



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 07:17 PM EST

PDB ID : 3U9T  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

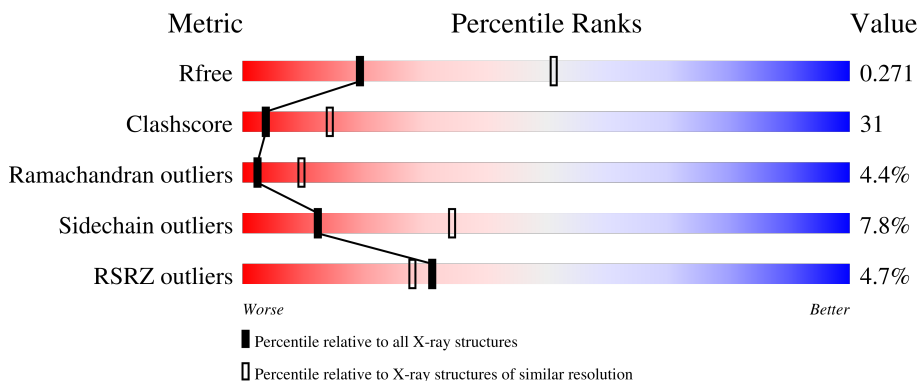
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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  $\geq 3$ , 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	
2	B	555	

## 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 Methylcrotonyl-CoA carboxylase, alpha-subunit.

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

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

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

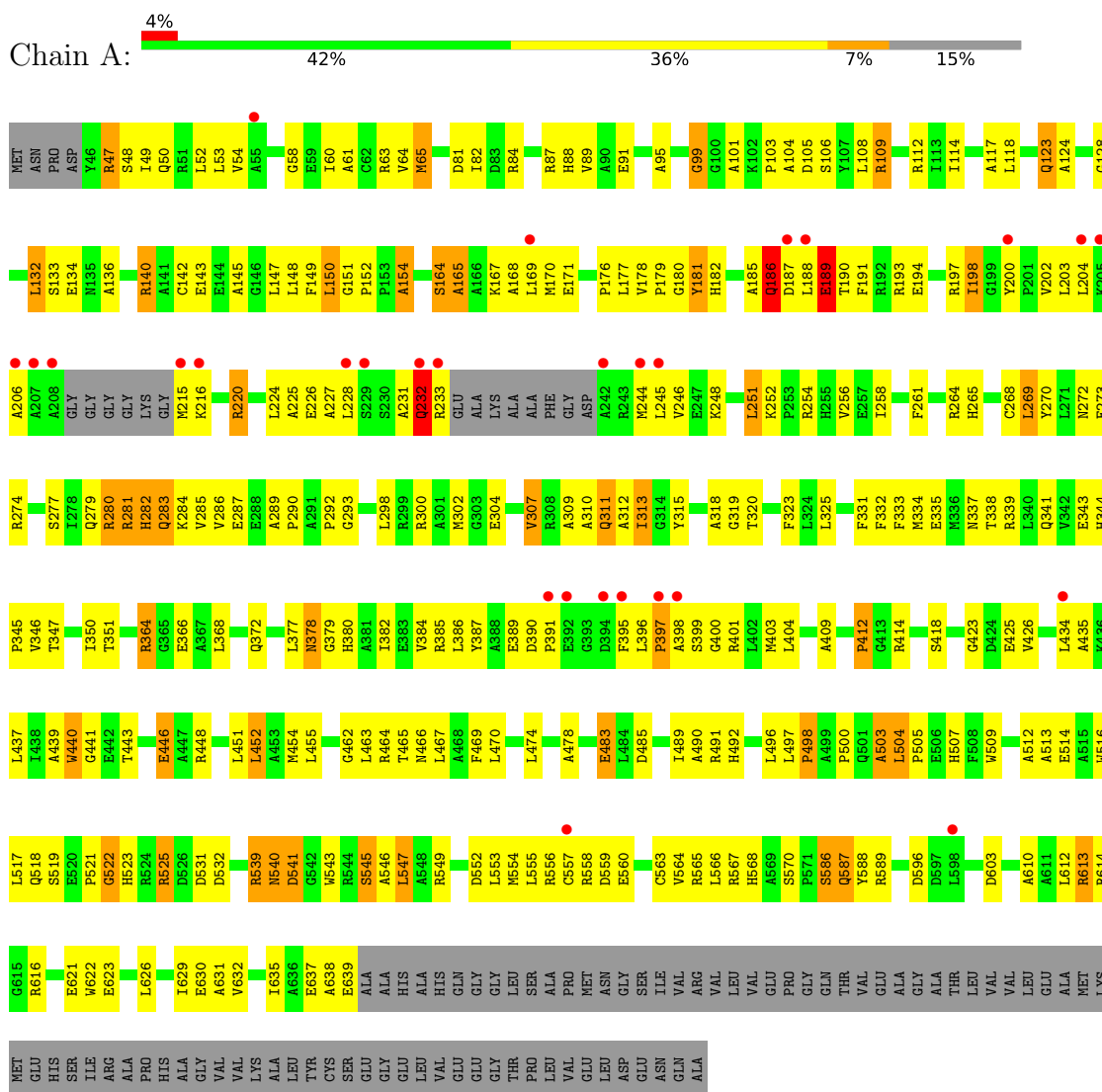
There are 20 discrepancies between the modelled and reference sequences:

