



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:46 PM GMT

PDB ID : 1B76
Title : GLYCYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS
COMPLEXED WITH ATP
Authors : Arnez, J.G.; Moras, D.
Deposited on : 1999-01-27
Resolution : 3.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

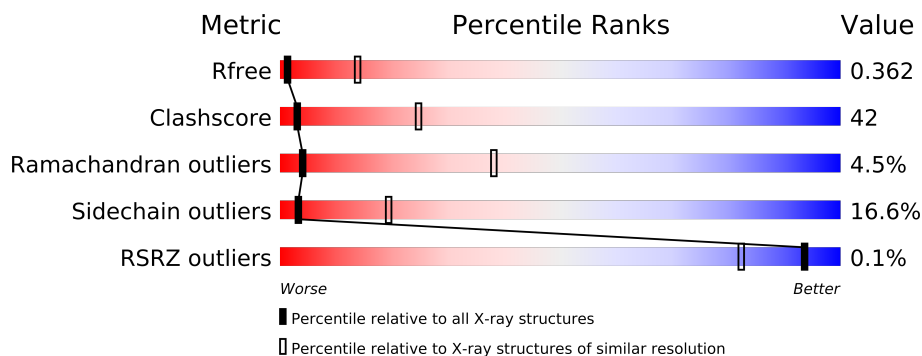
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	442	
1	B	442	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8961 atoms, of which 1686 are hydrogens and 0 are deuterium.

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.

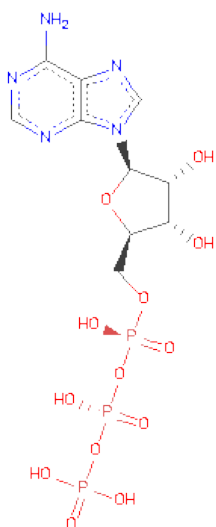
- Molecule 1 is a protein called PROTEIN (GLYCYL-TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	H	N	O	S	0	0	0
			4451	2297	841	649	656	8			
1	B	442	Total	C	H	N	O	S	0	0	0
			4440	2288	839	649	656	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	GAP	UNP P56206
A	?	-	ILE	GAP	UNP P56206
A	91	ALA	THR	conflict	UNP P56206
A	93	ALA	LYS	conflict	UNP P56206
B	?	-	ARG	GAP	UNP P56206
B	?	-	ILE	GAP	UNP P56206
B	91	ALA	THR	conflict	UNP P56206
B	93	ALA	LYS	conflict	UNP P56206

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			34	10	3	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			34	10	3	5	13	3		

- Molecule 3 is water.

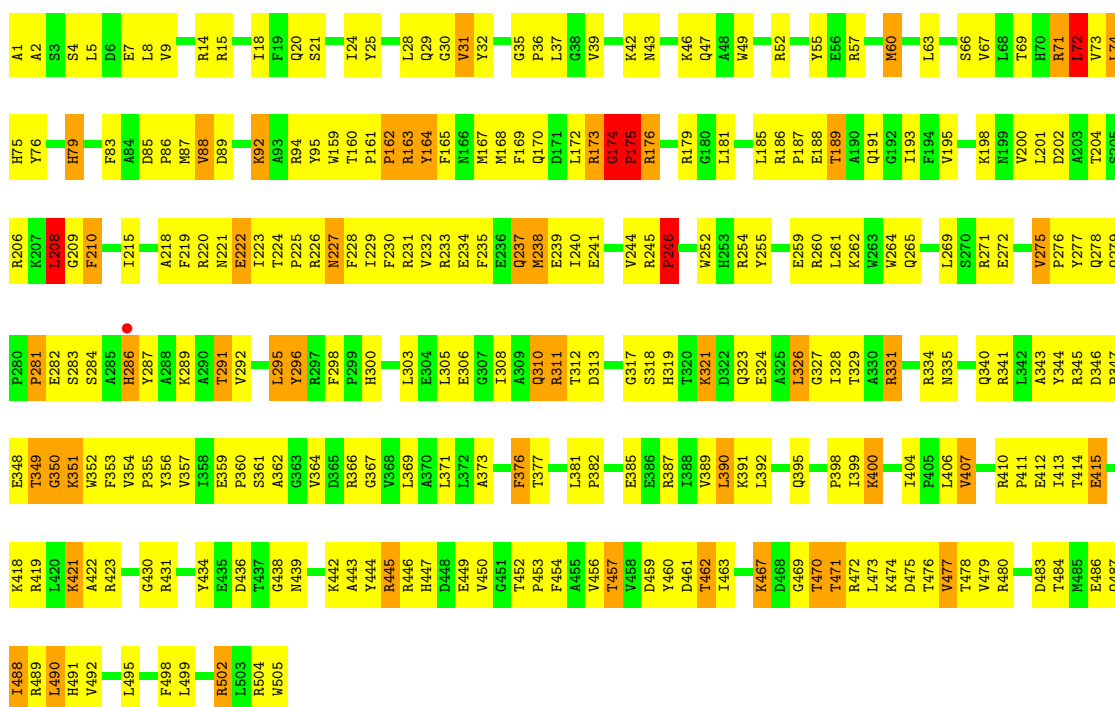
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		

3 Residue-property plots

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.

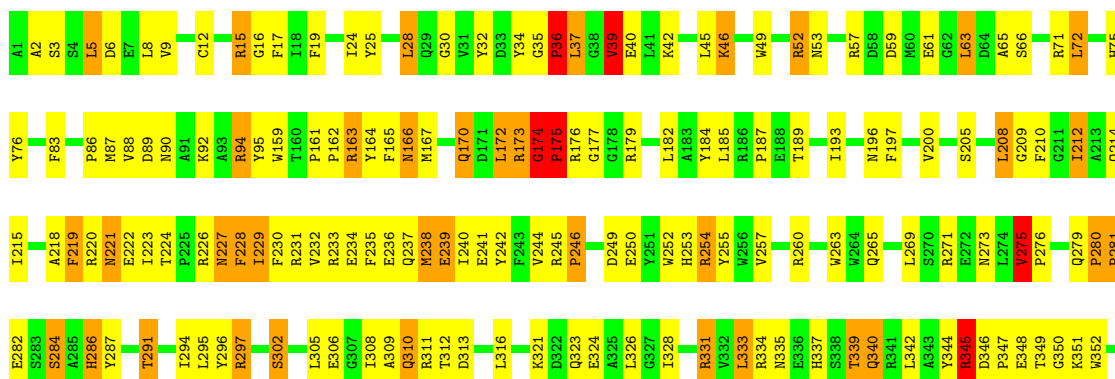
• Molecule 1: PROTEIN (GLYCYL-TRNA SYNTHETASE)

Chain A:



• Molecule 1: PROTEIN (GLYCYL-TRNA SYNTHETASE)

Chain B:



Q487	R423	Y366
I488	L424	Y367
R489	A425	I368
L490	A426	E369
H491	L427	P360
V492	G428	S361
D493	L429	A362
E494	G430	G363
L495	R431	V364
E496	V432	D365
G497	L433	
F498	T434	V368
L499	E435	L369
R500	D436	
R502	T437	L372
L503	G438	A373
E504	M439	E374
#505	T440	A375
	K441	F376
	K442	T377
	A443	R378
	Y444	E380
	R445	E379
	R446	L381
	H447	P382
	V450	E385
	G451	E386
	T452	R387
	P453	L388
	V454	V389
	A455	L390
	A456	K391
	T457	L392
	V458	K393
	D459	P394
	Y460	Q395
	D461	
	T462	P398
	I463	I399
		K400
		V401
	S466	L404
	K467	P405
	D468	L406
	G469	V407
	T470	K408
	T471	M409
	R472	L410
	K473	P411
	D475	E412
	T476	I413
	V477	T414
	T478	E415
	V479	Y416
	R480	A417
		K418
		L419
	M485	T420

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.80Å 250.90Å 105.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 3.40 12.16 – 3.30	Depositor EDS
% Data completeness (in resolution range)	83.0 (9.00-3.40) 80.4 (12.16-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	9.50	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.28Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.227 , 0.318 0.297 , 0.362	Depositor DCC
R_{free} test set	784 reflections (3.95%)	DCC
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 66.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	1 of 19864 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	8961	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.71	0/3696	0.92	6/4999 (0.1%)
1	B	0.66	0/3686	0.91	9/4986 (0.2%)
All	All	0.69	0/7382	0.91	15/9985 (0.2%)

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	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	GLY	C-N-CD	-9.31	100.11	120.60
1	A	174	GLY	C-N-CD	-8.00	102.99	120.60
1	B	39	VAL	CB-CA-C	-7.07	97.96	111.40
1	A	208	LEU	N-CA-C	6.75	129.23	111.00
1	B	208	LEU	N-CA-C	6.64	128.94	111.00
1	B	227	ASN	N-CA-C	5.80	126.67	111.00
1	B	345	ARG	N-CA-C	5.60	126.11	111.00
1	A	74	LEU	CA-CB-CG	-5.52	102.60	115.30
1	A	72	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	275	VAL	C-N-CD	-5.33	108.87	120.60
1	B	28	LEU	N-CA-C	-5.30	96.68	111.00
1	A	275	VAL	C-N-CD	-5.27	109.01	120.60
1	B	212	ILE	CB-CA-C	-5.17	101.25	111.60
1	B	280	PRO	C-N-CD	-5.17	109.23	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	ILE	CB-CA-C	-5.06	101.48	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3610	841	2725	306	0
1	B	3601	839	2709	322	0
2	A	31	3	9	5	0
2	B	31	3	9	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	7275	1686	5452	600	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 42.

