



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:15 AM UTC

PDB ID : 3OW7 / pdb_00003ow7
Title : Crystal structure of the membrane fusion protein CusB from Escherichia coli.
Authors : Su, C.-C.
Deposited on : 2010-09-17
Resolution : 3.78 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

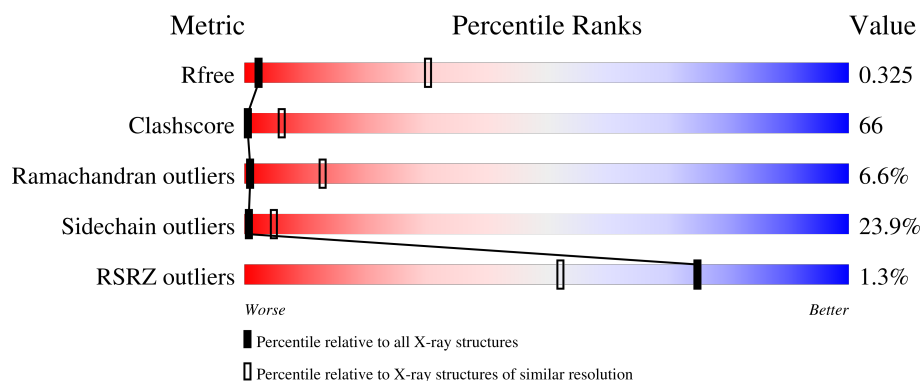
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 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 (3.94-3.62)
Clashscore	190562	1029 (3.92-3.64)
Ramachandran outliers	187476	1064 (3.94-3.62)
Sidechain outliers	187428	1059 (3.94-3.62)
RSRZ outliers	180081	1084 (3.94-3.62)

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	413	22%35%14%•28%
1	B	413	20%38%13%•28%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4545 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 Cation efflux system protein cusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2267	1444	391	427	5			
1	B	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	HIS	-	expression tag	UNP P77239
A	409	HIS	-	expression tag	UNP P77239
A	410	HIS	-	expression tag	UNP P77239
A	411	HIS	-	expression tag	UNP P77239
A	412	HIS	-	expression tag	UNP P77239
A	413	HIS	-	expression tag	UNP P77239
B	408	HIS	-	expression tag	UNP P77239
B	409	HIS	-	expression tag	UNP P77239
B	410	HIS	-	expression tag	UNP P77239
B	411	HIS	-	expression tag	UNP P77239
B	412	HIS	-	expression tag	UNP P77239
B	413	HIS	-	expression tag	UNP P77239

- Molecule 2 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	84.24Å 111.01Å 258.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.63 – 3.78 36.63 – 3.78	Depositor EDS
% Data completeness (in resolution range)	82.8 (36.63-3.78) 95.1 (36.63-3.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.66Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.280 , 0.324 0.288 , 0.325	Depositor DCC
R_{free} test set	588 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	148.8	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 223.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4545	wwPDB-VP
Average B, all atoms (Å ²)	227.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CU1

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	0.51	0/2306	1.02	10/3142 (0.3%)
1	B	0.48	1/2313 (0.0%)	1.01	16/3152 (0.5%)
All	All	0.50	1/4619 (0.0%)	1.01	26/6294 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	ASP	C-N	-5.70	1.25	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	LYS	N-CA-C	11.09	126.71	111.74
1	A	252	GLU	N-CA-C	9.16	121.26	111.28
1	A	251	PRO	N-CA-C	-7.71	98.13	111.32
1	B	110	PHE	CA-C-N	7.47	127.75	119.90
1	B	110	PHE	C-N-CA	7.47	127.75	119.90
1	A	257	LEU	N-CA-C	6.89	118.79	111.28
1	B	335	THR	N-CA-C	-6.73	104.20	114.16
1	B	142	ASP	N-CA-C	6.67	119.91	110.23
1	B	308	LYS	CA-C-N	6.64	128.14	119.84
1	B	308	LYS	C-N-CA	6.64	128.14	119.84
1	B	217	VAL	N-CA-C	6.63	118.02	108.48
1	A	245	TRP	N-CA-C	6.28	118.64	108.41
1	A	257	LEU	CA-C-N	6.06	129.62	120.77
1	A	257	LEU	C-N-CA	6.06	129.62	120.77
1	B	141	GLY	N-CA-C	5.62	119.47	112.73
1	B	215	ASP	CA-C-N	5.47	132.12	121.41
1	B	215	ASP	C-N-CA	5.47	132.12	121.41
1	B	300	VAL	N-CA-C	5.40	115.73	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	ALA	N-CA-C	5.37	117.13	111.28
1	A	333	ILE	N-CA-C	5.33	114.88	108.06
1	A	190	MET	N-CA-C	5.23	117.01	109.48
1	B	155	ILE	CA-C-N	5.18	126.31	119.84
1	B	155	ILE	C-N-CA	5.18	126.31	119.84
1	B	333	ILE	N-CA-C	5.15	115.54	108.12
1	A	337	SER	N-CA-C	-5.15	106.77	113.16
1	B	231	LYS	N-CA-C	5.14	115.61	108.00

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	2267	0	2336	347	0
1	B	2274	0	2342	278	0
2	A	2	0	0	1	0
2	B	2	0	0	0	0
All	All	4545	0	4678	612	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 66.