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



VAL	GLU	GLU	ALA	LYS	LYS	ALA	PRO	ILE	LEU	GLN	TYR	GLU	H515	G516	H517	H518	F519	Y520	Y521	S522	S523	A524	R525	L526	W527	P534	A535	Q536	E539	A544	L545	P552	L553	E554	H563																		
K436	V439	L440	L441	G442	G443	SER	PHE	GLY	ALA	ASN	TYR	G451	M452	C453	G454	R455	A456	Y457	R460	W463	M464	M467	A468	R469	ILE	GLY	VAL	MET	GLY	GLY	GLU	GLN	ALA	ALA	VAL	LEU	ALA	GLN	VAL	VAL	LYS	ARG	GLU	GLN	ALA	ALA	ARG	ALA	GLY	GLN	LEU	GLY	
S342	E343	K348	F351	T354	L355	H361	G364	I369	L370	A371	N372	N373	G374	I375	L376	A381	Q382	K383	F387	P397	L398	L399	F400	L401	Q402	N403	I404	T405	G406	PHE	VAL	GLY	GLN	LYS	TYR	GLU	ALA	GLY	G417	I418	A419	K420	L425	V429	R433								
A176	M177	L178	P179	ARG	GLN	ASP	GLU	H190	F191	G192	R193	F196	M197	N200	Y108	V109	G111	E112	E113	A114	A115	M213	G214	S215	C216	G219	G220	A221	Y222	V223	P224	A225	M232	V233	R234	E235	Q236	A237	T238	I239	F240	L241	ALA	GLY	PRO	PRO	LEU	VAL	LYS	ALA	ALA		
THR	GLY	GLU	VAL	VAL	SER	ALA	GLU	GLU	LEU	GLY	GLY	ALA	ASP	VAL	HIS	C267	K268	V269	S270	G271	V272	A273	Y276	A277	D280	D281	H282	A283	L284	V291	L294	K298	Q299	Q301	R305	A309	P310	L311	E315	E316	L317	Y318	G319	V320	Q327	E333	A336						
A77	R78	G79	R80	L81	L82	E85	R86	R89	P93	F97	L103	A104	A105	H106	E107	Y108	G111	E112	E113	A114	A115	M116	A117	G118	I119	G122	G135	M136	T139	V140	K141	G142	K152	Q157	A160	L161	R164	L165	P166	C167	I168	D172	S173	G174	G175								
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	A29	I30	L31	I35	N36	P37	R38	S39	A40	F41	F42	A43	A44	N45	A46	A47	T48	M49	L50	E51	Q52	V53	R57	T58	L59	L60	H64	E65	G66	A70	A71	R74	H75	S76

