Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:37 PM GMT

PDB ID	:	4CTS
Title	:	CRYSTAL STRUCTURE ANALYSIS AND MOLECULAR MODEL OF A COMPLEX OF CITRATE SYNTHASE WITH OXALOACETATE AND S-ACETONYL-COENZYME A
Authors	:	Remington, S.; Wiegand, G.; Huber, R.
Deposited on	:	1984-01-27
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

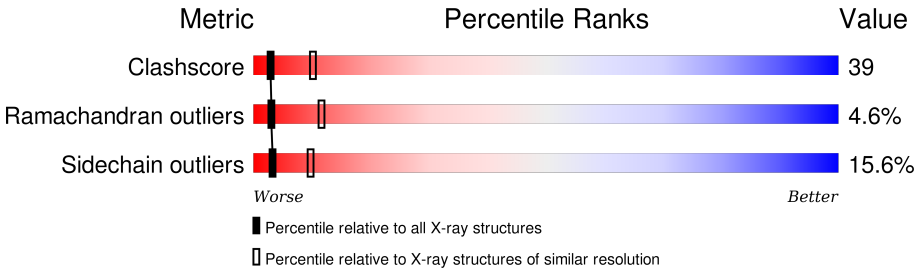
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	437	30% 41% 23% 6%
1	B	437	32% 40% 22% 7%

2 Entry composition

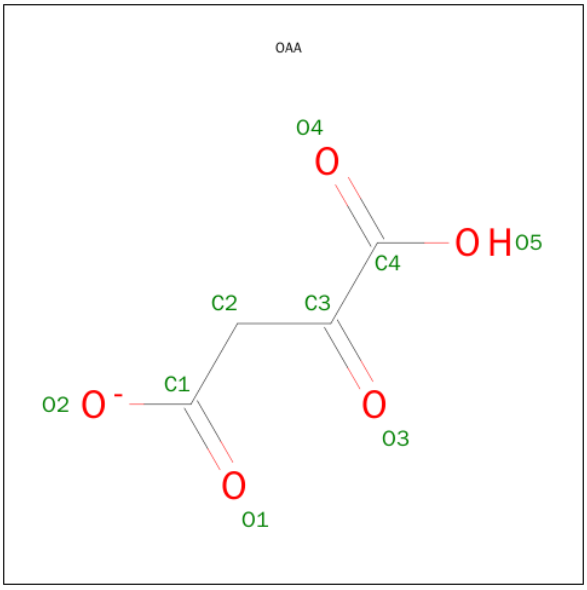
There are 3 unique types of molecules in this entry. The entry contains 7002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	227	0	0
			3444	2200	591	634	19			
1	B	437	Total	C	N	O	S	230	0	0
			3444	2200	591	634	19			

- Molecule 2 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O		0	0
			9	4	5			
2	B	1	Total	C	O		0	0
			9	4	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	49	Total O 49 49	0	0
3	B	47	Total O 47 47	0	0

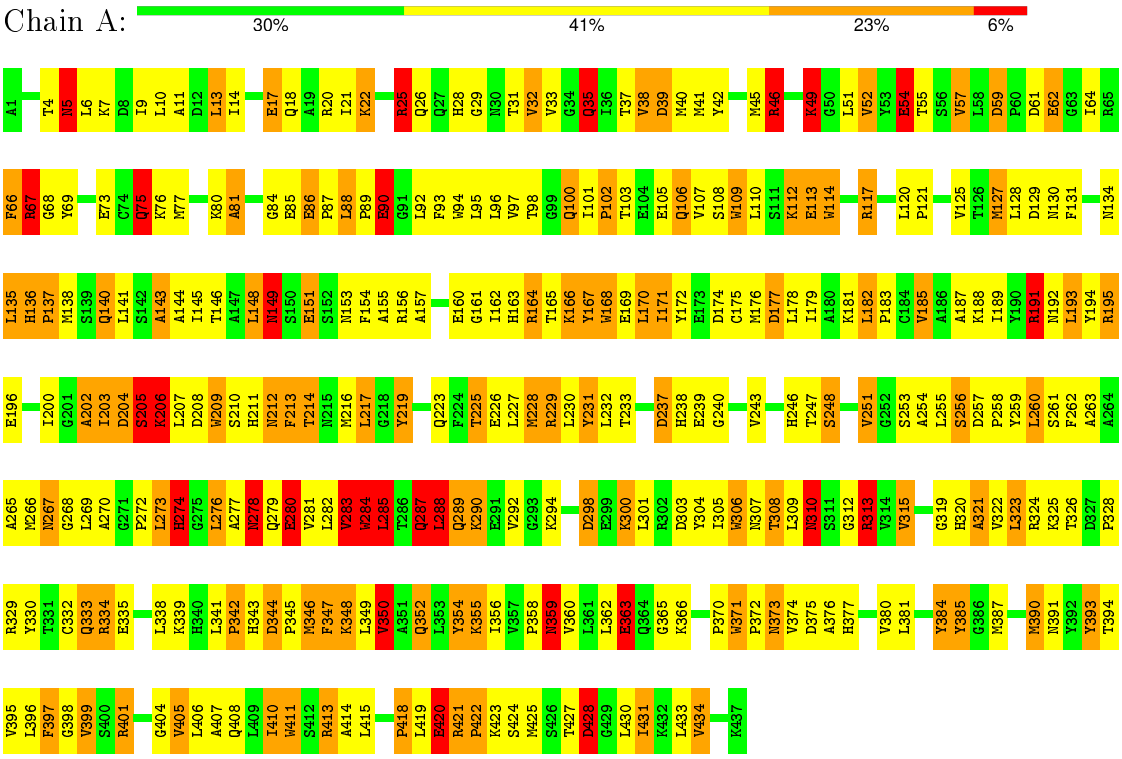
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

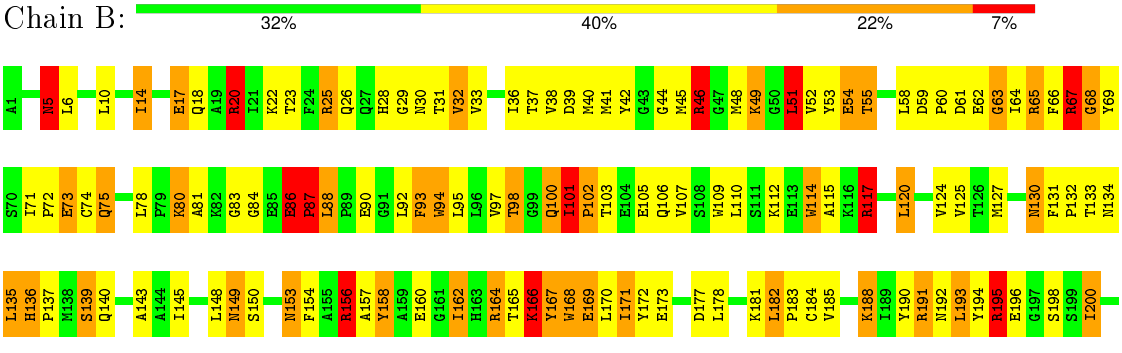
- Molecule 1: CITRATE SYNTHASE

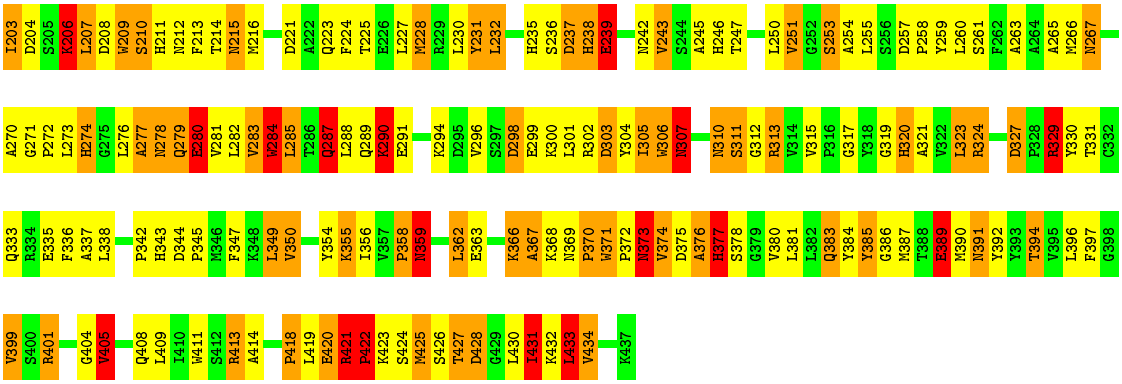
Chain A:



- Molecule 1: CITRATE SYNTHASE

Chain B:




I203 D204 S205 K206 L207 D208 W209 S210 H211 N212 F213 T214 N215 M216 D221 A222 Q223 F224 T225 E226 L227 M228 R229 L230 Y231 L232 H235 S236 D237 H238 E239 N242 V243 S244 A245 H246 T247 L250 V251 G252 S253 A254 L255 S256 D257 P258 Y259 L260 S261 F262 A263 A264 A265 M266 N267
A270 G271 P272 L273 H274 G275 L276 A277 N278 Q279 E280 V281 L282 V283 W284 L285 T286 Q287 L288 Q289 K290 E291 K294 D295 V296 S297 D298 E299 K300 L301 R302 D303 Y304 I305 W306 N307 N310 S311 G312 R313 V314 V315 P316 G317 Y318 G319 H320 A321 V322 L323 R324 D327 P328 R329 Y330 T331 G332
Q333 R334 E335 F336 A337 L338 P342 H343 D344 P345 N346 F347 K348 L349 V350 Y354 K355 I356 V357 P358 N359 L362 E363 K366 A367 K368 N369 P370 W371 P372 N373 V374 D375 A376 H377 S378 G379 V380 L381 L382 Q383 Y384 Y385 G386 M387 T388 E389 M390 N391 Y392 Y393 T394 V395 L396 F397 G398
V399 S400 R401 G404 Y405 Q408 L409 I410 W411 S412 R413 A414 P418 L419 E420 R421 P422 K423 S424 M425 S426 T427 D428 G429 L430 I431 K432 I433 V434 K437