All (612) 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:250:ILE:CG2	1:A:255:ALA:HB2	1.57	1.34
1:A:256:TRP:CH2	1:A:257:LEU:HD22	1.64	1.32
1:A:251:PRO:HG2	1:A:254:ILE:CG2	1.66	1.23
1:A:256:TRP:CZ3	1:A:257:LEU:HD22	1.75	1.20
1:A:257:LEU:O	1:A:259:LYS:HD3	1.42	1.19
1:A:368:ARG:HA	1:A:368:ARG:NE	1.52	1.18
1:A:256:TRP:CH2	1:A:257:LEU:CD2	2.30	1.15
1:A:256:TRP:CZ2	1:A:257:LEU:CD2	2.30	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLN:HG2	1:B:240:GLY:HA3	1.27	1.14
1:B:146:LYS:HD3	1:B:147:GLY:H	1.04	1.13
1:A:148:THR:HB	1:A:149:PRO:HD3	1.31	1.13
1:A:228:ASN:C	1:A:229:ILE:HD12	1.74	1.11
1:A:251:PRO:CG	1:A:254:ILE:CG2	2.30	1.08
1:A:250:ILE:HG23	1:A:251:PRO:HD2	1.28	1.08
1:A:251:PRO:HG2	1:A:254:ILE:HG22	1.29	1.07
1:A:250:ILE:HG21	1:A:255:ALA:CB	1.83	1.07
1:B:132:ILE:HB	1:B:226:GLY:HA2	1.35	1.04
1:A:250:ILE:HG21	1:A:255:ALA:HB2	1.05	1.04
1:B:241:MET:HE3	1:B:305:GLU:HG3	1.39	1.04
1:A:251:PRO:HD2	1:A:254:ILE:CG2	1.87	1.04
1:A:251:PRO:CG	1:A:254:ILE:HG21	1.89	1.03
1:A:251:PRO:CD	1:A:254:ILE:CG2	2.38	1.01
1:A:256:TRP:CZ2	1:A:257:LEU:HD22	1.89	1.01
1:B:154:THR:HG22	1:B:207:ARG:HB3	1.41	1.00
1:B:331:ALA:O	1:B:341:VAL:HG11	1.61	0.99
1:A:136:TYR:HB3	1:A:138:LEU:HD21	1.44	0.98
1:B:341:VAL:HG12	1:B:342:ILE:H	1.23	0.98
1:A:368:ARG:HA	1:A:368:ARG:CZ	1.93	0.98
1:B:258:VAL:HG13	1:B:259:LYS:H	1.26	0.98
1:B:146:LYS:HD3	1:B:147:GLY:N	1.79	0.97
1:A:235:VAL:HG22	1:A:235:VAL:O	1.61	0.97
1:B:166:LEU:HD21	1:B:202:GLN:NE2	1.82	0.95
1:A:256:TRP:CZ2	1:A:257:LEU:HD21	2.02	0.93
1:A:129:ALA:CB	1:A:230:ALA:HA	1.99	0.93
1:A:251:PRO:CG	1:A:254:ILE:HG22	1.94	0.92
1:B:241:MET:CE	1:B:305:GLU:HG3	1.99	0.92
1:A:231:LYS:O	1:A:232:ASP:HB2	1.66	0.92
1:A:246:VAL:HG22	1:A:298:LEU:HB2	1.51	0.92
1:A:106:PHE:CD2	1:B:253:SER:HA	2.04	0.92
1:A:368:ARG:NE	1:A:368:ARG:CA	2.29	0.90
1:B:205:GLN:HA	1:B:205:GLN:OE1	1.70	0.90
1:A:256:TRP:CE3	1:A:257:LEU:HA	2.07	0.90
1:A:229:ILE:HD12	1:A:229:ILE:N	1.84	0.89
1:B:331:ALA:O	1:B:341:VAL:CG1	2.20	0.89
1:A:221:PHE:O	1:A:222:ASP:HB3	1.72	0.89
1:A:229:ILE:N	1:A:229:ILE:CD1	2.34	0.89
1:B:142:ASP:O	1:B:218:ILE:CD1	2.21	0.88
1:A:284:LEU:HD21	1:A:297:ARG:HD2	1.52	0.87
1:A:132:ILE:HG23	1:A:227:MET:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:PHE:HD2	1:A:368:ARG:NE	1.72	0.87
1:A:250:ILE:HG22	1:A:255:ALA:HB2	1.53	0.86
1:A:256:TRP:CE3	1:A:256:TRP:C	2.53	0.86
1:A:256:TRP:CE3	1:A:257:LEU:HD22	2.09	0.86
1:A:235:VAL:O	1:A:236:ALA:CB	2.20	0.86
1:B:368:ARG:HE	1:B:368:ARG:HA	1.40	0.86
1:B:192:GLU:O	1:B:196:ARG:HG3	1.76	0.85
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.58	0.85
1:A:153:LEU:HD21	1:A:208:PHE:HD1	1.41	0.85
1:A:250:ILE:O	1:A:293:THR:HA	1.76	0.85
1:A:251:PRO:CD	1:A:254:ILE:HG21	2.05	0.85
1:A:332:LEU:HA	1:A:341:VAL:CG1	2.07	0.84
1:B:344:VAL:HG12	1:B:346:ALA:H	1.41	0.84
1:A:129:ALA:HB2	1:A:230:ALA:HA	1.59	0.83
1:A:368:ARG:HA	1:A:368:ARG:HE	1.43	0.83
1:B:305:GLU:O	1:B:305:GLU:HG2	1.78	0.83
1:A:256:TRP:CZ3	1:A:257:LEU:HA	2.14	0.83
1:B:340:ARG:HB3	1:B:353:LYS:O	1.79	0.82
1:A:153:LEU:HD23	1:A:155:ILE:HG13	1.61	0.82
1:B:132:ILE:HD11	1:B:229:ILE:HD11	1.61	0.82
1:A:219:THR:HG23	1:A:237:LYS:HB3	1.61	0.82
1:A:256:TRP:CE2	1:A:257:LEU:HD22	2.15	0.81
1:A:250:ILE:CG2	1:A:251:PRO:HD2	2.10	0.81
1:A:358:PHE:CD2	1:A:368:ARG:NE	2.49	0.81
1:A:250:ILE:HG23	1:A:251:PRO:CD	2.10	0.81
1:B:340:ARG:HG2	1:B:354:ARG:HA	1.61	0.81
1:A:256:TRP:CE2	1:A:257:LEU:CD2	2.64	0.80
1:B:120:GLN:HG2	1:B:240:GLY:CA	2.09	0.80
1:A:165:TYR:HB2	1:A:181:ILE:HG21	1.62	0.80
1:B:252:GLU:OE1	1:B:292:ARG:HB3	1.82	0.80
1:B:142:ASP:O	1:B:218:ILE:HD13	1.83	0.79
1:A:90:GLN:HG2	1:A:383:PHE:CE1	2.17	0.79
1:B:144:VAL:O	1:B:144:VAL:CG2	2.30	0.79
1:A:308:LYS:HB3	1:A:309:PRO:CD	2.13	0.79
1:A:136:TYR:HB3	1:A:138:LEU:CD2	2.12	0.78
1:A:166:LEU:HD12	1:A:204:ILE:HG13	1.65	0.78
1:B:162:GLN:HE21	1:B:185:LEU:HD21	1.46	0.78
1:A:153:LEU:HD21	1:A:208:PHE:CD1	2.19	0.78
1:A:147:GLY:HA3	1:A:212:ALA:O	1.83	0.78
1:A:340:ARG:HB2	1:A:353:LYS:O	1.84	0.76
1:B:223:LEU:HD23	1:B:223:LEU:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD11	1:A:208:PHE:HB2	1.67	0.76
1:A:242:ASP:HB3	1:A:243:PRO:HD3	1.67	0.76
1:B:327:ILE:HD12	1:B:328:PRO:O	1.86	0.76
1:A:148:THR:HB	1:A:149:PRO:CD	2.14	0.75
1:B:148:THR:HB	1:B:149:PRO:HD2	1.66	0.75
1:B:150:LEU:HD11	1:B:212:ALA:HB2	1.66	0.75
1:A:219:THR:HG21	1:A:239:GLN:HG2	1.66	0.75
1:B:120:GLN:CG	1:B:240:GLY:HA3	2.14	0.75
1:A:244:VAL:HG11	1:A:307:LEU:HG	1.68	0.75
1:A:108:GLN:O	1:A:316:GLN:HA	1.87	0.75
1:A:255:ALA:O	1:A:258:VAL:HG23	1.86	0.74
1:A:256:TRP:C	1:A:256:TRP:HE3	1.93	0.74
1:A:251:PRO:HD2	1:A:254:ILE:HG22	1.69	0.74
1:A:190:MET:SD	2:A:414:CU1:CU	1.76	0.74
1:B:339:GLN:HE21	1:B:339:GLN:HA	1.51	0.73
1:B:144:VAL:O	1:B:144:VAL:HG23	1.86	0.73
1:A:256:TRP:CE3	1:A:257:LEU:N	2.56	0.73
1:A:319:THR:HG22	1:A:320:ALA:H	1.52	0.73
1:B:270:ALA:C	1:B:271:ARG:HG3	2.13	0.73
1:B:142:ASP:O	1:B:218:ILE:HD12	1.88	0.73
1:B:334:ASP:HB2	1:B:338:GLU:O	1.89	0.73
1:A:103:PRO:HB3	1:A:321:SER:O	1.89	0.73
1:A:165:TYR:HE2	1:A:178:THR:HG1	1.36	0.72
1:A:129:ALA:CA	1:A:230:ALA:HA	2.19	0.72
1:A:235:VAL:O	1:A:235:VAL:CG2	2.35	0.72
1:A:251:PRO:HG2	1:A:254:ILE:HG21	1.53	0.72
1:A:284:LEU:HD21	1:A:297:ARG:CD	2.20	0.72
1:A:131:PHE:CZ	1:A:228:ASN:OD1	2.43	0.71
1:A:148:THR:CB	1:A:149:PRO:HD3	2.16	0.71
1:B:152:ASP:C	1:B:153:LEU:HD13	2.15	0.71
1:B:223:LEU:HD23	1:B:223:LEU:N	2.05	0.71
