



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:39 AM UTC

PDB ID : 3KCV / pdb_00003kcv
Title : Structure of formate channel
Authors : Wang, Y.; Huang, Y.; Wang, J.; Yan, N.; Shi, Y.
Deposited on : 2009-10-22
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

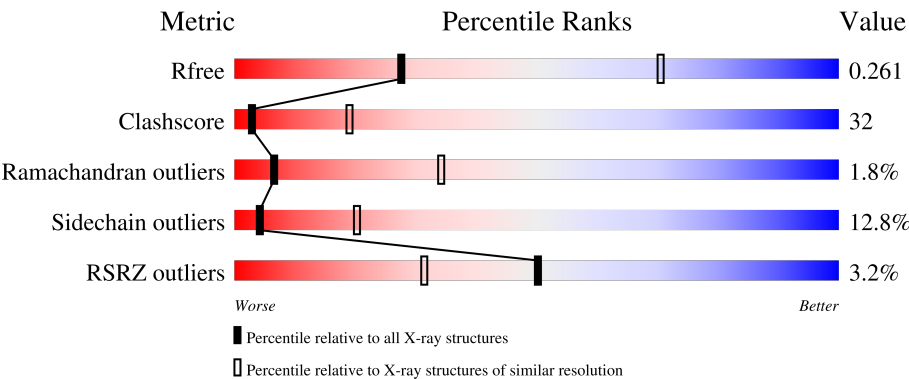
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	285	% 40% 38% 9% 12%
1	B	285	2% 45% 35% 8% 12%
1	C	285	3% 44% 35% 8% 12%
1	D	285	3% 37% 44% 7% 12%
1	E	285	5% 39% 42% 7% 12%

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Mol	Chain	Length	Quality of chain
1	F	285	
1	G	285	
1	H	285	
1	I	285	
1	J	285	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19120 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.

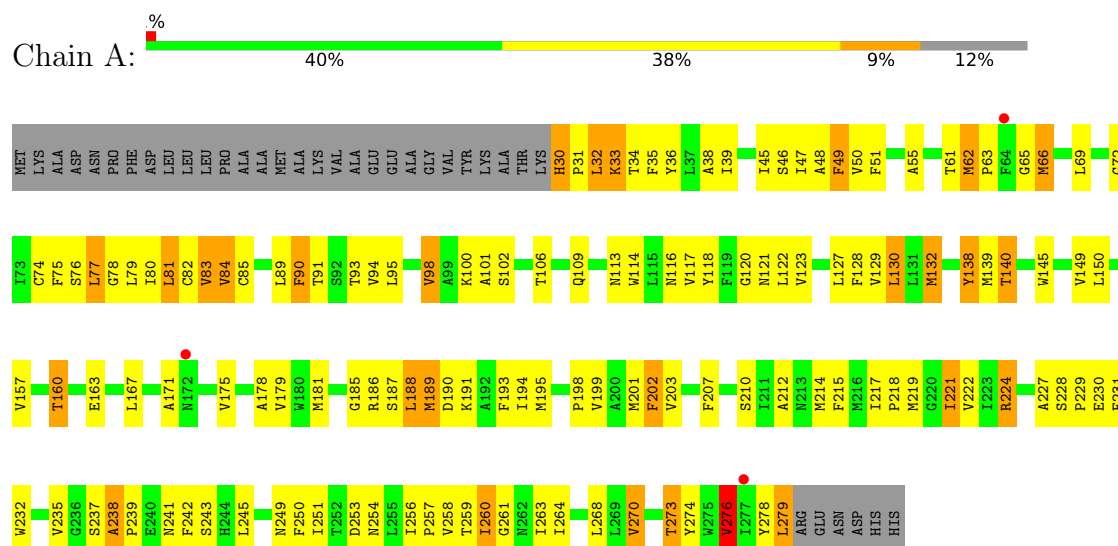
- Molecule 1 is a protein called Probable formate transporter 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1907	1269	298	322	18			
1	B	250	Total	C	N	O	S	0	0	0
			1907	1269	298	322	18			
1	C	250	Total	C	N	O	S	0	0	0
			1907	1269	298	322	18			
1	D	251	Total	C	N	O	S	0	0	0
			1912	1272	299	323	18			
1	E	252	Total	C	N	O	S	0	0	0
			1917	1275	300	324	18			
1	F	252	Total	C	N	O	S	0	0	0
			1917	1275	300	324	18			
1	G	252	Total	C	N	O	S	0	0	0
			1917	1275	300	324	18			
1	H	252	Total	C	N	O	S	0	0	0
			1917	1275	300	324	18			
1	I	252	Total	C	N	O	S	0	0	0
			1917	1275	300	324	18			
1	J	249	Total	C	N	O	S	0	0	0
			1902	1267	297	320	18			

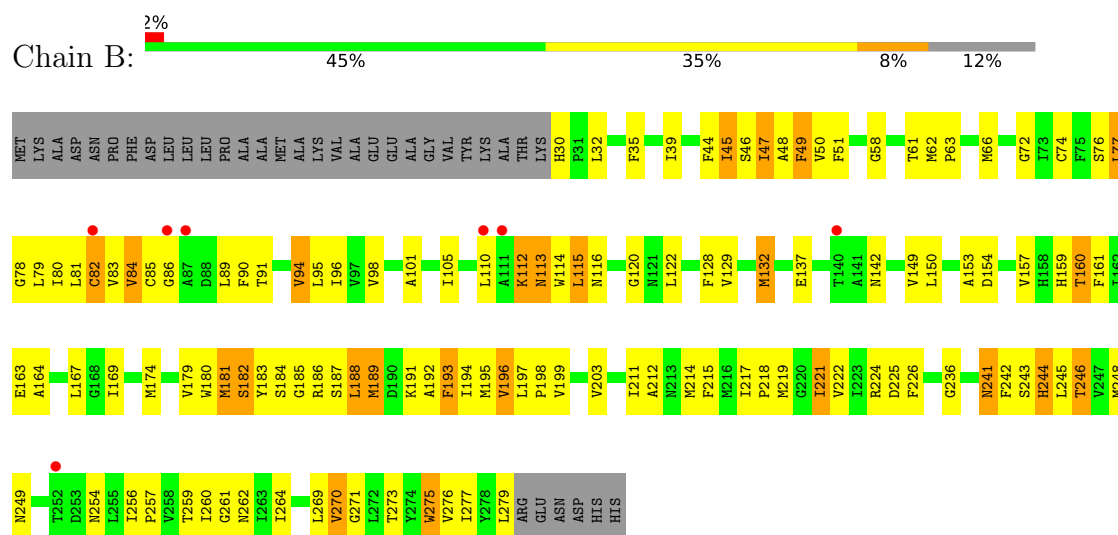
3 Residue-property plots

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

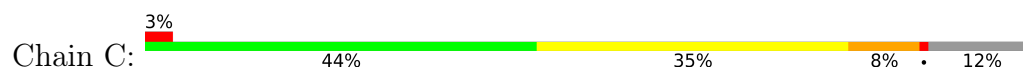
• Molecule 1: Probable formate transporter 1

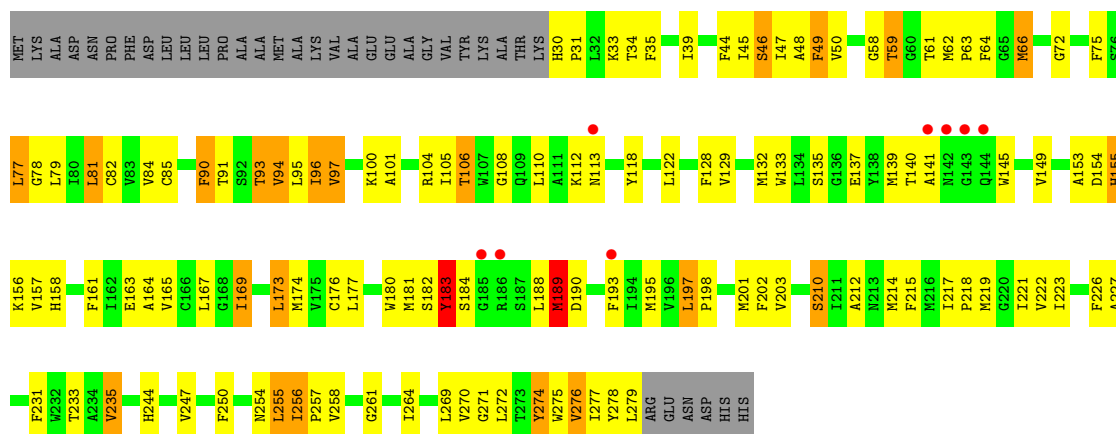


• Molecule 1: Probable formate transporter 1

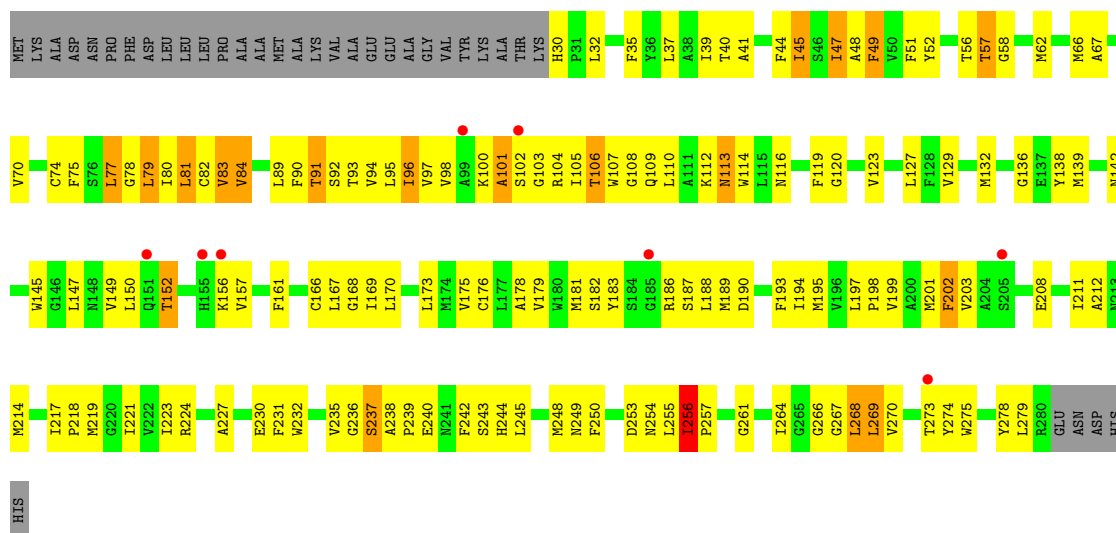


• Molecule 1: Probable formate transporter 1

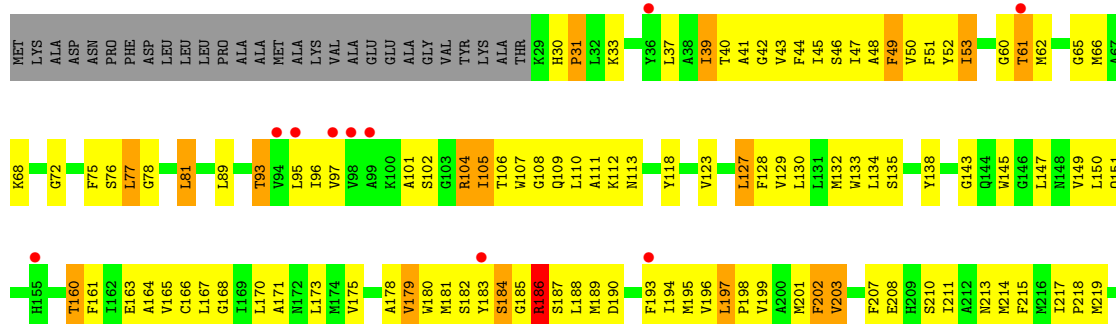




● Molecule 1: Probable formate transporter 1

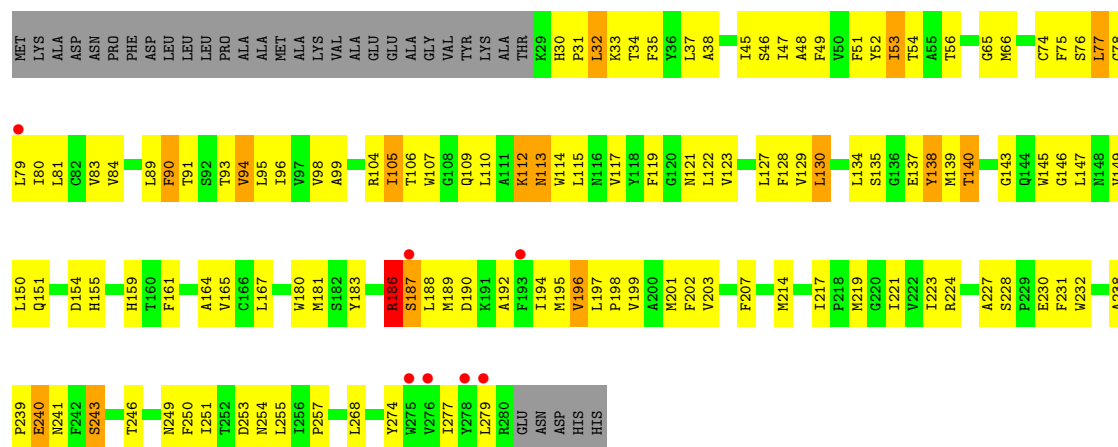
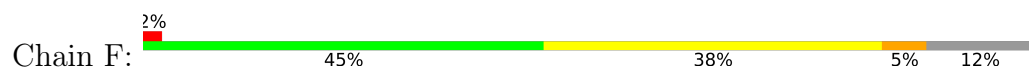


● Molecule 1: Probable formate transporter 1

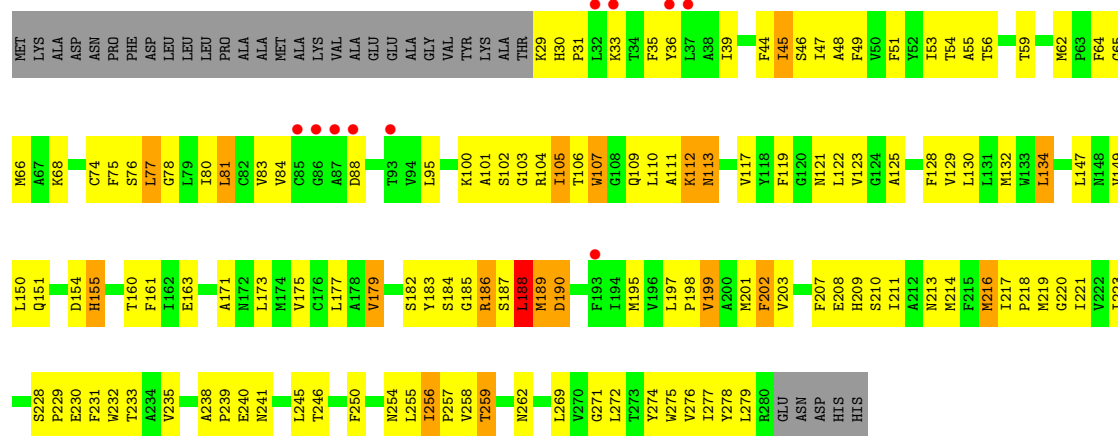




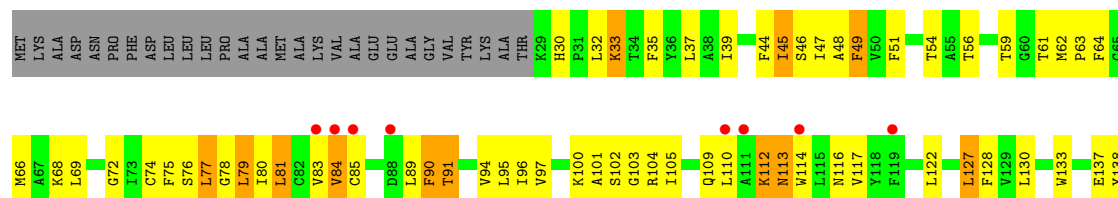
• Molecule 1: Probable formate transporter 1

