



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:39 PM UTC

PDB ID : 4A2Q / pdb_00004a2q
Title : Structure of duck RIG-I tandem CARDS and helicase domain
Authors : Kowalinski, E.; Lunardi, T.; McCarthy, A.A.; Cusack, S.
Deposited on : 2011-09-28
Resolution : 3.40 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

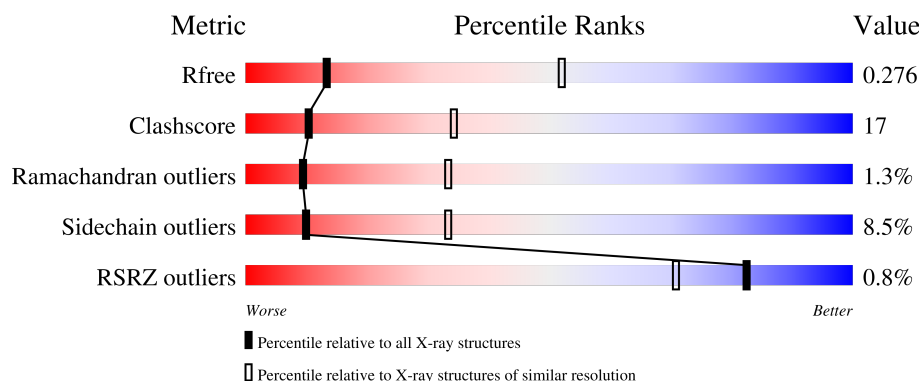
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	797	
1	B	797	
1	D	797	
1	E	797	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21661 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 RETINOIC ACID INDUCIBLE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5425	3430	933	1028	34			
1	B	675	Total	C	N	O	S	0	0	0
			5436	3436	937	1029	34			
1	D	671	Total	C	N	O	S	0	0	0
			5404	3417	930	1024	33			
1	E	670	Total	C	N	O	S	0	0	0
			5396	3413	929	1021	33			

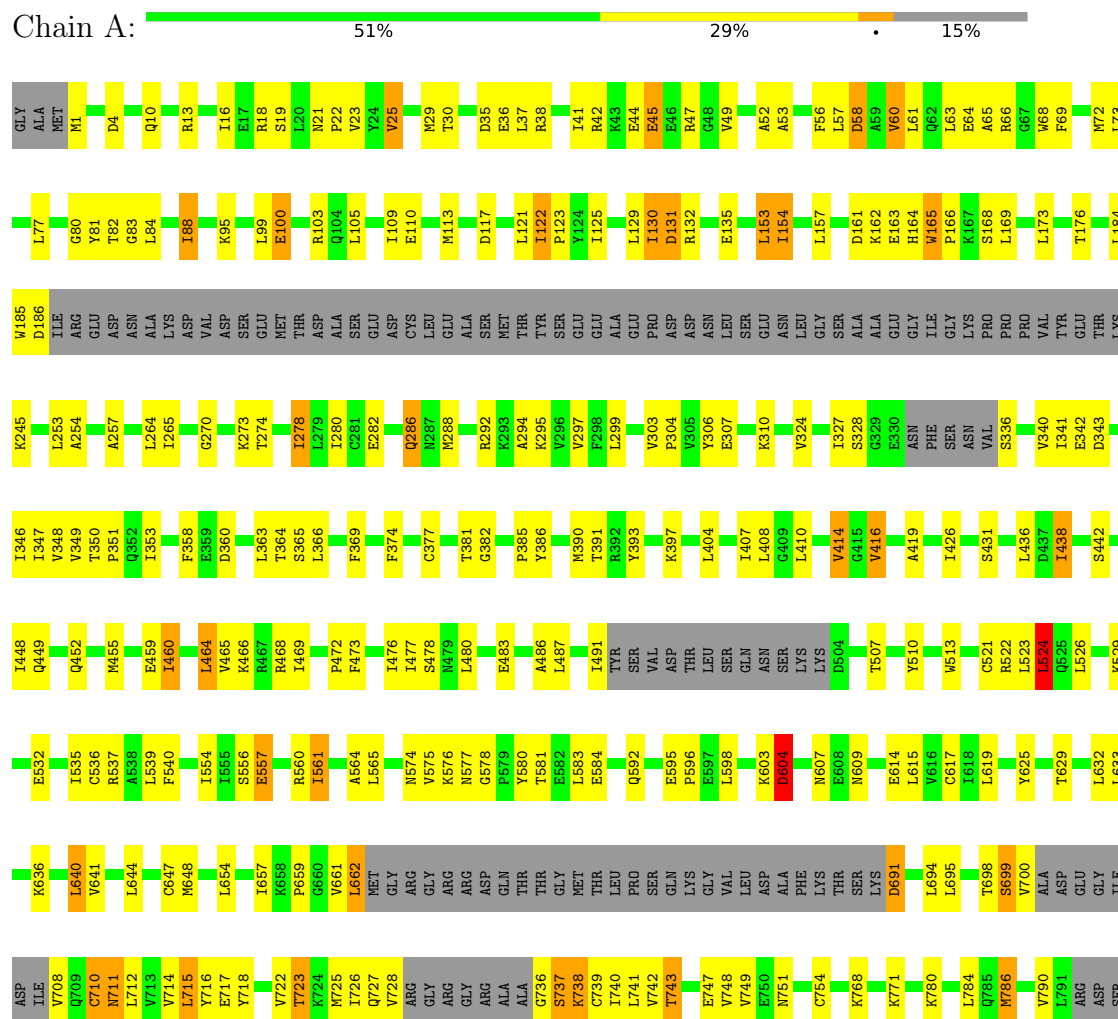
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D3TI84
A	-1	ALA	-	expression tag	UNP D3TI84
A	0	MET	-	expression tag	UNP D3TI84
B	-2	GLY	-	expression tag	UNP D3TI84
B	-1	ALA	-	expression tag	UNP D3TI84
B	0	MET	-	expression tag	UNP D3TI84
D	-2	GLY	-	expression tag	UNP D3TI84
D	-1	ALA	-	expression tag	UNP D3TI84
D	0	MET	-	expression tag	UNP D3TI84
E	-2	GLY	-	expression tag	UNP D3TI84
E	-1	ALA	-	expression tag	UNP D3TI84
E	0	MET	-	expression tag	UNP D3TI84

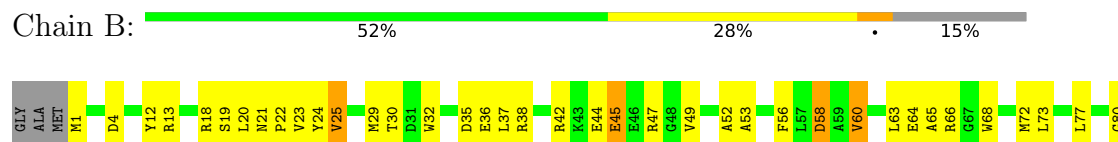
3 Residue-property plots

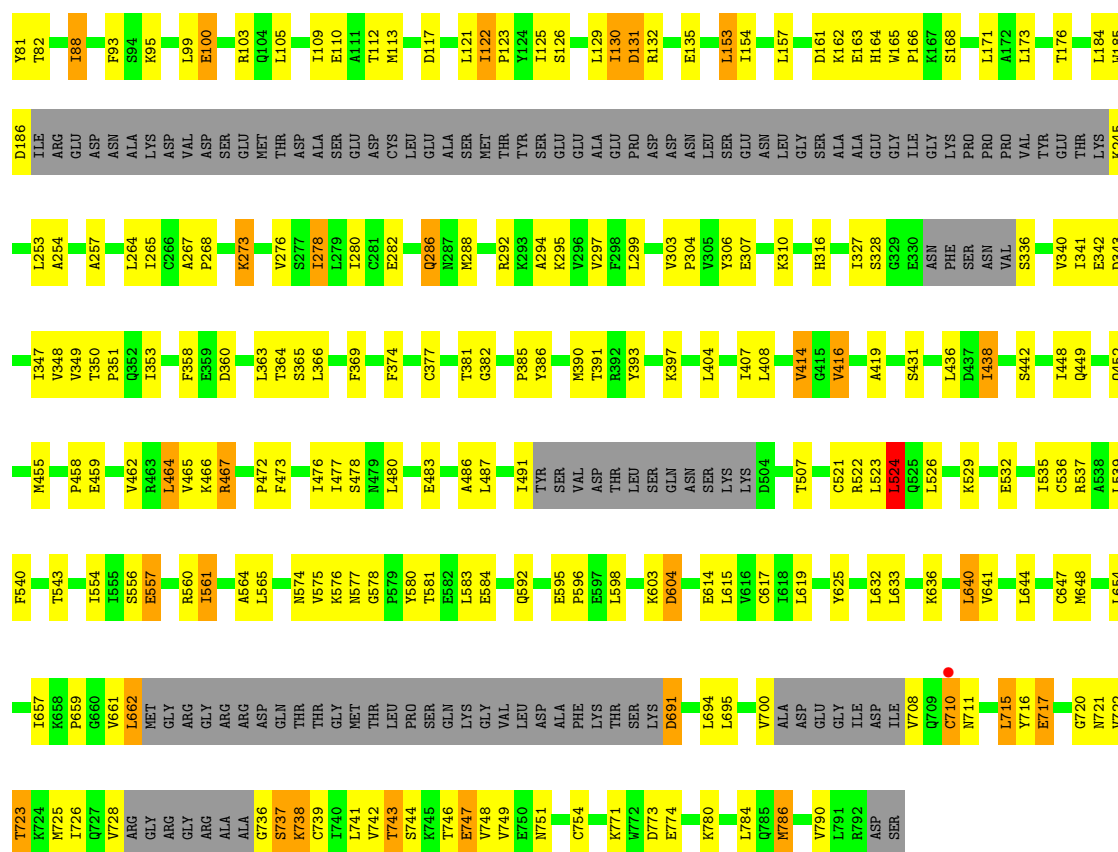
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

