



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:00 PM UTC

PDB ID : 3U9T / pdb_00003u9t
Title : Crystal structure of P. aeruginosa 3-methylcrotonyl-CoA carboxylase (MCC)
750 kD holoenzyme, free enzyme
Authors : Huang, C.S.; Tong, L.
Deposited on : 2011-10-19
Resolution : 2.90 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

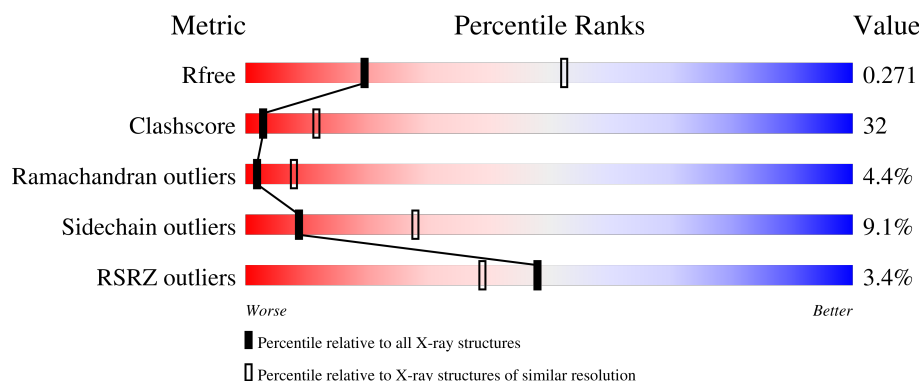
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	655	5% 39% 38% 8% 15%
2	B	555	5% 42% 32% 5% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7635 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 Methyldcrotonyl-CoA carboxylase, alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4323	2693	815	797	18			

- Molecule 2 is a protein called Methyldcrotonyl-CoA carboxylase, beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	437	Total	C	N	O	S	0	0	0
			3312	2101	600	592	19			

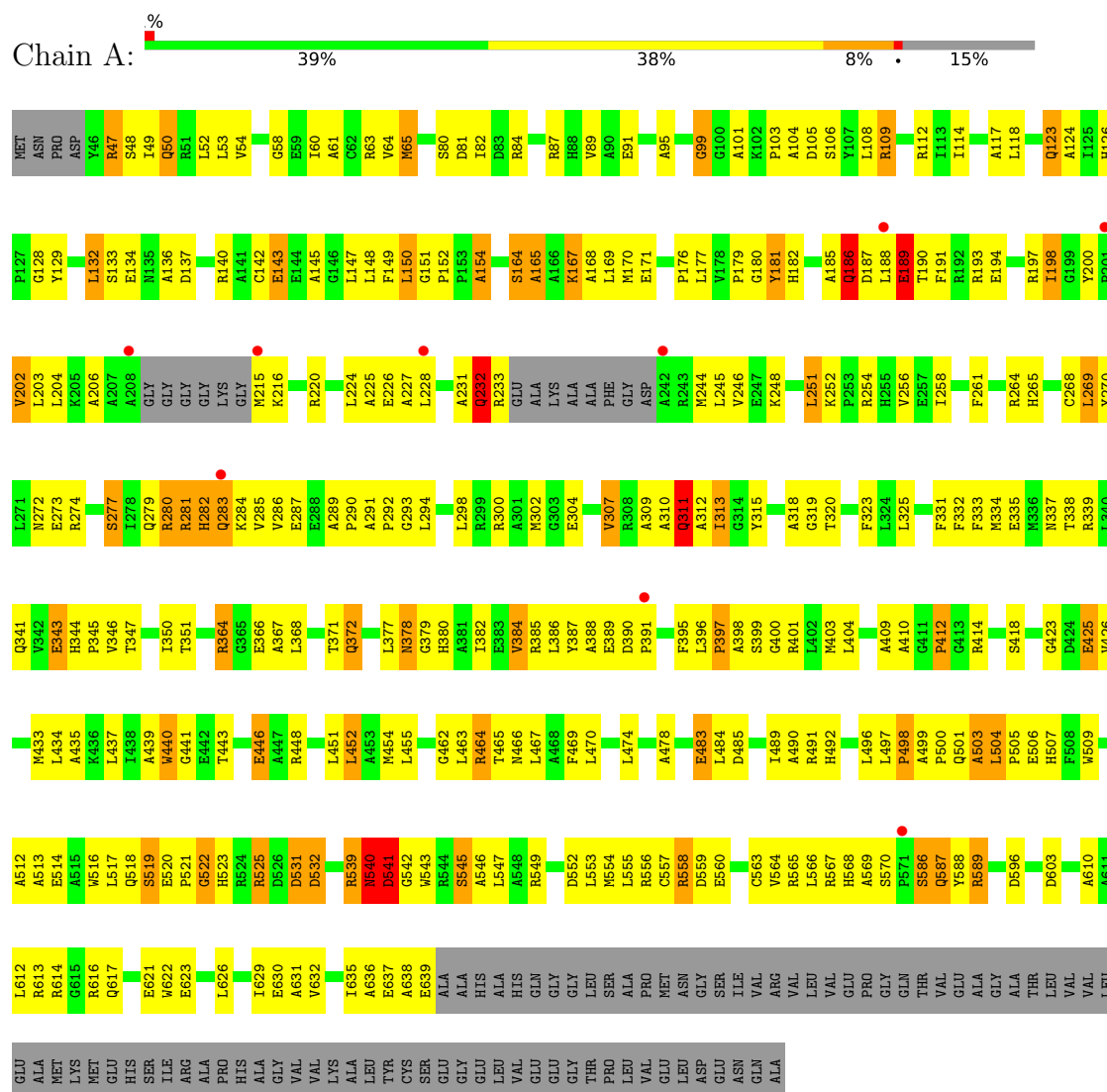
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	expression tag	UNP Q9I297
B	9	GLY	-	expression tag	UNP Q9I297
B	10	SER	-	expression tag	UNP Q9I297
B	11	SER	-	expression tag	UNP Q9I297
B	12	HIS	-	expression tag	UNP Q9I297
B	13	HIS	-	expression tag	UNP Q9I297
B	14	HIS	-	expression tag	UNP Q9I297
B	15	HIS	-	expression tag	UNP Q9I297
B	16	HIS	-	expression tag	UNP Q9I297
B	17	HIS	-	expression tag	UNP Q9I297
B	18	SER	-	expression tag	UNP Q9I297
B	19	SER	-	expression tag	UNP Q9I297
B	20	GLY	-	expression tag	UNP Q9I297
B	21	LEU	-	expression tag	UNP Q9I297
B	22	VAL	-	expression tag	UNP Q9I297
B	23	PRO	-	expression tag	UNP Q9I297
B	24	ARG	-	expression tag	UNP Q9I297
B	25	GLY	-	expression tag	UNP Q9I297
B	26	SER	-	expression tag	UNP Q9I297
B	27	HIS	-	expression tag	UNP Q9I297

