



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:43 PM UTC

PDB ID : 1L7J / pdb_00001l7j
Title : X-ray structure of galactose mutarotase from *Lactococcus lactis* (apo)
Authors : Holden, H.M.; Thoden, J.B.
Deposited on : 2002-03-15
Resolution : 1.90 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

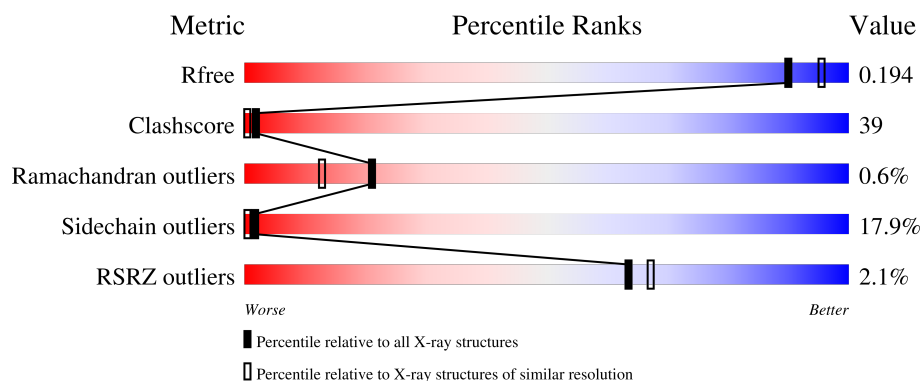
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	4% 35% 44% 16% • •
1	B	347	49% 36% 11% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6065 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 galactose mutarotase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	3	0
			2650	1673	447	527	3			
1	B	338	Total	C	N	O	S	0	2	0
			2645	1667	446	529	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	GLU	engineered mutation	UNP Q9ZB17
A	340	LEU	-	expression tag	UNP Q9ZB17
A	341	GLU	-	expression tag	UNP Q9ZB17
A	342	HIS	-	expression tag	UNP Q9ZB17
A	343	HIS	-	expression tag	UNP Q9ZB17
A	344	HIS	-	expression tag	UNP Q9ZB17
A	345	HIS	-	expression tag	UNP Q9ZB17
A	346	HIS	-	expression tag	UNP Q9ZB17
A	347	HIS	-	expression tag	UNP Q9ZB17
B	2	SER	GLU	engineered mutation	UNP Q9ZB17
B	340	LEU	-	expression tag	UNP Q9ZB17
B	341	GLU	-	expression tag	UNP Q9ZB17
B	342	HIS	-	expression tag	UNP Q9ZB17
B	343	HIS	-	expression tag	UNP Q9ZB17
B	344	HIS	-	expression tag	UNP Q9ZB17
B	345	HIS	-	expression tag	UNP Q9ZB17
B	346	HIS	-	expression tag	UNP Q9ZB17
B	347	HIS	-	expression tag	UNP Q9ZB17

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	376	Total	O	0	0
			376	376		

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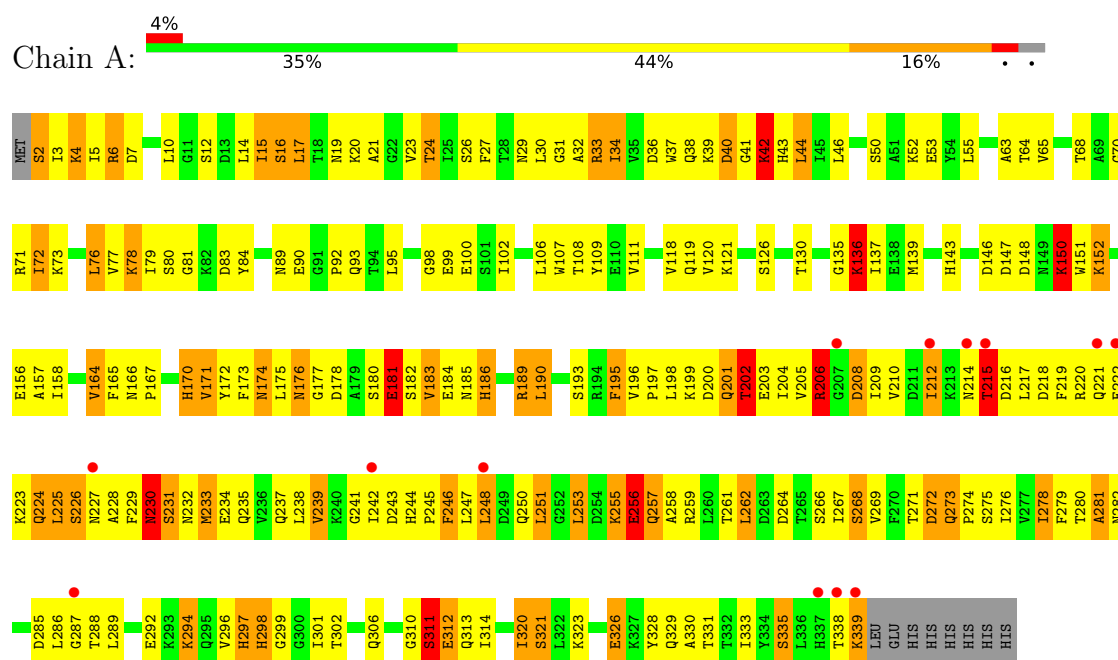
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	394	Total 394	O 394	0	0

