ASN:HD21	1:E:224:SER:N	2.07	0.40
1:G:135:TRP:HB2	1:G:136:THR:H	1.67	0.40
1:D:257:CYS:SG	1:D:270:LEU:HG	2.61	0.40
1:B:252:TYR:CE2	1:B:275:MET:HG3	2.56	0.40
1:F:143:ASN:C	1:F:143:ASN:HD22	2.25	0.40
1:D:216:LYS:HD3	1:D:223:THR:HB	2.03	0.40
1:E:134:LEU:HA	1:E:134:LEU:HD12	1.87	0.40
1:B:235:PRO:HG2	1:B:277:ASN:OD1	2.21	0.40
1:B:191:ASN:OD1	1:B:294:ASN:OD1	2.40	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%)	12	26
1	B	175/196 (89%)	159 (91%)	16 (9%)	12	26
1	D	175/196 (89%)	155 (89%)	20 (11%)	7	16
1	E	175/196 (89%)	156 (89%)	19 (11%)	8	18
1	F	175/196 (89%)	153 (87%)	22 (13%)	5	13
1	G	175/196 (89%)	161 (92%)	14 (8%)	15	33
All	All	1050/1176 (89%)	943 (90%)	107 (10%)	9	21

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

Some 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	192/220 (87%)	1.22	34 (17%) 2 1	34, 79, 108, 113	72 (37%)
1	B	192/220 (87%)	1.17	33 (17%) 2 1	41, 83, 108, 113	77 (40%)
1	D	192/220 (87%)	1.39	48 (25%) 1 1	51, 90, 108, 113	62 (32%)
1	E	192/220 (87%)	1.14	35 (18%) 2 1	42, 79, 108, 113	70 (36%)
1	F	192/220 (87%)	1.19	40 (20%) 1 1	42, 80, 108, 113	69 (35%)
1	G	192/220 (87%)	1.31	47 (24%) 1 1	55, 89, 108, 113	69 (35%)
All	All	1152/1320 (87%)	1.24	237 (20%) 1 1	34, 83, 108, 113	419 (36%)

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	GLU	22.0
1	F	246	THR	18.2
1	A	224	SER	14.0
1	E	225	GLU	13.3
1	D	228	ALA	12.8
1	B	246	THR	12.6
1	D	223	THR	12.6
1	D	245	THR	12.4
1	B	245	THR	11.9
1	A	246	THR	11.2
1	E	224	SER	10.9
1	G	228	ALA	10.0
1	G	224	SER	10.0
1	A	223	THR	9.3
1	E	246	THR	9.2
1	F	223	THR	9.2
1	F	222	ALA	8.9
1	A	243	ASN	8.7
1	E	223	THR	8.6