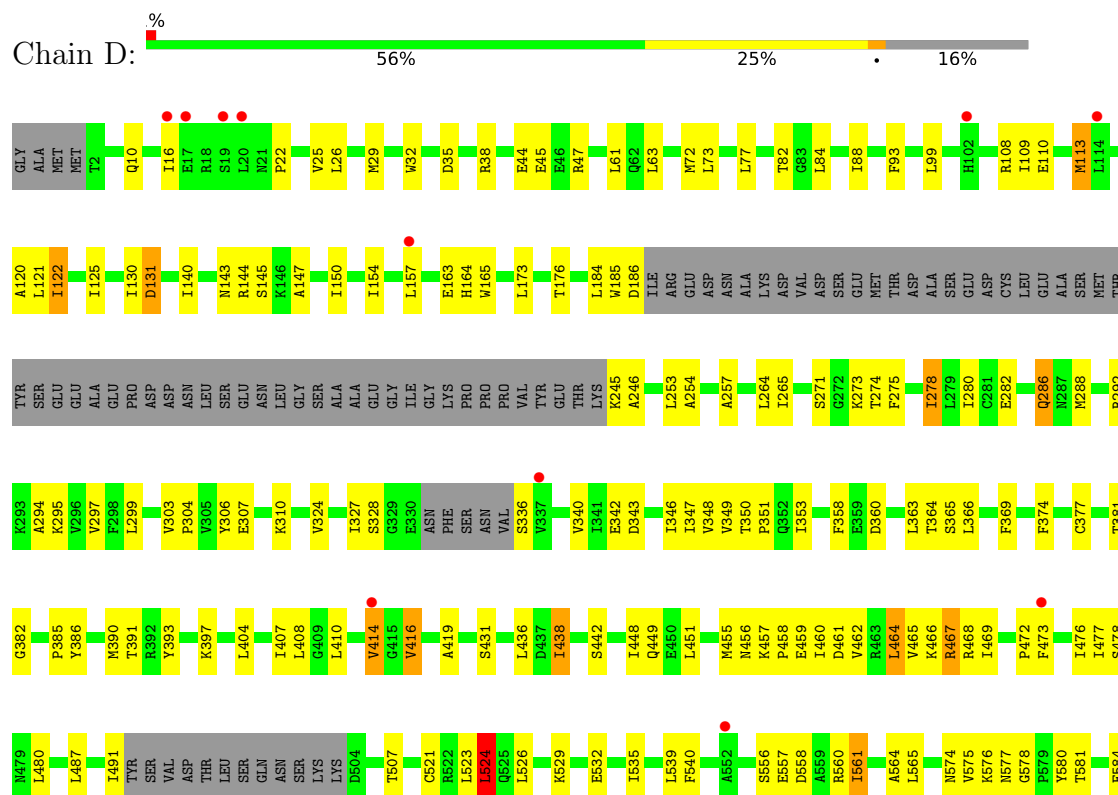


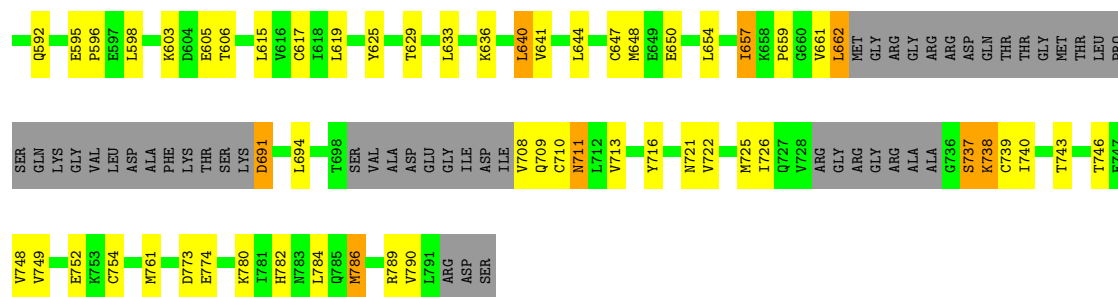
• Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I



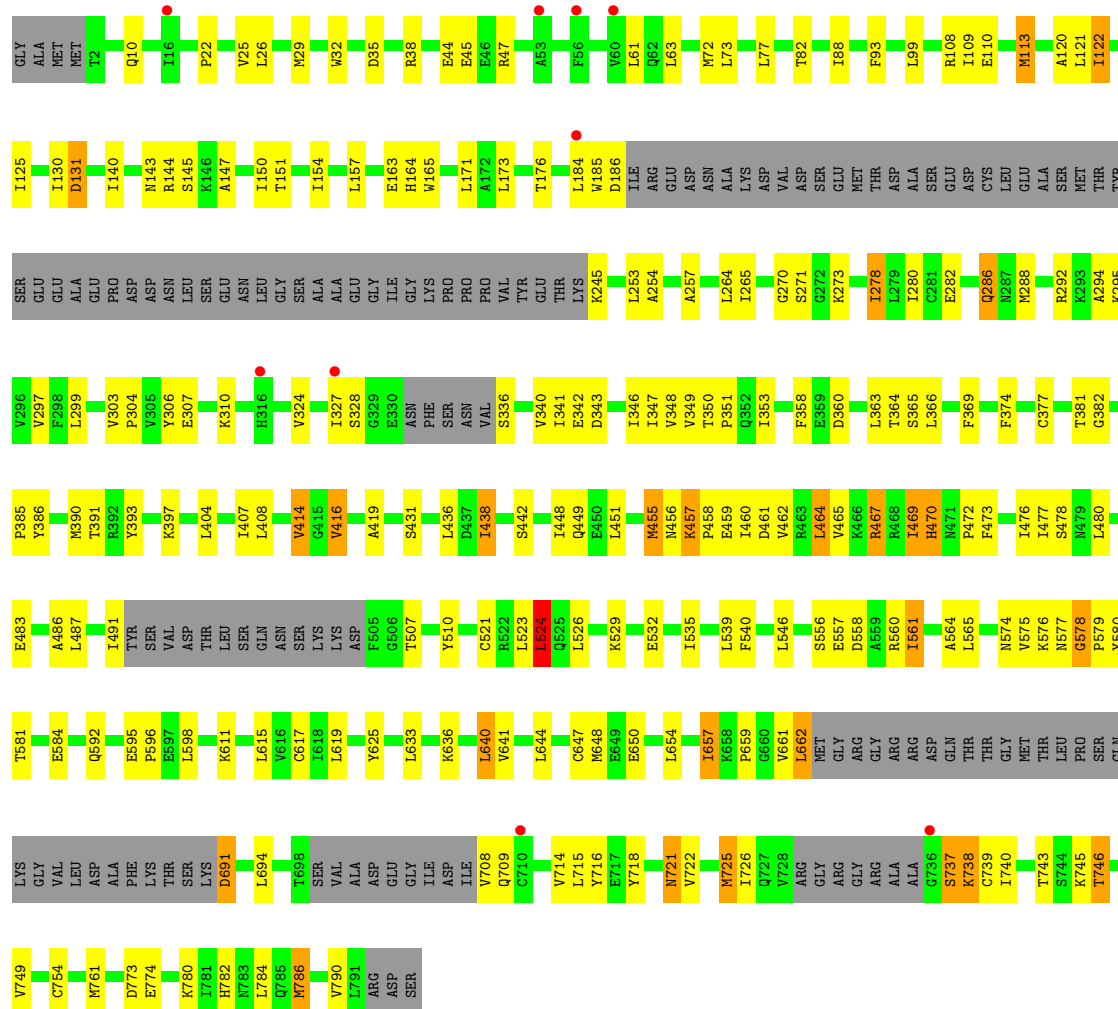


- Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I





• Molecule 1: RETINOIC ACID INDUCIBLE PROTEIN I



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	314.97Å 134.49Å 102.26Å 90.00° 92.17° 90.00°	Depositor
Resolution (Å)	157.37 – 3.40 157.37 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (157.37-3.40) 97.6 (157.37-3.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.239 , 0.276 0.241 , 0.276	Depositor DCC
R_{free} test set	2904 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	97.2	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 104.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21661	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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	0.69	0/5510	0.86	5/7434 (0.1%)
1	B	0.69	0/5521	0.87	4/7448 (0.1%)
1	D	0.59	0/5489	0.80	4/7406 (0.1%)
1	E	0.60	0/5481	0.80	6/7395 (0.1%)
All	All	0.64	0/22001	0.83	19/29683 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ILE	N-CA-C	5.77	115.04	106.85
1	D	122	ILE	CB-CA-C	-5.56	108.42	113.70
1	B	126	SER	N-CA-C	5.46	117.23	111.28
1	E	457	LYS	CA-C-N	-5.33	114.43	119.76
1	E	457	LYS	C-N-CA	-5.33	114.43	119.76
1	E	122	ILE	CB-CA-C	-5.25	108.71	113.70
1	A	578	GLY	CA-C-N	5.15	125.19	119.32
1	A	578	GLY	C-N-CA	5.15	125.19	119.32
1	B	720	GLY	N-CA-C	-5.14	107.07	111.95
1	B	578	GLY	CA-C-N	5.13	125.17	119.32
1	B	578	GLY	C-N-CA	5.13	125.17	119.32
1	D	578	GLY	CA-C-N	5.10	125.13	119.32
1	D	578	GLY	C-N-CA	5.10	125.13	119.32
1	E	657	ILE	N-CA-C	5.06	115.32	107.78
1	D	657	ILE	N-CA-C	5.05	115.31	107.78
1	A	165	TRP	CA-C-N	-5.02	113.57	119.84
1	A	165	TRP	C-N-CA	-5.02	113.57	119.84
1	E	578	GLY	CA-C-N	5.01	125.03	119.32
1	E	578	GLY	C-N-CA	5.01	125.03	119.32

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	5425	0	5473	204	0
1	B	5436	0	5486	213	0
1	D	5404	0	5447	167	0
1	E	5396	0	5443	166	0
All	All	21661	0	21849	741	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 17.