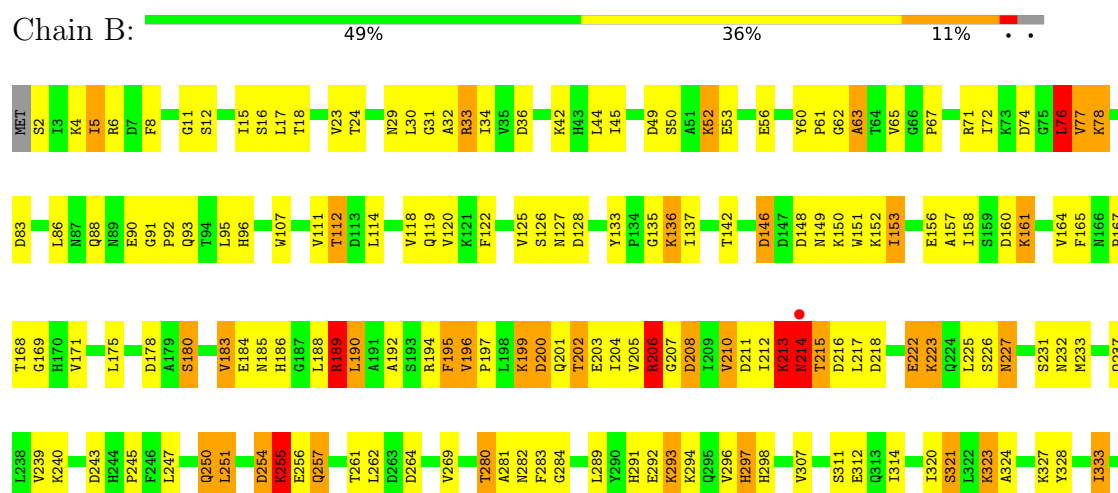
3 Residue-property plots

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: galactose mutarotase



• Molecule 1: galactose mutarotase



L336	H337	T338	K339	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.50Å 76.10Å 206.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.00-1.90) 92.6 (30.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.79Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.189 , 0.267 0.195 , 0.194	Depositor DCC
R_{free} test set	5844 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.815	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 123.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6065	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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	1.19	0/2714	1.77	46/3672 (1.3%)
1	B	1.24	0/2705	1.70	29/3661 (0.8%)
All	All	1.22	0/5419	1.73	75/7333 (1.0%)

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	LYS	N-CA-CB	-9.66	94.08	110.50
1	B	135	GLY	CA-C-N	9.42	138.66	121.70
1	B	135	GLY	C-N-CA	9.42	138.66	121.70
1	B	136	LYS	N-CA-CB	-7.96	96.97	110.50
1	A	272	ASP	N-CA-C	-7.49	104.28	113.41
1	A	202	THR	N-CA-C	-7.38	103.25	111.82
1	A	214	ASN	CA-C-N	7.14	135.18	121.54
1	A	214	ASN	C-N-CA	7.14	135.18	121.54
1	A	272	ASP	N-CA-CB	-7.10	100.11	110.47
1	A	135	GLY	CA-C-N	7.05	134.39	121.70
1	A	135	GLY	C-N-CA	7.05	134.39	121.70
1	A	255	LYS	N-CA-C	7.05	120.71	110.28
1	A	208	ASP	CB-CA-C	-6.83	97.87	109.83
1	B	210	VAL	N-CA-C	6.70	118.44	108.46
1	A	108	THR	N-CA-C	-6.70	101.89	110.53
1	A	231	SER	N-CA-C	6.68	119.15	110.53
1	A	229	PHE	CA-CB-CG	-6.68	107.12	113.80
1	B	76	LEU	N-CA-C	6.65	119.57	108.73
1	A	298	HIS	CA-CB-CG	-6.59	107.21	113.80
1	A	209	ILE	CA-C-N	-6.46	113.38	122.75
1	A	209	ILE	C-N-CA	-6.46	113.38	122.75
1	A	273	GLN	CA-C-N	6.38	127.30	120.47
1	A	273	GLN	C-N-CA	6.38	127.30	120.47
1	A	42	LYS	CB-CA-C	-6.35	99.39	109.80
1	A	135	GLY	O-C-N	-6.34	114.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ASP	CB-CA-C	-6.34	98.53	110.51
1	B	307	VAL	N-CA-C	-6.33	100.61	109.21
1	B	128	ASP	CA-CB-CG	6.26	118.86	112.60
1	B	63	ALA	N-CA-C	6.15	119.62	110.52
1	A	210	VAL	N-CA-C	6.02	116.96	108.17
1	B	297	HIS	N-CA-C	-5.94	101.86	110.24
1	B	23	VAL	CB-CA-C	-5.86	103.54	111.15
1	A	209	ILE	N-CA-C	-5.82	99.75	108.12
1	A	201	GLN	CA-C-N	5.74	129.03	120.31
1	A	201	GLN	C-N-CA	5.74	129.03	120.31
1	A	278	ILE	N-CA-C	5.67	114.91	106.85
1	B	214	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	256	GLU	N-CA-C	-5.58	101.59	109.96
1	B	136	LYS	CB-CA-C	-5.52	99.60	110.10
1	A	64	THR	N-CA-C	-5.49	100.23	108.96
1	A	174	ASN	N-CA-CB	5.46	119.72	110.49
1	B	213	LYS	N-CA-C	-5.46	102.19	110.28
1	A	215	THR	N-CA-CB	-5.45	101.28	110.49
1	A	170	HIS	N-CA-C	5.44	119.64	112.25
1	B	196	VAL	N-CA-CB	-5.42	104.57	111.23
1	B	227	ASN	CA-CB-CG	-5.42	107.19	112.60
1	B	333	ILE	N-CA-C	5.41	116.53	108.46
1	A	269	VAL	N-CA-C	5.39	116.34	108.53
1	B	96	HIS	N-CA-C	5.37	118.98	111.74
1	B	261	THR	N-CA-C	5.37	118.20	109.24
1	B	33	ARG	CD-NE-CZ	5.33	131.87	124.40
1	B	280	THR	CA-CB-OG1	-5.31	101.64	109.60
1	B	180	SER	CA-C-N	-5.29	115.64	123.05
1	B	180	SER	C-N-CA	-5.29	115.64	123.05
1	B	91	GLY	N-CA-C	-5.28	101.57	112.34
1	A	41	GLY	N-CA-C	-5.17	108.12	115.30
1	B	146	ASP	N-CA-C	5.17	118.08	110.59
1	A	176	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	92	PRO	N-CA-CB	5.15	107.08	101.88
1	B	255	LYS	N-CA-C	5.15	118.33	110.20
1	A	173	PHE	CA-CB-CG	-5.14	108.66	113.80
1	A	244	HIS	O-C-N	5.13	126.55	121.57
1	A	268	SER	N-CA-C	5.09	118.42	110.32
1	A	150	LYS	N-CA-C	5.09	116.81	108.52
1	A	181	GLU	N-CA-CB	5.09	118.59	110.65
1	A	206	ARG	CA-C-N	-5.08	117.39	123.08
1	A	206	ARG	C-N-CA	-5.08	117.39	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ASN	CB-CA-C	5.08	119.75	110.36
1	B	206	ARG	CB-CA-C	5.08	117.94	109.56
1	A	102	ILE	N-CA-C	5.07	119.89	109.34
1	B	189	ARG	CB-CA-C	5.06	118.24	110.14
1	A	229	PHE	N-CA-C	5.05	116.47	111.07
1	B	269	VAL	N-CA-C	5.04	115.10	107.75
1	A	297	HIS	N-CA-C	-5.03	103.14	110.24
1	A	326	GLU	N-CA-CB	5.02	117.35	109.97

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	2650	0	2592	251	0
1	B	2645	0	2576	161	0
2	A	376	0	0	29	0
2	B	394	0	0	23	0
All	All	6065	0	5168	409	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 39.