All (600) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:88:VAL:HG22	1:B:162:PRO:HB3	1.26	1.09
1:B:413:ILE:HG12	1:B:463:ILE:HD11	1.35	1.04
1:A:366:ARG:NH1	2:A:1552:ATP:H2'	1.72	1.02
1:A:400:LYS:HD3	1:A:430:GLY:HA3	1.43	1.00
1:B:442:LYS:HA	1:B:445:ARG:HD3	1.46	0.96
1:B:331:ARG:HB3	1:B:331:ARG:HH11	1.32	0.93
1:B:245:ARG:HH21	1:B:347:PRO:HA	1.35	0.90
1:A:173:ARG:NH1	1:A:173:ARG:HB2	1.86	0.90
1:A:413:ILE:CG1	1:A:463:ILE:HD11	2.04	0.88
1:A:244:VAL:HG21	1:A:252:TRP:CD1	2.09	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:387:ARG:HD2	1:A:445:ARG:HH21	1.41	0.84
1:A:444:TYR:CE1	1:A:480:ARG:HD3	2.12	0.83
1:A:326:LEU:HD23	1:A:341:ARG:HH22	1.44	0.82
1:B:316:LEU:HD22	1:B:342:LEU:HG	1.59	0.82
1:B:253:HIS:CD2	1:B:310:GLN:HB2	2.14	0.80
1:B:287:TYR:HD2	1:B:311:ARG:HG2	1.45	0.80
1:B:200:VAL:HG11	1:B:212:ILE:HD11	1.61	0.80
1:B:5:LEU:O	1:B:9:VAL:HG23	1.83	0.79
1:B:457:THR:HG23	1:B:478:THR:HG23	1.63	0.79
1:A:395:GLN:HB3	1:A:505:TRP:CE2	2.16	0.78
1:A:312:THR:O	1:A:356:TYR:HA	1.83	0.78
1:B:502:ARG:HD3	1:B:502:ARG:N	1.98	0.78
1:B:312:THR:O	1:B:356:TYR:HA	1.82	0.78
1:B:413:ILE:HG12	1:B:463:ILE:CD1	2.13	0.78
1:A:230:PHE:HE2	1:A:303:LEU:HD13	1.47	0.78
1:A:15:ARG:O	1:A:37:LEU:HD12	1.83	0.78
1:A:25:TYR:HD2	1:B:72:LEU:HD12	1.46	0.78
1:A:456:VAL:HG21	1:A:495:LEU:HD21	1.66	0.77
1:B:245:ARG:HH12	1:B:347:PRO:HB3	1.48	0.77
1:A:323:GLN:NE2	1:A:335:ASN:H	1.82	0.77
1:A:413:ILE:HG13	1:A:463:ILE:HD11	1.63	0.77
1:A:366:ARG:HH11	2:A:1552:ATP:H2'	1.51	0.76
1:A:410:ARG:HB3	1:A:412:GLU:OE1	1.86	0.74
1:A:410:ARG:NE	1:A:460:TYR:HE1	1.86	0.74
1:B:2:ALA:HB2	1:B:376:PHE:HB3	1.67	0.74
1:B:423:ARG:NH1	1:B:496:GLU:HG3	2.03	0.74
1:B:220:ARG:O	1:B:233:ARG:HA	1.88	0.73
1:B:364:VAL:O	1:B:368:VAL:HG23	1.89	0.73
1:A:173:ARG:HH11	1:A:173:ARG:HB2	1.54	0.72
1:A:277:TYR:HB3	1:A:295:LEU:HD21	1.70	0.72
1:A:351:LYS:HG3	1:A:352:TRP:N	2.03	0.72
1:A:2:ALA:HB2	1:A:376:PHE:HB3	1.72	0.72
1:A:79:HIS:HA	1:A:83:PHE:HB2	1.72	0.71
1:B:461:ASP:HB2	1:B:473:LEU:HB3	1.71	0.71
1:A:88:VAL:HB	1:A:159:TRP:CZ3	2.26	0.71
1:A:244:VAL:HG21	1:A:252:TRP:NE1	2.06	0.71
1:A:413:ILE:HG12	1:A:463:ILE:HD11	1.73	0.70
1:B:287:TYR:CD2	1:B:311:ARG:HG2	2.25	0.70
1:B:15:ARG:O	1:B:37:LEU:HD23	1.92	0.70
1:A:189:THR:HG23	1:A:237:GLN:NE2	2.06	0.70
1:A:313:ASP:HB2	1:A:354:VAL:HG12	1.73	0.70
1:A:241:GLU:OE1	1:A:359:GLU:HG3	1.92	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:208:LEU:HG	1:B:344:TYR:CE2	2.27	0.70
1:A:450:VAL:HG23	1:A:452:THR:HG23	1.74	0.69
1:A:223:ILE:HG22	1:A:224:THR:HG23	1.73	0.69
1:B:244:VAL:HG21	1:B:252:TRP:CD1	2.28	0.69
1:A:28:LEU:O	1:A:31:VAL:HG13	1.92	0.69
1:B:189:THR:HG22	1:B:214:GLN:OE1	1.93	0.69
1:A:404:ILE:HD13	1:A:443:ALA:HB1	1.75	0.69
1:B:87:MET:O	1:B:162:PRO:HA	1.92	0.68
1:B:331:ARG:NH1	1:B:331:ARG:HB3	2.08	0.68
1:B:165:PHE:O	1:B:167:MET:SD	2.51	0.68
1:B:344:TYR:CD1	1:B:345:ARG:N	2.62	0.68
1:B:208:LEU:HG	1:B:344:TYR:CD2	2.28	0.68
1:B:411:PRO:O	1:B:415:GLU:HG2	1.93	0.68
1:B:399:ILE:HD13	1:B:433:LEU:HD13	1.75	0.68
1:B:52:ARG:HG2	1:B:263:TRP:CD1	2.28	0.68
1:A:410:ARG:O	1:A:413:ILE:HB	1.94	0.68
1:A:340:GLN:HB2	1:B:24:ILE:HG22	1.75	0.68
1:A:208:LEU:O	1:A:210:PHE:N	2.27	0.67
1:B:410:ARG:HD2	1:B:412:GLU:HB2	1.76	0.67
1:B:440:ILE:HD11	1:B:444:TYR:CE2	2.29	0.67
1:B:423:ARG:HH12	1:B:496:GLU:HG3	1.59	0.67
1:B:406:LEU:HB2	1:B:459:ASP:HB3	1.77	0.67
1:A:88:VAL:HA	1:A:163:ARG:NH1	2.10	0.67
1:A:189:THR:HG23	1:A:237:GLN:HE21	1.60	0.67
1:B:265:GLN:OE1	1:B:271:ARG:HB2	1.95	0.67
1:A:5:LEU:HD23	1:A:227:ASN:HB2	1.77	0.67
1:B:244:VAL:HG11	1:B:252:TRP:HD1	1.60	0.67
1:A:323:GLN:HE22	1:A:334:ARG:HA	1.60	0.66
1:B:454:PHE:HE1	1:B:503:LEU:HD21	1.59	0.66
1:B:323:GLN:NE2	1:B:335:ASN:H	1.93	0.66
1:A:287:TYR:CE2	1:A:311:ARG:CZ	2.79	0.66
1:B:345:ARG:HD3	1:B:346:ASP:N	2.10	0.66
1:A:480:ARG:HG2	1:A:480:ARG:HH11	1.60	0.66
1:B:399:ILE:CD1	1:B:433:LEU:HD13	2.26	0.66
1:A:381:LEU:HD21	1:A:387:ARG:HD3	1.77	0.66
1:A:460:TYR:HA	1:A:463:ILE:HD12	1.76	0.66
1:A:79:HIS:O	1:A:83:PHE:HB3	1.96	0.66
1:A:174:GLY:H	1:B:221:ASN:HD22	1.44	0.66
1:A:480:ARG:NH1	1:A:480:ARG:HG2	2.11	0.65
1:A:281:PRO:HG2	1:A:282:GLU:OE1	1.96	0.65
1:B:310:GLN:HG2	1:B:358:ILE:CD1	2.27	0.65
1:B:83:PHE:CG	1:B:166:ASN:HA	2.31	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:323:GLN:NE2	1:B:334:ARG:HA	2.12	0.65
1:A:88:VAL:HB	1:A:159:TRP:HZ3	1.61	0.65
1:A:87:MET:SD	1:A:165:PHE:HB2	2.37	0.65
1:A:176:ARG:HE	1:B:163:ARG:HH12	1.46	0.64
1:B:394:PRO:HB2	1:B:395:GLN:OE1	1.98	0.64
1:A:323:GLN:NE2	1:A:334:ARG:HA	2.13	0.64
1:A:296:TYR:HD2	1:A:298:PHE:CD1	2.15	0.64
1:A:457:THR:O	1:A:477:VAL:HG12	1.98	0.64
1:A:381:LEU:HB2	1:A:385:GLU:O	1.98	0.63
1:A:25:TYR:CD2	1:B:72:LEU:HD12	2.32	0.63
1:B:65:ALA:H	1:B:214:GLN:NE2	1.97	0.63
1:A:461:ASP:O	1:A:474:LYS:HA	1.98	0.63
1:A:410:ARG:HD2	1:A:412:GLU:OE1	1.99	0.63
1:A:169:PHE:HE1	1:B:173:ARG:HH22	1.46	0.63
1:B:414:THR:O	1:B:418:LYS:HG3	1.99	0.63
1:B:287:TYR:CE2	1:B:311:ARG:NH1	2.67	0.63
1:A:445:ARG:HA	1:A:445:ARG:NE	2.14	0.62
1:B:287:TYR:HE2	1:B:311:ARG:NH1	1.97	0.62
1:A:24:ILE:HG13	1:A:25:TYR:CD1	2.34	0.62
1:B:405:PRO:HD2	1:B:435:GLU:O	2.00	0.62
1:B:395:GLN:N	1:B:395:GLN:OE1	2.31	0.62
1:A:72:LEU:HD12	1:B:25:TYR:CG	2.34	0.62
1:A:484:THR:CB	1:A:486:GLU:HG2	2.28	0.62
1:A:246:PRO:HA	1:A:356:TYR:CD1	2.34	0.62