3 Residue-property plots [i](#)

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

- Molecule 1: Methylcrotonyl-CoA carboxylase, alpha-subunit



- Molecule 2: Methylcrotonyl-CoA carboxylase, beta-subunit





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	158.93Å 158.93Å 311.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.23 – 2.90 46.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.9 (46.23-2.90) 92.9 (46.23-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.209 , 0.269 0.208 , 0.271	Depositor DCC
R_{free} test set	1674 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7635	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.61	0/4406	1.12	32/5958 (0.5%)
2	B	0.72	0/3380	1.17	22/4580 (0.5%)
All	All	0.66	0/7786	1.15	54/10538 (0.5%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ASP	CA-C-N	12.36	133.81	119.47
1	A	532	ASP	C-N-CA	12.36	133.81	119.47
2	B	193	ARG	N-CA-C	-9.89	100.50	111.28
1	A	569	ALA	N-CA-C	-9.01	102.84	112.93
2	B	270	SER	N-CA-C	-8.29	102.04	112.90
2	B	146	TYR	N-CA-C	-8.23	99.33	110.36
1	A	80	SER	N-CA-C	-7.64	99.81	110.35
1	A	410	ALA	N-CA-C	-7.43	100.02	110.50
1	A	540	ASN	N-CA-C	-7.38	104.67	112.93
2	B	306	ALA	CA-C-N	7.15	127.18	119.89
2	B	306	ALA	C-N-CA	7.15	127.18	119.89
2	B	176	ALA	N-CA-C	-7.09	103.94	112.59
1	A	506	GLU	N-CA-C	-7.07	104.39	112.87
1	A	540	ASN	CA-C-N	6.93	129.90	120.54
1	A	540	ASN	C-N-CA	6.93	129.90	120.54
1	A	294	LEU	N-CA-C	6.72	119.72	110.24
1	A	541	ASP	N-CA-C	6.71	119.16	111.11
2	B	96	PRO	N-CA-C	-6.67	101.89	111.22
1	A	499	ALA	CA-C-N	6.47	127.92	119.84
1	A	499	ALA	C-N-CA	6.47	127.92	119.84
2	B	55	ALA	N-CA-C	-6.45	104.16	111.07
2	B	339	VAL	N-CA-C	6.30	118.18	109.80
2	B	95	SER	N-CA-C	6.27	116.81	109.60
1	A	291	ALA	CA-C-N	6.25	127.65	119.84
1	A	291	ALA	C-N-CA	6.25	127.65	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	THR	N-CA-C	-6.20	101.03	110.14
1	A	311	GLN	N-CA-C	-5.98	104.76	111.28
2	B	454	GLY	N-CA-C	5.93	127.24	113.18
1	A	143	GLU	N-CA-C	-5.81	104.86	111.07
1	A	501	GLN	N-CA-C	5.80	118.31	110.88
2	B	296	TRP	N-CA-C	5.76	119.31	110.20
1	A	50	GLN	N-CA-C	-5.75	105.94	113.12
2	B	555	PRO	N-CA-C	-5.65	102.98	111.57
2	B	404	ILE	N-CA-C	5.63	115.76	107.15
1	A	202	VAL	N-CA-C	5.57	117.36	108.89
1	A	558	ARG	CB-CA-C	-5.54	109.69	117.23
1	A	519	SER	N-CA-C	-5.54	106.19	113.17
1	A	167	LYS	N-CA-C	-5.52	105.42	111.82
2	B	41	GLU	N-CA-C	-5.51	105.38	111.71
1	A	464	ARG	N-CA-C	-5.47	100.78	109.76
2	B	465	TRP	N-CA-C	-5.46	102.28	110.24
1	A	126	HIS	N-CA-C	-5.36	100.82	109.40
1	A	531	ASP	CB-CA-C	-5.36	101.57	110.68
1	A	484	LEU	N-CA-C	5.32	118.48	109.76
1	A	388	ALA	N-CA-C	-5.31	103.96	110.65
2	B	85	GLU	N-CA-C	-5.29	105.56	112.23
2	B	312	TYR	CA-C-N	5.15	125.09	119.78
2	B	312	TYR	C-N-CA	5.15	125.09	119.78
1	A	542	GLY	N-CA-C	-5.14	108.13	115.64
2	B	547	ALA	N-CA-C	-5.10	105.61	111.07
2	B	30	ILE	N-CA-C	5.07	119.88	109.34
2	B	218	ALA	CB-CA-C	-5.06	110.35	117.23
1	A	277	SER	N-CA-C	5.05	116.59	111.14
1	A	589	ARG	N-CA-C	-5.01	101.82	108.74

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	4323	0	4267	317	0
2	B	3312	0	3308	188	0
All	All	7635	0	7575	493	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 32.