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Mol	Chain	Res	Type	RSRZ
1	D	226	THR	8.6
1	G	223	THR	8.2
1	G	305	ILE	8.2
1	A	245	THR	8.2
1	D	222	ALA	8.2
1	G	226	THR	8.0
1	E	243	ASN	7.9
1	F	247	ARG	7.8
1	B	247	ARG	7.5
1	F	245	THR	7.5
1	F	227	VAL	7.4
1	A	227	VAL	7.3
1	B	222	ALA	7.3
1	B	219	SER	6.8
1	E	222	ALA	6.8
1	D	305	ILE	6.7
1	G	150	THR	6.5
1	B	227	VAL	6.5
1	A	305	ILE	6.4
1	D	221	THR	6.2
1	G	222	ALA	6.2
1	D	224	SER	6.1
1	F	248	ASP	6.1
1	F	226	THR	6.0
1	E	247	ARG	5.8
1	D	225	GLU	5.8
1	G	245	THR	5.8
1	B	150	THR	5.7
1	B	228	ALA	5.7
1	F	228	ALA	5.7
1	F	221	THR	5.7
1	G	221	THR	5.6
1	A	226	THR	5.6
1	F	305	ILE	5.5
1	F	219	SER	5.3
1	E	244	THR	5.2
1	G	263	TYR	5.1
1	E	245	THR	5.0
1	E	305	ILE	4.9
1	E	316	SER	4.9
1	D	150	THR	4.8
1	B	225	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	G	225	GLU	4.8
1	D	297	ALA	4.8
1	E	226	THR	4.8
1	E	221	THR	4.8
1	G	151	ASN	4.7
1	F	225	GLU	4.7
1	D	181	VAL	4.6
1	F	150	THR	4.6
1	G	297	ALA	4.5
1	F	151	ASN	4.5
1	B	221	THR	4.4
1	B	149	ASN	4.3
1	A	306	ALA	4.3
1	G	246	THR	4.2
1	B	226	THR	4.2
1	D	151	ASN	4.2
1	F	149	ASN	4.2
1	B	299	GLU	4.1
1	G	306	ALA	4.1
1	A	316	SER	4.1
1	A	247	ARG	4.0
1	A	244	THR	4.0
1	D	302	GLU	4.0
1	D	246	THR	4.0
1	G	243	ASN	3.9
1	G	184	MET	3.9
1	D	189	THR	3.8
1	D	149	ASN	3.8
1	B	151	ASN	3.8
1	B	315	PHE	3.8
1	B	314	PHE	3.7
1	B	305	ILE	3.7
1	B	263	TYR	3.6
1	A	263	TYR	3.6
1	D	227	VAL	3.6
1	G	300	SER	3.5
1	D	220	SER	3.5
1	D	184	MET	3.5
1	F	185	PHE	3.5
1	F	259	TYR	3.5
1	G	147	VAL	3.5
1	G	302	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	306	ALA	3.4
1	B	185	PHE	3.4
1	D	243	ASN	3.4
1	G	295	LEU	3.4
1	G	152	THR	3.4
1	D	263	TYR	3.4
1	G	189	THR	3.4
1	B	259	TYR	3.3
1	D	304	ASN	3.3
1	A	281	ILE	3.3
1	E	227	VAL	3.3
1	G	170	GLY	3.2
1	D	187	GLN	3.2
1	A	150	THR	3.1
1	A	253	ILE	3.1
1	D	185	PHE	3.1
1	D	183	GLN	3.1
1	G	301	PRO	3.1
1	G	185	PHE	3.1
1	G	282	SER	3.0
1	D	316	SER	3.0
1	D	147	VAL	3.0
1	G	227	VAL	3.0
1	D	152	THR	3.0
1	A	222	ALA	3.0
1	D	280	MET	3.0
1	D	282	SER	3.0
1	E	264	ASP	3.0
1	B	306	ALA	3.0
1	B	154	ASP	3.0
1	G	220	SER	2.9
1	D	300	SER	2.9
1	F	306	ALA	2.9
1	A	248	ASP	2.9
1	G	312	PRO	2.9
1	G	183	GLN	2.9
1	D	295	LEU	2.8
1	D	244	THR	2.8
1	E	154	ASP	2.8
1	G	313	PHE	2.8
1	G	303	SER	2.8
1	D	229	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	224	SER	2.8
1	F	187	GLN	2.8
1	A	228	ALA	2.8
1	G	146	ILE	2.7
1	G	315	PHE	2.7
1	A	206	THR	2.7
1	F	170	GLY	2.7
1	G	247	ARG	2.7
1	E	281	ILE	2.7
1	E	302	GLU	2.7
1	E	220	SER	2.6
1	F	268	PHE	2.6
1	A	169	ASN	2.6
1	E	257	CYS	2.6
1	G	316	SER	2.6
1	A	221	THR	2.6
1	G	186	THR	2.6
1	E	299	GLU	2.6
1	G	181	VAL	2.6
1	D	283	SER	2.6
1	D	238	THR	2.6
1	F	261	THR	2.6
1	G	280	MET	2.6
1	B	223	THR	2.5
1	E	312	PRO	2.5
1	F	142	PRO	2.5
1	E	255	GLY	2.5
1	A	302	GLU	2.5
1	E	149	ASN	2.5
1	E	208	GLU	2.5
1	D	254	HIS	2.5
1	B	316	SER	2.5
1	G	285	VAL	2.4
1	A	299	GLU	2.4
1	G	244	THR	2.4
1	D	153	ASN	2.4
1	D	315	PHE	2.4
1	F	314	PHE	2.4
1	G	229	SER	2.4
1	B	301	PRO	2.4
1	F	316	SER	2.4
1	A	233	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	263	TYR	2.4
1	G	304	ASN	2.4
1	B	190	ALA	2.3
1	G	262	SER	2.3
1	B	248	ASP	2.3
1	B	189	THR	2.3
1	A	312	PRO	2.3
1	F	301	PRO	2.3
1	E	169	ASN	2.3
1	F	152	THR	2.3
1	A	220	SER	2.3
1	D	257	CYS	2.3
1	G	283	SER	2.3
1	B	220	SER	2.3
1	F	250	GLU	2.3
1	F	312	PRO	2.3
1	E	253	ILE	2.3
1	F	263	TYR	2.3
1	A	301	PRO	2.2
1	A	313	PHE	2.2
1	B	313	PHE	2.2
1	B	170	GLY	2.2
1	F	249	SER	2.2
1	D	312	PRO	2.2
1	G	149	ASN	2.2
1	F	299	GLU	2.2
1	F	216	LYS	2.2
1	F	220	SER	2.1
1	A	322	ASP	2.1
1	A	282	SER	2.1
1	D	146	ILE	2.1
1	E	183	GLN	2.1
1	E	150	THR	2.1
1	D	170	GLY	2.1
1	E	301	PRO	2.1
1	A	264	ASP	2.1
1	B	261	THR	2.1
1	B	224	SER	2.1
1	D	303	SER	2.1
1	F	229	SER	2.1
1	E	171	TYR	2.1
1	E	170	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	131	ILE	2.1
1	F	300	SER	2.1
1	A	132	ASN	2.0
1	D	248	ASP	2.0
1	F	264	ASP	2.0
1	E	249	SER	2.0
1	D	247	ARG	2.0
1	F	313	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.