1:B:323:GLN:HE22	1:B:334:ARG:HA	1.63	0.62
1:A:456:VAL:CG2	1:A:495:LEU:HD21	2.28	0.62
1:B:257:VAL:HG22	1:B:308:ILE:HB	1.82	0.62
1:B:16:GLY:HA2	1:B:19:PHE:CE1	2.35	0.61
1:B:87:MET:HB3	1:B:94:ARG:NH2	2.15	0.61
1:A:410:ARG:HG3	1:A:460:TYR:OH	2.01	0.61
1:B:2:ALA:CB	1:B:8:LEU:HD21	2.29	0.61
1:A:57:ARG:HD3	1:A:60:MET:HG3	1.82	0.61
1:B:197:PHE:O	1:B:200:VAL:HG12	1.98	0.61
1:A:234:GLU:OE1	1:B:66:SER:HB2	2.00	0.61
1:B:480:ARG:HB2	1:B:487:GLN:HG3	1.80	0.61
1:B:456:VAL:HG22	1:B:479:VAL:HG12	1.81	0.61
1:A:475:ASP:O	1:A:492:VAL:HG23	2.01	0.61
1:A:462:THR:HG23	1:A:476:THR:O	2.00	0.61
1:A:172:LEU:HB3	1:A:181:LEU:CD1	2.31	0.61
1:A:9:VAL:HG22	1:A:228:PHE:CD2	2.36	0.61
1:B:466:SER:HB2	1:B:470:THR:O	2.01	0.61
1:A:387:ARG:HB2	1:A:445:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:450:VAL:HG23	1:B:452:THR:HG23	1.81	0.60
1:A:484:THR:OG1	1:A:486:GLU:HG2	2.01	0.60
1:B:347:PRO:O	1:B:348:GLU:HG2	2.00	0.60
1:B:219:PHE:N	1:B:219:PHE:CD1	2.69	0.60
1:A:89:ASP:N	1:A:159:TRP:CZ3	2.70	0.60
1:B:229:ILE:HG23	1:B:229:ILE:O	2.01	0.60
1:A:265:GLN:HA	1:A:269:LEU:O	2.02	0.60
1:A:474:LYS:O	1:A:475:ASP:HB2	2.02	0.60
1:B:2:ALA:HB3	1:B:8:LEU:HD21	1.83	0.60
1:A:407:VAL:HG21	1:A:460:TYR:CE2	2.37	0.60
1:B:52:ARG:HH11	1:B:52:ARG:HG3	1.67	0.60
1:A:348:GLU:HG3	1:A:349:THR:HG23	1.84	0.59
1:A:79:HIS:HB3	1:A:168:MET:HE1	1.84	0.59
1:B:460:TYR:HA	1:B:463:ILE:HD12	1.84	0.59
1:A:418:LYS:O	1:A:421:LYS:HE2	2.01	0.59
1:B:208:LEU:O	1:B:210:PHE:N	2.35	0.59
1:A:484:THR:HB	1:A:486:GLU:HG2	1.84	0.59
1:A:410:ARG:NE	1:A:460:TYR:CE1	2.69	0.59
1:B:71:ARG:HE	1:B:182:LEU:HD23	1.67	0.59
1:B:36:PRO:O	1:B:39:VAL:HG23	2.02	0.59
1:B:363:GLY:HA3	2:B:2552:ATP:H1'	1.85	0.59
1:B:57:ARG:HH22	1:B:242:TYR:HE1	1.50	0.59
1:B:427:LEU:CD2	1:B:496:GLU:HG2	2.32	0.59
1:A:223:ILE:CD1	1:B:175:PRO:HD3	2.33	0.59
1:A:4:SER:OG	1:A:7:GLU:HG3	2.02	0.59
2:A:1552:ATP:H3'	2:A:1552:ATP:O1B	2.03	0.59
1:A:351:LYS:HG3	1:A:352:TRP:O	2.02	0.59
1:B:308:ILE:H	1:B:308:ILE:HD12	1.67	0.58
1:A:24:ILE:HG22	1:B:340:GLN:NE2	2.18	0.58
1:B:237:GLN:HA	1:B:364:VAL:HG23	1.84	0.58
1:A:69:THR:HB	1:A:74:LEU:HD11	1.85	0.58
1:B:265:GLN:HA	1:B:269:LEU:O	2.03	0.58
1:A:175:PRO:HD3	1:B:223:ILE:HD13	1.85	0.58
1:A:208:LEU:HD11	1:A:355:PRO:HB3	1.84	0.58
1:B:242:TYR:HD2	1:B:244:VAL:HG23	1.69	0.58
1:B:219:PHE:HD1	1:B:219:PHE:N	2.01	0.58
1:A:331:ARG:HG2	1:A:331:ARG:O	2.03	0.58
1:B:347:PRO:HG3	1:B:351:LYS:HB3	1.86	0.58
1:B:410:ARG:HG3	1:B:413:ILE:HG13	1.84	0.58
1:A:447:HIS:HA	1:A:450:VAL:HG22	1.86	0.58
1:A:504:ARG:NH1	1:A:504:ARG:HB3	2.18	0.58
1:B:260:ARG:HD3	1:B:306:GLU:OE2	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:PHE:CZ	1:A:303:LEU:HB3	2.40	0.57
1:B:253:HIS:HE1	1:B:308:ILE:O	1.86	0.57
1:B:495:LEU:O	1:B:499:LEU:HG	2.04	0.57
1:B:72:LEU:O	1:B:75:HIS:HB3	2.04	0.57
1:B:446:ARG:O	1:B:450:VAL:HG22	2.05	0.57
1:B:252:TRP:CZ3	1:B:255:TYR:CD2	2.93	0.57
1:B:245:ARG:HH12	1:B:347:PRO:CB	2.18	0.57
1:A:462:THR:HG21	1:A:477:VAL:HG13	1.87	0.57
1:A:204:THR:OG1	1:A:206:ARG:HG2	2.04	0.57
1:A:74:LEU:HB3	1:A:168:MET:HE1	1.85	0.57
1:B:46:LYS:HE3	1:B:236:GLU:OE2	2.04	0.57
1:B:252:TRP:HZ3	1:B:255:TYR:CD2	2.23	0.57
1:B:424:LEU:HA	1:B:427:LEU:HG	1.87	0.57
1:A:76:TYR:O	1:A:318:SER:HB3	2.04	0.56
1:B:473:LEU:CD2	1:B:489:ARG:HD3	2.35	0.56
1:B:71:ARG:HH22	1:B:179:ARG:HE	1.52	0.56
1:A:42:LYS:O	1:A:46:LYS:HG3	2.05	0.56
1:A:287:TYR:HE2	1:A:311:ARG:CZ	2.18	0.56
1:A:279:GLN:HG3	1:A:291:THR:HG23	1.87	0.56
1:B:86:PRO:HG3	1:B:164:TYR:HE1	1.69	0.56
1:B:173:ARG:NH1	1:B:173:ARG:N	2.53	0.56
1:B:46:LYS:HG2	1:B:215:ILE:HG21	1.88	0.56
1:B:321:LYS:HD3	1:B:339:THR:O	2.06	0.56
1:B:454:PHE:CE2	1:B:498:PHE:HE1	2.23	0.56
1:B:390:LEU:HD13	1:B:392:LEU:HD11	1.88	0.56
1:A:480:ARG:HD2	1:A:487:GLN:HE21	1.70	0.55
1:B:475:ASP:O	1:B:492:VAL:HG23	2.06	0.55
1:A:376:PHE:CD1	1:A:376:PHE:C	2.79	0.55
1:B:378:ARG:HH22	1:B:388:ILE:HD11	1.71	0.55
1:B:349:THR:OG1	1:B:350:GLY:N	2.39	0.55
1:A:245:ARG:HG2	1:A:246:PRO:HD2	1.88	0.55
1:B:297:ARG:CZ	1:B:302:SER:HB2	2.37	0.55
1:A:71:ARG:HE	1:A:179:ARG:HE	1.53	0.55
1:A:230:PHE:CE1	1:A:366:ARG:CZ	2.89	0.55
1:B:200:VAL:HG11	1:B:212:ILE:CD1	2.34	0.55
1:A:1:ALA:N	1:A:377:THR:HG22	2.22	0.55
1:B:94:ARG:O	1:B:95:TYR:CB	2.55	0.55
1:B:345:ARG:O	1:B:347:PRO:HD3	2.06	0.55
1:A:87:MET:SD	1:A:165:PHE:CB	2.95	0.55
1:B:472:ARG:O	1:B:472:ARG:HD2	2.07	0.55
1:A:240:ILE:HB	1:A:360:PRO:HD2	1.87	0.55
1:A:444:TYR:CD1	1:A:480:ARG:HD3	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:294:ILE:HD11	1:B:308:ILE:HD11	1.90	0.54
1:A:390:LEU:HG	1:A:449:GLU:O	2.06	0.54
1:A:504:ARG:HB3	1:A:504:ARG:HH11	1.73	0.54
1:A:221:ASN:HD22	1:B:174:GLY:HA3	1.71	0.54
1:B:32:TYR:HB2	1:B:229:ILE:HD13	1.88	0.54
1:A:201:LEU:HD12	1:A:206:ARG:HB2	1.90	0.54
1:B:57:ARG:NH2	1:B:242:TYR:HE1	2.05	0.54
1:A:476:THR:OG1	1:A:489:ARG:NH1	2.37	0.54
1:A:215:ILE:HA	1:A:238:MET:HA	1.89	0.54
1:A:230:PHE:CE1	1:A:366:ARG:NE	2.76	0.54
1:A:460:TYR:HA	1:A:463:ILE:CD1	2.38	0.54
1:A:262:LYS:HB2	1:A:262:LYS:NZ	2.23	0.54
1:A:413:ILE:HG22	1:A:414:THR:N	2.23	0.54
1:A:295:LEU:HD22	1:A:295:LEU:N	2.23	0.54
1:B:497:GLY:O	1:B:500:ARG:HB2	2.07	0.54
1:A:72:LEU:O	1:A:75:HIS:HB3	2.08	0.53
1:B:189:THR:HB	1:B:239:GLU:OE1	2.07	0.53
1:A:490:LEU:CD1	1:A:495:LEU:HD13	2.38	0.53
1:B:52:ARG:CG	1:B:52:ARG:HH11	2.21	0.53
1:A:296:TYR:HD2	1:A:298:PHE:CE1	2.26	0.53
