



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:48 PM UTC

PDB ID : 2ZJB / pdb_00002zjb
Title : Crystal structure of the human Dmc1-M200V polymorphic variant
Authors : Hikiba, J.; Hirota, K.; Kagawa, W.; Ikawa, S.; Kinebuchi, T.; Sakane, I.; Takizawa, Y.; Yokoyama, S.; Mandon-Pepin, B.; Nicolas, A.; Shibata, T.; Ohta, K.; Kurumizaka, H.
Deposited on : 2008-03-02
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

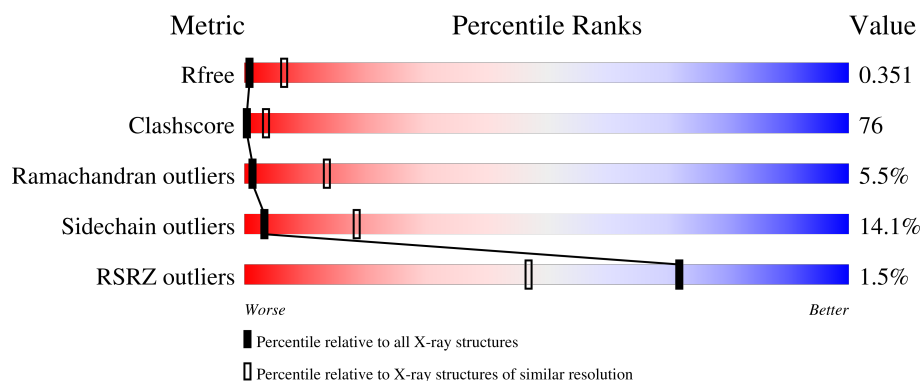
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	343	13% 43% 12% • 30%
1	B	343	18% 41% 11% 30%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3748 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 Meiotic recombination protein DMC1/LIM15 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1874	1186	325	356	7			
1	B	239	Total	C	N	O	S	0	0	0
			1874	1186	325	356	7			

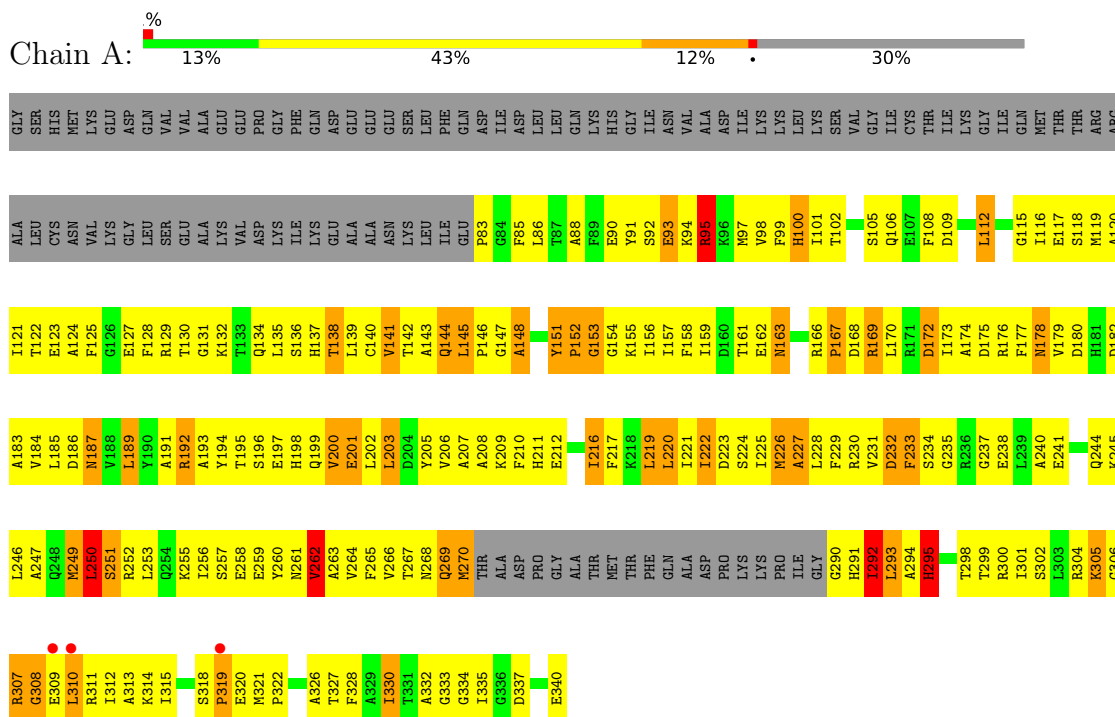
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q14565
A	-1	SER	-	expression tag	UNP Q14565
A	0	HIS	-	expression tag	UNP Q14565
A	200	VAL	MET	SEE REMARK 999	UNP Q14565
B	-2	GLY	-	expression tag	UNP Q14565
B	-1	SER	-	expression tag	UNP Q14565
B	0	HIS	-	expression tag	UNP Q14565
B	200	VAL	MET	SEE REMARK 999	UNP Q14565

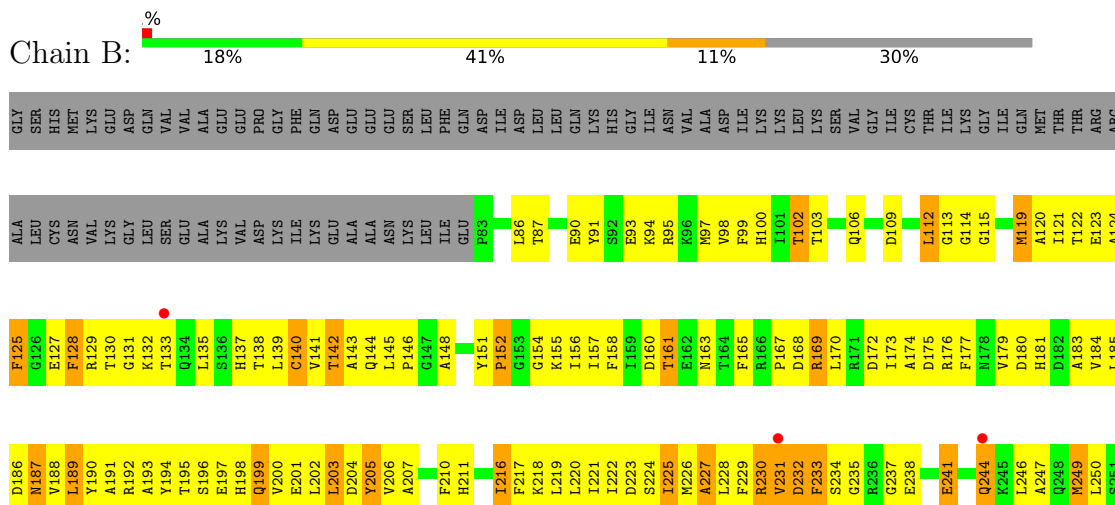
3 Residue-property plots

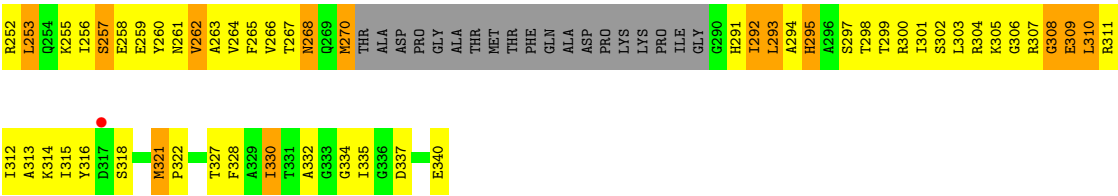
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Meiotic recombination protein DMC1/LIM15 homolog



• Molecule 1: Meiotic recombination protein DMC1/LIM15 homolog





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.09Å 124.09Å 217.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.50) 99.2 (20.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.53 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.294 , 0.351 0.293 , 0.351	Depositor DCC
R_{free} test set	1138 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	92.9	Xtriage
Anisotropy	0.978	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 110.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3748	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/1907	1.06	13/2564 (0.5%)
1	B	0.51	1/1907 (0.1%)	1.03	11/2564 (0.4%)
All	All	0.51	1/3814 (0.0%)	1.04	24/5128 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	MET	SD-CE	6.66	1.96	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	GLY	N-CA-C	-8.50	103.49	112.08
1	B	186	ASP	N-CA-C	-8.14	103.36	113.38
1	B	225	ILE	N-CA-C	7.52	118.45	111.45
1	B	103	THR	N-CA-C	-7.25	104.58	113.50
1	B	295	HIS	N-CA-C	-7.13	103.68	112.38
1	B	140	CYS	N-CA-C	-7.01	104.59	113.01
1	B	161	THR	N-CA-C	-6.97	103.41	112.68
1	A	154	GLY	N-CA-C	6.57	120.06	110.80
1	A	269	GLN	N-CA-C	6.21	118.94	110.06
1	A	201	GLU	N-CA-C	-6.14	103.90	111.33
1	A	295	HIS	N-CA-C	-6.07	104.73	111.71
1	A	187	ASN	N-CA-C	5.87	120.44	113.28
1	A	250	LEU	N-CA-C	-5.69	105.43	112.38
1	A	141	VAL	N-CA-C	5.64	116.47	111.90
1	B	309	GLU	N-CA-C	5.57	117.82	111.02
1	B	268	ASN	N-CA-C	5.55	115.71	107.88
1	A	144	GLN	N-CA-C	-5.33	106.71	114.12
1	B	205	TYR	N-CA-C	-5.29	107.37	113.88
1	A	151	TYR	CA-C-N	5.17	126.30	119.84
1	A	151	TYR	C-N-CA	5.17	126.30	119.84
1	B	321	MET	N-CA-C	5.08	116.30	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	SER	N-CA-C	-5.05	105.24	111.40
1	B	230	ARG	N-CA-C	-5.03	105.93	111.71
1	A	93	GLU	N-CA-C	-5.01	105.73	111.14

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	1874	0	1856	306	0
1	B	1874	0	1856	276	0
All	All	3748	0	3712	569	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 76.

All (569) 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:247:ALA:HB2	1:A:292:ILE:HD11	1.24	1.11
1:B:304:ARG:HG3	1:B:312:ILE:HB	1.45	0.99
1:A:141:VAL:O	1:A:145:LEU:HD22	1.63	0.98
1:A:119:MET:HG2	1:A:258:GLU:HA	1.45	0.96