1:A:285:PRO:HG2	1:B:357:VAL:HG23	1.72	0.71
1:A:228:ASN:C	1:A:229:ILE:CD1	2.59	0.71
1:A:235:VAL:O	1:A:236:ALA:HB2	1.89	0.71
1:B:198:LEU:O	1:B:202:GLN:HA	1.89	0.71
1:B:92:LEU:HD22	1:B:92:LEU:H	1.54	0.71
1:B:122:ALA:HB3	1:B:214:ILE:HD12	1.71	0.71
1:A:256:TRP:CD2	1:A:257:LEU:HD22	2.26	0.70
1:B:146:LYS:CD	1:B:147:GLY:H	1.95	0.70
1:B:368:ARG:HA	1:B:368:ARG:NE	2.04	0.70
1:A:158:TRP:O	1:A:162:GLN:HG2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LYS:NZ	1:B:241:MET:HE1	2.06	0.70
1:A:153:LEU:CD1	1:A:208:PHE:HB2	2.22	0.70
1:A:131:PHE:CE2	1:A:228:ASN:OD1	2.44	0.70
1:B:135:VAL:HG21	1:B:224:ARG:HA	1.74	0.69
1:B:377:VAL:HG22	1:B:378:VAL:H	1.58	0.69
1:A:162:GLN:HE22	1:A:190:MET:HE1	1.56	0.69
1:A:256:TRP:HE3	1:A:256:TRP:O	1.76	0.69
1:B:214:ILE:HD11	1:B:238:ILE:HB	1.74	0.69
1:A:129:ALA:HA	1:A:230:ALA:HA	1.74	0.69
1:A:256:TRP:CE3	1:A:257:LEU:CA	2.76	0.69
1:B:302:ASN:ND2	1:B:307:LEU:HG	2.08	0.68
1:B:340:ARG:CG	1:B:354:ARG:HA	2.22	0.68
1:B:166:LEU:HD21	1:B:202:GLN:HE22	1.57	0.68
1:A:251:PRO:CD	1:A:254:ILE:HG22	2.13	0.68
1:B:132:ILE:HG13	1:B:227:MET:H	1.59	0.68
1:B:278:ILE:HD12	1:B:298:LEU:HD21	1.75	0.68
1:B:343:THR:HB	1:B:351:VAL:HG13	1.75	0.68
1:A:129:ALA:HB2	1:A:230:ALA:CA	2.24	0.68
1:A:227:MET:O	1:A:229:ILE:HD13	1.94	0.68
1:B:308:LYS:H	1:B:311:MET:HE3	1.58	0.68
1:B:228:ASN:C	1:B:229:ILE:HD12	2.19	0.67
1:A:219:THR:CG2	1:A:239:GLN:HG2	2.23	0.67
1:A:284:LEU:N	1:A:284:LEU:HD22	2.09	0.67
1:A:296:LEU:HD23	1:A:296:LEU:O	1.95	0.67
1:A:368:ARG:CA	1:A:368:ARG:HE	1.97	0.67
1:B:250:ILE:O	1:B:293:THR:HA	1.93	0.67
1:B:258:VAL:HG13	1:B:259:LYS:N	2.04	0.67
1:B:121:TYR:CZ	1:B:237:LYS:HD2	2.30	0.66
1:A:257:LEU:O	1:A:259:LYS:CD	2.34	0.66
1:A:153:LEU:C	1:A:153:LEU:HD22	2.21	0.66
1:B:377:VAL:HG22	1:B:378:VAL:N	2.11	0.66
1:B:95:LYS:HB2	1:B:380:SER:HB2	1.78	0.65
1:B:339:GLN:C	1:B:340:ARG:HG3	2.21	0.65
1:A:167:LEU:HD12	1:A:167:LEU:C	2.21	0.65
1:B:142:ASP:OD1	1:B:142:ASP:N	2.30	0.65
1:A:166:LEU:CD1	1:A:204:ILE:HG13	2.26	0.65
1:A:149:PRO:C	1:A:150:LEU:HD12	2.21	0.65
1:A:358:PHE:HD2	1:A:368:ARG:CD	2.10	0.65
1:B:358:PHE:HB2	1:B:368:ARG:HB2	1.80	0.64
1:A:107:ALA:O	1:A:108:GLN:HG3	1.97	0.64
1:A:132:ILE:CG2	1:A:227:MET:H	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:HB	1:A:177:GLN:HE21	1.61	0.64
1:A:94:VAL:HG13	1:A:381:GLY:HA3	1.78	0.64
1:A:235:VAL:O	1:A:236:ALA:HB3	1.97	0.64
1:A:129:ALA:HA	1:A:229:ILE:O	1.98	0.64
1:B:347:ASP:HB2	1:B:349:ARG:CD	2.27	0.64
1:A:256:TRP:CH2	1:A:257:LEU:HD21	2.22	0.64
1:A:165:TYR:HE2	1:A:178:THR:OG1	1.81	0.64
1:A:167:LEU:O	1:A:171:THR:HG23	1.98	0.64
1:A:218:ILE:HD12	1:A:218:ILE:H	1.62	0.63
1:A:91:ASN:ND2	1:A:93:GLY:H	1.97	0.63
1:B:117:ASN:OD1	1:B:117:ASN:N	2.27	0.63
1:A:347:ASP:O	1:A:349:ARG:HG2	1.99	0.63
1:B:341:VAL:HG12	1:B:342:ILE:N	2.04	0.63
1:A:153:LEU:HD13	1:A:153:LEU:H	1.64	0.63
1:B:132:ILE:CG1	1:B:227:MET:H	2.11	0.63
1:B:298:LEU:HD23	1:B:299:GLU:H	1.63	0.63
1:A:251:PRO:CD	1:A:251:PRO:O	2.47	0.62
1:A:174:THR:HG22	1:A:176:THR:H	1.64	0.62
1:A:307:LEU:HD12	1:A:308:LYS:O	1.99	0.62
1:A:119:TYR:CE1	1:A:245:TRP:HH2	2.16	0.62
1:A:332:LEU:HA	1:A:341:VAL:HG11	1.80	0.62
1:B:355:VAL:HG11	1:B:371:LEU:HG	1.81	0.62
1:B:278:ILE:CG1	1:B:298:LEU:HD21	2.30	0.61
1:B:332:LEU:HA	1:B:341:VAL:CG2	2.30	0.61
1:A:129:ALA:CB	1:A:230:ALA:CA	2.76	0.61
1:A:321:SER:HA	1:B:256:TRP:CE2	2.35	0.61
1:A:284:LEU:HD23	1:A:295:GLN:HB3	1.82	0.61
1:A:307:LEU:HD12	1:A:307:LEU:C	2.24	0.61
1:B:214:ILE:HD13	1:B:214:ILE:H	1.64	0.61
1:A:250:ILE:CG2	1:A:255:ALA:CB	2.52	0.61
1:A:250:ILE:HG22	1:A:251:PRO:O	2.00	0.61
1:A:256:TRP:CZ3	1:A:257:LEU:CD2	2.67	0.61
1:A:307:LEU:HD12	1:A:308:LYS:N	2.14	0.61
1:A:253:SER:HA	1:B:106:PHE:CE2	2.36	0.61
1:A:253:SER:HB3	1:B:106:PHE:CD2	2.36	0.61
1:A:122:ALA:HB2	1:A:214:ILE:HD11	1.83	0.60
1:A:266:LEU:HD23	1:A:278:ILE:HD11	1.83	0.60
1:A:296:LEU:HD23	1:A:296:LEU:C	2.26	0.60
1:B:190:MET:HE2	1:B:195:ILE:HG23	1.82	0.60
1:B:152:ASP:CG	1:B:209:THR:HG22	2.27	0.60
1:B:279:ARG:HD2	1:B:301:ASP:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:TRP:HE1	1:A:299:GLU:HG2	1.65	0.60
1:B:306:ALA:C	1:B:307:LEU:HD23	2.26	0.60
1:B:339:GLN:HA	1:B:339:GLN:NE2	2.16	0.60
1:B:343:THR:OG1	1:B:353:LYS:HB2	2.01	0.60
1:A:213:PRO:O	1:A:214:ILE:HG12	2.02	0.60
1:B:319:THR:HG22	1:B:320:ALA:H	1.67	0.60
1:B:166:LEU:HD12	1:B:204:ILE:HG12	1.84	0.60
1:B:168:LEU:HD23	1:B:178:THR:HG22	1.84	0.60
1:A:150:LEU:HD21	1:A:212:ALA:HB2	1.83	0.60
1:B:208:PHE:CD1	1:B:208:PHE:N	2.67	0.60
1:B:183:GLU:O	1:B:187:LEU:HB3	2.02	0.59
1:A:165:TYR:CE1	1:A:198:LEU:HD21	2.37	0.59
1:A:165:TYR:OH	1:A:199:ILE:HG13	2.02	0.59
1:A:278:ILE:HD13	1:A:298:LEU:CD1	2.32	0.59
1:A:308:LYS:HB3	1:A:309:PRO:HD3	1.84	0.59
1:B:331:ALA:HB2	1:B:379:SER:HA	1.83	0.59
1:A:287:VAL:HG12	1:A:294:LEU:HD21	1.84	0.59
1:B:355:VAL:CG1	1:B:371:LEU:HG	2.32	0.59
1:A:284:LEU:HD21	1:A:297:ARG:HG3	1.83	0.59
1:B:153:LEU:HD13	1:B:153:LEU:N	2.17	0.59
1:A:251:PRO:O	1:A:254:ILE:HG22	2.03	0.59
1:B:288:ASP:HB2	1:B:293:THR:HB	1.85	0.59
1:A:340:ARG:HD3	1:A:354:ARG:HG3	1.85	0.59
1:B:154:THR:HG22	1:B:207:ARG:CB	2.26	0.59
1:A:382:LEU:HD23	1:A:383:PHE:N	2.17	0.59
1:B:229:ILE:HG23	1:B:233:ASN:OD1	2.03	0.59
1:A:117:ASN:ND2	1:A:243:PRO:HB2	2.18	0.58
1:A:317:LEU:C	1:A:317:LEU:HD12	2.28	0.58
1:B:104:LEU:O	1:B:320:ALA:HA	2.04	0.58
1:A:150:LEU:O	1:A:151:LEU:O	2.21	0.58
1:B:122:ALA:CB	1:B:214:ILE:HD12	2.34	0.58
