



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:07 PM UTC

PDB ID : 7ZQ7 / pdb_00007zq7
Title : Structure of RpF-1
Authors : Sanchez-Alba, L.; Reverter, D.; Conchillo, O.; Yero, D.; Daura, X.; Gibert, I.
Deposited on : 2022-04-29
Resolution : 3.00 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

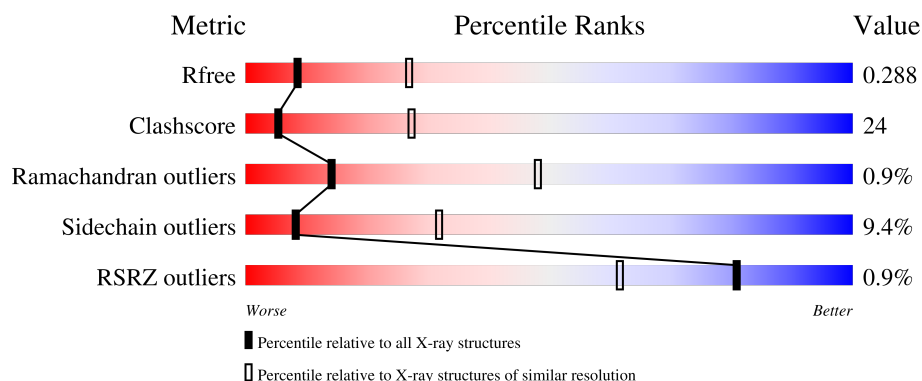
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	305	
1	B	305	
1	C	305	
1	D	305	
1	E	305	

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Mol	Chain	Length	Quality of chain
1	F	305	2% 38% 42% 7% 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12431 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 Crotonase/enoyl-CoA hydratase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2076	1306	375	379	16			
1	D	267	Total	C	N	O	S	0	0	0
			2075	1306	374	379	16			
1	C	267	Total	C	N	O	S	0	0	0
			2075	1306	374	379	16			
1	B	267	Total	C	N	O	S	0	0	0
			2075	1306	374	379	16			
1	E	264	Total	C	N	O	S	0	0	0
			2055	1294	370	375	16			
1	F	267	Total	C	N	O	S	0	0	0
			2075	1306	374	379	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q19VG8
A	-14	GLY	-	expression tag	UNP Q19VG8
A	-13	SER	-	expression tag	UNP Q19VG8
A	-12	SER	-	expression tag	UNP Q19VG8
A	-11	HIS	-	expression tag	UNP Q19VG8
A	-10	HIS	-	expression tag	UNP Q19VG8
A	-9	HIS	-	expression tag	UNP Q19VG8
A	-8	HIS	-	expression tag	UNP Q19VG8
A	-7	HIS	-	expression tag	UNP Q19VG8
A	-6	HIS	-	expression tag	UNP Q19VG8
A	-5	SER	-	expression tag	UNP Q19VG8
A	-4	GLN	-	expression tag	UNP Q19VG8
A	-3	ASP	-	expression tag	UNP Q19VG8
A	-2	PRO	-	expression tag	UNP Q19VG8
A	-1	ASN	-	expression tag	UNP Q19VG8
A	0	SER	-	expression tag	UNP Q19VG8
D	-15	MET	-	initiating methionine	UNP Q19VG8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	GLY	-	expression tag	UNP Q19VG8
D	-13	SER	-	expression tag	UNP Q19VG8
D	-12	SER	-	expression tag	UNP Q19VG8
D	-11	HIS	-	expression tag	UNP Q19VG8
D	-10	HIS	-	expression tag	UNP Q19VG8
D	-9	HIS	-	expression tag	UNP Q19VG8
D	-8	HIS	-	expression tag	UNP Q19VG8
D	-7	HIS	-	expression tag	UNP Q19VG8
D	-6	HIS	-	expression tag	UNP Q19VG8
D	-5	SER	-	expression tag	UNP Q19VG8
D	-4	GLN	-	expression tag	UNP Q19VG8
D	-3	ASP	-	expression tag	UNP Q19VG8
D	-2	PRO	-	expression tag	UNP Q19VG8
D	-1	ASN	-	expression tag	UNP Q19VG8
D	0	SER	-	expression tag	UNP Q19VG8
C	-15	MET	-	initiating methionine	UNP Q19VG8
C	-14	GLY	-	expression tag	UNP Q19VG8
C	-13	SER	-	expression tag	UNP Q19VG8
C	-12	SER	-	expression tag	UNP Q19VG8
C	-11	HIS	-	expression tag	UNP Q19VG8
C	-10	HIS	-	expression tag	UNP Q19VG8
C	-9	HIS	-	expression tag	UNP Q19VG8
C	-8	HIS	-	expression tag	UNP Q19VG8
C	-7	HIS	-	expression tag	UNP Q19VG8
C	-6	HIS	-	expression tag	UNP Q19VG8
C	-5	SER	-	expression tag	UNP Q19VG8
C	-4	GLN	-	expression tag	UNP Q19VG8
C	-3	ASP	-	expression tag	UNP Q19VG8
C	-2	PRO	-	expression tag	UNP Q19VG8
C	-1	ASN	-	expression tag	UNP Q19VG8
C	0	SER	-	expression tag	UNP Q19VG8
B	-15	MET	-	initiating methionine	UNP Q19VG8
B	-14	GLY	-	expression tag	UNP Q19VG8
B	-13	SER	-	expression tag	UNP Q19VG8
B	-12	SER	-	expression tag	UNP Q19VG8
B	-11	HIS	-	expression tag	UNP Q19VG8
B	-10	HIS	-	expression tag	UNP Q19VG8
B	-9	HIS	-	expression tag	UNP Q19VG8
B	-8	HIS	-	expression tag	UNP Q19VG8
B	-7	HIS	-	expression tag	UNP Q19VG8
B	-6	HIS	-	expression tag	UNP Q19VG8
B	-5	SER	-	expression tag	UNP Q19VG8

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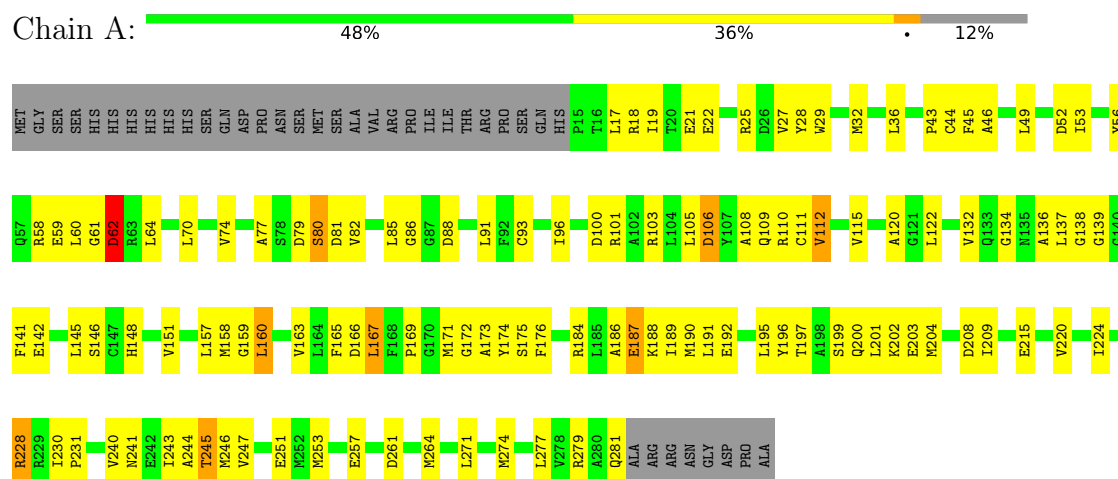
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLN	-	expression tag	UNP Q19VG8
B	-3	ASP	-	expression tag	UNP Q19VG8
B	-2	PRO	-	expression tag	UNP Q19VG8
B	-1	ASN	-	expression tag	UNP Q19VG8
B	0	SER	-	expression tag	UNP Q19VG8
E	-15	MET	-	initiating methionine	UNP Q19VG8
E	-14	GLY	-	expression tag	UNP Q19VG8
E	-13	SER	-	expression tag	UNP Q19VG8
E	-12	SER	-	expression tag	UNP Q19VG8
E	-11	HIS	-	expression tag	UNP Q19VG8
E	-10	HIS	-	expression tag	UNP Q19VG8
E	-9	HIS	-	expression tag	UNP Q19VG8
E	-8	HIS	-	expression tag	UNP Q19VG8
E	-7	HIS	-	expression tag	UNP Q19VG8
E	-6	HIS	-	expression tag	UNP Q19VG8
E	-5	SER	-	expression tag	UNP Q19VG8
E	-4	GLN	-	expression tag	UNP Q19VG8
E	-3	ASP	-	expression tag	UNP Q19VG8
E	-2	PRO	-	expression tag	UNP Q19VG8
E	-1	ASN	-	expression tag	UNP Q19VG8
E	0	SER	-	expression tag	UNP Q19VG8
F	-15	MET	-	initiating methionine	UNP Q19VG8
F	-14	GLY	-	expression tag	UNP Q19VG8
F	-13	SER	-	expression tag	UNP Q19VG8
F	-12	SER	-	expression tag	UNP Q19VG8
F	-11	HIS	-	expression tag	UNP Q19VG8
F	-10	HIS	-	expression tag	UNP Q19VG8
F	-9	HIS	-	expression tag	UNP Q19VG8
F	-8	HIS	-	expression tag	UNP Q19VG8
F	-7	HIS	-	expression tag	UNP Q19VG8
F	-6	HIS	-	expression tag	UNP Q19VG8
F	-5	SER	-	expression tag	UNP Q19VG8
F	-4	GLN	-	expression tag	UNP Q19VG8
F	-3	ASP	-	expression tag	UNP Q19VG8
F	-2	PRO	-	expression tag	UNP Q19VG8
F	-1	ASN	-	expression tag	UNP Q19VG8
F	0	SER	-	expression tag	UNP Q19VG8