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.54Å 101.54Å 224.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.22	11/3528 (0.3%)	1.77	41/4786 (0.9%)
1	B	1.22	11/3528 (0.3%)	1.77	54/4786 (1.1%)
All	All	1.22	22/7056 (0.3%)	1.77	95/9572 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	105
1	B	2	104
All	All	3	209

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	TRP	NE1-CE2	-8.77	1.26	1.37
1	B	109	TRP	NE1-CE2	-8.18	1.26	1.37
1	A	114	TRP	NE1-CE2	-7.93	1.27	1.37
1	A	168	TRP	NE1-CE2	-7.85	1.27	1.37
1	A	371	TRP	NE1-CE2	-7.65	1.27	1.37
1	B	371	TRP	NE1-CE2	-7.61	1.27	1.37
1	A	109	TRP	NE1-CE2	-7.47	1.27	1.37
1	B	94	TRP	NE1-CE2	-7.29	1.28	1.37
1	B	168	TRP	NE1-CE2	-7.26	1.28	1.37
1	A	209	TRP	NE1-CE2	-7.25	1.28	1.37
1	A	411	TRP	NE1-CE2	-7.14	1.28	1.37
1	B	411	TRP	NE1-CE2	-7.08	1.28	1.37
1	A	94	TRP	NE1-CE2	-6.98	1.28	1.37
1	B	284	TRP	NE1-CE2	-6.83	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	306	TRP	NE1-CE2	-6.81	1.28	1.37
1	B	384	TYR	CZ-OH	6.56	1.49	1.37
1	B	209	TRP	NE1-CE2	-6.52	1.29	1.37
1	A	306	TRP	NE1-CE2	-6.32	1.29	1.37
1	A	284	TRP	NE1-CE2	-5.64	1.30	1.37
1	A	231	TYR	CZ-OH	5.53	1.47	1.37
1	B	167	TYR	CZ-OH	5.04	1.46	1.37
1	A	393	TYR	CZ-OH	5.03	1.46	1.37

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	ARG	NE-CZ-NH2	-17.05	111.78	120.30
1	B	65	ARG	NE-CZ-NH1	14.64	127.62	120.30
1	A	191	ARG	NE-CZ-NH2	-11.17	114.72	120.30
1	A	67	ARG	NE-CZ-NH1	-10.86	114.87	120.30
1	B	20	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	B	46	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	B	324	ARG	NE-CZ-NH1	-9.03	115.79	120.30
1	B	20	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	A	205	SER	N-CA-CB	-8.67	97.50	110.50
1	B	117	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	B	283	VAL	CA-CB-CG1	8.30	123.35	110.90
1	B	65	ARG	CD-NE-CZ	7.93	134.70	123.60
1	A	278	ASN	C-N-CA	7.79	141.17	121.70
1	B	329	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	B	195	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	334	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	46	ARG	NE-CZ-NH1	-7.19	116.71	120.30
1	A	280	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	B	421	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	B	401	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	428	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	B	401	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	A	25	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	B	88	LEU	N-CA-CB	-6.70	97.00	110.40
1	B	167	TYR	CB-CG-CD1	-6.56	117.06	121.00
1	A	28	HIS	CA-CB-CG	-6.52	102.52	113.60
1	B	46	ARG	CD-NE-CZ	6.38	132.53	123.60
1	B	433	LEU	C-N-CA	-6.36	105.79	121.70
1	A	229	ARG	CD-NE-CZ	6.28	132.39	123.60
1	B	28	HIS	CA-CB-CG	-6.20	103.06	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	385	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	B	427	THR	N-CA-CB	6.10	121.89	110.30
1	A	90	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	A	298	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	385	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	B	405	VAL	CA-CB-CG1	5.82	119.64	110.90
1	A	177	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	156	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	324	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	274	HIS	CA-CB-CG	-5.78	103.77	113.60
1	A	208	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	377	HIS	N-CA-CB	-5.74	100.28	110.60
1	B	203	ILE	CA-CB-CG2	5.73	122.36	110.90
1	A	370	PRO	N-CA-CB	5.71	110.15	103.30
1	A	248	SER	O-C-N	5.69	131.81	122.70
1	A	422	PRO	N-CA-CB	5.67	110.11	103.30
1	B	165	THR	C-N-CA	5.66	135.84	121.70
1	B	373	ASN	CB-CA-C	-5.63	99.14	110.40
1	B	53	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	B	51	LEU	O-C-N	-5.62	113.71	122.70
1	B	358	PRO	C-N-CA	5.62	135.75	121.70
1	B	327	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	164	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	65	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	290	LYS	CA-C-N	-5.55	105.00	117.20
1	B	83	GLY	C-N-CA	5.54	133.94	122.30
1	B	206	LYS	CA-C-N	-5.53	105.03	117.20
1	B	359	ASN	N-CA-CB	-5.53	100.65	110.60
1	B	68	GLY	N-CA-C	-5.48	99.39	113.10
1	B	345	PRO	N-CA-CB	5.48	109.87	103.30
1	B	427	THR	OG1-CB-CG2	-5.46	97.44	110.00
1	B	280	GLU	OE1-CD-OE2	-5.45	116.77	123.30
1	B	156	ARG	CD-NE-CZ	5.40	131.16	123.60
1	A	363	GLU	C-N-CA	5.36	135.11	121.70
1	A	185	VAL	CA-CB-CG1	5.35	118.92	110.90
1	B	87	PRO	N-CA-CB	5.33	109.70	103.30
1	A	415	LEU	C-N-CA	5.28	133.39	122.30
1	A	100	GLN	N-CA-CB	-5.28	101.10	110.60
1	A	278	ASN	O-C-N	5.25	131.10	122.70
1	B	359	ASN	CA-C-N	-5.25	105.65	117.20
1	A	59	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	168	TRP	O-C-N	5.24	131.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	VAL	C-N-CA	5.22	134.76	121.70
1	B	209	TRP	O-C-N	5.22	131.05	122.70
1	B	422	PRO	N-CA-CB	5.21	109.56	103.30
1	A	117	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	A	285	LEU	CB-CA-C	5.20	120.09	110.20
1	A	288	LEU	CB-CG-CD1	5.20	119.84	111.00
1	B	67	ARG	CA-C-N	-5.20	105.81	116.20
1	A	170	LEU	CA-CB-CG	-5.17	103.42	115.30
1	A	278	ASN	CA-C-N	-5.17	105.84	117.20
1	A	334	ARG	CD-NE-CZ	5.16	130.83	123.60
1	B	396	LEU	O-C-N	5.14	130.93	122.70
1	B	25	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	73	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	A	22	LYS	N-CA-CB	5.08	119.73	110.60
1	A	46	ARG	NH1-CZ-NH2	5.07	124.97	119.40
1	B	370	PRO	N-CA-CB	5.07	109.38	103.30
1	A	183	PRO	N-CA-CB	5.05	109.36	103.30
1	B	54	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	B	253	SER	N-CA-CB	5.05	118.07	110.50
1	A	313	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	B	94	TRP	CA-CB-CG	-5.03	104.15	113.70
1	A	359	ASN	CA-C-N	-5.02	106.16	117.20
1	A	280	GLU	N-CA-CB	5.01	119.62	110.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	37	THR	CB
1	B	37	THR	CB
1	B	307	ASN	CA

