



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID : 1LBI
Title : LAC REPRESSOR
Authors : Lewis, M.; Chang, G.; Horton, N.C.; Kercher, M.A.; Pace, H.C.; Lu, P.
Deposited on : 1996-02-17
Resolution : 2.70 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

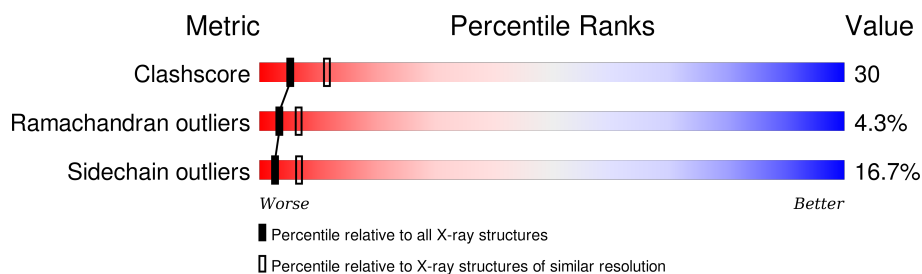
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	360	
1	B	360	
1	C	360	
1	D	360	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8872 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 LAC REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			
1	B	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			
1	C	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			
1	D	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			

There are 8 discrepancies between the modelled and reference sequences:

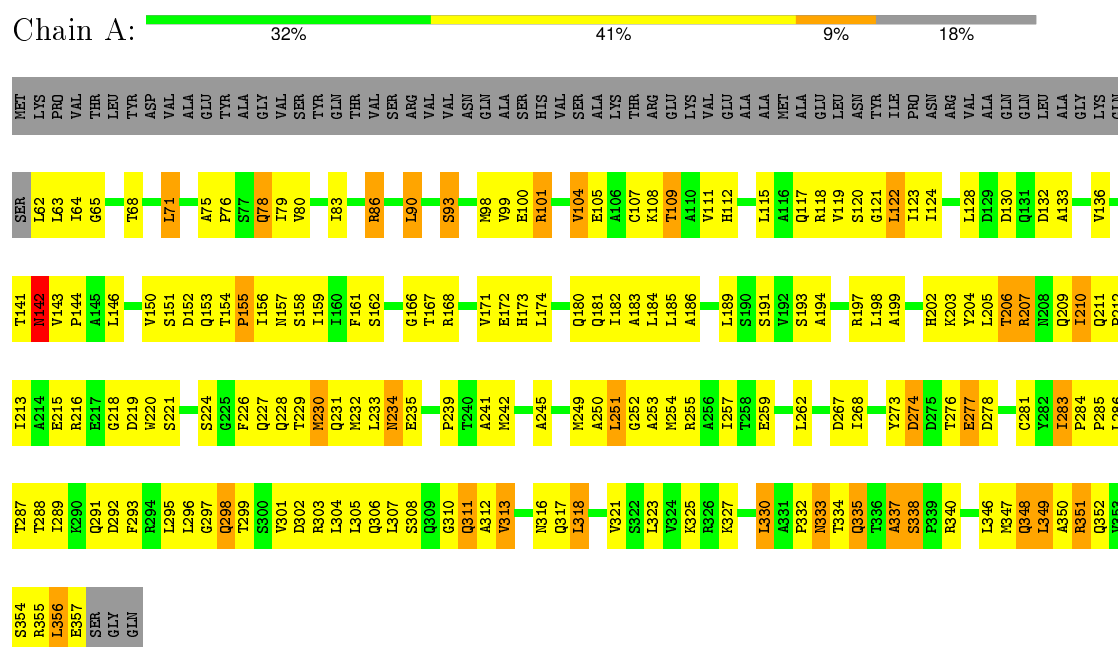
Chain	Residue	Modelled	Actual	Comment	Reference
A	109	THR	ALA	CONFLICT	UNP P03023
A	286	LEU	SER	CONFLICT	UNP P03023
B	109	THR	ALA	CONFLICT	UNP P03023
B	286	LEU	SER	CONFLICT	UNP P03023
C	109	THR	ALA	CONFLICT	UNP P03023
C	286	LEU	SER	CONFLICT	UNP P03023
D	109	THR	ALA	CONFLICT	UNP P03023
D	286	LEU	SER	CONFLICT	UNP P03023

3 Residue-property plots

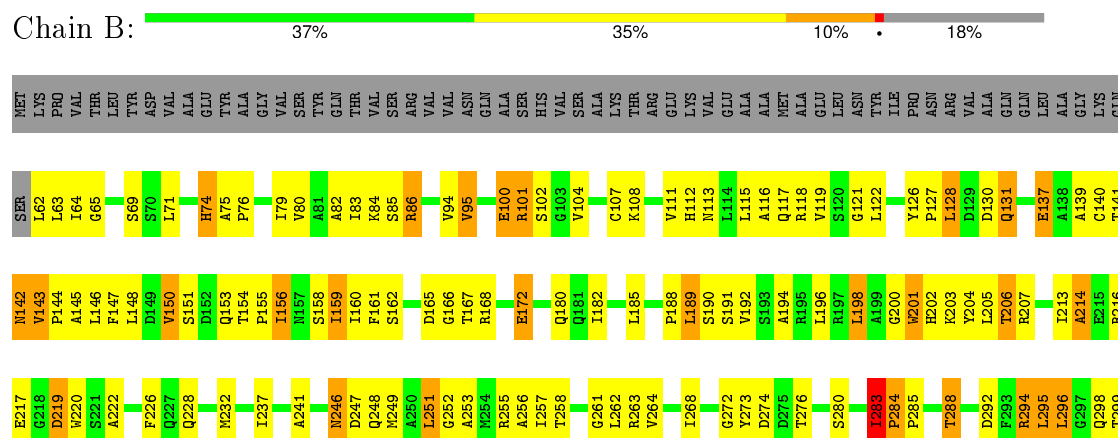
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

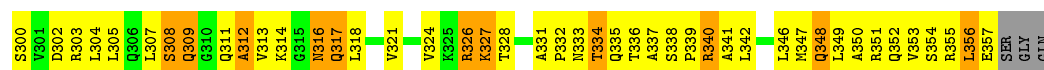
Note EDS was not executed.

• Molecule 1: LAC REPRESSOR



• Molecule 1: LAC REPRESSOR





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.30 Å 73.30 Å 147.80 Å 90.00° 120.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.250 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8872	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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	0.78	0/2247	1.04	4/3055 (0.1%)
1	B	0.82	0/2247	1.11	10/3055 (0.3%)
1	C	0.84	1/2247 (0.0%)	1.04	9/3055 (0.3%)
1	D	0.85	0/2247	0.99	3/3055 (0.1%)
All	All	0.82	1/8988 (0.0%)	1.05	26/12220 (0.2%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	TRP	CB-CG	6.07	1.61	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ILE	C-N-CD	-19.64	77.40	120.60
1	B	283	ILE	C-N-CA	10.29	165.20	122.00
1	C	330	LEU	CA-CB-CG	7.59	132.76	115.30
1	C	283	ILE	C-N-CD	7.05	143.21	128.40
1	B	336	THR	N-CA-C	-6.62	93.13	111.00
1	B	335	GLN	N-CA-C	6.47	128.46	111.00
1	C	333	ASN	N-CA-C	6.31	128.03	111.00
1	C	284	PRO	N-CA-C	-6.09	96.28	112.10
1	B	284	PRO	CA-N-CD	-5.94	103.19	111.50
1	A	351	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	326	ARG	NE-CZ-NH2	-5.83	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	104	VAL	CB-CA-C	-5.71	100.55	111.40
1	B	330	LEU	CA-CB-CG	5.68	128.37	115.30
1	D	283	ILE	C-N-CD	5.53	140.02	128.40
1	B	294	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	313	VAL	N-CA-C	-5.40	96.42	111.00
1	C	286	LEU	CA-CB-CG	5.39	127.71	115.30
1	A	65	GLY	N-CA-C	-5.39	99.62	113.10
1	C	309	GLN	N-CA-C	-5.29	96.71	111.00
1	D	148	LEU	CA-CB-CG	5.27	127.42	115.30
1	B	283	ILE	N-CA-C	5.06	124.66	111.00
1	C	185	LEU	N-CA-C	-5.02	97.45	111.00
1	C	314	LYS	N-CA-C	5.02	124.55	111.00
1	B	219	ASP	CB-CG-OD1	5.00	122.80	118.30
1	C	283	ILE	C-N-CA	-5.00	100.98	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	126	TYR	Sidechain

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	2218	0	2269	158	0
1	B	2218	0	2269	140	0
1	C	2218	0	2269	148	0
1	D	2218	0	2269	145	0
All	All	8872	0	9076	544	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 30.