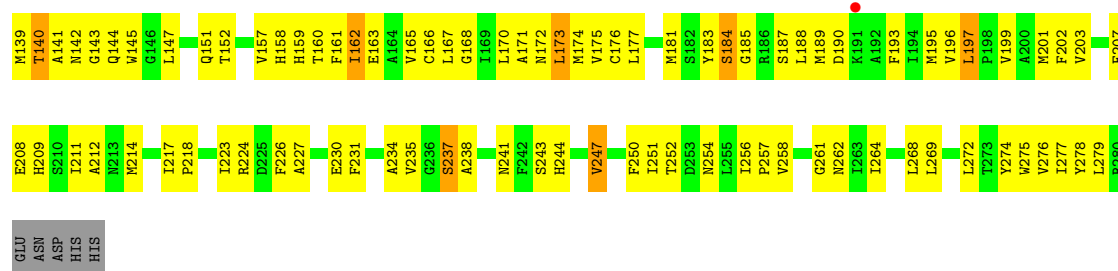


• Molecule 1: Probable formate transporter 1

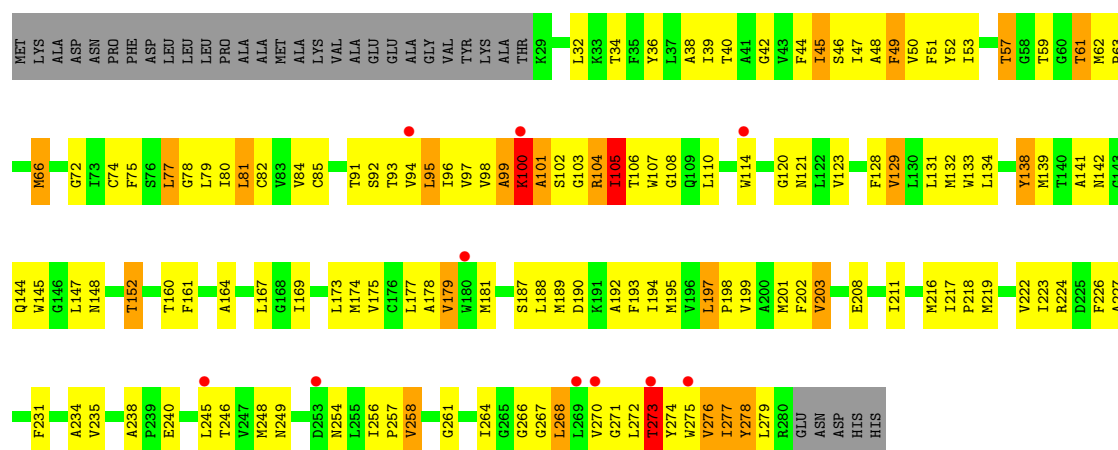


• Molecule 1: Probable formate transporter 1

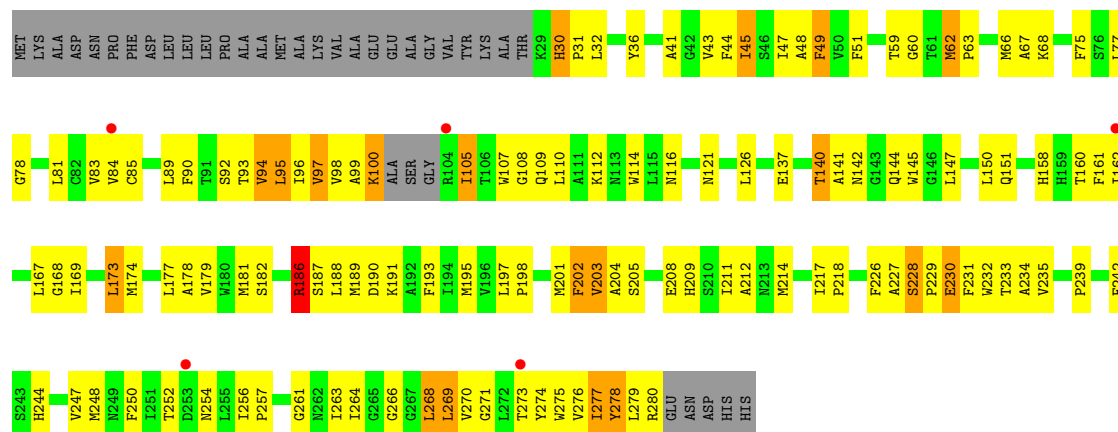




• Molecule 1: Probable formate transporter 1



• Molecule 1: Probable formate transporter 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	107.03Å 107.03Å 285.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.61 – 3.20 48.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.4 (48.61-3.20) 99.6 (48.61-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.193 , 0.260 0.199 , 0.261	Depositor DCC
R_{free} test set	3238 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 92.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.027 for h,-h-k,-l 0.009 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19120	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, 0.333 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	0.55	1/1958 (0.1%)	0.97	7/2670 (0.3%)
1	B	0.55	0/1958	0.87	0/2670
1	C	0.52	0/1958	0.90	0/2670
1	D	0.52	0/1963	0.92	4/2677 (0.1%)
1	E	0.58	0/1968	0.96	2/2684 (0.1%)
1	F	0.59	0/1968	0.93	4/2684 (0.1%)
1	G	0.59	0/1968	0.94	2/2684 (0.1%)
1	H	0.56	0/1968	0.94	3/2684 (0.1%)
1	I	0.63	0/1968	1.12	8/2684 (0.3%)
1	J	0.58	0/1952	0.99	6/2661 (0.2%)
All	All	0.57	1/19629 (0.0%)	0.96	36/26768 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	VAL	CA-C	5.08	1.59	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	100	LYS	N-CA-C	24.29	141.04	111.40
1	I	100	LYS	CB-CA-C	-10.81	92.63	110.79
1	I	100	LYS	CA-C-N	8.01	136.84	121.54
1	I	100	LYS	C-N-CA	8.01	136.84	121.54
1	J	30	HIS	CA-C-N	7.17	126.70	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	30	HIS	C-N-CA	7.17	126.70	119.24
1	J	62	MET	CA-C-N	7.05	127.47	119.93
1	J	62	MET	C-N-CA	7.05	127.47	119.93
1	A	62	MET	CA-C-N	6.12	126.43	119.83
1	A	62	MET	C-N-CA	6.12	126.43	119.83
1	I	175	VAL	CB-CA-C	-5.95	104.26	111.88
1	D	30	HIS	CA-C-N	5.84	125.31	119.24
1	D	30	HIS	C-N-CA	5.84	125.31	119.24
1	G	216	MET	N-CA-C	5.82	117.63	111.28
1	A	221	ILE	CB-CA-C	-5.80	104.45	112.04
1	A	238	ALA	CA-C-N	5.78	127.07	119.84
1	A	238	ALA	C-N-CA	5.78	127.07	119.84
1	E	238	ALA	CA-C-N	5.78	127.06	119.84
1	E	238	ALA	C-N-CA	5.78	127.06	119.84
1	J	228	SER	CA-C-N	5.71	125.56	119.28
1	J	228	SER	C-N-CA	5.71	125.56	119.28
1	D	256	ILE	CB-CA-C	-5.70	108.28	113.70
1	I	99	ALA	N-CA-C	-5.51	104.70	111.75
1	F	112	LYS	N-CA-C	5.45	116.91	110.97
1	H	94	VAL	N-CA-C	5.44	116.82	110.62
1	D	101	ALA	N-CA-C	-5.37	106.57	113.01
1	F	238	ALA	CA-C-N	5.29	126.45	119.84
1	F	238	ALA	C-N-CA	5.29	126.45	119.84
1	H	33	LYS	N-CA-C	-5.22	105.59	111.28
1	I	276	VAL	N-CA-C	5.19	115.41	110.42
1	A	30	HIS	CA-C-N	5.16	124.61	119.24
1	A	30	HIS	C-N-CA	5.16	124.61	119.24
1	G	188	LEU	N-CA-C	-5.11	105.79	111.36
1	I	273	THR	N-CA-CB	5.09	117.53	109.94
1	H	196	VAL	N-CA-C	5.05	115.27	110.42
1	F	251	ILE	N-CA-C	5.05	115.72	110.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	100	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1946	138	0
1	B	1907	0	1946	114	0
1	C	1907	0	1946	138	0
1	D	1912	0	1948	177	0
1	E	1917	0	1950	149	0
1	F	1917	0	1950	119	0
1	G	1917	0	1950	138	0
1	H	1917	0	1950	171	0
1	I	1917	0	1950	167	0
1	J	1902	0	1936	130	0
All	All	19120	0	19472	1253	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ILE:O	1:C:227:ALA:HB2	1.39	1.23
1:D:101:ALA:O	1:D:104:ARG:HB2	1.45	1.13
1:H:95:LEU:HD21	1:H:269:LEU:HB3	1.37	1.05
1:I:271:GLY:O	1:I:275:TRP:HD1	1.38	1.04
1:C:201:MET:HE3	1:D:47:ILE:HG23	1.39	1.03
1:C:274:TYR:O	1:C:278:TYR:HB3	1.59	1.02
1:D:98:VAL:HG11	1:D:270:VAL:HG13	1.36	1.02
1:D:264:ILE:O	1:D:268:LEU:HB3	1.61	1.00
1:E:101:ALA:O	1:E:104:ARG:HB2	1.62	0.98
1:C:140:THR:O	1:C:145:TRP:HB2	1.66	0.95
1:C:106:THR:O	1:C:110:LEU:HB2	1.66	0.95
1:A:190:ASP:OD2	1:B:187:SER:HB2	1.68	0.92
1:I:271:GLY:O	1:I:275:TRP:CD1	2.22	0.92
1:G:190:ASP:HB3	1:H:188:LEU:HB3	1.53	0.90
1:F:33:LYS:HD2	1:J:280:ARG:HA	1.53	0.90
1:I:268:LEU:O	1:I:272:LEU:HD13	1.70	0.89
1:J:271:GLY:O	1:J:274:TYR:HB3	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:LEU:HD21	1:C:269:LEU:HB3	1.55	0.89
1:E:95:LEU:HD21	1:E:269:LEU:HB3	1.54	0.88
1:D:102:SER:HB2	1:D:104:ARG:HD3	1.56	0.87
1:D:98:VAL:HG21	1:D:270:VAL:CG2	2.04	0.86
1:H:66:MET:H	1:H:66:MET:HE2	1.41	0.85
1:J:97:VAL:HB	1:J:270:VAL:HG11	1.58	0.85
1:A:190:ASP:HB3	1:B:188:LEU:HB2	1.58	0.84
1:B:129:VAL:HG22	1:B:219:MET:HE2	1.56	0.84
1:H:264:ILE:O	1:H:268:LEU:HG	1.77	0.84
1:D:264:ILE:O	1:D:268:LEU:CB	2.26	0.83
1:C:223:ILE:O	1:C:227:ALA:CB	2.22	0.83
1:D:181:MET:HE3	1:D:194:ILE:HG13	1.60	0.82
1:D:186:ARG:HH12	1:H:230:GLU:HG3	1.43	0.82
1:D:275:TRP:HA	1:D:278:TYR:HB3	1.60	0.82
1:G:48:ALA:HB2	1:G:78:GLY:HA3	1.61	0.82
1:F:33:LYS:HB2	1:J:279:LEU:HB2	1.60	0.82
1:H:109:GLN:HA	1:H:112:LYS:HE3	1.62	0.81
1:H:197:LEU:HB3	1:I:77:LEU:HG	1.63	0.81
1:C:274:TYR:O	1:C:278:TYR:CB	2.27	0.81
1:H:95:LEU:HD11	1:H:269:LEU:HD13	1.62	0.81
1:I:201:MET:HA	1:J:51:PHE:CE1	2.16	0.81
1:D:98:VAL:HG21	1:D:270:VAL:HG21	1.64	0.80
1:D:96:ILE:HD12	1:D:96:ILE:H	1.45	0.80
1:D:94:VAL:HG11	1:D:266:GLY:HA2	1.63	0.80
1:G:275:TRP:O	1:G:279:LEU:HB2	1.82	0.80
1:I:94:VAL:HG23	1:I:114:TRP:CZ2	2.17	0.80
1:A:188:LEU:HD23	1:E:190:ASP:HB3	1.64	0.80
1:F:186:ARG:HD3	1:F:187:SER:N	1.97	0.79
1:A:48:ALA:HB2	1:A:78:GLY:HA3	1.62	0.79
1:H:45:ILE:HG21	1:H:211:ILE:HG22	1.63	0.79
1:I:94:VAL:HG23	1:I:114:TRP:HZ2	1.45	0.79
1:A:193:PHE:HZ	1:E:193:PHE:O	1.65	0.79
1:B:101:ALA:HB1	1:B:105:ILE:HB	1.65	0.79
1:I:274:TYR:O	1:I:278:TYR:HB3	1.81	0.78
1:G:101:ALA:O	1:G:104:ARG:HG2	1.83	0.78
1:F:66:MET:HE2	1:F:66:MET:N	1.99	0.78
1:I:177:LEU:HD13	1:J:81:LEU:HD21	1.65	0.78
1:C:271:GLY:O	1:C:274:TYR:HB3	1.84	0.78
1:A:274:TYR:O	1:A:278:TYR:CB	2.32	0.78
1:E:186:ARG:HH11	1:E:186:ARG:HA	1.47	0.77
1:H:122:LEU:HD13	1:H:214:MET:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ILE:HD12	1:C:250:PHE:CD1	2.18	0.77
1:J:256:ILE:HB	1:J:257:PRO:HD3	1.65	0.77
1:B:95:LEU:HD11	1:B:269:LEU:HB3	1.67	0.76
1:C:108:GLY:O	1:C:112:LYS:HG2	1.84	0.76
1:C:94:VAL:HG12	1:C:95:LEU:HD23	1.68	0.75
1:A:63:PRO:HB3	1:B:58:GLY:O	1.87	0.75
1:A:163:GLU:O	1:A:167:LEU:HG	1.86	0.74
1:I:101:ALA:HB2	1:I:110:LEU:CD2	2.18	0.74
1:A:249:ASN:O	1:A:253:ASP:HB2	1.87	0.74
1:C:106:THR:O	1:C:110:LEU:CB	2.35	0.74
1:F:254:ASN:O	1:F:257:PRO:HD2	1.88	0.74
1:A:98:VAL:HG11	1:A:273:THR:HG21	1.68	0.73
1:J:177:LEU:HD21	1:J:269:LEU:HD11	1.70	0.73
1:H:103:GLY:C	1:H:105:ILE:H	1.96	0.73
1:H:76:SER:HA	1:H:199:VAL:HG11	1.69	0.73
1:J:97:VAL:CB	1:J:270:VAL:HG11	2.19	0.73
1:A:224:ARG:HH21	1:A:243:SER:HA	1.53	0.72
1:C:48:ALA:HB2	1:C:78:GLY:HA3	1.72	0.72
1:D:268:LEU:HD23	1:D:269:LEU:N	2.05	0.72
1:A:274:TYR:O	1:A:278:TYR:HB3	1.90	0.72
1:E:179:VAL:O	1:E:182:SER:HB3	1.88	0.72
1:G:147:LEU:HD22	1:G:235:VAL:HB	1.70	0.72
1:I:238:ALA:HB1	1:I:240:GLU:OE1	1.90	0.72
1:D:94:VAL:HG11	1:D:266:GLY:CA	2.20	0.71
1:E:104:ARG:HD2	1:I:61:THR:HG22	1.71	0.71
1:J:97:VAL:CG1	1:J:270:VAL:HG11	2.20	0.71
1:C:278:TYR:CE2	1:C:279:LEU:HG	2.25	0.71
1:D:186:ARG:NH1	1:H:230:GLU:HG3	2.05	0.71
1:G:160:THR:OG1	1:G:163:GLU:HG3	1.90	0.71
1:A:186:ARG:HD2	1:A:186:ARG:N	2.06	0.71
1:D:223:ILE:O	1:D:227:ALA:HB2	1.91	0.71
1:C:218:PRO:O	1:C:222:VAL:HG23	1.91	0.71
1:B:197:LEU:HD23	1:C:77:LEU:HB2	1.71	0.70
1:D:250:PHE:CZ	1:D:255:LEU:HD22	2.26	0.70
1:F:138:TYR:CE1	1:F:139:MET:HG2	2.26	0.70
1:E:105:ILE:HG23	1:E:110:LEU:HD11	1.72	0.70
1:E:150:LEU:CD2	1:E:224:ARG:HB2	2.22	0.70
1:B:244:HIS:CD2	1:B:244:HIS:H	2.09	0.70
1:D:123:VAL:O	1:D:127:LEU:HG	1.90	0.70
1:E:46:SER:HB3	1:E:128:PHE:HD2	1.57	0.70
1:F:202:PHE:HB2	1:F:207:PHE:HD2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:O	1:B:115:LEU:HD12	1.92	0.70
1:D:110:LEU:C	1:D:110:LEU:HD23	2.17	0.70
1:F:48:ALA:HB2	1:F:78:GLY:HA3	1.73	0.69
1:A:185:GLY:HA2	1:B:188:LEU:HD22	1.72	0.69
1:I:279:LEU:HD22	1:J:30:HIS:CE1	2.27	0.69
1:G:75:PHE:CD2	1:G:203:VAL:HG21	2.27	0.69
1:D:98:VAL:HG21	1:D:270:VAL:HG22	1.74	0.69
1:I:101:ALA:HB2	1:I:110:LEU:HD21	1.73	0.69
1:C:181:MET:HG2	1:D:84:VAL:HG11	1.72	0.69
1:B:94:VAL:HG12	1:B:95:LEU:HD23	1.75	0.69
1:E:102:SER:HB2	1:E:104:ARG:HD3	1.73	0.69
1:I:95:LEU:CD1	1:I:179:VAL:HG12	2.23	0.69
1:I:195:MET:C	1:I:198:PRO:HD2	2.18	0.69
1:D:190:ASP:HB3	1:E:188:LEU:HB3	1.74	0.69
1:I:63:PRO:HB3	1:J:59:THR:HG22	1.73	0.69
1:D:103:GLY:C	1:D:105:ILE:H	1.99	0.69
1:H:166:CYS:SG	1:I:134:LEU:HB3	2.32	0.69
1:A:187:SER:HA	1:E:186:ARG:HG3	1.76	0.68
1:C:94:VAL:CG1	1:C:270:VAL:HG23	2.24	0.68
1:B:154:ASP:OD1	1:B:244:HIS:CD2	2.47	0.68
1:I:100:LYS:O	1:I:104:ARG:N	2.22	0.68
1:J:161:PHE:CD1	1:J:257:PRO:HG3	2.28	0.68
1:A:98:VAL:HG21	1:A:270:VAL:HG22	1.76	0.67
1:A:81:LEU:O	1:A:85:CYS:HB2	1.93	0.67
1:E:202:PHE:CZ	1:E:203:VAL:HG23	2.28	0.67
1:J:32:LEU:HD23	1:J:32:LEU:O	1.93	0.67
1:J:142:ASN:ND2	1:J:234:ALA:HB1	2.09	0.67
1:D:102:SER:C	1:D:104:ARG:H	2.02	0.67
1:C:274:TYR:HD2	1:C:275:TRP:N	1.92	0.67
1:E:186:ARG:HA	1:E:186:ARG:NH1	2.09	0.67
1:A:274:TYR:O	1:A:278:TYR:HB2	1.95	0.67
1:H:174:MET:SD	1:I:47:ILE:HD13	2.34	0.67
1:A:228:SER:O	1:A:231:PHE:HB3	1.95	0.67
1:E:96:ILE:HG12	1:E:183:TYR:CZ	2.30	0.67
1:F:75:PHE:CD2	1:F:203:VAL:HG21	2.30	0.67
1:A:32:LEU:HD12	1:A:32:LEU:H	1.59	0.67
1:B:154:ASP:HA	1:B:245:LEU:HD21	1.77	0.67
1:H:140:THR:HG22	1:H:145:TRP:HB2	1.76	0.67
1:I:66:MET:HE2	1:J:59:THR:HG21	1.75	0.66
1:D:96:ILE:HD12	1:D:96:ILE:N	2.10	0.66
1:A:50:VAL:HG11	1:A:132:MET:HE2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD13	1:A:242:PHE:CE2	2.30	0.66
1:D:62:MET:HE2	1:D:67:ALA:HB2	1.78	0.66
1:D:266:GLY:O	1:D:270:VAL:HG23	1.94	0.66
1:G:276:VAL:HG12	1:G:276:VAL:O	1.94	0.66