All (209) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLN	Mainchain
1	A	102	PRO	Mainchain
1	A	106	GLN	Mainchain,Peptide
1	A	11	ALA	Mainchain
1	A	113	GLU	Sidechain
1	A	134	ASN	Mainchain
1	A	135	LEU	Mainchain
1	A	140	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	A	143	ALA	Mainchain
1	A	144	ALA	Mainchain
1	A	160	GLU	Sidechain
1	A	161	GLY	Mainchain
1	A	165	THR	Mainchain
1	A	167	TYR	Sidechain
1	A	18	GLN	Sidechain
1	A	191	ARG	Sidechain
1	A	194	TYR	Sidechain
1	A	195	ARG	Mainchain
1	A	202	ALA	Mainchain,Peptide
1	A	204	ASP	Sidechain
1	A	206	LYS	Mainchain
1	A	213	PHE	Mainchain
1	A	219	TYR	Mainchain
1	A	223	GLN	Sidechain
1	A	237	ASP	Sidechain
1	A	25	ARG	Sidechain
1	A	251	VAL	Mainchain
1	A	254	ALA	Mainchain
1	A	256	SER	Mainchain
1	A	26	GLN	Sidechain
1	A	267	ASN	Sidechain
1	A	280	GLU	Sidechain,Mainchain,Peptide
1	A	283	VAL	Mainchain
1	A	284	TRP	Mainchain
1	A	285	LEU	Mainchain
1	A	287	GLN	Sidechain,Mainchain
1	A	289	GLN	Mainchain
1	A	290	LYS	Mainchain,Peptide
1	A	292	VAL	Mainchain
1	A	300	LYS	Mainchain
1	A	304	TYR	Mainchain
1	A	308	THR	Mainchain
1	A	310	ASN	Sidechain
1	A	315	VAL	Mainchain
1	A	32	VAL	Mainchain
1	A	324	ARG	Sidechain
1	A	326	THR	Mainchain
1	A	333	GLN	Sidechain
1	A	335	GLU	Sidechain
1	A	342	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	A	344	ASP	Mainchain
1	A	346	MET	Mainchain
1	A	347	PHE	Mainchain
1	A	348	LYS	Mainchain
1	A	35	GLN	Sidechain
1	A	350	VAL	Mainchain
1	A	352	GLN	Mainchain
1	A	354	TYR	Mainchain
1	A	365	GLY	Mainchain
1	A	366	LYS	Mainchain,Peptide
1	A	373	ASN	Sidechain,Mainchain
1	A	375	ASP	Sidechain
1	A	376	ALA	Mainchain
1	A	384	TYR	Sidechain,Mainchain
1	A	385	TYR	Mainchain
1	A	39	ASP	Sidechain
1	A	390	MET	Mainchain
1	A	394	THR	Mainchain
1	A	399	VAL	Mainchain
1	A	401	ARG	Mainchain
1	A	406	LEU	Mainchain
1	A	410	ILE	Mainchain
1	A	411	TRP	Mainchain
1	A	420	GLU	Sidechain
1	A	428	ASP	Sidechain,Mainchain
1	A	431	ILE	Mainchain
1	A	433	LEU	Mainchain
1	A	52	VAL	Mainchain
1	A	54	GLU	Sidechain
1	A	59	ASP	Sidechain
1	A	61	ASP	Sidechain
1	A	62	GLU	Sidechain
1	A	64	ILE	Mainchain
1	A	66	PHE	Mainchain,Peptide
1	A	67	ARG	Mainchain
1	A	68	GLY	Mainchain
1	A	73	GLU	Mainchain
1	A	75	GLN	Sidechain
1	A	81	ALA	Mainchain
1	A	84	GLY	Mainchain
1	A	85	GLU	Mainchain
1	A	88	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	90	GLU	Sidechain
1	A	93	PHE	Mainchain
1	B	100	GLN	Sidechain
1	B	101	ILE	Mainchain,Peptide
1	B	102	PRO	Mainchain
1	B	115	ALA	Mainchain,Peptide
1	B	117	ARG	Mainchain
1	B	130	ASN	Sidechain
1	B	139	SER	Mainchain
1	B	140	GLN	Sidechain
1	B	153	ASN	Sidechain
1	B	158	TYR	Sidechain
1	B	160	GLU	Sidechain
1	B	166	LYS	Mainchain
1	B	169	GLU	Mainchain
1	B	17	GLU	Sidechain
1	B	177	ASP	Mainchain
1	B	18	GLN	Sidechain
1	B	184	CYS	Mainchain
1	B	188	LYS	Mainchain
1	B	191	ARG	Sidechain
1	B	192	ASN	Sidechain
1	B	195	ARG	Mainchain
1	B	200	ILE	Mainchain
1	B	206	LYS	Mainchain
1	B	207	LEU	Mainchain
1	B	208	ASP	Mainchain
1	B	221	ASP	Sidechain
1	B	223	GLN	Sidechain
1	B	231	TYR	Sidechain
1	B	232	LEU	Mainchain
1	B	235	HIS	Mainchain
1	B	237	ASP	Sidechain
1	B	238	HIS	Mainchain
1	B	239	GLU	Sidechain
1	B	251	VAL	Mainchain
1	B	267	ASN	Mainchain
1	B	278	ASN	Mainchain
1	B	280	GLU	Sidechain
1	B	284	TRP	Mainchain
1	B	287	GLN	Sidechain
1	B	290	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	B	291	GLU	Mainchain
1	B	298	ASP	Sidechain
1	B	299	GLU	Mainchain
1	B	30	ASN	Mainchain
1	B	303	ASP	Sidechain
1	B	305	ILE	Mainchain
1	B	311	SER	Mainchain
1	B	312	GLY	Mainchain
1	B	32	VAL	Mainchain
1	B	321	ALA	Mainchain
1	B	327	ASP	Sidechain
1	B	329	ARG	Mainchain
1	B	330	TYR	Sidechain
1	B	335	GLU	Sidechain
1	B	349	LEU	Mainchain
1	B	350	VAL	Mainchain
1	B	358	PRO	Mainchain
1	B	359	ASN	Mainchain
1	B	362	LEU	Mainchain
1	B	363	GLU	Sidechain
1	B	366	LYS	Mainchain
1	B	367	ALA	Mainchain,Peptide
1	B	370	PRO	Mainchain
1	B	373	ASN	Sidechain,Mainchain
1	B	374	VAL	Mainchain
1	B	376	ALA	Mainchain,Peptide
1	B	383	GLN	Sidechain
1	B	385	TYR	Mainchain
1	B	386	GLY	Mainchain,Peptide
1	B	389	GLU	Sidechain
1	B	390	MET	Mainchain
1	B	391	ASN	Sidechain
1	B	394	THR	Mainchain
1	B	399	VAL	Mainchain
1	B	404	GLY	Mainchain
1	B	405	VAL	Mainchain
1	B	420	GLU	Sidechain
1	B	422	PRO	Mainchain,Peptide
1	B	425	MET	Mainchain
1	B	431	ILE	Mainchain
1	B	433	LEU	Mainchain
1	B	46	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	51	LEU	Mainchain,Peptide
1	B	54	GLU	Sidechain
1	B	55	THR	Mainchain
1	B	61	ASP	Sidechain
1	B	63	GLY	Mainchain
1	B	66	PHE	Mainchain,Peptide
1	B	67	ARG	Mainchain
1	B	73	GLU	Mainchain
1	B	80	LYS	Mainchain,Peptide
1	B	84	GLY	Mainchain
1	B	86	GLU	Mainchain
1	B	93	PHE	Mainchain

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	3444	0	3436	291	17
1	B	3444	0	3436	283	27
2	A	9	0	2	0	0
2	B	9	0	2	0	0
3	A	49	0	0	4	0
3	B	47	0	0	0	2
All	All	7002	0	6876	502	38

