



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:48 PM UTC

PDB ID : 6JZQ / pdb_00006jzq
Title : The crystal structure of acyl-acyl carrier protein (acyl-ACP) reductase (AAR)
Authors : Zhang, H.M.; Li, M.; Gao, Y.
Deposited on : 2019-05-03
Resolution : 2.80 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

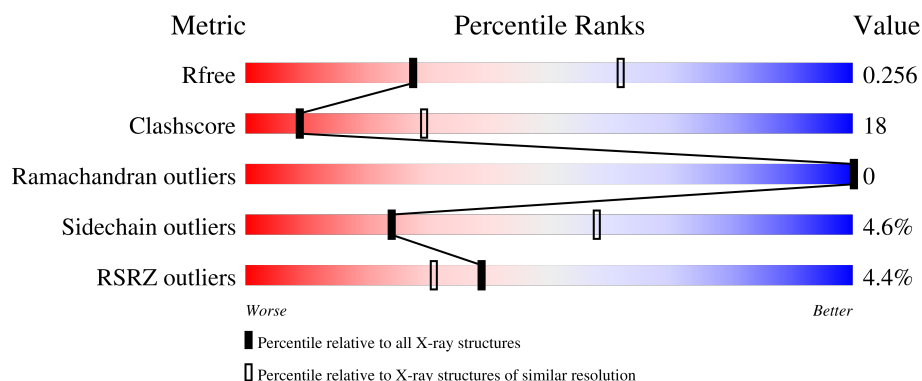
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	347	0% 77% 19% ..
1	B	347	3% 75% 24% ..
1	C	347	4% 66% 30% ..
1	D	347	3% 67% 27% ..
1	E	347	11% 64% 33% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12983 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 Long-chain acyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2610	1656	448	490	16			
1	B	345	Total	C	N	O	S	0	0	0
			2629	1673	444	496	16			
1	C	344	Total	C	N	O	S	0	0	0
			2609	1658	452	483	16			
1	D	339	Total	C	N	O	S	0	0	0
			2525	1611	426	472	16			
1	E	345	Total	C	N	O	S	0	1	0
			2562	1631	432	484	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	GLU	-	expression tag	UNP Q54765
A	343	ASN	-	expression tag	UNP Q54765
A	344	LEU	-	expression tag	UNP Q54765
A	345	TYR	-	expression tag	UNP Q54765
A	346	PHE	-	expression tag	UNP Q54765
A	347	GLN	-	expression tag	UNP Q54765
B	342	GLU	-	expression tag	UNP Q54765
B	343	ASN	-	expression tag	UNP Q54765
B	344	LEU	-	expression tag	UNP Q54765
B	345	TYR	-	expression tag	UNP Q54765
B	346	PHE	-	expression tag	UNP Q54765
B	347	GLN	-	expression tag	UNP Q54765
C	342	GLU	-	expression tag	UNP Q54765
C	343	ASN	-	expression tag	UNP Q54765
C	344	LEU	-	expression tag	UNP Q54765
C	345	TYR	-	expression tag	UNP Q54765
C	346	PHE	-	expression tag	UNP Q54765
C	347	GLN	-	expression tag	UNP Q54765
D	342	GLU	-	expression tag	UNP Q54765

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Chain	Residue	Modelled	Actual	Comment	Reference
D	343	ASN	-	expression tag	UNP Q54765
D	344	LEU	-	expression tag	UNP Q54765
D	345	TYR	-	expression tag	UNP Q54765
D	346	PHE	-	expression tag	UNP Q54765
D	347	GLN	-	expression tag	UNP Q54765
E	342	GLU	-	expression tag	UNP Q54765
E	343	ASN	-	expression tag	UNP Q54765
E	344	LEU	-	expression tag	UNP Q54765
E	345	TYR	-	expression tag	UNP Q54765
E	346	PHE	-	expression tag	UNP Q54765
E	347	GLN	-	expression tag	UNP Q54765

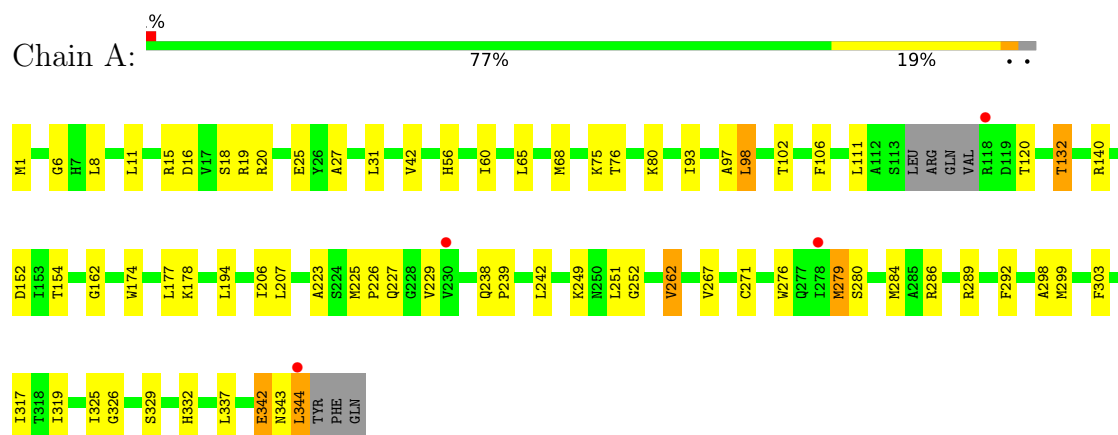
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	12	Total	O	0	0
			12	12		
2	C	4	Total	O	0	0
			4	4		
2	D	8	Total	O	0	0
			8	8		
2	E	3	Total	O	0	0
			3	3		

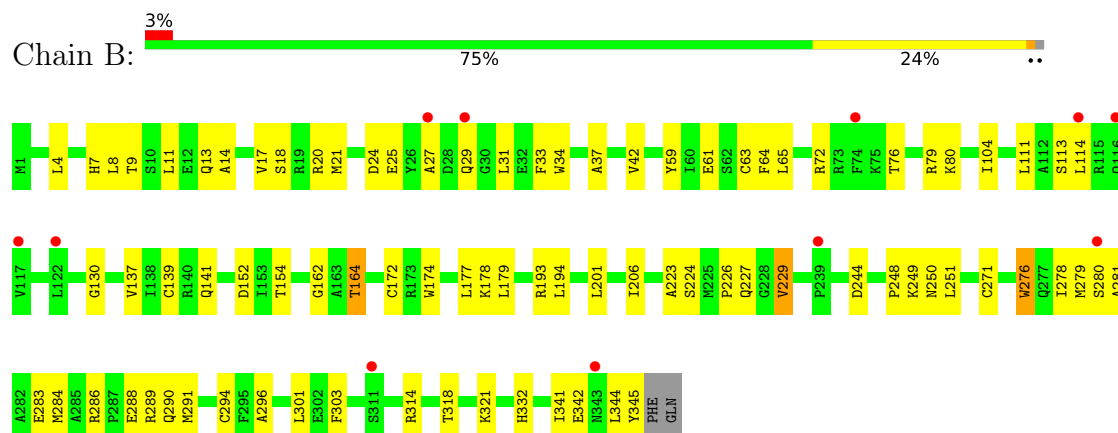
3 Residue-property plots [i](#)

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

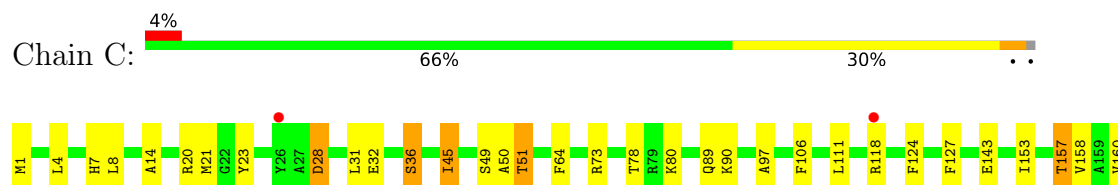
- Molecule 1: Long-chain acyl-[acyl-carrier-protein] reductase