1:A:254:ASN:O	1:A:257:PRO:HD2	1.96	0.66
1:F:66:MET:HE2	1:F:66:MET:H	1.61	0.66
1:J:274:TYR:CE2	1:J:275:TRP:CD1	2.84	0.66
1:G:190:ASP:OD2	1:H:188:LEU:N	2.26	0.65
1:J:84:VAL:HG11	1:J:188:LEU:HD11	1.78	0.65
1:B:261:GLY:HA2	1:B:264:ILE:HD12	1.78	0.65
1:C:90:PHE:CD2	1:C:91:THR:HG23	2.31	0.65
1:C:276:VAL:HG13	1:D:37:LEU:HD21	1.78	0.65
1:C:217:ILE:HB	1:C:218:PRO:HD3	1.78	0.65
1:H:48:ALA:HB2	1:H:78:GLY:HA3	1.77	0.65
1:H:256:ILE:HB	1:H:257:PRO:HD3	1.79	0.65
1:D:161:PHE:CE1	1:D:257:PRO:HG3	2.32	0.65
1:E:255:LEU:O	1:E:259:THR:HB	1.97	0.65
1:F:66:MET:HE1	1:G:55:ALA:O	1.97	0.65
1:G:202:PHE:HD1	1:G:207:PHE:HB2	1.62	0.65
1:H:66:MET:HE2	1:H:66:MET:N	2.10	0.65
1:H:66:MET:HE1	1:I:59:THR:HG21	1.78	0.65
1:A:201:MET:HE3	1:B:47:ILE:HG23	1.77	0.64
1:C:93:THR:O	1:C:97:VAL:HG23	1.97	0.64
1:G:189:MET:HG3	1:H:189:MET:HE2	1.77	0.64
1:H:189:MET:HG3	1:I:189:MET:HE2	1.77	0.64
1:A:279:LEU:HD11	1:B:32:LEU:HB3	1.80	0.64
1:C:145:TRP:O	1:C:149:VAL:HG23	1.97	0.64
1:D:119:PHE:O	1:D:123:VAL:HG23	1.96	0.64
1:I:99:ALA:O	1:I:103:GLY:HA3	1.97	0.64
1:E:60:GLY:C	1:E:62:MET:H	2.05	0.64
1:H:101:ALA:HB1	1:H:105:ILE:HB	1.78	0.64
1:C:193:PHE:CB	1:D:189:MET:HE1	2.28	0.64
1:E:43:VAL:O	1:E:47:ILE:HG13	1.98	0.64
1:J:43:VAL:O	1:J:47:ILE:HG13	1.97	0.64
1:A:175:VAL:O	1:A:179:VAL:HG23	1.98	0.64
1:C:35:PHE:O	1:C:39:ILE:HG13	1.98	0.64
1:C:274:TYR:C	1:C:274:TYR:CD2	2.75	0.64
1:H:46:SER:HB3	1:H:128:PHE:HD2	1.62	0.64
1:H:105:ILE:HG23	1:H:105:ILE:O	1.97	0.64
1:I:208:GLU:HB3	1:I:258:VAL:HG21	1.80	0.64
1:D:45:ILE:O	1:D:48:ALA:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ALA:HB3	1:D:105:ILE:HB	1.79	0.63
1:D:101:ALA:O	1:D:104:ARG:CB	2.36	0.63
1:H:274:TYR:O	1:H:278:TYR:HB3	1.99	0.63
1:A:187:SER:HB2	1:E:190:ASP:OD2	1.99	0.63
1:D:178:ALA:HB1	1:D:195:MET:HG2	1.81	0.63
1:E:93:THR:HG22	1:E:183:TYR:OH	1.97	0.63
1:I:38:ALA:O	1:I:121:ASN:ND2	2.29	0.63
1:E:48:ALA:HB2	1:E:78:GLY:HA3	1.80	0.63
1:F:30:HIS:CE1	1:F:32:LEU:HD22	2.34	0.63
1:G:155:HIS:C	1:G:155:HIS:HD1	2.06	0.63
1:A:129:VAL:HA	1:A:219:MET:CE	2.29	0.63
1:B:35:PHE:HB2	1:B:116:ASN:HD21	1.64	0.63
1:F:46:SER:HB3	1:F:128:PHE:CD2	2.34	0.63
1:B:63:PRO:HB3	1:C:58:GLY:O	1.99	0.62
1:H:97:VAL:HG12	1:H:110:LEU:HG	1.80	0.62
1:J:137:GLU:O	1:J:140:THR:HB	1.98	0.62
1:A:84:VAL:O	1:A:84:VAL:HG12	1.97	0.62
1:F:109:GLN:HA	1:F:112:LYS:HE3	1.81	0.62
1:H:133:TRP:CZ2	1:H:226:PHE:HB3	2.34	0.62
1:J:277:ILE:HG22	1:J:277:ILE:O	2.00	0.62
1:D:103:GLY:C	1:D:105:ILE:N	2.55	0.62
1:A:132:MET:HB3	1:A:219:MET:HE1	1.82	0.62
1:B:94:VAL:CG1	1:B:270:VAL:HG23	2.29	0.62
1:H:81:LEU:O	1:H:85:CYS:HB2	1.99	0.62
1:I:178:ALA:HB2	1:I:198:PRO:HB2	1.82	0.62
1:A:224:ARG:NH2	1:A:243:SER:HA	2.14	0.62
1:G:147:LEU:HG	1:G:151:GLN:OE1	2.00	0.62
1:A:76:SER:HA	1:A:199:VAL:HG11	1.81	0.62
1:A:77:LEU:HD21	1:E:198:PRO:HG3	1.82	0.62
1:J:177:LEU:CD2	1:J:269:LEU:HD11	2.29	0.62
1:H:217:ILE:HB	1:H:218:PRO:HD3	1.82	0.62
1:J:75:PHE:CD2	1:J:203:VAL:HG21	2.35	0.61
1:C:210:SER:O	1:C:214:MET:HG3	2.00	0.61
1:H:201:MET:HG2	1:I:51:PHE:CD1	2.35	0.61
1:A:129:VAL:HA	1:A:219:MET:HE2	1.80	0.61
1:H:75:PHE:CD2	1:H:203:VAL:HG21	2.35	0.61
1:D:186:ARG:HH12	1:H:230:GLU:HA	1.64	0.61
1:F:96:ILE:CD1	1:F:183:TYR:HB2	2.30	0.61
1:F:223:ILE:O	1:F:227:ALA:HB2	2.00	0.61
1:G:95:LEU:HD11	1:G:269:LEU:HB3	1.82	0.61
1:A:215:PHE:CE1	1:A:219:MET:HE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:VAL:HG12	1:B:84:VAL:N	2.14	0.61
1:B:161:PHE:CD1	1:B:257:PRO:HG3	2.35	0.61
1:C:176:CYS:HB2	1:C:269:LEU:HD12	1.82	0.61
1:D:186:ARG:HH12	1:H:230:GLU:CG	2.14	0.61
1:J:48:ALA:HB2	1:J:78:GLY:HA3	1.82	0.61
1:D:201:MET:HE3	1:E:47:ILE:HG23	1.82	0.61
1:H:84:VAL:HG12	1:H:84:VAL:O	1.99	0.61
1:I:100:LYS:O	1:I:104:ARG:C	2.43	0.61
1:I:48:ALA:HB2	1:I:78:GLY:HA3	1.83	0.61
1:C:96:ILE:O	1:C:100:LYS:HB3	2.00	0.61
1:D:179:VAL:O	1:D:182:SER:HB3	2.01	0.61
1:E:202:PHE:CE2	1:E:203:VAL:HG23	2.36	0.61
1:I:98:VAL:HA	1:I:101:ALA:HB3	1.81	0.61
1:C:256:ILE:HB	1:C:257:PRO:HD3	1.83	0.60
1:D:105:ILE:O	1:D:105:ILE:HG23	2.01	0.60
1:E:164:ALA:HA	1:E:167:LEU:HD12	1.82	0.60
1:G:101:ALA:C	1:G:103:GLY:H	2.08	0.60
1:G:202:PHE:HA	1:G:207:PHE:CD2	2.36	0.60
1:I:195:MET:O	1:I:198:PRO:HD2	2.01	0.60
1:C:217:ILE:HD12	1:C:254:ASN:HD22	1.66	0.60
1:D:79:LEU:HD21	1:D:175:VAL:HG13	1.84	0.60
1:G:66:MET:HE2	1:G:66:MET:H	1.65	0.60
1:H:189:MET:HG3	1:I:189:MET:CE	2.31	0.60
1:H:211:ILE:HD13	1:H:214:MET:CE	2.31	0.60
1:E:95:LEU:HD21	1:E:269:LEU:CB	2.31	0.60
1:H:166:CYS:O	1:H:170:LEU:HD12	2.00	0.60
1:B:275:TRP:O	1:B:279:LEU:HB2	2.02	0.60
1:H:190:ASP:OD2	1:I:188:LEU:N	2.32	0.60
1:I:95:LEU:HD12	1:I:179:VAL:HG12	1.83	0.60
1:E:167:LEU:HA	1:E:170:LEU:HD12	1.83	0.60
1:F:47:ILE:HG23	1:J:201:MET:HE3	1.83	0.60
1:J:105:ILE:HB	1:J:109:GLN:OE1	2.02	0.60
1:I:197:LEU:HB3	1:J:77:LEU:HD23	1.84	0.60
1:A:232:TRP:CE3	1:A:238:ALA:HA	2.37	0.59
1:D:149:VAL:HG11	1:D:219:MET:HG3	1.82	0.59
1:F:46:SER:HB3	1:F:128:PHE:HD2	1.67	0.59
1:A:66:MET:HE2	1:B:62:MET:SD	2.42	0.59
1:F:188:LEU:N	1:J:190:ASP:OD2	2.29	0.59
1:B:217:ILE:O	1:B:221:ILE:HG13	2.03	0.59
1:H:252:THR:HA	1:H:256:ILE:HD12	1.82	0.59
1:C:90:PHE:CD1	1:C:118:TYR:HD1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:GLY:O	1:D:112:LYS:HE3	2.03	0.59
1:C:161:PHE:CE1	1:C:257:PRO:HG3	2.37	0.59
1:F:198:PRO:HG3	1:G:77:LEU:HD21	1.83	0.59
1:J:275:TRP:HZ3	1:J:279:LEU:HD21	1.67	0.59
1:A:83:VAL:HG12	1:A:84:VAL:N	2.17	0.59
1:B:215:PHE:CE1	1:B:219:MET:HE3	2.37	0.59
1:H:224:ARG:NH2	1:H:243:SER:HA	2.16	0.59
1:J:141:ALA:O	1:J:144:GLN:HB2	2.03	0.59
1:C:227:ALA:HB1	1:C:231:PHE:CD2	2.37	0.59
1:A:230:GLU:CD	1:A:230:GLU:H	2.11	0.59
1:H:80:ILE:HA	1:H:195:MET:HE1	1.84	0.59
1:G:190:ASP:HB3	1:H:188:LEU:CB	2.30	0.59
1:B:275:TRP:HA	1:B:275:TRP:CE3	2.38	0.58
1:G:254:ASN:O	1:G:257:PRO:HD2	2.03	0.58
1:C:75:PHE:CD2	1:C:203:VAL:HG21	2.38	0.58
1:D:98:VAL:HG13	1:D:105:ILE:HG21	1.84	0.58
1:B:50:VAL:HG21	1:B:132:MET:HE2	1.85	0.58
1:B:77:LEU:O	1:B:81:LEU:HB2	2.03	0.58
1:D:110:LEU:HD23	1:D:110:LEU:O	2.03	0.58
1:E:178:ALA:HB2	1:E:198:PRO:HB2	1.86	0.58
1:I:93:THR:C	1:I:95:LEU:N	2.60	0.58
1:E:183:TYR:C	1:E:185:GLY:H	2.11	0.58
1:F:52:TYR:O	1:F:56:THR:HG23	2.03	0.58
1:B:179:VAL:O	1:B:182:SER:HB3	2.03	0.58
1:E:102:SER:C	1:E:104:ARG:H	2.11	0.58
1:A:122:LEU:HD13	1:A:214:MET:SD	2.43	0.58
1:D:91:THR:O	1:D:94:VAL:HB	2.03	0.58
1:F:217:ILE:O	1:F:221:ILE:HG13	2.04	0.58
1:H:30:HIS:CE1	1:H:32:LEU:H	2.22	0.58
1:H:72:GLY:HA2	1:H:203:VAL:CG1	2.34	0.58
1:E:179:VAL:HG12	1:E:180:TRP:N	2.18	0.58
1:J:217:ILE:HG21	1:J:250:PHE:HB2	1.86	0.58
1:C:72:GLY:HA2	1:C:203:VAL:CG1	2.34	0.58
1:D:48:ALA:HB2	1:D:78:GLY:HA3	1.85	0.58
1:D:227:ALA:HB1	1:D:231:PHE:CD2	2.39	0.58
1:C:271:GLY:O	1:C:275:TRP:CD1	2.57	0.57
1:D:129:VAL:HA	1:D:219:MET:CE	2.34	0.57
1:A:100:LYS:C	1:A:102:SER:H	2.11	0.57
1:B:242:PHE:HA	1:B:244:HIS:NE2	2.18	0.57
1:C:270:VAL:O	1:C:274:TYR:CB	2.52	0.57
1:D:103:GLY:HA2	1:D:105:ILE:HG22	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ARG:HG3	1:D:242:PHE:HB2	1.86	0.57
1:D:238:ALA:HB1	1:D:240:GLU:OE1	2.04	0.57
1:E:150:LEU:HD21	1:E:224:ARG:HB2	1.85	0.57
1:F:186:ARG:HB3	1:F:190:ASP:OD2	2.03	0.57
1:F:201:MET:HB2	1:G:51:PHE:CE2	2.39	0.57
1:H:168:GLY:HA2	1:H:208:GLU:O	2.04	0.57
1:C:201:MET:HA	1:D:51:PHE:CE1	2.39	0.57
1:D:96:ILE:HG12	1:D:183:TYR:OH	2.05	0.57
1:B:161:PHE:CE1	1:B:257:PRO:HG3	2.39	0.57
1:B:167:LEU:HD23	1:C:135:SER:HB2	1.86	0.57
1:B:242:PHE:HA	1:B:244:HIS:CD2	2.39	0.57
1:D:106:THR:HG22	1:D:109:GLN:HB3	1.86	0.57
1:E:223:ILE:O	1:E:227:ALA:HB2	2.04	0.57
1:G:66:MET:CE	1:H:59:THR:HG22	2.35	0.57
1:J:161:PHE:CE1	1:J:257:PRO:HG3	2.40	0.57
1:B:246:THR:OG1	1:B:249:ASN:ND2	2.37	0.57
1:B:256:ILE:HB	1:B:257:PRO:HD3	1.87	0.57
1:F:187:SER:HB2	1:J:190:ASP:OD2	2.05	0.57
1:H:44:PHE:CD2	1:H:81:LEU:HB3	2.40	0.57
1:E:123:VAL:HG12	1:E:127:LEU:HD12	1.87	0.57
1:B:260:ILE:HG22	1:B:264:ILE:HD11	1.87	0.57
1:H:138:TYR:HD2	1:H:223:ILE:HG23	1.67	0.57
1:I:94:VAL:O	1:I:98:VAL:HG22	2.04	0.57
1:E:46:SER:CB	1:E:128:PHE:CD2	2.88	0.57
1:I:266:GLY:O	1:I:270:VAL:HG23	2.05	0.57
1:F:181:MET:SD	1:G:81:LEU:HD12	2.45	0.57
1:G:101:ALA:HB1	1:G:104:ARG:HG3	1.87	0.57
1:H:237:SER:OG	1:H:241:ASN:ND2	2.36	0.57
1:A:189:MET:HG2	1:B:189:MET:HG2	1.87	0.56
1:D:242:PHE:HB3	1:D:245:LEU:HD12	1.87	0.56
1:E:76:SER:OG	1:E:196:VAL:HG22	2.04	0.56
1:E:161:PHE:CD1	1:E:257:PRO:HG3	2.39	0.56
1:A:181:MET:HE3	1:A:194:ILE:HG13	1.86	0.56
1:A:185:GLY:CA	1:B:188:LEU:HD22	2.36	0.56
1:B:46:SER:HB3	1:B:128:PHE:CD2	2.40	0.56
1:F:30:HIS:CD2	1:J:279:LEU:HD22	2.41	0.56
1:F:129:VAL:HG13	1:F:219:MET:SD	2.45	0.56
1:J:121:ASN:HB3	1:J:211:ILE:HD12	1.86	0.56
1:G:161:PHE:CD1	1:G:257:PRO:HG3	2.40	0.56
1:G:201:MET:HE3	1:H:47:ILE:HG23	1.87	0.56
1:I:106:THR:O	1:I:110:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ALA:O	1:A:175:VAL:HG23	2.05	0.56
1:E:108:GLY:C	1:E:110:LEU:H	2.14	0.56
1:E:231:PHE:O	1:E:235:VAL:HG22	2.05	0.56
1:G:190:ASP:OD2	1:H:187:SER:HB2	2.05	0.56
1:A:128:PHE:O	1:A:132:MET:HB2	2.05	0.56
1:I:142:ASN:ND2	1:I:234:ALA:HB1	2.21	0.56
1:H:211:ILE:HD13	1:H:214:MET:HE1	1.88	0.56
1:A:46:SER:HB3	1:A:128:PHE:CD2	2.41	0.56
1:A:160:THR:OG1	1:A:163:GLU:HG3	2.04	0.56
1:D:249:ASN:O	1:D:253:ASP:HB2	2.06	0.56
1:E:68:LYS:HD2	1:E:68:LYS:N	2.19	0.56
1:H:49:PHE:CE2	1:H:212:ALA:HB1	2.41	0.56
1:I:199:VAL:HG13	1:I:202:PHE:HE2	1.71	0.56
1:A:32:LEU:HD12	1:A:32:LEU:N	2.20	0.56
1:B:76:SER:OG	1:B:196:VAL:HG23	2.06	0.56
1:C:227:ALA:HB1	1:C:231:PHE:HD2	1.71	0.56
1:D:217:ILE:HB	1:D:218:PRO:HD3	1.87	0.56
1:A:259:THR:O	1:A:263:ILE:HG13	2.05	0.55
1:D:95:LEU:HD21	1:D:269:LEU:CB	2.36	0.55
1:E:111:ALA:O	1:E:112:LYS:C	2.49	0.55
1:I:81:LEU:O	1:I:85:CYS:HB2	2.05	0.55
1:I:101:ALA:HA	1:I:105:ILE:HG22	1.88	0.55
1:I:193:PHE:CD1	1:J:189:MET:HE1	2.41	0.55
1:F:224:ARG:NH2	1:F:243:SER:HA	2.20	0.55