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (502) 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:268:GLY:HA2	1:B:251:VAL:HG13	1.47	0.96
1:A:419:LEU:HD11	1:B:243:VAL:HG22	1.51	0.92
1:B:58:LEU:HD12	1:B:63:GLY:HA2	1.53	0.90
1:A:280:GLU:HA	1:A:283:VAL:HB	1.54	0.90
1:A:75:GLN:HA	1:A:87:PRO:HG3	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LYS:HB2	1:B:200:ILE:HD13	1.54	0.88
1:A:55:THR:HG21	1:A:407:ALA:HB1	1.57	0.86
1:B:272:PRO:HA	1:B:276:LEU:HB2	1.56	0.86
1:A:288:LEU:HD22	1:A:301:LEU:HD11	1.57	0.86
1:A:81:ALA:HB2	1:A:88:LEU:HD13	1.59	0.85
1:A:434:VAL:HG23	1:B:31:THR:HG21	1.57	0.84
1:A:273:LEU:HD22	1:B:255:LEU:HG	1.60	0.84
1:A:6:LEU:HD21	1:A:97:VAL:HG11	1.58	0.84
1:B:75:GLN:HA	1:B:87:PRO:HG3	1.59	0.83
1:B:298:ASP:HA	1:B:301:LEU:HB3	1.61	0.83
1:B:359:ASN:HA	1:B:362:LEU:HD12	1.60	0.82
1:A:434:VAL:CG2	1:B:31:THR:HG21	2.10	0.81
1:A:168:TRP:HB3	1:A:414:ALA:HB2	1.64	0.80
1:B:282:LEU:HD12	1:B:285:LEU:HB3	1.64	0.80
1:A:167:TYR:HB3	1:A:413:ARG:HG3	1.62	0.79
1:A:281:VAL:HG12	1:A:285:LEU:HD22	1.63	0.79
1:A:359:ASN:HA	1:A:362:LEU:HB2	1.64	0.78
1:A:138:MET:HG2	1:A:395:VAL:HG22	1.66	0.78
1:B:86:GLU:HG2	1:B:230:LEU:HB2	1.65	0.78
1:A:137:PRO:HB2	1:A:395:VAL:HG21	1.64	0.77
1:B:250:LEU:HD13	1:B:420:GLU:HB3	1.66	0.77
1:A:267:ASN:HB3	1:B:260:LEU:HG	1.67	0.76
1:A:81:ALA:HB2	1:A:88:LEU:CD1	2.16	0.76
1:A:200:ILE:O	1:A:216:MET:HG2	1.86	0.76
1:A:162:ILE:HD13	1:A:170:LEU:HD12	1.68	0.75
1:B:120:LEU:HD21	1:B:185:VAL:HG22	1.69	0.74
1:B:282:LEU:HA	1:B:285:LEU:HB2	1.68	0.74
1:A:137:PRO:HB3	1:A:189:ILE:CG2	2.17	0.74
1:A:419:LEU:HD11	1:B:243:VAL:CG2	2.18	0.73
1:B:17:GLU:HA	1:B:20:ARG:HB2	1.70	0.73
1:B:90:GLU:HB2	1:B:107:VAL:HG13	1.69	0.73
1:A:350:VAL:HG21	1:A:380:VAL:HG21	1.71	0.72
1:B:78:LEU:CD2	1:B:101:ILE:HD13	2.20	0.72
1:B:282:LEU:HD12	1:B:285:LEU:CB	2.20	0.71
1:B:425:MET:HG2	1:B:430:LEU:HG	1.71	0.71
1:B:300:LYS:HA	1:B:303:ASP:HB2	1.72	0.71
1:B:145:ILE:HG22	1:B:263:ALA:HB2	1.72	0.71
1:A:57:VAL:HG21	1:B:426:SER:HB3	1.71	0.70
1:A:298:ASP:OD2	1:A:301:LEU:HD23	1.92	0.69
1:A:171:ILE:HD11	1:A:410:ILE:HA	1.74	0.69
1:B:86:GLU:HG3	1:B:87:PRO:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LEU:CD1	1:B:420:GLU:HB3	2.21	0.69
1:B:298:ASP:O	1:B:302:ARG:HB2	1.93	0.69
1:A:424:SER:CB	1:B:51:LEU:HB2	2.23	0.69
1:A:49:LYS:HA	1:B:423:LYS:HB3	1.75	0.69
1:B:342:PRO:HA	1:B:347:PHE:CE1	2.28	0.68
1:A:273:LEU:HB2	1:B:254:ALA:O	1.94	0.68
1:B:148:LEU:HB3	1:B:259:TYR:CD1	2.28	0.68
1:B:103:THR:H	1:B:106:GLN:HG2	1.57	0.68
1:A:14:ILE:HG21	1:A:414:ALA:HB1	1.75	0.68
1:B:243:VAL:HB	1:B:274:HIS:CD2	2.28	0.67
1:B:67:ARG:HB3	1:B:69:TYR:CD1	2.30	0.67
1:A:298:ASP:HA	1:A:301:LEU:HB3	1.77	0.67
1:B:190:TYR:HB2	1:B:392:TYR:CE1	2.31	0.66
1:B:81:ALA:HB2	1:B:88:LEU:HD13	1.76	0.66
1:A:171:ILE:HG21	1:A:413:ARG:HG2	1.76	0.66
1:A:120:LEU:HD23	1:A:125:VAL:HG22	1.77	0.66
1:B:272:PRO:HA	1:B:276:LEU:CB	2.26	0.66
1:B:78:LEU:HD23	1:B:101:ILE:HD13	1.78	0.66
1:B:324:ARG:HE	1:B:368:LYS:HD3	1.61	0.66
1:B:276:LEU:O	1:B:280:GLU:HG2	1.96	0.66
1:B:344:ASP:HB3	1:B:347:PHE:HB3	1.79	0.65
1:A:51:LEU:HB2	1:B:424:SER:CB	2.27	0.65
1:B:127:MET:HE2	1:B:143:ALA:HB1	1.77	0.65
1:A:67:ARG:HB3	1:A:69:TYR:CD1	2.32	0.64
1:B:228:MET:HA	1:B:228:MET:CE	2.26	0.64
1:B:59:ASP:HB3	1:B:63:GLY:N	2.12	0.64
1:B:425:MET:CG	1:B:430:LEU:HG	2.27	0.64
1:B:45:MET:HG2	1:B:48:MET:CE	2.28	0.64
1:A:146:THR:HG23	1:A:260:LEU:HD12	1.79	0.64
1:B:90:GLU:HG3	1:B:114:TRP:CZ3	2.33	0.64
1:A:45:MET:HE2	1:B:422:PRO:HB3	1.80	0.64
1:A:52:VAL:HG22	1:B:430:LEU:CD1	2.28	0.64
1:B:371:TRP:HB3	1:B:372:PRO:HD2	1.79	0.64
1:A:138:MET:HA	1:A:141:LEU:HB3	1.79	0.64
1:A:282:LEU:HB3	1:A:390:MET:SD	2.37	0.63
1:A:168:TRP:CB	1:A:414:ALA:HB2	2.27	0.63
1:A:398:GLY:HA2	1:A:401:ARG:HB3	1.80	0.63
1:B:169:GLU:O	1:B:172:TYR:HB3	1.98	0.63
1:A:41:MET:HG2	1:B:52:VAL:HG23	1.79	0.63
1:A:300:LYS:HA	1:A:303:ASP:HB2	1.80	0.63
1:B:162:ILE:HD11	1:B:167:TYR:HD1	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLY:O	1:B:164:ARG:HD2	1.99	0.63
1:A:52:VAL:HA	1:B:425:MET:O	1.99	0.62
1:B:276:LEU:C	1:B:280:GLU:HG2	2.20	0.62
1:B:228:MET:HA	1:B:228:MET:HE2	1.79	0.62
1:A:247:THR:HG21	1:A:265:ALA:HA	1.80	0.62
1:A:178:LEU:HG	1:A:182:LEU:HD12	1.81	0.62
1:A:420:GLU:HG2	1:A:422:PRO:HD3	1.82	0.62
1:A:421:ARG:HH22	1:B:239:GLU:CG	2.12	0.62
1:B:135:LEU:HD22	1:B:139:SER:HB2	1.81	0.62
1:A:41:MET:SD	1:A:430:LEU:HD11	2.40	0.62
1:B:22:LYS:O	1:B:26:GLN:HG3	2.00	0.62
1:A:103:THR:HG22	1:A:105:GLU:HB3	1.82	0.61
1:A:284:TRP:CH2	1:A:305:ILE:HG12	2.36	0.61
1:A:31:THR:HG21	1:B:434:VAL:HB	1.81	0.61
1:A:276:LEU:O	1:A:279:GLN:HB3	2.01	0.61
1:B:344:ASP:HB3	1:B:347:PHE:CB	2.31	0.61
1:B:281:VAL:HG12	1:B:285:LEU:HD22	1.81	0.61
1:B:55:THR:HG23	1:B:408:GLN:OE1	2.01	0.60
1:B:166:LYS:O	1:B:169:GLU:HB2	2.00	0.60
1:B:430:LEU:O	1:B:434:VAL:HG12	2.02	0.60
1:B:157:ALA:HB1	1:B:162:ILE:HG21	1.84	0.60
1:A:341:LEU:HD13	1:A:384:TYR:CG	2.36	0.60
1:B:276:LEU:O	1:B:279:GLN:HB3	2.00	0.60
1:A:52:VAL:HG23	1:B:41:MET:HG2	1.83	0.60
1:A:4:THR:HG21	1:A:106:GLN:CB	2.32	0.60
1:A:209:TRP:HZ3	1:A:232:LEU:HD23	1.67	0.60
1:A:6:LEU:O	1:A:9:ILE:HB	2.02	0.60
1:A:231:TYR:HD1	1:A:232:LEU:HD12	1.67	0.59
1:A:341:LEU:HD22	1:A:384:TYR:CD2	2.37	0.59
1:B:133:THR:HG23	1:B:193:LEU:HD12	1.84	0.59
1:A:55:THR:HG22	1:A:96:LEU:HB3	1.83	0.59
1:B:279:GLN:O	1:B:283:VAL:HG23	2.02	0.59
1:A:51:LEU:HB2	1:B:424:SER:HA	1.84	0.59
1:B:59:ASP:HB3	1:B:63:GLY:H	1.65	0.58
1:A:288:LEU:CD2	1:A:301:LEU:HD11	2.31	0.58
1:A:350:VAL:CG2	1:A:380:VAL:HG21	2.32	0.58
1:A:90:GLU:HB2	1:A:107:VAL:HG13	1.85	0.58
1:A:163:HIS:O	1:A:166:LYS:HB2	2.03	0.58
1:A:425:MET:O	1:B:52:VAL:HA	2.03	0.58
1:A:425:MET:HG2	1:A:430:LEU:HG	1.83	0.58
1:A:55:THR:O	1:A:96:LEU:HD22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:O	1:A:193:LEU:HB2	2.04	0.58
1:A:52:VAL:HG23	1:B:41:MET:O	2.04	0.58
1:A:86:GLU:HG2	1:A:230:LEU:HB2	1.86	0.57
1:B:167:TYR:HB3	1:B:413:ARG:HG3	1.86	0.57
1:B:354:TYR:O	1:B:355:LYS:HD3	2.04	0.57
1:B:324:ARG:HA	1:B:369:ASN:HB2	1.86	0.57
1:A:207:LEU:HD12	1:A:212:ASN:ND2	2.19	0.57
1:B:190:TYR:HB2	1:B:392:TYR:CZ	2.39	0.57
1:A:103:THR:CG2	1:A:105:GLU:HB3	2.35	0.57
1:A:255:LEU:HD12	1:B:273:LEU:HD13	1.87	0.57
1:B:78:LEU:HD21	1:B:101:ILE:HD13	1.87	0.57
1:A:57:VAL:CG2	1:B:426:SER:HB3	2.35	0.56
1:B:103:THR:CG2	1:B:105:GLU:HB3	2.35	0.56
1:B:127:MET:HE2	1:B:143:ALA:CB	2.35	0.56
1:B:162:ILE:HD11	1:B:167:TYR:CD1	2.39	0.56
1:B:157:ALA:HB1	1:B:162:ILE:CG2	2.35	0.56
1:B:171:ILE:HD11	1:B:409:LEU:O	2.06	0.56
1:A:282:LEU:HA	1:A:285:LEU:HB2	1.87	0.56
1:A:284:TRP:CZ2	1:A:305:ILE:HG12	2.41	0.56
1:A:154:PHE:HD1	1:A:170:LEU:HB2	1.70	0.56
1:A:267:ASN:N	1:A:267:ASN:HD22	2.04	0.55
1:A:280:GLU:CA	1:A:283:VAL:HB	2.33	0.55
1:A:37:THR:CG2	1:A:40:MET:HG3	2.37	0.55
1:A:204:ASP:H	1:A:212:ASN:HD21	1.54	0.55
1:A:240:GLY:O	1:A:246:HIS:HB2	2.06	0.55
1:B:231:TYR:HD1	1:B:232:LEU:HD12	1.72	0.55
1:A:52:VAL:HG22	1:B:430:LEU:HD11	1.89	0.55
1:B:103:THR:HG22	1:B:105:GLU:H	1.72	0.55
1:B:236:SER:O	1:B:401:ARG:HD3	2.07	0.55
1:A:178:LEU:HD13	1:A:259:TYR:CE1	2.41	0.55
1:A:209:TRP:CZ3	1:A:232:LEU:HD23	2.42	0.55
1:A:321:ALA:HB1	1:A:322:VAL:HG23	1.89	0.55
1:B:72:PRO:HA	1:B:75:GLN:HB2	1.88	0.55
1:A:182:LEU:HD21	1:A:262:PHE:HE2	1.70	0.55
1:B:103:THR:HB	1:B:106:GLN:H	1.72	0.55
1:A:371:TRP:HB3	1:A:372:PRO:HD2	1.89	0.55
1:B:37:THR:HG22	1:B:40:MET:HG3	1.89	0.54