1:A:247:ALA:HB2	1:A:292:ILE:CD1	1.96	0.95
1:B:119:MET:HG2	1:B:258:GLU:HA	1.48	0.95
1:B:268:ASN:HD22	1:B:270:MET:HE1	1.31	0.95
1:B:141:VAL:HG12	1:B:145:LEU:HD21	1.51	0.92
1:A:196:SER:N	1:A:228:LEU:HD21	1.85	0.92
1:A:141:VAL:HG12	1:A:145:LEU:HD21	1.52	0.91
1:A:216:ILE:HD13	1:A:216:ILE:H	1.34	0.90
1:A:121:ILE:HA	1:A:264:VAL:HG23	1.53	0.90
1:B:226:MET:HB2	1:B:268:ASN:ND2	1.88	0.89
1:B:219:LEU:HD23	1:B:220:LEU:N	1.88	0.88
1:A:157:ILE:HB	1:A:220:LEU:HD23	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ALA:HB3	1:B:267:THR:HA	1.59	0.84
1:B:234:SER:HB2	1:B:238:GLU:HB3	1.58	0.84
1:A:234:SER:HB2	1:A:238:GLU:CB	2.07	0.84
1:B:144:GLN:NE2	1:B:187:ASN:HB3	1.92	0.83
1:B:157:ILE:HD13	1:B:189:LEU:CB	2.08	0.83
1:B:157:ILE:HD13	1:B:189:LEU:HB3	1.61	0.82
1:B:247:ALA:HB2	1:B:292:ILE:HD11	1.61	0.82
1:B:90:GLU:O	1:B:93:GLU:HB2	1.80	0.81
1:B:234:SER:HB2	1:B:238:GLU:CB	2.10	0.81
1:A:225:ILE:HG23	1:A:226:MET:H	1.44	0.81
1:A:228:LEU:O	1:A:228:LEU:HD23	1.81	0.81
1:B:305:LYS:HE3	1:B:311:ARG:HG3	1.61	0.81
1:A:234:SER:HB2	1:A:238:GLU:HB3	1.64	0.80
1:B:130:THR:HA	1:B:311:ARG:NH2	1.97	0.79
1:B:221:ILE:HD12	1:B:265:PHE:O	1.81	0.79
1:B:220:LEU:HB3	1:B:264:VAL:HG12	1.65	0.79
1:B:247:ALA:HB2	1:B:292:ILE:CD1	2.13	0.79
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.48	0.79
1:A:216:ILE:HD13	1:A:217:PHE:H	1.47	0.79
1:A:247:ALA:CB	1:A:292:ILE:HD11	2.09	0.78
1:A:146:PRO:HG3	1:A:152:PRO:O	1.84	0.78
1:B:216:ILE:HD13	1:B:216:ILE:H	1.46	0.78
1:A:216:ILE:H	1:A:216:ILE:CD1	1.96	0.78
1:A:121:ILE:HD13	1:A:253:LEU:HD22	1.66	0.77
1:A:174:ALA:HB2	1:A:184:VAL:HG21	1.63	0.77
1:A:130:THR:HA	1:A:311:ARG:HH22	1.49	0.77
1:B:130:THR:HA	1:B:311:ARG:HH22	1.49	0.77
1:B:129:ARG:HE	1:B:129:ARG:HA	1.50	0.77
1:A:220:LEU:HB3	1:A:264:VAL:HG12	1.66	0.76
1:B:180:ASP:O	1:B:184:VAL:HG23	1.84	0.76
1:A:253:LEU:HA	1:A:256:ILE:HD12	1.65	0.76
1:A:135:LEU:HD22	1:A:265:PHE:CE2	2.21	0.76
1:A:174:ALA:CB	1:A:184:VAL:HG21	2.16	0.76
1:B:144:GLN:OE1	1:B:184:VAL:HG13	1.87	0.75
1:B:313:ALA:HB2	1:B:328:PHE:HE2	1.50	0.75
1:A:182:ASP:O	1:A:186:ASP:HB2	1.87	0.74
1:A:121:ILE:CD1	1:A:253:LEU:HD22	2.16	0.74
1:A:203:LEU:HD21	1:A:222:ILE:HD11	1.69	0.74
1:B:142:THR:HA	1:B:145:LEU:HD23	1.67	0.74
1:A:226:MET:HB2	1:A:268:ASN:ND2	2.02	0.74
1:B:139:LEU:HA	1:B:142:THR:OG1	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:O	1:A:97:MET:HG2	1.88	0.73
1:B:120:ALA:HB1	1:B:298:THR:OG1	1.88	0.73
1:B:216:ILE:H	1:B:216:ILE:CD1	2.02	0.72
1:B:86:LEU:HD23	1:B:86:LEU:H	1.54	0.72
1:B:112:LEU:HB3	1:B:115:GLY:O	1.90	0.71
1:B:154:GLY:HA3	1:B:218:LYS:HG2	1.72	0.71
1:B:131:GLY:H	1:B:311:ARG:CZ	2.04	0.70
1:A:112:LEU:HD23	1:A:115:GLY:HA2	1.73	0.70
1:A:228:LEU:HD23	1:A:228:LEU:C	2.17	0.70
1:B:121:ILE:HD13	1:B:253:LEU:HD13	1.73	0.69
1:B:228:LEU:HD23	1:B:228:LEU:O	1.92	0.69
1:B:135:LEU:HD22	1:B:265:PHE:CE2	2.28	0.69
1:B:145:LEU:HG	1:B:177:PHE:HD2	1.57	0.69
1:A:226:MET:HB2	1:A:268:ASN:CG	2.18	0.69
1:A:138:THR:HG23	1:A:334:GLY:HA3	1.74	0.69
1:B:200:VAL:HG12	1:B:204:ASP:OD2	1.93	0.69
1:B:211:HIS:HA	1:B:260:TYR:HE2	1.58	0.69
1:B:231:VAL:HG12	1:B:232:ASP:N	2.06	0.69
1:A:136:SER:HB3	1:A:158:PHE:HE1	1.58	0.69
1:B:305:LYS:HD3	1:B:310:LEU:O	1.93	0.68
1:A:129:ARG:HE	1:A:129:ARG:HA	1.58	0.68
1:A:233:PHE:C	1:A:233:PHE:CD2	2.71	0.68
1:A:141:VAL:HG22	1:A:184:VAL:CG1	2.24	0.68
1:B:238:GLU:HG3	1:B:241:GLU:HB2	1.74	0.68
1:A:158:PHE:HA	1:A:221:ILE:HG23	1.75	0.68
1:A:262:VAL:HG23	1:A:263:ALA:N	2.07	0.68
1:B:268:ASN:HD22	1:B:270:MET:CE	2.07	0.68
1:A:95:ARG:NH1	1:A:98:VAL:HG21	2.10	0.67
1:A:132:LYS:HD2	1:A:267:THR:HB	1.77	0.67
1:A:255:LYS:O	1:A:259:GLU:HB3	1.94	0.67
1:A:306:GLY:O	1:A:307:ARG:HB2	1.95	0.67
1:A:85:PHE:CE1	1:B:189:LEU:HD12	2.30	0.67
1:A:221:ILE:HD13	1:A:265:PHE:HB3	1.77	0.67
1:B:145:LEU:HG	1:B:177:PHE:CD2	2.30	0.67