All (544) 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:A:144:PRO:HG2	1:A:308:SER:HA	1.24	1.13
1:A:115:LEU:HD11	1:A:143:VAL:HG11	1.18	1.10
1:C:283:ILE:HG22	1:C:284:PRO:HD3	1.43	1.01
1:B:189:LEU:HD13	1:B:217:GLU:HG3	1.40	0.99
1:A:144:PRO:HB3	1:A:307:LEU:HD22	1.44	0.98
1:C:97:SER:HB2	1:C:114:LEU:HD21	1.48	0.95
1:B:216:ARG:HB3	1:B:228:GLN:HE21	1.30	0.94
1:D:138:ALA:HA	1:D:141:THR:HG23	1.52	0.90
1:C:107:CYS:O	1:C:111:VAL:HG23	1.73	0.88
1:B:338:SER:O	1:B:342:LEU:HD12	1.73	0.88
1:D:105:GLU:O	1:D:109:THR:HG23	1.73	0.87
1:B:214:ALA:HB2	1:B:237:ILE:HG21	1.55	0.87
1:B:339:PRO:HA	1:D:357:GLU:OE1	1.76	0.85
1:A:104:VAL:HG13	1:A:132:ASP:HB3	1.55	0.85
1:C:104:VAL:HG21	1:C:135:ALA:HB3	1.57	0.85
1:B:115:LEU:HG	1:B:143:VAL:HG21	1.56	0.84
1:C:63:LEU:HG	1:C:119:VAL:HG12	1.59	0.84
1:D:71:LEU:HD11	1:D:101:ARG:HG3	1.60	0.84
1:A:245:ALA:O	1:A:273:TYR:HB3	1.76	0.83
1:B:113:ASN:O	1:B:117:GLN:HG2	1.79	0.83
1:B:115:LEU:HD11	1:B:122:LEU:HD21	1.59	0.82
1:C:349:LEU:HD13	1:D:346:LEU:HD23	1.61	0.82
1:B:222:ALA:HA	1:B:248:GLN:O	1.79	0.81
1:B:108:LYS:NZ	1:B:139:ALA:HB2	1.94	0.81
1:B:216:ARG:HH11	1:B:228:GLN:NE2	1.78	0.80
1:C:283:ILE:HG22	1:C:284:PRO:CD	2.13	0.79
1:B:86:ARG:HG3	1:B:298:GLN:HA	1.63	0.79
1:C:342:LEU:HD21	1:D:352:GLN:HB3	1.64	0.79
1:A:253:ALA:O	1:A:257:ILE:HG12	1.82	0.79
1:C:312:ALA:HB1	1:C:314:LYS:NZ	1.97	0.79
1:C:147:PHE:CD2	1:C:156:ILE:HD12	2.16	0.79
1:B:168:ARG:O	1:B:172:GLU:HB2	1.83	0.78
1:B:350:ALA:HA	1:D:346:LEU:HD12	1.67	0.77
1:A:239:PRO:O	1:A:268:ILE:HG12	1.85	0.77
1:B:76:PRO:O	1:B:80:VAL:HG23	1.85	0.77
1:A:283:ILE:HG22	1:A:284:PRO:HD3	1.65	0.77
1:A:63:LEU:HD23	1:A:119:VAL:HA	1.66	0.76
1:C:202:HIS:O	1:C:206:THR:HG23	1.84	0.76
1:C:246:ASN:OD1	1:C:249:MET:HB2	1.85	0.76
1:A:62:LEU:N	1:A:120:SER:HG	1.83	0.76
1:C:353:VAL:O	1:C:356:LEU:HB2	1.86	0.76
1:C:117:GLN:O	1:C:118:ARG:HD2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:HG21	1:B:156:ILE:HD11	1.68	0.75
1:A:346:LEU:HD23	1:B:349:LEU:HD13	1.67	0.75
1:A:347:MET:O	1:A:351:ARG:HG3	1.87	0.75
1:A:168:ARG:O	1:A:172:GLU:HG3	1.86	0.75
1:A:206:THR:HB	1:A:211:GLN:HE22	1.51	0.74
1:D:86:ARG:HG3	1:D:86:ARG:O	1.85	0.74
1:D:348:GLN:O	1:D:352:GLN:HG2	1.86	0.74
1:C:323:LEU:HD21	1:C:325:LYS:HG2	1.67	0.73
1:D:348:GLN:HG3	1:D:351:ARG:HH21	1.53	0.73
1:B:64:ILE:HD11	1:B:94:VAL:HG22	1.70	0.73
1:C:126:TYR:CD1	1:C:127:PRO:HD2	2.23	0.73
1:A:63:LEU:HD12	1:A:93:SER:HB3	1.70	0.73
1:A:191:SER:HB3	1:A:194:ALA:HB3	1.71	0.73
1:C:216:ARG:HB3	1:C:228:GLN:HE21	1.52	0.72
1:B:115:LEU:HD21	1:B:140:CYS:HA	1.71	0.71
1:C:168:ARG:O	1:C:172:GLU:HG2	1.89	0.71
1:C:312:ALA:HB1	1:C:314:LYS:HZ3	1.54	0.71
1:B:346:LEU:HD12	1:D:350:ALA:HA	1.71	0.71
1:A:64:ILE:HG13	1:A:304:LEU:HD23	1.72	0.71
1:C:70:SER:HB2	1:D:84:LYS:HG2	1.72	0.70
1:C:334:THR:C	1:C:336:THR:H	1.95	0.70
1:B:108:LYS:HZ2	1:B:139:ALA:HB2	1.54	0.70
1:A:316:ASN:HD21	1:A:318:LEU:HD12	1.55	0.70
1:A:250:ALA:O	1:A:254:MET:HG3	1.91	0.69
1:D:123:ILE:CG2	1:D:148:LEU:HD22	2.22	0.69
1:A:203:LYS:O	1:A:207:ARG:HD3	1.92	0.69
1:C:306:GLN:OE1	1:C:313:VAL:HG11	1.92	0.69
1:A:144:PRO:CG	1:A:308:SER:HA	2.14	0.69
1:B:188:PRO:HD3	1:B:219:ASP:HA	1.74	0.69
1:A:146:LEU:HD11	1:A:159:ILE:HG13	1.76	0.68
1:A:104:VAL:HG12	1:A:136:VAL:CG2	2.24	0.68
1:D:216:ARG:HH11	1:D:228:GLN:NE2	1.91	0.68
1:D:97:SER:HB2	1:D:114:LEU:HG	1.75	0.67
1:A:283:ILE:HG22	1:A:284:PRO:CD	2.24	0.67
1:D:181:GLN:HG2	1:D:213:ILE:HD13	1.75	0.67
1:B:213:ILE:HG13	1:B:213:ILE:O	1.95	0.67
1:A:79:ILE:HG22	1:A:83:ILE:HD13	1.76	0.67
1:B:216:ARG:HB3	1:B:228:GLN:NE2	2.05	0.67
1:A:98:MET:O	1:B:84:LYS:HE3	1.93	0.67
1:A:356:LEU:HD13	1:B:342:LEU:CD1	2.25	0.67
1:B:246:ASN:OD1	1:B:249:MET:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TYR:CG	1:C:127:PRO:HD2	2.30	0.66
1:A:229:THR:HG23	1:A:232:MET:HE1	1.76	0.66
1:C:63:LEU:CG	1:C:119:VAL:HG12	2.26	0.66
1:A:146:LEU:HD21	1:A:159:ILE:HD12	1.78	0.66
1:C:144:PRO:HG3	1:C:308:SER:HB3	1.77	0.66
1:B:357:GLU:OE2	1:D:340:ARG:HA	1.96	0.66
1:C:254:MET:CE	1:C:286:LEU:HD13	2.26	0.65
1:C:273:TYR:O	1:C:274:ASP:HB2	1.95	0.65
1:A:203:LYS:O	1:A:207:ARG:HB2	1.96	0.65
1:C:332:PRO:O	1:C:333:ASN:HB2	1.95	0.65
1:A:348:GLN:O	1:A:352:GLN:HG3	1.96	0.65
1:A:104:VAL:HG12	1:A:136:VAL:HG23	1.78	0.65
1:A:104:VAL:CG1	1:A:132:ASP:HB3	2.27	0.65
1:B:339:PRO:HA	1:D:357:GLU:CD	2.17	0.65
1:D:122:LEU:CD1	1:D:140:CYS:HB2	2.26	0.65
1:D:191:SER:O	1:D:195:ARG:HB2	1.97	0.64
1:C:323:LEU:CD2	1:C:325:LYS:HG2	2.27	0.64
1:B:160:ILE:HG22	1:B:161:PHE:O	1.98	0.64
1:D:132:ASP:O	1:D:136:VAL:HG23	1.98	0.64
1:B:338:SER:HB2	1:B:342:LEU:HD12	1.79	0.64
1:A:86:ARG:NH2	1:A:90:LEU:HD13	2.12	0.64
1:A:186:ALA:HA	1:A:245:ALA:HB2	1.80	0.63
1:B:283:ILE:O	1:B:283:ILE:HG22	1.97	0.63
1:A:352:GLN:HB2	1:B:342:LEU:HD21	1.79	0.63
1:D:254:MET:HE2	1:D:284:PRO:HD2	1.81	0.63
1:D:324:VAL:HG11	1:D:326:ARG:NH1	2.13	0.63
1:B:338:SER:HB2	1:B:342:LEU:CD1	2.29	0.63
1:D:275:ASP:HB3	1:D:290:LYS:HG3	1.81	0.63
1:D:71:LEU:HD11	1:D:101:ARG:CG	2.29	0.62
1:D:90:LEU:HD23	1:D:305:LEU:HD11	1.82	0.62
1:B:104:VAL:O	1:B:108:LYS:HG2	1.99	0.62
1:D:168:ARG:HH11	1:D:168:ARG:HG2	1.64	0.62
1:B:216:ARG:NH1	1:B:228:GLN:NE2	2.48	0.62
1:A:356:LEU:HD13	1:B:342:LEU:HD13	1.82	0.61
1:A:283:ILE:O	1:A:285:PRO:N	2.33	0.61
1:C:290:LYS:O	1:C:321:VAL:HG22	2.00	0.61
1:A:226:PHE:HA	1:A:252:GLY:O	2.00	0.61
1:A:109:THR:HA	1:A:112:HIS:CD2	2.35	0.61
1:C:313:VAL:O	1:C:313:VAL:HG22	2.00	0.61
1:C:185:LEU:HB3	1:C:244:VAL:HG13	1.80	0.61
1:B:311:GLN:O	1:B:313:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD12	1:C:350:ALA:HA	1.83	0.61
1:C:162:SER:HB3	1:C:165:ASP:HB2	1.83	0.61
1:B:207:ARG:HG2	1:B:207:ARG:O	2.00	0.61
1:A:150:VAL:HG11	1:A:156:ILE:HD11	1.83	0.61
1:A:283:ILE:CG2	1:A:284:PRO:HD3	2.31	0.61
1:C:254:MET:HE1	1:C:286:LEU:HD13	1.82	0.61
1:A:104:VAL:O	1:A:108:LYS:HG2	2.01	0.60
1:B:111:VAL:O	1:B:115:LEU:HD13	2.01	0.60
1:C:70:SER:HB3	1:C:98:MET:HB3	1.82	0.60
1:B:146:LEU:HD13	1:B:307:LEU:HD11	1.82	0.60
1:A:152:ASP:HA	1:A:316:ASN:OD1	2.01	0.60
1:D:70:SER:HB3	1:D:98:MET:HB3	1.83	0.60