1:D:95:LEU:HD21	1:D:269:LEU:HB3	1.86	0.55
1:G:76:SER:CB	1:G:199:VAL:HG11	2.36	0.55
1:A:251:ILE:O	1:A:256:ILE:HG13	2.07	0.55
1:G:44:PHE:CD2	1:G:81:LEU:HB3	2.41	0.55
1:G:160:THR:HG23	1:G:163:GLU:OE2	2.06	0.55
1:H:72:GLY:HA2	1:H:203:VAL:HG11	1.87	0.55
1:J:121:ASN:CB	1:J:211:ILE:HD12	2.36	0.55
1:J:274:TYR:HE2	1:J:275:TRP:NE1	2.05	0.55
1:B:81:LEU:O	1:B:85:CYS:HB2	2.06	0.55
1:D:186:ARG:NH1	1:H:230:GLU:HA	2.21	0.55
1:G:219:MET:O	1:G:223:ILE:HG13	2.07	0.55
1:H:105:ILE:HG23	1:H:110:LEU:HD12	1.86	0.55
1:I:174:MET:SD	1:J:47:ILE:HD13	2.46	0.55
1:I:187:SER:HB3	1:I:190:ASP:H	1.71	0.55
1:A:273:THR:HG22	1:A:274:TYR:N	2.21	0.55
1:G:185:GLY:HA2	1:G:190:ASP:HB2	1.89	0.55
1:D:106:THR:HG22	1:D:109:GLN:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:VAL:HG12	1:D:127:LEU:HD11	1.89	0.55
1:J:95:LEU:O	1:J:98:VAL:HG22	2.06	0.55
1:J:274:TYR:CD2	1:J:275:TRP:CD1	2.94	0.55
1:B:110:LEU:HD23	1:B:110:LEU:O	2.06	0.55
1:B:244:HIS:O	1:B:249:ASN:ND2	2.39	0.55
1:F:140:THR:HG22	1:F:145:TRP:HB2	1.87	0.55
1:F:195:MET:O	1:F:199:VAL:HG23	2.06	0.55
1:G:105:ILE:HG23	1:G:105:ILE:O	2.07	0.55
1:I:278:TYR:CE2	1:I:279:LEU:HD23	2.42	0.55
1:F:249:ASN:O	1:F:253:ASP:HB2	2.07	0.55
1:G:119:PHE:O	1:G:123:VAL:HG23	2.06	0.55
1:H:183:TYR:C	1:H:185:GLY:H	2.14	0.55
1:C:154:ASP:O	1:C:157:VAL:HG22	2.06	0.55
1:C:164:ALA:CB	1:C:257:PRO:HB2	2.36	0.55
1:I:95:LEU:HD11	1:I:179:VAL:HG12	1.88	0.55
1:E:229:PRO:HD2	1:E:230:GLU:OE2	2.07	0.54
1:I:138:TYR:CE1	1:I:139:MET:HG2	2.41	0.54
1:I:193:PHE:CG	1:J:189:MET:HE1	2.43	0.54
1:I:222:VAL:O	1:I:226:PHE:HB2	2.08	0.54
1:B:189:MET:HE3	1:B:193:PHE:CE2	2.42	0.54
1:D:109:GLN:HA	1:D:112:LYS:HD2	1.88	0.54
1:B:174:MET:SD	1:C:47:ILE:HD13	2.47	0.54
1:C:50:VAL:HG13	1:C:145:TRP:HZ2	1.72	0.54
1:D:147:LEU:HD22	1:D:235:VAL:HB	1.90	0.54
1:F:186:ARG:HD3	1:F:186:ARG:C	2.32	0.54
1:G:76:SER:HA	1:G:199:VAL:HG11	1.88	0.54
1:A:39:ILE:HA	1:A:120:GLY:O	2.06	0.54
1:B:48:ALA:HB2	1:B:78:GLY:HA3	1.89	0.54
1:C:96:ILE:HG13	1:C:183:TYR:CG	2.43	0.54
1:G:125:ALA:O	1:G:129:VAL:HG23	2.08	0.54
1:I:161:PHE:CE1	1:I:257:PRO:HG3	2.43	0.54
1:E:143:GLY:HA3	1:E:235:VAL:HG13	1.89	0.54
1:H:175:VAL:HG21	1:H:209:HIS:CD2	2.43	0.54
1:F:161:PHE:CE1	1:F:257:PRO:HG3	2.43	0.54
1:H:96:ILE:HD12	1:H:96:ILE:N	2.23	0.54
1:I:264:ILE:O	1:I:268:LEU:HB2	2.08	0.54
1:B:94:VAL:HG11	1:B:270:VAL:HG23	1.88	0.54
1:C:97:VAL:HG12	1:C:105:ILE:HD13	1.90	0.54
1:F:240:GLU:N	1:F:240:GLU:CD	2.66	0.54
1:G:130:LEU:HG	1:G:134:LEU:HD12	1.89	0.54
1:G:184:SER:HB2	1:H:188:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:MET:CE	1:J:59:THR:HG21	2.37	0.54
1:I:187:SER:HB3	1:I:190:ASP:CG	2.33	0.54
1:D:189:MET:HG3	1:E:189:MET:HE2	1.89	0.54
1:F:147:LEU:O	1:F:151:GLN:HG3	2.07	0.54
1:D:57:THR:OG1	1:D:145:TRP:HA	2.08	0.53
1:D:198:PRO:HG3	1:E:77:LEU:HD21	1.89	0.53
1:H:143:GLY:HA3	1:H:235:VAL:HG12	1.90	0.53
1:H:272:LEU:HD21	1:I:40:THR:OG1	2.08	0.53
1:G:208:GLU:HB3	1:G:258:VAL:HG11	1.90	0.53
1:H:113:ASN:O	1:H:117:VAL:HG23	2.07	0.53
1:F:51:PHE:CD2	1:F:74:CYS:O	2.61	0.53
1:G:53:ILE:HD11	1:G:216:MET:HE1	1.90	0.53
1:I:44:PHE:HD2	1:I:82:CYS:HA	1.73	0.53
1:J:178:ALA:HB1	1:J:195:MET:HG2	1.89	0.53
1:A:91:THR:HG22	1:A:114:TRP:CZ2	2.44	0.53
1:A:190:ASP:CB	1:B:188:LEU:HB2	2.36	0.53
1:D:35:PHE:HE1	1:D:119:PHE:CD2	2.26	0.53
1:A:46:SER:HB3	1:A:128:PHE:HD2	1.74	0.53
1:B:49:PHE:CE2	1:B:212:ALA:HB1	2.43	0.53
1:B:163:GLU:O	1:B:167:LEU:HG	2.07	0.53
1:A:217:ILE:HG21	1:A:250:PHE:CD1	2.44	0.53
1:G:155:HIS:C	1:G:155:HIS:ND1	2.65	0.53
1:C:63:PRO:HB3	1:D:58:GLY:O	2.09	0.53
1:C:95:LEU:HD11	1:C:269:LEU:HD13	1.91	0.53
1:D:83:VAL:HG12	1:D:84:VAL:N	2.24	0.53
1:F:38:ALA:O	1:F:121:ASN:ND2	2.42	0.53
1:A:66:MET:SD	1:A:66:MET:N	2.81	0.53
1:E:179:VAL:HG13	1:E:183:TYR:HE2	1.74	0.53
1:D:193:PHE:CG	1:E:189:MET:HE1	2.44	0.53
1:D:201:MET:HG3	1:E:51:PHE:HB2	1.90	0.53
1:H:96:ILE:HG21	1:H:183:TYR:OH	2.09	0.53
1:C:94:VAL:HG11	1:C:270:VAL:HG23	1.91	0.52
1:D:103:GLY:CA	1:D:105:ILE:HG22	2.39	0.52
1:D:173:LEU:C	1:D:173:LEU:HD13	2.34	0.52
1:D:201:MET:HA	1:E:51:PHE:CE1	2.44	0.52
1:D:254:ASN:O	1:D:257:PRO:HD2	2.08	0.52
1:I:141:ALA:O	1:I:144:GLN:HG2	2.08	0.52
1:I:231:PHE:O	1:I:235:VAL:HG22	2.09	0.52
1:B:129:VAL:HA	1:B:219:MET:HE1	1.91	0.52
1:C:140:THR:O	1:C:141:ALA:HB3	2.09	0.52
1:D:39:ILE:HA	1:D:120:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:81:LEU:O	1:J:85:CYS:HB2	2.09	0.52
1:C:94:VAL:HG13	1:C:270:VAL:HG23	1.92	0.52
1:D:49:PHE:CE2	1:D:212:ALA:HB1	2.44	0.52
1:H:138:TYR:HE2	1:H:227:ALA:HB1	1.75	0.52
1:C:272:LEU:HD21	1:D:40:THR:OG1	2.09	0.52
1:G:101:ALA:HB1	1:G:104:ARG:CG	2.39	0.52
1:G:250:PHE:CZ	1:G:255:LEU:HD22	2.45	0.52
1:H:96:ILE:HG12	1:H:183:TYR:CE2	2.44	0.52
1:B:45:ILE:HG21	1:B:211:ILE:HG22	1.91	0.52
1:G:217:ILE:HB	1:G:218:PRO:HD3	1.91	0.52
1:I:84:VAL:HG12	1:I:84:VAL:O	2.08	0.52
1:J:45:ILE:HG21	1:J:211:ILE:HG22	1.91	0.52
1:B:46:SER:HB3	1:B:128:PHE:HD2	1.75	0.52
1:B:149:VAL:HG11	1:B:219:MET:HG3	1.92	0.52
1:D:93:THR:HB	1:D:96:ILE:HD13	1.92	0.52
1:G:187:SER:HB2	1:G:190:ASP:OD1	2.09	0.52
1:I:101:ALA:HB2	1:I:110:LEU:HD22	1.92	0.52
1:C:176:CYS:HB2	1:C:269:LEU:CD1	2.38	0.52
1:C:190:ASP:OD2	1:D:187:SER:HB2	2.10	0.52
1:C:217:ILE:HG21	1:C:250:PHE:HB2	1.92	0.52
1:E:46:SER:HB2	1:E:128:PHE:CD2	2.45	0.52
1:H:173:LEU:HD13	1:H:173:LEU:C	2.34	0.52
1:H:181:MET:CE	1:I:81:LEU:HD13	2.40	0.52
1:J:217:ILE:HB	1:J:218:PRO:HD3	1.92	0.52
1:H:224:ARG:HH21	1:H:243:SER:HA	1.75	0.52
1:B:270:VAL:O	1:B:273:THR:HB	2.10	0.52
1:H:202:PHE:HB2	1:H:207:PHE:HD2	1.75	0.52
1:D:49:PHE:CD2	1:D:212:ALA:HB1	2.45	0.52
1:D:102:SER:C	1:D:104:ARG:N	2.67	0.52
1:G:189:MET:HG3	1:H:189:MET:CE	2.40	0.52
1:I:91:THR:O	1:I:94:VAL:HB	2.10	0.52
1:A:36:TYR:CE2	1:E:279:LEU:HD12	2.46	0.51
1:C:270:VAL:O	1:C:274:TYR:HB3	2.09	0.51
1:I:92:SER:O	1:I:179:VAL:HG11	2.09	0.51
1:C:46:SER:HB3	1:C:128:PHE:CD2	2.45	0.51
1:C:161:PHE:CD1	1:C:257:PRO:HG3	2.46	0.51
1:D:94:VAL:HG23	1:D:114:TRP:HZ2	1.75	0.51
1:E:45:ILE:HG21	1:E:211:ILE:HG22	1.92	0.51
1:G:68:LYS:N	1:G:68:LYS:HD2	2.25	0.51
1:J:110:LEU:C	1:J:110:LEU:HD23	2.35	0.51
1:C:181:MET:HG2	1:D:84:VAL:CG1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:TRP:HE3	1:D:107:TRP:H	1.55	0.51
1:D:230:GLU:H	1:D:230:GLU:CD	2.19	0.51
1:H:51:PHE:CD2	1:H:74:CYS:HB3	2.45	0.51
1:A:190:ASP:OD2	1:B:188:LEU:N	2.44	0.51
1:B:225:ASP:O	1:B:226:PHE:CD2	2.63	0.51
1:C:274:TYR:CD2	1:C:275:TRP:N	2.76	0.51
1:F:187:SER:HA	1:J:186:ARG:HG3	1.91	0.51
1:G:76:SER:CA	1:G:199:VAL:HG11	2.41	0.51
1:G:161:PHE:CE1	1:G:257:PRO:HG3	2.45	0.51
1:J:278:TYR:C	1:J:278:TYR:CD2	2.88	0.51
1:B:46:SER:CB	1:B:128:PHE:CD2	2.94	0.51
1:E:50:VAL:CG2	1:E:132:MET:HE2	2.41	0.51
1:E:160:THR:HG23	1:E:163:GLU:OE2	2.10	0.51
1:F:30:HIS:CG	1:J:279:LEU:HD22	2.45	0.51
1:H:35:PHE:HB2	1:H:116:ASN:HD21	1.75	0.51
1:J:158:HIS:NE2	1:J:244:HIS:CD2	2.79	0.51
1:D:96:ILE:O	1:D:100:LYS:HB2	2.11	0.51
1:E:161:PHE:O	1:E:165:VAL:HG23	2.09	0.51
1:A:256:ILE:HB	1:A:257:PRO:HD3	1.91	0.51
1:C:163:GLU:O	1:C:167:LEU:HG	2.11	0.51
1:C:217:ILE:CD1	1:C:254:ASN:ND2	2.74	0.51
1:D:108:GLY:O	1:D:112:LYS:HG2	2.11	0.51
1:H:101:ALA:CB	1:H:105:ILE:HB	2.41	0.51
1:I:201:MET:HG2	1:J:51:PHE:CD1	2.46	0.51
1:J:44:PHE:CD1	1:J:81:LEU:HD23	2.46	0.51
1:C:217:ILE:O	1:C:221:ILE:HG13	2.09	0.51
1:D:193:PHE:HB3	1:E:193:PHE:CZ	2.46	0.51
1:F:119:PHE:O	1:F:123:VAL:HG23	2.10	0.51
1:G:195:MET:C	1:G:198:PRO:HD2	2.36	0.51
1:C:95:LEU:HD12	1:C:180:TRP:HB2	1.92	0.51
1:D:152:THR:O	1:D:156:LYS:HG3	2.10	0.51
1:B:72:GLY:HA2	1:B:203:VAL:HG11	1.93	0.51
1:D:186:ARG:NH2	1:H:230:GLU:O	2.44	0.51
1:G:105:ILE:O	1:G:105:ILE:CG2	2.59	0.51
1:H:238:ALA:H	1:H:241:ASN:ND2	2.09	0.51
1:I:75:PHE:CD2	1:I:203:VAL:HG21	2.46	0.51
1:A:51:PHE:CD2	1:E:201:MET:HB2	2.46	0.50
1:A:221:ILE:HG12	1:A:245:LEU:O	2.10	0.50
1:B:181:MET:HG2	1:C:84:VAL:CG1	2.42	0.50
1:B:186:ARG:NH1	1:G:240:GLU:HB3	2.27	0.50
1:H:77:LEU:HD22	1:H:81:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:68:LYS:HD2	1:J:68:LYS:N	2.26	0.50
1:A:91:THR:HG22	1:A:114:TRP:CE2	2.47	0.50
1:A:132:MET:HB3	1:A:219:MET:CE	2.41	0.50
1:H:181:MET:HE2	1:I:81:LEU:CD1	2.41	0.50
1:H:279:LEU:HD11	1:I:36:TYR:HE2	1.77	0.50
1:B:91:THR:HG22	1:B:114:TRP:CZ2	2.46	0.50
1:B:94:VAL:CG2	1:B:114:TRP:HZ2	2.24	0.50
1:B:98:VAL:HG11	1:B:273:THR:HG21	1.92	0.50
1:B:195:MET:C	1:B:198:PRO:HD2	2.35	0.50
1:C:72:GLY:HA2	1:C:203:VAL:HG11	1.93	0.50
1:J:140:THR:HG22	1:J:145:TRP:HB2	1.93	0.50
1:A:130:LEU:C	1:A:130:LEU:HD12	2.37	0.50
1:C:35:PHE:CE2	1:C:39:ILE:HD11	2.47	0.50
1:F:190:ASP:HB3	1:G:188:LEU:CB	2.42	0.50
1:G:100:LYS:C	1:G:102:SER:H	2.19	0.50
1:G:201:MET:HA	1:H:51:PHE:CE1	2.47	0.50
1:E:147:LEU:HA	1:E:150:LEU:HD12	1.92	0.50
1:E:186:ARG:HB2	1:E:190:ASP:OD2	2.12	0.50
1:I:142:ASN:CG	1:I:142:ASN:O	2.53	0.50
1:C:217:ILE:HD11	1:C:254:ASN:ND2	2.27	0.50
1:E:33:LYS:O	1:E:37:LEU:HG	2.12	0.50
1:I:72:GLY:HA2	1:I:203:VAL:HG11	1.92	0.50
1:J:186:ARG:HH11	1:J:186:ARG:HB3	1.75	0.50
1:J:228:SER:O	1:J:231:PHE:HB3	2.11	0.50
1:G:66:MET:HE1	1:H:59:THR:HG22	1.93	0.50
1:H:279:LEU:HD22	1:I:32:LEU:HD23	1.93	0.50
1:C:97:VAL:HG12	1:C:105:ILE:CD1	2.42	0.50
1:C:231:PHE:O	1:C:235:VAL:HG13	2.11	0.50
1:D:193:PHE:HD1	1:E:193:PHE:CZ	2.30	0.50
1:F:250:PHE:O	1:F:254:ASN:HB3	2.12	0.50
1:D:97:VAL:HG12	1:D:97:VAL:O	2.11	0.50
1:A:34:THR:HG21	1:A:113:ASN:ND2	2.27	0.49
1:A:140:THR:HG22	1:A:145:TRP:HB2	1.94	0.49
1:C:217:ILE:CD1	1:C:254:ASN:HD22	2.24	0.49
1:D:201:MET:CE	1:E:47:ILE:HG23	2.42	0.49
1:D:223:ILE:O	1:D:227:ALA:CB	2.60	0.49
1:G:66:MET:HE3	1:H:62:MET:SD	2.52	0.49
1:G:111:ALA:O	1:G:113:ASN:N	2.44	0.49
1:H:138:TYR:HE2	1:H:227:ALA:CB	2.25	0.49
1:I:98:VAL:HG21	1:I:270:VAL:HG22	1.94	0.49
1:J:232:TRP:HZ3	1:J:242:PHE:HE2	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:PRO:HA	1:B:77:LEU:HD11	1.93	0.49