All (409) 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:216:ASP:HB2	1:A:233:MET:HE2	1.32	1.10
1:B:151:TRP:HH2	1:B:171:VAL:HG21	1.11	1.10
1:A:46[A]:LEU:HD13	1:A:172:TYR:HB3	1.32	1.07
1:A:19:ASN:HD21	1:A:21:ALA:HB3	1.21	1.03
1:A:151:TRP:HH2	1:A:171:VAL:HG21	1.28	0.97
1:A:166:ASN:HD22	1:A:320:ILE:HD11	1.29	0.94
1:B:151:TRP:CH2	1:B:171:VAL:HG21	2.03	0.92
1:B:202:THR:HG21	1:B:204:ILE:HG12	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:ND2	1:A:320:ILE:HD11	1.84	0.91
1:B:184:GLU:HG3	1:B:226:SER:HB3	1.50	0.91
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.35	0.89
1:A:151:TRP:CH2	1:A:171:VAL:HG21	2.10	0.87
1:B:216:ASP:HB2	1:B:233:MET:HE2	1.56	0.86
1:A:215:THR:HG23	1:A:233:MET:SD	2.16	0.84
1:A:6:ARG:HD3	1:A:14:LEU:HD23	1.60	0.84
1:A:46[A]:LEU:HD13	1:A:172:TYR:CB	2.07	0.84
1:A:195:PHE:CD2	1:A:212:ILE:HD12	2.13	0.84
1:A:183:VAL:HG13	1:A:225:LEU:HD23	1.61	0.81
1:A:200:ASP:HB2	1:A:202:THR:HB	1.63	0.81
1:B:202:THR:CG2	1:B:204:ILE:HG12	2.11	0.79
1:A:223:LYS:HB2	2:A:656:HOH:O	1.82	0.79
1:A:33:ARG:HB3	1:A:63:ALA:HA	1.65	0.78
1:A:250:GLN:HB3	1:A:255:LYS:HE2	1.65	0.78
1:B:71:ARG:HG2	1:B:95:LEU:HD13	1.65	0.78
1:A:217:LEU:HG	1:A:233:MET:CE	2.14	0.77
1:B:202:THR:HG23	1:B:204:ILE:H	1.48	0.77
1:A:296:VAL:HG23	1:A:297:HIS:O	1.83	0.77
1:A:19:ASN:ND2	1:A:21:ALA:HB3	2.00	0.77
1:A:287:GLY:O	1:A:294:LYS:HG3	1.85	0.76
1:A:248:LEU:HD13	1:A:257:GLN:HG2	1.66	0.75
1:A:217:LEU:HG	1:A:233:MET:HE3	1.68	0.75
1:A:216:ASP:HB2	1:A:233:MET:CE	2.13	0.74
1:A:321:SER:HB2	2:A:464:HOH:O	1.86	0.74
1:B:148:ASP:OD1	1:B:150:LYS:HE3	1.87	0.74
1:A:289:LEU:HD23	1:A:294:LYS:HA	1.69	0.74
1:A:7:ASP:HB2	2:A:515:HOH:O	1.87	0.74
1:A:37:TRP:O	1:A:44:LEU:HG	1.88	0.74
1:B:171:VAL:HG23	2:B:699:HOH:O	1.86	0.74
1:B:250:GLN:NE2	1:B:255:LYS:HE3	2.04	0.73
1:A:212:ILE:HD11	1:A:217:LEU:CB	2.19	0.73
1:B:146:ASP:HB2	1:B:150:LYS:H	1.52	0.73
1:A:217:LEU:N	1:A:233:MET:HE1	2.03	0.72
1:B:239:VAL:HG13	2:B:604:HOH:O	1.88	0.72
1:A:247:LEU:HD22	2:A:394:HOH:O	1.87	0.72
1:B:86:LEU:HD13	1:B:133:TYR:CZ	2.23	0.72
1:A:78:LYS:HG3	1:A:83:ASP:OD1	1.90	0.72
1:A:248:LEU:HD21	1:A:276:ILE:HD12	1.70	0.72
1:A:248:LEU:HD11	1:A:276:ILE:CD1	2.20	0.71
1:B:202:THR:CG2	1:B:204:ILE:H	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:HD2	1:A:147:ASP:OD2	1.90	0.70
1:A:136:LYS:NZ	2:A:402:HOH:O	2.24	0.70
1:B:208:ASP:HA	2:B:548:HOH:O	1.91	0.70
1:A:33:ARG:NH1	1:A:63:ALA:HB2	2.07	0.70
1:B:146:ASP:OD2	1:B:150:LYS:HB2	1.91	0.69
1:B:71:ARG:CG	1:B:95:LEU:HD13	2.23	0.69
1:A:39:LYS:O	1:A:42:LYS:HB2	1.91	0.69
1:A:39:LYS:NZ	1:A:338:THR:HG21	2.08	0.69
1:B:33:ARG:NH1	1:B:63:ALA:HB2	2.08	0.69
1:A:17:LEU:HD13	1:A:118:VAL:HB	1.76	0.68
1:B:217:LEU:HG	1:B:233:MET:HE1	1.76	0.68
1:A:250:GLN:O	1:A:257:GLN:NE2	2.27	0.68
1:B:289:LEU:HD11	1:B:294:LYS:HG3	1.74	0.68
1:B:190:LEU:HD13	1:B:192:ALA:HB3	1.76	0.67
1:B:126:SER:HB3	1:B:137:ILE:HB	1.75	0.67
1:A:280:THR:HG22	1:A:301:ILE:HD12	1.75	0.67
1:A:151:TRP:HH2	1:A:171:VAL:CG2	2.07	0.67
1:A:232:ASN:O	1:A:237:GLN:NE2	2.28	0.66
1:B:189:ARG:NH2	1:B:256:GLU:O	2.29	0.66
1:B:33:ARG:CZ	1:B:63:ALA:HB2	2.25	0.66
1:B:34:ILE:CG2	1:B:171:VAL:HG22	2.26	0.66
1:B:65:VAL:HG23	1:B:168:THR:HG22	1.77	0.66
1:A:2:SER:N	2:A:659:HOH:O	2.28	0.65
1:A:248:LEU:HD11	1:A:276:ILE:HD12	1.76	0.65
1:A:6:ARG:NH2	2:A:361:HOH:O	2.28	0.65
1:A:242:ILE:HG22	1:A:278:ILE:O	1.97	0.65
1:A:71:ARG:NH1	1:A:90:GLU:OE1	2.29	0.65
1:A:6:ARG:NH1	1:A:7:ASP:O	2.29	0.65
1:B:112:THR:OG1	1:B:119:GLN:HB2	1.96	0.65
1:B:17:LEU:HD13	1:B:118:VAL:HB	1.78	0.64
1:A:39:LYS:HZ2	1:A:338:THR:HG21	1.61	0.64
1:A:212:ILE:HD11	1:A:217:LEU:HB2	1.77	0.64
1:B:65:VAL:CG2	1:B:168:THR:HG22	2.26	0.64
1:A:232:ASN:ND2	2:A:389:HOH:O	2.29	0.64
1:B:321:SER:OG	1:B:323:LYS:NZ	2.31	0.64
1:A:165:PHE:CE2	1:A:167:PRO:HG3	2.32	0.64
1:A:152:LYS:HG3	1:A:333:ILE:CG1	2.28	0.63
1:A:100:GLU:OE2	1:B:125:VAL:HG21	1.98	0.63
1:A:19:ASN:OD1	1:A:23:VAL:N	2.30	0.63
1:B:338:THR:HB	2:B:732:HOH:O	1.98	0.63
1:B:311:SER:OG	1:B:320:ILE:HD12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD23	1:A:44:LEU:N	2.14	0.62
1:A:180:SER:HA	1:A:296:VAL:HG13	1.81	0.62
1:A:206:ARG:HD2	1:A:208:ASP:OD1	1.99	0.62
1:B:52:LYS:NZ	2:B:697:HOH:O	2.32	0.62
1:A:310:GLY:O	1:A:312:GLU:N	2.31	0.62
1:B:111:VAL:HG13	1:B:120:VAL:HG22	1.80	0.62
1:B:212:ILE:C	1:B:215:THR:HG23	2.24	0.62
1:B:156:GLU:OE2	1:B:327:LYS:HE2	2.00	0.62
1:A:282:ASN:HA	1:A:297:HIS:CE1	2.35	0.61
1:A:222:GLU:HG2	2:A:715:HOH:O	1.99	0.61
1:A:183:VAL:O	1:A:225:LEU:HD23	2.00	0.61