1:B:86:PRO:O	1:B:87:MET:SD	2.67	0.53
1:B:228:PHE:O	1:B:230:PHE:N	2.40	0.53
1:A:344:TYR:HD2	1:A:353:PHE:CE1	2.26	0.53
1:B:173:ARG:HA	1:B:173:ARG:CZ	2.39	0.53
1:A:319:HIS:HA	1:A:335:ASN:HD22	1.74	0.53
1:A:490:LEU:HD11	1:A:495:LEU:HD13	1.91	0.53
1:A:174:GLY:N	1:B:221:ASN:HD22	2.05	0.53
1:A:470:THR:HG22	1:A:471:THR:N	2.23	0.53
1:A:287:TYR:O	1:A:311:ARG:HA	2.09	0.53
1:B:226:ARG:HG3	1:B:231:ARG:HH22	1.73	0.53
1:B:410:ARG:CD	1:B:412:GLU:HB2	2.38	0.53
1:B:476:THR:HG22	1:B:489:ARG:HG3	1.90	0.53
1:A:277:TYR:CB	1:A:295:LEU:HD21	2.38	0.53
1:B:406:LEU:CB	1:B:459:ASP:HB3	2.39	0.53
1:A:412:GLU:H	1:A:412:GLU:CD	2.12	0.52
1:A:387:ARG:HB2	1:A:445:ARG:CZ	2.39	0.52
1:B:394:PRO:O	1:B:400:LYS:HD2	2.08	0.52
1:A:221:ASN:HD22	1:B:174:GLY:CA	2.22	0.52
1:B:381:LEU:HD21	1:B:387:ARG:HG2	1.92	0.52
1:B:310:GLN:HG2	1:B:358:ILE:HD12	1.90	0.52
1:A:15:ARG:NH2	1:A:449:GLU:HG3	2.24	0.52
1:B:427:LEU:HD13	1:B:429:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:427:LEU:HD22	1:B:496:GLU:HG2	1.92	0.52
1:A:220:ARG:O	1:A:233:ARG:HA	2.08	0.52
1:B:173:ARG:CA	1:B:173:ARG:CZ	2.88	0.52
1:A:366:ARG:CZ	2:A:1552:ATP:H2'	2.37	0.52
1:A:279:GLN:HG2	1:A:291:THR:O	2.10	0.52
1:B:89:ASP:HB2	1:B:94:ARG:NH2	2.25	0.51
1:B:287:TYR:CE2	1:B:311:ARG:CZ	2.93	0.51
1:A:74:LEU:HD13	1:A:168:MET:HE2	1.92	0.51
1:B:89:ASP:HB2	1:B:94:ARG:HH22	1.76	0.51
1:B:249:ASP:OD1	1:B:310:GLN:NE2	2.43	0.51
1:B:57:ARG:NH2	1:B:242:TYR:CE1	2.78	0.51
1:A:28:LEU:HD23	1:A:31:VAL:HG11	1.92	0.51
1:B:215:ILE:HA	1:B:238:MET:HA	1.93	0.51
1:A:170:GLN:OE1	1:A:170:GLN:N	2.44	0.51
1:A:173:ARG:CZ	1:A:173:ARG:HB2	2.40	0.51
1:B:230:PHE:O	2:B:2552:ATP:C2	2.64	0.51
1:A:89:ASP:N	1:A:159:TRP:HZ3	2.07	0.51
1:A:340:GLN:HB2	1:B:24:ILE:CG2	2.41	0.51
1:A:230:PHE:CD1	1:A:366:ARG:NE	2.79	0.51
1:A:76:TYR:CE1	1:A:335:ASN:HA	2.46	0.51
1:A:165:PHE:HZ	1:A:221:ASN:HD21	1.58	0.51
1:A:313:ASP:HB2	1:A:354:VAL:CG1	2.40	0.51
1:A:491:HIS:CD2	1:A:492:VAL:N	2.78	0.51
1:A:67:VAL:HA	1:A:186:ARG:HG2	1.92	0.51
1:B:76:TYR:CE1	1:B:335:ASN:HA	2.46	0.51
1:A:8:LEU:HD11	1:A:373:ALA:HA	1.91	0.51
1:B:296:TYR:OH	1:B:374:GLU:HB2	2.11	0.51
1:B:220:ARG:HD3	1:B:222:GLU:OE2	2.11	0.50
1:B:63:LEU:HD21	1:B:196:ASN:HD21	1.75	0.50
1:A:230:PHE:HE1	1:A:366:ARG:CZ	2.22	0.50
1:B:404:ILE:HD12	1:B:404:ILE:N	2.27	0.50
1:B:333:LEU:H	1:B:333:LEU:CD2	2.24	0.50
1:A:305:LEU:HD11	1:A:367:GLY:HA2	1.93	0.50
1:A:5:LEU:CD2	1:A:227:ASN:HB2	2.40	0.50
1:A:173:ARG:CB	1:A:173:ARG:CZ	2.89	0.50
1:A:287:TYR:HD2	1:A:311:ARG:NE	2.09	0.50
1:B:492:VAL:O	1:B:495:LEU:HB3	2.12	0.50
1:A:24:ILE:HA	1:B:339:THR:OG1	2.12	0.50
1:B:417:ALA:HB2	1:B:458:VAL:HG21	1.93	0.50
1:B:310:GLN:HG2	1:B:358:ILE:HD11	1.92	0.50
1:B:244:VAL:HG11	1:B:252:TRP:CD1	2.44	0.50
1:B:491:HIS:O	1:B:494:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:GLU:O	1:B:212:ILE:HA	2.12	0.50
1:A:395:GLN:HB3	1:A:505:TRP:NE1	2.26	0.50
1:B:321:LYS:HB2	1:B:339:THR:O	2.11	0.50
1:A:5:LEU:O	1:A:9:VAL:HG23	2.12	0.49
1:B:71:ARG:NE	1:B:182:LEU:HD23	2.27	0.49
1:A:225:PRO:HA	1:A:231:ARG:HG2	1.94	0.49
1:A:35:GLY:O	1:A:39:VAL:HG23	2.12	0.49
1:B:410:ARG:HD2	1:B:412:GLU:OE1	2.13	0.49
1:A:43:ASN:O	1:A:47:GLN:HG3	2.12	0.49
1:B:409:ASN:CG	1:B:410:ARG:N	2.65	0.49
1:A:245:ARG:CG	1:A:246:PRO:HD2	2.42	0.49
1:B:420:LEU:O	1:B:424:LEU:HG	2.13	0.49
1:A:208:LEU:HG	1:A:344:TYR:CD2	2.48	0.49
1:A:165:PHE:HZ	1:A:221:ASN:ND2	2.11	0.49
1:A:279:GLN:HB2	1:A:283:SER:OG	2.12	0.49
1:B:287:TYR:O	1:B:311:ARG:HA	2.12	0.49
1:A:88:VAL:CB	1:A:159:TRP:HZ3	2.24	0.49
1:B:291:THR:HB	1:B:309:ALA:HA	1.94	0.49
1:B:427:LEU:HD21	1:B:496:GLU:HG2	1.94	0.49
1:A:215:ILE:HG12	1:A:238:MET:HB3	1.95	0.49
1:B:189:THR:HG21	1:B:214:GLN:HG2	1.95	0.49
1:A:319:HIS:HA	1:A:335:ASN:ND2	2.28	0.49
1:B:416:TYR:CE2	1:B:462:THR:HG22	2.47	0.49
1:A:287:TYR:CD2	1:A:311:ARG:CZ	2.96	0.49
1:A:421:LYS:HE3	1:A:422:ALA:N	2.27	0.49
1:B:378:ARG:NH2	1:B:388:ILE:HD11	2.28	0.49
1:A:391:LYS:HG2	1:A:483:ASP:OD1	2.12	0.49
1:B:2:ALA:HB2	1:B:376:PHE:CB	2.39	0.49
1:A:187:PRO:HA	1:A:219:PHE:O	2.12	0.49
1:B:454:PHE:CE1	1:B:503:LEU:HD21	2.45	0.48
1:B:333:LEU:H	1:B:333:LEU:HD23	1.78	0.48
1:A:406:LEU:HD23	1:A:459:ASP:HB2	1.94	0.48
1:A:28:LEU:HB3	1:A:31:VAL:CG1	2.42	0.48
1:A:287:TYR:CD2	1:A:311:ARG:NE	2.81	0.48
1:A:73:VAL:HA	1:B:25:TYR:HE2	1.78	0.48
1:B:331:ARG:HH11	1:B:331:ARG:CB	2.15	0.48
1:B:473:LEU:HD22	1:B:489:ARG:HH11	1.78	0.48
1:B:87:MET:HB3	1:B:94:ARG:HH21	1.76	0.48
1:B:454:PHE:CE2	1:B:498:PHE:CE1	3.01	0.48
1:B:407:VAL:HG12	1:B:409:ASN:H	1.79	0.48
1:A:326:LEU:HD22	1:A:343:ALA:HB2	1.95	0.48
1:B:476:THR:HB	1:B:489:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:235:PHE:HB2	1:B:365:ASP:OD2	2.14	0.48
1:B:381:LEU:HB3	1:B:382:PRO:HD2	1.96	0.48
1:A:36:PRO:HB3	1:B:61:GLU:HG3	1.94	0.48
1:B:273:ASN:HB3	1:B:296:TYR:CE1	2.49	0.48
1:A:286:HIS:CG	1:A:287:TYR:H	2.32	0.48
1:A:25:TYR:CE2	1:B:76:TYR:CD2	3.02	0.48
1:B:2:ALA:HB2	1:B:376:PHE:CG	2.48	0.48
1:A:279:GLN:CG	1:A:291:THR:HG23	2.43	0.48
1:A:92:LYS:HD2	1:A:95:TYR:CE2	2.48	0.47
1:A:24:ILE:HG13	1:A:25:TYR:HD1	1.76	0.47
1:A:418:LYS:HG3	1:A:434:TYR:CE2	2.48	0.47
1:A:18:ILE:HG21	1:A:229:ILE:HD11	1.95	0.47
1:B:435:GLU:OE2	1:B:447:HIS:NE2	2.47	0.47
1:B:444:TYR:CE1	1:B:480:ARG:HD3	2.49	0.47
1:A:246:PRO:HD3	1:A:353:PHE:CE2	2.50	0.47
1:B:410:ARG:HD3	1:B:411:PRO:HD2	1.95	0.47