1:C:46:SER:OG	1:C:215:PHE:HB2	2.12	0.49
1:C:164:ALA:HB1	1:C:257:PRO:HB2	1.93	0.49
1:F:201:MET:HE3	1:G:47:ILE:HG23	1.93	0.49
1:H:102:SER:C	1:H:104:ARG:H	2.20	0.49
1:I:44:PHE:CD2	1:I:82:CYS:HA	2.46	0.49
1:A:113:ASN:O	1:A:117:VAL:HG23	2.12	0.49
1:A:229:PRO:HA	1:A:232:TRP:HD1	1.76	0.49
1:A:260:ILE:HG22	1:A:261:GLY:N	2.28	0.49
1:H:96:ILE:HD12	1:H:96:ILE:H	1.77	0.49
1:I:98:VAL:HB	1:I:270:VAL:HG22	1.94	0.49
1:I:199:VAL:HG13	1:I:202:PHE:CE2	2.46	0.49
1:D:66:MET:HE2	1:D:66:MET:H	1.78	0.49
1:D:217:ILE:HD12	1:D:250:PHE:CD1	2.47	0.49
1:E:132:MET:HB2	1:E:219:MET:CE	2.42	0.49
1:A:47:ILE:HG23	1:E:201:MET:HE3	1.93	0.49
1:A:51:PHE:CE2	1:E:201:MET:HB2	2.48	0.49
1:F:54:THR:HG21	1:J:204:ALA:C	2.38	0.49
1:F:96:ILE:HD11	1:F:183:TYR:HB2	1.94	0.49
1:G:276:VAL:O	1:G:276:VAL:CG1	2.60	0.49
1:H:84:VAL:O	1:H:84:VAL:CG1	2.60	0.49
1:A:84:VAL:O	1:A:84:VAL:CG1	2.61	0.49
1:A:138:TYR:CE1	1:A:139:MET:HG2	2.47	0.49
1:B:112:LYS:HG3	1:B:113:ASN:H	1.78	0.49
1:C:81:LEU:O	1:C:85:CYS:HB2	2.13	0.49
1:E:149:VAL:HG11	1:E:219:MET:HG3	1.93	0.49
1:F:190:ASP:HB3	1:G:188:LEU:HB3	1.95	0.49
1:H:68:LYS:O	1:H:69:LEU:C	2.55	0.49
1:I:93:THR:O	1:I:95:LEU:N	2.46	0.49
1:F:84:VAL:CG1	1:J:181:MET:HG2	2.42	0.49
1:G:208:GLU:HB3	1:G:258:VAL:CG1	2.43	0.49
1:G:256:ILE:HG22	1:G:257:PRO:N	2.27	0.49
1:H:138:TYR:CD2	1:H:223:ILE:HG23	2.47	0.49
1:H:247:VAL:O	1:H:251:ILE:HG12	2.12	0.49
1:I:273:THR:HG23	1:I:277:ILE:HG22	1.94	0.49
1:C:44:PHE:CD2	1:C:82:CYS:HA	2.48	0.49
1:A:210:SER:HB3	1:A:258:VAL:HG12	1.94	0.49
1:B:169:ILE:HG12	1:B:264:ILE:HB	1.94	0.49
1:C:197:LEU:HB3	1:D:77:LEU:HG	1.95	0.49
1:E:275:TRP:CE3	1:E:278:TYR:HB3	2.48	0.49
1:E:165:VAL:O	1:E:261:GLY:HA3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:PHE:HD2	1:I:57:THR:HG22	1.78	0.49
1:F:51:PHE:HD2	1:F:74:CYS:O	1.96	0.48
1:F:80:ILE:HG12	1:F:192:ALA:HB1	1.95	0.48
1:F:190:ASP:OD2	1:G:188:LEU:N	2.42	0.48
1:G:107:TRP:O	1:G:110:LEU:HB2	2.13	0.48
1:I:174:MET:HE1	1:J:77:LEU:HD11	1.95	0.48
1:B:192:ALA:C	1:B:194:ILE:H	2.20	0.48
1:E:179:VAL:HG13	1:E:183:TYR:CE2	2.48	0.48
1:H:161:PHE:CD1	1:H:257:PRO:HG3	2.48	0.48
1:A:31:PRO:HB2	1:A:32:LEU:HD12	1.94	0.48
1:A:202:PHE:CE2	1:A:203:VAL:HG23	2.48	0.48
1:C:49:PHE:CE2	1:C:212:ALA:HB1	2.48	0.48
1:G:59:THR:HB	1:G:62:MET:HB2	1.94	0.48
1:D:98:VAL:HG11	1:D:270:VAL:CG1	2.24	0.48
1:D:267:GLY:HA2	1:D:270:VAL:HB	1.95	0.48
1:G:75:PHE:CG	1:G:203:VAL:HG21	2.48	0.48
1:C:90:PHE:CE2	1:C:91:THR:HG23	2.48	0.48
1:D:129:VAL:HA	1:D:219:MET:HE2	1.94	0.48
1:B:222:VAL:O	1:B:226:PHE:HB2	2.13	0.48
1:E:112:LYS:HG3	1:E:113:ASN:N	2.28	0.48
1:F:190:ASP:OD2	1:G:187:SER:HB3	2.13	0.48
1:J:62:MET:HE2	1:J:67:ALA:HA	1.95	0.48
1:J:191:LYS:O	1:J:195:MET:HE2	2.14	0.48
1:A:36:TYR:HE2	1:E:279:LEU:HD12	1.78	0.48
1:E:183:TYR:C	1:E:185:GLY:N	2.71	0.48
1:G:160:THR:HG23	1:G:163:GLU:CD	2.38	0.48
1:I:80:ILE:HA	1:I:195:MET:HE1	1.96	0.48
1:I:164:ALA:CB	1:I:257:PRO:HB2	2.43	0.48
1:I:246:THR:O	1:I:249:ASN:HB2	2.14	0.48
1:B:154:ASP:O	1:B:157:VAL:HG22	2.13	0.48
1:C:250:PHE:CZ	1:C:255:LEU:HD22	2.49	0.48
1:G:95:LEU:HD21	1:G:269:LEU:HB3	1.95	0.48
1:J:147:LEU:HG	1:J:151:GLN:NE2	2.29	0.48
1:B:217:ILE:HB	1:B:218:PRO:HD3	1.96	0.48
1:C:94:VAL:HG13	1:C:270:VAL:CG2	2.44	0.48
1:C:101:ALA:CB	1:C:105:ILE:HB	2.44	0.48
1:C:139:MET:HE3	1:C:139:MET:HB3	1.71	0.48
1:E:232:TRP:CE2	1:E:239:PRO:HD3	2.49	0.48
1:F:232:TRP:CD2	1:F:239:PRO:HD3	2.49	0.48
1:C:217:ILE:HD12	1:C:250:PHE:HD1	1.75	0.48
1:G:177:LEU:HD23	1:G:177:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:ILE:O	1:H:163:GLU:C	2.57	0.48
1:H:173:LEU:HD22	1:H:173:LEU:O	2.14	0.48
1:H:193:PHE:CD1	1:I:189:MET:HE1	2.49	0.48
1:H:279:LEU:HD13	1:I:32:LEU:HG	1.94	0.48
1:I:49:PHE:O	1:I:50:VAL:C	2.56	0.48
1:J:30:HIS:CD2	1:J:31:PRO:HD2	2.48	0.48
1:A:130:LEU:HD12	1:A:130:LEU:O	2.13	0.47
1:B:39:ILE:HA	1:B:120:GLY:O	2.14	0.47
1:C:132:MET:HE1	1:C:137:GLU:HG2	1.95	0.47
1:C:133:TRP:CZ2	1:C:226:PHE:HB3	2.49	0.47
1:D:110:LEU:C	1:D:110:LEU:CD2	2.86	0.47
1:E:76:SER:HA	1:E:199:VAL:HG11	1.96	0.47
1:B:129:VAL:HA	1:B:219:MET:CE	2.44	0.47
1:E:133:TRP:HZ3	1:E:223:ILE:HG12	1.79	0.47
1:F:123:VAL:O	1:F:127:LEU:HD12	2.13	0.47
1:H:63:PRO:HG2	1:I:62:MET:SD	2.54	0.47
1:J:41:ALA:HA	1:J:44:PHE:HB2	1.95	0.47
1:J:173:LEU:O	1:J:177:LEU:HG	2.14	0.47
1:C:132:MET:HB3	1:C:219:MET:HE2	1.97	0.47
1:D:166:CYS:SG	1:E:134:LEU:HB3	2.54	0.47
1:E:96:ILE:HG12	1:E:183:TYR:CE1	2.49	0.47
1:J:227:ALA:HB1	1:J:231:PHE:CD2	2.49	0.47
1:A:35:PHE:HD1	1:A:116:ASN:OD1	1.96	0.47
1:E:248:MET:O	1:E:252:THR:HG23	2.14	0.47
1:G:190:ASP:CB	1:H:188:LEU:HB3	2.33	0.47
1:G:213:ASN:ND2	1:G:254:ASN:HD21	2.12	0.47
1:J:231:PHE:CE1	1:J:235:VAL:HG11	2.49	0.47
1:B:44:PHE:CD2	1:B:82:CYS:HA	2.50	0.47
1:B:259:THR:O	1:B:262:ASN:HB2	2.14	0.47
1:C:182:SER:C	1:C:184:SER:H	2.22	0.47
1:D:109:GLN:HA	1:D:112:LYS:CD	2.45	0.47
1:E:132:MET:HB2	1:E:219:MET:HE1	1.96	0.47
1:E:256:ILE:HB	1:E:257:PRO:HD3	1.95	0.47
1:A:201:MET:HA	1:B:51:PHE:CE1	2.49	0.47
1:D:186:ARG:HH12	1:H:230:GLU:CA	2.28	0.47
1:E:40:THR:HG22	1:E:44:PHE:CE2	2.50	0.47
1:E:129:VAL:HA	1:E:219:MET:CE	2.44	0.47
1:H:137:GLU:HG3	1:H:137:GLU:O	2.13	0.47
1:B:241:ASN:OD1	1:B:241:ASN:N	2.47	0.47
1:C:182:SER:HB2	1:C:195:MET:HG3	1.95	0.47
1:D:169:ILE:HG13	1:D:261:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ALA:HB1	1:E:89:LEU:HD12	1.96	0.47
1:F:115:LEU:HD12	1:F:115:LEU:O	2.15	0.47
1:F:190:ASP:CG	1:G:187:SER:HB3	2.40	0.47
1:F:279:LEU:HD13	1:G:33:LYS:HB2	1.97	0.47
1:G:254:ASN:C	1:G:257:PRO:HD2	2.40	0.47
1:H:161:PHE:CE1	1:H:257:PRO:HG3	2.50	0.47
1:H:162:ILE:HG22	1:H:163:GLU:N	2.30	0.47
1:I:51:PHE:HD2	1:I:74:CYS:O	1.98	0.47
1:J:100:LYS:HE2	1:J:107:TRP:CE2	2.49	0.47
1:J:266:GLY:O	1:J:270:VAL:HG13	2.14	0.47
1:A:32:LEU:H	1:A:32:LEU:CD1	2.24	0.47
1:A:33:LYS:N	1:E:279:LEU:HD13	2.30	0.47
1:B:150:LEU:O	1:B:154:ASP:HB2	2.14	0.47
1:B:181:MET:HG2	1:C:84:VAL:HG12	1.97	0.47
1:C:129:VAL:CG1	1:C:222:VAL:HG21	2.45	0.47
1:G:160:THR:O	1:G:161:PHE:C	2.55	0.47
1:I:94:VAL:O	1:I:98:VAL:HG13	2.15	0.47
1:J:179:VAL:O	1:J:182:SER:HB3	2.14	0.47
1:D:66:MET:HE2	1:D:66:MET:N	2.29	0.47
1:D:217:ILE:O	1:D:221:ILE:HG13	2.15	0.47
1:H:147:LEU:HG	1:H:151:GLN:HE21	1.78	0.47
1:A:46:SER:CB	1:A:128:PHE:CD2	2.98	0.47
1:B:63:PRO:HB3	1:C:59:THR:HG23	1.97	0.47
1:C:174:MET:SD	1:D:47:ILE:HD13	2.55	0.47
1:D:168:GLY:HA2	1:D:208:GLU:O	2.16	0.47
1:D:197:LEU:HB3	1:E:77:LEU:HD23	1.96	0.47
1:F:47:ILE:HD13	1:J:174:MET:SD	2.54	0.47
1:F:105:ILE:HA	1:F:109:GLN:OE1	2.16	0.47
1:G:149:VAL:HG12	1:G:220:GLY:HA2	1.96	0.47
1:G:277:ILE:C	1:G:279:LEU:H	2.23	0.47
1:A:178:ALA:HB1	1:A:195:MET:HG2	1.96	0.46
1:B:137:GLU:O	1:B:137:GLU:HG3	2.15	0.46
1:D:186:ARG:HH21	1:H:234:ALA:HB2	1.79	0.46
1:H:197:LEU:HD12	1:H:197:LEU:HA	1.70	0.46
1:J:97:VAL:HG12	1:J:270:VAL:HG21	1.97	0.46
1:J:97:VAL:HG12	1:J:270:VAL:HG11	1.97	0.46
1:A:75:PHE:CD2	1:A:203:VAL:HG21	2.49	0.46
1:C:195:MET:C	1:C:198:PRO:HD2	2.40	0.46
1:C:197:LEU:HD12	1:C:197:LEU:HA	1.70	0.46
1:F:164:ALA:HB3	1:F:257:PRO:HB2	1.97	0.46
1:H:176:CYS:HB2	1:H:269:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:267:GLY:O	1:I:270:VAL:HB	2.15	0.46
1:A:109:GLN:HG3	1:F:241:ASN:ND2	2.31	0.46
1:F:122:LEU:CD1	1:F:214:MET:HG2	2.45	0.46
1:F:181:MET:HG2	1:G:84:VAL:HG12	1.97	0.46
1:I:98:VAL:C	1:I:100:LYS:N	2.70	0.46
1:A:193:PHE:CZ	1:E:193:PHE:O	2.56	0.46
1:C:270:VAL:O	1:C:271:GLY:C	2.58	0.46
1:D:96:ILE:H	1:D:96:ILE:CD1	2.21	0.46
1:E:217:ILE:HB	1:E:218:PRO:HD3	1.97	0.46
1:I:46:SER:HB3	1:I:128:PHE:HD2	1.80	0.46
1:I:98:VAL:CB	1:I:270:VAL:HG22	2.46	0.46
1:J:230:GLU:CD	1:J:230:GLU:H	2.24	0.46
1:A:138:TYR:HE2	1:A:227:ALA:HB1	1.81	0.46
1:C:154:ASP:O	1:C:156:LYS:N	2.49	0.46
1:D:166:CYS:O	1:D:170:LEU:HD12	2.16	0.46
1:F:65:GLY:HA2	1:G:54:THR:O	2.16	0.46
1:I:169:ILE:HD11	1:I:264:ILE:HD13	1.97	0.46
1:C:133:TRP:HZ2	1:C:226:PHE:HB3	1.81	0.46
1:F:159:HIS:CE1	1:F:167:LEU:HD11	2.50	0.46
1:H:167:LEU:HA	1:H:170:LEU:HD12	1.97	0.46
1:J:45:ILE:O	1:J:48:ALA:HB3	2.15	0.46
1:C:108:GLY:C	1:C:110:LEU:H	2.24	0.46
1:D:232:TRP:CE2	1:D:239:PRO:HG3	2.51	0.46
1:F:34:THR:HG21	1:F:113:ASN:OD1	2.16	0.46
1:F:76:SER:HA	1:F:199:VAL:HG11	1.98	0.46
1:F:201:MET:HB2	1:G:51:PHE:CD2	2.51	0.46
1:H:56:THR:HA	1:H:59:THR:CG2	2.45	0.46
1:I:104:ARG:O	1:I:105:ILE:CD1	2.64	0.46
1:J:97:VAL:HB	1:J:270:VAL:CG1	2.38	0.46
1:J:195:MET:C	1:J:198:PRO:HD2	2.41	0.46
1:C:219:MET:O	1:C:223:ILE:HG13	2.16	0.46
1:D:96:ILE:CG1	1:D:183:TYR:CE2	2.98	0.46
1:D:254:ASN:C	1:D:257:PRO:HD2	2.40	0.46
1:F:99:ALA:HB2	1:F:180:TRP:CH2	2.51	0.46
1:G:65:GLY:O	1:G:66:MET:C	2.58	0.46
1:C:261:GLY:HA2	1:C:264:ILE:HD12	1.97	0.46
1:E:96:ILE:N	1:E:96:ILE:HD12	2.30	0.46
1:G:121:ASN:HB3	1:G:211:ILE:HG23	1.98	0.46
1:I:98:VAL:CG2	1:I:270:VAL:HG22	2.45	0.46
1:I:106:THR:HG22	1:I:108:GLY:H	1.81	0.46
1:I:208:GLU:CB	1:I:258:VAL:HG21	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:256:ILE:CB	1:J:257:PRO:HD3	2.41	0.46
1:B:45:ILE:HD12	1:B:45:ILE:HA	1.66	0.46
1:C:275:TRP:HA	1:C:278:TYR:CD2	2.51	0.46
1:E:160:THR:O	1:E:161:PHE:C	2.59	0.46
1:H:176:CYS:CB	1:H:269:LEU:HD12	2.46	0.46
1:I:53:ILE:HG22	1:I:145:TRP:NE1	2.31	0.46
1:F:130:LEU:O	1:F:134:LEU:HG	2.17	0.45
1:F:188:LEU:HD12	1:F:188:LEU:HA	1.67	0.45
1:I:79:LEU:HD21	1:I:179:VAL:HG23	1.98	0.45
1:I:102:SER:O	1:I:103:GLY:C	2.59	0.45
1:I:132:MET:CB	1:I:219:MET:HE1	2.46	0.45
1:E:39:ILE:O	1:E:42:GLY:N	2.49	0.45
1:C:94:VAL:HG12	1:C:95:LEU:N	2.31	0.45
1:D:193:PHE:HD1	1:E:193:PHE:CE1	2.35	0.45
1:D:217:ILE:HD12	1:D:250:PHE:CE1	2.51	0.45
1:F:105:ILE:HG23	1:F:105:ILE:O	2.17	0.45
1:F:135:SER:HB2	1:J:167:LEU:CD2	2.46	0.45
1:G:179:VAL:O	1:G:182:SER:HB3	2.16	0.45
1:H:110:LEU:O	1:H:110:LEU:HD23	2.16	0.45
1:I:49:PHE:O	1:I:52:TYR:N	2.50	0.45