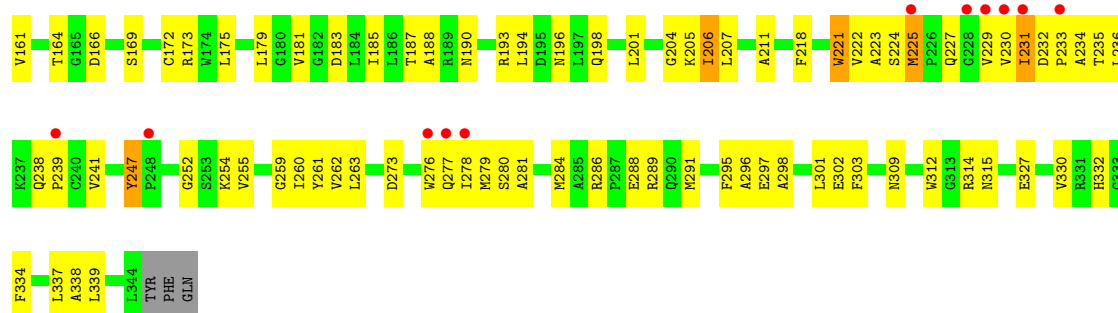


- Molecule 1: Long-chain acyl-[acyl-carrier-protein] reductase

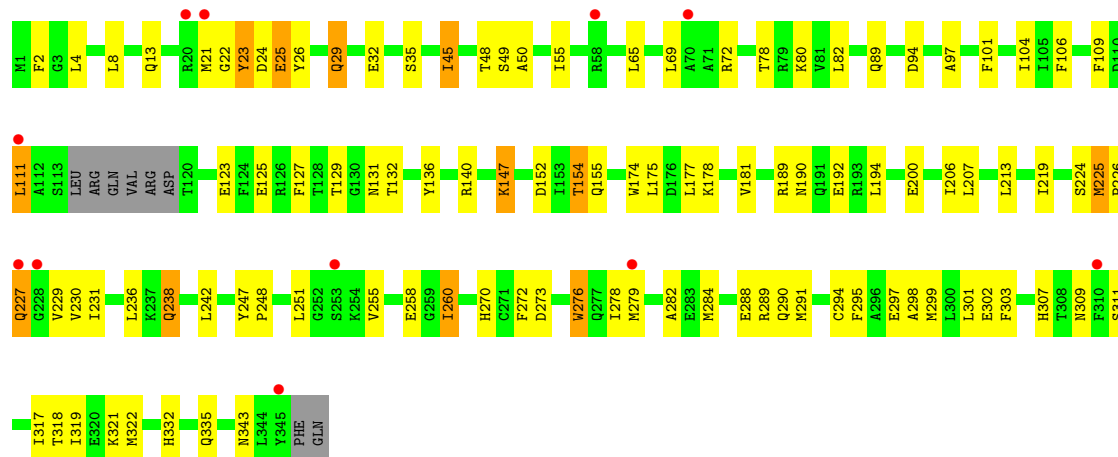


- Molecule 1: Long-chain acyl-[acyl-carrier-protein] reductase

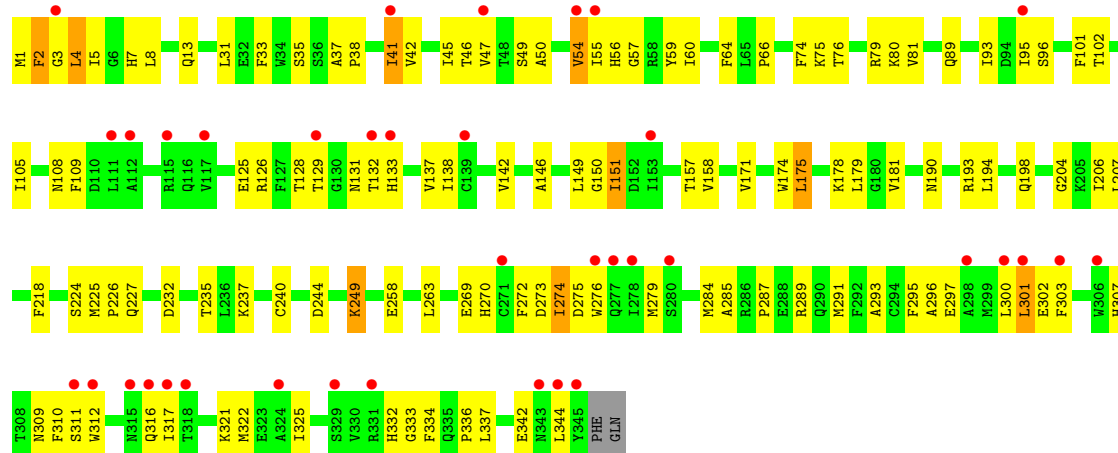




• Molecule 1: Long-chain acyl-[acyl-carrier-protein] reductase



• Molecule 1: Long-chain acyl-[acyl-carrier-protein] reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.17Å 201.44Å 124.58Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	46.11 – 2.80 46.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.11-2.80) 98.9 (46.11-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.218 , 0.254 0.222 , 0.256	Depositor DCC
R_{free} test set	1998 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12983	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.81	0/2661	1.00	4/3607 (0.1%)
1	B	0.74	0/2682	0.95	2/3642 (0.1%)
1	C	0.77	1/2660 (0.0%)	1.01	3/3609 (0.1%)
1	D	0.68	0/2576	0.94	6/3504 (0.2%)
1	E	0.66	0/2615	0.95	3/3561 (0.1%)
All	All	0.73	1/13194 (0.0%)	0.97	18/17923 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	221	TRP	C-O	-5.29	1.17	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	PRO	N-CA-C	-8.62	102.64	113.84
1	B	281	ALA	N-CA-C	8.13	120.14	111.28
1	E	227	GLN	N-CA-C	7.54	119.13	111.07
1	A	238	GLN	CA-C-N	-7.08	110.99	119.84
1	A	238	GLN	C-N-CA	-7.08	110.99	119.84
1	D	224	SER	N-CA-C	6.12	118.81	110.55
1	C	28	ASP	CB-CA-C	5.96	119.57	109.80
1	A	279	MET	N-CA-C	5.69	117.48	111.28
1	A	342	GLU	N-CA-C	-5.40	105.13	112.26
1	D	23	TYR	CA-C-N	5.39	127.94	120.29
1	D	23	TYR	C-N-CA	5.39	127.94	120.29
1	B	227	GLN	N-CA-C	5.31	117.14	111.36
1	E	225	MET	CA-C-N	5.23	125.14	119.85
1	E	225	MET	C-N-CA	5.23	125.14	119.85
1	C	247	TYR	CA-CB-CG	-5.21	104.51	113.90
1	D	238	GLN	CA-C-N	-5.17	113.38	119.84
1	D	238	GLN	C-N-CA	-5.17	113.38	119.84
1	D	229	VAL	N-CA-C	5.15	116.22	109.58

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	2610	0	2574	49	0
1	B	2629	0	2575	79	0
1	C	2609	0	2571	102	0
1	D	2525	0	2428	91	0
1	E	2562	0	2437	166	0
2	A	21	0	0	2	0
2	B	12	0	0	0	0
2	C	4	0	0	0	0
2	D	8	0	0	2	0
2	E	3	0	0	0	0
All	All	12983	0	12585	472	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 18.