All (493) 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:465:THR:HG22	1:A:467:LEU:H	1.15	1.11
1:A:274:ARG:HH22	1:A:320:THR:HG21	1.16	1.10
2:B:157:GLN:NE2	2:B:197:ASN:HD22	1.50	1.10
1:A:47:ARG:HH11	1:A:47:ARG:HB2	1.16	1.07
1:A:379:GLY:HA3	1:A:440:TRP:CH2	1.92	1.03
1:A:549:ARG:HH11	1:A:549:ARG:HG3	1.27	0.97
2:B:433:ARG:HH21	2:B:554:GLU:HG3	1.30	0.97
2:B:35:ILE:HD13	2:B:320:VAL:HG22	1.45	0.96
2:B:267:CYS:HA	2:B:273:ALA:HB3	1.48	0.95
1:A:274:ARG:NH2	1:A:320:THR:HG21	1.81	0.94
1:A:179:PRO:HB2	1:A:198:ILE:HG23	1.52	0.91
1:A:47:ARG:HG3	1:A:48:SER:H	1.36	0.91
2:B:82:LEU:HB2	2:B:85:GLU:HG3	1.55	0.88
1:A:465:THR:HG22	1:A:467:LEU:N	1.91	0.86
1:A:186:GLN:NE2	1:A:190:THR:H	1.73	0.85
1:A:539:ARG:HB3	1:A:541:ASP:HB2	1.59	0.85
1:A:261:PHE:CE1	1:A:318:ALA:HB2	2.12	0.84
2:B:232:MET:HE1	2:B:239:ILE:HD11	1.60	0.83
1:A:540:ASN:H	1:A:540:ASN:ND2	1.80	0.79
1:A:554:MET:HE3	1:A:632:VAL:HG21	1.64	0.79
2:B:315:GLU:CD	2:B:315:GLU:H	1.89	0.79
1:A:334:MET:HE2	1:A:334:MET:HA	1.63	0.79
1:A:505:PRO:HG2	1:A:507:HIS:HB3	1.65	0.79
1:A:182:HIS:HA	1:A:245:LEU:HD22	1.66	0.78
1:A:47:ARG:HB2	1:A:47:ARG:NH1	1.98	0.78
1:A:566:LEU:O	1:A:567:ARG:HD3	1.82	0.78
1:A:47:ARG:HG3	1:A:48:SER:N	1.99	0.78
1:A:272:ASN:ND2	1:A:377:LEU:HD22	1.99	0.77
1:A:565:ARG:HD3	1:A:567:ARG:NH2	2.00	0.77
2:B:267:CYS:SG	2:B:276:TYR:HB3	2.25	0.76
2:B:232:MET:HE3	2:B:232:MET:HA	1.66	0.76
2:B:518:HIS:CD2	2:B:520:TYR:HB2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:GLN:HE21	2:B:197:ASN:HD22	1.34	0.76
2:B:207:PRO:HG3	2:B:294:LEU:HD22	1.68	0.75
1:A:540:ASN:H	1:A:540:ASN:HD22	1.29	0.75
1:A:518:GLN:HE22	1:A:589:ARG:HA	1.50	0.74
2:B:354:THR:HG21	2:B:375:ILE:O	1.88	0.74
2:B:369:ILE:C	2:B:370:LEU:HD12	2.13	0.73
2:B:234:ARG:O	2:B:235:GLU:HG2	1.88	0.73
1:A:254:ARG:HH22	1:A:293:GLY:H	1.34	0.73
2:B:35:ILE:CD1	2:B:320:VAL:HG22	2.19	0.72
1:A:272:ASN:HD22	1:A:377:LEU:HD22	1.54	0.72
2:B:49:MET:HE1	2:B:467:ASN:HB3	1.71	0.72
1:A:540:ASN:HD22	1:A:540:ASN:N	1.86	0.72
2:B:75:HIS:CE1	2:B:80:LYS:HE2	2.24	0.72
2:B:30:ILE:HD13	2:B:343:GLU:HG2	1.72	0.71
1:A:272:ASN:HD21	1:A:377:LEU:HB2	1.55	0.71
2:B:425:LEU:O	2:B:429:VAL:HG23	1.89	0.71
2:B:467:ASN:HD22	2:B:468:ALA:N	1.88	0.71
2:B:74:ARG:O	2:B:77:ALA:HB3	1.92	0.70
2:B:433:ARG:NH2	2:B:554:GLU:HG3	2.06	0.70
2:B:44:ALA:O	2:B:47:ALA:HB3	1.91	0.70
1:A:152:PRO:HG2	1:A:338:THR:HB	1.73	0.70
2:B:160:ALA:CB	2:B:201:MET:HE1	2.21	0.70
1:A:285:VAL:HG12	1:A:286:VAL:HG23	1.74	0.70
2:B:420:LYS:O	2:B:420:LYS:HD3	1.90	0.70
1:A:198:ILE:CG2	1:A:248:LYS:HB2	2.22	0.69
1:A:282:HIS:O	1:A:283:GLN:HB2	1.90	0.69
1:A:347:THR:O	1:A:351:THR:HG23	1.92	0.69
1:A:404:LEU:HD23	1:A:626:LEU:HD21	1.73	0.69
1:A:304:GLU:O	1:A:307:VAL:HG12	1.92	0.69
1:A:586:SER:O	1:A:587:GLN:HB2	1.92	0.69
1:A:191:PHE:CZ	1:A:244:MET:HB3	2.28	0.69
2:B:212:VAL:HB	2:B:232:MET:CE	2.22	0.68
2:B:440:LEU:HB2	2:B:464:MET:HG2	1.74	0.68
2:B:518:HIS:ND1	2:B:519:PRO:HD2	2.08	0.68
1:A:224:LEU:HD23	1:A:224:LEU:O	1.93	0.68
2:B:48:THR:O	2:B:52:GLN:HG3	1.94	0.67
1:A:47:ARG:HH11	1:A:47:ARG:CB	2.02	0.66
1:A:50:GLN:HB2	1:A:123:GLN:NE2	2.11	0.66
2:B:78:ARG:HG3	2:B:78:ARG:HH11	1.60	0.66
1:A:186:GLN:HE22	1:A:189:GLU:H	1.42	0.66
2:B:232:MET:CE	2:B:239:ILE:HD11	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:SER:HB2	1:A:613:ARG:HG3	1.76	0.66
1:A:325:LEU:HD23	1:A:325:LEU:H	1.60	0.65
1:A:549:ARG:HG3	1:A:549:ARG:NH1	2.05	0.65
1:A:274:ARG:HH22	1:A:320:THR:CG2	2.01	0.65
1:A:48:SER:HA	1:A:364:ARG:HD3	1.77	0.65
2:B:212:VAL:CG1	2:B:232:MET:HE1	2.27	0.64
2:B:212:VAL:HB	2:B:232:MET:HE3	1.79	0.64
2:B:305:ARG:HG3	2:B:361:HIS:CD2	2.32	0.64
1:A:337:ASN:HD22	1:A:341:GLN:NE2	1.96	0.64
1:A:136:ALA:HB1	1:A:154:ALA:HB1	1.80	0.63
1:A:310:ALA:O	1:A:313:ILE:HD12	1.99	0.63
1:A:525:ARG:NH1	1:A:531:ASP:CG	2.57	0.63
1:A:378:ASN:O	1:A:440:TRP:CH2	2.51	0.62
1:A:165:ALA:O	1:A:168:ALA:HB3	2.00	0.62
2:B:451:GLY:O	2:B:452:MET:HB2	1.98	0.62
1:A:50:GLN:H	1:A:123:GLN:HG3	1.63	0.61
1:A:302:MET:HG2	1:A:331:PHE:CD2	2.36	0.61
1:A:549:ARG:HH11	1:A:549:ARG:CG	2.05	0.61
1:A:280:ARG:O	1:A:281:ARG:C	2.43	0.61
2:B:160:ALA:HB3	2:B:201:MET:HE1	1.82	0.61
1:A:128:GLY:O	1:A:133:SER:HB3	2.00	0.61
1:A:315:TYR:OH	1:A:338:THR:HA	2.01	0.61
1:A:302:MET:HE3	1:A:331:PHE:HB2	1.83	0.61
1:A:343:GLU:CD	1:A:343:GLU:H	2.08	0.61
2:B:31:LEU:HD13	2:B:336:ALA:HB2	1.82	0.61
1:A:565:ARG:HG2	1:A:567:ARG:NE	2.16	0.60
2:B:157:GLN:NE2	2:B:197:ASN:ND2	2.35	0.60
1:A:418:SER:HB3	1:A:435:ALA:HB2	1.83	0.60
1:A:390:ASP:CG	1:A:464:ARG:HD2	2.27	0.60
1:A:485:ASP:CG	1:A:491:ARG:HH22	2.10	0.60
2:B:53:VAL:HG12	2:B:57:ARG:NH1	2.16	0.59
1:A:82:ILE:HD11	1:A:101:ALA:CB	2.32	0.59
2:B:521:TYR:CE1	2:B:525:ARG:CZ	2.85	0.59
2:B:89:ARG:HH21	2:B:89:ARG:HG3	1.67	0.59
1:A:50:GLN:H	1:A:123:GLN:CG	2.15	0.59
1:A:272:ASN:ND2	1:A:377:LEU:HB2	2.18	0.59
1:A:186:GLN:HE22	1:A:190:THR:H	1.51	0.59
1:A:337:ASN:ND2	1:A:341:GLN:NE2	2.51	0.59
2:B:103:LEU:O	2:B:524:ALA:HA	2.03	0.59
1:A:269:LEU:HB2	1:A:372:GLN:NE2	2.18	0.58
1:A:384:VAL:CG1	1:A:470:LEU:HD13	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:HIS:C	1:A:570:SER:H	2.10	0.58
1:A:489:ILE:CG2	1:A:490:ALA:N	2.66	0.58
1:A:545:SER:O	2:B:536:GLN:NE2	2.33	0.58
2:B:403:ASN:C	2:B:403:ASN:HD22	2.10	0.58
1:A:99:GLY:HA2	1:A:112:ARG:HH12	1.69	0.58
1:A:310:ALA:HA	1:A:313:ILE:HD11	1.85	0.58
2:B:35:ILE:O	2:B:37:PRO:HD3	2.03	0.58
2:B:463:TRP:HH2	2:B:544:ALA:HB2	1.69	0.58
2:B:82:LEU:O	2:B:86:ARG:HG3	2.04	0.58
2:B:216:CYS:SG	2:B:239:ILE:HD12	2.44	0.58
1:A:198:ILE:HG22	1:A:248:LYS:HB2	1.85	0.58
1:A:635:ILE:O	1:A:639:GLU:HG3	2.04	0.58
2:B:86:ARG:NH2	2:B:280:ASP:OD2	2.30	0.58
2:B:440:LEU:HD12	2:B:464:MET:CG	2.34	0.58
1:A:437:LEU:HD22	1:A:455:LEU:HD23	1.86	0.57
1:A:232:GLN:HG2	1:A:233:ARG:N	2.19	0.57
1:A:637:GLU:O	1:A:638:ALA:C	2.48	0.57
1:A:186:GLN:HB3	1:A:190:THR:HB	1.86	0.57
2:B:239:ILE:HG22	2:B:239:ILE:O	2.03	0.57
2:B:348:LYS:O	2:B:383:LYS:HE2	2.04	0.57
2:B:152:LYS:HA	2:B:526:LEU:HD11	1.85	0.57
2:B:376:LEU:HD21	2:B:425:LEU:HD23	1.85	0.57
1:A:280:ARG:NH1	1:A:283:GLN:HE22	2.03	0.56
1:A:377:LEU:O	1:A:377:LEU:HG	2.03	0.56
2:B:403:ASN:CG	2:B:442:GLY:HA3	2.29	0.56
1:A:203:LEU:HD11	1:A:215:MET:HG2	1.87	0.56
1:A:99:GLY:HA2	1:A:112:ARG:NH1	2.20	0.56
1:A:105:ASP:HA	1:A:109:ARG:HD2	1.88	0.56
1:A:269:LEU:CD2	1:A:368:LEU:HD13	2.35	0.56
1:A:285:VAL:HG12	1:A:286:VAL:CG2	2.34	0.56
2:B:152:LYS:CA	2:B:526:LEU:HD11	2.35	0.56
1:A:149:PHE:O	1:A:151:GLY:N	2.38	0.56
1:A:188:LEU:H	1:A:188:LEU:HD23	1.70	0.56
1:A:400:GLY:CA	1:A:463:LEU:HD21	2.35	0.56
1:A:53:LEU:C	1:A:53:LEU:HD23	2.31	0.56
1:A:563:CYS:SG	2:B:89:ARG:NH1	2.78	0.56
1:A:390:ASP:OD1	1:A:464:ARG:HD2	2.05	0.56
1:A:514:GLU:HG3	1:A:588:TYR:CD1	2.41	0.56
2:B:272:VAL:O	2:B:272:VAL:CG1	2.54	0.56
1:A:350:ILE:HD12	1:A:377:LEU:CD1	2.35	0.56
1:A:198:ILE:HG22	1:A:198:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ALA:CB	1:A:564:VAL:HG11	2.36	0.55
2:B:381:ALA:HA	2:B:425:LEU:HD22	1.88	0.55
2:B:403:ASN:ND2	2:B:443:GLY:H	2.04	0.55
1:A:185:ALA:HB1	1:A:244:MET:H	1.71	0.55
1:A:290:PRO:HD2	1:A:380:HIS:ND1	2.21	0.55
2:B:42:PHE:CE1	2:B:319:GLY:HA3	2.42	0.55
1:A:525:ARG:HH12	1:A:531:ASP:CG	2.14	0.55
1:A:54:VAL:CG1	1:A:64:VAL:HG11	2.37	0.55
1:A:169:LEU:HD13	1:A:313:ILE:HG23	1.89	0.55