1:A:226:MET:HG3	1:A:270:MET:SD	2.35	0.66
1:B:305:LYS:CE	1:B:311:ARG:HG3	2.24	0.66
1:A:141:VAL:O	1:A:145:LEU:CD2	2.41	0.66
1:A:95:ARG:HH11	1:A:98:VAL:HG21	1.59	0.66
1:A:193:ALA:HA	1:A:198:HIS:HD2	1.61	0.66
1:A:252:ARG:CA	1:A:252:ARG:HH11	2.08	0.66
1:B:160:ASP:HB2	1:B:190:TYR:HE1	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD23	1:B:292:ILE:HD13	1.78	0.66
1:A:192:ARG:HG2	1:A:192:ARG:NH1	2.09	0.66
1:A:137:HIS:O	1:A:140:CYS:HB2	1.96	0.66
1:B:226:MET:CG	1:B:293:LEU:HD12	2.25	0.66
1:B:201:GLU:OE1	1:B:201:GLU:HA	1.96	0.66
1:B:142:THR:CA	1:B:145:LEU:HD23	2.26	0.65
1:B:252:ARG:HA	1:B:252:ARG:HH11	1.61	0.65
1:B:102:THR:HG23	1:B:142:THR:HB	1.79	0.65
1:B:172:ASP:OD2	1:B:332:ALA:HB1	1.96	0.65
1:B:304:ARG:CG	1:B:312:ILE:HB	2.26	0.65
1:B:200:VAL:O	1:B:201:GLU:C	2.38	0.65
1:A:233:PHE:C	1:A:233:PHE:HD2	2.04	0.65
1:A:226:MET:O	1:A:228:LEU:N	2.30	0.64
1:B:94:LYS:O	1:B:97:MET:HG2	1.97	0.64
1:A:101:ILE:HG21	1:A:143:ALA:HB2	1.79	0.64
1:B:192:ARG:HG2	1:B:192:ARG:HH11	1.62	0.64
1:A:83:PRO:HB3	1:B:205:TYR:OH	1.96	0.64
1:A:88:ALA:HB2	1:B:188:VAL:HB	1.79	0.64
1:A:130:THR:HA	1:A:311:ARG:NH2	2.12	0.64
1:A:252:ARG:HH11	1:A:252:ARG:HA	1.62	0.64
1:A:252:ARG:O	1:A:256:ILE:HG13	1.97	0.64
1:B:125:PHE:CB	1:B:302:SER:HA	2.28	0.64
1:A:85:PHE:HB2	1:B:190:TYR:O	1.99	0.63
1:A:253:LEU:HD23	1:A:253:LEU:O	1.97	0.63
1:B:303:LEU:HD23	1:B:313:ALA:HB2	1.80	0.63
1:B:137:HIS:O	1:B:140:CYS:N	2.32	0.63
1:A:121:ILE:HG12	1:A:264:VAL:HG21	1.81	0.63
1:B:123:GLU:HA	1:B:266:VAL:O	1.98	0.63
1:B:194:TYR:H	1:B:198:HIS:HD2	1.45	0.63
1:A:131:GLY:O	1:A:134:GLN:HB2	1.97	0.62
1:B:121:ILE:HA	1:B:264:VAL:HG23	1.79	0.62
1:B:203:LEU:HA	1:B:206:VAL:HG23	1.81	0.62
1:A:130:THR:HG22	1:A:132:LYS:H	1.64	0.62
1:A:253:LEU:HA	1:A:256:ILE:CD1	2.29	0.62
1:A:219:LEU:HD23	1:A:220:LEU:N	2.15	0.62
1:A:246:LEU:HD23	1:A:292:ILE:HD13	1.81	0.62
1:B:137:HIS:O	1:B:140:CYS:HB2	1.99	0.62
1:B:238:GLU:HG3	1:B:238:GLU:O	1.99	0.62
1:A:203:LEU:HD21	1:A:222:ILE:CD1	2.28	0.62
1:B:125:PHE:HB3	1:B:302:SER:HA	1.79	0.62
1:A:227:ALA:H	1:A:268:ASN:HD21	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ALA:CB	1:B:292:ILE:HD11	2.30	0.62
1:A:138:THR:HA	1:A:173:ILE:HD13	1.80	0.62
1:A:183:ALA:O	1:A:187:ASN:HB2	2.00	0.61
1:A:192:ARG:HE	1:A:194:TYR:HE2	1.47	0.61
1:A:201:GLU:HA	1:A:201:GLU:OE1	1.98	0.61
1:A:85:PHE:HE1	1:B:189:LEU:HD12	1.64	0.61
1:A:192:ARG:NE	1:A:194:TYR:HE2	1.99	0.61
1:B:268:ASN:ND2	1:B:270:MET:HE1	2.09	0.61
1:A:180:ASP:O	1:A:184:VAL:HG23	2.00	0.61
1:B:252:ARG:HH11	1:B:252:ARG:CA	2.13	0.61
1:A:131:GLY:H	1:A:311:ARG:CZ	2.14	0.61
1:B:146:PRO:HA	1:B:152:PRO:O	2.01	0.61
1:B:216:ILE:HD13	1:B:217:PHE:H	1.66	0.61
1:A:86:LEU:HD23	1:A:86:LEU:H	1.66	0.61
1:A:252:ARG:O	1:A:252:ARG:NH1	2.33	0.61
1:A:310:LEU:N	1:A:310:LEU:HD12	2.16	0.61
1:B:216:ILE:HD13	1:B:216:ILE:N	2.16	0.61
1:B:121:ILE:CD1	1:B:253:LEU:HD13	2.31	0.60
1:A:125:PHE:HB2	1:A:302:SER:HA	1.83	0.60
1:A:159:ILE:HB	1:A:222:ILE:HG12	1.84	0.60
1:B:233:PHE:C	1:B:233:PHE:CD2	2.79	0.60
1:A:227:ALA:H	1:A:268:ASN:ND2	1.98	0.60
1:A:304:ARG:HG3	1:A:312:ILE:HB	1.83	0.60
1:B:194:TYR:H	1:B:198:HIS:CD2	2.20	0.60
1:B:193:ALA:HA	1:B:198:HIS:HD2	1.67	0.59
1:A:144:GLN:OE1	1:A:184:VAL:HG13	2.02	0.59
1:A:310:LEU:HD12	1:A:310:LEU:H	1.67	0.59
1:B:226:MET:O	1:B:229:PHE:N	2.32	0.59
1:A:95:ARG:NH1	1:A:119:MET:HE2	2.18	0.59
1:A:136:SER:HB3	1:A:158:PHE:CE1	2.37	0.59
1:B:305:LYS:HE3	1:B:311:ARG:NE	2.17	0.59
1:A:156:ILE:HG23	1:A:219:LEU:HB3	1.84	0.59
1:B:200:VAL:HG22	1:B:249:MET:HG3	1.84	0.58
1:A:156:ILE:HG22	1:A:157:ILE:N	2.18	0.58
1:A:157:ILE:HD13	1:A:189:LEU:HB3	1.84	0.58
1:A:241:GLU:HA	1:A:241:GLU:OE1	2.02	0.58
1:B:226:MET:HB2	1:B:268:ASN:HD21	1.67	0.58
1:A:138:THR:OG1	1:A:335:ILE:HD13	2.02	0.58
1:B:303:LEU:HD23	1:B:313:ALA:CB	2.33	0.58
1:A:138:THR:HG21	1:A:335:ILE:H	1.67	0.58