1:A:156:ARG:HD2	3:A:467:HOH:O	2.07	0.54
1:A:257:ASP:HB2	1:A:258:PRO:HD2	1.88	0.54
1:B:93:PHE:O	1:B:97:VAL:HG23	2.06	0.54
1:B:284:TRP:HA	1:B:287:GLN:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HG	1:B:273:LEU:HD22	1.90	0.54
1:A:238:HIS:HE1	1:A:320:HIS:CE1	2.24	0.54
1:B:257:ASP:HB2	1:B:258:PRO:HD2	1.90	0.54
1:B:427:THR:HG22	1:B:431:ILE:HD12	1.89	0.54
1:A:248:SER:OG	1:A:405:VAL:HG22	2.08	0.54
1:A:164:ARG:HA	1:A:167:TYR:CE1	2.43	0.53
1:A:427:THR:HG22	1:A:431:ILE:HD12	1.90	0.53
1:B:319:GLY:HA2	1:B:369:ASN:O	2.09	0.53
1:A:42:TYR:CE1	1:B:52:VAL:HG11	2.43	0.53
1:A:423:LYS:HB3	1:B:49:LYS:HA	1.90	0.53
1:B:300:LYS:O	1:B:304:TYR:HB2	2.09	0.53
1:B:154:PHE:O	1:B:157:ALA:HB3	2.08	0.53
1:B:227:LEU:HB2	1:B:336:PHE:CZ	2.43	0.53
1:B:279:GLN:HG2	1:B:280:GLU:OE2	2.09	0.53
1:B:92:LEU:HD12	1:B:95:LEU:HD23	1.91	0.53
1:B:124:VAL:O	1:B:127:MET:HB3	2.08	0.53
1:A:266:MET:HE2	1:A:269:LEU:HD23	1.91	0.53
1:A:319:GLY:O	1:A:320:HIS:HB2	2.08	0.53
1:A:273:LEU:HD22	1:B:255:LEU:CG	2.36	0.52
1:B:67:ARG:H	1:B:69:TYR:H	1.56	0.52
1:A:129:ASP:HA	1:A:192:ASN:HD21	1.75	0.52
1:A:128:LEU:HD11	1:A:185:VAL:HG13	1.92	0.52
1:A:285:LEU:O	1:A:289:GLN:HB2	2.09	0.52
1:A:268:GLY:CA	1:B:251:VAL:HG13	2.31	0.52
1:B:277:ALA:HA	1:B:280:GLU:HB2	1.91	0.52
1:A:425:MET:HG2	1:A:430:LEU:CD2	2.38	0.52
1:B:167:TYR:O	1:B:171:ILE:HG23	2.09	0.52
1:A:37:THR:HA	1:B:31:THR:O	2.09	0.52
1:A:309:LEU:HD21	1:A:315:VAL:HG21	1.92	0.52
1:A:37:THR:HG22	1:A:40:MET:HG3	1.92	0.52
1:A:137:PRO:HB2	1:A:395:VAL:CG2	2.37	0.52
1:B:10:LEU:O	1:B:14:ILE:HG13	2.10	0.52
1:A:273:LEU:HB3	1:B:419:LEU:HD22	1.92	0.52
1:A:354:TYR:C	1:A:355:LYS:HD3	2.30	0.52
1:A:86:GLU:CG	1:A:230:LEU:HB2	2.41	0.51
1:B:333:GLN:OE1	1:B:378:SER:HB3	2.10	0.51
1:B:319:GLY:O	1:B:320:HIS:HB2	2.10	0.51
1:B:69:TYR:CD1	1:B:95:LEU:HD11	2.45	0.51
1:A:90:GLU:HG3	1:A:114:TRP:CZ3	2.45	0.51
1:A:38:VAL:HG22	1:B:33:VAL:HG23	1.91	0.51
1:A:136:HIS:HE1	1:A:279:GLN:HE22	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASN:HA	1:A:362:LEU:CB	2.38	0.51
1:B:132:PRO:HB2	1:B:134:ASN:OD1	2.11	0.51
1:A:344:ASP:O	1:A:348:LYS:HG3	2.10	0.51
1:A:29:GLY:HA3	1:B:39:ASP:OD2	2.11	0.51
1:A:277:ALA:HA	1:A:280:GLU:HG2	1.91	0.51
1:A:137:PRO:HB3	1:A:189:ILE:HG22	1.92	0.51
1:A:130:ASN:HD21	1:B:130:ASN:ND2	2.09	0.51
1:B:425:MET:HG2	1:B:430:LEU:CG	2.40	0.51
1:B:224:PHE:CE1	1:B:227:LEU:HD23	2.45	0.51
1:A:157:ALA:CB	1:A:170:LEU:HD13	2.40	0.51
1:B:157:ALA:CB	1:B:170:LEU:HD13	2.41	0.51
1:A:330:TYR:HE1	1:A:334:ARG:HH11	1.59	0.51
1:A:155:ALA:HB1	3:A:487:HOH:O	2.10	0.51
1:A:434:VAL:HG23	1:B:31:THR:CG2	2.36	0.50
1:A:424:SER:HA	1:B:51:LEU:HB2	1.93	0.50
1:A:108:SER:O	1:A:112:LYS:HB3	2.11	0.50
1:A:280:GLU:HB3	1:A:283:VAL:HB	1.92	0.50
1:B:266:MET:O	1:B:270:ALA:HB2	2.11	0.50
1:B:288:LEU:HD21	1:B:301:LEU:HD11	1.93	0.50
1:A:354:TYR:O	1:A:355:LYS:HD3	2.10	0.50
1:B:242:ASN:ND2	1:B:245:ALA:HB3	2.26	0.50
1:A:51:LEU:HB2	1:B:424:SER:HB2	1.93	0.50
1:A:54:GLU:H	1:A:408:GLN:CD	2.15	0.50
1:B:324:ARG:HD3	1:B:369:ASN:HB2	1.94	0.50
1:A:69:TYR:HD1	1:A:95:LEU:HD11	1.77	0.50
1:B:428:ASP:O	1:B:431:ILE:HG22	2.12	0.50
1:B:37:THR:HG22	1:B:40:MET:CE	2.42	0.50
1:B:74:CYS:HA	1:B:78:LEU:HG	1.93	0.50
1:B:350:VAL:HG21	1:B:380:VAL:HG21	1.93	0.50
1:A:153:ASN:HB2	1:A:174:ASP:OD1	2.12	0.50
1:B:65:ARG:HB3	1:B:68:GLY:C	2.32	0.50
1:B:103:THR:HG22	1:B:105:GLU:HB3	1.93	0.49
1:A:51:LEU:HB2	1:B:424:SER:CA	2.42	0.49
1:A:51:LEU:HD12	1:B:424:SER:HB3	1.93	0.49
1:A:38:VAL:HG22	1:B:33:VAL:CG2	2.41	0.49
1:B:285:LEU:O	1:B:289:GLN:HB2	2.12	0.49
1:B:171:ILE:HD12	1:B:409:LEU:HG	1.95	0.49
1:B:65:ARG:HB3	1:B:68:GLY:HA2	1.95	0.49
1:B:371:TRP:HA	1:B:371:TRP:CE3	2.46	0.49
1:A:428:ASP:O	1:A:431:ILE:HB	2.13	0.49
1:A:214:THR:HG21	1:A:225:THR:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:PRO:HA	1:B:347:PHE:HE1	1.71	0.49
1:B:347:PHE:HA	1:B:380:VAL:HG11	1.94	0.49
1:A:145:ILE:O	1:A:148:LEU:HB2	2.12	0.49
1:A:4:THR:HG21	1:A:106:GLN:HB2	1.95	0.49
1:A:113:GLU:O	1:A:117:ARG:HG3	2.13	0.49
1:B:71:ILE:HB	1:B:72:PRO:HD3	1.94	0.49
1:A:422:PRO:HG3	1:B:45:MET:HE1	1.93	0.49
1:B:317:GLY:O	1:B:373:ASN:HB2	2.12	0.49
1:B:92:LEU:O	1:B:95:LEU:HB3	2.12	0.49
1:B:342:PRO:HA	1:B:347:PHE:CD1	2.47	0.49
1:B:320:HIS:ND1	1:B:323:LEU:HB2	2.27	0.49
1:A:387:MET:HG2	1:A:393:TYR:HE1	1.77	0.49
1:A:334:ARG:O	1:A:338:LEU:HG	2.13	0.48
1:A:137:PRO:HB3	1:A:189:ILE:HG21	1.92	0.48
1:A:148:LEU:HB3	1:A:259:TYR:CD1	2.48	0.48
1:B:188:LYS:HB2	1:B:200:ILE:CD1	2.36	0.48
1:A:121:PRO:HG3	1:A:151:GLU:HG3	1.95	0.48
1:B:5:ASN:HD22	1:B:5:ASN:C	2.16	0.48
1:A:342:PRO:HA	1:A:347:PHE:CE1	2.48	0.48
1:A:174:ASP:CB	1:A:258:PRO:HG2	2.43	0.48
1:B:359:ASN:HA	1:B:362:LEU:HB2	1.95	0.48
1:B:148:LEU:C	1:B:150:SER:H	2.17	0.48
1:A:103:THR:HB	1:A:106:GLN:HG2	1.95	0.48
1:B:354:TYR:C	1:B:355:LYS:HD3	2.34	0.48
1:B:14:ILE:CG2	1:B:414:ALA:HB1	2.43	0.48
1:A:280:GLU:CB	1:A:283:VAL:HB	2.44	0.48
1:A:17:GLU:O	1:A:21:ILE:HG13	2.14	0.48
1:A:210:SER:O	1:A:213:PHE:HB3	2.14	0.48
1:B:148:LEU:HB3	1:B:259:TYR:CE1	2.49	0.47
1:B:182:LEU:HD23	1:B:399:VAL:HG22	1.96	0.47
1:A:86:GLU:HG3	1:A:230:LEU:HD13	1.97	0.47
1:B:359:ASN:CA	1:B:362:LEU:HD12	2.38	0.47
1:B:281:VAL:O	1:B:285:LEU:HB2	2.14	0.47
1:A:328:PRO:O	1:A:332:CYS:HB2	2.14	0.47
1:B:277:ALA:HA	1:B:280:GLU:CG	2.45	0.47
1:B:304:TYR:O	1:B:307:ASN:HA	2.15	0.47
1:A:39:ASP:OD2	1:B:29:GLY:HA3	2.14	0.47
1:A:419:LEU:O	1:B:46:ARG:NH1	2.48	0.47
1:B:92:LEU:CD1	1:B:95:LEU:HD23	2.45	0.47
1:A:31:THR:HB	1:B:38:VAL:HG23	1.95	0.47
1:A:25:ARG:HD2	1:B:42:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:PRO:HB3	1:B:45:MET:HE2	1.96	0.47
1:A:25:ARG:HH21	1:B:39:ASP:HA	1.79	0.47
1:A:371:TRP:CE3	1:A:371:TRP:HA	2.49	0.47
1:A:238:HIS:HE1	1:A:320:HIS:HE1	1.62	0.47
1:B:181:LYS:C	1:B:183:PRO:HD2	2.35	0.47
1:A:323:LEU:HD22	1:A:325:LYS:O	2.15	0.47
1:A:137:PRO:O	1:A:141:LEU:HB2	2.14	0.47
1:A:188:LYS:HB2	1:A:200:ILE:HD13	1.97	0.47
1:B:209:TRP:CZ3	1:B:232:LEU:HD23	2.50	0.47
1:A:90:GLU:CB	1:A:107:VAL:HG13	2.44	0.47
1:B:14:ILE:HG21	1:B:414:ALA:HB1	1.97	0.47
1:B:425:MET:HG2	1:B:430:LEU:CD2	2.44	0.47
1:A:267:ASN:CB	1:B:260:LEU:HG	2.39	0.47
1:A:21:ILE:O	1:A:25:ARG:HG3	2.15	0.47
1:A:52:VAL:CG2	1:B:41:MET:HG2	2.45	0.47
1:A:421:ARG:HH22	1:B:239:GLU:HG2	1.80	0.47
1:A:86:GLU:HB2	1:A:226:GLU:OE1	2.15	0.47
1:A:33:VAL:HG13	1:B:433:LEU:HD23	1.97	0.47
1:B:320:HIS:CG	1:B:323:LEU:HB2	2.50	0.46
1:A:228:MET:O	1:A:232:LEU:HB2	2.15	0.46
1:B:227:LEU:HD13	1:B:381:LEU:HD23	1.96	0.46
1:B:127:MET:CE	1:B:143:ALA:HB1	2.42	0.46
1:A:308:THR:HG22	1:A:313:ARG:HB2	1.96	0.46
1:A:227:LEU:O	1:A:230:LEU:HB3	2.16	0.46
1:A:346:MET:O	1:A:350:VAL:HB	2.15	0.46
1:B:359:ASN:HA	1:B:362:LEU:CD1	2.38	0.46
1:A:177:ASP:O	1:A:181:LYS:HD2	2.16	0.46
1:A:359:ASN:CA	1:A:362:LEU:HB2	2.39	0.46
1:B:383:GLN:HA	1:B:387:MET:O	2.15	0.46
1:B:162:ILE:HD13	1:B:170:LEU:CD1	2.46	0.46
1:B:194:TYR:CD2	1:B:389:GLU:HG3	2.51	0.46
1:A:217:LEU:HB3	1:A:219:TYR:HD2	1.81	0.46
1:A:284:TRP:HH2	1:A:305:ILE:HG12	1.80	0.46
1:B:182:LEU:N	1:B:183:PRO:HD2	2.31	0.46
1:A:172:TYR:CE2	1:A:176:MET:HG3	2.50	0.46
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.67	0.46
1:B:37:THR:HG22	1:B:40:MET:SD	2.57	0.45
1:A:213:PHE:CE2	1:A:399:VAL:HG11	2.51	0.45
1:A:39:ASP:OD1	1:B:25:ARG:NH2	2.48	0.45
1:B:377:HIS:O	1:B:381:LEU:HD13	2.16	0.45
1:B:253:SER:HB2	1:B:418:PRO:O	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:MET:HG2	1:A:430:LEU:CG	2.47	0.45