1:A:186:GLN:CG	1:A:187:ASP:H	2.19	0.55
1:A:466:ASN:O	1:A:470:LEU:HG	2.07	0.55
1:A:378:ASN:O	1:A:440:TRP:HH2	1.88	0.55
1:A:496:LEU:C	1:A:498:PRO:HD3	2.32	0.55
2:B:160:ALA:HB1	2:B:201:MET:HE1	1.89	0.54
1:A:198:ILE:HD12	1:A:246:VAL:HG12	1.89	0.54
2:B:157:GLN:HE22	2:B:197:ASN:HD22	1.50	0.54
2:B:351:PHE:O	2:B:383:LYS:HE3	2.07	0.54
1:A:384:VAL:HG13	1:A:470:LEU:HD22	1.90	0.54
1:A:176:PRO:C	1:A:177:LEU:HD23	2.33	0.54
1:A:554:MET:HG2	2:B:89:ARG:HH11	1.73	0.54
1:A:189:GLU:HA	1:A:189:GLU:OE1	2.06	0.54
1:A:104:ALA:HA	1:A:108:LEU:HD12	1.90	0.54
1:A:268:CYS:CB	1:A:311:GLN:HE22	2.21	0.54
1:A:53:LEU:HD13	1:A:117:ALA:HB2	1.90	0.54
1:A:82:ILE:HD11	1:A:101:ALA:HB1	1.90	0.54
1:A:186:GLN:CD	1:A:187:ASP:H	2.15	0.54
1:A:232:GLN:N	1:A:232:GLN:NE2	2.55	0.54
2:B:291:VAL:HG13	2:B:294:LEU:HD12	1.90	0.54
2:B:375:ILE:HD12	2:B:375:ILE:N	2.23	0.54
1:A:231:ALA:C	1:A:232:GLN:HE21	2.15	0.53
1:A:485:ASP:OD1	1:A:491:ARG:NH2	2.39	0.53
2:B:219:GLY:O	2:B:221:ALA:N	2.41	0.53
2:B:467:ASN:C	2:B:467:ASN:ND2	2.66	0.53
2:B:467:ASN:HD22	2:B:467:ASN:C	2.16	0.53
1:A:546:ALA:HB3	2:B:60:LEU:CD1	2.39	0.53
2:B:42:PHE:O	2:B:45:ASN:N	2.42	0.53
1:A:220:ARG:HA	1:A:220:ARG:CZ	2.38	0.53
1:A:251:LEU:CD1	1:A:251:LEU:N	2.72	0.53
1:A:284:LYS:O	1:A:385:ARG:HD2	2.09	0.53
2:B:382:GLN:O	2:B:383:LYS:C	2.52	0.53
2:B:525:ARG:HH11	2:B:525:ARG:HG3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PRO:HA	1:A:106:SER:OG	2.08	0.53
1:A:269:LEU:HA	1:A:372:GLN:HE22	1.74	0.53
2:B:71:ALA:HA	2:B:74:ARG:HD3	1.91	0.53
1:A:251:LEU:O	1:A:252:LYS:C	2.51	0.53
1:A:302:MET:HE3	1:A:331:PHE:CB	2.39	0.52
1:A:302:MET:HE2	1:A:323:PHE:CD2	2.44	0.52
1:A:320:THR:HG21	1:A:341:GLN:HG3	1.91	0.52
1:A:265:HIS:N	1:A:265:HIS:CD2	2.75	0.52
1:A:565:ARG:CD	1:A:567:ARG:NH2	2.72	0.52
2:B:201:MET:HE2	2:B:206:ILE:HG21	1.92	0.52
1:A:134:GLU:HG2	1:A:338:THR:OG1	2.09	0.52
2:B:221:ALA:CB	2:B:241:LEU:HD23	2.40	0.52
1:A:114:ILE:HG13	1:A:147:LEU:CD1	2.40	0.52
1:A:513:ALA:HA	1:A:555:LEU:HD11	1.91	0.52
2:B:440:LEU:HD12	2:B:464:MET:HG2	1.91	0.52
2:B:464:MET:HE2	2:B:519:PRO:HB3	1.92	0.52
2:B:119:ILE:HG23	2:B:152:LYS:HE2	1.91	0.52
1:A:140:ARG:C	1:A:140:ARG:HD3	2.35	0.52
2:B:464:MET:HE3	2:B:468:ALA:HB3	1.92	0.52
2:B:522:SER:HB2	2:B:527:TRP:HB2	1.90	0.52
1:A:81:ASP:O	1:A:84:ARG:HG2	2.09	0.51
1:A:325:LEU:HD23	1:A:325:LEU:N	2.25	0.51
2:B:519:PRO:O	2:B:523:SER:HB2	2.10	0.51
1:A:280:ARG:NH1	1:A:283:GLN:NE2	2.58	0.51
1:A:379:GLY:CA	1:A:440:TRP:CH2	2.82	0.51
1:A:622:TRP:CD1	1:A:623:GLU:HG2	2.46	0.51
2:B:212:VAL:HB	2:B:232:MET:HE1	1.90	0.51
1:A:47:ARG:HG2	1:A:148:LEU:HD11	1.92	0.51
1:A:517:LEU:HB2	1:A:553:LEU:HD11	1.92	0.51
1:A:596:ASP:HB3	1:A:612:LEU:HG	1.93	0.51
2:B:420:LYS:C	2:B:420:LYS:CD	2.84	0.51
1:A:204:LEU:HB2	1:A:216:LYS:HB3	1.93	0.51
1:A:333:PHE:CZ	1:A:335:GLU:HA	2.46	0.51
2:B:216:CYS:SG	2:B:239:ILE:CD1	2.99	0.51
1:A:261:PHE:O	1:A:269:LEU:HD23	2.11	0.51
2:B:105:ALA:O	2:B:106:HIS:C	2.54	0.51
2:B:403:ASN:C	2:B:403:ASN:ND2	2.66	0.51
1:A:441:GLY:HA3	1:A:446:GLU:HB3	1.93	0.50
1:A:554:MET:HG2	2:B:89:ARG:NH1	2.26	0.50
1:A:114:ILE:CD1	1:A:142:CYS:HA	2.42	0.50
1:A:200:TYR:O	1:A:202:VAL:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:ASN:ND2	2:B:468:ALA:N	2.58	0.50
1:A:108:LEU:HD23	1:A:132:LEU:HD13	1.92	0.50
1:A:302:MET:HG2	1:A:331:PHE:CE2	2.46	0.50
2:B:376:LEU:HD21	2:B:425:LEU:CD2	2.42	0.50
1:A:549:ARG:NH1	1:A:549:ARG:CG	2.66	0.50
1:A:566:LEU:C	1:A:567:ARG:HD3	2.35	0.49
1:A:150:LEU:HD12	1:A:150:LEU:H	1.76	0.49
1:A:182:HIS:HA	1:A:245:LEU:CD2	2.41	0.49
1:A:191:PHE:CE2	1:A:244:MET:HB3	2.47	0.49
1:A:350:ILE:HD12	1:A:377:LEU:HD13	1.94	0.49
2:B:212:VAL:O	2:B:233:VAL:HG23	2.12	0.49
2:B:369:ILE:HG22	2:B:370:LEU:N	2.27	0.49
1:A:232:GLN:N	1:A:232:GLN:HE21	2.10	0.49
1:A:280:ARG:HH11	1:A:283:GLN:HE22	1.59	0.49
2:B:232:MET:SD	2:B:239:ILE:HG13	2.52	0.49
1:A:565:ARG:CG	1:A:567:ARG:HH21	2.26	0.49
1:A:531:ASP:OD2	2:B:298:LYS:N	2.34	0.49
2:B:220:GLY:O	2:B:224:PRO:HD2	2.12	0.49
1:A:114:ILE:HG13	1:A:147:LEU:HD12	1.94	0.48
1:A:505:PRO:C	1:A:507:HIS:N	2.66	0.48
2:B:30:ILE:CD1	2:B:343:GLU:HG2	2.40	0.48
2:B:403:ASN:ND2	2:B:442:GLY:HA3	2.28	0.48
1:A:64:VAL:HG13	1:A:65:MET:N	2.28	0.48
1:A:194:GLU:O	1:A:197:ARG:HG2	2.13	0.48
1:A:565:ARG:HG2	1:A:567:ARG:CZ	2.43	0.48
2:B:239:ILE:HG21	2:B:270:SER:OG	2.13	0.48
2:B:468:ALA:O	2:B:519:PRO:HG3	2.13	0.48
1:A:522:GLY:O	1:A:523:HIS:HB3	2.13	0.48
2:B:468:ALA:O	2:B:469:ARG:NH2	2.46	0.48
1:A:152:PRO:HG3	1:A:315:TYR:OH	2.14	0.48
1:A:505:PRO:C	1:A:507:HIS:H	2.20	0.48
1:A:525:ARG:NH1	2:B:298:LYS:HG3	2.28	0.48
2:B:53:VAL:HG21	2:B:318:TYR:CE1	2.48	0.48
1:A:440:TRP:CD1	1:A:440:TRP:C	2.90	0.48
1:A:554:MET:HE3	1:A:632:VAL:CG2	2.39	0.48
1:A:187:ASP:OD1	1:A:188:LEU:HD23	2.14	0.48
1:A:587:GLN:HB3	1:A:588:TYR:CD1	2.49	0.48
2:B:152:LYS:HA	2:B:526:LEU:CD1	2.44	0.48
1:A:169:LEU:HD13	1:A:313:ILE:CG2	2.44	0.47
1:A:513:ALA:HB2	1:A:564:VAL:HG11	1.95	0.47
1:A:565:ARG:CG	1:A:567:ARG:NH2	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:LYS:HD3	2:B:420:LYS:C	2.39	0.47
1:A:478:ALA:O	1:A:483:GLU:HG3	2.14	0.47
1:A:152:PRO:HB3	1:A:315:TYR:CE2	2.50	0.47
1:A:170:MET:HB3	1:A:177:LEU:HD21	1.97	0.47
1:A:206:ALA:O	1:A:245:LEU:HG	2.15	0.47
1:A:281:ARG:O	1:A:282:HIS:O	2.33	0.47
1:A:378:ASN:O	1:A:440:TRP:CZ3	2.67	0.47
1:A:401:ARG:NE	1:A:423:GLY:O	2.48	0.47
1:A:332:PHE:CD1	1:A:332:PHE:N	2.82	0.47
1:A:554:MET:HG2	2:B:89:ARG:HE	1.80	0.47
2:B:31:LEU:CD1	2:B:336:ALA:HB2	2.44	0.47
2:B:89:ARG:HG3	2:B:89:ARG:NH2	2.29	0.47
2:B:316:GLU:O	2:B:320:VAL:HG23	2.15	0.47
1:A:256:VAL:O	1:A:323:PHE:HB2	2.14	0.47
1:A:516:TRP:CZ3	1:A:630:GLU:HA	2.50	0.47
1:A:274:ARG:HG2	1:A:289:ALA:HB2	1.96	0.46
1:A:439:ALA:HB3	1:A:451:LEU:HB2	1.96	0.46
1:A:513:ALA:O	1:A:514:GLU:C	2.57	0.46
2:B:354:THR:HG22	2:B:374:GLY:HA3	1.97	0.46
2:B:402:GLN:NE2	2:B:440:LEU:HD22	2.31	0.46
1:A:251:LEU:N	1:A:251:LEU:HD12	2.29	0.46
1:A:319:GLY:HA2	1:A:339:ARG:O	2.16	0.46
2:B:468:ALA:O	2:B:519:PRO:CG	2.64	0.46
1:A:399:SER:HB3	1:A:426:VAL:O	2.15	0.46
2:B:49:MET:HE1	2:B:467:ASN:CB	2.43	0.46
1:A:546:ALA:HB3	2:B:60:LEU:HD12	1.96	0.46
2:B:48:THR:O	2:B:51:GLU:HB3	2.15	0.46
1:A:465:THR:CG2	1:A:467:LEU:HB2	2.45	0.46
2:B:35:ILE:HD11	2:B:320:VAL:HG13	1.98	0.46
2:B:161:LEU:N	2:B:201:MET:HE3	2.31	0.46
2:B:212:VAL:CB	2:B:232:MET:HE1	2.46	0.46
1:A:273:GLU:OE1	1:A:273:GLU:N	2.44	0.46
1:A:181:TYR:HB3	1:A:246:VAL:HB	1.98	0.46
1:A:187:ASP:OD1	1:A:188:LEU:N	2.49	0.46
1:A:203:LEU:HG	1:A:204:LEU:H	1.81	0.46
1:A:396:LEU:O	1:A:398:ALA:N	2.49	0.46
1:A:287:GLU:HG2	1:A:343:GLU:CB	2.46	0.46
1:A:539:ARG:C	1:A:541:ASP:H	2.21	0.46
2:B:97:PHE:CZ	2:B:122:GLY:HA3	2.51	0.46
2:B:219:GLY:O	2:B:220:GLY:C	2.59	0.46
1:A:309:ALA:O	1:A:312:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:PHE:CZ	1:A:489:ILE:HD11	2.51	0.46
2:B:276:TYR:CD2	2:B:276:TYR:N	2.81	0.46
1:A:87:ARG:O	1:A:91:GLU:HG3	2.16	0.45
1:A:198:ILE:HD12	1:A:246:VAL:CG1	2.46	0.45
1:A:226:GLU:CD	1:A:226:GLU:O	2.60	0.45
1:A:610:ALA:HB3	1:A:621:GLU:HB2	1.98	0.45
2:B:440:LEU:HD12	2:B:464:MET:SD	2.56	0.45
1:A:164:SER:O	1:A:167:LYS:N	2.49	0.45
1:A:503:ALA:C	1:A:504:LEU:HG	2.41	0.45
1:A:300:ARG:O	1:A:304:GLU:HG3	2.17	0.45
1:A:637:GLU:C	1:A:639:GLU:N	2.73	0.45
2:B:222:TYR:O	2:B:223:VAL:C	2.59	0.45