All (472) 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:300:LEU:HD13	1:E:325:ILE:CG1	1.45	1.42
1:E:95:ILE:CG2	1:E:301:LEU:HD23	1.49	1.40
1:E:95:ILE:CG2	1:E:301:LEU:CD2	2.19	1.21
1:E:300:LEU:CD1	1:E:325:ILE:CG1	2.25	1.15
1:E:300:LEU:CD1	1:E:325:ILE:HG12	1.75	1.14
1:E:95:ILE:HG23	1:E:301:LEU:CD2	1.78	1.13
1:E:95:ILE:HG23	1:E:301:LEU:HD23	1.19	1.12
1:E:2:PHE:CE1	1:E:57:GLY:HA3	1.88	1.07
1:E:95:ILE:HG21	1:E:301:LEU:HD23	1.33	1.04
1:E:95:ILE:HG21	1:E:301:LEU:CD2	1.85	1.02
1:C:231:ILE:HD12	1:C:254:LYS:HD2	1.42	1.01
1:B:29:GLN:HB2	1:B:33:PHE:HD2	1.22	0.97
1:C:20:ARG:HH12	1:C:277:GLN:HB3	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:LEU:CD1	1:E:325:ILE:HG13	1.96	0.95
1:E:276:TRP:HH2	1:E:291:MET:SD	1.91	0.94
1:E:4:LEU:HD13	1:E:295:PHE:CD1	2.03	0.94
1:C:225:MET:SD	1:C:225:MET:N	2.39	0.94
1:E:95:ILE:HG21	1:E:301:LEU:HB3	1.48	0.94
1:E:300:LEU:HD13	1:E:325:ILE:HG12	0.95	0.93
1:E:4:LEU:HD13	1:E:295:PHE:CG	2.04	0.93
1:C:194:LEU:HB3	1:C:206:ILE:HD11	1.49	0.92
1:C:231:ILE:HD12	1:C:254:LYS:CD	2.00	0.92
1:B:280:SER:HB3	1:B:284:MET:HE2	1.52	0.91
1:B:29:GLN:NE2	1:B:34:TRP:CZ2	2.41	0.89
1:E:190:ASN:HD22	1:E:193:ARG:HG3	1.38	0.89
1:E:95:ILE:CD1	1:E:307:HIS:HD2	1.85	0.87
1:E:2:PHE:HD1	1:E:2:PHE:H	1.21	0.87
1:E:2:PHE:CD1	1:E:57:GLY:HA3	2.09	0.87
1:B:113:SER:C	1:B:114:LEU:HD12	2.00	0.86
1:E:300:LEU:HD13	1:E:325:ILE:HG13	1.49	0.85
1:E:158:VAL:HG22	1:E:218:PHE:HB2	1.60	0.82
1:E:310:PHE:HE2	1:E:325:ILE:HB	1.45	0.81
1:B:29:GLN:HB2	1:B:33:PHE:CD2	2.14	0.81
1:E:300:LEU:HD23	1:E:300:LEU:O	1.81	0.80
1:D:190:ASN:OD1	1:D:192:GLU:HG2	1.82	0.80
1:E:174:TRP:CE3	1:E:322:MET:HE2	2.18	0.79
1:E:95:ILE:HG21	1:E:301:LEU:CB	2.12	0.79
1:A:252:GLY:HA2	1:A:262:VAL:HG11	1.65	0.78
1:C:232:ASP:CB	1:C:235:THR:OG1	2.33	0.77
1:B:29:GLN:CB	1:B:33:PHE:HD2	1.98	0.77
1:C:157:THR:HG22	1:C:183:ASP:HB2	1.67	0.77
1:B:7:HIS:H	1:B:279:MET:HE2	1.48	0.77
1:C:158:VAL:HG22	1:C:218:PHE:HB2	1.68	0.76
1:E:276:TRP:CH2	1:E:291:MET:SD	2.75	0.76
1:D:225:MET:HE1	1:D:251:LEU:HD13	1.67	0.76
1:E:55:ILE:HG21	1:E:302:GLU:HG2	1.68	0.76
1:D:89:GLN:HE22	1:D:123:GLU:H	1.33	0.76
1:B:8:LEU:HB2	1:B:65:LEU:HD22	1.68	0.75
1:C:45:ILE:HG22	1:C:276:TRP:HB3	1.71	0.73
1:C:286:ARG:HD3	1:C:289:ARG:HG3	1.68	0.73
1:E:2:PHE:CE1	1:E:57:GLY:CA	2.70	0.73
1:E:95:ILE:CG2	1:E:301:LEU:HD22	2.18	0.73
1:D:106:PHE:HA	1:D:111:LEU:HD22	1.69	0.73
1:E:190:ASN:ND2	1:E:193:ARG:HG3	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:NH2	1:A:289:ARG:HH21	1.88	0.72
1:C:221:TRP:NE1	1:C:223:ALA:O	2.23	0.72
1:D:29:GLN:HE21	1:D:29:GLN:N	1.87	0.72
1:A:6:GLY:CA	1:A:279:MET:HE2	2.20	0.71
1:A:6:GLY:HA3	1:A:279:MET:HE2	1.73	0.71
1:C:205:LYS:HD3	1:C:207:LEU:HD11	1.73	0.70
1:E:178:LYS:HG3	1:E:179:LEU:HD12	1.74	0.70
1:E:95:ILE:HD11	1:E:307:HIS:HA	1.73	0.70
1:D:219:ILE:HB	1:D:242:LEU:HD23	1.73	0.70
1:D:318:THR:HG22	1:D:321:LYS:HD3	1.74	0.69
1:E:7:HIS:H	1:E:279:MET:CE	2.05	0.69
1:E:125:GLU:HG3	1:E:309:ASN:ND2	2.07	0.69
1:D:2:PHE:CZ	1:D:45:ILE:HD11	2.28	0.69
1:A:177:LEU:HD23	1:A:319:ILE:HG13	1.74	0.69
1:E:74:PHE:HB3	1:E:109:PHE:HE2	1.59	0.68
1:B:152:ASP:CG	1:C:32:GLU:HG3	2.19	0.68
1:C:20:ARG:NH1	1:C:277:GLN:HB3	2.05	0.68
1:A:132:THR:HG23	1:A:317:ILE:HG23	1.76	0.67
1:E:133:HIS:ND1	1:E:293:ALA:HB1	2.09	0.67
1:E:95:ILE:HG13	1:E:307:HIS:CD2	2.29	0.67
1:E:300:LEU:HD13	1:E:325:ILE:CD1	2.23	0.67
1:E:132:THR:HB	1:E:317:ILE:HD12	1.77	0.67
1:C:276:TRP:CZ2	1:C:278:ILE:HD13	2.29	0.66
1:B:8:LEU:HD22	1:B:65:LEU:HD21	1.75	0.66
1:C:231:ILE:CD1	1:C:254:LYS:HD2	2.21	0.66
1:C:231:ILE:HD13	1:C:231:ILE:N	2.10	0.66
1:C:291:MET:HE3	1:C:296:ALA:HB2	1.77	0.66
1:E:291:MET:HE3	1:E:296:ALA:HB2	1.77	0.66
1:B:24:ASP:HB3	1:B:27:ALA:HB2	1.78	0.66
1:E:232:ASP:O	1:E:235:THR:HG22	1.95	0.66
1:E:1:MET:C	1:E:302:GLU:OE1	2.39	0.66
1:E:7:HIS:H	1:E:279:MET:HE2	1.60	0.66
1:B:114:LEU:HD12	1:B:114:LEU:N	2.10	0.66
1:B:224:SER:HB3	1:E:344:LEU:HB2	1.75	0.66
1:E:95:ILE:CG1	1:E:307:HIS:HA	2.26	0.65
1:B:72:ARG:HH12	1:E:258:GLU:HG3	1.61	0.65
1:B:278:ILE:HG23	1:B:280:SER:H	1.61	0.65
1:E:175:LEU:O	1:E:181:VAL:HG23	1.97	0.65
1:E:133:HIS:O	1:E:137:VAL:HG23	1.96	0.65
1:E:342:GLU:OE1	1:E:342:GLU:N	2.23	0.65
1:E:5:ILE:HG23	1:E:60:ILE:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:MET:HE3	1:E:291:MET:HA	1.79	0.65
1:C:231:ILE:CD1	1:C:254:LYS:CD	2.75	0.64
1:E:297:GLU:O	1:E:301:LEU:HB2	1.96	0.64
1:E:303:PHE:HB3	1:E:332:HIS:NE2	2.11	0.64
1:D:49:SER:O	1:D:272:PHE:HE2	1.81	0.64
1:B:130:GLY:HA3	1:B:294:CYS:HB2	1.80	0.64
1:A:75:LYS:HD3	1:A:75:LYS:C	2.22	0.64
1:E:35:SER:O	1:E:80:LYS:NZ	2.31	0.64
1:D:194:LEU:HB3	1:D:206:ILE:HD13	1.80	0.64
1:E:270:HIS:ND1	1:E:333:GLY:O	2.29	0.63
1:B:20:ARG:HH21	1:B:42:VAL:HG11	1.63	0.63
1:B:194:LEU:HB3	1:B:206:ILE:HD13	1.80	0.63
1:D:132:THR:HG23	1:D:317:ILE:HG23	1.81	0.63
1:B:29:GLN:CD	1:B:34:TRP:CZ2	2.77	0.63
1:C:166:ASP:HB3	1:C:315:ASN:H	1.62	0.63
1:A:75:LYS:HD3	1:A:75:LYS:O	1.99	0.62
1:D:21:MET:HG2	1:D:22:GLY:N	2.15	0.62
1:E:128:THR:HG22	1:E:311:SER:H	1.64	0.62
1:E:311:SER:HA	1:E:317:ILE:HD11	1.81	0.62
1:B:8:LEU:HD12	1:B:61:GLU:OE2	2.00	0.62
1:D:189:ARG:HA	1:D:189:ARG:NE	2.14	0.62
1:E:300:LEU:HD23	1:E:300:LEU:C	2.24	0.62
1:D:78:THR:O	1:D:82:LEU:HD12	2.00	0.62
1:C:207:LEU:HD23	1:C:211:ALA:HB1	1.80	0.61