1:B:178:LEU:HG	1:B:182:LEU:HD12	1.97	0.45
1:A:135:LEU:HB3	1:A:140:GLN:HG3	1.98	0.45
1:A:251:VAL:HG13	1:B:267:ASN:C	2.36	0.45
1:B:125:VAL:HG13	1:B:188:LYS:HE2	1.97	0.45
1:B:298:ASP:OD2	1:B:301:LEU:HD23	2.15	0.45
1:A:420:GLU:HA	1:B:44:GLY:O	2.17	0.45
1:A:247:THR:CG2	1:A:265:ALA:HA	2.46	0.45
1:A:349:LEU:C	1:A:352:GLN:H	2.20	0.45
1:A:175:CYS:O	1:A:179:ILE:HG13	2.16	0.45
1:A:92:LEU:HD22	1:A:233:THR:HG23	1.99	0.45
1:A:168:TRP:HA	1:A:413:ARG:HB3	1.98	0.45
1:B:86:GLU:CG	1:B:230:LEU:HB2	2.43	0.45
1:A:137:PRO:HG3	1:A:193:LEU:HD23	1.99	0.45
1:A:151:GLU:HB3	3:A:465:HOH:O	2.17	0.45
1:B:329:ARG:O	1:B:374:VAL:HG23	2.16	0.45
1:A:14:ILE:CG2	1:A:414:ALA:HB1	2.43	0.45
1:A:187:ALA:O	1:A:191:ARG:HB2	2.17	0.45
1:A:329:ARG:HB3	1:A:374:VAL:CG2	2.47	0.45
1:B:276:LEU:HD23	1:B:280:GLU:OE1	2.17	0.45
1:A:128:LEU:HD23	1:A:131:PHE:CD2	2.52	0.45
1:B:210:SER:O	1:B:213:PHE:HB3	2.16	0.45
1:B:277:ALA:HB3	1:B:375:ASP:OD1	2.17	0.44
1:B:65:ARG:HB3	1:B:68:GLY:CA	2.47	0.44
1:A:5:ASN:C	1:A:5:ASN:HD22	2.20	0.44
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.61	0.44
1:A:172:TYR:HA	1:A:410:ILE:CD1	2.47	0.44
1:B:6:LEU:HB2	1:B:94:TRP:CH2	2.52	0.44
1:B:260:LEU:HD12	1:B:260:LEU:HA	1.72	0.44
1:A:45:MET:HE2	1:B:422:PRO:CB	2.47	0.44
1:A:136:HIS:CE1	1:A:279:GLN:HE22	2.34	0.44
1:A:272:PRO:CB	1:B:158:TYR:CE1	3.00	0.44
1:B:6:LEU:HB2	1:B:94:TRP:CZ3	2.52	0.44
1:B:421:ARG:HA	1:B:422:PRO:HD2	1.89	0.44
1:A:204:ASP:OD2	1:A:206:LYS:HG3	2.18	0.44
1:A:109:TRP:CZ3	1:A:110:LEU:HD12	2.53	0.44
1:B:59:ASP:H	1:B:63:GLY:HA2	1.82	0.44
1:A:9:ILE:CG2	1:A:13:LEU:HD13	2.48	0.44
1:B:67:ARG:HB3	1:B:69:TYR:HD1	1.77	0.44
1:A:228:MET:CE	1:A:228:MET:HA	2.48	0.44
1:A:228:MET:HE2	1:A:228:MET:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:THR:HA	1:B:193:LEU:HD11	2.00	0.44
1:B:366:LYS:HB3	1:B:367:ALA:H	1.64	0.44
1:B:117:ARG:HH11	1:B:117:ARG:HD3	1.56	0.44
1:B:45:MET:HG2	1:B:48:MET:SD	2.58	0.44
1:B:178:LEU:CD1	1:B:182:LEU:HD12	2.48	0.44
1:B:200:ILE:O	1:B:216:MET:HG2	2.17	0.44
1:B:303:ASP:O	1:B:307:ASN:HB2	2.18	0.44
1:B:168:TRP:CE2	1:B:169:GLU:HG3	2.53	0.44
1:B:23:THR:O	1:B:26:GLN:HB2	2.18	0.44
1:A:86:GLU:HG3	1:A:87:PRO:HD2	2.00	0.44
1:A:281:VAL:O	1:A:285:LEU:HB2	2.18	0.44
1:A:69:TYR:CD1	1:A:95:LEU:HD11	2.53	0.44
1:B:204:ASP:OD2	1:B:206:LYS:HG3	2.18	0.44
1:B:98:THR:C	1:B:100:GLN:H	2.21	0.44
1:A:66:PHE:HD1	1:A:96:LEU:HD21	1.83	0.43
1:A:425:MET:CG	1:A:430:LEU:HG	2.48	0.43
1:B:288:LEU:O	1:B:288:LEU:HD12	2.18	0.43
1:A:422:PRO:HG3	1:B:45:MET:CE	2.48	0.43
1:A:421:ARG:HH12	1:B:239:GLU:CD	2.21	0.43
1:B:59:ASP:OD2	1:B:62:GLU:HG2	2.18	0.43
1:A:418:PRO:HB2	1:A:419:LEU:H	1.49	0.43
1:B:132:PRO:HD2	1:B:135:LEU:HD12	1.99	0.43
1:A:178:LEU:HG	1:A:182:LEU:CD1	2.47	0.43
1:A:46:ARG:HH22	1:B:418:PRO:CB	2.32	0.43
1:A:35:GLN:HB3	1:B:32:VAL:HG23	2.00	0.43
1:A:424:SER:HB2	1:B:51:LEU:HB2	1.96	0.43
1:A:396:LEU:HA	1:A:396:LEU:HD23	1.87	0.43
1:A:227:LEU:HD13	1:A:381:LEU:HD23	2.01	0.43
1:A:298:ASP:HA	1:A:301:LEU:CB	2.47	0.43
1:A:10:LEU:HA	1:A:10:LEU:HD23	1.77	0.43
1:A:9:ILE:HG22	1:A:13:LEU:HD13	2.01	0.43
1:B:347:PHE:O	1:B:350:VAL:HB	2.19	0.43
1:A:149:ASN:HB3	1:A:259:TYR:HB2	2.01	0.43
1:A:269:LEU:HA	1:A:274:HIS:CD2	2.53	0.43
1:A:101:ILE:HA	1:A:102:PRO:HD3	1.94	0.43
1:B:300:LYS:HA	1:B:303:ASP:CB	2.46	0.43
1:B:313:ARG:HE	1:B:313:ARG:HB2	1.65	0.43
1:A:155:ALA:HB2	1:A:257:ASP:OD2	2.19	0.43
1:B:324:ARG:HG3	1:B:368:LYS:HE2	2.00	0.43
1:A:272:PRO:CB	1:B:158:TYR:HE1	2.32	0.43
1:B:173:GLU:OE2	1:B:173:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HA	1:A:285:LEU:HD12	1.81	0.42
3:A:471:HOH:O	1:B:419:LEU:HD21	2.19	0.42
1:A:6:LEU:HB3	1:A:172:TYR:OH	2.18	0.42
1:B:120:LEU:HA	1:B:120:LEU:HD12	1.78	0.42
1:B:101:ILE:HA	1:B:102:PRO:HD3	1.54	0.42
1:A:17:GLU:HA	1:A:20:ARG:HB2	2.00	0.42
1:A:145:ILE:HG12	1:A:148:LEU:HD12	2.00	0.42
1:A:127:MET:CE	1:B:127:MET:HE3	2.49	0.42
1:A:145:ILE:HG22	1:A:263:ALA:HB2	2.01	0.42
1:A:272:PRO:HA	1:A:276:LEU:HB3	2.01	0.42
1:A:174:ASP:HB3	1:A:258:PRO:HG2	2.01	0.42
1:A:253:SER:HB2	1:A:418:PRO:O	2.19	0.42
1:A:138:MET:HE3	1:A:270:ALA:HB2	2.00	0.42
1:B:120:LEU:HD21	1:B:185:VAL:CG2	2.45	0.42
1:A:266:MET:CE	1:A:269:LEU:HD23	2.48	0.42
1:A:404:GLY:O	1:A:407:ALA:HB3	2.19	0.42
1:A:278:ASN:HD21	1:A:397:PHE:HD2	1.67	0.42
1:B:157:ALA:HB2	1:B:170:LEU:HD13	2.02	0.42
1:A:131:PHE:HZ	1:A:143:ALA:HB3	1.84	0.42
1:A:89:PRO:HG3	1:A:229:ARG:O	2.19	0.42
1:A:284:TRP:HE3	1:A:285:LEU:HD13	1.84	0.42
1:A:52:VAL:HG11	1:B:42:TYR:CE1	2.55	0.42
1:B:284:TRP:CZ2	1:B:305:ILE:HG12	2.53	0.42
1:B:271:GLY:HA2	1:B:272:PRO:HD3	1.90	0.42
1:A:168:TRP:HB3	1:A:414:ALA:CB	2.42	0.42
1:B:162:ILE:HD13	1:B:170:LEU:HD12	2.02	0.42
1:A:418:PRO:HB2	1:B:46:ARG:HH22	1.84	0.42
1:B:103:THR:HG21	1:B:105:GLU:HB3	2.02	0.42
1:A:420:GLU:OE1	1:B:246:HIS:HE1	2.03	0.42
1:B:258:PRO:HA	1:B:261:SER:OG	2.20	0.42
1:A:211:HIS:O	1:A:214:THR:HG22	2.20	0.42
1:A:225:THR:O	1:A:229:ARG:HG3	2.20	0.42
1:B:329:ARG:HB3	1:B:374:VAL:CG2	2.50	0.42
1:A:6:LEU:O	1:A:10:LEU:HG	2.20	0.41
1:B:148:LEU:HB3	1:B:259:TYR:HD1	1.82	0.41
1:B:324:ARG:HA	1:B:324:ARG:HD3	1.69	0.41
1:A:260:LEU:HA	1:A:260:LEU:HD12	1.80	0.41
1:B:204:ASP:N	1:B:212:ASN:HD21	2.18	0.41
1:B:215:ASN:HD22	1:B:215:ASN:N	2.18	0.41
1:A:112:LYS:HE2	1:A:112:LYS:HB2	1.88	0.41
1:A:308:THR:HG23	1:A:313:ARG:HE	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:VAL:HA	1:A:363:GLU:HB2	2.01	0.41
1:A:41:MET:O	1:B:52:VAL:HG23	2.20	0.41
1:A:172:TYR:HA	1:A:410:ILE:HD13	2.03	0.41
1:A:333:GLN:NE2	1:A:377:HIS:HB3	2.35	0.41
1:B:64:ILE:CD1	1:B:238:HIS:HA	2.50	0.41
1:A:430:LEU:HA	1:A:430:LEU:HD23	1.83	0.41
1:A:413:ARG:HH11	1:A:413:ARG:HD3	1.62	0.41
1:A:391:ASN:N	1:A:391:ASN:HD22	2.17	0.41
1:B:247:THR:HG21	1:B:265:ALA:HA	2.03	0.41
1:A:305:ILE:O	1:A:309:LEU:HD12	2.20	0.41
1:B:86:GLU:HG3	1:B:230:LEU:HD13	2.02	0.41
1:B:207:LEU:HD13	1:B:211:HIS:ND1	2.35	0.41
1:B:209:TRP:HZ3	1:B:232:LEU:HD23	1.85	0.41
1:A:272:PRO:HB2	1:B:158:TYR:CE1	2.56	0.41
1:B:204:ASP:CG	1:B:206:LYS:H	2.24	0.41
1:B:59:ASP:H	1:B:63:GLY:CA	2.34	0.41
1:A:404:GLY:HA2	1:A:407:ALA:HB3	2.02	0.41
1:A:273:LEU:HD12	1:A:273:LEU:HA	1.82	0.41
1:A:427:THR:HG21	1:B:20:ARG:NH2	2.35	0.41
1:B:114:TRP:CE3	1:B:209:TRP:CD1	3.09	0.41
1:B:95:LEU:HD13	1:B:101:ILE:HG12	2.03	0.41
1:A:178:LEU:HD13	1:A:259:TYR:CD1	2.55	0.41
1:A:214:THR:HG21	1:A:225:THR:OG1	2.21	0.41
1:A:157:ALA:HB2	1:A:170:LEU:HD13	2.02	0.41
1:A:344:ASP:HB3	1:A:347:PHE:HB2	2.03	0.41
1:A:330:TYR:CD2	1:A:372:PRO:HB2	2.56	0.41
1:B:227:LEU:HA	1:B:336:PHE:CE2	2.56	0.41
1:A:174:ASP:HB2	1:A:258:PRO:HG2	2.02	0.40
1:A:167:TYR:HE2	1:A:255:LEU:HD11	1.86	0.40
1:B:423:LYS:HD2	1:B:423:LYS:HA	1.89	0.40
1:B:131:PHE:HD1	1:B:131:PHE:HA	1.73	0.40
1:B:136:HIS:HE1	1:B:279:GLN:HE22	1.68	0.40
1:B:81:ALA:CB	1:B:88:LEU:HD13	2.46	0.40
1:A:178:LEU:O	1:A:182:LEU:HB2	2.21	0.40
1:B:245:ALA:HA	1:B:405:VAL:CG2	2.52	0.40
1:A:5:ASN:HD22	1:A:7:LYS:H	1.69	0.40
1:A:301:LEU:O	1:A:305:ILE:HG13	2.21	0.40
1:B:344:ASP:HB3	1:B:347:PHE:HB2	2.04	0.40
1:B:337:ALA:HB1	1:B:347:PHE:CE2	2.56	0.40
1:A:430:LEU:O	1:A:434:VAL:HG12	2.22	0.40
1:A:347:PHE:C	1:A:350:VAL:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:CD1	1:B:424:SER:HB3	2.52	0.40
1:B:171:ILE:HG21	1:B:171:ILE:HD13	1.80	0.40
1:B:178:LEU:O	1:B:178:LEU:HD12	2.21	0.40
1:A:308:THR:O	1:A:313:ARG:HB2	2.21	0.40
1:A:77:MET:CB	1:A:101:ILE:HD13	2.51	0.40