1:A:142:ASN:ND2	1:A:143:VAL:N	2.48	0.60
1:C:97:SER:HB2	1:C:114:LEU:CD2	2.28	0.60
1:A:202:HIS:O	1:A:206:THR:HG23	2.01	0.60
1:B:222:ALA:O	1:B:252:GLY:HA3	2.01	0.60
1:B:148:LEU:HD12	1:B:159:ILE:CG2	2.32	0.60
1:D:90:LEU:HD23	1:D:305:LEU:CD1	2.31	0.59
1:C:86:ARG:HD2	1:C:298:GLN:HB2	1.83	0.59
1:C:333:ASN:HB3	1:C:336:THR:OG1	2.02	0.59
1:C:336:THR:O	1:D:356:LEU:HD22	2.02	0.59
1:A:288:THR:HG22	1:A:289:ILE:N	2.16	0.59
1:C:183:ALA:HB3	1:C:242:MET:HG2	1.83	0.59
1:D:227:GLN:O	1:D:231:GLN:HG3	2.02	0.59
1:D:339:PRO:C	1:D:341:ALA:H	2.05	0.59
1:D:103:GLY:O	1:D:105:GLU:N	2.36	0.59
1:D:104:VAL:HG23	1:D:136:VAL:CG2	2.32	0.59
1:C:114:LEU:O	1:C:119:VAL:HG22	2.02	0.59
1:A:205:LEU:HD12	1:A:212:PRO:HG3	1.85	0.59
1:C:126:TYR:O	1:C:149:ASP:HB3	2.03	0.59
1:B:323:LEU:HD23	1:B:325:LYS:HG3	1.85	0.59
1:C:342:LEU:CD2	1:D:352:GLN:HB3	2.32	0.58
1:C:118:ARG:HH22	1:D:118:ARG:HE	1.51	0.58
1:D:222:ALA:HA	1:D:248:GLN:O	2.03	0.58
1:B:122:LEU:HD23	1:B:140:CYS:HB3	1.85	0.58
1:A:281:CYS:O	1:B:251:LEU:HD22	2.04	0.58
1:C:128:LEU:HD21	1:C:136:VAL:HG21	1.86	0.58
1:A:115:LEU:HD13	1:A:122:LEU:HD11	1.84	0.58
1:D:111:VAL:CG2	1:D:140:CYS:HB3	2.33	0.58
1:B:330:LEU:HD12	1:B:331:ALA:H	1.67	0.58
1:C:133:ALA:HB1	1:C:156:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:NH1	1:B:280:SER:O	2.37	0.58
1:A:295:LEU:O	1:A:299:THR:HG23	2.04	0.58
1:B:202:HIS:O	1:B:206:THR:HG23	2.04	0.57
1:C:95:VAL:HG13	1:D:95:VAL:HG22	1.86	0.57
1:D:138:ALA:HA	1:D:141:THR:CG2	2.31	0.57
1:D:111:VAL:HG21	1:D:140:CYS:HB3	1.86	0.57
1:A:347:MET:HG2	1:C:347:MET:HG2	1.86	0.57
1:C:346:LEU:HD13	1:D:349:LEU:HD13	1.85	0.57
1:C:117:GLN:HG3	1:D:117:GLN:NE2	2.20	0.57
1:C:167:THR:HA	1:C:201:TRP:CZ3	2.38	0.57
1:A:157:ASN:HD22	1:A:307:LEU:HD11	1.70	0.57
1:D:171:VAL:O	1:D:175:VAL:HG23	2.05	0.57
1:D:111:VAL:O	1:D:115:LEU:HB2	2.04	0.57
1:A:262:LEU:HD12	1:A:267:ASP:HB3	1.86	0.57
1:A:193:SER:O	1:A:197:ARG:HB2	2.05	0.57
1:A:183:ALA:HB3	1:A:242:MET:HG2	1.86	0.57
1:A:273:TYR:N	1:A:288:THR:HG23	2.20	0.56
1:B:108:LYS:HZ1	1:B:139:ALA:HB2	1.69	0.56
1:C:118:ARG:HH22	1:D:118:ARG:NE	2.02	0.56
1:B:216:ARG:HH11	1:B:228:GLN:HE22	1.50	0.56
1:B:64:ILE:CD1	1:B:94:VAL:HG22	2.35	0.56
1:B:148:LEU:HD12	1:B:159:ILE:HG23	1.86	0.56
1:B:167:THR:HA	1:B:201:TRP:CZ3	2.41	0.56
1:C:255:ARG:O	1:C:259:GLU:HG3	2.05	0.56
1:A:273:TYR:O	1:A:274:ASP:HB2	2.06	0.56
1:C:214:ALA:HB2	1:C:237:ILE:HD13	1.88	0.56
1:A:219:ASP:O	1:A:220:TRP:HB2	2.04	0.56
1:C:161:PHE:CG	1:C:291:GLN:HG2	2.41	0.56
1:C:104:VAL:CG2	1:C:136:VAL:HG23	2.35	0.56
1:B:357:GLU:CD	1:D:340:ARG:HA	2.25	0.56
1:D:265:GLY:HA2	1:D:328:THR:O	2.05	0.55
1:C:223:MET:O	1:C:227:GLN:HG3	2.05	0.55
1:A:267:ASP:OD1	1:A:333:ASN:ND2	2.39	0.55
1:D:121:GLY:HA3	1:D:304:LEU:HD21	1.87	0.55
1:D:102:SER:HB2	1:D:106:ALA:HB2	1.87	0.55
1:D:254:MET:CE	1:D:284:PRO:HD2	2.36	0.55
1:B:119:VAL:HG23	1:B:143:VAL:HG11	1.88	0.55
1:C:336:THR:C	1:C:338:SER:H	2.10	0.55
1:B:75:ALA:HB3	1:B:76:PRO:HD3	1.88	0.55
1:D:347:MET:O	1:D:350:ALA:HB3	2.07	0.55
1:B:253:ALA:O	1:B:257:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLN:HA	1:A:228:GLN:OE1	2.06	0.55
1:C:215:GLU:C	1:C:216:ARG:HD2	2.28	0.54
1:B:102:SER:HA	1:B:126:TYR:OH	2.07	0.54
1:D:86:ARG:HE	1:D:89:GLN:NE2	2.04	0.54
1:B:159:ILE:HD11	1:B:299:THR:CG2	2.36	0.54
1:C:123:ILE:HG23	1:C:148:LEU:CD1	2.36	0.54
1:D:122:LEU:HD13	1:D:140:CYS:HB2	1.89	0.54
1:A:303:ARG:O	1:A:307:LEU:HB2	2.07	0.54
1:B:216:ARG:NH1	1:B:228:GLN:HE22	2.05	0.54
1:A:357:GLU:HB2	1:C:339:PRO:HB3	1.90	0.54
1:C:329:THR:O	1:C:330:LEU:HD22	2.08	0.54
1:D:108:LYS:HE2	1:D:139:ALA:HB2	1.89	0.54
1:D:99:VAL:HG13	1:D:106:ALA:O	2.08	0.54
1:A:174:LEU:HD22	1:A:241:ALA:HB1	1.88	0.54
1:A:206:THR:HB	1:A:211:GLN:NE2	2.22	0.54
1:C:101:ARG:HD3	1:C:102:SER:N	2.23	0.54
1:D:192:VAL:O	1:D:196:LEU:HD12	2.08	0.54
1:C:283:ILE:O	1:C:285:PRO:HD3	2.08	0.54
1:C:150:VAL:HG21	1:C:156:ILE:HD11	1.90	0.54
1:A:98:MET:HB2	1:B:84:LYS:HG2	1.89	0.53
1:C:185:LEU:HD11	1:C:225:GLY:HA2	1.90	0.53
1:B:346:LEU:HD21	1:C:346:LEU:HG	1.90	0.53
1:C:273:TYR:O	1:C:274:ASP:CB	2.56	0.53
1:D:283:ILE:O	1:D:285:PRO:HD3	2.08	0.53
1:C:192:VAL:HG13	1:C:193:SER:N	2.24	0.53
1:B:263:ARG:NH2	1:B:336:THR:HB	2.22	0.53
1:A:76:PRO:O	1:A:80:VAL:HG23	2.08	0.53
1:C:75:ALA:HB3	1:C:76:PRO:HD3	1.89	0.53
1:A:298:GLN:O	1:A:302:ASP:HB2	2.07	0.53
1:C:85:SER:O	1:C:88:ASP:HB2	2.09	0.53
1:A:146:LEU:HD21	1:A:159:ILE:CD1	2.39	0.53
1:D:144:PRO:HG2	1:D:308:SER:HA	1.89	0.53
1:A:311:GLN:O	1:A:313:VAL:HG22	2.09	0.53
1:A:287:THR:HG23	1:A:325:LYS:HA	1.90	0.53
1:B:159:ILE:HD11	1:B:299:THR:HG22	1.91	0.53
1:B:343:ALA:HB2	1:D:354:SER:HB3	1.91	0.53
1:C:186:ALA:N	1:C:216:ARG:O	2.42	0.53
1:A:133:ALA:HB1	1:A:156:ILE:CD1	2.39	0.53
1:D:327:LYS:NZ	1:D:327:LYS:HB3	2.23	0.53
1:D:253:ALA:O	1:D:257:ILE:HG13	2.09	0.53
1:A:161:PHE:HZ	1:A:292:ASP:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ARG:O	1:D:172:GLU:HG3	2.09	0.53
1:D:235:GLU:HG2	1:D:235:GLU:O	2.08	0.53
1:A:332:PRO:O	1:A:334:THR:N	2.42	0.53
1:C:297:GLY:O	1:C:301:VAL:HG23	2.08	0.52
1:B:146:LEU:HD13	1:B:307:LEU:CD1	2.40	0.52
1:D:162:SER:HA	1:D:318:LEU:HD12	1.91	0.52
1:B:86:ARG:O	1:B:86:ARG:HD3	2.09	0.52
1:C:84:LYS:HD3	1:D:98:MET:HB2	1.91	0.52
1:C:104:VAL:HG22	1:C:136:VAL:HG23	1.90	0.52
1:A:245:ALA:O	1:A:273:TYR:CB	2.55	0.52
1:B:226:PHE:HA	1:B:252:GLY:O	2.09	0.52
1:A:231:GLN:O	1:A:235:GLU:HB2	2.10	0.52
1:C:333:ASN:HB3	1:C:336:THR:CB	2.40	0.52
1:D:104:VAL:HG23	1:D:136:VAL:HG22	1.91	0.52
1:A:337:ALA:O	1:A:338:SER:HB2	2.10	0.51
1:A:283:ILE:O	1:A:285:PRO:CD	2.58	0.51
1:A:350:ALA:CB	1:C:347:MET:HG3	2.40	0.51
1:C:284:PRO:HB2	1:C:328:THR:HG22	1.91	0.51
1:D:312:ALA:C	1:D:314:LYS:N	2.62	0.51
1:D:168:ARG:HG2	1:D:168:ARG:NH1	2.26	0.51
1:C:118:ARG:HG2	1:C:118:ARG:O	2.11	0.51
1:C:333:ASN:OD1	1:C:335:GLN:N	2.42	0.51
1:D:86:ARG:HH21	1:D:89:GLN:NE2	2.09	0.51
1:D:337:ALA:O	1:D:338:SER:C	2.49	0.51
1:D:133:ALA:O	1:D:137:GLU:HB2	2.11	0.51
1:B:296:LEU:HD22	1:B:296:LEU:O	2.10	0.51
1:A:283:ILE:O	1:A:284:PRO:C	2.49	0.51