1:B:339:LYS:HE3	2:B:735:HOH:O	1.99	0.61
1:A:10:LEU:HD11	1:A:52[B]:LYS:HG2	1.82	0.61
1:A:16:SER:HB3	1:A:26:SER:HB3	1.82	0.61
1:A:177:GLY:HA2	2:A:359:HOH:O	2.00	0.61
1:B:216:ASP:O	1:B:223:LYS:NZ	2.29	0.60
1:A:185:ASN:OD1	1:A:186:HIS:ND1	2.31	0.60
1:A:282:ASN:ND2	1:A:298:HIS:NE2	2.49	0.60
1:A:253:LEU:HD21	1:A:333:ILE:CD1	2.31	0.60
1:A:218:ASP:O	1:A:223:LYS:HD3	2.01	0.60
1:B:164:VAL:HB	1:B:320:ILE:HG22	1.84	0.60
1:B:34:ILE:HG21	1:B:171:VAL:HG22	1.82	0.60
1:B:197:PRO:HD2	1:B:208:ASP:O	2.01	0.60
1:A:202:THR:HG22	1:A:204:ILE:H	1.66	0.60
1:A:310:GLY:O	1:A:311:SER:C	2.45	0.60
1:A:231:SER:OG	1:A:232:ASN:N	2.30	0.60
1:A:16:SER:C	1:A:17:LEU:HD23	2.26	0.59
1:A:212:ILE:HD11	1:A:217:LEU:HB3	1.84	0.59
1:A:83:ASP:HB2	2:A:469:HOH:O	2.02	0.59
1:A:239:VAL:HG21	1:A:243:ASP:HB3	1.84	0.59
1:B:194:ARG:NH2	2:B:705:HOH:O	2.30	0.59
1:A:78:LYS:HG2	1:A:81:GLY:O	2.02	0.59
1:B:2:SER:OG	1:B:18:THR:HB	2.02	0.58
1:A:6:ARG:HB3	2:A:352:HOH:O	2.03	0.58
1:A:273:GLN:HG3	1:A:306:GLN:HA	1.85	0.58
1:A:10:LEU:N	1:A:10:LEU:HD23	2.19	0.58
1:A:190:LEU:HD23	1:A:257:GLN:O	2.04	0.58
1:A:217:LEU:H	1:A:233:MET:HE1	1.67	0.58
1:B:8:PHE:HB3	1:B:12:SER:OG	2.04	0.58
1:A:15:ILE:N	1:A:15:ILE:HD12	2.19	0.57
1:A:216:ASP:O	1:A:223:LYS:NZ	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:HD21	1:A:276:ILE:CD1	2.34	0.57
1:A:280:THR:CG2	1:A:301:ILE:HD12	2.33	0.57
1:B:199:LYS:HB3	1:B:206:ARG:HB3	1.85	0.57
1:A:200:ASP:CB	1:A:202:THR:HB	2.34	0.57
1:B:217:LEU:N	1:B:233:MET:HE1	2.20	0.57
1:A:190:LEU:HD23	1:A:258:ALA:HB2	1.86	0.57
1:B:18:THR:OG1	1:B:24:THR:HG22	2.05	0.57
1:A:152:LYS:HG3	1:A:333:ILE:HG12	1.86	0.57
1:B:207:GLY:HA2	1:B:314:ILE:CD1	2.34	0.57
1:A:230:ASN:ND2	2:A:531:HOH:O	2.37	0.56
1:A:36:ASP:OD1	1:A:37:TRP:N	2.31	0.56
1:B:149:ASN:HB3	1:B:336:LEU:HB3	1.87	0.56
1:A:323:LYS:HD2	1:A:326:GLU:OE1	2.05	0.56
1:B:33:ARG:HB3	1:B:63:ALA:HA	1.87	0.56
1:B:92:PRO:HG3	2:B:692:HOH:O	2.05	0.56
1:A:20:LYS:HB2	2:A:574:HOH:O	2.04	0.56
1:A:185:ASN:OD1	1:A:185:ASN:N	2.35	0.56
1:B:289:LEU:HD11	1:B:294:LYS:CG	2.34	0.56
1:A:282:ASN:HD22	1:A:298:HIS:CD2	2.24	0.56
1:A:256:GLU:HG2	1:A:268:SER:OG	2.05	0.56
1:B:74:ASP:HA	1:B:92:PRO:O	2.06	0.56
1:B:217:LEU:HG	1:B:233:MET:CE	2.36	0.56
1:A:216:ASP:C	1:A:223:LYS:HZ1	2.10	0.56
1:B:199:LYS:HD2	1:B:200:ASP:OD2	2.06	0.56
1:B:255:LYS:HG3	1:B:257:GLN:HE22	1.71	0.56
1:B:5:ILE:HD13	1:B:15:ILE:HG23	1.87	0.56
1:B:206:ARG:HD2	1:B:208:ASP:HB2	1.88	0.56
1:A:6:ARG:HH11	1:A:6:ARG:CG	2.13	0.55
1:A:166:ASN:HB2	1:A:320:ILE:HG12	1.86	0.55
1:A:232:ASN:HB2	1:A:237:GLN:NE2	2.21	0.55
1:A:261:THR:HG22	1:A:266:SER:HB2	1.88	0.55
1:A:272:ASP:OD2	1:A:330:ALA:HA	2.06	0.55
1:A:253:LEU:HD11	1:A:331:THR:HB	1.88	0.55
1:B:78:LYS:HD3	1:B:83:ASP:OD1	2.07	0.55
1:B:196:VAL:HB	1:B:245:PRO:HG2	1.88	0.55
1:A:193[A]:SER:OG	1:A:220:ARG:HD2	2.08	0.54
1:A:338:THR:HG22	1:A:338:THR:O	2.06	0.54
1:A:72:ILE:HD13	1:A:312:GLU:OE2	2.06	0.54
1:B:213:LYS:O	1:B:214:ASN:ND2	2.39	0.54
1:B:201:GLN:HG2	2:B:724:HOH:O	2.07	0.54
1:B:34:ILE:HG21	1:B:171:VAL:CG2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:HA	1:A:42:LYS:O	2.08	0.53
1:A:174:ASN:ND2	1:A:299:GLY:O	2.32	0.53
1:A:189:ARG:O	1:A:258:ALA:HA	2.08	0.53
1:A:12:SER:HB3	1:A:106:LEU:HD21	1.90	0.53
1:A:199:LYS:HE3	1:A:200:ASP:OD2	2.07	0.53
1:A:227:ASN:N	1:A:227:ASN:HD22	2.05	0.53
1:B:188:LEU:HG	1:B:189:ARG:N	2.23	0.53
1:B:207:GLY:HA2	1:B:314:ILE:HG12	1.90	0.53
1:A:237:GLN:NE2	2:A:546:HOH:O	2.40	0.53
1:B:289:LEU:HD12	1:B:294:LYS:HA	1.90	0.53
1:B:71:ARG:HG2	1:B:95:LEU:CD1	2.39	0.53
1:A:77:VAL:HA	2:A:495:HOH:O	2.08	0.53
1:A:182:SER:C	1:A:184:GLU:H	2.17	0.53
1:B:200:ASP:C	1:B:202:THR:H	2.14	0.53
1:A:232:ASN:CA	1:A:237:GLN:HE21	2.21	0.52
1:A:146:ASP:HB3	2:A:680:HOH:O	2.08	0.52
1:A:248:LEU:HD11	1:A:276:ILE:HD11	1.91	0.52
1:A:170:HIS:O	1:A:170:HIS:ND1	2.39	0.52
1:B:296:VAL:HG12	2:B:444:HOH:O	2.08	0.52
1:A:197:PRO:HG2	1:A:208:ASP:HB2	1.91	0.52
1:A:282:ASN:ND2	1:A:298:HIS:CD2	2.78	0.52
1:B:88:GLN:HA	1:B:93:GLN:O	2.10	0.52
1:A:190:LEU:CD2	1:A:258:ALA:HB2	2.40	0.52
1:A:130:THR:HG23	1:B:127:ASN:HB2	1.92	0.52
1:A:280:THR:O	1:A:298:HIS:HD2	1.92	0.52
1:B:146:ASP:HB3	1:B:148:ASP:H	1.74	0.52
1:B:207:GLY:CA	1:B:314:ILE:HD11	2.40	0.52
1:B:250:GLN:HE21	1:B:255:LYS:HE3	1.74	0.51
1:A:17:LEU:HD23	1:A:17:LEU:N	2.26	0.51
1:B:165:PHE:CE2	1:B:167:PRO:HG3	2.46	0.51
1:B:282:ASN:HD22	1:B:298:HIS:CD2	2.28	0.51
1:A:296:VAL:O	1:A:297:HIS:C	2.53	0.51
1:B:86:LEU:HD13	1:B:133:TYR:CE2	2.45	0.51