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.93Å 158.93Å 311.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.23 – 2.90 46.22 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.9 (46.23-2.90) 93.0 (46.22-2.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.91Å)	Xtrriage
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 <sup>2</sup> )	70.2	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.49	0/4406	0.76	1/5958 (0.0%)
2	B	0.59	0/3380	0.79	1/4580 (0.0%)
All	All	0.54	0/7786	0.78	2/10538 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	454	GLY	N-CA-C	5.66	127.24	113.10
1	A	547	LEU	CA-CB-CG	-5.26	103.20	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	305	0
2	B	3312	0	3308	175	0
All	All	7635	0	7575	468	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 31.

All (468) 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
2:B:212:VAL:HB	2:B:232:MET:HE3	1.37	1.06
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
2:B:232:MET:HE1	2:B:239:ILE:HD11	1.50	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
1:A:540:ASN:H	1:A:540:ASN:ND2	1.80	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:518:HIS:CD2	2:B:520:TYR:HB2	2.20	0.76
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
2:B:315:GLU:CD	2:B:315:GLU:H	1.89	0.74
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:464:MET:HE2	2:B:519:PRO:HB3	1.72	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:334:MET:HE2	1:A:334:MET:HA	1.73	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:369:ILE:C	2:B:370:LEU:HD12	2.13	0.69
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:212:VAL:HB	2:B:232:MET:CE	2.22	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
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:232:MET:CE	2:B:239:ILE:HD11	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
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
1:A:525:ARG:NH1	1:A:531:ASP:CG	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:O	1:A:281:ARG:C	2.43	0.56
1:A:377:LEU:O	1:A:377:LEU:HG	2.03	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: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
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:485:ASP:CG	1:A:491:ARG:HH22	2.10	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:390:ASP:CG	1:A:464:ARG:HD2	2.27	0.55
1:A:466:ASN:O	1:A:470:LEU:HG	2.07	0.55
1:A:343:GLU:CD	1:A:343:GLU:H	2.08	0.55
1:A:378:ASN:O	1:A:440:TRP:HH2	1.88	0.55
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:554:MET:HG2	2:B:89:ARG:HH11	1.73	0.54
2:B:238:THR:HG1	2:B:240:PHE:HE2	1.54	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:568:HIS:C	1:A:570:SER:H	2.10	0.54
1:A:268:CYS:CB	1:A:311:GLN:HE22	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:403:ASN:C	2:B:403:ASN:HD22	2.10	0.54
1:A:554:MET:HE3	1:A:632:VAL:HG21	1.89	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
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:525:ARG:HH11	2:B:525:ARG:HG3	1.73	0.53
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:320:THR:HG21	1:A:341:GLN:HG3	1.91	0.52
2:B:213:MET:HE3	2:B:284:LEU:HG	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
1:A:637:GLU:O	1:A:638:ALA:C	2.48	0.52
2:B:403:ASN:CG	2:B:442:GLY:HA3	2.29	0.52
2:B:464:MET:HE3	2:B:468:ALA:HB3	1.90	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:119:ILE:HG23	2:B:152:LYS:HE2	1.91	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:53:LEU:C	1:A:53:LEU:HD23	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ASP:HB3	1:A:612:LEU:HG	1.93	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
1:A:441:GLY:HA3	1:A:446:GLU:HB3	1.93	0.50
1:A:554:MET:CE	1:A:632:VAL:HG21	2.41	0.50
1:A:525:ARG:HH12	1:A:531:ASP:CG	2.14	0.50
1:A:554:MET:HG2	2:B:89:ARG:NH1	2.26	0.50
2:B:160:ALA:HB3	2:B:201:MET:HE3	1.93	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
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