1:C:333:ASN:OD1	1:C:334:THR:N	2.43	0.51
1:A:233:LEU:HD11	1:A:257:ILE:HD13	1.93	0.51
1:C:154:THR:HG23	1:C:156:ILE:HG12	1.93	0.50
1:C:86:ARG:HG2	1:C:301:VAL:HB	1.92	0.50
1:D:247:ASP:OD1	1:D:288:THR:HG21	2.11	0.50
1:B:64:ILE:CG1	1:B:94:VAL:HG22	2.41	0.50
1:A:86:ARG:NH1	1:A:302:ASP:OD1	2.44	0.50
1:C:173:HIS:CE1	1:C:177:LEU:HD11	2.46	0.50
1:B:158:SER:OG	1:B:316:ASN:HB3	2.11	0.50
1:B:115:LEU:CD1	1:B:122:LEU:HD21	2.36	0.50
1:C:336:THR:O	1:C:338:SER:N	2.43	0.50
1:C:307:LEU:HD23	1:C:313:VAL:HG13	1.94	0.50
1:B:340:ARG:O	1:B:343:ALA:HB3	2.12	0.50
1:A:117:GLN:HB3	1:B:117:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:MET:O	1:D:84:LYS:HE3	2.10	0.50
1:A:83:ILE:HD12	1:A:297:GLY:HA2	1.92	0.50
1:D:332:PRO:C	1:D:334:THR:H	2.14	0.50
1:C:147:PHE:CG	1:C:156:ILE:HD12	2.46	0.50
1:B:191:SER:O	1:B:194:ALA:HB3	2.12	0.49
1:B:100:GLU:CD	1:B:100:GLU:H	2.16	0.49
1:D:219:ASP:O	1:D:220:TRP:HB2	2.12	0.49
1:A:199:ALA:O	1:A:202:HIS:HB2	2.11	0.49
1:A:204:TYR:HA	1:A:207:ARG:HB2	1.95	0.49
1:D:129:ASP:O	1:D:131:GLN:N	2.45	0.49
1:C:158:SER:O	1:C:303:ARG:NH2	2.45	0.49
1:B:115:LEU:HG	1:B:143:VAL:CG2	2.37	0.49
1:A:133:ALA:HB1	1:A:156:ILE:HD13	1.94	0.49
1:B:201:TRP:HE3	1:B:201:TRP:HA	1.77	0.49
1:B:191:SER:HB3	1:B:194:ALA:CB	2.42	0.49
1:B:191:SER:HB3	1:B:194:ALA:HB2	1.93	0.49
1:A:86:ARG:HG2	1:A:298:GLN:HA	1.93	0.49
1:D:182:ILE:HA	1:D:241:ALA:O	2.12	0.49
1:B:127:PRO:O	1:B:128:LEU:HD13	2.13	0.49
1:C:269:SER:HA	1:C:328:THR:O	2.11	0.49
1:C:312:ALA:HB1	1:C:314:LYS:HZ2	1.77	0.49
1:C:95:VAL:HG13	1:D:95:VAL:CG2	2.42	0.49
1:A:68:THR:HG23	1:A:98:MET:HE2	1.94	0.49
1:B:303:ARG:HE	1:B:317:GLN:NE2	2.11	0.49
1:A:352:GLN:CB	1:B:342:LEU:HD21	2.43	0.48
1:B:74:HIS:ND1	1:B:74:HIS:N	2.61	0.48
1:B:350:ALA:CA	1:D:346:LEU:HD12	2.38	0.48
1:A:79:ILE:O	1:A:83:ILE:HD13	2.13	0.48
1:A:184:LEU:HG	1:A:212:PRO:HB3	1.95	0.48
1:A:75:ALA:HB3	1:A:76:PRO:HD3	1.95	0.48
1:B:343:ALA:CB	1:D:354:SER:HB3	2.43	0.48
1:A:167:THR:O	1:A:171:VAL:HG23	2.13	0.48
1:D:148:LEU:HD11	1:D:300:SER:HB3	1.94	0.48
1:B:285:PRO:HB2	1:B:326:ARG:HG2	1.94	0.48
1:A:105:GLU:O	1:A:109:THR:HG22	2.13	0.48
1:C:84:LYS:HE2	1:C:88:ASP:OD1	2.14	0.48
1:A:229:THR:HG23	1:A:232:MET:CE	2.43	0.48
1:C:105:GLU:O	1:C:109:THR:HG22	2.13	0.48
1:B:338:SER:HB3	1:B:341:ALA:HB3	1.96	0.48
1:A:254:MET:CE	1:A:286:LEU:HD13	2.44	0.48
1:B:201:TRP:CE3	1:B:201:TRP:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:PHE:O	1:D:158:SER:HA	2.13	0.47
1:D:356:LEU:O	1:D:357:GLU:HB3	2.14	0.47
1:B:219:ASP:O	1:B:220:TRP:HB2	2.14	0.47
1:D:200:GLY:O	1:D:201:TRP:C	2.53	0.47
1:C:203:LYS:O	1:C:207:ARG:HD3	2.14	0.47
1:B:137:GLU:HB3	1:B:147:PHE:CZ	2.48	0.47
1:A:181:GLN:NE2	1:A:213:ILE:HG21	2.28	0.47
1:C:103:GLY:C	1:C:105:GLU:H	2.17	0.47
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.75	0.47
1:B:63:LEU:HB3	1:B:119:VAL:HA	1.96	0.47
1:D:141:THR:C	1:D:143:VAL:H	2.18	0.47
1:C:334:THR:C	1:C:336:THR:N	2.66	0.47
1:A:288:THR:CG2	1:A:289:ILE:N	2.77	0.47
1:A:283:ILE:HG22	1:A:284:PRO:N	2.29	0.47
1:C:103:GLY:C	1:C:105:GLU:N	2.67	0.47
1:A:313:VAL:HG23	1:A:313:VAL:O	2.14	0.47
1:B:304:LEU:HA	1:B:307:LEU:HD12	1.96	0.47
1:A:166:GLY:CA	1:A:321:VAL:HG11	2.45	0.47
1:A:276:THR:O	1:A:278:ASP:N	2.48	0.47
1:C:344:ASP:O	1:C:348:GLN:HG3	2.15	0.47
1:D:303:ARG:NH1	1:D:317:GLN:HB2	2.29	0.47
1:C:118:ARG:NH2	1:D:118:ARG:NE	2.62	0.46
1:C:254:MET:HE2	1:C:286:LEU:HD13	1.95	0.46
1:B:232:MET:HG2	1:B:237:ILE:HB	1.96	0.46
1:A:78:GLN:HE21	1:A:293:PHE:HD2	1.63	0.46
1:A:221:SER:O	1:A:249:MET:HG2	2.14	0.46
1:A:337:ALA:O	1:A:338:SER:CB	2.63	0.46
1:A:151:SER:HB3	1:A:154:THR:OG1	2.15	0.46
1:C:290:LYS:HB2	1:C:324:VAL:CG2	2.46	0.46
1:B:202:HIS:O	1:B:204:TYR:N	2.48	0.46
1:C:123:ILE:HG23	1:C:148:LEU:HD13	1.96	0.46
1:C:70:SER:CB	1:C:98:MET:HB3	2.44	0.46
1:C:101:ARG:NH1	1:C:102:SER:O	2.48	0.46
1:D:116:ALA:C	1:D:118:ARG:H	2.19	0.46
1:D:220:TRP:CZ3	1:D:246:ASN:HB3	2.51	0.46
1:B:131:GLN:CD	1:B:131:GLN:H	2.19	0.46
1:D:82:ALA:O	1:D:294:ARG:NH2	2.49	0.46
1:D:216:ARG:NH1	1:D:228:GLN:NE2	2.60	0.46
1:C:86:ARG:NH1	1:C:90:LEU:HD11	2.30	0.46
1:D:141:THR:C	1:D:142:ASN:ND2	2.69	0.46
1:C:126:TYR:HD2	1:C:128:LEU:HD13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:GLY:HA3	1:C:288:THR:HG22	1.98	0.46
1:D:247:ASP:OD2	1:D:279:SER:OG	2.25	0.46
1:D:165:ASP:O	1:D:166:GLY:C	2.54	0.46
1:A:207:ARG:C	1:A:209:GLN:H	2.19	0.46
1:D:201:TRP:HA	1:D:201:TRP:CE3	2.51	0.46
1:D:282:TYR:O	1:D:283:ILE:O	2.34	0.46
1:A:173:HIS:CG	1:A:323:LEU:HD21	2.51	0.46
1:C:213:ILE:HD11	1:C:239:PRO:HB3	1.97	0.46
1:D:202:HIS:O	1:D:206:THR:HG23	2.15	0.46
1:B:160:ILE:HG22	1:B:161:PHE:N	2.31	0.45
1:B:202:HIS:C	1:B:206:THR:HG23	2.36	0.45
1:D:167:THR:O	1:D:171:VAL:HG23	2.16	0.45
1:B:137:GLU:HB3	1:B:147:PHE:CE1	2.50	0.45
1:A:182:ILE:N	1:A:182:ILE:HD12	2.31	0.45
1:D:296:LEU:O	1:D:296:LEU:HD22	2.16	0.45
1:C:64:ILE:HG12	1:C:94:VAL:HG22	1.99	0.45
1:A:213:ILE:HD11	1:A:239:PRO:HB3	1.99	0.45
1:D:349:LEU:O	1:D:353:VAL:HG23	2.17	0.45
1:D:97:SER:CB	1:D:114:LEU:HG	2.45	0.45
1:B:182:ILE:HA	1:B:241:ALA:O	2.15	0.45
1:A:273:TYR:O	1:A:274:ASP:CB	2.64	0.45
1:B:146:LEU:HD11	1:B:303:ARG:HD3	1.98	0.45
1:D:272:GLY:C	1:D:288:THR:HG22	2.37	0.45
1:C:180:GLN:HG2	1:C:210:ILE:HD11	1.99	0.45
1:B:272:GLY:C	1:B:288:THR:HG22	2.37	0.45
1:C:107:CYS:HB3	1:C:136:VAL:HG21	1.99	0.45
1:D:100:GLU:HA	1:D:101:ARG:HH21	1.81	0.45
1:A:68:THR:O	1:A:98:MET:HA	2.16	0.45
1:B:253:ALA:O	1:B:256:ALA:HB3	2.17	0.45
1:B:142:ASN:O	1:B:144:PRO:N	2.50	0.45
1:D:273:TYR:CE2	1:D:289:ILE:HG21	2.52	0.45
1:C:161:PHE:CD2	1:C:291:GLN:HG2	2.52	0.45
1:C:250:ALA:O	1:C:254:MET:HG3	2.17	0.45
1:B:121:GLY:HA3	1:B:304:LEU:HD21	1.99	0.45
1:C:326:ARG:C	1:C:327:LYS:HD2	2.38	0.45
1:A:197:ARG:NH2	1:A:273:TYR:CE1	2.85	0.44
1:A:171:VAL:HG21	1:A:204:TYR:HB2	1.99	0.44
1:C:307:LEU:CD2	1:C:313:VAL:HG13	2.47	0.44
1:B:160:ILE:O	1:B:318:LEU:HA	2.16	0.44
1:D:309:GLN:NE2	1:D:311:GLN:HE22	2.15	0.44
1:A:355:ARG:HH22	1:B:261:GLY:HA3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:SER:O	1:A:316:ASN:HA	2.17	0.44