1:B:187:LEU:HD12	1:B:187:LEU:C	2.29	0.58
1:A:137:PRO:O	1:A:138:LEU:HD13	2.02	0.58
1:B:256:TRP:CE2	1:B:257:LEU:HD22	2.37	0.58
1:B:258:VAL:CG1	1:B:259:LYS:H	2.09	0.58
1:B:205:GLN:OE1	1:B:205:GLN:CA	2.47	0.58
1:A:126:ALA:O	1:A:232:ASP:N	2.37	0.58
1:A:129:ALA:HB2	1:A:230:ALA:CB	2.34	0.58
1:A:358:PHE:HD1	1:A:359:GLN:HG3	1.67	0.58
1:A:127:ARG:HA	1:A:232:ASP:OD1	2.03	0.58
1:A:148:THR:CB	1:A:149:PRO:CD	2.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ILE:HD12	1:B:327:ILE:C	2.29	0.58
1:A:246:VAL:CG2	1:A:298:LEU:HB2	2.31	0.57
1:B:288:ASP:CB	1:B:293:THR:HB	2.33	0.57
1:A:91:ASN:CG	1:A:92:LEU:N	2.60	0.57
1:A:333:ILE:HD12	1:A:334:ASP:H	1.69	0.57
1:B:202:GLN:O	1:B:203:LYS:C	2.47	0.57
1:B:156:PRO:O	1:B:157:ASP:C	2.47	0.57
1:B:94:VAL:HG12	1:B:381:GLY:HA2	1.86	0.57
1:B:319:THR:HG22	1:B:320:ALA:N	2.20	0.57
1:A:280:LYS:HA	1:A:280:LYS:HE3	1.87	0.57
1:A:251:PRO:HD2	1:A:251:PRO:O	2.03	0.57
1:B:198:LEU:HD12	1:B:198:LEU:C	2.30	0.57
1:A:358:PHE:CD2	1:A:368:ARG:CD	2.87	0.57
1:B:347:ASP:HB2	1:B:349:ARG:HD3	1.87	0.57
1:A:104:LEU:O	1:A:320:ALA:HA	2.04	0.56
1:B:198:LEU:O	1:B:202:GLN:CA	2.52	0.56
1:A:90:GLN:HG2	1:A:383:PHE:HE1	1.68	0.56
1:B:132:ILE:CD1	1:B:227:MET:H	2.17	0.56
1:A:148:THR:O	1:A:211:LYS:HA	2.04	0.56
1:B:221:PHE:CG	1:B:221:PHE:O	2.58	0.56
1:B:156:PRO:O	1:B:158:TRP:N	2.38	0.56
1:A:250:ILE:CG2	1:A:251:PRO:CD	2.79	0.56
1:B:278:ILE:CD1	1:B:298:LEU:HD21	2.35	0.56
1:B:288:ASP:HB3	1:B:291:THR:O	2.06	0.56
1:B:332:LEU:HA	1:B:341:VAL:HG22	1.88	0.56
1:A:125:GLN:HB2	1:A:232:ASP:O	2.06	0.56
1:A:134:LYS:O	1:A:135:VAL:HB	2.06	0.55
1:A:162:GLN:HE22	1:A:190:MET:CE	2.17	0.55
1:A:256:TRP:HD1	1:B:106:PHE:HE2	1.54	0.55
1:A:358:PHE:CD2	1:A:368:ARG:HD2	2.41	0.55
1:A:94:VAL:HG22	1:A:382:LEU:H	1.72	0.55
1:B:178:THR:O	1:B:181:ILE:HG22	2.06	0.55
1:B:178:THR:O	1:B:182:LEU:HD13	2.06	0.55
1:A:283:LEU:O	1:A:285:PRO:HD3	2.06	0.55
1:B:106:PHE:HZ	1:B:359:GLN:HE22	1.53	0.55
1:B:136:TYR:H	1:B:136:TYR:HD2	1.52	0.55
1:B:146:LYS:CD	1:B:147:GLY:N	2.62	0.55
1:A:97:ALA:HB3	1:A:377:VAL:HG13	1.88	0.55
1:A:253:SER:HB3	1:B:106:PHE:HD2	1.72	0.55
1:A:162:GLN:O	1:A:165:TYR:HB3	2.07	0.55
1:A:91:ASN:O	1:A:92:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HB2	1:A:221:PHE:HE1	1.71	0.55
1:B:143:LYS:HZ3	1:B:241:MET:HE1	1.69	0.55
1:A:285:PRO:CG	1:B:357:VAL:HG23	2.36	0.55
1:A:114:VAL:HG21	1:A:307:LEU:HD13	1.89	0.54
1:A:256:TRP:HD1	1:B:106:PHE:CE2	2.25	0.54
1:B:95:LYS:O	1:B:378:VAL:HG23	2.07	0.54
1:A:284:LEU:HD21	1:A:297:ARG:CG	2.36	0.54
1:A:142:ASP:HB2	1:A:218:ILE:HD13	1.90	0.54
1:A:319:THR:HG22	1:A:320:ALA:N	2.22	0.54
1:B:274:LYS:H	1:B:274:LYS:HD2	1.72	0.54
1:A:92:LEU:O	1:A:92:LEU:HD22	2.08	0.54
1:B:298:LEU:HD23	1:B:299:GLU:N	2.23	0.54
1:B:340:ARG:NH2	1:B:354:ARG:HH22	2.06	0.54
1:A:114:VAL:HB	1:A:307:LEU:HD11	1.90	0.54
1:A:332:LEU:HA	1:A:341:VAL:HG12	1.88	0.54
1:A:146:LYS:O	1:A:146:LYS:HG2	2.08	0.53
1:B:144:VAL:CG1	1:B:218:ILE:HD11	2.38	0.53
1:B:194:ASP:OD2	1:B:208:PHE:HB3	2.07	0.53
1:B:305:GLU:O	1:B:305:GLU:CG	2.54	0.53
1:A:121:TYR:HD1	1:A:121:TYR:H	1.56	0.53
1:A:251:PRO:HD2	1:A:254:ILE:HG23	1.81	0.53
1:B:283:LEU:HD23	1:B:294:LEU:HD12	1.90	0.53
1:A:332:LEU:HG	1:A:333:ILE:N	2.23	0.53
1:A:283:LEU:HD11	1:A:296:LEU:HD12	1.91	0.53
1:B:342:ILE:HB	1:B:378:VAL:HG12	1.90	0.53
1:A:117:ASN:C	1:A:119:TYR:H	2.17	0.53
1:A:260:ASP:O	1:A:263:GLN:HG2	2.09	0.53
1:B:347:ASP:HB2	1:B:349:ARG:HD2	1.90	0.53
1:A:218:ILE:HD12	1:A:218:ILE:N	2.23	0.52
1:B:140:VAL:HG13	1:B:220:ALA:H	1.72	0.52
1:A:302:ASN:OD1	1:A:302:ASN:C	2.52	0.52
1:A:150:LEU:C	1:A:151:LEU:HD23	2.35	0.52
1:B:148:THR:CB	1:B:149:PRO:HD2	2.38	0.52
1:B:317:LEU:HD12	1:B:318:ASN:H	1.75	0.52
1:A:249:ALA:HB1	1:A:293:THR:OG1	2.10	0.52
1:B:203:LYS:O	1:B:204:ILE:C	2.53	0.52
1:A:284:LEU:O	1:A:286:GLY:N	2.43	0.52
1:B:193:ALA:O	1:B:197:ARG:HG3	2.09	0.52
1:B:302:ASN:ND2	1:B:305:GLU:HA	2.25	0.52
1:A:94:VAL:HG22	1:A:382:LEU:N	2.25	0.52
1:A:114:VAL:HG21	1:A:311:MET:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ALA:HB3	1:B:231:LYS:O	2.09	0.52
1:A:305:GLU:O	1:A:306:ALA:HB3	2.10	0.52
1:A:315:LEU:HG	1:A:315:LEU:O	2.10	0.52
1:B:230:ALA:O	1:B:231:LYS:HG3	2.10	0.52
1:A:115:SER:N	1:A:245:TRP:O	2.43	0.52
1:A:244:VAL:HG11	1:A:307:LEU:CG	2.38	0.52
1:A:250:ILE:CG2	1:A:251:PRO:O	2.58	0.52
1:B:147:GLY:HA3	1:B:212:ALA:O	2.10	0.52
1:B:112:ALA:HB3	1:B:313:ALA:O	2.10	0.51
1:B:165:TYR:CD2	1:B:182:LEU:HD11	2.45	0.51
1:B:221:PHE:O	1:B:221:PHE:CD1	2.64	0.51
1:B:241:MET:HE3	1:B:305:GLU:CG	2.26	0.51
1:A:117:ASN:N	1:A:117:ASN:OD1	2.42	0.51
1:B:106:PHE:HZ	1:B:359:GLN:NE2	2.08	0.51
1:B:308:LYS:HG2	1:B:311:MET:HE3	1.92	0.51
1:A:284:LEU:CD2	1:A:297:ARG:HD2	2.35	0.51
1:A:284:LEU:HD11	1:A:297:ARG:HD2	1.92	0.51
1:A:304:ASP:O	1:A:305:GLU:HB2	2.09	0.51
1:B:210:LEU:HD12	1:B:210:LEU:C	2.36	0.51
1:B:229:ILE:HD12	1:B:229:ILE:N	2.26	0.51
1:A:227:MET:C	1:A:229:ILE:CD1	2.83	0.51
1:A:232:ASP:O	1:A:233:ASN:C	2.52	0.51
1:B:174:THR:HG23	1:B:177:GLN:HB3	1.93	0.51
1:B:198:LEU:HD12	1:B:199:ILE:N	2.26	0.51
1:B:223:LEU:HB3	1:B:227:MET:SD	2.51	0.51
1:A:119:TYR:CE1	1:A:245:TRP:CH2	2.99	0.51
1:B:148:THR:HB	1:B:149:PRO:CD	2.39	0.51
1:A:135:VAL:HG12	1:A:136:TYR:O	2.11	0.51
1:B:271:ARG:NH1	1:B:306:ALA:HB1	2.26	0.51
1:B:281:TRP:HZ3	1:B:283:LEU:CD1	2.23	0.51
1:A:231:LYS:O	1:A:232:ASP:CB	2.44	0.51
1:A:334:ASP:HB2	1:A:338:GLU:O	2.11	0.51