1:A:314:LYS:HG2	1:A:315:ILE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LYS:HB3	1:B:217:PHE:CE2	2.38	0.58
1:B:330:ILE:HD12	1:B:330:ILE:H	1.68	0.58
1:A:108:PHE:O	1:A:112:LEU:HD22	2.04	0.58
1:A:224:SER:HB2	1:A:267:THR:O	2.03	0.58
1:A:119:MET:HB3	1:A:258:GLU:HG2	1.84	0.58
1:B:252:ARG:O	1:B:256:ILE:HG13	2.04	0.58
1:B:180:ASP:HB3	1:B:183:ALA:CB	2.34	0.57
1:B:157:ILE:HD13	1:B:189:LEU:HB2	1.86	0.57
1:A:90:GLU:O	1:A:93:GLU:HB2	2.05	0.57
1:B:106:GLN:N	1:B:337:ASP:OD1	2.37	0.57
1:B:121:ILE:HD11	1:B:253:LEU:HB3	1.85	0.57
1:B:129:ARG:HA	1:B:129:ARG:NE	2.18	0.57
1:B:141:VAL:O	1:B:142:THR:C	2.48	0.57
1:A:195:THR:H	1:A:198:HIS:HB3	1.70	0.57
1:A:155:LYS:HB3	1:A:217:PHE:CE2	2.40	0.57
1:B:252:ARG:NH1	1:B:252:ARG:HB3	2.20	0.57
1:A:198:HIS:O	1:A:201:GLU:HB2	2.05	0.57
1:B:210:PHE:HB3	1:B:260:TYR:CD2	2.40	0.57
1:A:95:ARG:HH11	1:A:98:VAL:CG2	2.17	0.56
1:A:216:ILE:HD13	1:A:216:ILE:N	2.10	0.56
1:B:86:LEU:HD11	1:B:91:TYR:HA	1.87	0.56
1:B:253:LEU:HA	1:B:256:ILE:HD12	1.87	0.56
1:A:250:LEU:HD11	1:A:293:LEU:HG	1.88	0.56
1:B:193:ALA:HA	1:B:198:HIS:CD2	2.39	0.56
1:A:124:ALA:HB3	1:A:267:THR:HG22	1.86	0.56
1:B:233:PHE:HD2	1:B:233:PHE:O	1.89	0.56
1:A:238:GLU:O	1:A:238:GLU:HG3	2.05	0.56
1:B:305:LYS:HE3	1:B:311:ARG:CG	2.34	0.56
1:A:220:LEU:O	1:A:264:VAL:HA	2.04	0.56
1:A:226:MET:CE	1:A:270:MET:HG2	2.35	0.56
1:A:225:ILE:HG23	1:A:226:MET:N	2.15	0.56
1:B:332:ALA:C	1:B:334:GLY:H	2.12	0.56
1:A:138:THR:HA	1:A:173:ILE:CD1	2.35	0.56
1:A:147:GLY:O	1:A:148:ALA:O	2.23	0.56
1:A:221:ILE:HD13	1:A:265:PHE:CD2	2.41	0.56
1:A:123:GLU:OE1	1:A:293:LEU:HD22	2.06	0.55
1:B:124:ALA:HB3	1:B:267:THR:CA	2.32	0.55
1:B:262:VAL:HG23	1:B:263:ALA:N	2.20	0.55
1:B:203:LEU:HA	1:B:206:VAL:CG2	2.37	0.55
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.72	0.55
1:A:119:MET:CG	1:A:258:GLU:HA	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:C	1:A:135:LEU:HD23	2.32	0.55
1:A:193:ALA:HA	1:A:198:HIS:CD2	2.41	0.55
1:A:202:LEU:O	1:A:206:VAL:HG23	2.06	0.55
1:A:221:ILE:HD12	1:A:265:PHE:O	2.07	0.55
1:B:203:LEU:HD21	1:B:222:ILE:HD11	1.88	0.55
1:A:122:THR:O	1:A:266:VAL:HG22	2.07	0.55
1:A:241:GLU:O	1:A:245:LYS:HB2	2.07	0.55
1:A:172:ASP:OD2	1:A:332:ALA:HB1	2.07	0.55
1:B:119:MET:CG	1:B:258:GLU:HA	2.31	0.55
1:B:196:SER:N	1:B:228:LEU:HD22	2.22	0.55
1:A:211:HIS:HA	1:A:260:TYR:HE2	1.72	0.55
1:A:196:SER:HA	1:A:228:LEU:CD2	2.35	0.55
1:A:124:ALA:HB3	1:A:267:THR:HA	1.88	0.55
1:A:169:ARG:HG3	1:A:169:ARG:HH11	1.72	0.55
1:B:137:HIS:O	1:B:138:THR:C	2.50	0.54
1:A:100:HIS:HA	1:A:116:ILE:O	2.07	0.54
1:A:161:THR:HG21	1:A:224:SER:O	2.07	0.54
1:B:176:ARG:HH21	1:B:177:PHE:HZ	1.55	0.54
1:B:310:LEU:HD12	1:B:310:LEU:N	2.22	0.54
1:A:140:CYS:O	1:A:144:GLN:NE2	2.40	0.54
1:A:92:SER:HB2	1:B:167:PRO:CB	2.38	0.54
1:B:145:LEU:N	1:B:145:LEU:HD22	2.22	0.54
1:B:176:ARG:HE	1:B:177:PHE:HE1	1.53	0.54
1:A:196:SER:CA	1:A:228:LEU:HD21	2.37	0.54
1:A:229:PHE:C	1:A:231:VAL:H	2.15	0.54
1:B:335:ILE:N	1:B:335:ILE:HD12	2.22	0.54
1:B:226:MET:HE2	1:B:291:HIS:CE1	2.43	0.54
1:B:226:MET:HG2	1:B:293:LEU:HD12	1.89	0.54
1:B:305:LYS:HE2	1:B:308:GLY:O	2.07	0.54
1:B:314:LYS:HG2	1:B:315:ILE:N	2.23	0.54
1:B:130:THR:HG22	1:B:132:LYS:H	1.72	0.54
1:B:294:ALA:HA	1:B:300:ARG:NH1	2.22	0.54
1:B:135:LEU:HD23	1:B:135:LEU:O	2.08	0.53
1:A:177:PHE:O	1:A:179:VAL:HG23	2.07	0.53
1:A:197:GLU:O	1:A:201:GLU:HG2	2.08	0.53
1:B:140:CYS:HA	1:B:156:ILE:CD1	2.38	0.53
1:A:167:PRO:HB3	1:A:185:LEU:HD11	1.90	0.53
1:A:196:SER:CA	1:A:228:LEU:CD2	2.87	0.53
1:A:222:ILE:O	1:A:222:ILE:HG22	2.07	0.53
1:B:196:SER:CA	1:B:228:LEU:HD22	2.38	0.53
1:B:221:ILE:HD13	1:B:265:PHE:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ALA:N	1:B:292:ILE:HD11	2.24	0.53
1:A:137:HIS:O	1:A:138:THR:C	2.51	0.53
1:A:238:GLU:HG3	1:A:241:GLU:HB2	1.91	0.53
1:B:145:LEU:O	1:B:146:PRO:C	2.51	0.53