1:D:114:LEU:HD13	1:D:122:LEU:CD2	2.47	0.44
1:A:231:GLN:HG2	1:A:235:GLU:OE1	2.16	0.44
1:B:349:LEU:O	1:B:353:VAL:HG23	2.16	0.44
1:B:154:THR:HA	1:B:155:PRO:HD3	1.58	0.44
1:B:65:GLY:HA2	1:B:95:VAL:O	2.18	0.44
1:B:116:ALA:C	1:B:118:ARG:H	2.21	0.44
1:D:352:GLN:HA	1:D:352:GLN:OE1	2.16	0.44
1:D:167:THR:HA	1:D:201:TRP:CZ3	2.52	0.44
1:D:141:THR:O	1:D:142:ASN:ND2	2.51	0.44
1:D:71:LEU:HD21	1:D:101:ARG:HG2	1.99	0.44
1:D:264:VAL:HB	1:D:284:PRO:HG2	1.98	0.44
1:B:202:HIS:O	1:B:205:LEU:N	2.50	0.44
1:D:201:TRP:HA	1:D:201:TRP:HE3	1.82	0.44
1:A:121:GLY:HA2	1:A:143:VAL:CG2	2.48	0.44
1:C:275:ASP:HB3	1:C:290:LYS:HG3	1.99	0.44
1:D:137:GLU:HG3	1:D:156:ILE:HG22	1.99	0.44
1:A:143:VAL:HA	1:A:144:PRO:HD3	1.86	0.44
1:D:123:ILE:HG23	1:D:148:LEU:HD22	1.96	0.44
1:C:273:TYR:CD1	1:C:291:GLN:NE2	2.86	0.44
1:A:205:LEU:HB3	1:A:210:ILE:O	2.17	0.44
1:C:163:HIS:CD2	1:C:163:HIS:H	2.36	0.44
1:A:230:MET:O	1:A:234:ASN:HB2	2.17	0.44
1:D:309:GLN:HB3	1:D:311:GLN:OE1	2.18	0.44
1:C:96:VAL:HB	1:D:96:VAL:HB	2.00	0.43
1:C:189:LEU:HD21	1:C:198:LEU:HD12	2.00	0.43
1:A:349:LEU:HD13	1:B:342:LEU:HD23	1.99	0.43
1:B:264:VAL:HA	1:B:268:ILE:O	2.18	0.43
1:A:348:GLN:NE2	1:B:258:THR:O	2.51	0.43
1:A:104:VAL:HG13	1:A:132:ASP:CB	2.38	0.43
1:D:76:PRO:O	1:D:80:VAL:HG23	2.19	0.43
1:C:70:SER:HB2	1:D:84:LYS:CG	2.44	0.43
1:D:115:LEU:HD13	1:D:122:LEU:HD11	2.00	0.43
1:D:264:VAL:CG1	1:D:328:THR:HG22	2.48	0.43
1:A:174:LEU:HD22	1:A:241:ALA:CB	2.47	0.43
1:A:283:ILE:O	1:A:285:PRO:HD3	2.18	0.43
1:C:70:SER:HA	1:C:98:MET:HE3	2.01	0.43
1:A:330:LEU:HD11	1:A:340:ARG:NH1	2.34	0.43
1:A:303:ARG:HA	1:A:306:GLN:HE21	1.84	0.43
1:C:128:LEU:HG	1:C:132:ASP:HB3	2.01	0.43
1:D:111:VAL:CG1	1:D:140:CYS:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:VAL:HG12	1:D:328:THR:HG22	2.00	0.43
1:A:205:LEU:HA	1:A:205:LEU:HD23	1.59	0.43
1:B:166:GLY:CA	1:B:321:VAL:HG11	2.49	0.43
1:C:129:ASP:O	1:C:132:ASP:HB2	2.19	0.43
1:C:265:GLY:HA2	1:C:328:THR:O	2.19	0.43
1:C:206:THR:HG22	1:C:211:GLN:OE1	2.19	0.43
1:A:301:VAL:O	1:A:305:LEU:HG	2.19	0.43
1:B:79:ILE:O	1:B:83:ILE:HG13	2.19	0.43
1:A:206:THR:CB	1:A:211:GLN:HE22	2.27	0.42
1:D:140:CYS:SG	1:D:140:CYS:O	2.76	0.42
1:D:339:PRO:C	1:D:341:ALA:N	2.72	0.42
1:B:285:PRO:CB	1:B:326:ARG:HG2	2.49	0.42
1:C:100:GLU:H	1:C:100:GLU:CD	2.22	0.42
1:C:62:LEU:HB3	1:C:63:LEU:H	1.56	0.42
1:A:183:ALA:HB2	1:A:239:PRO:HB3	2.01	0.42
1:A:251:LEU:HA	1:A:254:MET:HE3	2.02	0.42
1:D:216:ARG:HB3	1:D:228:GLN:NE2	2.34	0.42
1:C:286:LEU:HG	1:C:288:THR:HG23	2.01	0.42
1:C:273:TYR:CE1	1:C:291:GLN:NE2	2.88	0.42
1:C:167:THR:HA	1:C:201:TRP:HZ3	1.82	0.42
1:B:166:GLY:HA2	1:B:321:VAL:HG11	2.00	0.42
1:A:350:ALA:HB3	1:C:347:MET:HG3	2.01	0.42
1:D:168:ARG:HD3	1:D:204:TYR:CE1	2.54	0.42
1:D:331:ALA:C	1:D:333:ASN:H	2.21	0.42
1:A:122:LEU:HD22	1:A:124:ILE:HD11	2.01	0.42
1:A:104:VAL:HG23	1:A:105:GLU:N	2.34	0.42
1:C:154:THR:HA	1:C:155:PRO:HD2	1.87	0.42
1:B:273:TYR:N	1:B:288:THR:HG22	2.34	0.42
1:D:154:THR:HA	1:D:155:PRO:HD3	1.80	0.42
1:A:111:VAL:HG21	1:A:136:VAL:HG13	2.01	0.42
1:C:123:ILE:HG23	1:C:148:LEU:HD11	2.01	0.42
1:C:102:SER:O	1:C:103:GLY:O	2.37	0.42
1:B:330:LEU:HD12	1:B:331:ALA:N	2.33	0.42
1:D:239:PRO:O	1:D:268:ILE:HG12	2.20	0.42
1:C:265:GLY:O	1:C:330:LEU:HB2	2.19	0.42
1:A:349:LEU:HA	1:A:349:LEU:HD22	1.75	0.42
1:C:327:LYS:HG3	1:C:340:ARG:NH1	2.35	0.42
1:A:218:GLY:HA2	1:A:224:SER:HB2	2.00	0.42
1:D:141:THR:O	1:D:142:ASN:CG	2.58	0.42
1:B:192:VAL:HG22	1:B:196:LEU:HD11	2.01	0.42
1:A:142:ASN:CG	1:A:143:VAL:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HG12	1:A:100:GLU:O	2.20	0.41
1:D:141:THR:HB	1:D:142:ASN:H	1.63	0.41
1:D:229:THR:OG1	1:D:253:ALA:HA	2.20	0.41
1:A:307:LEU:O	1:A:310:GLY:N	2.53	0.41
1:B:62:LEU:HG	1:B:63:LEU:N	2.35	0.41
1:D:104:VAL:O	1:D:108:LYS:HG3	2.20	0.41
1:A:86:ARG:HB3	1:A:301:VAL:HG21	2.02	0.41
1:D:144:PRO:HB2	1:D:304:LEU:HD11	2.03	0.41
1:D:246:ASN:OD1	1:D:249:MET:HG3	2.20	0.41
1:B:82:ALA:O	1:B:85:SER:HB2	2.20	0.41
1:A:283:ILE:HA	1:B:255:ARG:HG2	2.03	0.41
1:D:86:ARG:HD3	1:D:302:ASP:OD1	2.20	0.41
1:B:167:THR:HG21	1:B:200:GLY:HA3	2.01	0.41
1:D:120:SER:O	1:D:144:PRO:HD2	2.21	0.41
1:D:99:VAL:HG13	1:D:106:ALA:C	2.39	0.41
1:C:210:ILE:HG23	1:C:210:ILE:HD12	1.77	0.41
1:B:162:SER:OG	1:B:165:ASP:HB2	2.20	0.41
1:C:191:SER:HB3	1:C:194:ALA:HB2	2.02	0.41
1:A:143:VAL:O	1:A:143:VAL:HG13	2.20	0.41
1:B:86:ARG:CG	1:B:298:GLN:HA	2.40	0.41
1:A:184:LEU:O	1:A:215:GLU:HA	2.21	0.41
1:D:152:ASP:HB2	1:D:316:ASN:ND2	2.36	0.41
1:A:274:ASP:OD1	1:A:291:GLN:NE2	2.52	0.41
1:A:327:LYS:HA	1:A:340:ARG:HH22	1.85	0.41
1:B:292:ASP:HB3	1:B:295:LEU:HB3	2.02	0.41
1:B:247:ASP:OD1	1:B:288:THR:HG21	2.20	0.41
1:A:115:LEU:CD1	1:A:122:LEU:HD11	2.50	0.41
1:A:349:LEU:HD22	1:B:342:LEU:HD23	2.03	0.41
1:B:142:ASN:O	1:B:143:VAL:C	2.59	0.41
1:B:222:ALA:CA	1:B:248:GLN:O	2.61	0.41
1:B:213:ILE:O	1:B:213:ILE:CG1	2.66	0.41
1:C:290:LYS:HB2	1:C:324:VAL:HG23	2.01	0.41
1:A:332:PRO:C	1:A:334:THR:N	2.74	0.41
1:D:79:ILE:O	1:D:83:ILE:HG13	2.21	0.41
1:B:151:SER:C	1:B:153:GLN:H	2.23	0.41
1:B:122:LEU:O	1:B:145:ALA:HA	2.21	0.41
1:D:104:VAL:HG21	1:D:135:ALA:HB3	2.04	0.40
1:A:255:ARG:O	1:A:259:GLU:HG3	2.20	0.40
1:C:153:GLN:HG2	1:C:153:GLN:H	1.64	0.40
1:B:352:GLN:O	1:B:355:ARG:HB2	2.22	0.40
1:C:63:LEU:CD1	1:C:119:VAL:HG12	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:HIS:CE1	1:C:332:PRO:HD3	2.56	0.40
1:D:148:LEU:HD11	1:D:300:SER:CB	2.52	0.40
1:C:253:ALA:O	1:C:257:ILE:HG13	2.21	0.40
1:B:338:SER:HA	1:B:339:PRO:HD2	1.69	0.40
1:A:150:VAL:CG2	1:A:158:SER:CB	3.00	0.40
1:A:205:LEU:CD1	1:A:212:PRO:HG3	2.50	0.40
1:A:107:CYS:O	1:A:111:VAL:HG23	2.22	0.40
1:C:353:VAL:HG22	1:D:342:LEU:HD13	2.04	0.40
1:D:275:ASP:CB	1:D:290:LYS:HG3	2.49	0.40
1:B:198:LEU:HD23	1:B:201:TRP: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	294/360 (82%)	244 (83%)	32 (11%)	18 (6%)	2	3
1	B	294/360 (82%)	247 (84%)	31 (10%)	16 (5%)	2	4
1	C	294/360 (82%)	260 (88%)	26 (9%)	8 (3%)	6	16
1	D	294/360 (82%)	247 (84%)	38 (13%)	9 (3%)	5	12
All	All	1176/1440 (82%)	998 (85%)	127 (11%)	51 (4%)	3	7