1:B:410:ARG:HA	1:B:411:PRO:HD3	1.78	0.47
1:B:405:PRO:HA	1:B:458:VAL:CG2	2.44	0.47
1:B:254:ARG:HG3	1:B:255:TYR:N	2.30	0.47
1:B:90:ASN:HB2	1:B:159:TRP:CZ3	2.48	0.47
1:A:400:LYS:HD3	1:A:430:GLY:CA	2.30	0.47
1:A:479:VAL:CG1	1:A:490:LEU:HD11	2.44	0.47
1:A:323:GLN:HB3	1:A:328:ILE:HD12	1.95	0.47
1:B:406:LEU:HD12	1:B:406:LEU:O	2.14	0.47
1:A:223:ILE:HD11	1:B:175:PRO:HD3	1.97	0.47
1:A:63:LEU:HD12	1:B:35:GLY:HA2	1.97	0.47
1:B:253:HIS:CE1	1:B:308:ILE:O	2.67	0.47
1:B:479:VAL:HG21	1:B:498:PHE:CE2	2.50	0.47
1:B:323:GLN:O	1:B:326:LEU:O	2.32	0.47
1:B:376:PHE:CD1	1:B:376:PHE:C	2.88	0.47
1:B:52:ARG:HG2	1:B:263:TRP:HD1	1.75	0.47
1:A:454:PHE:CE1	1:A:498:PHE:HE1	2.32	0.47
1:A:89:ASP:O	1:A:159:TRP:CE3	2.68	0.47
1:A:264:TRP:HH2	1:A:367:GLY:HA3	1.80	0.47
1:B:294:ILE:CD1	1:B:308:ILE:HD11	2.45	0.46
1:B:473:LEU:HD21	1:B:489:ARG:HD3	1.95	0.46
1:B:87:MET:C	1:B:162:PRO:HA	2.35	0.46
1:A:5:LEU:HD12	1:A:5:LEU:HA	1.74	0.46
1:B:57:ARG:NH2	1:B:59:ASP:OD1	2.48	0.46
1:B:476:THR:HB	1:B:489:ARG:NH1	2.30	0.46
1:A:176:ARG:NE	1:B:163:ARG:HH21	2.13	0.46
1:A:238:MET:SD	1:A:364:VAL:HG22	2.55	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:461:ASP:HB2	1:B:473:LEU:CB	2.43	0.46
1:A:376:PHE:HD1	1:A:376:PHE:C	2.18	0.46
1:B:30:GLY:O	1:B:232:VAL:HB	2.14	0.46
1:A:387:ARG:CZ	1:A:389:VAL:HG21	2.46	0.46
1:B:229:ILE:HG13	1:B:365:ASP:HB3	1.97	0.46
1:B:473:LEU:HD22	1:B:489:ARG:HD3	1.96	0.46
1:A:346:ASP:HA	1:A:350:GLY:HA2	1.96	0.46
1:A:186:ARG:HD2	1:A:189:THR:HA	1.97	0.46
1:A:86:PRO:HA	1:A:164:TYR:HA	1.96	0.46
1:A:230:PHE:CD2	1:A:300:HIS:CE1	3.04	0.46
1:A:173:ARG:CB	1:A:173:ARG:NH1	2.70	0.46
1:B:244:VAL:CG2	1:B:252:TRP:CD1	2.99	0.46
1:B:49:TRP:CZ2	1:B:238:MET:HB2	2.50	0.46
1:A:366:ARG:HD2	2:A:1552:ATP:O2'	2.15	0.46
1:B:442:LYS:CA	1:B:445:ARG:HD3	2.32	0.46
1:A:326:LEU:HD23	1:A:341:ARG:NH2	2.22	0.46
1:A:395:GLN:HB3	1:A:505:TRP:CZ2	2.51	0.46
1:B:49:TRP:CE2	1:B:238:MET:HB2	2.51	0.46
1:B:467:LYS:C	1:B:469:GLY:H	2.19	0.46
1:A:231:ARG:O	1:A:231:ARG:HG2	2.16	0.46
1:A:480:ARG:HG2	1:A:480:ARG:O	2.16	0.45
1:B:447:HIS:HA	1:B:450:VAL:HG22	1.98	0.45
1:B:241:GLU:OE1	1:B:359:GLU:HG3	2.16	0.45
1:B:71:ARG:HH22	1:B:179:ARG:HH22	1.64	0.45
1:B:408:LYS:HE2	1:B:436:ASP:O	2.16	0.45
1:A:191:GLN:O	1:A:195:VAL:HG22	2.15	0.45
1:B:86:PRO:HG3	1:B:164:TYR:CE1	2.50	0.45
1:A:295:LEU:CD2	1:A:295:LEU:N	2.80	0.45
1:B:408:LYS:HE2	1:B:437:THR:O	2.16	0.45
1:A:260:ARG:HD3	1:A:306:GLU:OE2	2.16	0.45
1:A:467:LYS:C	1:A:469:GLY:H	2.19	0.45
1:A:245:ARG:NH2	1:A:347:PRO:O	2.49	0.45
1:B:313:ASP:HB3	1:B:356:TYR:CD1	2.52	0.45
1:B:447:HIS:HB3	1:B:452:THR:OG1	2.16	0.45
1:B:379:GLU:O	1:B:386:GLU:HA	2.17	0.45
1:A:55:TYR:HE1	1:B:40:GLU:OE2	1.99	0.45
1:B:173:ARG:O	1:B:175:PRO:HD2	2.17	0.45
1:B:193:ILE:HD11	1:B:214:GLN:HB3	1.99	0.45
1:A:172:LEU:HD23	1:A:181:LEU:HD12	1.98	0.45
1:A:278:GLN:NE2	1:A:292:VAL:HG22	2.31	0.45
1:B:161:PRO:HA	1:B:162:PRO:HD2	1.68	0.45
1:A:49:TRP:CH2	1:A:238:MET:HB2	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:GLU:O	1:A:262:LYS:HB3	2.17	0.45
1:A:52:ARG:HD3	1:A:52:ARG:O	2.16	0.45
1:A:447:HIS:HB3	1:A:452:THR:OG1	2.16	0.45
1:A:230:PHE:CE2	1:A:303:LEU:HD13	2.38	0.45
1:B:479:VAL:HG23	1:B:479:VAL:O	2.17	0.45
1:B:498:PHE:CD1	1:B:498:PHE:C	2.90	0.45
1:A:92:LYS:HD2	1:A:95:TYR:HE2	1.82	0.45
1:B:344:TYR:HD1	1:B:345:ARG:N	2.10	0.45
1:A:479:VAL:HG12	1:A:490:LEU:HD11	1.98	0.45
1:B:83:PHE:CB	1:B:166:ASN:HA	2.47	0.45
1:A:222:GLU:HG2	1:A:231:ARG:CD	2.47	0.45
1:B:219:PHE:CE2	1:B:234:GLU:OE1	2.71	0.44
1:B:316:LEU:HD22	1:B:342:LEU:CG	2.41	0.44
1:B:456:VAL:HG11	1:B:495:LEU:HD21	1.99	0.44
1:B:472:ARG:C	1:B:472:ARG:HD2	2.38	0.44
1:B:224:THR:OG1	1:B:231:ARG:NH2	2.50	0.44
1:B:9:VAL:HG22	1:B:228:PHE:CD2	2.53	0.44
1:B:187:PRO:HA	1:B:219:PHE:O	2.17	0.44
1:A:72:LEU:HD12	1:B:25:TYR:HB3	1.99	0.44
1:B:427:LEU:CD1	1:B:429:LEU:HD12	2.47	0.44
1:A:74:LEU:HB3	1:A:168:MET:CE	2.48	0.44
1:A:28:LEU:HB3	1:A:31:VAL:HG13	2.00	0.44
1:A:173:ARG:CA	1:A:173:ARG:CZ	2.95	0.44
1:A:289:LYS:HE2	1:A:310:GLN:OE1	2.17	0.44
1:A:228:PHE:CG	1:A:229:ILE:N	2.85	0.44
1:A:399:ILE:O	1:A:452:THR:HB	2.18	0.44
1:A:167:MET:O	1:A:221:ASN:HB3	2.18	0.44
1:B:401:VAL:CG1	1:B:456:VAL:HG23	2.47	0.44
1:B:53:ASN:N	1:B:53:ASN:HD21	2.16	0.44
1:A:434:TYR:CE1	1:A:436:ASP:HB3	2.52	0.44
1:A:406:LEU:CD2	1:A:459:ASP:HB2	2.48	0.44
1:A:310:GLN:HE21	1:A:310:GLN:CA	2.31	0.44
1:A:18:ILE:CG2	1:A:32:TYR:HD2	2.31	0.44
1:A:42:LYS:HD3	1:A:46:LYS:CE	2.48	0.44
1:B:240:ILE:HB	1:B:360:PRO:HD2	2.00	0.44
1:A:400:LYS:O	1:A:453:PRO:HG2	2.18	0.44
1:A:452:THR:HA	1:A:453:PRO:HD2	1.77	0.44
1:A:328:ILE:CG2	1:A:329:THR:N	2.81	0.44
1:A:346:ASP:N	1:A:347:PRO:HD3	2.32	0.43
1:B:498:PHE:CE1	1:B:502:ARG:CZ	3.00	0.43
1:A:88:VAL:C	1:A:159:TRP:HZ3	2.21	0.43
1:B:387:ARG:CZ	1:B:485:MET:SD	3.06	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:473:LEU:HA	1:A:473:LEU:HD23	1.79	0.43
1:A:252:TRP:O	1:A:255:TYR:HB3	2.18	0.43
1:B:253:HIS:HB2	1:B:310:GLN:HG3	2.00	0.43
1:A:72:LEU:HB3	1:B:25:TYR:CD2	2.53	0.43
1:A:172:LEU:HB3	1:A:181:LEU:HD12	2.00	0.43
1:B:279:GLN:HG3	1:B:291:THR:O	2.18	0.43
1:A:15:ARG:HH22	1:A:449:GLU:HG3	1.81	0.43
1:B:452:THR:HA	1:B:453:PRO:HD3	1.82	0.43
1:B:179:ARG:NE	1:B:182:LEU:HD22	2.33	0.43
1:B:275:VAL:HG23	1:B:295:LEU:HB2	2.01	0.43
1:B:170:GLN:NE2	1:B:184:TYR:CE2	2.86	0.43