1:B:218:ILE:HD12	1:B:218:ILE:H	1.76	0.51
1:A:122:ALA:HB3	1:A:238:ILE:HB	1.91	0.50
1:A:144:VAL:HG13	1:A:218:ILE:HD11	1.93	0.50
1:B:152:ASP:HA	1:B:209:THR:HG22	1.93	0.50
1:A:358:PHE:HD2	1:A:368:ARG:HD2	1.76	0.50
1:A:129:ALA:CB	1:A:230:ALA:CB	2.89	0.50
1:A:221:PHE:O	1:A:222:ASP:CB	2.52	0.50
1:A:126:ALA:O	1:A:232:ASP:HA	2.11	0.50
1:A:129:ALA:CA	1:A:229:ILE:O	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASP:O	1:A:335:THR:HG23	2.12	0.50
1:A:382:LEU:HD23	1:A:382:LEU:C	2.37	0.50
1:B:132:ILE:HG13	1:B:227:MET:N	2.27	0.50
1:B:122:ALA:HB3	1:B:214:ILE:CD1	2.39	0.50
1:B:158:TRP:CH2	1:B:188:ALA:HB1	2.47	0.50
1:B:380:SER:O	1:B:382:LEU:HD23	2.11	0.50
1:A:221:PHE:CG	1:A:222:ASP:N	2.79	0.50
1:A:244:VAL:HG23	1:A:302:ASN:HB3	1.93	0.50
1:A:266:LEU:HD22	1:A:315:LEU:HD13	1.92	0.50
1:A:377:VAL:HG22	1:A:378:VAL:N	2.26	0.50
1:B:198:LEU:O	1:B:202:GLN:N	2.43	0.50
1:B:345:ASP:O	1:B:346:ALA:HB3	2.12	0.50
1:B:341:VAL:CG1	1:B:342:ILE:H	2.04	0.50
1:A:150:LEU:HD12	1:A:150:LEU:N	2.27	0.49
1:A:114:VAL:HG11	1:A:307:LEU:HD22	1.95	0.49
1:A:153:LEU:C	1:A:153:LEU:CD2	2.85	0.49
1:A:316:GLN:O	1:A:316:GLN:HG3	2.12	0.49
1:A:368:ARG:HA	1:A:368:ARG:NH2	2.24	0.49
1:B:308:LYS:O	1:B:311:MET:HG3	2.12	0.49
1:B:337:SER:O	1:B:339:GLN:HG2	2.12	0.49
1:B:340:ARG:HA	1:B:355:VAL:HG22	1.95	0.49
1:B:345:ASP:OD1	1:B:345:ASP:N	2.45	0.49
1:A:119:TYR:HE1	1:A:245:TRP:HH2	1.56	0.49
1:A:214:ILE:HG13	1:A:215:ASP:O	2.12	0.49
1:B:135:VAL:HG12	1:B:135:VAL:O	2.12	0.49
1:B:136:TYR:O	1:B:138:LEU:N	2.44	0.49
1:B:302:ASN:CG	1:B:305:GLU:HA	2.36	0.49
1:A:278:ILE:HG21	1:A:298:LEU:HD13	1.95	0.49
1:A:121:TYR:HA	1:A:238:ILE:O	2.12	0.49
1:A:256:TRP:CD1	1:B:106:PHE:HE2	2.30	0.49
1:B:121:TYR:CE2	1:B:237:LYS:HD2	2.48	0.49
1:B:230:ALA:O	1:B:233:ASN:OD1	2.30	0.49
1:A:135:VAL:O	1:A:136:TYR:CB	2.59	0.49
1:B:206:THR:HG23	1:B:207:ARG:H	1.77	0.49
1:B:327:ILE:HD12	1:B:328:PRO:C	2.38	0.49
1:B:169:ARG:NH1	1:B:202:GLN:HG2	2.27	0.49
1:A:179:GLU:OE2	1:A:179:GLU:HA	2.13	0.49
1:A:201:THR:C	1:A:203:LYS:H	2.21	0.49
1:A:265:THR:HB	1:A:316:GLN:HG2	1.94	0.49
1:A:229:ILE:N	1:A:229:ILE:HD13	2.27	0.48
1:B:106:PHE:CZ	1:B:359:GLN:NE2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLN:HG3	1:A:146:LYS:N	2.28	0.48
1:A:227:MET:O	1:A:229:ILE:CD1	2.61	0.48
1:A:213:PRO:C	1:A:214:ILE:HG12	2.38	0.48
1:B:325:LEU:O	1:B:366:ALA:HA	2.14	0.48
1:B:139:THR:N	1:B:142:ASP:OD2	2.39	0.48
1:B:157:ASP:O	1:B:158:TRP:C	2.56	0.48
1:B:192:GLU:HA	1:B:195:ILE:HD11	1.95	0.48
1:B:342:ILE:O	1:B:377:VAL:HG23	2.13	0.48
1:A:104:LEU:HD12	1:A:324:MET:HE1	1.94	0.48
1:A:267:THR:HG23	1:A:314:TRP:HB2	1.95	0.48
1:A:307:LEU:CD1	1:A:308:LYS:O	2.61	0.48
1:B:165:TYR:CD1	1:B:165:TYR:C	2.92	0.48
1:A:91:ASN:O	1:A:92:LEU:CB	2.62	0.48
1:A:273:ASP:HB3	1:A:274:LYS:H	1.47	0.48
1:B:136:TYR:CZ	1:B:149:PRO:HB2	2.49	0.48
1:A:112:ALA:HB3	1:A:313:ALA:O	2.13	0.47
1:A:358:PHE:CD1	1:A:359:GLN:HG3	2.48	0.47
1:A:106:PHE:HD2	1:B:253:SER:HA	1.67	0.47
1:A:198:LEU:C	1:A:198:LEU:HD23	2.39	0.47
1:B:278:ILE:O	1:B:278:ILE:HG12	2.11	0.47
1:B:377:VAL:CG2	1:B:378:VAL:H	2.23	0.47
1:B:117:ASN:HD21	1:B:243:PRO:HG2	1.79	0.47
1:B:254:ILE:O	1:B:254:ILE:HG22	2.14	0.47
1:A:237:LYS:HG2	1:A:238:ILE:N	2.30	0.47
1:B:339:GLN:HB3	1:B:355:VAL:O	2.14	0.47
1:A:291:THR:CG2	1:A:293:THR:HB	2.45	0.47
1:B:152:ASP:CG	1:B:209:THR:CG2	2.88	0.47
1:A:297:ARG:C	1:A:298:LEU:HD23	2.39	0.47
1:A:136:TYR:CD1	1:A:137:PRO:HD2	2.50	0.47
1:A:245:TRP:CZ3	1:A:297:ARG:NH2	2.82	0.47
1:B:345:ASP:C	1:B:347:ASP:H	2.21	0.47
1:A:91:ASN:CB	1:A:382:LEU:HD22	2.45	0.46
1:A:96:THR:OG1	1:A:376:LYS:HD3	2.15	0.46
1:A:122:ALA:HB2	1:A:214:ILE:CD1	2.45	0.46
1:A:150:LEU:N	1:A:150:LEU:CD1	2.78	0.46
1:A:224:ARG:HG2	1:A:225:ALA:N	2.30	0.46
1:A:358:PHE:CD2	1:A:368:ARG:CZ	2.97	0.46
1:A:120:GLN:HG2	1:A:240:GLY:HA3	1.97	0.46
1:A:260:ASP:OD1	1:A:262:SER:N	2.36	0.46
1:A:343:THR:O	1:A:350:PHE:HA	2.15	0.46
1:B:112:ALA:HB3	1:B:313:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ALA:HB1	1:B:246:VAL:HG23	1.97	0.46
1:B:327:ILE:HD11	1:B:332:LEU:HB2	1.95	0.46
1:A:132:ILE:HG23	1:A:227:MET:N	2.20	0.46
1:B:235:VAL:CG2	1:B:236:ALA:N	2.78	0.46
1:A:284:LEU:HD22	1:A:284:LEU:H	1.78	0.46
1:A:292:ARG:HD2	1:A:292:ARG:HA	1.71	0.46
1:B:219:THR:O	1:B:220:ALA:HB3	2.15	0.46
1:B:271:ARG:HB2	1:B:273:ASP:OD1	2.16	0.46
1:B:327:ILE:CD1	1:B:328:PRO:O	2.61	0.46
1:B:377:VAL:CG2	1:B:378:VAL:N	2.77	0.46
1:A:156:PRO:O	1:A:159:VAL:HG22	2.15	0.46
1:A:167:LEU:C	1:A:167:LEU:CD1	2.88	0.46
1:A:190:MET:HA	1:A:191:PRO:HD2	1.78	0.46
1:B:332:LEU:HA	1:B:341:VAL:HG21	1.96	0.46
1:B:127:ARG:O	1:B:128:ALA:HB2	2.16	0.46
1:B:274:LYS:HD2	1:B:274:LYS:N	2.31	0.46
1:A:137:PRO:C	1:A:138:LEU:HD13	2.41	0.46
1:B:275:THR:HG23	1:B:277:THR:HG23	1.97	0.46
1:B:132:ILE:HG13	1:B:227:MET:O	2.16	0.46
1:B:132:ILE:HD12	1:B:227:MET:H	1.80	0.46
1:B:153:LEU:HD22	1:B:208:PHE:O	2.15	0.46
1:A:253:SER:HA	1:B:106:PHE:HE2	1.81	0.45
1:B:302:ASN:HD21	1:B:307:LEU:HG	1.79	0.45
1:B:166:LEU:CD1	1:B:204:ILE:HG12	2.47	0.45
1:A:367:LEU:O	1:A:368:ARG:NH2	2.49	0.45
1:B:282:THR:OG1	1:B:283:LEU:N	2.49	0.45
1:A:266:LEU:CD2	1:A:315:LEU:HD13	2.46	0.45
1:B:304:ASP:O	1:B:305:GLU:HB3	2.17	0.45
1:A:135:VAL:O	1:A:136:TYR:HB2	2.15	0.45
1:A:259:LYS:HE2	1:A:259:LYS:HB2	1.75	0.45
1:B:132:ILE:HG22	1:B:133:ASP:N	2.32	0.45
1:A:339:GLN:O	1:A:340:ARG:HB3	2.15	0.45
1:B:254:ILE:O	1:B:254:ILE:CG2	2.64	0.45
1:B:115:SER:N	1:B:245:TRP:O	2.50	0.45