1:A:152:PRO:HG3	1:A:315:TYR:CZ	2.51	0.45
2:B:455:ARG:HH22	2:B:529:ASP:CG	2.24	0.45
1:A:150:LEU:HD12	1:A:150:LEU:N	2.31	0.45
1:A:194:GLU:O	1:A:198:ILE:HG13	2.16	0.45
1:A:396:LEU:HA	1:A:397:PRO:HD3	1.89	0.45
1:A:497:LEU:O	1:A:498:PRO:O	2.35	0.45
1:A:613:ARG:O	1:A:614:ARG:HD2	2.17	0.45
1:A:532:ASP:OD1	2:B:298:LYS:NZ	2.44	0.45
2:B:225:ALA:HA	2:B:272:VAL:HG22	1.99	0.45
2:B:397:PRO:HG2	2:B:545:LEU:HD21	1.99	0.45
1:A:232:GLN:HG2	1:A:233:ARG:H	1.82	0.45
1:A:287:GLU:CD	1:A:343:GLU:HB3	2.41	0.45
1:A:232:GLN:C	1:A:233:ARG:HG2	2.42	0.45
2:B:193:ARG:O	2:B:196:PHE:HB3	2.16	0.45
1:A:103:PRO:HA	1:A:106:SER:HG	1.81	0.44
1:A:287:GLU:HG2	1:A:343:GLU:HG3	1.99	0.44
1:A:465:THR:HG21	1:A:467:LEU:HB2	1.99	0.44
1:A:539:ARG:HH12	1:A:543:TRP:HB2	1.81	0.44
2:B:212:VAL:HG11	2:B:232:MET:HE1	2.00	0.44
1:A:186:GLN:NE2	1:A:187:ASP:N	2.65	0.44
1:A:190:THR:HA	1:A:193:ARG:NH1	2.32	0.44
1:A:269:LEU:HB2	1:A:372:GLN:HE22	1.81	0.44
1:A:516:TRP:CZ2	1:A:631:ALA:HB2	2.53	0.44
1:A:469:PHE:HZ	1:A:489:ILE:HD11	1.83	0.44
1:A:491:ARG:HD2	1:A:492:HIS:CE1	2.52	0.44
2:B:291:VAL:HA	2:B:294:LEU:CD1	2.48	0.44
1:A:451:LEU:HG	1:A:474:LEU:CD1	2.48	0.44
1:A:503:ALA:O	1:A:504:LEU:CB	2.65	0.44
1:A:140:ARG:O	1:A:143:GLU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLU:O	1:A:346:VAL:HG22	2.17	0.44
1:A:552:ASP:O	1:A:553:LEU:HD23	2.18	0.44
1:A:378:ASN:C	1:A:440:TRP:HH2	2.26	0.44
1:A:462:GLY:O	1:A:463:LEU:HD23	2.17	0.44
2:B:464:MET:HE2	2:B:464:MET:HB3	1.75	0.44
1:A:61:ALA:O	1:A:65:MET:HB2	2.18	0.44
2:B:207:PRO:CG	2:B:294:LEU:HD22	2.42	0.44
1:A:565:ARG:HG2	1:A:567:ARG:HE	1.80	0.44
2:B:136:ASN:HB2	2:B:172:ASP:O	2.18	0.44
1:A:269:LEU:CB	1:A:372:GLN:HE22	2.31	0.43
1:A:382:ILE:HD12	1:A:448:ARG:HA	2.00	0.43
2:B:66:GLY:HA2	2:B:115:ALA:HB3	1.99	0.43
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.84	0.43
1:A:176:PRO:O	1:A:177:LEU:HD23	2.17	0.43
1:A:344:HIS:N	1:A:345:PRO:CD	2.81	0.43
1:A:525:ARG:HH11	1:A:531:ASP:HB2	1.83	0.43
1:A:49:ILE:HD13	1:A:124:ALA:CB	2.49	0.43
2:B:35:ILE:HD12	2:B:333:GLU:HB3	2.00	0.43
1:A:367:ALA:O	1:A:368:LEU:C	2.61	0.43
1:A:554:MET:HG2	2:B:89:ARG:NE	2.33	0.43
1:A:565:ARG:HD3	1:A:567:ARG:HH21	1.81	0.43
1:A:298:LEU:O	1:A:302:MET:HG3	2.19	0.43
2:B:166:PRO:HB3	2:B:207:PRO:HG2	2.00	0.43
2:B:369:ILE:O	2:B:370:LEU:HD12	2.18	0.43
1:A:108:LEU:HD23	1:A:132:LEU:CD1	2.48	0.43
1:A:547:LEU:HD12	2:B:64:HIS:CE1	2.53	0.43
1:A:268:CYS:HB3	1:A:311:GLN:HE22	1.84	0.43
2:B:178:LEU:HB2	2:B:179:PRO:HD3	2.01	0.43
1:A:49:ILE:HD13	1:A:124:ALA:HB3	2.00	0.43
2:B:119:ILE:HA	2:B:135:GLY:O	2.18	0.43
1:A:489:ILE:HG23	1:A:490:ALA:N	2.33	0.43
1:A:334:MET:HA	1:A:334:MET:CE	2.43	0.43
1:A:387:TYR:HB3	1:A:389:GLU:HG3	2.01	0.43
1:A:400:GLY:HA3	1:A:463:LEU:HD21	2.01	0.43
1:A:418:SER:HB3	1:A:435:ALA:CB	2.48	0.43
2:B:439:VAL:HA	2:B:463:TRP:O	2.18	0.43
1:A:53:LEU:HD23	1:A:54:VAL:N	2.34	0.42
1:A:414:ARG:HG2	1:A:454:MET:SD	2.59	0.42
1:A:452:LEU:HD12	1:A:474:LEU:HB2	2.00	0.42
2:B:105:ALA:O	2:B:108:VAL:HB	2.19	0.42
2:B:216:CYS:SG	2:B:239:ILE:HA	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:GLU:CD	2:B:315:GLU:N	2.67	0.42
2:B:305:ARG:O	2:B:364:GLY:HA3	2.19	0.42
1:A:386:LEU:HD11	1:A:465:THR:CG2	2.48	0.42
2:B:238:THR:HB	2:B:240:PHE:HD2	1.83	0.42
1:A:109:ARG:HH11	1:A:112:ARG:CZ	2.33	0.42
1:A:320:THR:CG2	1:A:341:GLN:HG3	2.49	0.42
1:A:512:ALA:HB1	1:A:629:ILE:HD13	2.02	0.42
1:A:556:ARG:HB2	1:A:632:VAL:HG22	2.01	0.42
1:A:557:CYS:O	1:A:558:ARG:HB2	2.20	0.42
2:B:114:VAL:HG12	2:B:117:ALA:HA	2.02	0.42
2:B:213:MET:CE	2:B:284:LEU:HG	2.50	0.42
2:B:232:MET:O	2:B:277:ALA:N	2.51	0.42
1:A:313:ILE:HD12	1:A:313:ILE:H	1.85	0.42
1:A:258:ILE:CG2	1:A:270:TYR:HB2	2.50	0.42
1:A:277:SER:O	1:A:279:GLN:HG3	2.19	0.42
1:A:437:LEU:HD12	1:A:437:LEU:N	2.34	0.42
2:B:521:TYR:CE1	2:B:525:ARG:NH2	2.88	0.42
1:A:114:ILE:HD11	1:A:142:CYS:HA	2.02	0.42
1:A:129:TYR:OH	1:A:433:MET:HE1	2.19	0.42
2:B:311:LEU:HG	2:B:342:SER:HB2	2.02	0.42
1:A:180:GLY:O	1:A:181:TYR:HB2	2.20	0.42
1:A:202:VAL:HG22	1:A:203:LEU:N	2.35	0.42
2:B:191:PHE:C	2:B:193:ARG:H	2.28	0.42
2:B:371:ALA:HB2	2:B:401:LEU:HB2	2.02	0.42
2:B:436:LYS:O	2:B:460:ARG:N	2.48	0.42
1:A:54:VAL:HG13	1:A:64:VAL:HG11	2.01	0.42
1:A:89:VAL:HG13	1:A:95:ALA:CB	2.50	0.42
2:B:418:ILE:HG23	2:B:419:ALA:H	1.84	0.42
1:A:52:LEU:HD12	1:A:53:LEU:N	2.34	0.41
1:A:167:LYS:HG3	1:A:177:LEU:CD1	2.50	0.41
1:A:171:GLU:HG3	1:A:177:LEU:HD11	2.01	0.41
2:B:142:GLY:O	2:B:174:GLY:N	2.52	0.41
2:B:168:ILE:HD11	2:B:291:VAL:HG21	2.01	0.41
2:B:402:GLN:NE2	2:B:440:LEU:CD2	2.83	0.41
2:B:459:PRO:O	2:B:460:ARG:C	2.63	0.41
1:A:186:GLN:CD	1:A:190:THR:H	2.23	0.41
1:A:505:PRO:CG	1:A:507:HIS:HB3	2.43	0.41
1:A:269:LEU:CB	1:A:372:GLN:NE2	2.83	0.41
1:A:311:GLN:CA	1:A:311:GLN:HE21	2.33	0.41
1:A:554:MET:CE	1:A:632:VAL:HG21	2.41	0.41
2:B:164:ARG:O	2:B:164:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:TYR:HA	2:B:225:ALA:HB3	2.02	0.41
2:B:226:MET:HE3	2:B:226:MET:HB3	1.88	0.41
1:A:177:LEU:O	1:A:179:PRO:HD3	2.20	0.41
1:A:440:TRP:CG	1:A:441:GLY:N	2.87	0.41
2:B:39:SER:OG	2:B:40:ALA:N	2.53	0.41
2:B:238:THR:HB	2:B:240:PHE:CD2	2.55	0.41
2:B:355:LEU:HD12	2:B:355:LEU:HA	1.88	0.41
1:A:114:ILE:HD12	1:A:142:CYS:HA	2.03	0.41
1:A:203:LEU:HG	1:A:204:LEU:N	2.35	0.41
1:A:344:HIS:ND1	1:A:345:PRO:HD3	2.36	0.41
1:A:519:SER:CB	1:A:613:ARG:HG3	2.46	0.41
2:B:536:GLN:HG2	2:B:539:GLU:OE1	2.20	0.41
1:A:224:LEU:HA	1:A:227:ALA:HB3	2.03	0.41
1:A:465:THR:HG22	1:A:467:LEU:CB	2.51	0.41
2:B:515:HIS:C	2:B:517:GLY:H	2.28	0.41
2:B:370:LEU:HD11	2:B:387:PHE:CD2	2.56	0.41
1:A:54:VAL:HG11	1:A:64:VAL:HG11	2.02	0.41
1:A:179:PRO:HD2	1:A:248:LYS:HD3	2.03	0.41
1:A:401:ARG:HD3	1:A:425:GLU:HG3	2.02	0.41
1:A:503:ALA:O	1:A:504:LEU:HB2	2.20	0.41
1:A:635:ILE:O	1:A:636:ALA:C	2.62	0.41
2:B:42:PHE:O	2:B:43:ALA:C	2.63	0.41
2:B:77:ALA:C	2:B:79:GLY:H	2.28	0.41
2:B:190:HIS:O	2:B:191:PHE:O	2.39	0.41
2:B:212:VAL:HG11	2:B:239:ILE:HD11	2.03	0.41
2:B:277:ALA:HB1	2:B:282:HIS:HB3	2.03	0.41
1:A:186:GLN:HB3	1:A:186:GLN:HE21	1.65	0.41
1:A:232:GLN:CG	1:A:233:ARG:H	2.34	0.41
1:A:333:PHE:CD1	1:A:333:PHE:C	2.99	0.41
1:A:364:ARG:NH1	1:A:366:GLU:OE1	2.54	0.41
1:A:386:LEU:HD11	1:A:465:THR:HG21	2.02	0.41
1:A:509:TRP:HB3	1:A:564:VAL:CG2	2.51	0.41
2:B:196:PHE:CZ	2:B:200:ASN:ND2	2.89	0.41
2:B:232:MET:SD	2:B:239:ILE:HD11	2.61	0.41
2:B:526:LEU:N	2:B:526:LEU:HD23	2.36	0.41
1:A:264:ARG:HH11	1:A:264:ARG:HG2	1.86	0.40
1:A:489:ILE:HG22	1:A:490:ALA:H	1.86	0.40
1:A:400:GLY:C	1:A:463:LEU:HD21	2.46	0.40
2:B:42:PHE:O	2:B:44:ALA:N	2.54	0.40
2:B:309:ALA:HA	2:B:310:PRO:HD3	1.92	0.40
2:B:525:ARG:HG3	2:B:525:ARG:NH1	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:O	1:A:63:ARG:HB3	2.22	0.40
1:A:269:LEU:CA	1:A:372:GLN:HE22	2.34	0.40
2:B:299:GLN:OE1	2:B:552:PRO:HD3	2.21	0.40
1:A:136:ALA:O	1:A:137:ASP:C	2.63	0.40
2:B:78:ARG:HG3	2:B:78:ARG:NH1	2.32	0.40
2:B:321:ILE:O	2:B:322:PRO:C	2.62	0.40
2:B:369:ILE:HG12	2:B:399:LEU:HB3	2.03	0.40
2:B:518:HIS:NE2	2:B:520:TYR:CG	2.89	0.40
1:A:372:GLN:HE21	1:A:372:GLN:HB2	1.68	0.40
2:B:59:LEU:HD12	2:B:59:LEU: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	552/655 (84%)	433 (78%)	88 (16%)	31 (6%)	1	4
2	B	425/555 (77%)	374 (88%)	39 (9%)	12 (3%)	4	15
All	All	977/1210 (81%)	807 (83%)	127 (13%)	43 (4%)	2	8