1:A:19:ARG:HB2	1:A:25:GLU:HG2	1.81	0.61
1:D:152:ASP:OD1	1:D:154:THR:HB	2.00	0.61
1:A:342:GLU:HG3	1:A:342:GLU:O	2.01	0.61
1:E:95:ILE:HG23	1:E:301:LEU:HD22	1.79	0.61
1:E:95:ILE:CD1	1:E:307:HIS:CD2	2.77	0.61
1:E:54:VAL:C	1:E:55:ILE:HD12	2.26	0.61
1:C:288:GLU:HG2	1:C:289:ARG:HG2	1.82	0.60
1:D:270:HIS:O	1:D:289:ARG:HG2	2.01	0.60
1:E:55:ILE:HD13	1:E:303:PHE:CE1	2.35	0.60
1:A:97:ALA:HB2	1:A:298:ALA:HB2	1.83	0.60
1:A:194:LEU:HB3	1:A:206:ILE:HD13	1.83	0.60
1:D:230:VAL:O	1:D:231:ILE:HG22	2.01	0.60
1:C:222:VAL:HG22	1:C:222:VAL:O	2.00	0.60
1:C:1:MET:N	1:C:302:GLU:OE2	2.21	0.60
1:D:175:LEU:O	1:D:181:VAL:HG23	2.02	0.59
1:D:35:SER:HA	1:D:80:LYS:HZ1	1.67	0.59
1:D:129:THR:HG22	1:D:311:SER:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ILE:HD13	1:C:231:ILE:H	1.66	0.59
1:D:189:ARG:NH2	2:D:401:HOH:O	2.36	0.59
1:E:95:ILE:CD1	1:E:307:HIS:HA	2.32	0.59
1:C:45:ILE:CG2	1:C:276:TRP:HB3	2.33	0.59
1:D:32:GLU:CD	1:D:32:GLU:H	2.11	0.59
1:A:8:LEU:HB2	1:A:65:LEU:HD13	1.84	0.58
1:A:162:GLY:HA3	1:A:223:ALA:HB2	1.85	0.58
1:C:291:MET:HE1	1:C:334:PHE:CE1	2.39	0.58
1:E:95:ILE:HD11	1:E:307:HIS:HD2	1.67	0.58
1:B:226:PRO:HG2	1:B:229:VAL:CG2	2.34	0.58
1:D:273:ASP:OD1	1:D:289:ARG:NE	2.36	0.58
1:E:132:THR:HG22	1:E:311:SER:HB3	1.85	0.58
1:E:146:ALA:HA	1:E:151:ILE:HD11	1.86	0.58
1:E:276:TRP:CH2	1:E:291:MET:HB3	2.39	0.58
1:B:152:ASP:OD1	1:B:154:THR:HB	2.04	0.57
1:C:254:LYS:O	1:C:254:LYS:HD3	2.04	0.57
1:A:280:SER:HG	1:A:292:PHE:HZ	1.51	0.57
1:A:227:GLN:NE2	1:D:343:ASN:HB3	2.19	0.57
1:C:238:GLN:O	1:C:259:GLY:HA3	2.05	0.57
1:C:252:GLY:HA2	1:C:262:VAL:HG11	1.87	0.57
1:D:225:MET:HE1	1:D:251:LEU:CD1	2.34	0.57
1:C:8:LEU:HD22	1:C:14:ALA:HA	1.87	0.57
1:D:129:THR:HG22	1:D:311:SER:CB	2.34	0.57
1:B:31:LEU:HD13	1:E:150:GLY:HA2	1.87	0.57
1:C:190:ASN:O	1:C:194:LEU:HD12	2.05	0.57
1:C:227:GLN:O	1:C:229:VAL:HG23	2.05	0.57
1:C:303:PHE:HB3	1:C:332:HIS:CE1	2.40	0.56
1:C:314:ARG:HG2	1:C:315:ASN:ND2	2.20	0.56
1:C:273:ASP:OD1	1:C:289:ARG:HD3	2.04	0.56
1:E:1:MET:N	1:E:302:GLU:OE1	2.34	0.56
1:E:244:ASP:OD2	1:E:249:LYS:HA	2.06	0.56
1:E:47:VAL:HG13	1:E:274:ILE:HG21	1.87	0.56
1:E:95:ILE:CG1	1:E:307:HIS:HD2	2.18	0.56
1:C:97:ALA:HB2	1:C:298:ALA:HB2	1.87	0.56
1:E:7:HIS:ND1	1:E:8:LEU:O	2.38	0.56
1:A:344:LEU:HD13	1:A:344:LEU:C	2.30	0.55
1:C:337:LEU:HD23	1:C:338:ALA:N	2.21	0.55
1:E:125:GLU:HG3	1:E:309:ASN:HD22	1.70	0.55
1:D:276:TRP:HH2	1:D:291:MET:HE3	1.72	0.55
1:D:55:ILE:HD13	1:D:302:GLU:HG3	1.87	0.55
1:A:60:ILE:HD11	1:A:93:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:CYS:O	1:A:289:ARG:NH1	2.29	0.55
1:B:37:ALA:O	1:B:80:LYS:NZ	2.38	0.55
1:B:137:VAL:O	1:B:141:GLN:HG3	2.07	0.55
1:C:185:ILE:HG23	1:C:207:LEU:HD13	1.87	0.55
1:E:151:ILE:HD11	1:E:218:PHE:HZ	1.71	0.55
1:D:2:PHE:HZ	1:D:45:ILE:HD11	1.71	0.55
1:C:231:ILE:CD1	1:C:231:ILE:H	2.19	0.54
1:C:45:ILE:HG21	1:C:276:TRP:HE3	1.71	0.54
1:E:95:ILE:HG21	1:E:301:LEU:CG	2.36	0.54
1:B:177:LEU:HB2	1:C:118:ARG:HD3	1.88	0.54
1:A:286:ARG:NH2	1:A:289:ARG:NH2	2.55	0.54
1:D:35:SER:HA	1:D:80:LYS:NZ	2.22	0.54
1:E:76:THR:O	1:E:80:LYS:HG2	2.08	0.54
1:B:29:GLN:CD	1:B:34:TRP:HZ2	2.14	0.54
1:C:263:LEU:HD13	1:C:339:LEU:HG	1.89	0.54
1:B:29:GLN:CB	1:B:33:PHE:CD2	2.84	0.54
1:A:242:LEU:HD23	1:A:251:LEU:HD23	1.89	0.53
1:B:31:LEU:HD12	1:B:31:LEU:H	1.73	0.53
1:C:247:TYR:OH	1:C:279:MET:HE2	2.08	0.53
1:D:55:ILE:HD13	1:D:302:GLU:CG	2.39	0.53
1:D:213:LEU:HD11	1:D:231:ILE:HD11	1.90	0.53
1:B:271:CYS:O	1:B:289:ARG:CZ	2.57	0.53
1:B:8:LEU:HB2	1:B:65:LEU:CD2	2.39	0.53
1:E:95:ILE:HD12	1:E:307:HIS:HD2	1.73	0.53
1:C:31:LEU:HD23	1:C:73:ARG:CZ	2.39	0.53
1:C:169:SER:O	1:C:172:CYS:HB2	2.08	0.53
1:E:7:HIS:CD2	1:E:279:MET:HE1	2.44	0.53
1:E:5:ILE:HA	1:E:60:ILE:HG13	1.90	0.53
1:B:9:THR:HG22	1:B:13:GLN:OE1	2.08	0.53
1:C:286:ARG:HD3	1:C:289:ARG:CG	2.38	0.53
1:E:269:GLU:HA	1:E:289:ARG:O	2.09	0.53
1:B:341:ILE:HA	1:B:344:LEU:HD12	1.92	0.52
1:C:206:ILE:O	1:C:207:LEU:HD12	2.09	0.52
1:D:97:ALA:HB2	1:D:298:ALA:HB2	1.91	0.52
1:D:276:TRP:CD1	1:D:278:ILE:CG1	2.92	0.52
1:B:224:SER:CB	1:E:344:LEU:HB2	2.39	0.52
1:E:237:LYS:O	1:E:240:CYS:HB2	2.10	0.52
1:E:108:ASN:C	1:E:109:PHE:HD1	2.16	0.52
1:B:114:LEU:N	1:B:114:LEU:CD1	2.73	0.52
1:C:20:ARG:NH1	1:C:277:GLN:CB	2.73	0.52
1:C:21:MET:HB2	1:C:23:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:LEU:HD11	1:E:325:ILE:HG13	1.84	0.52
1:D:94:ASP:HB3	1:D:307:HIS:HD2	1.74	0.52
1:A:174:TRP:CD2	1:A:178:LYS:HG3	2.45	0.52
1:C:153:ILE:HD13	1:C:179:LEU:HB3	1.92	0.51
1:C:205:LYS:HB3	1:C:207:LEU:CD1	2.41	0.51
1:E:129:THR:HG23	1:E:131:ASN:H	1.73	0.51
1:D:129:THR:HG23	1:D:131:ASN:H	1.75	0.51
1:E:95:ILE:HD11	1:E:307:HIS:CD2	2.45	0.51
1:B:20:ARG:HE	1:B:42:VAL:HG13	1.75	0.51
1:D:111:LEU:N	1:D:111:LEU:CD1	2.73	0.51
1:E:194:LEU:HB3	1:E:206:ILE:HD13	1.92	0.51
1:A:262:VAL:HG12	2:A:406:HOH:O	2.10	0.51
1:D:276:TRP:CD1	1:D:278:ILE:HG12	2.46	0.51
1:D:303:PHE:HB3	1:D:332:HIS:CD2	2.46	0.51
1:E:55:ILE:CG2	1:E:302:GLU:HG2	2.40	0.51
1:E:126:ARG:HH21	1:E:126:ARG:HG3	1.77	0.50
1:E:151:ILE:HD11	1:E:218:PHE:CZ	2.45	0.50
1:B:179:LEU:O	1:C:36:SER:HB3	2.11	0.50
1:D:49:SER:OG	1:D:50:ALA:N	2.45	0.50
1:D:226:PRO:O	1:D:227:GLN:CB	2.60	0.50
1:B:174:TRP:CE2	1:B:178:LYS:HG3	2.46	0.50
1:C:231:ILE:CD1	1:C:231:ILE:N	2.74	0.50
1:D:288:GLU:OE1	1:D:288:GLU:N	2.35	0.50