1:I:273:THR:O	1:I:274:TYR:C	2.57	0.45
1:I:275:TRP:CD1	1:I:275:TRP:H	2.35	0.45
1:J:229:PRO:HA	1:J:232:TRP:HD1	1.80	0.45
1:A:254:ASN:C	1:A:257:PRO:HD2	2.41	0.45
1:A:279:LEU:CD1	1:B:32:LEU:HB3	2.46	0.45
1:D:169:ILE:HG12	1:D:264:ILE:HB	1.98	0.45
1:F:189:MET:HB2	1:J:190:ASP:OD1	2.16	0.45
1:G:66:MET:HE1	1:H:59:THR:CG2	2.46	0.45
1:H:49:PHE:CD2	1:H:212:ALA:HB1	2.52	0.45
1:H:138:TYR:CE1	1:H:139:MET:HG2	2.52	0.45
1:J:84:VAL:HG12	1:J:84:VAL:O	2.16	0.45
1:J:93:THR:O	1:J:97:VAL:HG23	2.16	0.45
1:F:33:LYS:HB2	1:J:279:LEU:CB	2.38	0.45
1:F:122:LEU:HD13	1:F:214:MET:HG2	1.99	0.45
1:F:123:VAL:HG12	1:F:127:LEU:CD1	2.46	0.45
1:F:194:ILE:O	1:F:194:ILE:HG13	2.14	0.45
1:F:255:LEU:HD12	1:F:255:LEU:HA	1.82	0.45
1:G:107:TRP:HH2	1:G:271:GLY:HA2	1.82	0.45
1:I:66:MET:HE3	1:J:62:MET:SD	2.57	0.45
1:A:38:ALA:O	1:A:121:ASN:ND2	2.50	0.45
1:A:100:LYS:C	1:A:102:SER:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LEU:HD23	1:B:279:LEU:HA	1.68	0.45
1:C:110:LEU:O	1:C:110:LEU:HD23	2.16	0.45
1:D:129:VAL:O	1:D:219:MET:HE1	2.17	0.45
1:E:199:VAL:HA	1:E:202:PHE:HD2	1.81	0.45
1:E:201:MET:SD	1:E:201:MET:C	3.00	0.45
1:E:213:ASN:ND2	1:E:254:ASN:OD1	2.47	0.45
1:G:29:LYS:O	1:G:31:PRO:HD3	2.16	0.45
1:G:106:THR:HG22	1:G:109:GLN:OE1	2.16	0.45
1:G:107:TRP:HA	1:G:110:LEU:HD12	1.98	0.45
1:G:274:TYR:O	1:G:278:TYR:HB2	2.16	0.45
1:H:141:ALA:O	1:H:144:GLN:HB2	2.17	0.45
1:I:80:ILE:HD13	1:I:192:ALA:HB1	1.99	0.45
1:J:150:LEU:HD13	1:J:242:PHE:CE2	2.52	0.45
1:C:270:VAL:O	1:C:274:TYR:HB2	2.16	0.45
1:F:254:ASN:C	1:F:257:PRO:HD2	2.42	0.45
1:H:139:MET:SD	1:H:231:PHE:HB2	2.56	0.45
1:I:45:ILE:HD12	1:I:45:ILE:HA	1.77	0.45
1:J:202:PHE:O	1:J:202:PHE:CD1	2.69	0.45
1:B:66:MET:HE3	1:C:59:THR:HG21	1.99	0.45
1:B:270:VAL:HG12	1:B:271:GLY:N	2.31	0.45
1:D:35:PHE:HD1	1:D:116:ASN:OD1	1.99	0.45
1:E:160:THR:HG23	1:E:163:GLU:CD	2.42	0.45
1:F:146:GLY:O	1:F:149:VAL:HB	2.17	0.45
1:F:268:LEU:HD23	1:F:268:LEU:HA	1.85	0.45
1:H:275:TRP:HZ3	1:H:278:TYR:CE2	2.35	0.45
1:I:46:SER:CB	1:I:128:PHE:CD2	3.00	0.45
1:J:89:LEU:O	1:J:90:PHE:C	2.60	0.45
1:B:185:GLY:O	1:B:191:LYS:HE3	2.16	0.45
1:D:44:PHE:HD2	1:D:82:CYS:HA	1.82	0.45
1:D:96:ILE:HG12	1:D:183:TYR:CE2	2.51	0.45
1:D:169:ILE:HA	1:D:261:GLY:O	2.16	0.45
1:D:264:ILE:O	1:D:268:LEU:HB2	2.14	0.45
1:E:93:THR:HG22	1:E:183:TYR:HH	1.80	0.45
1:E:259:THR:HG22	1:E:260:ILE:N	2.31	0.45
1:G:101:ALA:C	1:G:103:GLY:N	2.75	0.45
1:I:77:LEU:O	1:I:81:LEU:HB2	2.17	0.45
1:I:198:PRO:HG3	1:J:77:LEU:HD21	1.99	0.45
1:C:193:PHE:HB3	1:D:189:MET:HE1	1.98	0.45
1:D:96:ILE:CG1	1:D:183:TYR:HE2	2.29	0.45
1:G:88:ASP:OD2	1:G:117:VAL:HG13	2.17	0.45
1:H:171:ALA:HB2	1:H:207:PHE:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:231:PHE:CE1	1:H:235:VAL:HG11	2.51	0.45
1:J:214:MET:O	1:J:218:PRO:HG2	2.17	0.45
1:D:75:PHE:CD2	1:D:203:VAL:HG21	2.52	0.44
1:E:39:ILE:HG22	1:E:40:THR:N	2.31	0.44
1:H:147:LEU:O	1:H:151:GLN:HG3	2.17	0.44
1:H:202:PHE:HB2	1:H:207:PHE:CD2	2.53	0.44
1:I:164:ALA:HB3	1:I:257:PRO:HB2	1.99	0.44
1:B:150:LEU:CD2	1:B:224:ARG:HB2	2.46	0.44
1:D:84:VAL:HG22	1:D:188:LEU:HD11	1.99	0.44
1:E:53:ILE:HG21	1:E:145:TRP:CE2	2.53	0.44
1:H:137:GLU:O	1:H:140:THR:HB	2.17	0.44
1:H:170:LEU:HG	1:I:131:LEU:HD21	1.99	0.44
1:H:195:MET:O	1:H:199:VAL:HG23	2.17	0.44
1:I:133:TRP:HA	1:I:133:TRP:CE3	2.52	0.44
1:A:118:TYR:O	1:A:121:ASN:HB2	2.18	0.44
1:E:102:SER:C	1:E:104:ARG:N	2.75	0.44
1:H:63:PRO:O	1:H:64:PHE:C	2.61	0.44
1:A:232:TRP:HA	1:A:235:VAL:HG22	1.98	0.44
1:B:254:ASN:O	1:B:257:PRO:HD2	2.18	0.44
1:E:250:PHE:CD1	1:E:250:PHE:C	2.94	0.44
1:G:221:ILE:HG12	1:G:245:LEU:O	2.17	0.44
1:I:217:ILE:HB	1:I:218:PRO:HD3	1.98	0.44
1:A:30:HIS:HA	1:A:31:PRO:HD3	1.90	0.44
1:A:51:PHE:CE1	1:E:201:MET:HA	2.52	0.44
1:B:79:LEU:N	1:B:79:LEU:HD22	2.32	0.44
1:C:189:MET:HG2	1:D:189:MET:HG2	1.99	0.44
1:D:35:PHE:HE1	1:D:119:PHE:HD2	1.64	0.44
1:E:60:GLY:C	1:E:62:MET:N	2.74	0.44
1:G:46:SER:HB2	1:G:128:PHE:CD2	2.53	0.44
1:G:132:MET:HB3	1:G:219:MET:CE	2.47	0.44
1:H:171:ALA:HB2	1:H:207:PHE:HB3	2.00	0.44
1:I:80:ILE:O	1:I:81:LEU:C	2.60	0.44
1:I:187:SER:HB3	1:I:190:ASP:CB	2.48	0.44
1:J:92:SER:C	1:J:94:VAL:H	2.25	0.44
1:A:232:TRP:CZ2	1:A:239:PRO:HG3	2.52	0.44
1:D:62:MET:HE2	1:D:62:MET:HB3	1.64	0.44
1:D:77:LEU:HD22	1:D:81:LEU:HD22	1.98	0.44
1:E:108:GLY:C	1:E:110:LEU:N	2.75	0.44
1:G:202:PHE:CD1	1:G:202:PHE:C	2.96	0.44
1:H:183:TYR:O	1:H:185:GLY:N	2.51	0.44
1:I:106:THR:HG22	1:I:107:TRP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:ARG:HD2	1:I:245:LEU:HB2	1.99	0.44
1:I:278:TYR:CD2	1:I:279:LEU:N	2.86	0.44
1:A:72:GLY:HA2	1:A:203:VAL:CG1	2.48	0.44
1:A:72:GLY:HA2	1:A:203:VAL:HG11	2.00	0.44
1:C:217:ILE:HD12	1:C:250:PHE:CE1	2.50	0.44
1:D:96:ILE:HG12	1:D:183:TYR:CZ	2.53	0.44
1:E:269:LEU:HD23	1:E:269:LEU:HA	1.84	0.44
1:G:238:ALA:O	1:G:241:ASN:HB2	2.18	0.44
1:H:172:ASN:HB2	1:H:262:ASN:ND2	2.33	0.44
1:H:189:MET:CG	1:I:189:MET:HE2	2.44	0.44
1:C:254:ASN:O	1:C:258:VAL:HG23	2.17	0.44
1:D:211:ILE:O	1:D:214:MET:HB2	2.17	0.44
1:F:240:GLU:CD	1:F:240:GLU:H	2.26	0.44
1:I:49:PHE:CE2	1:I:216:MET:HB2	2.52	0.44
1:J:169:ILE:HG13	1:J:261:GLY:HA2	2.00	0.44
1:D:84:VAL:CG2	1:D:188:LEU:HD11	2.48	0.44
1:E:181:MET:HE3	1:E:194:ILE:HG13	2.00	0.44
1:F:76:SER:OG	1:F:196:VAL:HG22	2.17	0.44
1:F:113:ASN:O	1:F:117:VAL:HG23	2.18	0.44
1:H:105:ILE:CG2	1:H:110:LEU:HD12	2.48	0.44
1:I:42:GLY:O	1:I:45:ILE:HG22	2.18	0.44
1:I:66:MET:HE3	1:J:62:MET:HE1	1.99	0.44
1:I:93:THR:C	1:I:95:LEU:H	2.24	0.44
1:A:149:VAL:HG11	1:A:219:MET:HG3	2.00	0.43
1:A:217:ILE:HB	1:A:218:PRO:HD3	1.99	0.43
1:B:122:LEU:HB2	1:B:214:MET:SD	2.58	0.43
1:C:66:MET:HE3	1:D:70:VAL:HG11	1.99	0.43
1:D:77:LEU:O	1:D:81:LEU:HB2	2.18	0.43
1:D:139:MET:HE3	1:D:139:MET:HB3	1.87	0.43
1:G:35:PHE:CE1	1:G:119:PHE:HD2	2.36	0.43
1:H:214:MET:O	1:H:218:PRO:HG2	2.18	0.43
1:I:46:SER:HB2	1:I:128:PHE:CD2	2.53	0.43
1:I:173:LEU:HD23	1:I:173:LEU:C	2.43	0.43
1:I:272:LEU:HD12	1:J:36:TYR:OH	2.17	0.43
1:J:62:MET:HG3	1:J:63:PRO:HD2	1.99	0.43
1:J:168:GLY:HA2	1:J:208:GLU:O	2.17	0.43
1:J:264:ILE:O	1:J:268:LEU:HB2	2.18	0.43
1:A:106:THR:HG21	1:F:241:ASN:OD1	2.16	0.43
1:A:123:VAL:O	1:A:127:LEU:HG	2.17	0.43
1:C:201:MET:HG2	1:D:51:PHE:CD1	2.52	0.43
1:D:193:PHE:CB	1:E:189:MET:HE1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:PHE:HD1	1:E:207:PHE:HB2	1.83	0.43
1:G:64:PHE:CD2	1:H:141:ALA:HB2	2.53	0.43
1:A:98:VAL:HG21	1:A:270:VAL:CG2	2.47	0.43
1:A:193:PHE:HB3	1:B:189:MET:HE1	2.00	0.43
1:A:195:MET:C	1:A:198:PRO:HD2	2.44	0.43
1:A:201:MET:HB2	1:B:51:PHE:CE2	2.53	0.43
1:C:256:ILE:CB	1:C:257:PRO:HD3	2.49	0.43
1:D:95:LEU:HD11	1:D:269:LEU:HD12	1.99	0.43
1:D:132:MET:HB2	1:D:219:MET:CE	2.48	0.43
1:E:72:GLY:O	1:E:75:PHE:HB3	2.17	0.43
1:G:129:VAL:HG13	1:G:219:MET:HA	1.98	0.43
1:H:202:PHE:HD1	1:H:207:PHE:HB2	1.82	0.43
1:B:186:ARG:HD3	1:B:186:ARG:HA	1.74	0.43
1:C:154:ASP:O	1:C:155:HIS:C	2.62	0.43
1:E:75:PHE:CD2	1:E:203:VAL:HG21	2.53	0.43
1:F:33:LYS:CD	1:J:280:ARG:HA	2.38	0.43
1:G:171:ALA:O	1:G:175:VAL:HG23	2.18	0.43
1:G:183:TYR:N	1:G:183:TYR:CD2	2.86	0.43
1:J:45:ILE:HD12	1:J:45:ILE:HA	1.77	0.43
1:J:94:VAL:O	1:J:98:VAL:HG13	2.18	0.43
1:B:89:LEU:O	1:B:90:PHE:C	2.61	0.43
1:D:232:TRP:NE1	1:D:239:PRO:HG3	2.34	0.43
1:E:188:LEU:HD12	1:E:188:LEU:HA	1.82	0.43
1:E:275:TRP:CH2	1:E:278:TYR:CD2	3.06	0.43
1:F:80:ILE:HA	1:F:195:MET:HE1	2.00	0.43
1:F:130:LEU:O	1:F:130:LEU:HD12	2.19	0.43
1:G:48:ALA:HB2	1:G:78:GLY:CA	2.42	0.43
1:G:51:PHE:CG	1:G:74:CYS:HB3	2.54	0.43
1:H:46:SER:HB3	1:H:128:PHE:CD2	2.48	0.43
1:H:66:MET:HE1	1:I:59:THR:CG2	2.47	0.43
1:I:132:MET:HB3	1:I:219:MET:CE	2.48	0.43
1:A:132:MET:HE1	1:E:207:PHE:CE1	2.54	0.43
1:B:76:SER:HA	1:B:199:VAL:HG11	2.01	0.43
1:C:96:ILE:HG13	1:C:183:TYR:CD1	2.54	0.43
1:D:95:LEU:HD11	1:D:269:LEU:CD1	2.48	0.43
1:E:171:ALA:HB2	1:E:207:PHE:HB3	2.01	0.43
1:G:84:VAL:CG2	1:G:188:LEU:HD11	2.48	0.43
1:G:109:GLN:HA	1:G:112:LYS:HE3	2.01	0.43
1:H:127:LEU:HD22	1:H:127:LEU:HA	1.53	0.43
1:J:49:PHE:CE2	1:J:212:ALA:HB1	2.54	0.43
1:J:226:PHE:O	1:J:227:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:HG22	1:C:219:MET:HB2	2.01	0.43
1:C:169:ILE:O	1:C:173:LEU:HB2	2.18	0.43
1:H:89:LEU:O	1:H:90:PHE:C	2.61	0.43
1:H:250:PHE:O	1:H:254:ASN:HB3	2.19	0.43
1:I:72:GLY:HA2	1:I:203:VAL:CG1	2.49	0.43
1:A:33:LYS:HE3	1:E:276:VAL:O	2.18	0.43
1:A:69:LEU:HD21	1:B:74:CYS:SG	2.59	0.43
1:D:181:MET:HE3	1:D:194:ILE:CG1	2.40	0.43
1:F:195:MET:C	1:F:198:PRO:HD2	2.43	0.43
1:G:122:LEU:HB2	1:G:214:MET:SD	2.59	0.43
1:H:79:LEU:HD11	1:H:175:VAL:HG13	2.01	0.43
1:I:62:MET:HE2	1:I:62:MET:HB3	1.85	0.43
1:I:195:MET:O	1:I:199:VAL:HG23	2.19	0.43
1:J:96:ILE:O	1:J:99:ALA:HB3	2.19	0.43
1:J:186:ARG:HB2	1:J:187:SER:H	1.61	0.43
1:D:35:PHE:CE1	1:D:119:PHE:CD2	3.07	0.43
1:E:130:LEU:HG	1:E:134:LEU:HD12	2.01	0.43
1:F:65:GLY:HA3	1:G:55:ALA:O	2.19	0.43
1:G:189:MET:HA	1:G:189:MET:HE3	1.99	0.43
1:A:79:LEU:HD12	1:A:79:LEU:HA	1.76	0.43
1:C:164:ALA:HB3	1:C:257:PRO:HB2	2.00	0.43
1:C:189:MET:O	1:C:190:ASP:C	2.62	0.43
1:D:44:PHE:CD2	1:D:82:CYS:HA	2.53	0.43
1:E:129:VAL:HG22	1:E:215:PHE:CD1	2.54	0.43
1:F:46:SER:CB	1:F:128:PHE:CD2	3.01	0.43
1:F:77:LEU:O	1:F:81:LEU:HB2	2.19	0.43
1:G:259:THR:O	1:G:262:ASN:HB2	2.18	0.43
1:H:81:LEU:HD12	1:H:81:LEU:HA	1.79	0.43
1:I:45:ILE:O	1:I:48:ALA:HB3	2.18	0.43
1:A:49:PHE:CD2	1:A:212:ALA:HB1	2.53	0.42
1:A:186:ARG:HD2	1:A:186:ARG:H	1.84	0.42
1:B:80:ILE:O	1:B:84:VAL:HB	2.18	0.42
1:D:41:ALA:HB1	1:D:89:LEU:HB2	2.00	0.42
1:D:147:LEU:HA	1:D:150:LEU:HD12	2.01	0.42
1:E:118:TYR:CE1	1:E:211:ILE:HD11	2.54	0.42
1:E:240:GLU:CD	1:E:240:GLU:N	2.77	0.42
1:F:35:PHE:O	1:F:38:ALA:N	2.52	0.42
1:H:202:PHE:CE2	1:H:203:VAL:HG23	2.54	0.42
1:I:129:VAL:HG21	1:I:218:PRO:HB2	2.01	0.42
1:I:254:ASN:O	1:I:257:PRO:HD2	2.19	0.42