1:B:216:ASP:CB	1:B:233:MET:HE2	2.34	0.51
1:A:43:HIS:C	1:A:44:LEU:HD23	2.36	0.51
1:A:203:GLU:OE2	1:A:243:ASP:OD2	2.29	0.51
1:B:36:ASP:HA	1:B:45:ILE:HD11	1.93	0.51
1:A:29:ASN:HB2	1:A:107:TRP:O	2.11	0.51
1:B:207:GLY:HA2	1:B:314:ILE:HD11	1.92	0.51
1:B:136:LYS:HE3	1:B:160:ASP:OD2	2.11	0.50
1:B:169:GLY:C	2:B:699:HOH:O	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ARG:HB3	1:B:222:GLU:HG3	1.93	0.50
1:A:278:ILE:CG2	1:A:301:ILE:HD11	2.42	0.50
1:B:72:ILE:HG23	1:B:312:GLU:OE1	2.10	0.50
1:B:297:HIS:CD2	1:B:298:HIS:CE1	3.00	0.50
1:A:242:ILE:O	1:A:279:PHE:HA	2.12	0.50
1:B:33:ARG:HB2	1:B:62:GLY:O	2.12	0.50
1:A:241:GLY:HA2	2:A:428:HOH:O	2.11	0.50
1:B:291:HIS:O	1:B:292:GLU:HB2	2.10	0.50
1:B:2:SER:HB3	2:B:546:HOH:O	2.12	0.50
1:A:253:LEU:HD21	1:A:333:ILE:HD12	1.93	0.49
1:A:256:GLU:CD	1:A:259:ARG:HE	2.20	0.49
1:A:39:LYS:O	1:A:40:ASP:HB2	2.12	0.49
1:A:121:LYS:HD2	2:A:714:HOH:O	2.12	0.49
1:B:338:THR:O	1:B:338:THR:HG22	2.10	0.49
1:A:157:ALA:C	1:A:158:ILE:HG13	2.37	0.49
1:B:180:SER:HA	1:B:296:VAL:HG13	1.94	0.49
1:A:171:VAL:O	1:A:302:THR:HG22	2.12	0.49
1:B:206:ARG:CD	1:B:208:ASP:HB2	2.42	0.49
1:A:271:THR:OG1	1:A:272:ASP:N	2.45	0.49
1:B:212:ILE:O	1:B:215:THR:HG23	2.12	0.49
1:A:27:PHE:CZ	1:A:143:HIS:HB3	2.47	0.49
1:A:286:LEU:O	1:A:286:LEU:HD23	2.13	0.49
1:A:150:LYS:HG2	1:A:335:SER:HB2	1.94	0.49
1:B:283:PHE:O	1:B:284:GLY:C	2.52	0.49
1:A:227:ASN:N	1:A:227:ASN:ND2	2.61	0.48
1:A:261:THR:HG22	1:A:266:SER:CB	2.44	0.48
1:B:178:ASP:OD1	1:B:180:SER:OG	2.28	0.48
1:B:199:LYS:HE2	2:B:684:HOH:O	2.13	0.48
1:A:217:LEU:HG	1:A:233:MET:HE1	1.95	0.48
1:A:55:LEU:HD22	2:A:681:HOH:O	2.14	0.48
1:A:183:VAL:HG13	1:A:183:VAL:O	2.14	0.48
1:B:232:ASN:CA	1:B:237:GLN:HE21	2.26	0.48
1:B:161:LYS:NZ	2:B:689:HOH:O	2.43	0.48
1:B:175:LEU:HB2	1:B:186:HIS:NE2	2.28	0.48
1:A:39:LYS:HZ2	1:A:338:THR:CG2	2.27	0.48
1:A:241:GLY:HA3	1:A:282:ASN:ND2	2.28	0.48
1:A:14:LEU:HD11	1:A:26:SER:HB2	1.96	0.47
1:A:23:VAL:HG13	1:A:38:GLN:O	2.13	0.47
1:A:175:LEU:HB2	1:A:262:LEU:HD12	1.96	0.47
1:A:205:VAL:HG12	1:A:206:ARG:N	2.27	0.47
1:A:196:VAL:HB	1:A:245:PRO:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LYS:HG3	2:B:675:HOH:O	2.14	0.47
1:A:76:LEU:HG	1:A:77:VAL:N	2.29	0.47
1:A:79:ILE:O	1:A:80:SER:C	2.56	0.47
1:B:71:ARG:NE	1:B:90:GLU:OE1	2.42	0.47
1:A:176:ASN:HD22	1:A:181:GLU:HB2	1.80	0.47
1:B:152:LYS:HB2	1:B:333:ILE:HG12	1.97	0.47
1:B:207:GLY:N	1:B:314:ILE:HD11	2.28	0.47
1:A:10:LEU:HD23	1:A:10:LEU:H	1.79	0.47
1:A:272:ASP:HB2	1:A:331:THR:O	2.15	0.47
1:B:29:ASN:HB2	1:B:107:TRP:O	2.15	0.47
1:B:212:ILE:HD12	1:B:218:ASP:HA	1.96	0.47
1:B:254:ASP:CG	1:B:255:LYS:HD3	2.40	0.47
1:B:194:ARG:HD3	2:B:663:HOH:O	2.15	0.47
1:B:282:ASN:ND2	1:B:298:HIS:CD2	2.82	0.47
1:A:152:LYS:HG3	1:A:333:ILE:HG13	1.96	0.46
1:A:286:LEU:HD23	1:A:286:LEU:C	2.39	0.46
1:A:289:LEU:CD2	1:A:294:LYS:N	2.79	0.46
1:B:280:THR:O	1:B:281:ALA:C	2.56	0.46
1:A:78:LYS:HE2	1:A:83:ASP:OD1	2.15	0.46
1:A:89:ASN:ND2	1:A:95:LEU:O	2.48	0.46
1:B:206:ARG:HD2	1:B:208:ASP:CB	2.45	0.46
1:A:72:ILE:O	1:A:93:GLN:HG3	2.16	0.46
1:A:311:SER:HB2	2:A:607:HOH:O	2.14	0.46
1:A:38:GLN:HE21	1:A:38:GLN:HB2	1.48	0.46
1:A:80:SER:N	2:A:567:HOH:O	2.39	0.46
1:B:212:ILE:HA	1:B:215:THR:HG21	1.98	0.46
1:A:219:PHE:O	1:A:220:ARG:C	2.58	0.46
1:B:207:GLY:HA2	1:B:314:ILE:CG1	2.45	0.46
1:B:264:ASP:O	1:B:338:THR:HA	2.16	0.46
1:A:182:SER:HA	1:A:298:HIS:O	2.16	0.46
1:A:248:LEU:HD13	1:A:257:GLN:CG	2.41	0.46
1:B:60:TYR:N	1:B:61:PRO:CD	2.79	0.46
1:B:216:ASP:HB2	1:B:233:MET:CE	2.37	0.46
1:B:239:VAL:O	1:B:240:LYS:HB2	2.17	0.45
1:A:212:ILE:O	1:A:212:ILE:HG23	2.13	0.45
1:A:278:ILE:HG23	1:A:301:ILE:HD11	1.98	0.45
1:B:194:ARG:HA	1:B:210:VAL:O	2.16	0.45
1:B:195:PHE:CD2	1:B:212:ILE:CG2	2.99	0.45
1:A:232:ASN:O	1:A:233:MET:C	2.56	0.45
1:B:17:LEU:HD22	1:B:118:VAL:HG11	1.97	0.45
1:B:239:VAL:CG1	1:B:243:ASP:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASP:HB3	1:A:202:THR:H	1.81	0.45
1:A:3:ILE:O	1:A:4:LYS:HG2	2.16	0.45
1:A:313:GLN:C	1:A:314:ILE:HG13	2.42	0.45
1:A:50:SER:OG	1:A:53:GLU:HG3	2.17	0.45
1:A:224:GLN:HB2	2:A:675:HOH:O	2.17	0.45
1:A:274:PRO:HB2	2:A:704:HOH:O	2.15	0.45
1:B:29:ASN:HA	1:B:122:PHE:CE2	2.52	0.45
1:A:137:ILE:HG22	1:A:139:MET:HG2	1.99	0.45
1:A:109:TYR:CE2	1:B:11:GLY:HA2	2.52	0.45
1:A:156:GLU:HG2	1:A:329:GLN:HG2	1.98	0.45
1:A:216:ASP:C	1:A:218:ASP:H	2.25	0.45
1:A:239:VAL:CG2	1:A:243:ASP:HB3	2.47	0.45
1:B:227:ASN:ND2	2:B:406:HOH:O	2.50	0.45
1:A:297:HIS:NE2	1:A:298:HIS:CE1	2.85	0.44
1:B:202:THR:HG23	1:B:204:ILE:N	2.24	0.44