1:C:193:ARG:HA	1:C:196:ASN:OD1	2.11	0.50
1:C:254:LYS:HD3	1:C:254:LYS:C	2.36	0.50
1:C:297:GLU:O	1:C:301:LEU:HG	2.12	0.50
1:E:2:PHE:CD1	1:E:2:PHE:N	2.72	0.50
1:B:72:ARG:NH1	1:E:258:GLU:HG3	2.26	0.50
1:C:20:ARG:HH12	1:C:277:GLN:CB	2.13	0.50
1:E:41:ILE:HG22	1:E:60:ILE:HG22	1.94	0.50
1:B:286:ARG:HG3	1:B:288:GLU:OE2	2.12	0.50
1:D:276:TRP:CH2	1:D:291:MET:HE3	2.47	0.50
1:E:276:TRP:CZ2	1:E:291:MET:HB3	2.47	0.50
1:A:11:LEU:HD23	1:A:65:LEU:HD21	1.94	0.50
1:A:344:LEU:C	1:A:344:LEU:CD1	2.85	0.50
1:D:8:LEU:HD12	1:D:65:LEU:HD21	1.92	0.50
1:E:291:MET:CE	1:E:296:ALA:HB2	2.41	0.50
1:D:136:TYR:CE1	1:D:140:ARG:HD3	2.46	0.50
1:E:95:ILE:CG1	1:E:307:HIS:CD2	2.94	0.50
1:E:95:ILE:HG12	1:E:307:HIS:HA	1.93	0.50
1:B:271:CYS:O	1:B:289:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ILE:CD1	1:C:254:LYS:HD3	2.42	0.49
1:D:177:LEU:HD22	1:D:319:ILE:HD12	1.93	0.49
1:E:49:SER:OG	1:E:50:ALA:N	2.45	0.49
1:E:175:LEU:HD12	1:E:181:VAL:HG21	1.93	0.49
1:E:95:ILE:HD13	1:E:301:LEU:CG	2.42	0.49
1:B:250:ASN:OD1	1:E:342:GLU:HG3	2.13	0.49
1:E:2:PHE:HE1	1:E:57:GLY:N	2.10	0.49
1:A:267:VAL:HG12	1:A:337:LEU:HB2	1.94	0.49
1:B:29:GLN:OE1	1:B:34:TRP:HZ2	1.96	0.49
1:D:213:LEU:CD1	1:D:231:ILE:HD11	2.43	0.49
1:A:15:ARG:NH2	1:A:27:ALA:O	2.46	0.49
1:D:206:ILE:O	1:D:207:LEU:HD23	2.13	0.49
1:C:221:TRP:CD1	1:C:223:ALA:O	2.66	0.49
1:E:291:MET:HE2	1:E:334:PHE:CE1	2.48	0.48
1:E:224:SER:O	1:E:226:PRO:HD3	2.13	0.48
1:D:278:ILE:HG22	1:D:279:MET:H	1.78	0.48
1:E:93:ILE:HD12	1:E:93:ILE:H	1.78	0.48
1:B:31:LEU:HD13	1:E:150:GLY:CA	2.43	0.48
1:B:139:CYS:HB3	1:B:174:TRP:CD1	2.49	0.48
1:C:143:GLU:HB2	1:C:179:LEU:HD21	1.95	0.48
1:D:278:ILE:HG22	1:D:279:MET:N	2.29	0.48
1:E:300:LEU:HD11	1:E:325:ILE:CG1	2.34	0.48
1:B:164:THR:HG21	1:B:193:ARG:HD3	1.96	0.48
1:B:226:PRO:HG2	1:B:229:VAL:HG21	1.96	0.48
1:C:172:CYS:HB3	1:C:201:LEU:HD21	1.95	0.48
1:E:59:TYR:OH	1:E:279:MET:HB3	2.14	0.48
1:E:95:ILE:HD13	1:E:301:LEU:CB	2.44	0.48
1:E:300:LEU:C	1:E:300:LEU:CD2	2.86	0.48
1:B:11:LEU:O	1:B:14:ALA:HB3	2.14	0.48
1:E:66:PRO:HB3	1:E:101:PHE:HE2	1.78	0.48
1:B:8:LEU:HD13	1:B:63:CYS:HA	1.96	0.48
1:C:164:THR:HG21	1:C:193:ARG:HD3	1.96	0.48
1:C:232:ASP:O	1:C:235:THR:N	2.43	0.48
1:B:164:THR:HG22	1:B:314:ARG:HH21	1.79	0.47
1:E:138:ILE:O	1:E:142:VAL:HG23	2.13	0.47
1:A:227:GLN:HE22	1:D:343:ASN:HB3	1.79	0.47
1:C:238:GLN:N	1:C:239:PRO:CD	2.78	0.47
1:E:41:ILE:O	1:E:41:ILE:HD12	2.14	0.47
1:D:294:CYS:O	1:D:297:GLU:HB3	2.14	0.47
1:E:81:VAL:HG22	1:E:102:THR:HG22	1.96	0.47
1:D:49:SER:HB2	1:D:303:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:HIS:HB2	1:C:64:PHE:O	2.14	0.47
1:C:291:MET:HE1	1:C:334:PHE:HE1	1.78	0.47
1:B:342:GLU:CD	1:B:342:GLU:H	2.23	0.47
1:C:49:SER:OG	1:C:50:ALA:N	2.46	0.47
1:A:206:ILE:O	1:A:207:LEU:HD12	2.15	0.47
1:B:276:TRP:HH2	1:B:291:MET:HB3	1.80	0.47
1:B:194:LEU:HD22	1:B:206:ILE:HG23	1.96	0.47
1:D:4:LEU:HD13	1:D:295:PHE:CD2	2.50	0.47
1:E:95:ILE:HD13	1:E:301:LEU:HB3	1.96	0.47
1:B:111:LEU:C	1:B:113:SER:N	2.71	0.46
1:C:4:LEU:HD22	1:C:295:PHE:CD1	2.49	0.46
1:D:247:TYR:HB3	1:D:248:PRO:HD3	1.98	0.46
1:E:7:HIS:HB2	1:E:64:PHE:O	2.15	0.46
1:E:175:LEU:CD1	1:E:181:VAL:HG21	2.45	0.46
1:A:343:ASN:O	1:A:344:LEU:HB3	2.13	0.46
1:C:231:ILE:HG13	1:C:255:VAL:CB	2.45	0.46
1:B:111:LEU:HA	1:B:114:LEU:HD13	1.96	0.46
1:A:19:ARG:HD2	1:A:25:GLU:OE2	2.14	0.46
1:A:225:MET:HE1	1:D:343:ASN:ND2	2.30	0.46
1:C:238:GLN:N	1:C:239:PRO:HD2	2.31	0.46
1:E:46:THR:HA	1:E:55:ILE:O	2.14	0.46
1:B:20:ARG:HE	1:B:42:VAL:CG1	2.28	0.46
1:E:2:PHE:HE1	1:E:56:HIS:C	2.24	0.46
1:A:31:LEU:HD11	1:A:68:MET:HG3	1.98	0.46
1:B:17:VAL:O	1:B:21:MET:HG3	2.15	0.46
1:D:284:MET:HG3	1:D:290:GLN:HB2	1.97	0.46
1:A:16:ASP:OD1	1:A:16:ASP:C	2.58	0.46
1:C:206:ILE:C	1:C:207:LEU:HD12	2.40	0.46
1:D:29:GLN:N	1:D:29:GLN:NE2	2.59	0.46
1:E:64:PHE:CZ	1:E:105:ILE:HD11	2.51	0.46
1:A:284:MET:HE2	1:A:284:MET:HA	1.97	0.46
1:D:72:ARG:HA	2:D:407:HOH:O	2.16	0.46
1:A:226:PRO:HD2	1:A:229:VAL:HG21	1.98	0.45
1:B:164:THR:CG2	1:B:193:ARG:HD3	2.47	0.45
1:B:278:ILE:HG12	1:B:279:MET:H	1.80	0.45
1:D:231:ILE:HG23	1:D:231:ILE:O	2.16	0.45
1:E:310:PHE:HZ	1:E:321:LYS:O	2.00	0.45
1:A:239:PRO:HG2	2:A:401:HOH:O	2.15	0.45
1:B:301:LEU:HD23	1:B:301:LEU:HA	1.71	0.45
1:C:227:GLN:HA	1:C:227:GLN:OE1	2.15	0.45
1:D:288:GLU:H	1:D:288:GLU:CD	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:PHE:HB3	1:A:332:HIS:CE1	2.52	0.45
1:B:64:PHE:C	1:B:65:LEU:HD23	2.42	0.45
1:D:2:PHE:CE2	1:D:299:MET:HG2	2.52	0.45
1:C:232:ASP:C	1:C:234:ALA:N	2.70	0.45
1:D:174:TRP:HE3	1:D:322:MET:HE3	1.82	0.45
1:A:106:PHE:HA	1:A:111:LEU:HD12	1.99	0.45
1:B:76:THR:HG22	1:B:79:ARG:NH2	2.32	0.45
1:D:32:GLU:HA	1:D:35:SER:OG	2.17	0.45
1:D:297:GLU:O	1:D:301:LEU:HG	2.16	0.45
1:B:14:ALA:O	1:B:18:SER:HB3	2.17	0.45
1:E:74:PHE:HB3	1:E:109:PHE:CE2	2.47	0.45
1:E:55:ILE:HD12	1:E:55:ILE:N	2.32	0.45
1:C:276:TRP:CE2	1:C:278:ILE:HD13	2.52	0.44
1:E:5:ILE:HD13	1:E:60:ILE:CD1	2.47	0.44
1:E:95:ILE:HD11	1:E:307:HIS:CA	2.45	0.44
1:E:171:VAL:O	1:E:175:LEU:HD23	2.16	0.44
1:C:45:ILE:HG21	1:C:276:TRP:CE3	2.52	0.44
1:A:152:ASP:OD1	1:A:154:THR:HB	2.17	0.44
1:C:124:PHE:HB3	1:C:312:TRP:CZ2	2.53	0.44
1:D:236:LEU:HD12	1:D:260:ILE:HG12	2.00	0.44
1:E:2:PHE:HE1	1:E:57:GLY:CA	2.28	0.44
1:E:4:LEU:CD1	1:E:295:PHE:CG	2.88	0.44
1:C:188:ALA:H	1:C:194:LEU:HD21	1.82	0.44