1:A:73:VAL:HG13	1:A:319:HIS:CE1	2.54	0.43
1:A:237:GLN:NE2	1:A:239:GLU:OE1	2.51	0.43
1:A:230:PHE:HZ	1:A:303:LEU:HB3	1.82	0.43
1:B:308:ILE:N	1:B:308:ILE:HD12	2.32	0.43
1:B:265:GLN:NE2	1:B:271:ARG:HD3	2.33	0.43
1:A:498:PHE:CE1	1:A:502:ARG:HD3	2.53	0.43
1:B:34:TYR:CZ	1:B:42:LYS:HD3	2.53	0.43
1:A:413:ILE:HG13	1:A:463:ILE:CD1	2.41	0.43
1:B:416:TYR:O	1:B:416:TYR:HD1	2.02	0.43
1:A:223:ILE:HA	1:A:223:ILE:HD13	1.88	0.43
1:B:221:ASN:O	1:B:221:ASN:OD1	2.37	0.43
1:B:45:LEU:HA	1:B:45:LEU:HD12	1.83	0.43
1:B:88:VAL:O	1:B:159:TRP:CZ3	2.71	0.43
1:A:5:LEU:HD22	1:A:300:HIS:HD2	1.84	0.43
1:B:224:THR:O	1:B:231:ARG:NH2	2.49	0.43
1:B:479:VAL:HG22	1:B:488:ILE:HG12	2.00	0.43
1:B:498:PHE:HD1	1:B:498:PHE:C	2.22	0.43
1:B:306:GLU:HG3	1:B:361:SER:O	2.18	0.43
1:A:480:ARG:HD2	1:A:487:GLN:NE2	2.33	0.43
1:B:15:ARG:HD3	1:B:450:VAL:HG13	1.99	0.43
1:B:241:GLU:OE2	1:B:359:GLU:HG3	2.19	0.43
1:B:46:LYS:HE3	1:B:236:GLU:CD	2.38	0.43
1:A:346:ASP:CG	1:A:346:ASP:O	2.57	0.43
1:B:381:LEU:HD11	1:B:387:ARG:HB3	2.00	0.43
1:A:29:GLN:O	1:A:233:ARG:NH1	2.52	0.43
1:A:169:PHE:CD2	1:A:219:PHE:HB3	2.54	0.42
1:A:312:THR:O	1:A:356:TYR:CA	2.62	0.42
1:A:87:MET:O	1:A:88:VAL:HG13	2.19	0.42
1:A:491:HIS:HD2	1:A:492:VAL:N	2.17	0.42
1:A:185:LEU:HD21	1:B:185:LEU:HD11	2.01	0.42
1:B:238:MET:HG2	1:B:238:MET:H	1.61	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:416:TYR:CE1	1:B:420:LEU:HD22	2.54	0.42
1:B:279:GLN:HA	1:B:280:PRO:HD3	1.73	0.42
1:B:376:PHE:C	1:B:376:PHE:HD1	2.22	0.42
1:B:423:ARG:O	1:B:426:ALA:HB3	2.19	0.42
1:B:405:PRO:HA	1:B:458:VAL:HG23	2.02	0.42
1:B:185:LEU:HD13	1:B:219:PHE:CD2	2.54	0.42
1:B:52:ARG:CG	1:B:52:ARG:NH1	2.80	0.42
1:B:179:ARG:HD2	1:B:179:ARG:HA	1.74	0.42
1:B:172:LEU:HD22	1:B:177:GLY:C	2.40	0.42
1:A:187:PRO:CD	1:A:188:GLU:H	2.32	0.42
1:B:390:LEU:HD13	1:B:392:LEU:CD1	2.50	0.42
1:B:390:LEU:HA	1:B:390:LEU:HD23	1.94	0.42
1:B:372:LEU:HA	1:B:372:LEU:HD23	1.64	0.42
1:B:410:ARG:HB3	1:B:413:ILE:CD1	2.50	0.42
1:B:174:GLY:O	1:B:175:PRO:C	2.57	0.42
1:B:280:PRO:CB	1:B:281:PRO:HD2	2.46	0.42
1:A:346:ASP:O	1:A:347:PRO:C	2.58	0.42
1:B:479:VAL:CG2	1:B:488:ILE:HG12	2.50	0.42
1:A:308:ILE:N	1:A:308:ILE:HD12	2.34	0.42
1:A:344:TYR:HD2	1:A:353:PHE:CZ	2.38	0.42
1:B:323:GLN:HE22	1:B:335:ASN:H	1.61	0.42
1:B:241:GLU:CD	1:B:359:GLU:HG3	2.39	0.42
1:B:260:ARG:HD3	1:B:306:GLU:CD	2.39	0.42
1:A:49:TRP:CZ2	1:A:238:MET:HB2	2.55	0.42
1:B:249:ASP:OD1	1:B:250:GLU:N	2.53	0.42
1:B:242:TYR:HD2	1:B:244:VAL:CG2	2.32	0.42
1:A:367:GLY:O	1:A:371:LEU:HG	2.20	0.42
1:B:459:ASP:O	1:B:462:THR:N	2.53	0.41
1:A:287:TYR:HD1	1:A:287:TYR:H	1.68	0.41
1:B:218:ALA:N	1:B:235:PHE:O	2.50	0.41
1:B:223:ILE:HD12	1:B:223:ILE:HA	1.75	0.41
1:B:393:LYS:HD3	1:B:394:PRO:HD2	2.02	0.41
1:A:415:GLU:OE2	1:A:419:ARG:HD2	2.20	0.41
1:B:473:LEU:HD23	1:B:473:LEU:HA	1.74	0.41
1:A:265:GLN:NE2	1:A:271:ARG:HD3	2.35	0.41
1:A:30:GLY:O	1:A:232:VAL:HB	2.20	0.41
1:A:387:ARG:CZ	1:A:389:VAL:CG2	2.98	0.41
1:B:313:ASP:HB3	1:B:356:TYR:CE1	2.54	0.41
1:A:175:PRO:HD3	1:B:223:ILE:CD1	2.49	0.41
1:A:321:LYS:NZ	1:A:321:LYS:HB3	2.35	0.41
1:A:198:LYS:HD2	1:A:202:ASP:OD1	2.20	0.41
1:B:65:ALA:N	1:B:214:GLN:NE2	2.67	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:63:LEU:HD23	1:B:214:GLN:NE2	2.35	0.41
1:B:163:ARG:HB3	1:B:163:ARG:HE	1.63	0.41
1:B:40:GLU:HB2	1:B:398:PRO:HB3	2.02	0.41
1:A:310:GLN:O	1:A:310:GLN:CG	2.69	0.41
1:A:94:ARG:HH12	1:B:176:ARG:HG3	1.84	0.41
1:A:395:GLN:HG2	1:A:505:TRP:CG	2.56	0.41
1:B:165:PHE:O	1:B:166:ASN:C	2.59	0.41
1:A:264:TRP:CH2	1:A:367:GLY:HA3	2.55	0.41
1:A:218:ALA:HB3	1:A:235:PHE:CE1	2.56	0.41
1:A:387:ARG:HD2	1:A:445:ARG:NH2	2.22	0.41
1:A:445:ARG:O	1:A:445:ARG:HD3	2.21	0.41
1:A:347:PRO:HD3	1:A:351:LYS:O	2.21	0.41
1:A:14:ARG:O	1:A:15:ARG:HD3	2.20	0.41
1:B:461:ASP:OD1	1:B:462:THR:N	2.54	0.41
1:B:12:CYS:HA	1:B:17:PHE:HB2	2.03	0.41
1:B:378:ARG:HB3	1:B:386:GLU:OE1	2.21	0.41
1:B:297:ARG:NE	1:B:302:SER:HB2	2.36	0.41
1:B:363:GLY:CA	2:B:2552:ATP:H1'	2.50	0.41
1:B:324:GLU:HB3	1:B:334:ARG:NH1	2.36	0.41
1:A:317:GLY:C	1:A:319:HIS:H	2.23	0.41
1:B:461:ASP:O	1:B:474:LYS:HA	2.20	0.41
1:A:470:THR:HG22	1:A:471:THR:H	1.85	0.41
1:A:161:PRO:HA	1:A:162:PRO:HD3	1.92	0.41
1:B:311:ARG:HB2	1:B:357:VAL:HG13	2.03	0.41
1:A:356:TYR:C	1:A:357:VAL:HG23	2.41	0.41
1:A:275:VAL:HB	1:A:295:LEU:HB2	2.03	0.41
1:A:21:SER:HB3	1:A:31:VAL:HG22	2.03	0.41
1:A:201:LEU:O	1:A:201:LEU:HG	2.21	0.41
1:B:297:ARG:CZ	1:B:302:SER:CB	2.99	0.41
1:A:306:GLU:CD	1:A:362:ALA:HB2	2.41	0.41
1:B:8:LEU:HA	1:B:8:LEU:HD13	1.88	0.40
1:A:187:PRO:HG2	1:A:188:GLU:HG2	2.03	0.40
1:B:252:TRP:O	1:B:255:TYR:HB3	2.21	0.40
1:A:410:ARG:HA	1:A:411:PRO:HD2	1.73	0.40
1:A:328:ILE:HG22	1:A:329:THR:N	2.36	0.40
1:A:89:ASP:H	1:A:160:THR:HG1	1.69	0.40
1:B:53:ASN:O	1:B:57:ARG:HG3	2.21	0.40
1:B:193:ILE:HD12	1:B:241:GLU:HG2	2.03	0.40
1:A:176:ARG:HE	1:B:163:ARG:NH1	2.15	0.40
1:A:200:VAL:O	1:A:204:THR:HG23	2.21	0.40
1:A:71:ARG:HH22	1:A:179:ARG:HH22	1.68	0.40
1:A:306:GLU:HG3	1:A:361:SER:O	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:323:GLN:HE22	1:A:334:ARG:CA	2.31	0.40
1:A:495:LEU:O	1:A:499:LEU:HG	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	438/442 (99%)	355 (81%)	65 (15%)	18 (4%)	4	42
1	B	438/442 (99%)	354 (81%)	63 (14%)	21 (5%)	4	36
All	All	876/884 (99%)	709 (81%)	128 (15%)	39 (4%)	4	38