1:B:52:LYS:O	1:B:56:GLU:HB2	2.16	0.44
1:B:114:LEU:HD23	1:B:114:LEU:HA	1.64	0.44
1:A:73:LYS:HA	1:A:93:GLN:OE1	2.17	0.44
1:A:126:SER:HB3	1:A:137:ILE:HB	1.99	0.44
1:A:312:GLU:H	1:A:312:GLU:HG2	1.24	0.44
1:A:339:LYS:HE3	1:A:339:LYS:HB2	1.55	0.44
1:A:232:ASN:HA	1:A:237:GLN:HE21	1.82	0.44
1:B:178:ASP:OD1	1:B:293:LYS:HD3	2.17	0.44
1:A:77:VAL:HG23	1:A:84:TYR:HB2	1.99	0.44
1:A:178:ASP:HB3	1:A:181:GLU:OE1	2.18	0.44
1:A:232:ASN:HB2	1:A:237:GLN:HE21	1.81	0.44
1:A:296:VAL:O	1:A:299:GLY:N	2.51	0.44
1:A:72:ILE:HG13	2:A:366:HOH:O	2.16	0.44
1:A:285:ASP:HB2	2:A:476:HOH:O	2.18	0.44
1:B:183:VAL:HG13	1:B:225:LEU:HD12	2.00	0.44
1:B:255:LYS:H	1:B:255:LYS:HG2	1.50	0.44
1:A:221:GLN:O	1:A:222:GLU:C	2.60	0.44
1:B:206:ARG:HD2	1:B:208:ASP:OD2	2.18	0.43
1:B:251:LEU:HA	2:B:389:HOH:O	2.18	0.43
1:A:27:PHE:HB3	1:A:33:ARG:O	2.17	0.43
1:A:178:ASP:HB3	1:A:181:GLU:HG3	1.99	0.43
1:A:280:THR:O	1:A:281:ALA:C	2.61	0.43
1:B:215:THR:HA	2:B:411:HOH:O	2.18	0.43
1:A:39:LYS:NZ	1:A:338:THR:CG2	2.80	0.43
1:A:274:PRO:HD2	1:A:306:GLN:O	2.19	0.43
1:B:111:VAL:HG22	1:B:120:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:O	1:A:34:ILE:HG23	2.17	0.43
1:A:36:ASP:HB2	2:A:358:HOH:O	2.17	0.43
1:A:152:LYS:CG	1:A:333:ILE:HG13	2.49	0.43
1:A:279:PHE:CZ	1:A:281:ALA:HA	2.53	0.43
1:B:52:LYS:HG3	1:B:53:GLU:N	2.33	0.43
1:B:323:LYS:O	1:B:324:ALA:C	2.61	0.43
1:A:31:GLY:O	1:A:32:ALA:C	2.62	0.43
1:B:185:ASN:OD1	1:B:186:HIS:ND1	2.51	0.43
1:B:189:ARG:NH2	1:B:256:GLU:HB3	2.33	0.43
1:B:200:ASP:C	1:B:202:THR:N	2.75	0.43
1:A:44:LEU:N	1:A:44:LEU:CD2	2.80	0.43
1:A:195:PHE:HZ	1:A:235:GLN:HG3	1.84	0.43
1:B:49:ASP:HB3	2:B:358:HOH:O	2.19	0.43
1:A:70:GLY:HA2	2:A:638:HOH:O	2.18	0.43
1:B:232:ASN:HB2	1:B:237:GLN:NE2	2.34	0.43
1:A:226:SER:O	1:A:227:ASN:C	2.62	0.43
1:A:176:ASN:ND2	1:A:181:GLU:HB2	2.34	0.43
1:A:289:LEU:CD2	1:A:294:LYS:HA	2.43	0.43
1:B:232:ASN:HB2	1:B:237:GLN:HE21	1.84	0.42
1:B:280:THR:O	1:B:298:HIS:HA	2.19	0.42
1:A:10:LEU:HD11	1:A:52[B]:LYS:CG	2.49	0.42
1:A:228:ALA:O	1:A:231:SER:HB3	2.18	0.42
1:B:239:VAL:HG11	1:B:243:ASP:HB2	2.00	0.42
1:A:246:PHE:O	1:A:275:SER:HB2	2.19	0.42
1:A:71:ARG:C	1:A:72:ILE:HG12	2.44	0.42
1:A:289:LEU:HD22	1:A:294:LYS:N	2.34	0.42
1:B:142:THR:O	1:B:153:ILE:HA	2.20	0.42
1:A:176:ASN:OD1	1:A:262:LEU:HD11	2.20	0.42
1:A:225:LEU:HD12	1:A:225:LEU:HA	1.62	0.42
1:A:10:LEU:HD11	1:A:52[A]:LYS:HG3	2.02	0.42
1:A:196:VAL:HG13	2:A:407:HOH:O	2.20	0.42
1:A:232:ASN:CB	1:A:237:GLN:HE21	2.33	0.42
1:A:323:LYS:HD3	1:A:326:GLU:OE2	2.20	0.42
1:B:6:ARG:NH2	2:B:556:HOH:O	2.52	0.42
1:B:33:ARG:CB	1:B:63:ALA:HA	2.47	0.42
1:A:79:ILE:HD11	1:A:164:VAL:HG13	2.02	0.42
1:A:310:GLY:C	1:A:312:GLU:N	2.77	0.42
1:A:39:LYS:NZ	1:A:338:THR:CB	2.82	0.41
1:A:197:PRO:HA	1:A:235:GLN:OE1	2.19	0.41
1:B:67:PRO:HG2	1:B:133:TYR:CE2	2.55	0.41
1:A:109:TYR:HA	1:A:121:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PRO:HG2	1:B:133:TYR:CZ	2.54	0.41
1:B:262:LEU:HD12	1:B:262:LEU:HA	1.92	0.41
1:A:10:LEU:HD11	1:A:52[A]:LYS:CG	2.50	0.41
1:A:24:THR:O	1:A:37:TRP:HD1	2.04	0.41
1:B:207:GLY:CA	1:B:314:ILE:CD1	2.99	0.41
1:B:251:LEU:HD11	2:B:605:HOH:O	2.19	0.41
1:A:68:THR:CG2	1:A:164:VAL:HG23	2.50	0.41
1:A:246:PHE:CD1	1:A:246:PHE:N	2.89	0.41
1:A:251:LEU:HD11	1:A:274:PRO:HA	2.03	0.41
1:A:289:LEU:CD2	1:A:294:LYS:CA	2.98	0.41
1:A:71:ARG:NH1	1:A:90:GLU:CD	2.79	0.41
1:A:111:VAL:HG22	1:A:120:VAL:HG22	2.02	0.41
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.87	0.41
1:A:235:GLN:O	1:A:238:LEU:HB3	2.20	0.41
1:A:273:GLN:HB3	1:A:274:PRO:HD2	2.03	0.41
1:B:76:LEU:HG	1:B:77:VAL:N	2.36	0.41
1:B:206:ARG:HG3	2:B:654:HOH:O	2.20	0.41
1:B:328:TYR:CD2	1:B:328:TYR:C	2.99	0.41
1:A:89:ASN:ND2	1:A:98:GLY:C	2.79	0.40
1:B:31:GLY:O	1:B:32:ALA:C	2.64	0.40
1:B:157:ALA:C	1:B:158:ILE:HG13	2.46	0.40
1:B:216:ASP:OD2	1:B:231:SER:HB2	2.22	0.40
1:B:217:LEU:CG	1:B:233:MET:HE1	2.48	0.40
1:A:164:VAL:HB	1:A:320:ILE:CG2	2.51	0.40
1:A:3:ILE:C	1:A:4:LYS:HG2	2.47	0.40
1:A:166:ASN:CB	1:A:320:ILE:CD1	3.00	0.40
1:A:248:LEU:HD22	1:A:257:GLN:HG2	2.02	0.40
1:A:273:GLN:HA	1:A:274:PRO:HD3	1.79	0.40
1:A:289:LEU:HD23	1:A:294:LYS:CA	2.46	0.40
1:B:212:ILE:HD12	1:B:217:LEU:O	2.21	0.40
1:A:328:TYR:CD2	1:A:328:TYR:C	2.99	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	339/347 (98%)	299 (88%)	36 (11%)	4 (1%)	10	4
1	B	338/347 (97%)	309 (91%)	29 (9%)	0	100	100
All	All	677/694 (98%)	608 (90%)	65 (10%)	4 (1%)	21	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	THR
1	A	311	SER
1	A	40	ASP
1	A	281	ALA