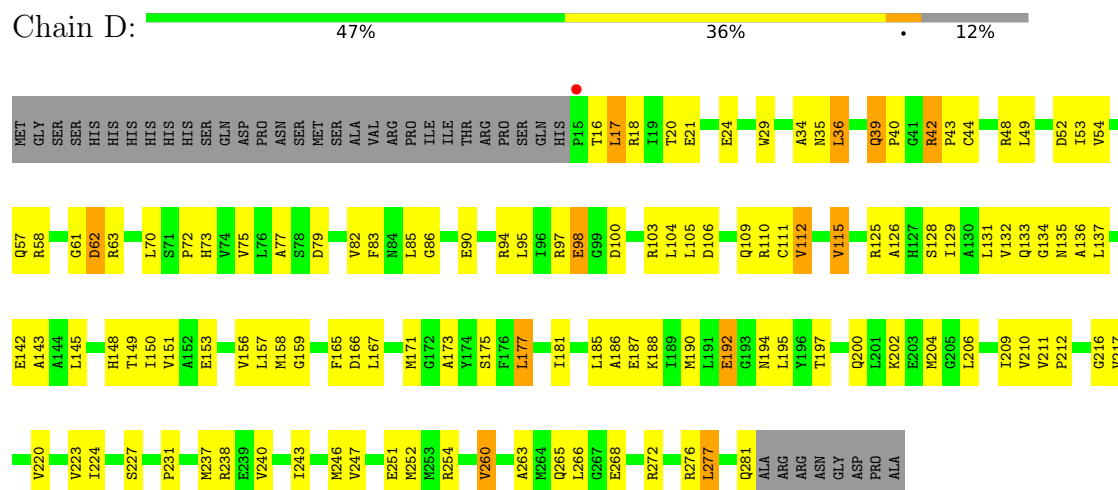
3 Residue-property plots

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: Crotonase/enoyl-CoA hydratase family protein

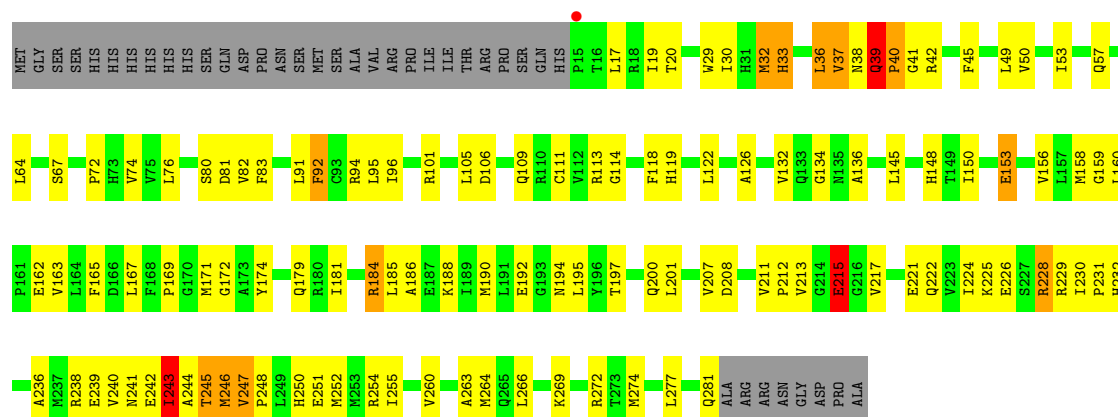


- Molecule 1: Crotonase/enoyl-CoA hydratase family protein

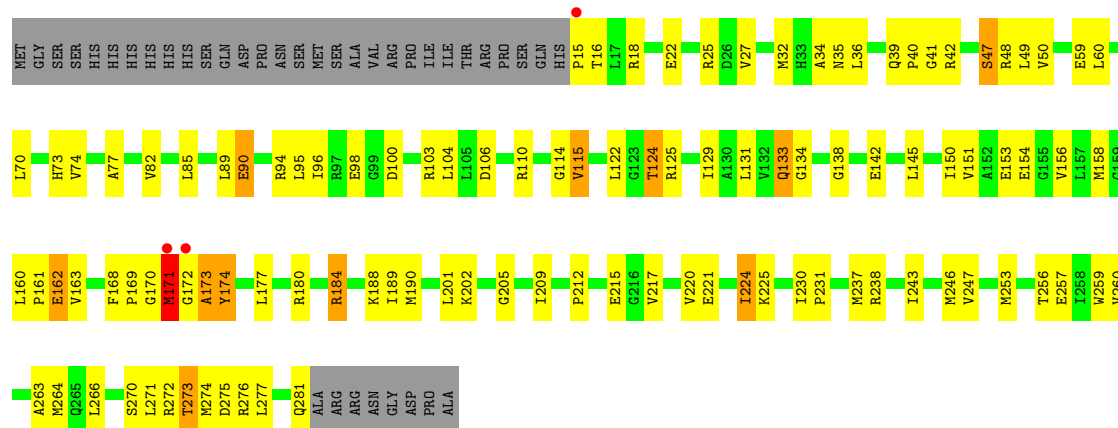


- Molecule 1: Crotonase/enoyl-CoA hydratase family protein

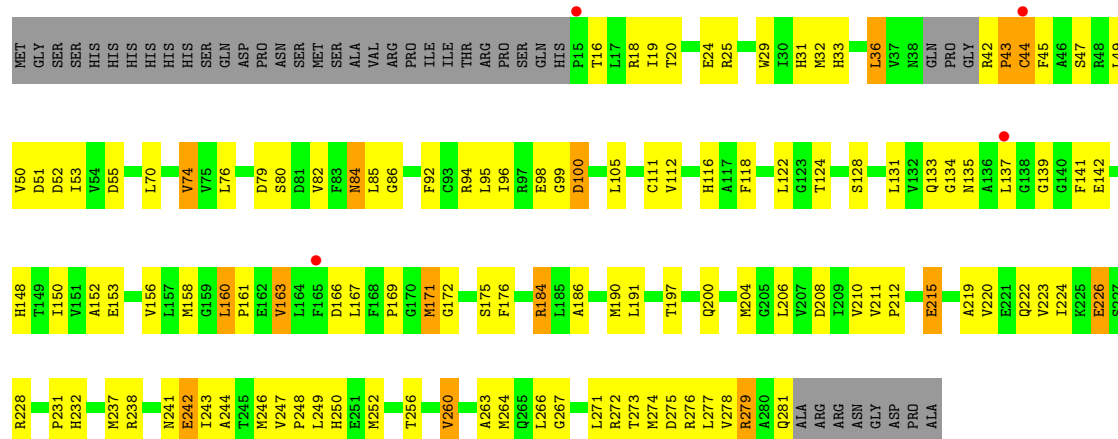




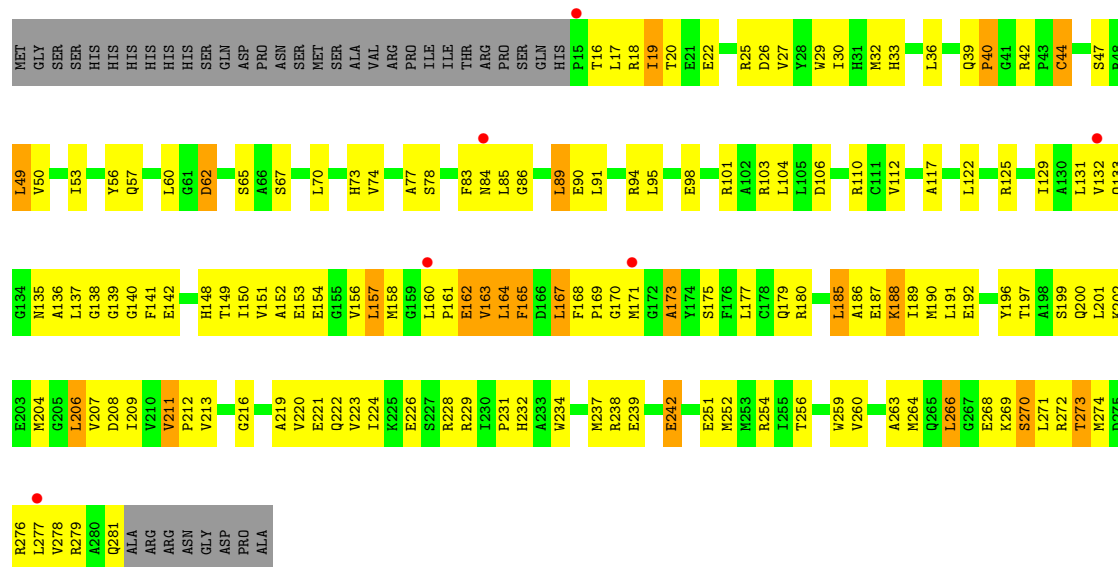
• Molecule 1: Crotonase/enoyl-CoA hydratase family protein