1:A:496:LEU:C	1:A:498:PRO:HD3	2.32	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: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:334:MET:HA	1:A:334:MET:CE	2.43	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:176:PRO:C	1:A:177:LEU:HD23	2.33	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:505:PRO:C	1:A:507:HIS:N	2.66	0.49
1:A:186:GLN:CD	1:A:187:ASP:H	2.15	0.49
1:A:565:ARG:CG	1:A:567:ARG:HH21	2.26	0.49
1:A:231:ALA:C	1:A:232:GLN:HE21	2.15	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
2:B:403:ASN:ND2	2:B:403:ASN:C	2.66	0.49
2:B:467:ASN:ND2	2:B:467:ASN:C	2.66	0.49
1:A:114:ILE:HG13	1:A:147:LEU:HD12	1.94	0.48
2:B:467:ASN:HD22	2:B:467:ASN:C	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:382:GLN:O	2:B:383:LYS:C	2.52	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:251:LEU:O	1:A:252:LYS:C	2.51	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: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
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:140:ARG:C	1:A:140:ARG:HD3	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:420:LYS:C	2:B:420:LYS:CD	2.84	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
2:B:105:ALA:O	2:B:106:HIS:C	2.54	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
2:B:97:PHE:CZ	2:B:122:GLY:HA3	2.51	0.46
1:A:309:ALA:O	1:A:312:ALA:HB3	2.15	0.46
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: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:300:ARG:O	1:A:304:GLU:HG3	2.17	0.45
1:A:152:PRO:HG3	1:A:315:TYR:CZ	2.51	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
2:B:464:MET:HE2	2:B:519:PRO:CB	2.44	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:566:LEU:C	1:A:567:ARG:HD3	2.35	0.45
1:A:65:MET:HE1	1:A:88:HIS:O	2.17	0.45
2:B:193:ARG:O	2:B:196:PHE:HB3	2.16	0.45
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:160:ALA:CB	2:B:201:MET:HE3	2.47	0.44
1:A:186:GLN:NE2	1:A:187:ASP:N	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:462:GLY:O	1:A:463:LEU:HD23	2.17	0.44
1:A:505:PRO:C	1:A:507:HIS:H	2.20	0.44
2:B:49:MET:CE	2:B:467:ASN:HB3	2.48	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: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
1:A:440:TRP:CD1	1:A:440:TRP:C	2.90	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
2:B:420:LYS:HD3	2:B:420:LYS:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:178:VAL:HG21	1:A:334:MET:HE1	2.01	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:315:GLU:CD	2:B:315:GLU:N	2.67	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
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
1:A:513:ALA:O	1:A:514:GLU:C	2.57	0.42
2:B:232:MET:HE2	2:B:233:VAL:H	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:ILE:HD11	2:B:291:VAL:HG21	2.01	0.41
2:B:213:MET:CE	2:B:284:LEU:HG	2.50	0.41
2:B:402:GLN:NE2	2:B:440:LEU:CD2	2.83	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:539:ARG:C	1:A:541:ASP:H	2.21	0.41
2:B:161:LEU:N	2:B:201:MET:HE3	2.34	0.41
2:B:164:ARG:O	2:B:164:ARG:HG2	2.20	0.41
2:B:222:TYR:HA	2:B:225:ALA:HB3	2.02	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:503:ALA:C	1:A:504:LEU:HG	2.41	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:219:GLY:O	2:B:220:GLY:C	2.59	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:226:GLU:O	1:A:226:GLU:CD	2.60	0.41
1:A:503:ALA:O	1:A:504:LEU:HB2	2.20	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: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
1:A:637:GLU:C	1:A:639:GLU:N	2.73	0.41
2:B:196:PHE:CZ	2:B:200:ASN:ND2	2.89	0.41
2:B:222:TYR:O	2:B:223:VAL:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:B:78:ARG:HG3	2:B:78:ARG:NH1	2.32	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:287:GLU:CD	1:A:343:GLU:HB3	2.41	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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	552/655 (84%)	433 (78%)	88 (16%)	31 (6%)	<b>2</b> <b>5</b>
2	B	425/555 (77%)	374 (88%)	39 (9%)	12 (3%)	<b>5</b> <b>19</b>
All	All	977/1210 (81%)	807 (83%)	127 (13%)	43 (4%)	<b>2</b> <b>10</b>