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	294/300 (98%)	232 (79%)	62 (21%)	1	0
1	B	293/300 (98%)	251 (86%)	42 (14%)	3	1
All	All	587/600 (98%)	483 (82%)	104 (18%)	2	0

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	4	LYS
1	A	5	ILE
1	A	6	ARG
1	A	15	ILE
1	A	16	SER
1	A	17	LEU
1	A	24	THR
1	A	30	LEU

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Mol	Chain	Res	Type
1	A	33	ARG
1	A	34	ILE
1	A	42	LYS
1	A	44	LEU
1	A	65	VAL
1	A	72	ILE
1	A	76	LEU
1	A	78	LYS
1	A	99	GLU
1	A	119	GLN
1	A	136	LYS
1	A	148	ASP
1	A	150	LYS
1	A	152	LYS
1	A	164	VAL
1	A	171	VAL
1	A	181	GLU
1	A	183	VAL
1	A	186	HIS
1	A	189	ARG
1	A	190	LEU
1	A	195	PHE
1	A	198	LEU
1	A	201	GLN
1	A	202	THR
1	A	206	ARG
1	A	212	ILE
1	A	215	THR
1	A	224	GLN
1	A	225	LEU
1	A	226	SER
1	A	230	ASN
1	A	233	MET
1	A	234	GLU
1	A	239	VAL
1	A	246	PHE
1	A	248	LEU
1	A	251	LEU
1	A	253	LEU
1	A	256	GLU
1	A	257	GLN
1	A	262	LEU