All (741) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:MET:HE1	1:E:173:LEU:HD21	1.45	0.99
1:D:524:LEU:HD23	1:D:526:LEU:HD12	1.45	0.98
1:E:524:LEU:HD23	1:E:526:LEU:HD12	1.47	0.97
1:A:524:LEU:HD23	1:A:526:LEU:HD12	1.48	0.95
1:B:524:LEU:HD23	1:B:526:LEU:HD12	1.48	0.95
1:D:113:MET:HE1	1:D:173:LEU:HD21	1.49	0.94
1:B:257:ALA:HB3	1:B:280:ILE:HD12	1.51	0.92
1:A:257:ALA:HB3	1:A:280:ILE:HD12	1.53	0.91
1:B:60:VAL:HG11	1:B:72:MET:CE	2.01	0.89
1:D:464:LEU:HD22	1:D:749:VAL:HG21	1.55	0.89
1:B:700:VAL:HG11	1:B:728:VAL:HG12	1.54	0.89
1:B:715:LEU:HD11	1:B:722:VAL:HG13	1.54	0.88
1:A:615:LEU:HD23	1:A:619:LEU:HD13	1.55	0.88
1:B:615:LEU:HD23	1:B:619:LEU:HD13	1.57	0.86
1:E:257:ALA:HB3	1:E:280:ILE:HD12	1.56	0.85
1:D:257:ALA:HB3	1:D:280:ILE:HD12	1.57	0.84
1:D:288:MET:HG3	1:D:294:ALA:HB2	1.61	0.83
1:E:327:ILE:HG22	1:E:349:VAL:HG22	1.59	0.83
1:B:60:VAL:HG11	1:B:72:MET:HE1	1.62	0.82
1:E:288:MET:HG3	1:E:294:ALA:HB2	1.61	0.82
1:D:327:ILE:HG22	1:D:349:VAL:HG22	1.61	0.82
1:E:288:MET:HE1	1:E:292:ARG:HG2	1.62	0.81
1:A:288:MET:HG3	1:A:294:ALA:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ILE:HG22	1:A:349:VAL:HG22	1.63	0.81
1:B:288:MET:HG3	1:B:294:ALA:HB2	1.63	0.81
1:A:60:VAL:HG11	1:A:72:MET:CE	2.11	0.81
1:A:328:SER:HA	1:A:353:ILE:HD11	1.62	0.81
1:D:328:SER:HA	1:D:353:ILE:HD11	1.63	0.80
1:B:288:MET:HE1	1:B:292:ARG:HG2	1.62	0.80
1:A:288:MET:HE1	1:A:292:ARG:HG2	1.63	0.80
1:B:327:ILE:HG22	1:B:349:VAL:HG22	1.63	0.79
1:A:13:ARG:NH2	1:A:58:ASP:OD1	2.15	0.79
1:E:77:LEU:HD23	1:E:82:THR:HG22	1.63	0.79
1:B:328:SER:HA	1:B:353:ILE:HD11	1.62	0.79
1:E:328:SER:HA	1:E:353:ILE:HD11	1.63	0.79
1:D:288:MET:HE1	1:D:292:ARG:HG2	1.64	0.79
1:B:700:VAL:HG11	1:B:728:VAL:CG1	2.14	0.77
1:E:121:LEU:HD11	1:E:173:LEU:HD12	1.64	0.77
1:B:13:ARG:NH2	1:B:58:ASP:OD1	2.18	0.77
1:D:561:ILE:HD12	1:D:561:ILE:H	1.50	0.77
1:A:715:LEU:HD11	1:A:722:VAL:HG13	1.66	0.77
1:D:460:ILE:HD13	1:D:722:VAL:HG11	1.67	0.77
1:D:77:LEU:HD23	1:D:82:THR:HG22	1.64	0.77
1:D:121:LEU:HD11	1:D:173:LEU:HD12	1.67	0.77
1:D:615:LEU:HD23	1:D:619:LEU:HD13	1.67	0.76
1:B:297:VAL:HG12	1:B:299:LEU:HD23	1.69	0.75
1:E:615:LEU:HD23	1:E:619:LEU:HD13	1.68	0.75
1:E:561:ILE:HD12	1:E:561:ILE:H	1.52	0.75
1:B:122:ILE:HA	1:B:125:ILE:HG22	1.69	0.74
1:A:743:THR:HG21	1:A:748:VAL:HB	1.67	0.74
1:A:60:VAL:HG11	1:A:72:MET:HE1	1.67	0.73
1:A:257:ALA:HB3	1:A:280:ILE:CD1	2.19	0.73
1:D:10:GLN:OE1	1:D:61:LEU:HD13	1.89	0.73
1:A:297:VAL:HG12	1:A:299:LEU:HD23	1.71	0.72
1:B:257:ALA:HB3	1:B:280:ILE:CD1	2.18	0.72
1:B:121:LEU:HD11	1:B:173:LEU:HD12	1.70	0.72
1:B:464:LEU:HD12	1:B:749:VAL:HG21	1.71	0.72
1:D:73:LEU:HD21	1:D:88:ILE:CD1	2.19	0.72
1:D:726:ILE:HD11	1:D:739:CYS:SG	2.30	0.72
1:A:105:LEU:HD23	1:A:185:TRP:CZ3	2.24	0.72
1:B:125:ILE:CD1	1:B:153:LEU:HD21	2.19	0.72
1:D:73:LEU:HD21	1:D:88:ILE:HD11	1.71	0.71
1:B:695:LEU:HD12	1:B:708:VAL:HG11	1.71	0.71
1:A:121:LEU:HD11	1:A:173:LEU:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:THR:HG21	1:B:748:VAL:HB	1.71	0.71
1:D:472:PRO:O	1:D:476:ILE:HD13	1.91	0.70
1:A:125:ILE:CD1	1:A:153:LEU:HD21	2.21	0.70
1:B:99:LEU:HD21	1:B:163:GLU:HA	1.73	0.70
1:E:472:PRO:O	1:E:476:ILE:HD13	1.92	0.70
1:A:122:ILE:HA	1:A:125:ILE:HG22	1.72	0.70
1:A:561:ILE:HD12	1:A:561:ILE:H	1.56	0.70
1:E:297:VAL:HG12	1:E:299:LEU:HD23	1.74	0.70
1:E:73:LEU:HD21	1:E:88:ILE:HD11	1.73	0.70
1:A:472:PRO:O	1:A:476:ILE:HD13	1.91	0.69
1:D:297:VAL:HG12	1:D:299:LEU:HD23	1.74	0.69
1:E:73:LEU:HD21	1:E:88:ILE:CD1	2.21	0.69
1:E:718:TYR:CE1	1:E:725:MET:HE2	2.28	0.69
1:B:561:ILE:HD12	1:B:561:ILE:H	1.56	0.69
1:A:265:ILE:HD13	1:A:442:SER:HB3	1.75	0.69
1:B:105:LEU:HD23	1:B:185:TRP:CZ3	2.28	0.69
1:E:257:ALA:HB3	1:E:280:ILE:CD1	2.21	0.69
1:B:465:VAL:HG13	1:B:614:GLU:HG3	1.73	0.69
1:A:592:GLN:OE1	1:B:592:GLN:OE1	2.10	0.68
1:D:257:ALA:HB3	1:D:280:ILE:CD1	2.22	0.68
1:A:615:LEU:HD22	1:A:648:MET:HE1	1.76	0.68
1:E:265:ILE:HD13	1:E:442:SER:HB3	1.73	0.68
1:D:265:ILE:HD13	1:D:442:SER:HB3	1.74	0.68
1:D:737:SER:O	1:D:738:LYS:HB2	1.95	0.67
1:B:737:SER:O	1:B:738:LYS:HB2	1.94	0.67
1:E:10:GLN:OE1	1:E:61:LEU:HD13	1.94	0.67
1:B:153:LEU:C	1:B:153:LEU:HD23	2.19	0.67
1:B:265:ILE:HD13	1:B:442:SER:HB3	1.75	0.67
1:D:73:LEU:CD2	1:D:88:ILE:HD11	2.25	0.66
1:E:654:LEU:HD22	1:E:657:ILE:HD12	1.77	0.66
1:D:615:LEU:HD22	1:D:648:MET:HE1	1.78	0.66
1:A:153:LEU:HD23	1:A:153:LEU:C	2.20	0.66
1:A:737:SER:O	1:A:738:LYS:HB2	1.94	0.66
1:B:700:VAL:CG1	1:B:728:VAL:HG12	2.25	0.65
1:A:99:LEU:HD21	1:A:163:GLU:HA	1.77	0.65
1:A:722:VAL:HG21	1:A:741:LEU:HD22	1.79	0.65
1:D:29:MET:HE1	1:D:72:MET:HA	1.79	0.65
1:E:615:LEU:HD22	1:E:648:MET:HE1	1.79	0.65
1:E:73:LEU:CD2	1:E:88:ILE:HD11	2.26	0.65
1:B:615:LEU:HD22	1:B:648:MET:HE1	1.79	0.65
1:E:737:SER:O	1:E:738:LYS:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:HD11	1:A:157:LEU:CD1	2.28	0.64
1:A:165:TRP:O	1:A:166:PRO:C	2.40	0.64
1:D:278:ILE:C	1:D:278:ILE:HD12	2.22	0.64
1:E:278:ILE:C	1:E:278:ILE:HD12	2.21	0.63
1:D:122:ILE:HA	1:D:125:ILE:HG22	1.81	0.63
1:D:264:LEU:HD13	1:D:377:CYS:SG	2.39	0.63
1:B:25:VAL:HG13	1:B:29:MET:CE	2.29	0.63
1:E:416:VAL:HG13	1:E:419:ALA:HB3	1.81	0.63
1:B:165:TRP:O	1:B:166:PRO:C	2.38	0.63
1:B:472:PRO:O	1:B:476:ILE:HD13	1.98	0.63
1:E:122:ILE:HA	1:E:125:ILE:HG22	1.81	0.63
1:B:416:VAL:HG13	1:B:419:ALA:HB3	1.81	0.63
1:A:416:VAL:HG13	1:A:419:ALA:HB3	1.80	0.63
1:D:654:LEU:HD22	1:D:657:ILE:HD12	1.80	0.63
1:A:44:GLU:OE2	1:A:47:ARG:NH1	2.32	0.62
1:B:726:ILE:HD11	1:B:739:CYS:SG	2.39	0.62
1:B:654:LEU:HD22	1:B:657:ILE:HD12	1.81	0.62
1:A:715:LEU:HD12	1:A:722:VAL:HG22	1.81	0.62
1:D:416:VAL:HG13	1:D:419:ALA:HB3	1.81	0.62
1:A:88:ILE:HD12	1:A:88:ILE:C	2.23	0.62
1:A:278:ILE:HD12	1:A:278:ILE:C	2.25	0.62
1:A:487:LEU:O	1:A:491:ILE:HD13	1.99	0.62
1:D:108:ARG:NH2	1:D:532:GLU:OE2	2.32	0.62
1:A:654:LEU:HD22	1:A:657:ILE:HD12	1.81	0.61
1:E:726:ILE:HD11	1:E:739:CYS:SG	2.40	0.61
1:A:603:LYS:O	1:A:604:ASP:C	2.42	0.61
1:B:88:ILE:C	1:B:88:ILE:HD12	2.26	0.61
1:E:264:LEU:HD13	1:E:377:CYS:SG	2.40	0.61
1:B:44:GLU:OE2	1:B:47:ARG:NH1	2.34	0.61
1:A:615:LEU:HD12	1:A:716:TYR:CD1	2.36	0.61
1:A:264:LEU:HD13	1:A:377:CYS:SG	2.40	0.61
1:B:393:TYR:CD1	1:B:404:LEU:HD22	2.36	0.61
1:D:606:THR:O	1:D:606:THR:HG22	2.01	0.61
1:B:487:LEU:O	1:B:491:ILE:HD13	2.01	0.60
1:E:487:LEU:O	1:E:491:ILE:HD13	2.01	0.60
1:A:700:VAL:HG21	1:A:728:VAL:C	2.26	0.60
1:B:278:ILE:C	1:B:278:ILE:HD12	2.26	0.60
1:B:581:THR:HB	1:B:584:GLU:HG3	1.83	0.60
1:B:328:SER:HA	1:B:353:ILE:CD1	2.30	0.60
1:D:393:TYR:CD1	1:D:404:LEU:HD22	2.37	0.60
1:A:726:ILE:HD11	1:A:739:CYS:SG	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:LEU:HD12	1:B:722:VAL:HG22	1.83	0.59
1:E:29:MET:HE1	1:E:72:MET:HA	1.84	0.59
1:E:328:SER:HA	1:E:353:ILE:CD1	2.32	0.59
1:B:130:ILE:O	1:B:131:ASP:C	2.45	0.59
1:E:416:VAL:CG1	1:E:416:VAL:O	2.50	0.59
1:A:125:ILE:HD11	1:A:157:LEU:HD13	1.83	0.59
1:A:393:TYR:CD1	1:A:404:LEU:HD22	2.38	0.59
1:A:595:GLU:OE1	1:B:576:LYS:NZ	2.34	0.59
1:D:147:ALA:O	1:D:150:ILE:HG22	2.02	0.59
1:B:297:VAL:HG12	1:B:299:LEU:CD2	2.32	0.59
1:E:393:TYR:CD1	1:E:404:LEU:HD22	2.37	0.59
1:A:25:VAL:HG13	1:A:29:MET:CE	2.33	0.58
1:A:581:THR:HB	1:A:584:GLU:HG3	1.84	0.58
1:B:288:MET:HE2	1:B:294:ALA:CA	2.34	0.58
1:D:109:ILE:HG22	1:D:109:ILE:O	2.02	0.58
1:B:615:LEU:HD12	1:B:716:TYR:CD1	2.38	0.58
1:D:143:ASN:CG	1:E:650:GLU:HG2	2.28	0.58
1:A:288:MET:HE2	1:A:294:ALA:CA	2.33	0.58
1:A:615:LEU:HD12	1:A:716:TYR:CG	2.39	0.58
1:B:722:VAL:HG21	1:B:741:LEU:HD22	1.85	0.58
1:D:328:SER:HA	1:D:353:ILE:CD1	2.33	0.58
1:E:469:ILE:O	1:E:470:HIS:CG	2.56	0.58
1:D:416:VAL:O	1:D:416:VAL:CG1	2.51	0.58
1:D:288:MET:HE2	1:D:294:ALA:CA	2.34	0.58
1:A:21:ASN:OD1	1:A:23:VAL:HG23	2.04	0.58
1:B:21:ASN:OD1	1:B:23:VAL:HG23	2.04	0.57
1:D:487:LEU:O	1:D:491:ILE:HD13	2.04	0.57
1:D:558:ASP:HB2	1:D:640:LEU:HD11	1.86	0.57
1:E:560:ARG:HG3	1:E:647:CYS:SG	2.43	0.57
1:A:328:SER:HA	1:A:353:ILE:CD1	2.32	0.57
1:A:416:VAL:O	1:A:416:VAL:CG1	2.53	0.57
1:E:147:ALA:O	1:E:150:ILE:HG22	2.04	0.57
1:E:288:MET:HE2	1:E:294:ALA:CA	2.35	0.57
1:B:264:LEU:HD13	1:B:377:CYS:SG	2.44	0.57
1:D:364:THR:HG22	1:D:364:THR:O	2.04	0.57
1:E:109:ILE:HG22	1:E:109:ILE:O	2.02	0.57
1:A:130:ILE:O	1:A:131:ASP:C	2.47	0.57
1:B:125:ILE:HD11	1:B:157:LEU:CD1	2.35	0.57