1:A:142:ASP:OD2	1:A:142:ASP:N	2.51	0.44
1:B:166:LEU:HD23	1:B:166:LEU:HA	1.62	0.44
1:B:210:LEU:HD12	1:B:210:LEU:O	2.17	0.44
1:B:368:ARG:O	1:B:369:SER:CB	2.65	0.44
1:A:167:LEU:HD12	1:A:168:LEU:N	2.32	0.44
1:A:250:ILE:HG21	1:A:255:ALA:CA	2.44	0.44
1:A:297:ARG:O	1:A:298:LEU:HD23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:HB	1:A:378:VAL:HG12	1.98	0.44
1:A:132:ILE:HD12	1:A:151:LEU:HD12	1.98	0.44
1:A:253:SER:HA	1:A:256:TRP:CD1	2.52	0.44
1:B:156:PRO:O	1:B:159:VAL:N	2.34	0.44
1:A:183:GLU:OE1	1:A:183:GLU:HA	2.16	0.44
1:B:246:VAL:HG13	1:B:298:LEU:HB3	1.99	0.44
1:B:92:LEU:HD22	1:B:92:LEU:N	2.28	0.44
1:B:102:GLY:O	1:B:323:PRO:HA	2.17	0.44
1:B:132:ILE:HG22	1:B:133:ASP:H	1.82	0.44
1:A:91:ASN:CG	1:A:93:GLY:H	2.24	0.44
1:A:144:VAL:HG22	1:A:216:GLY:O	2.18	0.44
1:B:159:VAL:HG23	1:B:160:GLU:N	2.32	0.44
1:A:272:PRO:O	1:A:273:ASP:C	2.61	0.44
1:A:91:ASN:HB2	1:A:382:LEU:HD22	2.00	0.44
1:A:291:THR:HG22	1:A:293:THR:HB	2.00	0.44
1:B:133:ASP:HB3	1:B:152:ASP:HB2	1.99	0.44
1:A:260:ASP:OD1	1:A:260:ASP:C	2.60	0.43
1:B:147:GLY:CA	1:B:212:ALA:O	2.66	0.43
1:B:155:ILE:HG13	1:B:208:PHE:HE1	1.82	0.43
1:B:155:ILE:O	1:B:159:VAL:HG13	2.18	0.43
1:B:159:VAL:O	1:B:160:GLU:C	2.60	0.43
1:B:190:MET:HA	1:B:191:PRO:HD2	1.79	0.43
1:B:307:LEU:HD23	1:B:307:LEU:N	2.33	0.43
1:A:258:VAL:HA	1:A:263:GLN:OE1	2.18	0.43
1:B:104:LEU:HD12	1:B:104:LEU:HA	1.74	0.43
1:B:136:TYR:CD2	1:B:136:TYR:N	2.86	0.43
1:B:139:THR:O	1:B:142:ASP:OD1	2.36	0.43
1:B:256:TRP:CE2	1:B:257:LEU:CD2	3.00	0.43
1:A:120:GLN:CG	1:A:240:GLY:HA3	2.49	0.43
1:A:196:ARG:O	1:A:199:ILE:HG22	2.18	0.43
1:B:231:LYS:CG	1:B:232:ASP:H	2.31	0.43
1:B:234:VAL:HG13	1:B:234:VAL:O	2.19	0.43
1:A:340:ARG:CD	1:A:354:ARG:HG3	2.47	0.43
1:B:144:VAL:O	1:B:144:VAL:HG22	2.15	0.43
1:B:317:LEU:C	1:B:318:ASN:HD22	2.27	0.43
1:B:340:ARG:HH21	1:B:354:ARG:HH22	1.66	0.43
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.36	0.43
1:B:339:GLN:O	1:B:340:ARG:HG3	2.18	0.43
1:B:342:ILE:HG23	1:B:350:PHE:HB3	2.00	0.43
1:A:134:LYS:O	1:A:135:VAL:CB	2.67	0.43
1:A:256:TRP:HA	1:B:358:PHE:HZ	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:O	1:A:272:PRO:HD2	2.18	0.43
1:A:114:VAL:HG12	1:A:246:VAL:HG12	2.01	0.43
1:A:153:LEU:O	1:A:207:ARG:HA	2.19	0.43
1:A:250:ILE:HD13	1:A:250:ILE:HA	1.88	0.43
1:A:269:PRO:O	1:A:270:ALA:C	2.61	0.43
1:A:130:GLY:HA3	1:A:155:ILE:HG12	2.01	0.42
1:A:155:ILE:HG22	1:A:157:ASP:H	1.84	0.42
1:B:256:TRP:CD2	1:B:257:LEU:HD22	2.54	0.42
1:B:331:ALA:O	1:B:341:VAL:HG13	2.12	0.42
1:B:339:GLN:C	1:B:340:ARG:CG	2.92	0.42
1:A:231:LYS:HD2	1:A:231:LYS:HA	1.63	0.42
1:B:166:LEU:HD21	1:B:202:GLN:CD	2.43	0.42
1:B:275:THR:HG23	1:B:277:THR:OG1	2.18	0.42
1:A:174:THR:N	1:A:177:GLN:HG3	2.34	0.42
1:A:244:VAL:HG12	1:A:245:TRP:N	2.35	0.42
1:A:256:TRP:C	1:A:256:TRP:CD2	2.91	0.42
1:A:284:LEU:HD23	1:A:295:GLN:CB	2.49	0.42
1:B:224:ARG:O	1:B:225:ALA:HB3	2.20	0.42
1:A:132:ILE:HG13	1:A:133:ASP:N	2.35	0.42
1:A:266:LEU:HD13	1:A:266:LEU:HA	1.92	0.42
1:B:232:ASP:OD1	1:B:232:ASP:N	2.53	0.42
1:B:317:LEU:HD12	1:B:318:ASN:N	2.35	0.42
1:A:138:LEU:HB2	1:A:221:PHE:CE1	2.53	0.42
1:A:150:LEU:O	1:A:151:LEU:C	2.62	0.42
1:A:264:PHE:HE1	1:A:281:TRP:CG	2.37	0.42
1:A:244:VAL:HG12	1:A:245:TRP:H	1.85	0.42
1:B:329:SER:O	1:B:330:GLN:C	2.61	0.42
1:A:130:GLY:N	1:A:229:ILE:O	2.52	0.41
1:A:150:LEU:CD2	1:A:212:ALA:HB2	2.50	0.41
1:A:287:VAL:HG12	1:A:294:LEU:CD2	2.49	0.41
1:B:250:ILE:HG22	1:B:294:LEU:HB2	2.02	0.41
1:B:351:VAL:HA	1:B:352:PRO:HD3	1.94	0.41
1:A:159:VAL:HG23	1:A:160:GLU:N	2.36	0.41
1:A:182:LEU:HD21	1:A:199:ILE:HD12	2.01	0.41
1:A:91:ASN:ND2	1:A:93:GLY:N	2.66	0.41
1:A:177:GLN:H	1:A:177:GLN:HG2	1.63	0.41
1:A:250:ILE:HG23	1:A:254:ILE:HG23	2.02	0.41
1:A:284:LEU:N	1:A:284:LEU:CD2	2.79	0.41
1:B:278:ILE:HG13	1:B:298:LEU:HD21	2.03	0.41
1:A:241:MET:SD	1:A:305:GLU:OE1	2.78	0.41
1:A:244:VAL:HG21	1:A:302:ASN:HD22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:HG22	1:A:176:THR:N	2.34	0.41
1:B:144:VAL:HG12	1:B:218:ILE:HD11	2.02	0.41
1:B:174:THR:O	1:B:178:THR:HG23	2.20	0.41
1:A:117:ASN:C	1:A:119:TYR:N	2.79	0.41
1:A:168:LEU:HD12	1:A:173:GLY:HA3	2.03	0.41
1:B:95:LYS:HB2	1:B:379:SER:O	2.21	0.41
1:A:155:ILE:HA	1:A:156:PRO:HD3	1.71	0.41
1:B:113:ASN:OD1	1:B:113:ASN:C	2.63	0.41
1:B:331:ALA:HB2	1:B:379:SER:CA	2.49	0.41
1:B:140:VAL:CG1	1:B:220:ALA:H	2.34	0.41
1:B:288:ASP:HB3	1:B:293:THR:HB	2.00	0.41
1:A:254:ILE:HG23	1:A:255:ALA:N	2.36	0.40
1:A:342:ILE:CG2	1:A:350:PHE:HB3	2.51	0.40
1:B:102:GLY:C	1:B:323:PRO:HA	2.47	0.40
1:B:128:ALA:CB	1:B:158:TRP:CZ3	3.04	0.40
1:B:260:ASP:OD1	1:B:260:ASP:C	2.63	0.40
1:B:275:THR:HG23	1:B:277:THR:CG2	2.51	0.40
1:A:91:ASN:HD21	1:A:93:GLY:H	1.67	0.40
1:A:237:LYS:HG2	1:A:238:ILE:H	1.86	0.40
1:A:284:LEU:C	1:A:286:GLY:N	2.80	0.40
1:B:276:LEU:HA	1:B:276:LEU:HD13	1.83	0.40
1:B:384:LEU:C	1:B:384:LEU:HD12	2.46	0.40
1:A:104:LEU:HD21	1:A:364:VAL:HG23	2.01	0.40
1:A:159:VAL:CG2	1:A:160:GLU:N	2.85	0.40
1:A:160:GLU:CD	1:A:160:GLU:C	2.90	0.40
1:A:311:MET:HB3	1:A:312:ASN:H	1.66	0.40
1:B:104:LEU:N	1:B:321:SER:OG	2.55	0.40
1:B:223:LEU:N	1:B:223:LEU:CD2	2.75	0.40
1:B:230:ALA:O	1:B:231:LYS:CG	2.70	0.40
1:B:287:VAL:HA	1:B:293:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/413 (71%)	227 (77%)	44 (15%)	23 (8%)	1	11
1	B	295/413 (71%)	240 (81%)	39 (13%)	16 (5%)	1	16
All	All	589/826 (71%)	467 (79%)	83 (14%)	39 (7%)	1	13