1:C:181:MET:CG	1:D:84:VAL:HG11	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:THR:CA	1:D:96:ILE:HD13	2.50	0.42
1:D:186:ARG:HH12	1:H:230:GLU:CB	2.32	0.42
1:F:83:VAL:HG12	1:F:84:VAL:N	2.34	0.42
1:F:232:TRP:CZ2	1:F:239:PRO:HG3	2.54	0.42
1:G:105:ILE:HG13	1:G:109:GLN:NE2	2.35	0.42
1:G:183:TYR:N	1:G:183:TYR:HD2	2.16	0.42
1:H:269:LEU:HD23	1:H:269:LEU:HA	1.92	0.42
1:I:39:ILE:HA	1:I:120:GLY:O	2.19	0.42
1:J:232:TRP:CE2	1:J:239:PRO:HD3	2.54	0.42
1:A:65:GLY:O	1:A:66:MET:C	2.62	0.42
1:C:62:MET:HE2	1:C:62:MET:HB3	1.82	0.42
1:D:94:VAL:HG12	1:D:176:CYS:SG	2.59	0.42
1:F:33:LYS:HD2	1:J:280:ARG:CA	2.38	0.42
1:F:150:LEU:HD21	1:F:223:ILE:HG22	2.00	0.42
1:G:173:LEU:O	1:G:177:LEU:HG	2.19	0.42
1:H:201:MET:HG2	1:I:51:PHE:CG	2.54	0.42
1:H:201:MET:HA	1:I:51:PHE:CE1	2.55	0.42
1:A:201:MET:HB2	1:B:51:PHE:CD2	2.54	0.42
1:C:79:LEU:HD23	1:C:195:MET:SD	2.60	0.42
1:D:52:TYR:O	1:D:56:THR:HG23	2.20	0.42
1:G:214:MET:O	1:G:218:PRO:HG2	2.19	0.42
1:J:232:TRP:CD2	1:J:239:PRO:HD3	2.54	0.42
1:C:153:ALA:HB1	1:C:217:ILE:HA	1.99	0.42
1:E:49:PHE:O	1:E:52:TYR:HB3	2.20	0.42
1:F:37:LEU:HD23	1:F:37:LEU:HA	1.86	0.42
1:F:94:VAL:CG1	1:F:95:LEU:N	2.81	0.42
1:F:181:MET:HE3	1:F:194:ILE:HG13	2.00	0.42
1:F:195:MET:O	1:F:198:PRO:HD2	2.19	0.42
1:G:102:SER:O	1:G:277:ILE:HG21	2.19	0.42
1:H:223:ILE:O	1:H:227:ALA:HB2	2.20	0.42
1:I:132:MET:HB3	1:I:219:MET:HE1	2.00	0.42
1:I:181:MET:HB2	1:I:181:MET:HE3	1.68	0.42
1:J:62:MET:HE2	1:J:67:ALA:CA	2.50	0.42
1:J:248:MET:O	1:J:252:THR:HG23	2.19	0.42
1:J:274:TYR:CE2	1:J:275:TRP:NE1	2.84	0.42
1:D:202:PHE:CE2	1:D:203:VAL:HG23	2.54	0.42
1:E:30:HIS:HA	1:E:31:PRO:HD3	1.94	0.42
1:E:268:LEU:HD23	1:E:268:LEU:HA	1.86	0.42
1:F:98:VAL:HG23	1:F:110:LEU:HD21	2.01	0.42
1:G:190:ASP:OD1	1:G:190:ASP:N	2.52	0.42
1:G:228:SER:HB2	1:G:229:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:245:LEU:HD23	1:G:245:LEU:HA	1.81	0.42
1:H:91:THR:HB	1:H:172:ASN:HD21	1.84	0.42
1:A:39:ILE:HG12	1:A:120:GLY:O	2.20	0.42
1:A:55:ALA:O	1:E:65:GLY:HA3	2.19	0.42
1:C:122:LEU:HD12	1:C:122:LEU:O	2.20	0.42
1:C:214:MET:O	1:C:218:PRO:HG2	2.19	0.42
1:E:44:PHE:CE1	1:E:81:LEU:HG	2.54	0.42
1:E:166:CYS:O	1:E:170:LEU:HD12	2.20	0.42
1:H:63:PRO:HB3	1:I:59:THR:HG22	2.00	0.42
1:J:84:VAL:CG1	1:J:188:LEU:HD11	2.48	0.42
1:B:246:THR:HB	1:B:248:MET:SD	2.60	0.42
1:E:46:SER:HB3	1:E:128:PHE:CD2	2.42	0.42
1:F:66:MET:HE3	1:G:59:THR:HG22	2.01	0.42
1:G:106:THR:HG23	1:G:109:GLN:HB3	2.01	0.42
1:G:209:HIS:O	1:G:210:SER:C	2.61	0.42
1:H:83:VAL:C	1:H:85:CYS:H	2.28	0.42
1:H:201:MET:C	1:H:201:MET:SD	3.02	0.42
1:I:167:LEU:HD23	1:I:167:LEU:HA	1.70	0.42
1:D:195:MET:O	1:D:199:VAL:HG23	2.19	0.42
1:D:201:MET:HG2	1:E:51:PHE:CD1	2.55	0.42
1:E:178:ALA:O	1:E:195:MET:HG2	2.20	0.42
1:G:187:SER:HB3	1:G:189:MET:HB2	2.02	0.42
1:H:56:THR:HA	1:H:59:THR:HG21	2.02	0.42
1:H:112:LYS:C	1:H:114:TRP:H	2.28	0.42
1:J:32:LEU:HD23	1:J:32:LEU:C	2.43	0.42
1:C:165:VAL:O	1:C:169:ILE:HD12	2.20	0.41
1:C:197:LEU:HB2	1:C:198:PRO:HD3	2.02	0.41
1:D:80:ILE:HA	1:D:195:MET:HE1	2.01	0.41
1:D:214:MET:O	1:D:218:PRO:HG2	2.20	0.41
1:E:106:THR:HG22	1:E:109:GLN:HB3	2.01	0.41
1:F:230:GLU:CD	1:F:230:GLU:H	2.27	0.41
1:G:48:ALA:HB1	1:G:75:PHE:O	2.20	0.41
1:G:202:PHE:HA	1:G:207:PHE:HD2	1.81	0.41
1:H:183:TYR:C	1:H:185:GLY:N	2.78	0.41
1:H:231:PHE:CZ	1:H:235:VAL:HG11	2.55	0.41
1:H:279:LEU:CD1	1:I:36:TYR:HE2	2.33	0.41
1:I:147:LEU:HB2	1:I:235:VAL:HG11	2.02	0.41
1:B:211:ILE:O	1:B:214:MET:HB2	2.20	0.41
1:D:256:ILE:HB	1:D:257:PRO:HD3	2.02	0.41
1:F:30:HIS:CB	1:J:279:LEU:HD22	2.50	0.41
1:F:137:GLU:O	1:F:140:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:LYS:O	1:H:37:LEU:HG	2.20	0.41
1:J:112:LYS:O	1:J:116:ASN:HB2	2.20	0.41
1:A:194:ILE:HD12	1:A:194:ILE:HA	1.95	0.41
1:A:237:SER:OG	1:A:241:ASN:ND2	2.50	0.41
1:B:63:PRO:HG2	1:C:62:MET:HG3	2.02	0.41
1:E:246:THR:O	1:E:249:ASN:HB2	2.20	0.41
1:E:259:THR:O	1:E:262:ASN:HB2	2.20	0.41
1:F:135:SER:HB2	1:J:167:LEU:HD23	2.02	0.41
1:H:181:MET:HE2	1:I:81:LEU:HD13	2.02	0.41
1:H:208:GLU:HB3	1:H:258:VAL:CG2	2.50	0.41
1:I:192:ALA:C	1:I:194:ILE:H	2.29	0.41
1:I:268:LEU:O	1:I:272:LEU:CD1	2.57	0.41
1:A:80:ILE:HA	1:A:195:MET:HE1	2.02	0.41
1:C:158:HIS:CE1	1:C:244:HIS:CD2	3.08	0.41
1:D:90:PHE:C	1:D:92:SER:H	2.28	0.41
1:E:179:VAL:CG1	1:E:183:TYR:HE2	2.32	0.41
1:E:210:SER:O	1:E:214:MET:HG3	2.20	0.41
1:G:230:GLU:H	1:G:230:GLU:HG3	1.66	0.41
1:H:165:VAL:O	1:H:261:GLY:HA3	2.20	0.41
1:I:227:ALA:HB1	1:I:231:PHE:CD2	2.55	0.41
1:J:202:PHE:CD1	1:J:202:PHE:C	2.97	0.41
1:J:277:ILE:O	1:J:277:ILE:CG2	2.67	0.41
1:A:276:VAL:HG12	1:A:276:VAL:O	2.20	0.41
1:B:159:HIS:HB3	1:B:164:ALA:HB2	2.02	0.41
1:B:276:VAL:HG13	1:C:33:LYS:NZ	2.35	0.41
1:D:32:LEU:HA	1:D:32:LEU:HD12	1.85	0.41
1:D:181:MET:SD	1:E:81:LEU:HD12	2.61	0.41
1:D:236:GLY:O	1:D:237:SER:HB2	2.21	0.41
1:I:38:ALA:O	1:I:121:ASN:HA	2.21	0.41
1:C:140:THR:O	1:C:145:TRP:CB	2.54	0.41
1:D:51:PHE:CD2	1:D:74:CYS:HB3	2.56	0.41
1:D:167:LEU:CD2	1:E:135:SER:HB2	2.50	0.41
1:E:45:ILE:O	1:E:48:ALA:HB3	2.21	0.41
1:E:195:MET:C	1:E:198:PRO:HD2	2.45	0.41
1:E:197:LEU:HD12	1:E:197:LEU:HA	1.75	0.41
1:F:31:PRO:O	1:F:35:PHE:HB2	2.20	0.41
1:F:75:PHE:CG	1:F:203:VAL:HG21	2.56	0.41
1:F:123:VAL:HG12	1:F:127:LEU:HD12	2.02	0.41
1:G:155:HIS:ND1	1:G:155:HIS:O	2.53	0.41
1:G:240:GLU:H	1:G:240:GLU:CD	2.28	0.41
1:H:165:VAL:HA	1:H:257:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:197:LEU:HD12	1:I:197:LEU:HA	1.83	0.41
1:I:223:ILE:O	1:I:227:ALA:HB2	2.21	0.41
1:A:279:LEU:HD13	1:B:30:HIS:CE1	2.56	0.41
1:B:44:PHE:HD2	1:B:82:CYS:HA	1.84	0.41
1:E:223:ILE:O	1:E:227:ALA:CB	2.69	0.41
1:F:91:THR:HG22	1:F:114:TRP:CZ2	2.56	0.41
1:G:150:LEU:HD11	1:G:231:PHE:HE2	1.85	0.41
1:A:33:LYS:HB2	1:E:279:LEU:HB3	2.03	0.41
1:A:264:ILE:O	1:A:268:LEU:HG	2.20	0.41
1:G:45:ILE:HD12	1:G:45:ILE:HA	1.91	0.41
1:H:30:HIS:CE1	1:H:32:LEU:CB	3.03	0.41
1:H:64:PHE:HD2	1:I:57:THR:CG2	2.33	0.41
1:H:101:ALA:O	1:H:104:ARG:HB2	2.21	0.41
1:H:168:GLY:O	1:H:262:ASN:ND2	2.51	0.41
1:I:53:ILE:CG2	1:I:145:TRP:CE2	3.04	0.41
1:J:126:LEU:HD23	1:J:126:LEU:HA	1.87	0.41
1:A:89:LEU:O	1:A:90:PHE:C	2.64	0.41
1:A:189:MET:CG	1:B:189:MET:HG2	2.50	0.41
1:A:227:ALA:HB1	1:A:231:PHE:CD2	2.56	0.41
1:B:77:LEU:HD22	1:B:81:LEU:HD22	2.03	0.41
1:C:64:PHE:HB3	1:D:57:THR:HG22	2.03	0.41
1:C:90:PHE:CE1	1:C:118:TYR:HD1	2.39	0.41
1:E:44:PHE:CG	1:E:81:LEU:HB3	2.56	0.41
1:E:50:VAL:HG22	1:E:132:MET:HE2	2.01	0.41
1:E:151:GLN:HE21	1:E:151:GLN:HB2	1.67	0.41
1:F:89:LEU:O	1:F:90:PHE:C	2.64	0.41
1:F:154:ASP:O	1:F:155:HIS:C	2.64	0.41
1:G:232:TRP:CZ2	1:G:239:PRO:HG3	2.56	0.41
1:H:30:HIS:ND1	1:H:30:HIS:C	2.79	0.41
1:I:46:SER:HB3	1:I:128:PHE:CD2	2.56	0.41
1:I:93:THR:O	1:I:94:VAL:C	2.63	0.41
1:I:97:VAL:O	1:I:97:VAL:HG12	2.20	0.41
1:I:277:ILE:HG23	1:I:277:ILE:O	2.21	0.41
1:A:62:MET:HE2	1:A:62:MET:HB3	1.82	0.41
1:B:96:ILE:HD12	1:B:180:TRP:HE3	1.85	0.41
1:G:80:ILE:HA	1:G:195:MET:HE1	2.03	0.41
1:H:158:HIS:NE2	1:H:244:HIS:CG	2.88	0.41
1:I:261:GLY:HA2	1:I:264:ILE:HD12	2.02	0.41
1:J:107:TRP:O	1:J:108:GLY:C	2.64	0.41
1:D:132:MET:HB2	1:D:219:MET:HE1	2.03	0.40
1:D:232:TRP:HB3	1:D:237:SER:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ALA:O	1:E:175:VAL:HG23	2.20	0.40
1:F:81:LEU:HD11	1:J:177:LEU:HB3	2.02	0.40
1:G:130:LEU:HG	1:G:134:LEU:CD1	2.50	0.40
1:G:202:PHE:HB2	1:G:207:PHE:HD2	1.86	0.40
1:H:102:SER:C	1:H:104:ARG:N	2.79	0.40
1:I:189:MET:O	1:I:190:ASP:C	2.64	0.40
1:J:209:HIS:HE1	1:J:211:ILE:HB	1.86	0.40
1:A:51:PHE:CD2	1:A:74:CYS:HB3	2.56	0.40
1:B:153:ALA:HB1	1:B:217:ILE:HA	2.03	0.40
1:C:95:LEU:HD11	1:C:269:LEU:HD22	2.03	0.40
1:F:138:TYR:O	1:F:143:GLY:HA2	2.21	0.40
1:F:228:SER:O	1:F:231:PHE:HB3	2.20	0.40
1:H:217:ILE:HG21	1:H:250:PHE:CD1	2.56	0.40
1:I:148:ASN:O	1:I:152:THR:OG1	2.35	0.40
1:B:101:ALA:CB	1:B:105:ILE:HB	2.43	0.40
1:C:30:HIS:ND1	1:C:31:PRO:HD2	2.36	0.40
1:F:106:THR:HG22	1:F:109:GLN:HG3	2.04	0.40
1:G:130:LEU:O	1:G:134:LEU:HD12	2.21	0.40
1:H:101:ALA:O	1:H:104:ARG:CB	2.69	0.40
1:I:45:ILE:HG21	1:I:211:ILE:HG22	2.04	0.40
1:I:169:ILE:HG12	1:I:264:ILE:HB	2.02	0.40
1:J:60:GLY:C	1:J:62:MET:H	2.29	0.40
1:J:211:ILE:O	1:J:214:MET:HB2	2.21	0.40
1:A:98:VAL:CG1	1:A:273:THR:HG21	2.44	0.40
1:A:202:PHE:HB2	1:A:207:PHE:HD2	1.86	0.40
1:A:230:GLU:CD	1:A:230:GLU:N	2.78	0.40
1:B:160:THR:HG23	1:B:163:GLU:CD	2.47	0.40
1:D:273:THR:O	1:D:274:TYR:C	2.63	0.40
1:E:138:TYR:HA	1:E:145:TRP:HE3	1.86	0.40
1:E:168:GLY:HA2	1:E:208:GLU:O	2.22	0.40
1:G:274:TYR:O	1:G:278:TYR:CB	2.69	0.40
1:H:97:VAL:CG1	1:H:110:LEU:HG	2.50	0.40
1:I:94:VAL:HG21	1:I:266:GLY:HA3	2.03	0.40
1:J:114:TRP:HZ3	1:J:263:ILE:HG23	1.87	0.40
1:J:201:MET:O	1:J:205:SER:HB2	2.21	0.40
1:J:250:PHE:O	1:J:254:ASN:HB3	2.22	0.40
1:A:83:VAL:C	1:A:85:CYS:H	2.30	0.40
1:A:94:VAL:HG13	1:A:95:LEU:N	2.36	0.40
1:A:190:ASP:HB3	1:B:188:LEU:CB	2.40	0.40
1:D:89:LEU:O	1:D:90:PHE:C	2.64	0.40
1:E:232:TRP:CZ2	1:E:239:PRO:HD3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:ASN:O	1:E:257:PRO:HD2	2.21	0.40
1:F:53:ILE:HG22	1:F:145:TRP:CE2	2.57	0.40
1:G:56:THR:O	1:G:59:THR:HG23	2.21	0.40
1:I:66:MET:HE3	1:J:62:MET:CE	2.52	0.40
1:I:254:ASN:ND2	1:I:254:ASN:C	2.77	0.40
1:I:256:ILE:HB	1:I:257:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/285 (87%)	230 (93%)	15 (6%)	3 (1%)	10	42
1	B	248/285 (87%)	217 (88%)	26 (10%)	5 (2%)	6	31
1	C	248/285 (87%)	220 (89%)	23 (9%)	5 (2%)	6	31
1	D	249/285 (87%)	224 (90%)	20 (8%)	5 (2%)	6	31
1	E	250/285 (88%)	220 (88%)	23 (9%)	7 (3%)	4	25
1	F	250/285 (88%)	234 (94%)	12 (5%)	4 (2%)	7	36
1	G	250/285 (88%)	222 (89%)	25 (10%)	3 (1%)	10	42
1	H	250/285 (88%)	225 (90%)	19 (8%)	6 (2%)	4	28
1	I	250/285 (88%)	218 (87%)	28 (11%)	4 (2%)	7	36
1	J	245/285 (86%)	219 (89%)	22 (9%)	4 (2%)	7	36
All	All	2488/2850 (87%)	2229 (90%)	213 (9%)	46 (2%)	6	34