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	THR
1	A	142	ASN
1	A	162	SER
1	A	274	ASP
1	A	277	GLU

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Mol	Chain	Res	Type
1	A	283	ILE
1	A	311	GLN
1	A	338	SER
1	B	69	SER
1	B	101	ARG
1	B	141	THR
1	B	159	ILE
1	B	214	ALA
1	B	283	ILE
1	B	284	PRO
1	B	335	GLN
1	B	339	PRO
1	C	274	ASP
1	C	337	ALA
1	D	104	VAL
1	D	130	ASP
1	D	312	ALA
1	A	101	ARG
1	A	312	ALA
1	A	333	ASN
1	A	335	GLN
1	A	356	LEU
1	B	203	LYS
1	B	274	ASP
1	B	312	ALA
1	C	103	GLY
1	C	130	ASP
1	C	159	ILE
1	C	338	SER
1	D	274	ASP
1	A	71	LEU
1	A	337	ALA
1	B	130	ASP
1	B	314	LYS
1	D	63	LEU
1	D	283	ILE
1	A	155	PRO
1	B	100	GLU
1	C	283	ILE
1	D	102	SER
1	A	130	ASP
1	A	189	LEU

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Mol	Chain	Res	Type
1	C	189	LEU
1	D	141	THR
1	D	309	GLN
1	B	150	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/295 (82%)	208 (86%)	35 (14%)	4	10
1	B	243/295 (82%)	203 (84%)	40 (16%)	3	7
1	C	243/295 (82%)	201 (83%)	42 (17%)	2	6
1	D	243/295 (82%)	198 (82%)	45 (18%)	2	5
All	All	972/1180 (82%)	810 (83%)	162 (17%)	3	7