• Molecule 1: Crotonase/enoyl-CoA hydratase family protein



• Molecule 1: Crotonase/enoyl-CoA hydratase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.82Å 148.81Å 87.83Å 90.00° 112.11° 90.00°	Depositor
Resolution (Å)	81.37 – 3.00 81.37 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (81.37-3.00) 99.4 (81.37-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.216 , 0.289 0.223 , 0.288	Depositor DCC
R_{free} test set	1890 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12431	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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	0.52	0/2115	0.82	3/2863 (0.1%)
1	B	0.45	0/2113	0.72	6/2859 (0.2%)
1	C	0.52	0/2113	0.85	4/2859 (0.1%)
1	D	0.47	0/2113	0.70	0/2859
1	E	0.49	0/2091	0.72	5/2827 (0.2%)
1	F	0.51	0/2113	0.86	5/2859 (0.2%)
All	All	0.49	0/12658	0.78	23/17126 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	40	PRO	N-CA-C	16.40	136.33	113.53
1	F	40	PRO	CB-CA-C	-10.86	94.70	112.62
1	A	62	ASP	N-CA-C	-9.76	101.51	113.41
1	C	114	GLY	N-CA-C	9.58	123.61	112.50
1	F	173	ALA	CA-C-N	-8.37	109.25	120.63
1	F	173	ALA	C-N-CA	-8.37	109.25	120.63
1	B	115	VAL	N-CA-C	-8.04	103.06	111.58
1	C	215	GLU	N-CA-C	-7.89	97.78	109.62
1	A	61	GLY	N-CA-C	7.78	122.05	112.64
1	B	174	TYR	N-CA-C	-7.22	103.94	112.89
1	E	244	ALA	N-CA-C	7.20	122.25	112.68
1	B	114	GLY	N-CA-C	6.68	120.98	112.83
1	C	37	VAL	CB-CA-C	6.58	122.89	112.16
1	F	173	ALA	N-CA-C	-6.54	104.19	111.71
1	E	100	ASP	N-CA-C	-6.53	96.69	108.58
1	B	60	LEU	N-CA-C	-6.28	105.45	113.23
1	E	85	LEU	N-CA-CB	6.06	119.67	110.95
1	E	84	ASN	CB-CA-C	6.00	121.75	110.95
1	B	171	MET	N-CA-C	-5.79	98.46	110.80
1	B	59	GLU	N-CA-C	5.73	117.99	111.11
1	C	243	ILE	N-CA-C	-5.28	105.56	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	85	LEU	N-CA-C	-5.27	105.56	113.89
1	A	189	ILE	N-CA-C	-5.10	105.57	110.72

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	2076	0	2078	83	1
1	B	2075	0	2075	94	0
1	C	2075	0	2075	103	0
1	D	2075	0	2075	104	0
1	E	2055	0	2056	91	1
1	F	2075	0	2075	145	0
All	All	12431	0	12434	597	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 24.