1:B:227:ALA:H	1:B:268:ASN:HD21	1.55	0.53
1:A:163:ASN:OD1	1:A:192:ARG:HD2	2.09	0.53
1:A:185:LEU:C	1:A:187:ASN:H	2.16	0.53
1:A:185:LEU:C	1:A:187:ASN:N	2.66	0.53
1:B:156:ILE:HG22	1:B:157:ILE:N	2.24	0.53
1:B:299:THR:HA	1:B:318:SER:OG	2.09	0.53
1:A:320:GLU:O	1:A:322:PRO:HD3	2.09	0.52
1:B:196:SER:N	1:B:228:LEU:CD2	2.72	0.52
1:B:199:GLN:OE1	1:B:225:ILE:HG13	2.09	0.52
1:A:221:ILE:HD13	1:A:265:PHE:HD2	1.72	0.52
1:A:227:ALA:N	1:A:268:ASN:HD21	2.06	0.52
1:B:184:VAL:O	1:B:187:ASN:HB2	2.09	0.52
1:A:305:LYS:HE2	1:A:308:GLY:O	2.10	0.52
1:B:291:HIS:O	1:B:294:ALA:N	2.41	0.52
1:A:106:GLN:N	1:A:337:ASP:OD1	2.42	0.52
1:A:156:ILE:HG22	1:A:157:ILE:H	1.75	0.52
1:A:310:LEU:HD23	1:A:327:THR:CG2	2.40	0.52
1:B:140:CYS:SG	1:B:158:PHE:HD1	2.33	0.52
1:A:162:GLU:O	1:A:163:ASN:CB	2.58	0.52
1:B:127:GLU:OE2	1:B:128:PHE:HB2	2.10	0.52
1:B:167:PRO:HB3	1:B:185:LEU:CD1	2.40	0.52
1:A:145:LEU:HD13	1:A:145:LEU:N	2.24	0.52
1:A:95:ARG:NH1	1:A:98:VAL:CG2	2.72	0.52
1:B:202:LEU:O	1:B:205:TYR:N	2.32	0.52
1:A:233:PHE:HD2	1:A:233:PHE:O	1.93	0.51
1:A:314:LYS:HG2	1:A:315:ILE:H	1.74	0.51
1:A:155:LYS:HB3	1:A:217:PHE:HE2	1.74	0.51
1:A:166:ARG:O	1:A:169:ARG:N	2.42	0.51
1:A:196:SER:HA	1:A:228:LEU:HD22	1.92	0.51
1:B:207:ALA:O	1:B:210:PHE:HB2	2.09	0.51
1:B:267:THR:O	1:B:268:ASN:OD1	2.29	0.51
1:A:216:ILE:CD1	1:A:217:PHE:H	2.21	0.51
1:A:231:VAL:HG12	1:A:232:ASP:N	2.25	0.51
1:B:175:ASP:C	1:B:177:PHE:N	2.68	0.51
1:B:221:ILE:HD13	1:B:265:PHE:HB3	1.92	0.51
1:A:97:MET:O	1:A:99:PHE:HD2	1.94	0.51
1:A:195:THR:C	1:A:228:LEU:HD21	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:MET:O	1:A:229:PHE:N	2.25	0.51
1:B:121:ILE:HG22	1:B:297:SER:HB3	1.93	0.51
1:B:160:ASP:HB2	1:B:190:TYR:CE1	2.43	0.51
1:A:235:GLY:C	1:A:237:GLY:H	2.18	0.51
1:B:200:VAL:C	1:B:202:LEU:N	2.66	0.51
1:B:306:GLY:O	1:B:307:ARG:HB2	2.10	0.51
1:B:121:ILE:HG12	1:B:264:VAL:HG21	1.93	0.51
1:A:141:VAL:O	1:A:142:THR:C	2.54	0.51
1:B:250:LEU:HD11	1:B:293:LEU:HG	1.93	0.51
1:A:269:GLN:N	1:A:269:GLN:OE1	2.44	0.51
1:B:100:HIS:HB3	1:B:114:GLY:O	2.10	0.51
1:A:95:ARG:HH12	1:A:119:MET:HE2	1.76	0.50
1:B:203:LEU:HD21	1:B:222:ILE:CD1	2.41	0.50
1:B:211:HIS:CA	1:B:260:TYR:HE2	2.22	0.50
1:A:85:PHE:CG	1:B:191:ALA:HB2	2.47	0.50
1:A:210:PHE:HB3	1:A:260:TYR:CD2	2.46	0.50
1:B:102:THR:CG2	1:B:142:THR:HB	2.40	0.50
1:A:209:LYS:CG	1:A:217:PHE:HE1	2.24	0.50
1:A:330:ILE:HD12	1:A:330:ILE:O	2.10	0.50
1:B:196:SER:HB3	1:B:229:PHE:CE2	2.46	0.50
1:A:157:ILE:HD13	1:A:189:LEU:CB	2.41	0.50
1:B:174:ALA:HB2	1:B:184:VAL:HG21	1.93	0.50
1:A:216:ILE:CD1	1:A:216:ILE:N	2.69	0.50
1:A:293:LEU:O	1:A:300:ARG:NH1	2.44	0.50
1:B:124:ALA:CB	1:B:267:THR:HG22	2.42	0.50
1:A:138:THR:CG2	1:A:335:ILE:H	2.25	0.50
1:A:194:TYR:H	1:A:198:HIS:CD2	2.30	0.50
1:A:209:LYS:HG3	1:A:217:PHE:HE1	1.75	0.50
1:A:318:SER:O	1:A:319:PRO:C	2.54	0.50
1:B:249:MET:O	1:B:252:ARG:HB2	2.11	0.50
1:B:167:PRO:HB3	1:B:185:LEU:HD11	1.94	0.49
1:B:192:ARG:HH21	1:B:194:TYR:HE2	1.59	0.49
1:A:196:SER:HB3	1:A:229:PHE:CE2	2.48	0.49
1:B:305:LYS:CD	1:B:311:ARG:HG3	2.42	0.49
1:A:155:LYS:HB2	1:A:217:PHE:CD2	2.48	0.49
1:A:161:THR:HG22	1:A:193:ALA:HB3	1.93	0.49
1:A:226:MET:N	1:A:268:ASN:OD1	2.45	0.49
1:A:229:PHE:CD1	1:A:246:LEU:HD12	2.47	0.49
1:A:291:HIS:HD2	1:A:292:ILE:HG22	1.76	0.49
1:A:117:GLU:HG2	1:A:118:SER:N	2.27	0.49
1:A:142:THR:HA	1:A:145:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HD23	1:B:135:LEU:C	2.37	0.49
1:B:139:LEU:C	1:B:141:VAL:N	2.71	0.49
1:B:205:TYR:O	1:B:205:TYR:CD2	2.66	0.49
1:B:219:LEU:HD23	1:B:219:LEU:C	2.38	0.49
1:A:129:ARG:HA	1:A:129:ARG:NE	2.24	0.49
1:B:127:GLU:CD	1:B:128:PHE:H	2.21	0.49
1:B:165:PHE:HB3	1:B:190:TYR:CZ	2.48	0.49
1:B:169:ARG:O	1:B:172:ASP:HB3	2.13	0.49
1:B:226:MET:HG3	1:B:293:LEU:HD12	1.93	0.49
1:B:247:ALA:CA	1:B:292:ILE:HD11	2.42	0.49