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	PRO
1	A	281	PRO
1	A	286	HIS
1	A	438	GLY
1	B	92	LYS
1	B	175	PRO
1	B	227	ASN
1	B	281	PRO
1	B	284	SER
1	B	286	HIS
1	B	438	GLY
1	A	209	GLY
1	A	284	SER
1	A	327	GLY
1	A	349	THR
1	B	209	GLY
1	B	229	ILE
1	B	339	THR

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Mol	Chain	Res	Type
1	B	439	ASN
1	B	468	ASP
1	A	79	HIS
1	A	350	GLY
1	A	439	ASN
1	A	470	THR
1	B	166	ASN
1	B	276	PRO
1	B	302	SER
1	A	71	ARG
1	A	382	PRO
1	B	221	ASN
1	A	174	GLY
1	A	227	ASN
1	B	246	PRO
1	B	337	HIS
1	A	276	PRO
1	B	174	GLY
1	B	36	PRO
1	B	440	ILE
1	A	246	PRO

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	375/376 (100%)	315 (84%)	60 (16%)	3	21
1	B	374/376 (100%)	310 (83%)	64 (17%)	3	18
All	All	749/752 (100%)	625 (83%)	124 (17%)	3	19

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	31	VAL
1	A	60	MET
1	A	66	SER