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	151	LEU
1	A	204	ILE
1	A	214	ILE
1	A	236	ALA
1	B	156	PRO
1	B	157	ASP
1	B	221	PHE
1	A	91	ASN
1	A	92	LEU
1	A	148	THR
1	A	222	ASP
1	A	272	PRO
1	A	311	MET
1	A	335	THR
1	A	341	VAL
1	A	348	GLY
1	B	135	VAL
1	B	172	GLY
1	A	270	ALA
1	A	273	ASP
1	A	305	GLU
1	A	308	LYS
1	B	158	TRP
1	B	206	THR
1	A	221	PHE
1	A	225	ALA
1	A	285	PRO
1	A	290	ALA
1	B	369	SER
1	A	340	ARG
1	B	137	PRO
1	B	189	GLY

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Mol	Chain	Res	Type
1	B	213	PRO
1	B	220	ALA
1	B	341	VAL
1	B	204	ILE
1	B	309	PRO
1	B	370	GLY

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	242/338 (72%)	184 (76%)	58 (24%)	1	5
1	B	243/338 (72%)	185 (76%)	58 (24%)	1	5
All	All	485/676 (72%)	369 (76%)	116 (24%)	1	5

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	92	LEU
1	A	98	THR
1	A	100	THR
1	A	109	SER
1	A	116	TYR
1	A	117	ASN
1	A	121	TYR
1	A	132	ILE
1	A	135	VAL
1	A	138	LEU
1	A	142	ASP
1	A	150	LEU
1	A	153	LEU
1	A	167	LEU
1	A	168	LEU
1	A	171	THR