1:A:146:PRO:CG	1:A:152:PRO:O	2.60	0.49
1:B:255:LYS:O	1:B:259:GLU:HB3	2.13	0.49
1:A:141:VAL:HG22	1:A:184:VAL:HG11	1.95	0.49
1:B:132:LYS:HD2	1:B:267:THR:HB	1.94	0.49
1:B:161:THR:HG21	1:B:199:GLN:HE22	1.77	0.49
1:B:244:GLN:C	1:B:244:GLN:OE1	2.55	0.49
1:A:255:LYS:HG2	1:B:194:TYR:CE1	2.48	0.48
1:B:175:ASP:C	1:B:177:PHE:H	2.20	0.48
1:B:95:ARG:HH11	1:B:98:VAL:HG21	1.78	0.48
1:B:112:LEU:HD23	1:B:115:GLY:C	2.38	0.48
1:A:139:LEU:HA	1:A:142:THR:OG1	2.14	0.48
1:B:310:LEU:HD23	1:B:327:THR:CG2	2.43	0.48
1:B:122:THR:O	1:B:266:VAL:HG22	2.13	0.48
1:A:124:ALA:CB	1:A:267:THR:HG22	2.43	0.48
1:A:159:ILE:HA	1:A:191:ALA:O	2.14	0.48
1:A:176:ARG:HD3	1:A:333:GLY:O	2.13	0.48
1:B:157:ILE:HB	1:B:220:LEU:HD23	1.94	0.48
1:B:235:GLY:C	1:B:237:GLY:H	2.21	0.48
1:B:252:ARG:HH11	1:B:252:ARG:CB	2.27	0.48
1:B:180:ASP:HB3	1:B:183:ALA:HB3	1.94	0.48
1:B:200:VAL:O	1:B:202:LEU:N	2.47	0.48
1:A:95:ARG:NH1	1:A:95:ARG:HG2	2.27	0.48
1:A:127:GLU:O	1:A:128:PHE:C	2.57	0.48
1:B:180:ASP:HB3	1:B:183:ALA:HB2	1.96	0.48
1:B:121:ILE:HG22	1:B:297:SER:CB	2.44	0.48
1:B:144:GLN:HE21	1:B:187:ASN:HB3	1.74	0.48
1:B:219:LEU:HD21	1:B:221:ILE:HB	1.95	0.48
1:B:233:PHE:C	1:B:233:PHE:HD2	2.21	0.48
1:B:125:PHE:HB2	1:B:301:ILE:O	2.14	0.47
1:A:200:VAL:HA	1:A:203:LEU:HB2	1.96	0.47
1:A:231:VAL:C	1:A:233:PHE:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:PHE:O	1:A:178:ASN:C	2.57	0.47
1:A:229:PHE:C	1:A:231:VAL:N	2.72	0.47
1:A:291:HIS:CD2	1:A:292:ILE:HG22	2.49	0.47
1:B:219:LEU:HD23	1:B:220:LEU:C	2.40	0.47
1:B:309:GLU:HG3	1:B:310:LEU:HD12	1.95	0.47
1:A:216:ILE:HD13	1:A:217:PHE:N	2.24	0.47
1:A:238:GLU:OE1	1:A:238:GLU:HA	2.14	0.47
1:B:97:MET:O	1:B:99:PHE:HD2	1.97	0.47
1:A:141:VAL:HG12	1:A:145:LEU:CD2	2.36	0.47
1:B:165:PHE:HD1	1:B:190:TYR:CD1	2.33	0.47
1:B:226:MET:O	1:B:228:LEU:N	2.47	0.47
1:A:166:ARG:O	1:A:167:PRO:C	2.58	0.47
1:B:224:SER:HB2	1:B:267:THR:O	2.14	0.47
1:A:85:PHE:CB	1:B:191:ALA:HB2	2.45	0.47
1:A:118:SER:HA	1:A:262:VAL:O	2.15	0.47
1:A:112:LEU:HD11	1:A:301:ILE:HD11	1.96	0.47
1:A:309:GLU:HB3	1:A:310:LEU:HD12	1.95	0.47
1:B:121:ILE:HD11	1:B:253:LEU:HD22	1.97	0.47
1:A:132:LYS:HZ3	1:A:269:GLN:HG3	1.79	0.47
1:A:252:ARG:NH1	1:A:252:ARG:HB3	2.30	0.47
1:A:127:GLU:N	1:A:130:THR:OG1	2.44	0.46
1:A:176:ARG:NH2	1:A:177:PHE:CZ	2.81	0.46
1:A:340:GLU:OXT	1:A:340:GLU:HG2	2.15	0.46
1:B:158:PHE:HA	1:B:221:ILE:HG23	1.96	0.46
1:A:118:SER:O	1:A:119:MET:C	2.58	0.46
1:A:269:GLN:H	1:A:270:MET:CE	2.28	0.46
1:B:234:SER:HB2	1:B:238:GLU:HB2	1.94	0.46
1:A:95:ARG:C	1:A:97:MET:H	2.24	0.46
1:A:170:LEU:C	1:A:172:ASP:N	2.73	0.46
1:A:249:MET:HA	1:A:252:ARG:HB2	1.97	0.46
1:B:226:MET:SD	1:B:246:LEU:HD21	2.55	0.46
1:A:225:ILE:HG23	1:A:268:ASN:OD1	2.16	0.46
1:B:165:PHE:CD1	1:B:190:TYR:CD1	3.03	0.46
1:A:321:MET:O	1:A:321:MET:HG3	2.14	0.46
1:B:216:ILE:HG12	1:B:217:PHE:N	2.30	0.46
1:A:205:TYR:O	1:A:206:VAL:C	2.57	0.46
1:B:130:THR:HA	1:B:311:ARG:CZ	2.44	0.46
1:B:174:ALA:HB1	1:B:179:VAL:HB	1.97	0.46
1:B:163:ASN:O	1:B:163:ASN:CG	2.59	0.46
1:B:173:ILE:C	1:B:175:ASP:N	2.74	0.46
1:B:220:LEU:O	1:B:264:VAL:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HB	1:B:297:SER:HA	1.98	0.46
1:B:231:VAL:O	1:B:233:PHE:N	2.49	0.46
1:B:314:LYS:HG2	1:B:315:ILE:H	1.80	0.46
1:A:88:ALA:CB	1:B:188:VAL:HB	2.46	0.45
1:B:202:LEU:O	1:B:203:LEU:C	2.59	0.45
1:B:211:HIS:HB2	1:B:260:TYR:OH	2.16	0.45
1:A:86:LEU:HD12	1:A:90:GLU:HB3	1.96	0.45
1:A:155:LYS:O	1:A:217:PHE:HA	2.16	0.45
1:A:131:GLY:N	1:A:311:ARG:CZ	2.78	0.45
1:B:175:ASP:OD1	1:B:181:HIS:HE1	1.99	0.45
1:A:249:MET:O	1:A:253:LEU:N	2.50	0.45
1:A:195:THR:C	1:A:197:GLU:N	2.73	0.45
1:B:176:ARG:NE	1:B:177:PHE:HE1	2.14	0.45
1:B:216:ILE:CD1	1:B:217:PHE:H	2.30	0.45
1:A:100:HIS:N	1:A:100:HIS:CD2	2.83	0.45
1:B:291:HIS:HD2	1:B:292:ILE:HG22	1.80	0.45
1:A:219:LEU:HD23	1:A:263:ALA:O	2.16	0.45
1:A:295:HIS:ND1	1:A:295:HIS:C	2.73	0.45