1:E:465:VAL:HG11	1:E:611:LYS:HA	1.87	0.57
1:B:184:LEU:HD12	1:B:522:ARG:HD3	1.87	0.57
1:D:26:LEU:HD22	1:D:38:ARG:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LEU:HD22	1:E:38:ARG:HG2	1.87	0.57
1:A:184:LEU:HD12	1:A:522:ARG:HD3	1.87	0.56
1:B:364:THR:HG22	1:B:364:THR:O	2.05	0.56
1:D:565:LEU:HD12	1:D:598:LEU:HB3	1.87	0.56
1:A:560:ARG:HG3	1:A:647:CYS:SG	2.45	0.56
1:A:715:LEU:CD1	1:A:722:VAL:HG22	2.36	0.56
1:D:297:VAL:HG12	1:D:299:LEU:CD2	2.36	0.56
1:E:108:ARG:NH2	1:E:532:GLU:OE2	2.37	0.56
1:D:629:THR:HG23	1:D:711:ASN:OD1	2.06	0.56
1:E:364:THR:O	1:E:364:THR:HG22	2.04	0.56
1:E:297:VAL:HG12	1:E:299:LEU:CD2	2.36	0.56
1:A:297:VAL:HG12	1:A:299:LEU:CD2	2.35	0.56
1:D:99:LEU:HD22	1:D:165:TRP:NE1	2.21	0.56
1:D:560:ARG:HG3	1:D:647:CYS:SG	2.46	0.56
1:B:565:LEU:HD12	1:B:598:LEU:HB3	1.88	0.55
1:E:469:ILE:HD12	1:E:469:ILE:H	1.71	0.55
1:E:558:ASP:HB2	1:E:640:LEU:HD11	1.88	0.55
1:A:73:LEU:HD21	1:A:88:ILE:CG1	2.36	0.55
1:E:99:LEU:HD22	1:E:165:TRP:NE1	2.21	0.55
1:A:184:LEU:HD21	1:A:540:PHE:CE1	2.41	0.55
1:E:88:ILE:HG22	1:E:93:PHE:HZ	1.70	0.55
1:A:364:THR:HG22	1:A:364:THR:O	2.06	0.55
1:B:786:MET:HE2	1:B:786:MET:N	2.21	0.55
1:A:257:ALA:CB	1:A:280:ILE:HD12	2.33	0.55
1:A:786:MET:N	1:A:786:MET:HE2	2.22	0.55
1:D:615:LEU:HD12	1:D:716:TYR:CD1	2.40	0.55
1:E:565:LEU:HD12	1:E:598:LEU:HB3	1.87	0.55
1:D:464:LEU:CD2	1:D:749:VAL:HG21	2.34	0.55
1:A:698:THR:O	1:A:700:VAL:N	2.40	0.55
1:B:184:LEU:HD21	1:B:540:PHE:CE1	2.42	0.55
1:D:88:ILE:HG22	1:D:93:PHE:HZ	1.70	0.55
1:A:1:MET:HB2	1:A:4:ASP:HB2	1.89	0.54
1:B:22:PRO:HG3	1:B:53:ALA:HA	1.89	0.54
1:A:35:ASP:OD1	1:A:38:ARG:NH2	2.38	0.54
1:A:465:VAL:HG13	1:A:614:GLU:HG3	1.88	0.54
1:A:565:LEU:HD12	1:A:598:LEU:HB3	1.88	0.54
1:B:257:ALA:CB	1:B:280:ILE:HD12	2.32	0.54
1:B:416:VAL:CG1	1:B:416:VAL:O	2.55	0.54
1:D:786:MET:HE2	1:D:786:MET:N	2.23	0.54
1:B:477:ILE:O	1:B:480:LEU:N	2.40	0.54
1:E:581:THR:HB	1:E:584:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:MET:HE1	1:D:407:ILE:HD12	1.89	0.54
1:E:390:MET:HE1	1:E:407:ILE:HD12	1.90	0.54
1:D:521:CYS:SG	1:D:539:LEU:HD13	2.48	0.53
1:A:390:MET:HE1	1:A:407:ILE:HD12	1.91	0.53
1:D:110:GLU:HG3	1:D:154:ILE:HD11	1.91	0.53
1:B:23:VAL:HG13	1:B:42:ARG:HG2	1.90	0.53
1:D:581:THR:HB	1:D:584:GLU:HG3	1.90	0.53
1:E:633:LEU:HD12	1:E:714:VAL:HG12	1.89	0.53
1:E:461:ASP:HB3	1:E:740:ILE:HG23	1.91	0.53
1:E:464:LEU:HD12	1:E:465:VAL:N	2.24	0.53
1:B:73:LEU:HD21	1:B:88:ILE:CG1	2.39	0.53
1:B:129:LEU:HD21	1:B:157:LEU:HD13	1.91	0.53
1:A:73:LEU:HD21	1:A:88:ILE:HG13	1.91	0.52
1:B:603:LYS:O	1:B:604:ASP:C	2.52	0.52
1:D:461:ASP:CB	1:D:740:ILE:HG23	2.39	0.52
1:D:710:CYS:SG	1:D:711:ASN:N	2.82	0.52
1:A:129:LEU:HD21	1:A:157:LEU:HD13	1.90	0.52
1:B:523:LEU:O	1:B:524:LEU:C	2.53	0.52
1:E:140:ILE:HG23	1:E:144:ARG:HD3	1.92	0.52
1:B:125:ILE:HD11	1:B:157:LEU:HD13	1.91	0.52
1:E:349:VAL:HG12	1:E:350:THR:O	2.10	0.52
1:A:270:GLY:HA3	1:A:727:GLN:HE22	1.74	0.52
1:B:125:ILE:HD11	1:B:157:LEU:CD2	2.39	0.52
1:B:790:VAL:HG12	1:B:790:VAL:O	2.10	0.52
1:E:521:CYS:SG	1:E:539:LEU:HD13	2.49	0.52
1:A:358:PHE:CZ	1:A:366:LEU:HD13	2.45	0.52
1:B:1:MET:HB2	1:B:4:ASP:HB2	1.91	0.52
1:E:310:LYS:HA	1:E:348:VAL:HG21	1.91	0.52
1:B:25:VAL:HG13	1:B:29:MET:HE2	1.91	0.51
1:B:722:VAL:O	1:B:723:THR:C	2.53	0.51
1:B:477:ILE:O	1:B:478:SER:C	2.52	0.51
1:D:77:LEU:CD2	1:D:82:THR:HG22	2.39	0.51
1:E:77:LEU:CD2	1:E:82:THR:HG22	2.38	0.51
1:B:297:VAL:CG1	1:B:299:LEU:CD2	2.88	0.51
1:D:790:VAL:HG12	1:D:790:VAL:O	2.09	0.51
1:A:310:LYS:HA	1:A:348:VAL:HG21	1.92	0.51
1:B:73:LEU:HD21	1:B:88:ILE:HD11	1.92	0.51
1:B:358:PHE:CZ	1:B:366:LEU:HD13	2.45	0.51
1:E:786:MET:N	1:E:786:MET:HE2	2.24	0.51
1:A:110:GLU:HG3	1:A:154:ILE:HD11	1.91	0.51
1:B:615:LEU:HD11	1:B:633:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:LEU:HB2	1:B:710:CYS:SG	2.50	0.51
1:D:524:LEU:CD2	1:D:526:LEU:HD12	2.28	0.51
1:A:700:VAL:HG11	1:A:728:VAL:HG12	1.93	0.51
1:A:464:LEU:HD12	1:A:749:VAL:HG21	1.92	0.51
1:A:523:LEU:O	1:A:524:LEU:C	2.53	0.50
1:D:140:ILE:HG23	1:D:144:ARG:HD3	1.93	0.50
1:D:349:VAL:HG12	1:D:350:THR:O	2.10	0.50
1:A:73:LEU:HD21	1:A:88:ILE:HD11	1.92	0.50
1:A:349:VAL:HG12	1:A:350:THR:O	2.11	0.50
1:B:743:THR:HG21	1:B:748:VAL:CB	2.39	0.50
1:E:110:GLU:HG3	1:E:154:ILE:HD11	1.93	0.50
1:E:523:LEU:O	1:E:524:LEU:C	2.55	0.50
1:B:747:GLU:O	1:B:751:ASN:HB2	2.12	0.50
1:A:73:LEU:HD11	1:A:88:ILE:HD11	1.94	0.50
1:A:350:THR:HG23	1:A:351:PRO:HD2	1.93	0.50
1:B:350:THR:HG23	1:B:351:PRO:HD2	1.93	0.50
1:E:295:LYS:NZ	1:E:342:GLU:HA	2.27	0.50
1:E:390:MET:HE1	1:E:407:ILE:CD1	2.41	0.50
1:B:310:LYS:HA	1:B:348:VAL:HG21	1.92	0.50
1:A:60:VAL:HG13	1:A:68:TRP:CZ3	2.47	0.50
1:A:615:LEU:HD11	1:A:633:LEU:HD11	1.93	0.50
1:B:715:LEU:CD1	1:B:722:VAL:HG22	2.42	0.50
1:A:25:VAL:HG13	1:A:29:MET:HE2	1.94	0.50
1:A:436:LEU:CB	1:A:438:ILE:HD13	2.42	0.50
1:B:110:GLU:HG3	1:B:154:ILE:HD11	1.94	0.50
1:D:464:LEU:HD13	1:D:749:VAL:CG2	2.42	0.50
1:B:381:THR:HG22	1:B:382:GLY:N	2.27	0.50
1:B:574:ASN:O	1:B:575:VAL:C	2.55	0.50
1:B:347:ILE:HG22	1:B:349:VAL:CG2	2.42	0.50
1:B:390:MET:HE1	1:B:407:ILE:HD12	1.93	0.50
1:B:615:LEU:HD12	1:B:716:TYR:CG	2.47	0.50
1:D:358:PHE:CZ	1:D:366:LEU:HD13	2.47	0.50
1:A:63:LEU:HD23	1:A:68:TRP:CG	2.47	0.49
1:A:477:ILE:O	1:A:480:LEU:N	2.44	0.49
1:B:483:GLU:O	1:B:486:ALA:HB3	2.12	0.49
1:A:80:GLY:O	1:A:82:THR:N	2.45	0.49
1:A:714:VAL:HG22	1:A:740:ILE:HB	1.94	0.49
1:B:73:LEU:HD21	1:B:88:ILE:HG13	1.93	0.49
1:B:661:VAL:HG12	1:B:662:LEU:N	2.27	0.49
1:B:295:LYS:NZ	1:B:342:GLU:HA	2.27	0.49
1:D:295:LYS:NZ	1:D:342:GLU:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:HG3	1:A:154:ILE:CD1	2.42	0.49
1:A:465:VAL:HG21	1:A:742:VAL:HG13	1.94	0.49
1:A:615:LEU:HD22	1:A:648:MET:CE	2.41	0.49
1:B:328:SER:CA	1:B:353:ILE:HD11	2.37	0.49
1:E:32:TRP:HB3	1:E:63:LEU:HD21	1.94	0.49
1:A:297:VAL:CG1	1:A:299:LEU:CD2	2.90	0.49
1:B:336:SER:O	1:B:340:VAL:HG23	2.13	0.49
1:D:390:MET:HE1	1:D:407:ILE:CD1	2.42	0.49
1:A:295:LYS:NZ	1:A:342:GLU:HA	2.27	0.49
1:A:431:SER:HA	1:A:784:LEU:HD13	1.93	0.49
1:D:464:LEU:HD13	1:D:749:VAL:HG21	1.94	0.49
1:A:23:VAL:HG13	1:A:42:ARG:HG2	1.95	0.49
1:B:700:VAL:HG21	1:B:728:VAL:C	2.38	0.49
1:D:32:TRP:HB3	1:D:63:LEU:HD21	1.94	0.49
1:D:310:LYS:HA	1:D:348:VAL:HG21	1.94	0.49
1:B:60:VAL:HG13	1:B:68:TRP:CZ3	2.48	0.49
1:E:328:SER:CA	1:E:353:ILE:HD11	2.38	0.49
1:E:347:ILE:HG22	1:E:349:VAL:CG2	2.43	0.49
1:A:303:VAL:N	1:A:304:PRO:HD2	2.28	0.49
1:A:381:THR:HG22	1:A:382:GLY:N	2.28	0.49
1:A:629:THR:HG23	1:A:711:ASN:OD1	2.13	0.49
1:B:95:LYS:HD3	1:B:163:GLU:OE1	2.13	0.49
1:D:477:ILE:O	1:D:480:LEU:N	2.46	0.48
1:E:358:PHE:CZ	1:E:366:LEU:HD13	2.47	0.48
1:E:431:SER:HA	1:E:784:LEU:HD13	1.95	0.48
1:B:306:TYR:CZ	1:B:328:SER:HB2	2.48	0.48
1:B:385:PRO:O	1:B:386:TYR:C	2.54	0.48
1:B:35:ASP:OD1	1:B:38:ARG:NH2	2.41	0.48
1:B:595:GLU:N	1:B:596:PRO:CD	2.76	0.48
1:A:22:PRO:HG3	1:A:53:ALA:HA	1.95	0.48
1:A:385:PRO:O	1:A:386:TYR:C	2.56	0.48
1:A:615:LEU:HD23	1:A:619:LEU:CD1	2.37	0.48
1:B:303:VAL:N	1:B:304:PRO:HD2	2.28	0.48
1:D:650:GLU:HG2	1:E:143:ASN:CG	2.39	0.48
1:D:726:ILE:CD1	1:D:739:CYS:SG	3.00	0.48
1:A:477:ILE:O	1:A:478:SER:C	2.57	0.48
1:B:45:GLU:HG2	1:B:49:VAL:HG22	1.95	0.48
1:B:524:LEU:CD2	1:B:526:LEU:HD12	2.31	0.48
1:D:143:ASN:HB3	1:E:650:GLU:CD	2.38	0.48
1:D:306:TYR:CZ	1:D:328:SER:HB2	2.49	0.48
1:A:336:SER:O	1:A:340:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ILE:N	1:B:491:ILE:HD12	2.28	0.48
1:B:122:ILE:HA	1:B:125:ILE:CG2	2.40	0.48
1:B:349:VAL:HG12	1:B:350:THR:O	2.12	0.48
1:D:264:LEU:HD21	1:D:414:VAL:CG1	2.44	0.48
1:D:523:LEU:O	1:D:524:LEU:C	2.56	0.48
1:E:257:ALA:CB	1:E:280:ILE:HD12	2.36	0.48
1:A:60:VAL:CG1	1:A:68:TRP:CZ3	2.96	0.48
1:D:347:ILE:HG22	1:D:349:VAL:CG2	2.42	0.48
1:E:691:ASP:OD2	1:E:691:ASP:N	2.47	0.48
1:E:790:VAL:O	1:E:790:VAL:HG12	2.14	0.48
1:A:347:ILE:HG22	1:A:349:VAL:CG2	2.43	0.47
1:A:390:MET:HE1	1:A:407:ILE:CD1	2.44	0.47
1:A:483:GLU:O	1:A:486:ALA:HB3	2.14	0.47
1:D:661:VAL:HG12	1:D:662:LEU:N	2.29	0.47
1:E:278:ILE:HD12	1:E:278:ILE:O	2.14	0.47
1:E:381:THR:HG22	1:E:382:GLY:N	2.29	0.47
1:E:436:LEU:CB	1:E:438:ILE:HD13	2.44	0.47
1:A:632:LEU:HB2	1:A:710:CYS:SG	2.54	0.47
1:B:615:LEU:HD22	1:B:648:MET:CE	2.44	0.47
1:D:431:SER:HA	1:D:784:LEU:HD13	1.96	0.47