All (597) 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:D:39:GLN:CB	1:D:40:PRO:HD3	1.55	1.31
1:C:92:PHE:O	1:C:96:ILE:HD12	1.08	1.22
1:D:39:GLN:HB3	1:D:40:PRO:CD	1.68	1.18
1:F:160:LEU:HD11	1:F:190:MET:HA	1.17	1.13
1:A:112:VAL:HG11	1:A:253:MET:HE2	1.29	1.12
1:E:142:GLU:OE1	1:E:171:MET:O	1.71	1.08
1:C:92:PHE:O	1:C:96:ILE:CD1	2.01	1.08
1:A:112:VAL:HG11	1:A:253:MET:CE	1.82	1.08
1:F:271:LEU:HA	1:F:274:MET:HG3	1.27	1.07
1:D:173:ALA:O	1:D:177:LEU:HB2	1.53	1.06
1:D:16:THR:HA	1:D:35:ASN:HD21	1.23	1.01
1:F:84:ASN:HB3	1:F:140:GLY:HA3	1.36	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:GLN:CB	1:D:40:PRO:CD	2.26	0.98
1:F:132:VAL:HB	1:F:152:ALA:HA	1.48	0.95
1:A:188:LYS:O	1:A:192:GLU:HG3	1.68	0.93
1:C:39:GLN:CG	1:C:40:PRO:HD3	1.98	0.93
1:D:42:ARG:NH2	1:D:90:GLU:OE1	2.03	0.92
1:A:112:VAL:CG1	1:A:253:MET:CE	2.48	0.91
1:F:173:ALA:O	1:F:177:LEU:CD1	2.21	0.89
1:A:174:TYR:OH	1:C:241:ASN:OD1	1.91	0.89
1:F:132:VAL:HG11	1:F:156:VAL:HG21	1.56	0.87
1:D:173:ALA:O	1:D:177:LEU:CB	2.25	0.85
1:A:187:GLU:OE2	1:C:238:ARG:NH2	2.10	0.84
1:F:70:LEU:HD23	1:F:231:PRO:HB2	1.59	0.84
1:F:150:ILE:H	1:F:208:ASP:HB2	1.43	0.83
1:B:202:LYS:HE2	1:B:209:ILE:HD12	1.60	0.83
1:A:112:VAL:CG1	1:A:253:MET:HE1	2.10	0.81
1:C:184:ARG:HH21	1:C:188:LYS:HG3	1.45	0.80
1:B:133:GLN:HE21	1:B:153:GLU:HG3	1.46	0.80
1:C:174:TYR:HD1	1:C:190:MET:HE1	1.45	0.80
1:F:44:CYS:HA	1:F:85:LEU:HB2	1.62	0.79
1:D:42:ARG:HB2	1:D:281:GLN:OE1	1.83	0.78
1:A:160:LEU:HD13	1:A:169:PRO:HG2	1.63	0.78
1:F:173:ALA:O	1:F:177:LEU:HD12	1.82	0.78
1:B:94:ARG:HH22	1:B:103:ARG:HH11	1.29	0.78
1:F:129:ILE:HG12	1:F:149:THR:HB	1.66	0.77
1:F:173:ALA:O	1:F:177:LEU:HD13	1.84	0.77
1:F:151:VAL:HG22	1:F:209:ILE:CG2	2.15	0.77
1:A:101:ARG:NH2	1:A:261:ASP:OD1	2.17	0.77
1:D:39:GLN:HB3	1:D:40:PRO:HD3	0.80	0.76
1:C:174:TYR:CD1	1:C:190:MET:HE1	2.20	0.76
1:F:84:ASN:HB3	1:F:140:GLY:CA	2.15	0.76
1:C:39:GLN:HB3	1:C:40:PRO:CD	2.16	0.75
1:B:124:THR:O	1:B:124:THR:OG1	2.05	0.75
1:C:39:GLN:CB	1:C:40:PRO:CD	2.64	0.75
1:A:25:ARG:O	1:A:228:ARG:NH2	2.20	0.74
1:D:18:ARG:NH1	1:D:79:ASP:OD1	2.20	0.74
1:C:91:LEU:O	1:C:91:LEU:HD12	1.87	0.74
1:C:74:VAL:HG21	1:C:122:LEU:HD11	1.69	0.74
1:C:72:PRO:HG2	1:C:126:ALA:HB2	1.70	0.74
1:E:163:VAL:HG11	1:E:191:LEU:HA	1.69	0.73
1:D:39:GLN:HB2	1:D:40:PRO:CD	2.17	0.73
1:E:142:GLU:OE1	1:E:171:MET:HG3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:VAL:CG1	1:F:156:VAL:HG21	2.19	0.72
1:F:154:GLU:HB2	1:F:212:PRO:HA	1.71	0.72
1:D:20:THR:HB	1:D:29:TRP:HB2	1.71	0.72
1:D:106:ASP:OD1	1:D:110:ARG:NH1	2.23	0.72
1:B:42:ARG:HH22	1:B:90:GLU:HB2	1.54	0.72
1:F:219:ALA:HA	1:F:222:GLN:HB2	1.72	0.72
1:B:125:ARG:HG2	1:B:238:ARG:HB2	1.72	0.71
1:F:220:VAL:O	1:F:224:ILE:HG13	1.90	0.71
1:D:95:LEU:HD11	1:D:103:ARG:HB3	1.72	0.71
1:B:142:GLU:OE2	1:B:171:MET:HB2	1.90	0.71
1:F:160:LEU:HD13	1:F:169:PRO:HG2	1.72	0.71
1:D:181:ILE:HD12	1:D:185:LEU:HD23	1.73	0.71
1:F:22:GLU:OE2	1:F:25:ARG:HD2	1.91	0.71
1:B:94:ARG:HH22	1:B:103:ARG:NH1	1.88	0.71
1:B:95:LEU:HD21	1:B:103:ARG:HD3	1.73	0.71
1:A:142:GLU:OE1	1:A:171:MET:HB2	1.91	0.70
1:F:269:LYS:HA	1:F:272:ARG:HB2	1.73	0.70
1:A:60:LEU:HG	1:A:64:LEU:CD1	2.22	0.70
1:A:241:ASN:OD1	1:A:245:THR:HG21	1.91	0.69
1:B:25:ARG:NH1	1:B:221:GLU:OE2	2.16	0.69
1:A:142:GLU:OE1	1:A:171:MET:CB	2.41	0.69
1:F:148:HIS:CE1	1:F:238:ARG:HD2	2.28	0.69
1:B:22:GLU:OE1	1:B:25:ARG:NH2	2.13	0.68
1:D:39:GLN:HB2	1:D:40:PRO:HD3	1.71	0.68
1:D:220:VAL:HG12	1:D:224:ILE:HD11	1.75	0.68
1:C:101:ARG:HA	1:C:264:MET:HE2	1.74	0.68
1:F:83:PHE:CD2	1:F:132:VAL:HA	2.29	0.68
1:A:112:VAL:HG11	1:A:253:MET:HE1	1.72	0.68
1:C:163:VAL:HG21	1:C:190:MET:O	1.94	0.67
1:B:142:GLU:CD	1:B:171:MET:HB2	2.20	0.67
1:F:101:ARG:HA	1:F:264:MET:HE3	1.75	0.67
1:C:92:PHE:HB3	1:C:96:ILE:HD11	1.76	0.67
1:F:148:HIS:HE1	1:F:238:ARG:HD2	1.57	0.67
1:D:70:LEU:HD12	1:D:231:PRO:HB2	1.77	0.67
1:D:187:GLU:HA	1:D:190:MET:HE2	1.75	0.67
1:C:82:VAL:HA	1:C:134:GLY:HA3	1.75	0.66
1:C:39:GLN:HG2	1:C:40:PRO:HD3	1.78	0.66
1:F:271:LEU:CA	1:F:274:MET:HG3	2.16	0.66
1:E:33:HIS:HB3	1:E:36:LEU:HB2	1.77	0.66
1:B:158:MET:HB2	1:B:201:LEU:HD11	1.76	0.66
1:B:133:GLN:NE2	1:B:153:GLU:CG	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:GLU:HG2	1:F:25:ARG:HB3	1.78	0.65
1:C:136:ALA:HB3	1:C:158:MET:HG2	1.78	0.65
1:D:187:GLU:OE2	1:E:238:ARG:NH2	2.30	0.65
1:C:39:GLN:CB	1:C:40:PRO:HD3	2.24	0.65
1:A:188:LYS:NZ	1:C:208:ASP:OD1	2.28	0.64
1:B:133:GLN:HE21	1:B:153:GLU:CG	2.09	0.64
1:E:25:ARG:O	1:E:228:ARG:NH1	2.31	0.64
1:E:184:ARG:NH1	1:F:148:HIS:O	2.31	0.64
1:A:188:LYS:O	1:A:192:GLU:CG	2.43	0.64
1:B:89:LEU:HD22	1:B:274:MET:HG2	1.80	0.63
1:E:128:SER:OG	1:E:148:HIS:ND1	2.23	0.63
1:F:106:ASP:O	1:F:110:ARG:HG3	1.99	0.63
1:D:277:LEU:O	1:D:281:GLN:N	2.32	0.63
1:F:160:LEU:HD11	1:F:190:MET:CA	2.12	0.63
1:B:94:ARG:O	1:B:98:GLU:HG3	1.98	0.63
1:A:142:GLU:HG2	1:A:173:ALA:HB2	1.81	0.63
1:A:45:PHE:CD2	1:A:171:MET:HE1	2.34	0.63
1:E:160:LEU:HD22	1:E:169:PRO:HG3	1.79	0.63
1:F:47:SER:HA	1:F:50:VAL:HG12	1.81	0.63
1:D:18:ARG:HD3	1:D:79:ASP:OD2	1.99	0.62
1:B:160:LEU:HD12	1:B:160:LEU:O	1.99	0.62
1:C:92:PHE:C	1:C:96:ILE:HD12	2.14	0.62
1:C:162:GLU:HG3	1:C:169:PRO:HD3	1.80	0.62
1:A:136:ALA:HB3	1:A:158:MET:HG2	1.80	0.62
1:E:47:SER:O	1:E:51:ASP:HB2	1.99	0.62
1:E:222:GLN:O	1:E:226:GLU:HG3	2.00	0.62
1:A:74:VAL:HG21	1:A:122:LEU:HD11	1.82	0.62
1:E:184:ARG:HB2	1:F:179:GLN:O	2.00	0.62
1:D:128:SER:HB2	1:D:148:HIS:H	1.64	0.62
1:F:237:MET:HA	1:F:237:MET:HE2	1.81	0.62
1:D:105:LEU:HA	1:D:260:VAL:HG21	1.81	0.61
1:A:62:ASP:OD1	1:A:62:ASP:N	2.34	0.61
1:A:186:ALA:O	1:A:190:MET:HG3	2.00	0.61
1:A:240:VAL:O	1:A:243:ILE:HG12	2.00	0.61
1:D:167:LEU:HD21	1:D:263:ALA:HB2	1.83	0.61
1:D:190:MET:HE1	1:E:237:MET:SD	2.41	0.61
1:F:148:HIS:H	1:F:148:HIS:CD2	2.17	0.61
1:A:166:ASP:OD2	1:C:232:HIS:HB2	2.01	0.60
1:D:49:LEU:O	1:D:53:ILE:HG13	2.01	0.60
1:D:197:THR:HG22	1:D:200:GLN:OE1	2.01	0.60
1:E:200:GLN:O	1:E:204:MET:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:PHE:CE1	1:F:158:MET:HG3	2.37	0.60
1:C:145:LEU:HA	1:C:150:ILE:HD11	1.82	0.60
1:F:17:LEU:HD12	1:F:19:ILE:HG23	1.82	0.60
1:A:148:HIS:O	1:B:184:ARG:NH1	2.34	0.60
1:D:167:LEU:HG	1:D:266:LEU:HD11	1.83	0.60
1:C:20:THR:HB	1:C:29:TRP:HB2	1.83	0.60
1:B:133:GLN:NE2	1:B:153:GLU:CD	2.60	0.60
1:D:82:VAL:HA	1:D:134:GLY:HA3	1.83	0.60
1:C:39:GLN:HG3	1:C:40:PRO:HD3	1.83	0.60
1:F:84:ASN:CB	1:F:140:GLY:HA3	2.22	0.60
1:F:268:GLU:O	1:F:272:ARG:N	2.34	0.60
1:D:21:GLU:OE2	1:D:63:ARG:NH1	2.35	0.60
1:E:95:LEU:HD22	1:E:100:ASP:HB3	1.84	0.59
1:D:77:ALA:HB2	1:D:131:LEU:HB3	1.84	0.59
1:F:83:PHE:CE2	1:F:132:VAL:HA	2.37	0.59
1:C:150:ILE:HG22	1:C:207:VAL:HG13	1.83	0.59
1:B:104:LEU:HD23	1:B:264:MET:HE3	1.84	0.59
1:F:25:ARG:HG2	1:F:228:ARG:NH1	2.17	0.59
1:C:263:ALA:O	1:C:266:LEU:HG	2.01	0.59
1:E:142:GLU:OE1	1:E:171:MET:C	2.43	0.59
1:C:32:MET:HE1	1:C:83:PHE:CE1	2.38	0.58
1:E:160:LEU:HD13	1:E:190:MET:HA	1.85	0.58
1:F:256:THR:O	1:F:260:VAL:HG12	2.02	0.58
1:C:39:GLN:CG	1:C:40:PRO:CD	2.78	0.58
1:F:33:HIS:HB3	1:F:36:LEU:HB2	1.85	0.58
1:F:91:LEU:HD12	1:F:95:LEU:HD23	1.84	0.58
1:E:133:GLN:HA	1:E:133:GLN:OE1	2.04	0.58
1:A:165:PHE:CD2	1:A:274:MET:HE2	2.37	0.58
1:C:39:GLN:HB3	1:C:40:PRO:HD2	1.85	0.58
1:B:42:ARG:NH2	1:B:90:GLU:HB2	2.18	0.58
1:F:132:VAL:HG11	1:F:156:VAL:HG11	1.85	0.58
1:A:60:LEU:HG	1:A:64:LEU:HD12	1.84	0.58
1:B:133:GLN:NE2	1:B:153:GLU:HG3	2.16	0.58
1:F:201:LEU:HB3	1:F:207:VAL:HG23	1.84	0.58
1:C:91:LEU:HD11	1:C:95:LEU:HD13	1.86	0.58
1:C:197:THR:HG22	1:C:200:GLN:HG2	1.84	0.58
1:B:36:LEU:HA	1:B:39:GLN:HB2	1.86	0.58
1:F:20:THR:HB	1:F:29:TRP:HB2	1.86	0.58
1:A:163:VAL:HG11	1:A:191:LEU:HA	1.86	0.57
1:D:112:VAL:HG22	1:D:252:MET:HE2	1.84	0.57
1:B:173:ALA:O	1:B:177:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:HIS:CD2	1:F:148:HIS:N	2.72	0.57
1:C:72:PRO:HG2	1:C:126:ALA:CB	2.34	0.57
1:E:92:PHE:O	1:E:96:ILE:HG13	2.03	0.57
1:F:271:LEU:HA	1:F:274:MET:CG	2.18	0.57
1:C:229:ARG:HH11	1:C:229:ARG:HG3	1.69	0.57
1:E:82:VAL:HA	1:E:134:GLY:HA3	1.86	0.57
1:D:72:PRO:HG2	1:D:126:ALA:HB2	1.86	0.57
1:B:39:GLN:HB3	1:B:40:PRO:HD2	1.86	0.57
1:B:96:ILE:HA	1:B:264:MET:HE1	1.86	0.57
1:D:132:VAL:HG12	1:D:156:VAL:HG11	1.87	0.56
1:B:184:ARG:NH2	1:B:188:LYS:HG3	2.19	0.56
1:F:160:LEU:HD12	1:F:160:LEU:O	2.05	0.56
1:E:18:ARG:NH1	1:E:79:ASP:OD2	2.36	0.56
1:F:165:PHE:N	1:F:165:PHE:CD1	2.73	0.56
1:A:112:VAL:HG12	1:A:253:MET:HE1	1.86	0.56
1:E:16:THR:HG21	1:E:49:LEU:HA	1.86	0.56
1:E:219:ALA:O	1:E:223:VAL:HG23	2.06	0.56
1:F:104:LEU:HD23	1:F:260:VAL:HG23	1.86	0.56
1:E:128:SER:HG	1:E:148:HIS:CE1	2.20	0.56
1:C:217:VAL:O	1:C:221:GLU:HB2	2.05	0.56
1:B:16:THR:HG21	1:B:48:ARG:HB3	1.86	0.56
1:A:106:ASP:O	1:A:110:ARG:HG3	2.05	0.56
1:D:237:MET:CE	1:F:187:GLU:HA	2.35	0.56