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Mol	Chain	Res	Type
1	A	264	ASP
1	A	267	ILE
1	A	288	THR
1	A	292	GLU
1	A	294	LYS
1	A	311	SER
1	A	312	GLU
1	A	320	ILE
1	A	321	SER
1	A	335	SER
1	A	339	LYS
1	B	4	LYS
1	B	5	ILE
1	B	16	SER
1	B	30	LEU
1	B	42	LYS
1	B	44	LEU
1	B	50	SER
1	B	52	LYS
1	B	76	LEU
1	B	77	VAL
1	B	78	LYS
1	B	112	THR
1	B	153	ILE
1	B	161	LYS
1	B	183	VAL
1	B	189	ARG
1	B	190	LEU
1	B	195	PHE
1	B	199	LYS
1	B	200	ASP
1	B	202	THR
1	B	203	GLU
1	B	205	VAL
1	B	206	ARG
1	B	208	ASP
1	B	211	ASP
1	B	213	LYS
1	B	214	ASN
1	B	215	THR
1	B	222	GLU
1	B	223	LYS

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Mol	Chain	Res	Type
1	B	247	LEU
1	B	250	GLN
1	B	251	LEU
1	B	254	ASP
1	B	255	LYS
1	B	257	GLN
1	B	293	LYS
1	B	321	SER
1	B	323	LYS
1	B	338	THR
1	B	339	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	43	HIS
1	A	89	ASN
1	A	119	GLN
1	A	221	GLN
1	A	227	ASN
1	A	230	ASN
1	A	237	GLN
1	A	250	GLN
1	A	273	GLN
1	A	282	ASN
1	A	306	GLN
1	A	329	GLN
1	B	38	GLN
1	B	227	ASN
1	B	237	GLN
1	B	250	GLN
1	B	282	ASN
1	B	295	GLN
1	B	298	HIS
1	B	329	GLN

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 [i](#)

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

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	338/347 (97%)	0.23	13 (3%) 44 47	11, 28, 54, 90	3 (0%)
1	B	338/347 (97%)	-0.24	1 (0%) 90 91	9, 22, 45, 68	2 (0%)
All	All	676/694 (97%)	-0.00	14 (2%) 63 67	9, 24, 49, 90	5 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	ILE	4.0
1	A	215	THR	3.8
1	A	227	ASN	3.7
1	A	212	ILE	3.5
1	A	214	ASN	3.1
1	A	339	LYS	2.9
1	A	221	GLN	2.8
1	A	222	GLU	2.7
1	A	337	HIS	2.6
1	A	338	THR	2.3
1	A	207	GLY	2.2
1	A	287	GLY	2.2
1	B	214	ASN	2.1
1	A	248	LEU	2.1

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.