1:E:615:LEU:HD22	1:E:648:MET:CE	2.44	0.47
1:A:661:VAL:HG12	1:A:662:LEU:N	2.28	0.47
1:B:465:VAL:HG12	1:B:466:LYS:N	2.29	0.47
1:D:436:LEU:CB	1:D:438:ILE:HD13	2.45	0.47
1:E:306:TYR:CZ	1:E:328:SER:HB2	2.49	0.47
1:A:288:MET:HE2	1:A:294:ALA:HB2	1.96	0.47
1:A:521:CYS:SG	1:A:539:LEU:HD13	2.55	0.47
1:A:524:LEU:CD2	1:A:526:LEU:HD12	2.31	0.47
1:B:63:LEU:HD23	1:B:68:TRP:CG	2.50	0.47
1:D:328:SER:CA	1:D:353:ILE:HD11	2.38	0.47
1:E:125:ILE:HD11	1:E:157:LEU:CD2	2.45	0.47
1:E:524:LEU:CD2	1:E:526:LEU:HD12	2.29	0.47
1:A:328:SER:CA	1:A:353:ILE:HD11	2.39	0.47
1:E:303:VAL:N	1:E:304:PRO:HD2	2.29	0.47
1:A:306:TYR:CZ	1:A:328:SER:HB2	2.49	0.47
1:A:722:VAL:CG2	1:A:741:LEU:HD22	2.44	0.47
1:A:790:VAL:HG12	1:A:790:VAL:O	2.14	0.47
1:D:22:PRO:HA	1:D:25:VAL:HG12	1.97	0.47
1:D:297:VAL:CG1	1:D:299:LEU:CD2	2.93	0.47
1:D:303:VAL:N	1:D:304:PRO:HD2	2.29	0.47
1:D:574:ASN:O	1:D:575:VAL:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:615:LEU:HD22	1:D:648:MET:CE	2.44	0.47
1:E:282:GLU:O	1:E:286:GLN:HB2	2.14	0.47
1:E:299:LEU:HD12	1:E:374:PHE:CE1	2.50	0.47
1:E:477:ILE:O	1:E:478:SER:C	2.57	0.47
1:A:554:ILE:HG22	1:A:640:LEU:HD12	1.96	0.47
1:B:254:ALA:HA	1:B:280:ILE:HD11	1.97	0.47
1:B:436:LEU:CB	1:B:438:ILE:HD13	2.45	0.47
1:E:416:VAL:HG11	1:E:761:MET:CE	2.45	0.47
1:D:327:ILE:HG23	1:D:353:ILE:HD13	1.97	0.47
1:E:641:VAL:HG11	1:E:661:VAL:HG13	1.97	0.47
1:A:691:ASP:OD2	1:A:691:ASP:N	2.48	0.47
1:D:257:ALA:CB	1:D:280:ILE:HD12	2.37	0.47
1:E:393:TYR:CE1	1:E:404:LEU:HD22	2.50	0.47
1:E:661:VAL:HG12	1:E:662:LEU:N	2.29	0.47
1:A:278:ILE:HD12	1:A:278:ILE:O	2.15	0.46
1:B:295:LYS:HZ3	1:B:342:GLU:HA	1.80	0.46
1:D:278:ILE:HD12	1:D:278:ILE:O	2.15	0.46
1:D:336:SER:O	1:D:340:VAL:HG23	2.16	0.46
1:E:336:SER:O	1:E:340:VAL:HG23	2.16	0.46
1:A:576:LYS:NZ	1:B:595:GLU:OE1	2.37	0.46
1:B:458:PRO:HG2	1:B:726:ILE:HD13	1.97	0.46
1:B:473:PHE:CZ	1:B:564:ALA:HB1	2.50	0.46
1:D:385:PRO:O	1:D:386:TYR:C	2.58	0.46
1:E:297:VAL:CG1	1:E:299:LEU:CD2	2.93	0.46
1:A:574:ASN:O	1:A:575:VAL:C	2.58	0.46
1:B:431:SER:HA	1:B:784:LEU:HD13	1.97	0.46
1:B:641:VAL:HG11	1:B:661:VAL:HG13	1.98	0.46
1:B:80:GLY:O	1:B:82:THR:N	2.47	0.46
1:B:288:MET:HE2	1:B:294:ALA:HB2	1.97	0.46
1:D:184:LEU:HD21	1:D:540:PHE:CE1	2.50	0.46
1:D:282:GLU:O	1:D:286:GLN:HB2	2.14	0.46
1:D:691:ASP:OD2	1:D:691:ASP:N	2.48	0.46
1:E:574:ASN:O	1:E:575:VAL:C	2.58	0.46
1:A:448:ILE:O	1:A:449:GLN:C	2.59	0.46
1:D:73:LEU:CG	1:D:88:ILE:HD11	2.45	0.46
1:D:561:ILE:HD12	1:D:561:ILE:N	2.25	0.46
1:E:350:THR:HG23	1:E:351:PRO:HD2	1.97	0.46
1:E:477:ILE:O	1:E:480:LEU:N	2.48	0.46
1:A:125:ILE:HD11	1:A:157:LEU:CD2	2.46	0.46
1:B:390:MET:HE1	1:B:407:ILE:CD1	2.46	0.46
1:B:722:VAL:CG2	1:B:741:LEU:HD22	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:641:VAL:HG11	1:D:661:VAL:HG13	1.96	0.46
1:E:99:LEU:HD21	1:E:163:GLU:HA	1.98	0.46
1:A:469:ILE:HD12	1:A:469:ILE:H	1.80	0.46
1:B:691:ASP:N	1:B:691:ASP:OD2	2.49	0.46
1:A:69:PHE:CZ	1:A:88:ILE:HD13	2.51	0.46
1:A:95:LYS:HD3	1:A:163:GLU:OE1	2.16	0.46
1:A:436:LEU:HB2	1:A:438:ILE:HD13	1.98	0.46
1:A:576:LYS:CE	1:A:592:GLN:HE22	2.28	0.46
1:D:44:GLU:OE2	1:D:47:ARG:NH1	2.48	0.46
1:D:477:ILE:O	1:D:478:SER:C	2.58	0.46
1:D:574:ASN:O	1:D:577:ASN:N	2.48	0.46
1:E:22:PRO:HA	1:E:25:VAL:HG12	1.98	0.46
1:E:461:ASP:CB	1:E:740:ILE:HG23	2.46	0.46
1:E:708:VAL:CG1	1:E:709:GLN:N	2.79	0.46
1:B:60:VAL:CG1	1:B:68:TRP:CZ3	2.99	0.46
1:D:381:THR:HG22	1:D:382:GLY:N	2.31	0.46
1:E:73:LEU:CG	1:E:88:ILE:HD11	2.46	0.46
1:A:254:ALA:HA	1:A:280:ILE:HD11	1.99	0.45
1:A:595:GLU:N	1:A:596:PRO:CD	2.78	0.45
1:B:110:GLU:HG3	1:B:154:ILE:CD1	2.46	0.45
1:B:153:LEU:C	1:B:153:LEU:CD2	2.88	0.45
1:E:297:VAL:CG2	1:E:369:PHE:CE2	3.00	0.45
1:B:554:ILE:HG22	1:B:640:LEU:HD12	1.97	0.45
1:B:659:PRO:HB3	1:B:694:LEU:HD23	1.98	0.45
1:D:109:ILE:O	1:D:109:ILE:CG2	2.64	0.45
1:A:132:ARG:HA	1:A:135:GLU:HG2	1.98	0.45
1:B:125:ILE:HD11	1:B:157:LEU:HD22	1.97	0.45
1:B:165:TRP:O	1:B:168:SER:N	2.50	0.45
1:B:576:LYS:CE	1:B:592:GLN:HE22	2.30	0.45
1:D:393:TYR:CE1	1:D:404:LEU:HD22	2.51	0.45
1:D:725:MET:HE2	1:D:725:MET:HA	1.98	0.45
1:B:393:TYR:CE1	1:B:404:LEU:HD22	2.51	0.45
1:D:615:LEU:HD12	1:D:716:TYR:CG	2.52	0.45
1:A:327:ILE:HG23	1:A:353:ILE:HD13	1.98	0.45
1:A:491:ILE:HD12	1:A:491:ILE:N	2.32	0.45
1:B:37:LEU:O	1:B:38:ARG:C	2.59	0.45
1:B:467:ARG:NH1	1:B:557:GLU:OE2	2.50	0.45
1:B:560:ARG:HG3	1:B:647:CYS:SG	2.56	0.45
1:D:790:VAL:O	1:D:790:VAL:CG1	2.64	0.45
1:A:743:THR:HG21	1:A:748:VAL:CB	2.41	0.45
1:B:100:GLU:HA	1:B:103:ARG:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:HA	1:B:135:GLU:HG2	1.98	0.45
1:D:350:THR:HG23	1:D:351:PRO:HD2	1.99	0.45
1:A:288:MET:HE3	1:A:292:ARG:O	2.17	0.45
1:A:529:LYS:HA	1:A:532:GLU:HB3	1.98	0.45
1:B:278:ILE:HD12	1:B:278:ILE:O	2.17	0.45
1:E:385:PRO:O	1:E:386:TYR:C	2.59	0.45
1:E:491:ILE:N	1:E:491:ILE:HD12	2.32	0.45
1:A:153:LEU:C	1:A:153:LEU:CD2	2.89	0.45
1:A:299:LEU:HD12	1:A:374:PHE:CE1	2.51	0.45
1:B:529:LYS:HA	1:B:532:GLU:HB3	1.99	0.45
1:B:574:ASN:O	1:B:577:ASN:N	2.50	0.45
1:B:790:VAL:O	1:B:790:VAL:CG1	2.65	0.45
1:D:327:ILE:CG2	1:D:349:VAL:HG13	2.47	0.45
1:E:109:ILE:O	1:E:109:ILE:CG2	2.64	0.45
1:A:574:ASN:O	1:A:577:ASN:N	2.50	0.45
1:D:125:ILE:HD11	1:D:157:LEU:CD2	2.46	0.45
1:E:254:ALA:HA	1:E:280:ILE:HD11	1.99	0.45
1:E:529:LYS:HA	1:E:532:GLU:HB3	1.98	0.45
1:E:615:LEU:HD12	1:E:716:TYR:CD1	2.52	0.45
1:A:100:GLU:HA	1:A:103:ARG:HD3	1.99	0.45
1:A:254:ALA:CA	1:A:280:ILE:HD11	2.47	0.45
1:A:641:VAL:HG11	1:A:661:VAL:HG13	1.97	0.45
1:D:299:LEU:HD12	1:D:374:PHE:CE1	2.52	0.45
1:D:465:VAL:HG12	1:D:466:LYS:N	2.31	0.45
1:B:254:ALA:CA	1:B:280:ILE:HD11	2.46	0.44
1:B:288:MET:HE3	1:B:292:ARG:O	2.17	0.44
1:B:464:LEU:HD12	1:B:749:VAL:CG2	2.44	0.44
1:B:715:LEU:HD11	1:B:722:VAL:CG1	2.37	0.44
1:A:37:LEU:O	1:A:38:ARG:C	2.60	0.44
1:A:264:LEU:CD1	1:A:377:CYS:SG	3.04	0.44
1:D:461:ASP:HB2	1:D:740:ILE:HG23	1.99	0.44
1:E:184:LEU:HD21	1:E:540:PHE:CE1	2.51	0.44
1:B:109:ILE:O	1:B:110:GLU:C	2.61	0.44
1:D:469:ILE:HG22	1:D:469:ILE:O	2.17	0.44
1:E:254:ALA:CA	1:E:280:ILE:HD11	2.48	0.44
1:E:324:VAL:HG22	1:E:346:ILE:HB	2.00	0.44
1:E:574:ASN:O	1:E:577:ASN:N	2.49	0.44
1:A:41:ILE:HD13	1:A:56:PHE:HB2	2.00	0.44
1:B:615:LEU:CD2	1:B:619:LEU:HD13	2.39	0.44
1:E:464:LEU:HD22	1:E:749:VAL:HG21	1.99	0.44
1:D:99:LEU:HD21	1:D:163:GLU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:VAL:HG11	1:D:761:MET:CE	2.47	0.44
1:E:523:LEU:HD23	1:E:524:LEU:N	2.32	0.44
1:A:73:LEU:HD21	1:A:88:ILE:CD1	2.47	0.44
1:A:487:LEU:O	1:A:491:ILE:CD1	2.63	0.44
1:B:45:GLU:HA	1:B:52:ALA:HB2	2.00	0.44
1:B:278:ILE:HD13	1:B:316:HIS:NE2	2.32	0.44
1:B:282:GLU:O	1:B:286:GLN:HB2	2.16	0.44
1:D:297:VAL:CG2	1:D:369:PHE:CE2	3.01	0.44
1:D:529:LYS:HA	1:D:532:GLU:HB3	2.00	0.44
1:E:264:LEU:HD21	1:E:414:VAL:CG1	2.48	0.44
1:A:282:GLU:O	1:A:286:GLN:HB2	2.17	0.44
1:B:65:ALA:O	1:B:66:ARG:C	2.60	0.44
1:D:35:ASP:OD1	1:D:38:ARG:NH2	2.49	0.44
1:D:254:ALA:HA	1:D:280:ILE:HD11	2.00	0.44
1:A:125:ILE:HD12	1:A:153:LEU:HD21	1.97	0.44
1:B:161:ASP:C	1:B:162:LYS:HG2	2.41	0.44
1:B:717:GLU:OE2	1:B:744:SER:OG	2.18	0.44
1:D:265:ILE:HG12	1:D:408:LEU:HD11	2.00	0.44
1:E:44:GLU:OE2	1:E:47:ARG:NH1	2.50	0.44
1:A:185:TRP:O	1:A:186:ASP:C	2.60	0.44
1:B:73:LEU:HD21	1:B:88:ILE:CD1	2.48	0.44
1:E:35:ASP:OD1	1:E:38:ARG:NH2	2.50	0.44
1:A:83:GLY:O	1:A:84:LEU:C	2.62	0.43
1:B:110:GLU:OE2	1:B:154:ILE:HD11	2.18	0.43
1:D:185:TRP:O	1:D:186:ASP:C	2.60	0.43
1:D:324:VAL:HG22	1:D:346:ILE:HB	1.99	0.43
1:E:595:GLU:N	1:E:596:PRO:CD	2.81	0.43
1:D:523:LEU:HD23	1:D:524:LEU:N	2.33	0.43
1:E:436:LEU:HB2	1:E:438:ILE:HD13	1.99	0.43
1:A:536:CYS:O	1:A:537:ARG:C	2.62	0.43
1:A:565:LEU:C	1:A:565:LEU:HD23	2.44	0.43
1:B:448:ILE:O	1:B:449:GLN:C	2.61	0.43
1:D:436:LEU:HB2	1:D:438:ILE:HD13	2.00	0.43
1:E:469:ILE:O	1:E:470:HIS:CB	2.65	0.43
1:A:117:ASP:C	1:A:117:ASP:OD1	2.62	0.43
1:D:491:ILE:HD12	1:D:491:ILE:N	2.33	0.43
1:E:327:ILE:CG2	1:E:349:VAL:HG13	2.49	0.43
1:B:297:VAL:CG2	1:B:369:PHE:CE2	3.02	0.43
1:A:297:VAL:CG2	1:A:369:PHE:CE2	3.02	0.43
1:A:393:TYR:CE1	1:A:404:LEU:HD22	2.53	0.43
1:A:460:ILE:O	1:A:460:ILE:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:VAL:O	1:A:723:THR:C	2.61	0.43
1:B:122:ILE:O	1:B:125:ILE:HG22	2.17	0.43
1:B:297:VAL:HG11	1:B:299:LEU:HD21	2.00	0.43
1:D:461:ASP:HB3	1:D:740:ILE:HG23	1.99	0.43