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Mol	Chain	Res	Type
1	A	177	GLN
1	A	178	THR
1	A	198	LEU
1	A	204	ILE
1	A	206	THR
1	A	207	ARG
1	A	210	LEU
1	A	217	VAL
1	A	219	THR
1	A	222	ASP
1	A	224	ARG
1	A	229	ILE
1	A	231	LYS
1	A	234	VAL
1	A	235	VAL
1	A	246	VAL
1	A	252	GLU
1	A	256	TRP
1	A	258	VAL
1	A	260	ASP
1	A	271	ARG
1	A	276	LEU
1	A	280	LYS
1	A	282	THR
1	A	284	LEU
1	A	292	ARG
1	A	298	LEU
1	A	300	VAL
1	A	307	LEU
1	A	316	GLN
1	A	317	LEU
1	A	332	LEU
1	A	335	THR
1	A	347	ASP
1	A	350	PHE
1	A	351	VAL
1	A	353	LYS
1	A	355	VAL
1	A	368	ARG
1	A	378	VAL
1	A	385	ILE
1	B	91	ASN

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Mol	Chain	Res	Type
1	B	92	LEU
1	B	98	THR
1	B	100	THR
1	B	104	LEU
1	B	109	SER
1	B	117	ASN
1	B	121	TYR
1	B	123	ILE
1	B	125	GLN
1	B	132	ILE
1	B	142	ASP
1	B	143	LYS
1	B	144	VAL
1	B	146	LYS
1	B	148	THR
1	B	151	LEU
1	B	153	LEU
1	B	157	ASP
1	B	165	TYR
1	B	167	LEU
1	B	174	THR
1	B	176	THR
1	B	187	LEU
1	B	195	ILE
1	B	198	LEU
1	B	202	GLN
1	B	205	GLN
1	B	206	THR
1	B	208	PHE
1	B	214	ILE
1	B	223	LEU
1	B	232	ASP
1	B	235	VAL
1	B	239	GLN
1	B	246	VAL
1	B	250	ILE
1	B	260	ASP
1	B	265	THR
1	B	271	ARG
1	B	274	LYS
1	B	276	LEU
1	B	278	ILE

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Mol	Chain	Res	Type
1	B	282	THR
1	B	294	LEU
1	B	305	GLU
1	B	307	LEU
1	B	326	LEU
1	B	327	ILE
1	B	329	SER
1	B	334	ASP
1	B	340	ARG
1	B	345	ASP
1	B	347	ASP
1	B	365	THR
1	B	367	LEU
1	B	368	ARG
1	B	384	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	162	GLN
1	A	177	GLN
1	A	228	ASN
1	A	318	ASN
1	A	330	GLN
1	A	359	GLN
1	B	125	GLN
1	B	145	GLN
1	B	239	GLN
1	B	302	ASN
1	B	318	ASN
1	B	339	GLN
1	B	359	GLN
1	B	362	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	296/413 (71%)	-0.01	5 (1%)	69 46	133, 211, 301, 394	0
1	B	297/413 (71%)	-0.09	3 (1%)	79 57	135, 224, 341, 582	0
All	All	593/826 (71%)	-0.05	8 (1%)	75 52	133, 218, 329, 582	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	ARG	2.7
1	A	213	PRO	2.5
1	A	156	PRO	2.3
1	A	149	PRO	2.3
1	B	235	VAL	2.3
1	A	157	ASP	2.2
1	A	255	ALA	2.1
1	B	378	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CU1	A	415	1/1	0.58	0.23	247,247,247,247	0
2	CU1	B	415	1/1	0.64	0.23	547,547,547,547	0
2	CU1	A	414	1/1	0.93	0.21	452,452,452,452	0
2	CU1	B	414	1/1	0.94	0.11	296,296,296,296	0

6.5 Other polymers [i](#)

There are no such residues in this entry.