1:C:64:LEU:HD13	1:C:72:PRO:HG3	1.88	0.56
1:B:246:MET:HE3	1:B:247:VAL:O	2.05	0.56
1:A:28:TYR:CE2	1:A:60:LEU:HD11	2.39	0.56
1:A:70:LEU:CD2	1:A:231:PRO:HB2	2.36	0.56
1:A:251:GLU:HG3	1:C:243:ILE:CD1	2.35	0.56
1:B:82:VAL:HG21	1:B:85:LEU:HD21	1.88	0.56
1:A:60:LEU:HG	1:A:64:LEU:HD11	1.88	0.56
1:E:99:GLY:HA2	1:E:264:MET:HE1	1.88	0.56
1:F:200:GLN:O	1:F:204:MET:HG3	2.06	0.56
1:D:177:LEU:CD2	1:D:181:ILE:HD11	2.36	0.56
1:F:90:GLU:OE1	1:F:278:VAL:HG11	2.05	0.56
1:F:263:ALA:O	1:F:266:LEU:HB2	2.06	0.56
1:C:212:PRO:HD2	1:C:215:GLU:HG3	1.88	0.56
1:B:94:ARG:HH12	1:B:103:ARG:HH12	1.54	0.56
1:D:240:VAL:O	1:D:243:ILE:HG12	2.06	0.55
1:B:272:ARG:O	1:B:276:ARG:N	2.37	0.55
1:E:137:LEU:HD12	1:E:161:PRO:HG3	1.87	0.55
1:D:18:ARG:HB2	1:D:34:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:HIS:CE1	1:C:247:VAL:HG13	2.41	0.55
1:D:151:VAL:HG22	1:D:209:ILE:CG2	2.36	0.55
1:F:77:ALA:HB1	1:F:133:GLN:HG3	1.88	0.55
1:C:92:PHE:CD1	1:C:92:PHE:N	2.73	0.55
1:D:16:THR:HG23	1:D:52:ASP:OD2	2.06	0.55
1:F:150:ILE:H	1:F:208:ASP:CB	2.16	0.54
1:C:201:LEU:HB3	1:C:207:VAL:HG23	1.89	0.54
1:A:120:ALA:HA	1:A:246:MET:HE3	1.89	0.54
1:D:135:ASN:ND2	1:D:157:LEU:HB2	2.23	0.54
1:B:266:LEU:HD23	1:B:274:MET:HE1	1.90	0.54
1:E:267:GLY:O	1:E:271:LEU:HD12	2.08	0.54
1:A:105:LEU:O	1:A:109:GLN:HG3	2.06	0.54
1:A:251:GLU:HG3	1:C:243:ILE:HD11	1.89	0.54
1:E:211:VAL:HG21	1:E:215:GLU:HB3	1.88	0.54
1:F:219:ALA:O	1:F:223:VAL:HG22	2.07	0.54
1:A:142:GLU:OE1	1:A:171:MET:HB3	2.08	0.54
1:E:171:MET:O	1:E:171:MET:HG3	2.08	0.54
1:F:239:GLU:HA	1:F:242:GLU:HB2	1.90	0.54
1:A:108:ALA:O	1:A:111:CYS:HB2	2.07	0.54
1:F:188:LYS:HD3	1:F:192:GLU:CD	2.32	0.54
1:D:104:LEU:HG	1:D:260:VAL:HG22	1.90	0.54
1:D:237:MET:HE1	1:F:187:GLU:HA	1.88	0.54
1:E:166:ASP:OD2	1:F:232:HIS:HB2	2.08	0.54
1:A:21:GLU:HB2	1:A:28:TYR:CD2	2.43	0.53
1:C:241:ASN:OD1	1:C:245:THR:HB	2.07	0.53
1:B:180:ARG:HD3	1:B:205:GLY:O	2.07	0.53
1:F:89:LEU:HD23	1:F:278:VAL:HG22	1.89	0.53
1:F:186:ALA:O	1:F:190:MET:HG3	2.08	0.53
1:A:277:LEU:O	1:A:281:GLN:HG3	2.09	0.53
1:F:273:THR:HG23	1:F:276:ARG:HE	1.73	0.53
1:D:73:HIS:CD2	1:D:224:ILE:HG23	2.44	0.53
1:B:129:ILE:HG21	1:B:220:VAL:HG13	1.89	0.53
1:F:129:ILE:HD13	1:F:223:VAL:HG21	1.90	0.53
1:D:62:ASP:N	1:D:62:ASP:OD1	2.41	0.53
1:B:41:GLY:O	1:B:42:ARG:HG2	2.08	0.53
1:E:224:ILE:O	1:E:228:ARG:HG3	2.08	0.53
1:D:125:ARG:HA	1:D:238:ARG:HG2	1.89	0.53
1:C:172:GLY:HA2	1:C:252:MET:CE	2.39	0.53
1:A:100:ASP:OD2	1:A:103:ARG:HB2	2.09	0.53
1:D:36:LEU:HG	1:D:43:PRO:HB3	1.91	0.53
1:F:170:GLY:O	1:F:256:THR:CG2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ARG:HH12	1:B:103:ARG:NH1	2.06	0.53
1:B:160:LEU:HD22	1:B:169:PRO:HG3	1.89	0.53
1:A:112:VAL:HG12	1:A:253:MET:CE	2.37	0.53
1:C:160:LEU:HB3	1:C:169:PRO:HG3	1.91	0.53
1:B:160:LEU:HB2	1:B:162:GLU:OE1	2.09	0.53
1:D:129:ILE:HG23	1:D:149:THR:HB	1.91	0.53
1:D:237:MET:HG3	1:F:191:LEU:HD21	1.91	0.53
1:B:138:GLY:HA2	1:B:162:GLU:OE1	2.09	0.53
1:A:80:SER:OG	1:A:81:ASP:N	2.42	0.52
1:B:184:ARG:HH21	1:B:188:LYS:HG3	1.74	0.52
1:E:32:MET:HE1	1:E:84:ASN:HD22	1.74	0.52
1:E:172:GLY:O	1:E:176:PHE:CD2	2.62	0.52
1:F:151:VAL:HA	1:F:209:ILE:O	2.09	0.52
1:A:208:ASP:C	1:A:209:ILE:HD12	2.34	0.52
1:D:106:ASP:O	1:D:110:ARG:HG3	2.07	0.52
1:D:85:LEU:HD13	1:D:281:GLN:HG2	1.90	0.52
1:E:163:VAL:HA	1:E:167:LEU:O	2.09	0.52
1:E:273:THR:HA	1:E:276:ARG:HD2	1.90	0.52
1:A:230:ILE:HD12	1:A:230:ILE:O	2.09	0.52
1:D:97:ARG:HH21	1:D:268:GLU:CD	2.16	0.52
1:B:74:VAL:HG21	1:B:122:LEU:HD11	1.92	0.52
1:B:122:LEU:O	1:B:124:THR:HG22	2.10	0.52
1:E:152:ALA:O	1:E:210:VAL:HA	2.10	0.52
1:F:142:GLU:OE1	1:F:173:ALA:N	2.42	0.52
1:D:272:ARG:O	1:D:276:ARG:HG3	2.10	0.52
1:B:106:ASP:OD2	1:B:110:ARG:NH1	2.43	0.52
1:E:191:LEU:HD21	1:F:237:MET:HG3	1.92	0.52
1:F:22:GLU:HB3	1:F:27:VAL:O	2.09	0.52
1:F:171:MET:O	1:F:252:MET:HE1	2.08	0.52
1:C:222:GLN:O	1:C:226:GLU:HG3	2.10	0.52
1:B:256:THR:O	1:B:260:VAL:N	2.34	0.52
1:E:167:LEU:HD13	1:E:266:LEU:HD11	1.90	0.52
1:F:74:VAL:HG21	1:F:122:LEU:HD11	1.91	0.52
1:B:25:ARG:HG2	1:B:27:VAL:HG23	1.92	0.52
1:E:273:THR:HG22	1:E:276:ARG:HD2	1.90	0.52
1:A:175:SER:HB3	1:A:247:VAL:HG21	1.91	0.52
1:D:220:VAL:CG1	1:D:224:ILE:HD11	2.40	0.52
1:E:45:PHE:HB2	1:E:86:GLY:O	2.10	0.52
1:F:62:ASP:OD1	1:F:62:ASP:N	2.42	0.52
1:D:129:ILE:HD13	1:D:223:VAL:HG12	1.90	0.51
1:B:142:GLU:OE2	1:B:171:MET:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:HA	1:A:134:GLY:HA3	1.92	0.51
1:F:25:ARG:NH2	1:F:221:GLU:OE1	2.43	0.51
1:F:135:ASN:OD1	1:F:157:LEU:HB2	2.09	0.51
1:D:188:LYS:O	1:D:192:GLU:HB2	2.11	0.51
1:E:142:GLU:CD	1:E:171:MET:HG3	2.35	0.51
1:F:73:HIS:CD2	1:F:224:ILE:HG23	2.46	0.51
1:D:220:VAL:O	1:D:223:VAL:N	2.43	0.51
1:E:49:LEU:O	1:E:53:ILE:HG13	2.10	0.51
1:D:200:GLN:O	1:D:204:MET:HG3	2.10	0.51
1:C:83:PHE:HD2	1:C:132:VAL:HA	1.76	0.51
1:B:151:VAL:HG21	1:B:220:VAL:HG22	1.92	0.51
1:E:176:PHE:CE1	1:E:252:MET:HE1	2.45	0.51
1:F:86:GLY:HA2	1:F:139:GLY:H	1.76	0.51
1:C:236:ALA:O	1:C:240:VAL:HG23	2.11	0.51
1:E:76:LEU:HD22	1:E:118:PHE:CE2	2.46	0.51
1:C:153:GLU:O	1:C:156:VAL:HG23	2.11	0.50
1:C:165:PHE:CE1	1:C:167:LEU:HB2	2.46	0.50
1:A:158:MET:HB2	1:A:201:LEU:HD11	1.92	0.50
1:D:85:LEU:CD1	1:D:281:GLN:HG2	2.41	0.50
1:C:150:ILE:O	1:C:208:ASP:HB2	2.12	0.50
1:F:56:TYR:OH	1:F:60:LEU:HD22	2.11	0.50
1:F:95:LEU:HD11	1:F:103:ARG:HG2	1.93	0.50
1:F:150:ILE:N	1:F:208:ASP:HB2	2.21	0.50
1:D:136:ALA:O	1:D:158:MET:HA	2.11	0.50
1:C:150:ILE:N	1:C:208:ASP:OD2	2.43	0.50
1:E:211:VAL:CG2	1:E:215:GLU:HB3	2.42	0.50
1:C:49:LEU:O	1:C:53:ILE:HG13	2.11	0.50
1:C:277:LEU:O	1:C:281:GLN:HG3	2.12	0.50
1:E:94:ARG:O	1:E:98:GLU:HG3	2.11	0.50
1:F:164:LEU:N	1:F:164:LEU:HD23	2.27	0.50
1:C:192:GLU:HB3	1:C:194:ASN:OD1	2.11	0.50
1:E:186:ALA:O	1:E:190:MET:HG3	2.11	0.50
1:A:146:SER:HB3	1:A:176:PHE:CE2	2.46	0.50
1:F:83:PHE:HD2	1:F:132:VAL:HA	1.75	0.50
1:A:163:VAL:HA	1:A:167:LEU:O	2.11	0.50
1:D:131:LEU:HD13	1:D:220:VAL:HG23	1.94	0.50
1:D:142:GLU:OE1	1:D:173:ALA:N	2.45	0.50
1:C:174:TYR:HD1	1:C:190:MET:CE	2.19	0.50
1:C:269:LYS:HA	1:C:272:ARG:NH1	2.27	0.49
1:B:220:VAL:O	1:B:224:ILE:HG13	2.12	0.49
1:E:33:HIS:NE2	1:E:43:PRO:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:CYS:SG	1:E:45:PHE:N	2.85	0.49
1:C:83:PHE:CD2	1:C:132:VAL:HA	2.46	0.49
1:A:138:GLY:HA2	1:A:160:LEU:HB3	1.95	0.49
1:E:135:ASN:HB3	1:E:137:LEU:HD23	1.94	0.49
1:F:224:ILE:O	1:F:228:ARG:HG3	2.12	0.49
1:C:17:LEU:HD22	1:C:30:ILE:HG23	1.95	0.49
1:E:105:LEU:HA	1:E:260:VAL:HG21	1.93	0.49
1:E:275:ASP:HA	1:E:278:VAL:HB	1.94	0.49
1:B:100:ASP:CG	1:B:103:ARG:HB2	2.38	0.49
1:E:141:PHE:CE1	1:E:158:MET:HE2	2.48	0.49
1:E:175:SER:HB3	1:E:247:VAL:HG11	1.94	0.49
1:C:224:ILE:O	1:C:228:ARG:HG3	2.13	0.49
1:A:157:LEU:HD22	1:A:195:LEU:HD23	1.95	0.48
1:B:142:GLU:CG	1:B:173:ALA:HB2	2.43	0.48
1:E:32:MET:CE	1:E:84:ASN:HD22	2.26	0.48
1:F:266:LEU:HD13	1:F:270:SER:HB2	1.95	0.48
1:F:274:MET:O	1:F:278:VAL:HG23	2.13	0.48
1:C:50:VAL:HG21	1:C:111:CYS:SG	2.53	0.48
1:C:179:GLN:HE21	1:C:247:VAL:HG12	1.78	0.48
1:B:22:GLU:CD	1:B:25:ARG:HH21	2.13	0.48
1:F:160:LEU:HD13	1:F:169:PRO:CG	2.42	0.48
1:A:18:ARG:NH1	1:A:79:ASP:OD1	2.46	0.48
1:F:25:ARG:HG2	1:F:228:ARG:HH11	1.79	0.48
1:D:105:LEU:HG	1:D:109:GLN:HE21	1.78	0.48
1:A:96:ILE:HA	1:A:264:MET:HE1	1.95	0.48
1:B:70:LEU:CD2	1:B:231:PRO:HB2	2.43	0.48
1:E:277:LEU:O	1:E:281:GLN:N	2.41	0.48
1:B:122:LEU:HB2	1:B:124:THR:CG2	2.43	0.48
1:F:170:GLY:O	1:F:256:THR:HG22	2.14	0.48
1:A:151:VAL:HG13	1:A:209:ILE:HG22	1.96	0.48
1:E:211:VAL:HB	1:E:212:PRO:CD	2.44	0.48
1:E:275:ASP:HB3	1:E:279:ARG:NH1	2.29	0.48
1:B:173:ALA:O	1:B:177:LEU:CG	2.62	0.48
1:D:105:LEU:HG	1:D:109:GLN:NE2	2.29	0.48
1:B:18:ARG:HB2	1:B:34:ALA:HB2	1.95	0.48
1:F:62:ASP:HA	1:F:65:SER:HB3	1.96	0.48
1:F:86:GLY:HA2	1:F:139:GLY:N	2.29	0.48
1:E:166:ASP:CG	1:F:232:HIS:HB2	2.39	0.48
1:A:200:GLN:O	1:A:204:MET:HG3	2.14	0.47
1:F:196:TYR:HB2	1:F:201:LEU:HG	1.95	0.47
1:A:139:GLY:HA2	1:A:142:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:VAL:HG22	1:B:73:HIS:HB2	1.96	0.47
1:E:45:PHE:HA	1:E:49:LEU:HD23	1.96	0.47
1:D:202:LYS:NZ	1:D:210:VAL:HG22	2.29	0.47
1:F:148:HIS:HD1	1:F:234:TRP:HZ2	1.56	0.47
1:C:91:LEU:CD1	1:C:95:LEU:HD13	2.44	0.47
1:E:150:ILE:N	1:E:208:ASP:OD2	2.46	0.47
1:F:32:MET:N	1:F:78:SER:HA	2.30	0.47
1:F:106:ASP:OD2	1:F:110:ARG:NH1	2.43	0.47
1:F:136:ALA:O	1:F:158:MET:HB2	2.14	0.47
1:D:115:VAL:HG12	1:D:143:ALA:HA	1.95	0.47
1:C:92:PHE:N	1:C:92:PHE:HD1	2.11	0.47
1:B:172:GLY:O	1:B:174:TYR:N	2.46	0.47
1:E:242:GLU:HA	1:E:246:MET:HB2	1.97	0.47
1:F:141:PHE:CD1	1:F:158:MET:HG3	2.49	0.47
1:F:157:LEU:HD22	1:F:197:THR:HA	1.96	0.47
1:A:22:GLU:O	1:A:22:GLU:HG3	2.15	0.47
1:D:166:ASP:CG	1:E:231:PRO:HD2	2.39	0.47
1:A:137:LEU:HA	1:A:159:GLY:O	2.14	0.47
1:D:133:GLN:NE2	1:D:217:VAL:HG22	2.30	0.47