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	78	GLN
1	A	86	ARG
1	A	90	LEU
1	A	93	SER
1	A	101	ARG
1	A	109	THR
1	A	118	ARG
1	A	122	LEU
1	A	123	ILE
1	A	128	LEU
1	A	142	ASN
1	A	153	GLN
1	A	155	PRO
1	A	180	GLN
1	A	185	LEU
1	A	198	LEU

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Mol	Chain	Res	Type
1	A	206	THR
1	A	207	ARG
1	A	210	ILE
1	A	216	ARG
1	A	227	GLN
1	A	230	MET
1	A	234	ASN
1	A	251	LEU
1	A	277	GLU
1	A	296	LEU
1	A	298	GLN
1	A	317	GLN
1	A	318	LEU
1	A	330	LEU
1	A	335	GLN
1	A	348	GLN
1	A	349	LEU
1	A	354	SER
1	B	71	LEU
1	B	74	HIS
1	B	86	ARG
1	B	95	VAL
1	B	101	ARG
1	B	107	CYS
1	B	112	HIS
1	B	128	LEU
1	B	131	GLN
1	B	137	GLU
1	B	142	ASN
1	B	143	VAL
1	B	156	ILE
1	B	172	GLU
1	B	180	GLN
1	B	185	LEU
1	B	189	LEU
1	B	190	SER
1	B	198	LEU
1	B	201	TRP
1	B	206	THR
1	B	246	ASN
1	B	251	LEU
1	B	262	LEU