1:A:305:LYS:HD3	1:A:310:LEU:O	2.16	0.45
1:B:127:GLU:N	1:B:130:THR:OG1	2.50	0.45
1:B:141:VAL:O	1:B:143:ALA:N	2.50	0.45
1:B:195:THR:C	1:B:197:GLU:H	2.25	0.45
1:B:228:LEU:O	1:B:228:LEU:CD2	2.64	0.45
1:A:167:PRO:O	1:A:170:LEU:HB2	2.17	0.45
1:B:138:THR:OG1	1:B:335:ILE:HD13	2.17	0.45
1:A:120:ALA:N	1:A:257:SER:OG	2.50	0.44
1:B:131:GLY:N	1:B:311:ARG:CZ	2.75	0.44
1:B:176:ARG:NH2	1:B:177:PHE:CE1	2.79	0.44
1:B:86:LEU:H	1:B:86:LEU:CD2	2.27	0.44
1:A:299:THR:HA	1:A:318:SER:OG	2.17	0.44
1:A:225:ILE:CG2	1:A:268:ASN:OD1	2.65	0.44
1:A:291:HIS:O	1:A:292:ILE:C	2.59	0.44
1:A:112:LEU:HD22	1:A:112:LEU:H	1.81	0.44
1:A:169:ARG:HG3	1:A:169:ARG:NH1	2.32	0.44
1:A:200:VAL:O	1:A:201:GLU:C	2.60	0.44
1:A:112:LEU:HD13	1:A:112:LEU:N	2.33	0.44
1:B:140:CYS:O	1:B:144:GLN:NE2	2.51	0.44
1:B:202:LEU:O	1:B:205:TYR:HB3	2.17	0.44
1:A:135:LEU:CD2	1:A:139:LEU:HG	2.47	0.44
1:A:313:ALA:HB2	1:A:328:PHE:HE2	1.81	0.44
1:A:105:SER:OG	1:A:108:PHE:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ARG:NH1	1:A:335:ILE:O	2.49	0.44
1:A:200:VAL:CG1	1:A:249:MET:HB2	2.47	0.44
1:A:222:ILE:O	1:A:266:VAL:HA	2.18	0.44
1:A:258:GLU:OE2	1:B:192:ARG:NE	2.48	0.44
1:B:121:ILE:HG12	1:B:264:VAL:CG2	2.48	0.44
1:A:203:LEU:CD2	1:A:222:ILE:HD11	2.43	0.44
1:A:234:SER:HB2	1:A:238:GLU:HB2	1.94	0.44
1:B:194:TYR:N	1:B:198:HIS:HD2	2.14	0.44
1:B:225:ILE:HG13	1:B:249:MET:HE1	2.00	0.44
1:A:105:SER:O	1:A:108:PHE:N	2.50	0.43
1:A:159:ILE:HD12	1:A:222:ILE:HD11	2.00	0.43
1:A:92:SER:HB2	1:B:167:PRO:HB2	1.99	0.43
1:A:108:PHE:CE2	1:A:301:ILE:HD13	2.53	0.43
1:A:162:GLU:O	1:A:163:ASN:HB3	2.19	0.43
1:A:216:ILE:CG1	1:A:217:PHE:N	2.80	0.43
1:A:318:SER:O	1:A:321:MET:HB3	2.17	0.43
1:B:133:THR:O	1:B:137:HIS:ND1	2.51	0.43
1:B:192:ARG:NH2	1:B:194:TYR:HE2	2.16	0.43
1:A:170:LEU:C	1:A:172:ASP:H	2.26	0.43
1:B:183:ALA:O	1:B:184:VAL:C	2.62	0.43
1:B:216:ILE:CG1	1:B:217:PHE:N	2.82	0.43
1:A:194:TYR:H	1:A:198:HIS:HD2	1.67	0.43
1:A:291:HIS:O	1:A:294:ALA:N	2.52	0.43
1:B:199:GLN:HG2	1:B:249:MET:HE3	2.00	0.43
1:A:174:ALA:HB1	1:A:184:VAL:HG21	1.98	0.43
1:A:91:TYR:C	1:A:93:GLU:N	2.77	0.42
1:A:123:GLU:OE2	1:A:125:PHE:HE1	2.02	0.42
1:A:135:LEU:HD23	1:A:139:LEU:HG	2.01	0.42
1:B:226:MET:HG3	1:B:270:MET:SD	2.58	0.42
1:A:161:THR:OG1	1:A:162:GLU:N	2.51	0.42
1:A:205:TYR:C	1:A:205:TYR:CD2	2.96	0.42
1:A:249:MET:C	1:A:251:SER:N	2.72	0.42
1:B:256:ILE:O	1:B:257:SER:C	2.63	0.42
1:B:195:THR:C	1:B:197:GLU:N	2.76	0.42
1:B:203:LEU:CA	1:B:206:VAL:HG23	2.48	0.42
1:B:300:ARG:HH21	1:B:316:TYR:HE2	1.67	0.42
1:A:102:THR:HG1	1:A:109:ASP:CG	2.28	0.42
1:A:194:TYR:C	1:A:228:LEU:HD11	2.44	0.42
1:A:196:SER:OG	1:A:228:LEU:HD23	2.19	0.42
1:B:95:ARG:C	1:B:97:MET:N	2.77	0.42
1:B:205:TYR:O	1:B:205:TYR:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:NH1	1:B:252:ARG:CB	2.82	0.42
1:B:299:THR:HG23	1:B:318:SER:OG	2.20	0.42
1:A:144:GLN:C	1:A:145:LEU:HD13	2.45	0.42
1:A:312:ILE:HA	1:A:326:ALA:O	2.19	0.42
1:B:199:GLN:HE21	1:B:199:GLN:HB2	1.55	0.42
1:A:105:SER:O	1:A:106:GLN:C	2.61	0.42
1:A:151:TYR:CZ	1:A:153:GLY:HA2	2.55	0.42
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.22	0.42
1:A:200:VAL:HG13	1:A:249:MET:HG3	2.02	0.42
1:A:226:MET:O	1:A:227:ALA:C	2.62	0.42
1:B:129:ARG:HE	1:B:129:ARG:CA	2.28	0.42
1:B:221:ILE:HD13	1:B:265:PHE:HD2	1.84	0.42
1:B:321:MET:HA	1:B:322:PRO:HD3	1.83	0.42
1:A:123:GLU:HA	1:A:266:VAL:O	2.19	0.42
1:A:145:LEU:O	1:A:146:PRO:C	2.62	0.42
1:B:163:ASN:HB2	1:B:192:ARG:NH1	2.35	0.42
1:A:216:ILE:HG12	1:A:217:PHE:N	2.35	0.41
1:A:259:GLU:HG2	1:A:260:TYR:CD1	2.55	0.41
1:B:130:THR:HG23	1:B:311:ARG:NH1	2.35	0.41
1:A:83:PRO:C	1:A:85:PHE:H	2.27	0.41
1:A:290:GLY:HA3	1:B:230:ARG:NH2	2.35	0.41
1:B:125:PHE:HB2	1:B:302:SER:HA	2.01	0.41
1:B:156:ILE:O	1:B:189:LEU:HB2	2.21	0.41
1:B:140:CYS:HA	1:B:156:ILE:HD12	2.01	0.41