1:B:160:LEU:HD13	1:B:169:PRO:HG3	1.97	0.47
1:E:197:THR:HG23	1:E:200:GLN:OE1	2.14	0.47
1:F:163:VAL:HG23	1:F:163:VAL:O	2.14	0.47
1:E:18:ARG:HB3	1:E:31:HIS:HB2	1.96	0.47
1:C:248:PRO:HB3	1:C:250:HIS:CE1	2.49	0.47
1:E:44:CYS:HB2	1:E:86:GLY:O	2.14	0.47
1:F:228:ARG:HE	1:F:228:ARG:HB3	1.54	0.47
1:B:131:LEU:HB2	1:B:220:VAL:HG21	1.97	0.46
1:B:142:GLU:OE2	1:B:172:GLY:N	2.48	0.46
1:B:263:ALA:HA	1:B:266:LEU:HD13	1.97	0.46
1:F:131:LEU:HD13	1:F:220:VAL:HG21	1.97	0.46
1:A:93:CYS:SG	1:A:271:LEU:HD22	2.56	0.46
1:C:225:LYS:HB3	1:C:225:LYS:HE3	1.65	0.46
1:E:248:PRO:HB2	1:E:250:HIS:CE1	2.51	0.46
1:F:17:LEU:HD13	1:F:30:ILE:HG23	1.96	0.46
1:B:256:THR:HA	1:B:259:TRP:HB3	1.98	0.46
1:E:74:VAL:HG21	1:E:122:LEU:CD1	2.45	0.46
1:E:237:MET:HE2	1:E:237:MET:HA	1.97	0.46
1:D:17:LEU:CD2	1:D:52:ASP:HB3	2.45	0.46
1:B:273:THR:HA	1:B:276:ARG:HB2	1.97	0.46
1:D:246:MET:HG2	1:D:247:VAL:N	2.30	0.46
1:D:277:LEU:O	1:D:281:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:PRO:HG2	1:C:190:MET:HB3	1.98	0.46
1:C:197:THR:HG22	1:C:200:GLN:CG	2.46	0.46
1:D:177:LEU:HD21	1:D:181:ILE:HD11	1.98	0.46
1:A:44:CYS:HB2	1:A:86:GLY:O	2.16	0.46
1:A:184:ARG:NH2	1:C:148:HIS:O	2.48	0.46
1:C:163:VAL:HG12	1:B:230:ILE:HG21	1.98	0.46
1:B:94:ARG:NH2	1:B:103:ARG:HH11	2.07	0.46
1:E:176:PHE:CZ	1:E:252:MET:HE1	2.51	0.46
1:F:57:GLN:HG2	1:F:122:LEU:HD22	1.98	0.46
1:F:167:LEU:HD21	1:F:263:ALA:HB2	1.97	0.46
1:C:17:LEU:HD23	1:C:32:MET:HA	1.98	0.45
1:C:254:ARG:HD2	1:E:250:HIS:HB3	1.98	0.45
1:B:168:PHE:HB2	1:B:169:PRO:HD2	1.98	0.45
1:B:96:ILE:HG12	1:B:264:MET:HE2	1.98	0.45
1:B:145:LEU:HA	1:B:150:ILE:HD11	1.98	0.45
1:B:170:GLY:HA3	1:B:259:TRP:CD1	2.51	0.45
1:C:186:ALA:O	1:C:190:MET:HG3	2.17	0.45
1:C:211:VAL:HB	1:C:212:PRO:CD	2.46	0.45
1:E:116:HIS:CE1	1:E:249:LEU:HB2	2.51	0.45
1:E:153:GLU:O	1:E:156:VAL:HG23	2.15	0.45
1:A:46:ALA:O	1:A:49:LEU:N	2.50	0.45
1:A:88:ASP:OD2	1:A:91:LEU:HB2	2.16	0.45
1:D:95:LEU:CD1	1:D:103:ARG:HB3	2.43	0.45
1:C:57:GLN:NE2	1:C:118:PHE:CE1	2.85	0.45
1:C:167:LEU:HA	1:C:167:LEU:HD23	1.71	0.45
1:B:32:MET:HB3	1:B:49:LEU:HD21	1.98	0.45
1:B:82:VAL:HG21	1:B:85:LEU:CD2	2.46	0.45
1:C:163:VAL:HA	1:C:167:LEU:O	2.17	0.45
1:E:96:ILE:HD13	1:E:263:ALA:O	2.16	0.45
1:F:89:LEU:HD22	1:F:89:LEU:H	1.82	0.45
1:F:131:LEU:HD22	1:F:220:VAL:HG21	1.98	0.45
1:C:136:ALA:HB3	1:C:158:MET:CG	2.47	0.45
1:F:180:ARG:NH1	1:F:206:LEU:O	2.50	0.45
1:D:202:LYS:HZ3	1:D:210:VAL:HG22	1.83	0.44
1:A:188:LYS:C	1:A:192:GLU:HG3	2.39	0.44
1:F:138:GLY:HA2	1:F:162:GLU:OE1	2.17	0.44
1:F:94:ARG:O	1:F:98:GLU:HG3	2.17	0.44
1:B:15:PRO:HB2	1:B:16:THR:H	1.68	0.44
1:B:160:LEU:CD2	1:B:169:PRO:HG3	2.48	0.44
1:D:44:CYS:HB2	1:D:86:GLY:O	2.18	0.44
1:C:39:GLN:HG2	1:C:40:PRO:CD	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:ILE:HG13	1:C:244:ALA:N	2.33	0.44
1:B:95:LEU:HD23	1:B:95:LEU:HA	1.73	0.44
1:A:220:VAL:O	1:A:224:ILE:HG13	2.18	0.44
1:D:192:GLU:HG2	1:D:194:ASN:ND2	2.33	0.44
1:F:165:PHE:O	1:F:270:SER:HB3	2.18	0.44
1:D:54:VAL:O	1:D:58:ARG:HG2	2.18	0.44
1:D:177:LEU:HD23	1:D:181:ILE:HD11	1.99	0.44
1:E:204:MET:HB2	1:E:206:LEU:HD23	1.99	0.44
1:D:220:VAL:HG12	1:D:224:ILE:CD1	2.44	0.44
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.81	0.44
1:F:148:HIS:ND1	1:F:234:TRP:CZ2	2.81	0.44
1:C:230:ILE:HD12	1:C:230:ILE:O	2.17	0.43
1:F:117:ALA:HB1	1:F:122:LEU:HD23	1.99	0.43
1:F:164:LEU:N	1:F:164:LEU:CD2	2.81	0.43
1:B:253:MET:O	1:B:257:GLU:HG3	2.17	0.43
1:E:271:LEU:O	1:E:274:MET:HB2	2.19	0.43
1:A:132:VAL:HG11	1:A:158:MET:SD	2.57	0.43
1:A:139:GLY:HA3	1:A:171:MET:CE	2.49	0.43
1:A:32:MET:HG2	1:A:77:ALA:O	2.18	0.43
1:B:32:MET:HG3	1:B:77:ALA:O	2.18	0.43
1:F:16:THR:HG23	1:F:17:LEU:HD23	2.00	0.43
1:F:32:MET:H	1:F:78:SER:HA	1.84	0.43
1:D:57:GLN:O	1:D:61:GLY:N	2.49	0.43
1:B:35:ASN:ND2	1:B:36:LEU:HD22	2.33	0.43
1:F:95:LEU:HA	1:F:95:LEU:HD13	1.79	0.43
1:D:94:ARG:O	1:D:98:GLU:HG3	2.18	0.43
1:C:162:GLU:H	1:C:162:GLU:HG2	1.47	0.43
1:E:167:LEU:HD13	1:E:266:LEU:HD21	2.00	0.43
1:F:49:LEU:O	1:F:53:ILE:HG13	2.18	0.43
1:D:111:CYS:SG	1:D:171:MET:HE3	2.59	0.43
1:F:112:VAL:HG13	1:F:252:MET:HE3	2.01	0.43
1:A:175:SER:HB3	1:A:247:VAL:HG11	2.00	0.43
1:C:251:GLU:O	1:C:255:ILE:HG13	2.19	0.43
1:F:211:VAL:HG11	1:F:219:ALA:HB2	2.01	0.43
1:A:141:PHE:CE1	1:A:158:MET:HE2	2.54	0.43
1:F:216:GLY:O	1:F:220:VAL:HG23	2.19	0.43
1:A:17:LEU:HD11	1:A:52:ASP:HB3	2.01	0.43
1:C:228:ARG:O	1:C:231:PRO:HD3	2.19	0.43
1:E:70:LEU:HD21	1:E:232:HIS:CD2	2.54	0.43
1:D:238:ARG:NH2	1:F:187:GLU:OE2	2.51	0.42
1:B:225:LYS:HB3	1:B:225:LYS:HE2	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:PHE:HB3	1:C:136:ALA:HB2	2.01	0.42
1:E:242:GLU:HA	1:E:246:MET:HE2	2.01	0.42
1:F:150:ILE:O	1:F:208:ASP:HB2	2.18	0.42
1:F:226:GLU:O	1:F:229:ARG:HB3	2.19	0.42
1:F:277:LEU:O	1:F:281:GLN:HG3	2.19	0.42
1:A:29:TRP:CD1	1:A:29:TRP:N	2.87	0.42
1:D:72:PRO:HG2	1:D:126:ALA:CB	2.49	0.42
1:D:95:LEU:CD1	1:D:100:ASP:HB3	2.50	0.42
1:B:169:PRO:HG2	1:B:190:MET:HG2	2.00	0.42
1:E:79:ASP:N	1:E:79:ASP:OD1	2.51	0.42
1:F:39:GLN:HB3	1:F:40:PRO:HD2	2.01	0.42
1:B:189:ILE:HD13	1:B:189:ILE:HA	1.88	0.42
1:A:196:TYR:HB3	1:A:200:GLN:HE21	1.84	0.42
1:D:85:LEU:HD22	1:D:137:LEU:HD21	2.00	0.42
1:F:168:PHE:O	1:F:259:TRP:CD1	2.72	0.42
1:C:165:PHE:CE1	1:C:274:MET:HE2	2.54	0.42
1:B:82:VAL:HA	1:B:134:GLY:HA3	2.02	0.42
1:E:33:HIS:O	1:E:36:LEU:HB2	2.20	0.42
1:E:112:VAL:HG21	1:E:256:THR:CG2	2.50	0.42
1:F:169:PRO:HD2	1:F:190:MET:HE3	2.02	0.42
1:F:185:LEU:O	1:F:186:ALA:C	2.63	0.42
1:D:100:ASP:OD2	1:D:103:ARG:HB2	2.19	0.42
1:D:263:ALA:HA	1:D:266:LEU:HG	2.02	0.42
1:C:33:HIS:O	1:C:36:LEU:HB2	2.19	0.42
1:C:76:LEU:HD22	1:C:118:PHE:CZ	2.54	0.42
1:E:275:ASP:N	1:E:275:ASP:OD1	2.52	0.42
1:D:83:PHE:HB3	1:D:136:ALA:HB2	2.01	0.42
1:C:165:PHE:HE1	1:C:167:LEU:HD12	1.85	0.42
1:F:129:ILE:CG1	1:F:149:THR:HB	2.44	0.42
1:A:19:ILE:HG21	1:A:56:TYR:CZ	2.55	0.42
1:D:211:VAL:HG11	1:D:216:GLY:HA2	2.01	0.42
1:C:159:GLY:HA3	1:C:195:LEU:HD23	2.02	0.42
1:B:160:LEU:HA	1:B:161:PRO:HD3	1.89	0.42
1:E:139:GLY:HA2	1:E:142:GLU:OE2	2.19	0.42
1:D:42:ARG:HG3	1:D:42:ARG:HH11	1.85	0.42
1:D:105:LEU:HA	1:D:105:LEU:HD12	1.80	0.42
1:F:170:GLY:O	1:F:256:THR:HG23	2.20	0.42
1:F:185:LEU:O	1:F:189:ILE:HD12	2.19	0.42
1:B:95:LEU:HD22	1:B:100:ASP:HB3	2.02	0.41
1:E:20:THR:HB	1:E:29:TRP:HB2	2.02	0.41
1:F:22:GLU:CD	1:F:25:ARG:HD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:PHE:CD2	1:F:274:MET:HE3	2.55	0.41
1:A:43:PRO:HD2	1:A:85:LEU:HD12	2.02	0.41
1:D:24:GLU:CD	1:D:24:GLU:H	2.28	0.41
1:D:29:TRP:CZ3	1:D:75:VAL:HG11	2.55	0.41
1:D:125:ARG:HG2	1:D:238:ARG:HB3	2.01	0.41
1:D:153:GLU:O	1:D:156:VAL:HG23	2.20	0.41
1:C:109:GLN:O	1:C:113:ARG:HG3	2.20	0.41
1:F:17:LEU:CD1	1:F:30:ILE:HG23	2.50	0.41
1:C:19:ILE:HA	1:C:29:TRP:O	2.20	0.41
1:A:197:THR:HG23	1:A:200:GLN:HG3	2.01	0.41
1:D:159:GLY:HA3	1:D:195:LEU:HD12	2.01	0.41
1:B:153:GLU:HB2	1:B:156:VAL:HG23	2.02	0.41
1:E:19:ILE:H	1:E:19:ILE:HG13	1.65	0.41
1:F:39:GLN:OE1	1:F:40:PRO:HD2	2.20	0.41
1:A:27:VAL:C	1:A:28:TYR:CD1	2.99	0.41
1:D:145:LEU:HA	1:D:150:ILE:HD11	2.02	0.41
1:C:266:LEU:HD23	1:C:266:LEU:N	2.35	0.41
1:E:131:LEU:HD22	1:E:220:VAL:HG21	2.01	0.41
1:E:206:LEU:HA	1:E:206:LEU:HD13	1.79	0.41
1:C:40:PRO:HB2	1:C:41:GLY:H	1.60	0.41
1:C:246:MET:HE3	1:C:246:MET:HB3	1.75	0.41
1:F:32:MET:HB2	1:F:32:MET:HE2	1.77	0.41
1:D:211:VAL:HG22	1:D:212:PRO:HD2	2.03	0.41
1:C:101:ARG:CA	1:C:264:MET:HE2	2.49	0.41
1:F:25:ARG:HH22	1:F:221:GLU:CD	2.27	0.41
1:F:85:LEU:HD23	1:F:85:LEU:HA	1.80	0.41
1:B:122:LEU:HB2	1:B:124:THR:HG23	2.03	0.41
1:B:212:PRO:HG2	1:B:215:GLU:OE1	2.21	0.41
1:F:125:ARG:HG2	1:F:238:ARG:HB2	2.02	0.41
1:F:142:GLU:HG2	1:F:173:ALA:HB2	2.03	0.41
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.83	0.41
1:D:115:VAL:CG1	1:D:143:ALA:HA	2.50	0.41
1:B:237:MET:HE2	1:B:237:MET:HA	2.03	0.41
1:F:83:PHE:N	1:F:135:ASN:O	2.54	0.41
1:F:148:HIS:ND1	1:F:234:TRP:HZ2	2.17	0.41
1:F:151:VAL:HG22	1:F:209:ILE:HG23	1.99	0.41
1:D:177:LEU:CD2	1:D:186:ALA:HA	2.51	0.41
1:D:254:ARG:NH2	1:E:243:ILE:HB	2.35	0.41
1:C:215:GLU:H	1:C:215:GLU:HG2	1.52	0.41
1:B:47:SER:HA	1:B:50:VAL:HB	2.02	0.41
1:B:271:LEU:HA	1:B:274:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:SER:O	1:A:203:GLU:HG2	2.22	0.40
1:E:32:MET:HE3	1:E:33:HIS:CE1	2.56	0.40
1:D:175:SER:HB3	1:D:247:VAL:HG11	2.03	0.40
1:C:92:PHE:HB3	1:C:96:ILE:CD1	2.50	0.40
1:C:105:LEU:HG	1:C:109:GLN:HG3	2.03	0.40
1:C:132:VAL:O	1:C:132:VAL:HG12	2.21	0.40
1:B:142:GLU:OE1	1:B:171:MET:HB2	2.21	0.40
1:B:277:LEU:O	1:B:281:GLN:HB2	2.20	0.40
1:E:167:LEU:HD12	1:E:167:LEU:HA	1.74	0.40
1:A:49:LEU:O	1:A:53:ILE:HG13	2.21	0.40
1:C:239:GLU:O	1:C:242:GLU:HB2	2.22	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:215:GLU:OE1	1:E:272:ARG:NH2[1_554]	2.07	0.13