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ALA
1	A	164	SER
1	A	283	GLN
1	A	409	ALA
1	A	412	PRO
1	A	498	PRO
1	A	521	PRO
1	A	545	SER

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Mol	Chain	Res	Type
1	A	586	SER
2	B	191	PHE
2	B	452	MET
2	B	454	GLY
1	A	99	GLY
1	A	150	LEU
1	A	181	TYR
1	A	186	GLN
1	A	282	HIS
1	A	391	PRO
1	A	397	PRO
1	A	587	GLN
1	A	603	ASP
2	B	177	ASN
2	B	220	GLY
1	A	154	ALA
1	A	395	PHE
1	A	522	GLY
2	B	70	ALA
2	B	516	GLN
1	A	281	ARG
1	A	500	PRO
1	A	165	ALA
1	A	189	GLU
1	A	225	ALA
1	A	503	ALA
2	B	172	ASP
1	A	232	GLN
1	A	504	LEU
2	B	111	GLY
1	A	58	GLY
1	A	198	ILE
2	B	93	PRO
2	B	327	GLN
2	B	114	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	427/496 (86%)	387 (91%)	40 (9%)	8	26
2	B	331/418 (79%)	302 (91%)	29 (9%)	9	29
All	All	758/914 (83%)	689 (91%)	69 (9%)	9	28