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	186	ARG

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Mol	Chain	Res	Type
1	G	113	ASN
1	I	95	LEU
1	I	101	ALA
1	J	94	VAL
1	J	268	LEU
1	A	101	ALA
1	B	86	GLY
1	C	155	HIS
1	C	276	VAL
1	D	113	ASN
1	E	61	THR
1	G	112	LYS
1	G	186	ARG
1	H	112	LYS
1	H	184	SER
1	I	104	ARG
1	B	193	PHE
1	E	186	ARG
1	F	104	ARG
1	H	90	PHE
1	B	112	LYS
1	C	90	PHE
1	E	105	ILE
1	E	107	TRP
1	E	184	SER
1	F	90	PHE
1	J	186	ARG
1	A	84	VAL
1	A	90	PHE
1	C	183	TYR
1	C	189	MET
1	D	91	THR
1	D	279	LEU
1	E	104	ARG
1	H	113	ASN
1	I	105	ILE
1	B	221	ILE
1	D	136	GLY
1	F	105	ILE
1	B	236	GLY
1	H	162	ILE
1	E	31	PRO

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Mol	Chain	Res	Type
1	D	83	VAL
1	J	277	ILE
1	H	84	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/230 (88%)	174 (86%)	29 (14%)	3	16
1	B	203/230 (88%)	176 (87%)	27 (13%)	4	19
1	C	203/230 (88%)	171 (84%)	32 (16%)	2	13
1	D	203/230 (88%)	180 (89%)	23 (11%)	5	24
1	E	203/230 (88%)	180 (89%)	23 (11%)	5	24
1	F	203/230 (88%)	180 (89%)	23 (11%)	5	24
1	G	203/230 (88%)	177 (87%)	26 (13%)	4	20
1	H	203/230 (88%)	177 (87%)	26 (13%)	4	20
1	I	203/230 (88%)	177 (87%)	26 (13%)	4	20
1	J	202/230 (88%)	178 (88%)	24 (12%)	5	23
All	All	2029/2300 (88%)	1770 (87%)	259 (13%)	4	20

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	33	LYS
1	A	45	ILE
1	A	49	PHE
1	A	61	THR
1	A	66	MET
1	A	77	LEU
1	A	81	LEU
1	A	82	CYS
1	A	83	VAL

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Mol	Chain	Res	Type
1	A	93	THR
1	A	98	VAL
1	A	130	LEU
1	A	132	MET
1	A	138	TYR
1	A	140	THR
1	A	157	VAL
1	A	160	THR
1	A	188	LEU
1	A	189	MET
1	A	191	LYS
1	A	202	PHE
1	A	222	VAL
1	A	224	ARG
1	A	260	ILE
1	A	270	VAL
1	A	273	THR
1	A	276	VAL
1	A	279	LEU
1	B	45	ILE
1	B	47	ILE
1	B	49	PHE
1	B	61	THR
1	B	77	LEU
1	B	82	CYS
1	B	84	VAL
1	B	94	VAL
1	B	113	ASN
1	B	115	LEU
1	B	132	MET
1	B	142	ASN
1	B	160	THR
1	B	181	MET
1	B	182	SER
1	B	183	TYR
1	B	184	SER
1	B	188	LEU
1	B	189	MET
1	B	196	VAL
1	B	241	ASN
1	B	243	SER
1	B	244	HIS

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Mol	Chain	Res	Type
1	B	246	THR
1	B	270	VAL
1	B	275	TRP
1	B	277	ILE
1	C	34	THR
1	C	45	ILE
1	C	46	SER
1	C	49	PHE
1	C	59	THR
1	C	61	THR
1	C	66	MET
1	C	77	LEU
1	C	81	LEU
1	C	93	THR
1	C	94	VAL
1	C	96	ILE
1	C	97	VAL
1	C	104	ARG
1	C	106	THR
1	C	113	ASN
1	C	169	ILE
1	C	173	LEU
1	C	177	LEU
1	C	183	TYR
1	C	188	LEU
1	C	189	MET
1	C	197	LEU
1	C	202	PHE
1	C	210	SER
1	C	233	THR
1	C	235	VAL
1	C	247	VAL
1	C	255	LEU
1	C	256	ILE
1	C	274	TYR
1	C	277	ILE
1	D	45	ILE
1	D	47	ILE
1	D	49	PHE
1	D	57	THR
1	D	77	LEU
1	D	79	LEU

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Mol	Chain	Res	Type
1	D	81	LEU
1	D	84	VAL
1	D	96	ILE
1	D	106	THR
1	D	113	ASN
1	D	138	TYR
1	D	142	ASN
1	D	152	THR
1	D	157	VAL
1	D	202	PHE
1	D	237	SER
1	D	243	SER
1	D	244	HIS
1	D	248	MET
1	D	256	ILE
1	D	268	LEU
1	D	269	LEU
1	E	39	ILE
1	E	49	PHE
1	E	53	ILE
1	E	61	THR
1	E	66	MET
1	E	77	LEU
1	E	81	LEU
1	E	93	THR
1	E	97	VAL
1	E	127	LEU
1	E	160	THR
1	E	173	LEU
1	E	179	VAL
1	E	184	SER
1	E	186	ARG
1	E	187	SER
1	E	197	LEU
1	E	202	PHE
1	E	203	VAL
1	E	235	VAL
1	E	259	THR
1	E	273	THR
1	E	276	VAL
1	F	32	LEU
1	F	45	ILE

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Mol	Chain	Res	Type
1	F	49	PHE
1	F	53	ILE
1	F	77	LEU
1	F	79	LEU
1	F	93	THR
1	F	94	VAL
1	F	107	TRP
1	F	113	ASN
1	F	130	LEU
1	F	138	TYR
1	F	140	THR
1	F	165	VAL
1	F	186	ARG
1	F	187	SER
1	F	196	VAL
1	F	197	LEU
1	F	240	GLU
1	F	243	SER
1	F	246	THR
1	F	274	TYR
1	F	277	ILE
1	G	30	HIS
1	G	36	TYR
1	G	39	ILE
1	G	45	ILE
1	G	49	PHE
1	G	77	LEU
1	G	81	LEU
1	G	83	VAL
1	G	105	ILE
1	G	107	TRP
1	G	134	LEU
1	G	154	ASP
1	G	155	HIS
1	G	179	VAL
1	G	186	ARG
1	G	188	LEU
1	G	189	MET
1	G	190	ASP
1	G	197	LEU
1	G	199	VAL
1	G	202	PHE

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Mol	Chain	Res	Type
1	G	233	THR
1	G	246	THR
1	G	256	ILE
1	G	259	THR
1	G	272	LEU
1	H	39	ILE
1	H	45	ILE
1	H	49	PHE
1	H	54	THR
1	H	61	THR
1	H	77	LEU
1	H	79	LEU
1	H	81	LEU
1	H	91	THR
1	H	100	LYS
1	H	127	LEU
1	H	130	LEU
1	H	140	THR
1	H	142	ASN
1	H	152	THR
1	H	157	VAL
1	H	159	HIS
1	H	160	THR
1	H	173	LEU
1	H	177	LEU
1	H	184	SER
1	H	197	LEU
1	H	237	SER
1	H	247	VAL
1	H	276	VAL
1	H	277	ILE
1	I	34	THR
1	I	45	ILE
1	I	49	PHE
1	I	57	THR
1	I	61	THR
1	I	66	MET
1	I	77	LEU
1	I	81	LEU
1	I	96	ILE
1	I	100	LYS
1	I	105	ILE

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Mol	Chain	Res	Type
1	I	123	VAL
1	I	129	VAL
1	I	138	TYR
1	I	152	THR
1	I	160	THR
1	I	179	VAL
1	I	197	LEU
1	I	203	VAL
1	I	248	MET
1	I	258	VAL
1	I	268	LEU
1	I	273	THR
1	I	276	VAL
1	I	277	ILE
1	I	278	TYR
1	J	45	ILE
1	J	49	PHE
1	J	66	MET
1	J	83	VAL
1	J	95	LEU
1	J	97	VAL
1	J	100	LYS
1	J	105	ILE
1	J	140	THR
1	J	160	THR
1	J	162	ILE
1	J	173	LEU
1	J	186	ARG
1	J	193	PHE
1	J	197	LEU
1	J	202	PHE
1	J	203	VAL
1	J	230	GLU
1	J	233	THR
1	J	247	VAL
1	J	269	LEU
1	J	273	THR
1	J	276	VAL
1	J	278	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	109	GLN
1	A	142	ASN
1	A	144	GLN
1	A	158	HIS
1	A	241	ASN
1	B	113	ASN
1	B	116	ASN
1	B	142	ASN
1	B	144	GLN
1	B	151	GLN
1	B	249	ASN
1	C	142	ASN
1	C	144	GLN
1	C	155	HIS
1	C	158	HIS
1	C	159	HIS
1	C	244	HIS
1	C	254	ASN
1	D	142	ASN
1	D	151	GLN
1	D	172	ASN
1	D	213	ASN
1	D	244	HIS
1	E	142	ASN
1	E	144	GLN
1	E	151	GLN
1	E	249	ASN
1	F	142	ASN
1	F	148	ASN
1	F	155	HIS
1	F	159	HIS
1	F	209	HIS
1	F	213	ASN
1	F	249	ASN
1	F	254	ASN
1	G	113	ASN
1	G	158	HIS
1	G	209	HIS
1	G	213	ASN
1	G	241	ASN
1	G	244	HIS
1	G	254	ASN

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Mol	Chain	Res	Type
1	H	113	ASN
1	H	116	ASN
1	H	151	GLN
1	H	172	ASN
1	H	209	HIS
1	H	241	ASN
1	I	142	ASN
1	I	158	HIS
1	I	244	HIS
1	J	30	HIS
1	J	142	ASN
1	J	148	ASN
1	J	151	GLN
1	J	213	ASN
1	J	244	HIS

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 oligosaccharides 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	250/285 (87%)	-0.09	3 (1%) 76 58	54, 78, 115, 178	0
1	B	250/285 (87%)	-0.01	7 (2%) 55 35	57, 88, 164, 301	0
1	C	250/285 (87%)	0.04	8 (3%) 50 31	64, 98, 183, 259	0
1	D	251/285 (88%)	-0.02	8 (3%) 50 31	61, 91, 182, 314	0
1	E	252/285 (88%)	0.15	14 (5%) 30 19	44, 83, 175, 306	0
1	F	252/285 (88%)	-0.04	7 (2%) 55 35	47, 79, 135, 210	0
1	G	252/285 (88%)	0.05	10 (3%) 42 26	53, 84, 184, 236	0
1	H	252/285 (88%)	0.07	9 (3%) 46 28	59, 90, 192, 316	0
1	I	252/285 (88%)	0.02	10 (3%) 42 26	52, 85, 125, 224	0
1	J	249/285 (87%)	-0.10	5 (2%) 65 45	53, 84, 137, 223	0
All	All	2510/2850 (88%)	0.01	81 (3%) 50 31	44, 86, 166, 316	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	36	TYR	6.7
1	G	88	ASP	5.6
1	C	141	ALA	5.2
1	F	279	LEU	4.9
1	H	114	TRP	4.9
1	H	84	VAL	4.2
1	C	185	GLY	3.9
1	I	275	TRP	3.9
1	G	32	LEU	3.9
1	E	253	ASP	3.8
1	H	83	VAL	3.7
1	I	180	TRP	3.6
1	E	95	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	102	SER	3.5
1	B	86	GLY	3.5
1	B	252	THR	3.5
1	I	269	LEU	3.4
1	E	36	TYR	3.4
1	I	270	VAL	3.3
1	C	144	GLN	3.3
1	E	98	VAL	3.3
1	C	142	ASN	3.2
1	G	86	GLY	3.2
1	G	37	LEU	3.1
1	C	186	ARG	3.1
1	E	252	THR	3.0
1	B	82	CYS	2.9
1	B	87	ALA	2.9
1	G	87	ALA	2.8
1	E	94	VAL	2.8
1	I	94	VAL	2.8
1	A	64	PHE	2.8
1	C	143	GLY	2.8
1	D	155	HIS	2.8
1	F	276	VAL	2.8
1	G	93	THR	2.7
1	J	273	THR	2.7
1	I	273	THR	2.6
1	B	110	LEU	2.6
1	E	155	HIS	2.6
1	J	162	ILE	2.6
1	F	79	LEU	2.6
1	H	85	CYS	2.5
1	D	151	GLN	2.5
1	H	191	LYS	2.5
1	E	61	THR	2.5
1	H	119	PHE	2.4
1	E	249	ASN	2.4
1	C	113	ASN	2.4
1	E	245	LEU	2.4
1	D	185	GLY	2.4
1	I	100	LYS	2.4
1	B	140	THR	2.3
1	J	84	VAL	2.3
1	F	275	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	110	LEU	2.3
1	G	33	LYS	2.3
1	E	99	ALA	2.3
1	E	97	VAL	2.3
1	D	273	THR	2.2
1	D	205	SER	2.2
1	H	88	ASP	2.2
1	I	245	LEU	2.2
1	I	253	ASP	2.2
1	H	111	ALA	2.2
1	E	193	PHE	2.2
1	E	183	TYR	2.2
1	F	278	TYR	2.2
1	A	277	ILE	2.2
1	G	193	PHE	2.1
1	J	104	ARG	2.1
1	D	156	LYS	2.1
1	B	111	ALA	2.1
1	D	99	ALA	2.1
1	A	172	ASN	2.1
1	F	187	SER	2.0
1	I	114	TRP	2.0
1	J	253	ASP	2.0
1	G	85	CYS	2.0
1	C	193	PHE	2.0
1	F	193	PHE	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.