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	265/305 (87%)	249 (94%)	13 (5%)	3 (1%)	11	43
1	B	265/305 (87%)	245 (92%)	18 (7%)	2 (1%)	16	50
1	C	265/305 (87%)	244 (92%)	17 (6%)	4 (2%)	8	35
1	D	265/305 (87%)	250 (94%)	14 (5%)	1 (0%)	30	65
1	E	260/305 (85%)	246 (95%)	12 (5%)	2 (1%)	16	50
1	F	265/305 (87%)	248 (94%)	15 (6%)	2 (1%)	16	50
All	All	1585/1830 (87%)	1482 (94%)	89 (6%)	14 (1%)	14	48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	39	GLN
1	C	94	ARG
1	B	171	MET
1	A	245	THR
1	C	40	PRO
1	B	173	ALA
1	C	39	GLN
1	F	161	PRO
1	E	44	CYS
1	A	172	GLY
1	A	244	ALA
1	C	33	HIS
1	F	42	ARG
1	E	43	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	220/253 (87%)	205 (93%)	15 (7%)	14	45
1	B	219/253 (87%)	203 (93%)	16 (7%)	13	42
1	C	219/253 (87%)	194 (89%)	25 (11%)	5	24
1	D	219/253 (87%)	202 (92%)	17 (8%)	11	39
1	E	217/253 (86%)	197 (91%)	20 (9%)	8	33
1	F	219/253 (87%)	188 (86%)	31 (14%)	3	16
All	All	1313/1518 (86%)	1189 (91%)	124 (9%)	8	32