1:D:23:TYR:HE1	1:D:25:GLU:HG3	1.82	0.44
1:D:154:THR:HG22	1:D:155:GLN:HG3	1.99	0.44
1:E:7:HIS:O	1:E:279:MET:HE2	2.18	0.44
1:E:42:VAL:HG22	1:E:59:TYR:HD1	1.83	0.44
1:E:3:GLY:O	1:E:96:SER:HA	2.18	0.44
1:E:1:MET:SD	1:E:57:GLY:HA2	2.58	0.44
1:B:25:GLU:H	1:B:25:GLU:HG3	1.65	0.44
1:D:226:PRO:O	1:D:227:GLN:HG2	2.18	0.44
1:E:1:MET:HA	1:E:56:HIS:O	2.17	0.44
1:E:5:ILE:HD13	1:E:60:ILE:HG12	1.99	0.44
1:B:318:THR:OG1	1:B:321:LYS:HG3	2.18	0.43
1:E:41:ILE:CG2	1:E:60:ILE:HG22	2.48	0.43
1:C:106:PHE:HA	1:C:111:LEU:HD22	2.00	0.43
1:C:124:PHE:O	1:C:309:ASN:HB3	2.17	0.43
1:D:123:GLU:HG3	1:D:125:GLU:HG2	2.00	0.43
1:E:151:ILE:HD12	1:E:151:ILE:O	2.17	0.43
1:D:55:ILE:HG13	1:D:303:PHE:CE1	2.53	0.43
1:C:278:ILE:O	1:C:281:ALA:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ILE:HD11	1:D:303:PHE:HA	1.99	0.43
1:B:344:LEU:O	1:B:345:TYR:HB3	2.18	0.43
1:C:198:GLN:NE2	1:C:204:GLY:O	2.41	0.43
1:E:31:LEU:HD23	1:E:31:LEU:HA	1.66	0.43
1:E:137:VAL:HG13	1:E:336:PRO:HB3	2.01	0.43
1:D:69:LEU:HD23	1:D:69:LEU:HA	1.68	0.43
1:C:7:HIS:O	1:C:279:MET:HE3	2.18	0.43
1:C:127:PHE:O	1:C:309:ASN:HA	2.18	0.43
1:E:174:TRP:HE3	1:E:322:MET:HE2	1.73	0.43
1:B:162:GLY:HA3	1:B:223:ALA:HB2	2.00	0.43
1:B:248:PRO:HG3	1:E:342:GLU:HB2	2.00	0.43
1:D:276:TRP:CD1	1:D:278:ILE:HD11	2.54	0.43
1:D:303:PHE:HB3	1:D:332:HIS:NE2	2.33	0.43
1:E:64:PHE:HE2	1:E:101:PHE:CD2	2.36	0.43
1:C:161:VAL:O	1:C:222:VAL:HG12	2.18	0.43
1:C:232:ASP:O	1:C:235:THR:HB	2.19	0.43
1:D:29:GLN:NE2	1:D:29:GLN:CA	2.82	0.43
1:E:33:PHE:CD1	1:E:33:PHE:C	2.97	0.43
1:B:303:PHE:HB3	1:B:332:HIS:CE1	2.54	0.42
1:C:175:LEU:O	1:C:181:VAL:HG23	2.19	0.42
1:A:76:THR:O	1:A:80:LYS:HG2	2.19	0.42
1:B:276:TRP:CH2	1:B:291:MET:HB3	2.54	0.42
1:D:174:TRP:CZ2	1:D:178:LYS:HD3	2.55	0.42
1:E:263:LEU:HD11	1:E:337:LEU:HD23	2.00	0.42
1:B:291:MET:HE2	1:B:296:ALA:N	2.34	0.42
1:D:297:GLU:OE2	1:D:311:SER:OG	2.29	0.42
1:A:15:ARG:HA	1:A:18:SER:HB2	2.01	0.42
1:D:127:PHE:O	1:D:309:ASN:HA	2.19	0.42
1:E:64:PHE:HE2	1:E:101:PHE:HD2	1.66	0.42
1:E:95:ILE:CG1	1:E:301:LEU:HD23	2.49	0.42
1:B:286:ARG:HB3	1:B:290:GLN:CD	2.44	0.42
1:C:166:ASP:CB	1:C:315:ASN:H	2.31	0.42
1:C:280:SER:O	1:C:284:MET:HG2	2.20	0.42
1:C:80:LYS:HD2	1:C:80:LYS:HA	1.60	0.42
1:E:3:GLY:O	1:E:4:LEU:HD23	2.20	0.42
1:E:310:PHE:CZ	1:E:321:LYS:O	2.72	0.42
1:B:21:MET:HB3	1:B:21:MET:HE2	1.77	0.42
1:B:172:CYS:HB3	1:B:201:LEU:HD11	2.01	0.42
1:E:89:GLN:HG3	1:E:126:ARG:HH22	1.85	0.42
1:E:198:GLN:NE2	1:E:204:GLY:O	2.53	0.42
1:E:3:GLY:HA3	1:E:93:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:ILE:HA	1:E:60:ILE:CG1	2.49	0.42
1:A:276:TRP:CZ3	1:A:299:MET:HE1	2.55	0.42
1:A:325:ILE:HA	1:A:325:ILE:HD12	1.84	0.42
1:C:327:GLU:HA	1:C:330:VAL:HG12	2.02	0.42
1:E:55:ILE:HG22	1:E:56:HIS:N	2.35	0.42
1:B:14:ALA:HB1	1:B:34:TRP:CZ2	2.55	0.41
1:E:206:ILE:C	1:E:207:LEU:HD23	2.45	0.41
1:C:161:VAL:HA	1:C:187:THR:HB	2.02	0.41
1:D:258:GLU:O	1:D:260:ILE:HD12	2.20	0.41
1:A:140:ARG:HD2	1:A:140:ARG:HA	1.86	0.41
1:C:241:VAL:HA	1:C:261:TYR:O	2.19	0.41
1:E:50:ALA:HA	1:E:272:PHE:CE2	2.54	0.41
1:B:224:SER:HB3	1:E:344:LEU:HD22	2.03	0.41
1:E:50:ALA:HA	1:E:272:PHE:HE2	1.86	0.41
1:E:126:ARG:HG3	1:E:126:ARG:NH2	2.35	0.41
1:C:49:SER:OG	1:C:51:THR:N	2.54	0.41
1:D:226:PRO:O	1:D:227:GLN:CG	2.69	0.41
1:E:75:LYS:O	1:E:79:ARG:HG2	2.20	0.41
1:A:1:MET:HA	1:A:56:HIS:O	2.20	0.41
1:B:244:ASP:OD2	1:B:251:LEU:HB2	2.21	0.41
1:C:193:ARG:O	1:C:196:ASN:HB2	2.20	0.41
1:D:282:ALA:C	1:D:284:MET:H	2.28	0.41
1:E:95:ILE:HD13	1:E:301:LEU:HG	2.03	0.41
1:A:174:TRP:CE2	1:A:178:LYS:HG3	2.56	0.41
1:C:238:GLN:OE1	1:C:238:GLN:HA	2.21	0.41
1:D:25:GLU:H	1:D:25:GLU:HG2	1.65	0.41
1:D:147:LYS:HB2	1:D:147:LYS:HE2	1.72	0.41
1:C:284:MET:HE3	1:C:291:MET:HA	2.02	0.41
1:D:109:PHE:O	1:D:111:LEU:CD1	2.68	0.41
1:C:90:LYS:HD3	1:C:118:ARG:HH22	1.86	0.40
1:C:158:VAL:HG11	1:C:175:LEU:HD23	2.02	0.40
1:D:238:GLN:OE1	1:D:238:GLN:HA	2.21	0.40
1:E:76:THR:HA	1:E:79:ARG:HD3	2.03	0.40
1:E:149:LEU:HD23	1:E:149:LEU:HA	1.91	0.40
1:E:295:PHE:HD1	1:E:295:PHE:HA	1.72	0.40
1:A:98:LEU:HB3	1:A:102:THR:CG2	2.50	0.40
1:B:8:LEU:CD1	1:B:63:CYS:HA	2.50	0.40
1:D:29:GLN:HE21	1:D:29:GLN:CA	2.34	0.40
1:D:101:PHE:HD1	1:D:104:ILE:HD12	1.85	0.40
1:D:227:GLN:O	1:D:227:GLN:HG3	2.20	0.40
1:E:37:ALA:HA	1:E:38:PRO:HD3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:GLU:OE2	1:D:200:GLU:HA	2.22	0.40
1:E:285:ALA:O	1:E:287:PRO:HD3	2.20	0.40
1:A:326:GLY:O	1:A:329:SER:HB3	2.21	0.40
1:C:21:MET:HB2	1:C:23:TYR:CE2	2.56	0.40
1:C:153:ILE:CD1	1:C:179:LEU:HD23	2.50	0.40
1:C:229:VAL:HG12	1:C:230:VAL:N	2.37	0.40
1:D:335:GLN:OE1	1:D:335:GLN:HA	2.21	0.40
1:B:4:LEU:HB2	1:B:59:TYR:HD1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/347 (97%)	316 (94%)	20 (6%)	0	100	100
1	B	343/347 (99%)	329 (96%)	14 (4%)	0	100	100
1	C	342/347 (99%)	322 (94%)	20 (6%)	0	100	100
1	D	335/347 (96%)	319 (95%)	16 (5%)	0	100	100
1	E	344/347 (99%)	324 (94%)	20 (6%)	0	100	100
All	All	1700/1735 (98%)	1610 (95%)	90 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	271/281 (96%)	263 (97%)	8 (3%)	36	72
1	B	271/281 (96%)	265 (98%)	6 (2%)	45	78
1	C	266/281 (95%)	251 (94%)	15 (6%)	19	50
1	D	249/281 (89%)	234 (94%)	15 (6%)	17	47
1	E	252/281 (90%)	236 (94%)	16 (6%)	16	45
All	All	1309/1405 (93%)	1249 (95%)	60 (5%)	24	58