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Mol	Chain	Res	Type
1	B	276	THR
1	B	288	THR
1	B	294	ARG
1	B	295	LEU
1	B	296	LEU
1	B	309	GLN
1	B	321	VAL
1	B	323	LEU
1	B	325	LYS
1	B	326	ARG
1	B	327	LYS
1	B	338	SER
1	B	342	LEU
1	B	348	GLN
1	B	351	ARG
1	B	354	SER
1	C	69	SER
1	C	86	ARG
1	C	93	SER
1	C	97	SER
1	C	101	ARG
1	C	102	SER
1	C	105	GLU
1	C	107	CYS
1	C	109	THR
1	C	115	LEU
1	C	118	ARG
1	C	128	LEU
1	C	130	ASP
1	C	143	VAL
1	C	151	SER
1	C	154	THR
1	C	162	SER
1	C	164	GLU
1	C	185	LEU
1	C	198	LEU
1	C	201	TRP
1	C	206	THR
1	C	249	MET
1	C	251	LEU
1	C	262	LEU
1	C	271	VAL

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Mol	Chain	Res	Type
1	C	295	LEU
1	C	296	LEU
1	C	298	GLN
1	C	303	ARG
1	C	313	VAL
1	C	316	ASN
1	C	317	GLN
1	C	319	LEU
1	C	321	VAL
1	C	323	LEU
1	C	330	LEU
1	C	334	THR
1	C	338	SER
1	C	346	LEU
1	C	355	ARG
1	C	356	LEU
1	D	62	LEU
1	D	69	SER
1	D	71	LEU
1	D	90	LEU
1	D	93	SER
1	D	101	ARG
1	D	104	VAL
1	D	111	VAL
1	D	115	LEU
1	D	128	LEU
1	D	130	ASP
1	D	142	ASN
1	D	148	LEU
1	D	154	THR
1	D	156	ILE
1	D	184	LEU
1	D	185	LEU
1	D	190	SER
1	D	197	ARG
1	D	198	LEU
1	D	201	TRP
1	D	230	MET
1	D	251	LEU
1	D	255	ARG
1	D	262	LEU
1	D	276	THR

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Mol	Chain	Res	Type
1	D	277	GLU
1	D	288	THR
1	D	294	ARG
1	D	296	LEU
1	D	307	LEU
1	D	308	SER
1	D	313	VAL
1	D	316	ASN
1	D	317	GLN
1	D	321	VAL
1	D	326	ARG
1	D	327	LYS
1	D	334	THR
1	D	335	GLN
1	D	336	THR
1	D	340	ARG
1	D	348	GLN
1	D	355	ARG
1	D	356	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	113	ASN
1	A	142	ASN
1	A	157	ASN
1	A	181	GLN
1	A	202	HIS
1	A	231	GLN
1	A	234	ASN
1	A	306	GLN
1	A	311	GLN
1	A	316	ASN
1	B	113	ASN
1	B	125	ASN
1	B	142	ASN
1	B	228	GLN
1	B	317	GLN
1	C	163	HIS
1	C	181	GLN
1	C	202	HIS

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Mol	Chain	Res	Type
1	C	228	GLN
1	C	234	ASN
1	C	291	GLN
1	C	298	GLN
1	D	89	GLN
1	D	117	GLN
1	D	142	ASN
1	D	208	ASN
1	D	228	GLN
1	D	234	ASN
1	D	309	GLN
1	D	333	ASN
1	D	348	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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.