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	58	ARG
1	A	59	GLU

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Mol	Chain	Res	Type
1	A	62	ASP
1	A	80	SER
1	A	106	ASP
1	A	112	VAL
1	A	115	VAL
1	A	160	LEU
1	A	167	LEU
1	A	187	GLU
1	A	202	LYS
1	A	228	ARG
1	A	257	GLU
1	A	279	ARG
1	D	17	LEU
1	D	36	LEU
1	D	42	ARG
1	D	48	ARG
1	D	62	ASP
1	D	98	GLU
1	D	112	VAL
1	D	115	VAL
1	D	165	PHE
1	D	177	LEU
1	D	192	GLU
1	D	206	LEU
1	D	227	SER
1	D	251	GLU
1	D	260	VAL
1	D	265	GLN
1	D	277	LEU
1	C	32	MET
1	C	36	LEU
1	C	37	VAL
1	C	38	ASN
1	C	39	GLN
1	C	42	ARG
1	C	45	PHE
1	C	67	SER
1	C	80	SER
1	C	81	ASP
1	C	92	PHE
1	C	106	ASP
1	C	153	GLU

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Mol	Chain	Res	Type
1	C	171	MET
1	C	181	ILE
1	C	184	ARG
1	C	185	LEU
1	C	213	VAL
1	C	215	GLU
1	C	228	ARG
1	C	243	ILE
1	C	245	THR
1	C	246	MET
1	C	247	VAL
1	C	260	VAL
1	B	47	SER
1	B	90	GLU
1	B	115	VAL
1	B	124	THR
1	B	133	GLN
1	B	154	GLU
1	B	162	GLU
1	B	163	VAL
1	B	171	MET
1	B	184	ARG
1	B	217	VAL
1	B	224	ILE
1	B	243	ILE
1	B	270	SER
1	B	273	THR
1	B	275	ASP
1	E	24	GLU
1	E	36	LEU
1	E	42	ARG
1	E	50	VAL
1	E	52	ASP
1	E	55	ASP
1	E	74	VAL
1	E	80	SER
1	E	111	CYS
1	E	124	THR
1	E	160	LEU
1	E	163	VAL
1	E	171	MET
1	E	184	ARG

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Mol	Chain	Res	Type
1	E	215	GLU
1	E	226	GLU
1	E	241	ASN
1	E	242	GLU
1	E	260	VAL
1	E	279	ARG
1	F	18	ARG
1	F	19	ILE
1	F	26	ASP
1	F	44	CYS
1	F	49	LEU
1	F	62	ASP
1	F	67	SER
1	F	89	LEU
1	F	137	LEU
1	F	153	GLU
1	F	157	LEU
1	F	162	GLU
1	F	163	VAL
1	F	164	LEU
1	F	165	PHE
1	F	167	LEU
1	F	175	SER
1	F	185	LEU
1	F	188	LYS
1	F	199	SER
1	F	202	LYS
1	F	206	LEU
1	F	211	VAL
1	F	213	VAL
1	F	242	GLU
1	F	251	GLU
1	F	254	ARG
1	F	266	LEU
1	F	270	SER
1	F	273	THR
1	F	279	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN

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Mol	Chain	Res	Type
1	A	200	GLN
1	D	31	HIS
1	D	35	ASN
1	D	222	GLN
1	D	265	GLN
1	C	39	GLN
1	C	109	GLN
1	C	222	GLN
1	B	133	GLN
1	F	109	GLN
1	F	133	GLN
1	F	241	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	267/305 (87%)	-0.36	0 100 100	45, 57, 74, 118	0
1	B	267/305 (87%)	-0.20	3 (1%) 78 57	39, 67, 95, 118	0
1	C	267/305 (87%)	-0.29	1 (0%) 88 76	45, 67, 90, 112	0
1	D	267/305 (87%)	-0.17	1 (0%) 88 76	47, 67, 91, 111	0
1	E	264/305 (86%)	-0.14	4 (1%) 72 49	51, 77, 100, 122	0
1	F	267/305 (87%)	0.11	6 (2%) 62 39	60, 86, 114, 134	0
All	All	1599/1830 (87%)	-0.17	15 (0%) 81 61	39, 69, 102, 134	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	15	PRO	3.8
1	F	84	ASN	3.7
1	D	15	PRO	3.4
1	F	160	LEU	3.3
1	E	165	PHE	3.1
1	C	15	PRO	2.7
1	F	132	VAL	2.6
1	E	44	CYS	2.6
1	F	277	LEU	2.5
1	B	15	PRO	2.4
1	B	172	GLY	2.4
1	F	15	PRO	2.2
1	F	171	MET	2.1
1	E	137	LEU	2.0
1	B	171	MET	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 oligosaccharides 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.