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	65	MET
1	A	109	ARG
1	A	118	LEU
1	A	123	GLN
1	A	132	LEU
1	A	186	GLN
1	A	189	GLU
1	A	228	LEU
1	A	232	GLN
1	A	251	LEU
1	A	269	LEU
1	A	280	ARG
1	A	292	PRO
1	A	307	VAL
1	A	311	GLN
1	A	313	ILE
1	A	343	GLU
1	A	364	ARG
1	A	372	GLN
1	A	378	ASN
1	A	384	VAL
1	A	403	MET
1	A	412	PRO
1	A	425	GLU
1	A	434	LEU
1	A	440	TRP
1	A	443	THR
1	A	446	GLU
1	A	452	LEU
1	A	483	GLU
1	A	520	GLU
1	A	525	ARG
1	A	539	ARG

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Mol	Chain	Res	Type
1	A	540	ASN
1	A	541	ASP
1	A	559	ASP
1	A	560	GLU
1	A	616	ARG
1	A	617	GLN
2	B	30	ILE
2	B	48	THR
2	B	64	HIS
2	B	112	GLU
2	B	139	THR
2	B	141	LYS
2	B	148	LEU
2	B	213	MET
2	B	215	SER
2	B	216	CYS
2	B	234	ARG
2	B	270	SER
2	B	272	VAL
2	B	281	ASP
2	B	301	GLN
2	B	305	ARG
2	B	315	GLU
2	B	354	THR
2	B	373	ASN
2	B	403	ASN
2	B	418	ILE
2	B	420	LYS
2	B	455	ARG
2	B	467	ASN
2	B	523	SER
2	B	526	LEU
2	B	532	ILE
2	B	534	PRO
2	B	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	186	GLN
1	A	232	GLN