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Mol	Chain	Res	Type
1	A	72	LEU
1	A	85	ASP
1	A	88	VAL
1	A	92	LYS
1	A	162	PRO
1	A	163	ARG
1	A	164	TYR
1	A	173	ARG
1	A	175	PRO
1	A	176	ARG
1	A	189	THR
1	A	193	ILE
1	A	208	LEU
1	A	210	PHE
1	A	222	GLU
1	A	226	ARG
1	A	237	GLN
1	A	238	MET
1	A	246	PRO
1	A	254	ARG
1	A	261	LEU
1	A	272	GLU
1	A	291	THR
1	A	295	LEU
1	A	310	GLN
1	A	311	ARG
1	A	321	LYS
1	A	324	GLU
1	A	326	LEU
1	A	331	ARG
1	A	345	ARG
1	A	351	LYS
1	A	369	LEU
1	A	376	PHE
1	A	390	LEU
1	A	392	LEU
1	A	398	PRO
1	A	400	LYS
1	A	407	VAL
1	A	415	GLU
1	A	421	LYS
1	A	423	ARG

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Mol	Chain	Res	Type
1	A	431	ARG
1	A	442	LYS
1	A	445	ARG
1	A	446	ARG
1	A	457	THR
1	A	462	THR
1	A	467	LYS
1	A	471	THR
1	A	472	ARG
1	A	477	VAL
1	A	478	THR
1	A	488	ILE
1	A	490	LEU
1	A	502	ARG
1	B	3	SER
1	B	5	LEU
1	B	6	ASP
1	B	15	ARG
1	B	28	LEU
1	B	36	PRO
1	B	37	LEU
1	B	39	VAL
1	B	46	LYS
1	B	52	ARG
1	B	63	LEU
1	B	72	LEU
1	B	94	ARG
1	B	163	ARG
1	B	170	GLN
1	B	172	LEU
1	B	173	ARG
1	B	175	PRO
1	B	205	SER
1	B	219	PHE
1	B	228	PHE
1	B	238	MET
1	B	239	GLU
1	B	246	PRO
1	B	254	ARG
1	B	275	VAL
1	B	282	GLU
1	B	284	SER

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Mol	Chain	Res	Type
1	B	286	HIS
1	B	291	THR
1	B	297	ARG
1	B	305	LEU
1	B	310	GLN
1	B	328	ILE
1	B	331	ARG
1	B	333	LEU
1	B	340	GLN
1	B	345	ARG
1	B	352	TRP
1	B	357	VAL
1	B	369	LEU
1	B	376	PHE
1	B	385	GLU
1	B	386	GLU
1	B	398	PRO
1	B	400	LYS
1	B	406	LEU
1	B	409	ASN
1	B	412	GLU
1	B	416	TYR
1	B	420	LEU
1	B	431	ARG
1	B	433	LEU
1	B	440	ILE
1	B	442	LYS
1	B	467	LYS
1	B	470	THR
1	B	477	VAL
1	B	478	THR
1	B	488	ILE
1	B	490	LEU
1	B	496	GLU
1	B	498	PHE
1	B	502	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	199	ASN

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Mol	Chain	Res	Type
1	A	221	ASN
1	A	237	GLN
1	A	278	GLN
1	A	300	HIS
1	A	323	GLN
1	A	335	ASN
1	A	340	GLN
1	A	487	GLN
1	A	491	HIS
1	B	44	ASN
1	B	75	HIS
1	B	170	GLN
1	B	196	ASN
1	B	214	GLN
1	B	221	ASN
1	B	237	GLN
1	B	253	HIS
1	B	323	GLN
1	B	340	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	ATP	A	1552	-	33,33,33	0.82	0	52,52,52	0.72	0
2	ATP	B	2552	-	33,33,33	0.74	0	52,52,52	0.64	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	ATP	A	1552	-	-	0/22/38/38	0/1/3/3
2	ATP	B	2552	-	-	0/22/38/38	0/1/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	442/442 (100%)	-0.10	1 (0%) 93 77	14, 38, 78, 95	0
1	B	442/442 (100%)	-0.01	0 100 100	13, 41, 79, 96	0
All	All	884/884 (100%)	-0.06	1 (0%) 93 82	13, 40, 79, 96	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	HIS	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ATP	A	1552	31/31	0.25	1.01	0,42,82,84	0
2	ATP	B	2552	31/31	0.26	0.43	0,67,102,102	0

6.5 Other polymers ⓘ

There are no such residues in this entry.