1:B:167:PRO:O	1:B:170:LEU:N	2.50	0.41
1:A:120:ALA:HB1	1:A:298:THR:OG1	2.20	0.41
1:B:109:ASP:O	1:B:113:GLY:N	2.54	0.41
1:B:226:MET:CB	1:B:270:MET:SD	3.08	0.41
1:B:146:PRO:HA	1:B:151:TYR:O	2.19	0.41
1:A:135:LEU:O	1:A:136:SER:C	2.64	0.41
1:A:173:ILE:C	1:A:175:ASP:N	2.77	0.41
1:A:205:TYR:O	1:A:208:ALA:N	2.53	0.41
1:A:238:GLU:C	1:A:240:ALA:N	2.74	0.41
1:B:234:SER:C	1:B:235:GLY:O	2.63	0.41
1:A:125:PHE:CB	1:A:302:SER:HA	2.51	0.41
1:A:335:ILE:N	1:A:335:ILE:HD12	2.36	0.41
1:B:146:PRO:CA	1:B:152:PRO:O	2.68	0.41
1:B:192:ARG:HG2	1:B:192:ARG:NH1	2.31	0.41
1:A:220:LEU:HB3	1:A:264:VAL:CG1	2.45	0.41
1:A:226:MET:HE2	1:A:270:MET:HG2	2.02	0.41
1:A:226:MET:HE3	1:A:270:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:C	1:A:228:LEU:CD2	2.90	0.41
1:B:173:ILE:O	1:B:174:ALA:C	2.64	0.41
1:B:247:ALA:HA	1:B:250:LEU:HB2	2.02	0.41
1:B:305:LYS:HG2	1:B:311:ARG:CZ	2.51	0.41
1:A:219:LEU:C	1:A:219:LEU:CD2	2.94	0.41
1:B:177:PHE:O	1:B:179:VAL:HG23	2.21	0.41
1:B:340:GLU:OXT	1:B:340:GLU:HG2	2.21	0.41
1:A:210:PHE:CE2	1:A:262:VAL:HG11	2.55	0.40
1:A:225:ILE:O	1:A:226:MET:C	2.64	0.40
1:A:293:LEU:HD22	1:A:293:LEU:O	2.21	0.40
1:B:170:LEU:C	1:B:172:ASP:N	2.77	0.40
1:A:108:PHE:CE2	1:A:112:LEU:HD21	2.56	0.40
1:A:185:LEU:N	1:A:185:LEU:CD2	2.85	0.40
1:A:207:ALA:O	1:A:210:PHE:N	2.52	0.40
1:A:231:VAL:HG12	1:A:232:ASP:OD1	2.21	0.40
1:B:184:VAL:O	1:B:187:ASN:CB	2.69	0.40
1:B:161:THR:HG22	1:B:193:ALA:HB3	2.03	0.40
1:B:219:LEU:C	1:B:219:LEU:CD2	2.94	0.40
1:A:206:VAL:O	1:A:207:ALA:C	2.64	0.40
1:A:112:LEU:CB	1:A:115:GLY:O	2.70	0.40
1:B:95:ARG:HA	1:B:98:VAL:HG23	2.03	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	235/343 (68%)	184 (78%)	36 (15%)	15 (6%)	1	11
1	B	235/343 (68%)	188 (80%)	36 (15%)	11 (5%)	2	17
All	All	470/686 (68%)	372 (79%)	72 (15%)	26 (6%)	1	13

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
1	A	226	MET
1	A	227	ALA
1	B	227	ALA
1	A	95	ARG
1	A	163	ASN
1	A	292	ILE
1	A	307	ARG
1	B	148	ALA
1	B	231	VAL
1	B	232	ASP
1	B	308	GLY
1	A	212	GLU
1	A	232	ASP
1	A	261	ASN
1	A	308	GLY
1	B	142	THR
1	B	152	PRO
1	B	257	SER
1	B	261	ASN
1	A	152	PRO
1	B	102	THR
1	A	262	VAL
1	A	319	PRO
1	A	178	ASN
1	B	262	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	195/282 (69%)	163 (84%)	32 (16%)	2	14
1	B	195/282 (69%)	172 (88%)	23 (12%)	5	23
All	All	390/564 (69%)	335 (86%)	55 (14%)	3	18

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ARG
1	A	100	HIS
1	A	112	LEU
1	A	138	THR
1	A	145	LEU
1	A	167	PRO
1	A	168	ASP
1	A	169	ARG
1	A	172	ASP
1	A	189	LEU
1	A	192	ARG
1	A	199	GLN
1	A	200	VAL
1	A	203	LEU
1	A	216	ILE
1	A	219	LEU
1	A	220	LEU
1	A	222	ILE
1	A	223	ASP
1	A	230	ARG
1	A	233	PHE
1	A	244	GLN
1	A	249	MET
1	A	250	LEU
1	A	262	VAL
1	A	270	MET
1	A	292	ILE
1	A	293	LEU
1	A	295	HIS
1	A	305	LYS
1	A	310	LEU
1	A	330	ILE
1	B	87	THR
1	B	112	LEU
1	B	125	PHE
1	B	128	PHE
1	B	168	ASP
1	B	169	ARG
1	B	187	ASN
1	B	189	LEU
1	B	199	GLN
1	B	203	LEU

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Mol	Chain	Res	Type
1	B	216	ILE
1	B	223	ASP
1	B	233	PHE
1	B	241	GLU
1	B	244	GLN
1	B	249	MET
1	B	253	LEU
1	B	270	MET
1	B	292	ILE
1	B	293	LEU
1	B	295	HIS
1	B	310	LEU
1	B	330	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	181	HIS
1	A	187	ASN
1	A	198	HIS
1	A	254	GLN
1	A	291	HIS
1	B	100	HIS
1	B	163	ASN
1	B	181	HIS
1	B	187	ASN
1	B	198	HIS
1	B	244	GLN
1	B	268	ASN
1	B	291	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	239/343 (69%)	0.16	3 (1%)	75 50	32, 111, 173, 195	0
1	B	239/343 (69%)	0.12	4 (1%)	69 43	76, 119, 182, 198	0
All	All	478/686 (69%)	0.14	7 (1%)	72 47	32, 114, 176, 198	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	GLU	3.3
1	B	317	ASP	2.9
1	B	231	VAL	2.5
1	A	310	LEU	2.5
1	A	319	PRO	2.1
1	B	133	THR	2.1
1	B	244	GLN	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.