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	42	VAL
1	A	98	LEU
1	A	120	THR
1	A	132	THR
1	A	249	LYS
1	A	262	VAL
1	A	344	LEU
1	B	104	ILE
1	B	164	THR
1	B	229	VAL
1	B	249	LYS
1	B	276	TRP
1	B	283	GLU
1	C	28	ASP
1	C	36	SER
1	C	45	ILE
1	C	51	THR
1	C	78	THR
1	C	89	GLN
1	C	157	THR
1	C	160	VAL
1	C	173	ARG
1	C	206	ILE
1	C	224	SER
1	C	225	MET
1	C	231	ILE
1	C	236	LEU
1	C	260	ILE

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Mol	Chain	Res	Type
1	D	13	GLN
1	D	24	ASP
1	D	25	GLU
1	D	26	TYR
1	D	29	GLN
1	D	45	ILE
1	D	48	THR
1	D	111	LEU
1	D	147	LYS
1	D	154	THR
1	D	225	MET
1	D	227	GLN
1	D	255	VAL
1	D	260	ILE
1	D	276	TRP
1	E	2	PHE
1	E	4	LEU
1	E	13	GLN
1	E	41	ILE
1	E	45	ILE
1	E	54	VAL
1	E	151	ILE
1	E	157	THR
1	E	175	LEU
1	E	249	LYS
1	E	273	ASP
1	E	274	ILE
1	E	275	ASP
1	E	301	LEU
1	E	312	TRP
1	E	316	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	B	40	GLN
1	B	91	HIS
1	B	198	GLN
1	C	270	HIS
1	C	315	ASN
1	C	316	GLN