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ALA
1	A	164	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	283	GLN
1	A	409	ALA
1	A	412	PRO
1	A	498	PRO
1	A	521	PRO
1	A	545	SER
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%)	390 (91%)	37 (9%)	10	30
2	B	331/418 (79%)	309 (93%)	22 (7%)	16	44
All	All	758/914 (83%)	699 (92%)	59 (8%)	12	34

All (59) 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	140	ARG
1	A	186	GLN
1	A	189	GLU
1	A	220	ARG
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	364	ARG
1	A	378	ASN
1	A	403	MET
1	A	412	PRO
1	A	434	LEU
1	A	440	TRP
1	A	443	THR
1	A	446	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	452	LEU
1	A	483	GLU
1	A	525	ARG
1	A	539	ARG
1	A	540	ASN
1	A	541	ASP
1	A	559	ASP
1	A	560	GLU
1	A	613	ARG
1	A	616	ARG
2	B	36	ASN
2	B	48	THR
2	B	64	HIS
2	B	112	GLU
2	B	139	THR
2	B	141	LYS
2	B	215	SER
2	B	216	CYS
2	B	270	SER
2	B	281	ASP
2	B	301	GLN
2	B	305	ARG
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	534	PRO
2	B	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	50	GLN
1	A	186	GLN
1	A	232	GLN
1	A	265	HIS
1	A	272	ASN
1	A	283	GLN

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	337	ASN
1	A	372	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	157	GLN
2	B	198	GLN
2	B	327	GLN
2	B	361	HIS
2	B	373	ASN
2	B	382	GLN
2	B	393	GLN
2	B	402	GLN
2	B	403	ASN
2	B	467	ASN
2	B	536	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	558/655 (85%)	0.11	28 (5%) 28 25	48, 87, 147, 168	0
2	B	437/555 (78%)	-0.04	19 (4%) 35 31	40, 63, 123, 172	0
All	All	995/1210 (82%)	0.04	47 (4%) 31 28	40, 77, 142, 172	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	241	LEU	6.9
2	B	176	ALA	6.3
2	B	240	PHE	6.2
1	A	245	LEU	5.4
1	A	207	ALA	4.9
1	A	392	GLU	4.8
1	A	188	LEU	4.8
1	A	204	LEU	4.7
2	B	177	ASN	4.6
2	B	406	GLY	4.6
1	A	187	ASP	4.6
1	A	215	MET	4.4
1	A	391	PRO	4.3
1	A	394	ASP	4.3
2	B	451	GLY	4.2
2	B	175	GLY	4.1
2	B	267	CYS	3.9
2	B	268	LYS	3.7
1	A	228	LEU	3.6
2	B	405	THR	3.6
2	B	516	GLN	3.5
2	B	269	VAL	3.5
1	A	206	ALA	3.4
2	B	517	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	398	ALA	3.3
1	A	233	ARG	3.1
1	A	232	GLN	3.0
2	B	31	LEU	3.0
1	A	242	ALA	2.8
1	A	208	ALA	2.7
1	A	244	MET	2.6
2	B	457	TYR	2.6
1	A	169	LEU	2.5
1	A	55	ALA	2.5
2	B	29	ALA	2.3
1	A	205	LYS	2.3
1	A	434	LEU	2.2
1	A	229	SER	2.2
2	B	179	PRO	2.2
1	A	216	LYS	2.2
1	A	397	PRO	2.1
2	B	178	LEU	2.1
2	B	236	GLN	2.1
1	A	200	TYR	2.1
1	A	557	CYS	2.0
1	A	395	PHE	2.0
1	A	598	LEU	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 monosaccharides 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.