1:D:603:LYS:NZ	1:E:578:GLY:O	2.46	0.43
1:E:458:PRO:HG2	1:E:726:ILE:HG21	2.00	0.43
1:E:487:LEU:O	1:E:491:ILE:CD1	2.67	0.43
1:A:718:TYR:OH	1:A:725:MET:HE2	2.19	0.43
1:B:110:GLU:CD	1:B:154:ILE:HD11	2.43	0.43
1:B:436:LEU:HB2	1:B:438:ILE:HD13	2.01	0.43
1:B:747:GLU:O	1:B:751:ASN:CB	2.67	0.43
1:D:264:LEU:CD1	1:D:377:CYS:SG	3.06	0.43
1:E:271:SER:HB3	1:E:451:LEU:HD11	2.00	0.43
1:B:746:THR:O	1:B:747:GLU:C	2.61	0.43
1:D:254:ALA:CA	1:D:280:ILE:HD11	2.49	0.43
1:E:448:ILE:O	1:E:449:GLN:C	2.62	0.43
1:A:341:ILE:HG23	1:A:347:ILE:CD1	2.48	0.43
1:D:288:MET:HE2	1:D:294:ALA:HB2	1.99	0.43
1:E:565:LEU:C	1:E:565:LEU:HD23	2.44	0.43
1:B:521:CYS:SG	1:B:539:LEU:HD13	2.59	0.43
1:B:523:LEU:HD23	1:B:524:LEU:N	2.33	0.43
1:B:583:LEU:HD12	1:B:583:LEU:O	2.18	0.43
1:A:161:ASP:C	1:A:162:LYS:HG2	2.43	0.42
1:B:327:ILE:HG23	1:B:353:ILE:HD13	2.01	0.42
1:D:595:GLU:N	1:D:596:PRO:CD	2.82	0.42
1:E:708:VAL:HG12	1:E:709:GLN:N	2.34	0.42
1:A:109:ILE:O	1:A:110:GLU:C	2.62	0.42
1:A:473:PHE:CZ	1:A:564:ALA:HB1	2.53	0.42
1:D:130:ILE:O	1:D:131:ASP:C	2.62	0.42
1:A:45:GLU:HG2	1:A:49:VAL:HG22	1.99	0.42
1:A:157:LEU:HG	1:A:165:TRP:CE3	2.54	0.42
1:A:523:LEU:HD23	1:A:524:LEU:N	2.34	0.42
1:B:117:ASP:OD1	1:B:117:ASP:C	2.62	0.42
1:B:397:LYS:HB2	1:B:404:LEU:HD11	2.02	0.42
1:D:73:LEU:HD21	1:D:88:ILE:CG1	2.49	0.42
1:D:456:ASN:O	1:D:458:PRO:N	2.53	0.42
1:D:576:LYS:CE	1:D:592:GLN:HE22	2.33	0.42
1:D:650:GLU:CD	1:E:143:ASN:HB3	2.43	0.42
1:D:713:VAL:HG23	1:D:738:LYS:O	2.19	0.42
1:E:265:ILE:HG12	1:E:408:LEU:HD11	2.01	0.42
1:E:327:ILE:HG23	1:E:353:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LEU:HD12	1:A:583:LEU:O	2.19	0.42
1:B:184:LEU:O	1:B:522:ARG:HD2	2.20	0.42
1:B:536:CYS:O	1:B:537:ARG:C	2.62	0.42
1:A:122:ILE:HA	1:A:125:ILE:CG2	2.45	0.42
1:A:659:PRO:HB3	1:A:694:LEU:HD23	2.01	0.42
1:B:299:LEU:HD12	1:B:374:PHE:CE1	2.55	0.42
1:E:288:MET:HE2	1:E:294:ALA:HA	2.02	0.42
1:E:288:MET:HE2	1:E:294:ALA:HB2	2.01	0.42
1:A:265:ILE:HG12	1:A:408:LEU:HD11	2.00	0.42
1:A:465:VAL:HG12	1:A:466:LYS:N	2.35	0.42
1:A:695:LEU:HD12	1:A:708:VAL:HG11	2.00	0.42
1:E:615:LEU:HD11	1:E:633:LEU:HD11	2.02	0.42
1:E:721:ASN:C	1:E:721:ASN:ND2	2.78	0.42
1:A:16:ILE:HG21	1:A:57:LEU:HD13	2.01	0.42
1:A:661:VAL:CG1	1:A:662:LEU:N	2.83	0.42
1:B:539:LEU:O	1:B:543:THR:HG23	2.20	0.42
1:B:632:LEU:CB	1:B:710:CYS:SG	3.08	0.42
1:B:773:ASP:O	1:B:774:GLU:C	2.62	0.42
1:E:130:ILE:O	1:E:131:ASP:C	2.63	0.42
1:E:264:LEU:CD1	1:E:377:CYS:SG	3.06	0.42
1:A:10:GLN:OE1	1:A:61:LEU:CD1	2.68	0.42
1:A:45:GLU:HA	1:A:52:ALA:HB2	2.02	0.42
1:A:165:TRP:O	1:A:168:SER:N	2.52	0.42
1:A:288:MET:HE2	1:A:294:ALA:HA	2.01	0.42
1:A:297:VAL:HG11	1:A:299:LEU:HD21	2.01	0.42
1:D:640:LEU:HD23	1:D:644:LEU:HG	2.01	0.42
1:D:786:MET:SD	1:D:789:ARG:NH1	2.93	0.42
1:E:473:PHE:CZ	1:E:564:ALA:HB1	2.55	0.42
1:A:295:LYS:HZ3	1:A:342:GLU:HA	1.85	0.42
1:A:712:LEU:HD12	1:A:738:LYS:HG2	2.00	0.42
1:B:32:TRP:HB3	1:B:63:LEU:HD21	2.02	0.42
1:B:73:LEU:HD11	1:B:88:ILE:HD11	2.02	0.42
1:B:465:VAL:HG21	1:B:742:VAL:HG13	2.02	0.42
1:D:468:ARG:NH1	1:D:606:THR:O	2.52	0.42
1:E:782:HIS:CE1	1:E:786:MET:HE3	2.55	0.42
1:B:273:LYS:O	1:B:276:VAL:N	2.53	0.41
1:B:288:MET:HE2	1:B:294:ALA:HA	2.02	0.41
1:D:120:ALA:HB1	1:D:176:THR:HG21	2.01	0.41
1:E:73:LEU:HG	1:E:88:ILE:HD11	2.02	0.41
1:E:390:MET:HG3	1:E:436:LEU:HD23	2.02	0.41
1:E:416:VAL:HG13	1:E:416:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ILE:HG22	1:B:452:GLN:CD	2.46	0.41
1:B:661:VAL:CG1	1:B:662:LEU:N	2.83	0.41
1:D:25:VAL:HG22	1:D:25:VAL:O	2.20	0.41
1:E:640:LEU:HD23	1:E:644:LEU:HG	2.02	0.41
1:E:773:ASP:O	1:E:774:GLU:C	2.63	0.41
1:A:264:LEU:HD21	1:A:414:VAL:CG1	2.50	0.41
1:A:274:THR:O	1:A:278:ILE:HG23	2.21	0.41
1:A:468:ARG:NH2	1:A:609:ASN:HB2	2.35	0.41
1:A:640:LEU:O	1:A:641:VAL:C	2.60	0.41
1:B:157:LEU:HD12	1:B:157:LEU:HA	1.89	0.41
1:D:288:MET:HE2	1:D:294:ALA:HA	2.02	0.41
1:D:708:VAL:HG12	1:D:709:GLN:N	2.35	0.41
1:E:120:ALA:HB1	1:E:176:THR:HG21	2.01	0.41
1:B:109:ILE:O	1:B:109:ILE:HG22	2.20	0.41
1:B:157:LEU:HG	1:B:165:TRP:CE3	2.55	0.41
1:B:565:LEU:HD23	1:B:565:LEU:C	2.46	0.41
1:D:246:ALA:HB2	1:D:275:PHE:CZ	2.55	0.41
1:E:297:VAL:CG2	1:E:369:PHE:CD2	3.04	0.41
1:A:557:GLU:O	1:A:609:ASN:ND2	2.46	0.41
1:B:12:TYR:CG	1:B:93:PHE:CE2	3.09	0.41
1:B:21:ASN:HB3	1:B:24:TYR:CD2	2.56	0.41
1:D:110:GLU:CD	1:D:154:ILE:HD11	2.46	0.41
1:D:271:SER:HB3	1:D:451:LEU:HD11	2.02	0.41
1:D:487:LEU:O	1:D:491:ILE:CD1	2.68	0.41
1:D:576:LYS:NZ	1:E:595:GLU:CD	2.78	0.41
1:A:727:GLN:O	1:A:728:VAL:HG23	2.19	0.41
1:B:374:PHE:CZ	1:B:390:MET:HE2	2.55	0.41
1:B:722:VAL:O	1:B:725:MET:N	2.54	0.41
1:D:448:ILE:O	1:D:449:GLN:C	2.63	0.41
1:B:264:LEU:HD21	1:B:414:VAL:CG1	2.51	0.41
1:B:640:LEU:HD23	1:B:644:LEU:HG	2.03	0.41
1:D:390:MET:HG3	1:D:436:LEU:HD23	2.01	0.41
1:D:773:ASP:O	1:D:774:GLU:C	2.64	0.41
1:E:185:TRP:O	1:E:186:ASP:C	2.62	0.41
1:E:576:LYS:CE	1:E:592:GLN:HE22	2.34	0.41
1:A:122:ILE:N	1:A:123:PRO:HD2	2.36	0.41
1:A:397:LYS:HB2	1:A:404:LEU:HD11	2.03	0.41
1:D:297:VAL:CG2	1:D:369:PHE:CD2	3.04	0.41
1:D:473:PHE:CZ	1:D:564:ALA:HB1	2.55	0.41
1:D:782:HIS:CE1	1:D:786:MET:HE3	2.55	0.41
1:E:341:ILE:HG23	1:E:347:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ALA:O	1:A:66:ARG:C	2.64	0.41
1:A:448:ILE:HG22	1:A:452:GLN:CD	2.46	0.41
1:A:698:THR:HG23	1:A:699:SER:N	2.36	0.41
1:A:736:GLY:C	1:A:737:SER:OG	2.64	0.41
1:B:288:MET:HE2	1:B:294:ALA:N	2.36	0.41
1:B:341:ILE:HG23	1:B:347:ILE:CD1	2.50	0.41
1:B:487:LEU:O	1:B:491:ILE:CD1	2.68	0.41
1:D:16:ILE:HG12	1:D:84:LEU:HD22	2.03	0.41
1:D:461:ASP:HB2	1:D:740:ILE:HG12	2.02	0.41
1:D:469:ILE:HD12	1:D:469:ILE:H	1.85	0.41
1:E:73:LEU:HD21	1:E:88:ILE:CG1	2.50	0.41
1:A:426:ILE:HD11	1:A:768:LYS:HD3	2.02	0.41
1:A:640:LEU:HD23	1:A:644:LEU:HG	2.03	0.41
1:A:747:GLU:O	1:A:751:ASN:HB2	2.21	0.41
1:B:122:ILE:N	1:B:123:PRO:HD2	2.36	0.41
1:B:125:ILE:HD12	1:B:153:LEU:HD21	1.99	0.41
1:B:171:LEU:HD23	1:B:171:LEU:O	2.21	0.41
1:B:267:ALA:HB1	1:B:268:PRO:HD2	2.02	0.41
1:D:73:LEU:HG	1:D:88:ILE:HD11	2.01	0.41
1:D:659:PRO:HB3	1:D:694:LEU:HD23	2.03	0.41
1:D:661:VAL:CG1	1:D:662:LEU:N	2.84	0.41
1:E:25:VAL:O	1:E:25:VAL:HG22	2.21	0.41
1:E:640:LEU:O	1:E:641:VAL:C	2.64	0.41
1:E:745:LYS:C	1:E:746:THR:O	2.64	0.41
1:E:790:VAL:O	1:E:790:VAL:CG1	2.68	0.41
1:A:278:ILE:C	1:A:278:ILE:CD1	2.91	0.40
1:B:297:VAL:CG1	1:B:299:LEU:HD21	2.51	0.40
1:B:348:VAL:C	1:B:349:VAL:HG23	2.46	0.40
1:B:381:THR:CG2	1:B:382:GLY:N	2.84	0.40
1:D:265:ILE:HB	1:D:410:LEU:HD23	2.03	0.40
1:D:397:LYS:HB2	1:D:404:LEU:HD11	2.04	0.40
1:D:615:LEU:HD11	1:D:633:LEU:HD11	2.02	0.40
1:E:110:GLU:CD	1:E:154:ILE:HD11	2.46	0.40
1:E:171:LEU:HD23	1:E:171:LEU:O	2.21	0.40
1:E:726:ILE:CD1	1:E:739:CYS:SG	3.07	0.40
1:A:44:GLU:HA	1:A:47:ARG:NH1	2.36	0.40
1:A:288:MET:HE2	1:A:294:ALA:N	2.36	0.40
1:B:29:MET:HE3	1:B:56:PHE:CZ	2.57	0.40
1:B:109:ILE:HG22	1:B:112:THR:HB	2.03	0.40
1:E:295:LYS:HZ3	1:E:342:GLU:HA	1.86	0.40
1:E:397:LYS:HB2	1:E:404:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:ILE:HD13	1:E:722:VAL:HG11	2.03	0.40
1:E:659:PRO:HB3	1:E:694:LEU:HD23	2.03	0.40
1:B:736:GLY:C	1:B:737:SER:OG	2.65	0.40
1:D:462:VAL:HG21	1:D:752:GLU:OE1	2.21	0.40
1:E:151:THR:OG1	1:E:579:PRO:HD3	2.21	0.40
1:E:270:GLY:HA3	1:E:455:MET:HE1	2.03	0.40
1:A:157:LEU:HD21	1:A:169:LEU:HD13	2.02	0.40
1:A:265:ILE:HB	1:A:410:LEU:HD23	2.03	0.40
1:A:324:VAL:HG22	1:A:346:ILE:HB	2.04	0.40
1:A:374:PHE:CZ	1:A:390:MET:HE2	2.56	0.40
1:B:264:LEU:CD1	1:B:377:CYS:SG	3.08	0.40
1:B:265:ILE:HG12	1:B:408:LEU:HD11	2.02	0.40
1:B:374:PHE:CE2	1:B:390:MET:HE2	2.56	0.40
1:E:73:LEU:HD21	1:E:88:ILE:HG13	2.03	0.40
1:E:456:ASN:O	1:E:458:PRO:N	2.54	0.40
1:A:510:TYR:O	1:A:513:TRP:HB3	2.22	0.40
1:B:185:TRP:O	1:B:186:ASP:C	2.64	0.40
1:B:327:ILE:CG2	1:B:349:VAL:HG13	2.52	0.40
1:D:274:THR:O	1:D:278:ILE:HG23	2.22	0.40
1:E:483:GLU:O	1:E:486:ALA:HB3	2.22	0.40
1:E:510:TYR:OH	1:E:546:LEU:HD22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	660/797 (83%)	586 (89%)	64 (10%)	10 (2%)	8	30
1	B	661/797 (83%)	587 (89%)	65 (10%)	9 (1%)	9	31
1	D	657/797 (82%)	590 (90%)	60 (9%)	7 (1%)	11	38
1	E	656/797 (82%)	589 (90%)	59 (9%)	8 (1%)	10	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2634/3188 (83%)	2352 (89%)	248 (9%)	34 (1%)	9	33