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Mol	Chain	Res	Type
1	D	29	GLN
1	D	89	GLN
1	D	227	GLN
1	D	332	HIS
1	E	91	HIS
1	E	190	ASN
1	E	198	GLN
1	E	290	GLN
1	E	307	HIS
1	E	309	ASN
1	E	335	GLN

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	340/347 (97%)	-0.14	4 (1%) 76 68	38, 56, 88, 139	1 (0%)
1	B	345/347 (99%)	0.13	11 (3%) 50 40	39, 63, 105, 145	0
1	C	344/347 (99%)	0.32	13 (3%) 44 35	40, 70, 106, 145	0
1	D	339/347 (97%)	0.42	11 (3%) 50 40	24, 81, 107, 160	1 (0%)
1	E	345/347 (99%)	0.78	37 (10%) 11 8	46, 88, 109, 146	2 (0%)
All	All	1713/1735 (98%)	0.30	76 (4%) 39 31	24, 73, 106, 160	4 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	227	GLN	5.2
1	E	277	GLN	4.7
1	C	239	PRO	4.0
1	E	311	SER	3.7
1	E	344	LEU	3.6
1	A	344	LEU	3.5
1	E	345	TYR	3.4
1	C	277	GLN	3.4
1	C	248	PRO	3.3
1	E	312	TRP	3.2
1	C	278	ILE	3.2
1	E	301	LEU	3.2
1	E	343	ASN	3.1
1	B	280	SER	3.1
1	C	231	ILE	3.0
1	E	300	LEU	3.0
1	E	153	ILE	3.0
1	C	230	VAL	3.0
1	E	271	CYS	2.9
1	A	278	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	95	ILE	2.8
1	E	280	SER	2.8
1	E	303	PHE	2.8
1	D	345	TYR	2.7
1	E	316	GLN	2.7
1	B	117	VAL	2.7
1	E	298	ALA	2.7
1	C	276	TRP	2.7
1	E	315[A]	ASN	2.7
1	E	278	ILE	2.6
1	C	229	VAL	2.6
1	B	29	GLN	2.6
1	E	306	TRP	2.5
1	E	324	ALA	2.5
1	C	225	MET	2.4
1	E	129	THR	2.4
1	E	139	CYS	2.4
1	E	132	THR	2.4
1	E	117	VAL	2.4
1	E	317	ILE	2.4
1	D	20	ARG	2.4
1	C	26	TYR	2.3
1	E	55	ILE	2.3
1	B	116	GLN	2.3
1	B	114	LEU	2.3
1	D	111	LEU	2.3
1	D	21	MET	2.3
1	B	239	PRO	2.3
1	E	318	THR	2.3
1	C	233	PRO	2.3
1	C	228	GLY	2.2
1	E	111	LEU	2.2
1	D	70	ALA	2.2
1	B	311	SER	2.2
1	E	3	GLY	2.2
1	D	279	MET	2.2
1	E	112	ALA	2.2
1	B	122	LEU	2.2
1	D	228	GLY	2.2
1	D	253	SER	2.2
1	E	276	TRP	2.1
1	E	331	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	41	ILE	2.1
1	E	133	HIS	2.1
1	B	343	ASN	2.1
1	B	27	ALA	2.1
1	E	329	SER	2.1
1	C	118	ARG	2.1
1	E	47	VAL	2.1
1	B	74	PHE	2.1
1	E	54	VAL	2.0
1	D	310	PHE	2.0
1	E	115	ARG	2.0
1	A	118	ARG	2.0
1	A	230	VAL	2.0
1	D	58	ARG	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.