All (38) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:O	3:B:476:HOH:O[6_455]	0.90	1.30
1:B:153:ASN:OD1	1:B:306:TRP:CH2[3_544]	0.98	1.22
1:A:206:LYS:CD	1:B:191:ARG:NH2[6_455]	1.22	0.98
1:B:156:ARG:CZ	1:B:303:ASP:CB[3_544]	1.41	0.79
1:B:153:ASN:CG	1:B:306:TRP:CH2[3_544]	1.42	0.78
1:B:153:ASN:CB	1:B:306:TRP:CZ2[3_544]	1.45	0.75
1:B:170:LEU:CD2	1:B:310:ASN:OD1[3_544]	1.52	0.68
1:B:156:ARG:NH1	1:B:303:ASP:CB[3_544]	1.52	0.68
1:A:206:LYS:CE	1:B:198:SER:OG[6_455]	1.55	0.65
1:B:156:ARG:NH1	1:B:303:ASP:OD1[3_544]	1.59	0.61
1:A:203:ILE:C	3:B:476:HOH:O[6_455]	1.59	0.61
1:A:153:ASN:CG	1:A:306:TRP:CH2[4_555]	1.66	0.54
1:A:170:LEU:CD2	1:A:310:ASN:OD1[4_555]	1.67	0.53
1:B:156:ARG:NH1	1:B:303:ASP:CG[3_544]	1.69	0.51
1:B:153:ASN:OD1	1:B:306:TRP:CZ3[3_544]	1.69	0.51
1:B:162:ILE:CG2	1:B:311:SER:OG[3_544]	1.74	0.46
1:A:166:LYS:CD	1:A:310:ASN:O[4_555]	1.77	0.43
1:B:156:ARG:NE	1:B:303:ASP:CB[3_544]	1.79	0.41
1:B:157:ALA:CA	1:B:307:ASN:OD1[3_544]	1.80	0.40
1:A:153:ASN:ND2	1:A:306:TRP:CH2[4_555]	1.82	0.38
1:B:153:ASN:CB	1:B:306:TRP:CH2[3_544]	1.82	0.38
1:B:153:ASN:CG	1:B:306:TRP:CZ2[3_544]	1.84	0.36
1:A:206:LYS:NZ	1:B:191:ARG:NE[6_455]	1.87	0.33
1:A:206:LYS:CE	1:B:191:ARG:NH2[6_455]	1.92	0.28
1:A:153:ASN:OD1	1:A:306:TRP:CZ3[4_555]	1.92	0.28
1:B:156:ARG:NH2	1:B:300:LYS:O[3_544]	1.94	0.26
1:A:156:ARG:CZ	1:A:303:ASP:CB[4_555]	1.95	0.25
1:B:157:ALA:N	1:B:307:ASN:OD1[3_544]	1.95	0.25
1:B:156:ARG:O	1:B:307:ASN:OD1[3_544]	1.96	0.24
1:A:156:ARG:O	1:A:307:ASN:OD1[4_555]	1.97	0.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:C	1:B:307:ASN:OD1[3_544]	2.04	0.16
1:A:287:GLN:OE1	1:B:290:LYS:NZ[3_544]	2.05	0.15
1:A:153:ASN:OD1	1:A:306:TRP:CH2[4_555]	2.06	0.14
1:A:290:LYS:NZ	1:B:287:GLN:OE1[3_544]	2.08	0.12
1:A:156:ARG:NH2	1:A:303:ASP:CB[4_555]	2.11	0.09
1:B:153:ASN:CA	1:B:306:TRP:CH2[3_544]	2.16	0.04
1:B:166:LYS:CD	1:B:310:ASN:O[3_544]	2.16	0.04
1:B:153:ASN:OD1	1:B:306:TRP:CZ2[3_544]	2.18	0.02