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	LEU
1	A	699	SER
1	B	524	LEU
1	D	524	LEU
1	D	746	THR
1	E	470	HIS
1	E	524	LEU
1	A	81	TYR
1	A	131	ASP
1	A	604	ASP
1	A	717	GLU
1	A	738	LYS
1	B	81	TYR
1	B	131	ASP
1	B	717	GLU
1	B	738	LYS
1	D	738	LYS
1	E	738	LYS
1	E	746	THR
1	A	365	SER
1	A	723	THR
1	B	365	SER
1	B	723	THR
1	B	747	GLU
1	D	365	SER
1	E	365	SER
1	A	607	ASN
1	D	131	ASP
1	E	131	ASP
1	E	467	ARG
1	B	711	ASN
1	D	467	ARG
1	D	457	LYS
1	E	457	LYS

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	603/704 (86%)	545 (90%)	58 (10%)	8	28
1	B	604/704 (86%)	544 (90%)	60 (10%)	7	26
1	D	600/704 (85%)	557 (93%)	43 (7%)	13	39
1	E	599/704 (85%)	555 (93%)	44 (7%)	13	39
All	All	2406/2816 (85%)	2201 (92%)	205 (8%)	10	33

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	19	SER
1	A	25	VAL
1	A	30	THR
1	A	36	GLU
1	A	45	GLU
1	A	58	ASP
1	A	60	VAL
1	A	64	GLU
1	A	77	LEU
1	A	88	ILE
1	A	100	GLU
1	A	113	MET
1	A	122	ILE
1	A	130	ILE
1	A	153	LEU
1	A	154	ILE
1	A	164	HIS
1	A	176	THR
1	A	245	LYS
1	A	253	LEU
1	A	273	LYS
1	A	278	ILE
1	A	286	GLN