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Mol	Chain	Res	Type
1	A	265	HIS
1	A	272	ASN
1	A	283	GLN
1	A	311	GLN
1	A	337	ASN
1	A	372	GLN
1	A	493	GLN
1	A	501	GLN
1	A	507	HIS
1	A	518	GLN
1	A	540	ASN
1	A	617	GLN
2	B	36	ASN
2	B	64	HIS
2	B	106	HIS
2	B	157	GLN
2	B	177	ASN
2	B	236	GLN
2	B	301	GLN
2	B	327	GLN
2	B	361	HIS
2	B	373	ASN
2	B	402	GLN
2	B	403	ASN
2	B	467	ASN
2	B	536	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	558/655 (85%)	-0.01	9 (1%) 70 62	48, 87, 147, 168	0
2	B	437/555 (78%)	-0.18	25 (5%) 29 23	40, 63, 123, 172	0
All	All	995/1210 (82%)	-0.08	34 (3%) 48 39	40, 77, 142, 172	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	451	GLY	5.2
2	B	178	LEU	4.6
2	B	176	ALA	4.3
2	B	241	LEU	4.1
2	B	29	ALA	3.9
2	B	457	TYR	3.9
2	B	267	CYS	3.8
2	B	276	TYR	3.8
1	A	208	ALA	3.6
2	B	268	LYS	3.5
2	B	236	GLN	3.4
2	B	406	GLY	3.3
2	B	240	PHE	3.0
2	B	30	ILE	2.9
2	B	269	VAL	2.7
1	A	242	ALA	2.7
2	B	31	LEU	2.7
1	A	391	PRO	2.6
2	B	239	ILE	2.6
2	B	179	PRO	2.5
1	A	188	LEU	2.5
1	A	228	LEU	2.5
2	B	518	HIS	2.4
2	B	515	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	418	ILE	2.3
2	B	190	HIS	2.3
2	B	177	ASN	2.3
2	B	404	ILE	2.3
2	B	270	SER	2.2
2	B	405	THR	2.2
1	A	283	GLN	2.1
1	A	215	MET	2.1
1	A	201	PRO	2.1
1	A	571	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.