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	435/437 (100%)	359 (82%)	55 (13%)	21 (5%)	3	10
1	B	435/437 (100%)	357 (82%)	59 (14%)	19 (4%)	3	12
All	All	870/874 (100%)	716 (82%)	114 (13%)	40 (5%)	3	11

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	LYS
1	A	205	SER
1	A	239	GLU
1	B	166	LYS
1	B	239	GLU
1	B	278	ASN
1	B	376	ALA
1	A	5	ASN
1	A	75	GLN
1	A	148	LEU
1	A	149	ASN
1	A	196	GLU

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Mol	Chain	Res	Type
1	A	313	ARG
1	A	418	PRO
1	B	5	ASN
1	B	196	GLU
1	B	277	ALA
1	B	279	GLN
1	B	320	HIS
1	B	338	LEU
1	B	418	PRO
1	A	164	ARG
1	A	202	ALA
1	A	294	LYS
1	A	321	ALA
1	A	420	GLU
1	B	294	LYS
1	A	137	PRO
1	A	276	LEU
1	A	278	ASN
1	A	345	PRO
1	B	149	ASN
1	A	49	LYS
1	B	87	PRO
1	B	243	VAL
1	B	307	ASN
1	B	137	PRO
1	A	243	VAL
1	B	14	ILE
1	B	60	PRO

5.3.2 Protein sidechains (i)

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	371/371 (100%)	311 (84%)	60 (16%)	3 9
1	B	371/371 (100%)	315 (85%)	56 (15%)	3 11
All	All	742/742 (100%)	626 (84%)	116 (16%)	3 10

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

Mol	Chain	Res	Type
1	A	5	ASN
1	A	13	LEU
1	A	17	GLU
1	A	22	LYS
1	A	32	VAL
1	A	35	GLN
1	A	38	VAL
1	A	46	ARG
1	A	49	LYS
1	A	54	GLU
1	A	62	GLU
1	A	76	LYS
1	A	80	LYS
1	A	86	GLU
1	A	98	THR
1	A	112	LYS
1	A	127	MET
1	A	136	HIS
1	A	149	ASN
1	A	151	GLU
1	A	169	GLU
1	A	171	ILE
1	A	182	LEU
1	A	193	LEU
1	A	195	ARG
1	A	203	ILE
1	A	205	SER
1	A	206	LYS
1	A	212	ASN
1	A	214	THR
1	A	217	LEU
1	A	225	THR
1	A	228	MET
1	A	237	ASP
1	A	256	SER
1	A	260	LEU
1	A	261	SER
1	A	273	LEU
1	A	274	HIS
1	A	283	VAL
1	A	285	LEU
1	A	287	GLN

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Mol	Chain	Res	Type
1	A	288	LEU
1	A	310	ASN
1	A	313	ARG
1	A	323	LEU
1	A	339	LYS
1	A	343	HIS
1	A	350	VAL
1	A	355	LYS
1	A	356	ILE
1	A	358	PRO
1	A	359	ASN
1	A	363	GLU
1	A	373	ASN
1	A	397	PHE
1	A	405	VAL
1	A	413	ARG
1	A	421	ARG
1	A	434	VAL
1	B	5	ASN
1	B	20	ARG
1	B	36	ILE
1	B	46	ARG
1	B	49	LYS
1	B	75	GLN
1	B	80	LYS
1	B	86	GLU
1	B	98	THR
1	B	101	ILE
1	B	110	LEU
1	B	112	LYS
1	B	120	LEU
1	B	135	LEU
1	B	136	HIS
1	B	149	ASN
1	B	156	ARG
1	B	162	ILE
1	B	171	ILE
1	B	182	LEU
1	B	193	LEU
1	B	195	ARG
1	B	203	ILE
1	B	210	SER

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Mol	Chain	Res	Type
1	B	214	THR
1	B	215	ASN
1	B	225	THR
1	B	228	MET
1	B	237	ASP
1	B	274	HIS
1	B	285	LEU
1	B	287	GLN
1	B	296	VAL
1	B	307	ASN
1	B	310	ASN
1	B	313	ARG
1	B	315	VAL
1	B	323	LEU
1	B	331	THR
1	B	343	HIS
1	B	349	LEU
1	B	355	LYS
1	B	356	ILE
1	B	373	ASN
1	B	377	HIS
1	B	389	GLU
1	B	391	ASN
1	B	394	THR
1	B	397	PHE
1	B	405	VAL
1	B	413	ARG
1	B	421	ARG
1	B	428	ASP
1	B	431	ILE
1	B	432	LYS
1	B	434	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	27	GLN
1	A	30	ASN
1	A	140	GLN
1	A	149	ASN
1	A	211	HIS

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Mol	Chain	Res	Type
1	A	212	ASN
1	A	215	ASN
1	A	238	HIS
1	A	267	ASN
1	A	278	ASN
1	A	279	GLN
1	A	333	GLN
1	A	359	ASN
1	A	383	GLN
1	A	391	ASN
1	B	5	ASN
1	B	27	GLN
1	B	30	ASN
1	B	106	GLN
1	B	123	HIS
1	B	130	ASN
1	B	136	HIS
1	B	149	ASN
1	B	153	ASN
1	B	163	HIS
1	B	212	ASN
1	B	215	ASN
1	B	246	HIS
1	B	267	ASN
1	B	359	ASN
1	B	383	GLN
1	B	391	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OAA	A	438	-	2,8,8	1.28	0	2,10,10	1.97	1 (50%)
2	OAA	B	438	-	2,8,8	2.02	1 (50%)	2,10,10	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OAA	A	438	-	-	0/2/8/8	0/0/0/0
2	OAA	B	438	-	-	0/2/8/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	438	OAA	O3-C3	2.65	1.26	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	438	OAA	C1-C2-C3	-2.78	110.46	115.52

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

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.