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Mol	Chain	Res	Type
1	A	307	GLU
1	A	343	ASP
1	A	360	ASP
1	A	363	LEU
1	A	391	THR
1	A	414	VAL
1	A	416	VAL
1	A	438	ILE
1	A	455	MET
1	A	459	GLU
1	A	464	LEU
1	A	507	THR
1	A	524	LEU
1	A	535	ILE
1	A	556	SER
1	A	557	GLU
1	A	561	ILE
1	A	580	TYR
1	A	604	ASP
1	A	617	CYS
1	A	625	TYR
1	A	636	LYS
1	A	640	LEU
1	A	662	LEU
1	A	691	ASP
1	A	710	CYS
1	A	711	ASN
1	A	715	LEU
1	A	737	SER
1	A	743	THR
1	A	754	CYS
1	A	771	LYS
1	A	780	LYS
1	A	786	MET
1	B	18	ARG
1	B	19	SER
1	B	20	LEU
1	B	25	VAL
1	B	30	THR
1	B	36	GLU
1	B	45	GLU
1	B	58	ASP

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Mol	Chain	Res	Type
1	B	60	VAL
1	B	64	GLU
1	B	77	LEU
1	B	88	ILE
1	B	100	GLU
1	B	113	MET
1	B	122	ILE
1	B	130	ILE
1	B	153	LEU
1	B	164	HIS
1	B	176	THR
1	B	245	LYS
1	B	253	LEU
1	B	273	LYS
1	B	278	ILE
1	B	286	GLN
1	B	307	GLU
1	B	343	ASP
1	B	360	ASP
1	B	363	LEU
1	B	391	THR
1	B	414	VAL
1	B	416	VAL
1	B	438	ILE
1	B	455	MET
1	B	459	GLU
1	B	462	VAL
1	B	464	LEU
1	B	467	ARG
1	B	507	THR
1	B	524	LEU
1	B	535	ILE
1	B	556	SER
1	B	557	GLU
1	B	561	ILE
1	B	580	TYR
1	B	604	ASP
1	B	617	CYS
1	B	625	TYR
1	B	636	LYS
1	B	640	LEU
1	B	662	LEU

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Mol	Chain	Res	Type
1	B	691	ASP
1	B	710	CYS
1	B	715	LEU
1	B	721	ASN
1	B	737	SER
1	B	743	THR
1	B	754	CYS
1	B	771	LYS
1	B	780	LYS
1	B	786	MET
1	D	45	GLU
1	D	113	MET
1	D	145	SER
1	D	164	HIS
1	D	245	LYS
1	D	253	LEU
1	D	273	LYS
1	D	278	ILE
1	D	286	GLN
1	D	307	GLU
1	D	343	ASP
1	D	360	ASP
1	D	363	LEU
1	D	391	THR
1	D	414	VAL
1	D	416	VAL
1	D	438	ILE
1	D	455	MET
1	D	459	GLU
1	D	464	LEU
1	D	467	ARG
1	D	507	THR
1	D	524	LEU
1	D	535	ILE
1	D	556	SER
1	D	557	GLU
1	D	561	ILE
1	D	580	TYR
1	D	605	GLU
1	D	617	CYS
1	D	625	TYR
1	D	636	LYS

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Mol	Chain	Res	Type
1	D	640	LEU
1	D	662	LEU
1	D	691	ASP
1	D	711	ASN
1	D	721	ASN
1	D	737	SER
1	D	743	THR
1	D	748	VAL
1	D	754	CYS
1	D	780	LYS
1	D	786	MET
1	E	45	GLU
1	E	113	MET
1	E	145	SER
1	E	164	HIS
1	E	245	LYS
1	E	253	LEU
1	E	273	LYS
1	E	278	ILE
1	E	286	GLN
1	E	307	GLU
1	E	343	ASP
1	E	360	ASP
1	E	363	LEU
1	E	391	THR
1	E	414	VAL
1	E	416	VAL
1	E	438	ILE
1	E	455	MET
1	E	459	GLU
1	E	462	VAL
1	E	464	LEU
1	E	467	ARG
1	E	469	ILE
1	E	507	THR
1	E	524	LEU
1	E	535	ILE
1	E	556	SER
1	E	557	GLU
1	E	561	ILE
1	E	580	TYR
1	E	617	CYS

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Mol	Chain	Res	Type
1	E	625	TYR
1	E	636	LYS
1	E	640	LEU
1	E	662	LEU
1	E	691	ASP
1	E	715	LEU
1	E	721	ASN
1	E	725	MET
1	E	737	SER
1	E	743	THR
1	E	754	CYS
1	E	780	LYS
1	E	786	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	447	ASN
1	A	586	HIS
1	A	592	GLN
1	A	721	ASN
1	A	783	ASN
1	B	139	GLN
1	B	586	HIS
1	B	783	ASN
1	D	325	GLN
1	D	447	ASN
1	D	592	GLN
1	D	721	ASN
1	E	325	GLN
1	E	447	ASN
1	E	586	HIS
1	E	607	ASN

5.3.3 RNA ⓘ

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	674/797 (84%)	-0.38	0 100 100	52, 97, 153, 210	0
1	B	675/797 (84%)	-0.39	1 (0%) 92 91	53, 96, 155, 220	0
1	D	671/797 (84%)	0.16	11 (1%) 70 56	109, 192, 271, 320	0
1	E	670/797 (84%)	0.18	9 (1%) 75 61	104, 199, 292, 359	0
All	All	2690/3188 (84%)	-0.11	21 (0%) 82 71	52, 145, 273, 359	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	ILE	5.1
1	D	19	SER	4.0
1	E	16	ILE	3.9
1	D	473	PHE	3.6
1	E	56	PHE	3.4
1	E	184	LEU	3.3
1	E	53	ALA	3.0
1	D	414	VAL	2.8
1	E	60	VAL	2.8
1	E	710	CYS	2.7
1	D	20	LEU	2.7
1	E	736	GLY	2.5
1	D	157	LEU	2.5
1	D	17	GLU	2.4
1	D	102	HIS	2.3
1	B	710	CYS	2.3
1	D	552	ALA	2.3
1	E	316	HIS	2.2
1	E	327	ILE	2.1
1	D	114	LEU	2.1
1	D	337	VAL	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.