



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:31 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 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

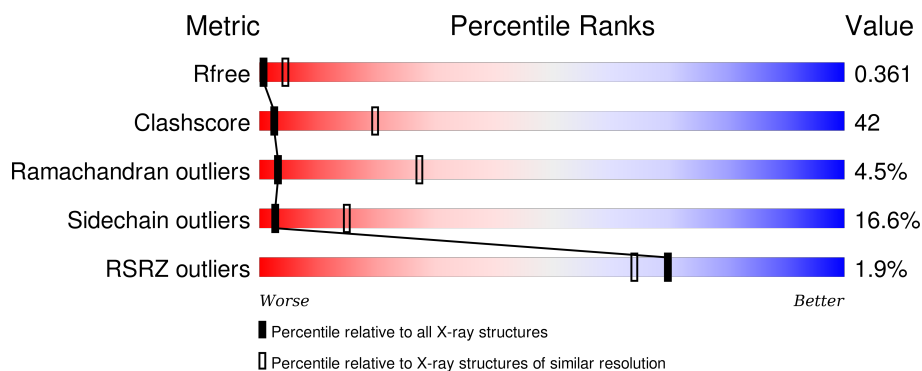
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	442	<div> <div>2%</div> <div>39%</div> <div>49%</div> <div>11%</div> <div>.</div> </div>
1	B	442	<div> <div>2%</div> <div>39%</div> <div>47%</div> <div>13%</div> <div>.</div> </div>

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 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 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: $C_{10}H_{16}N_5O_{13}P_3$).



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		

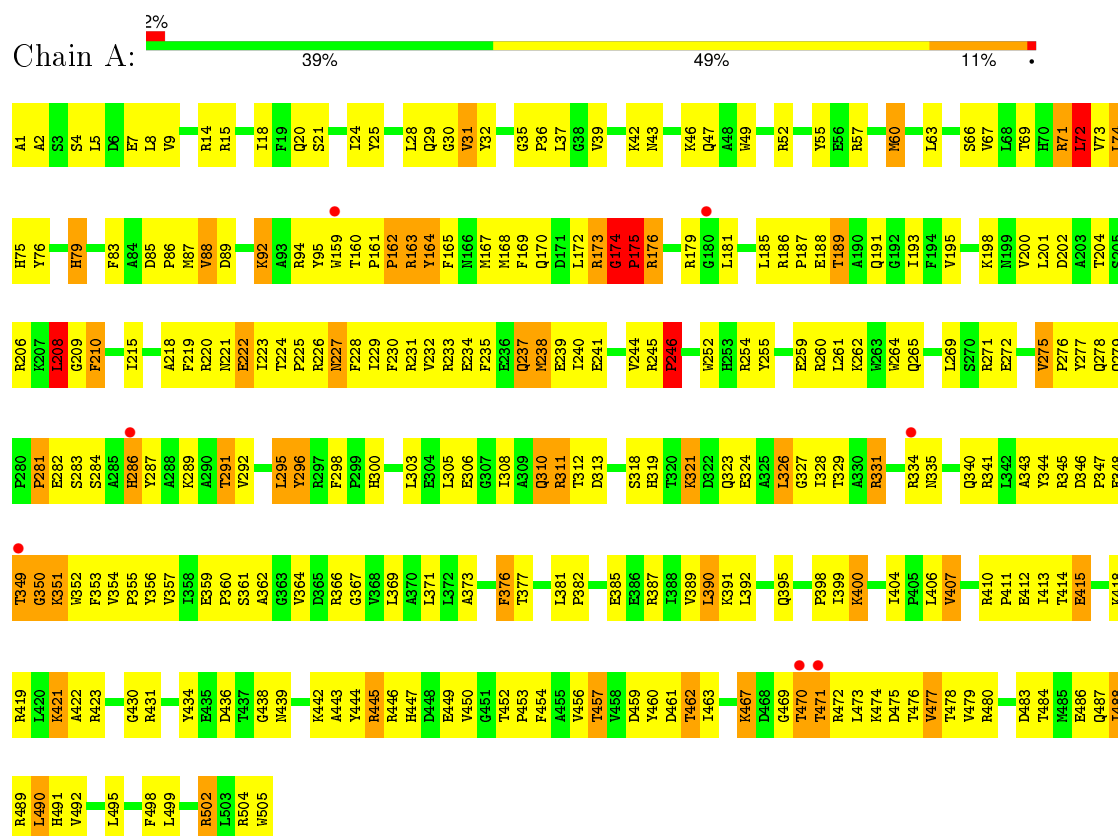
- Molecule 3 is water.

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

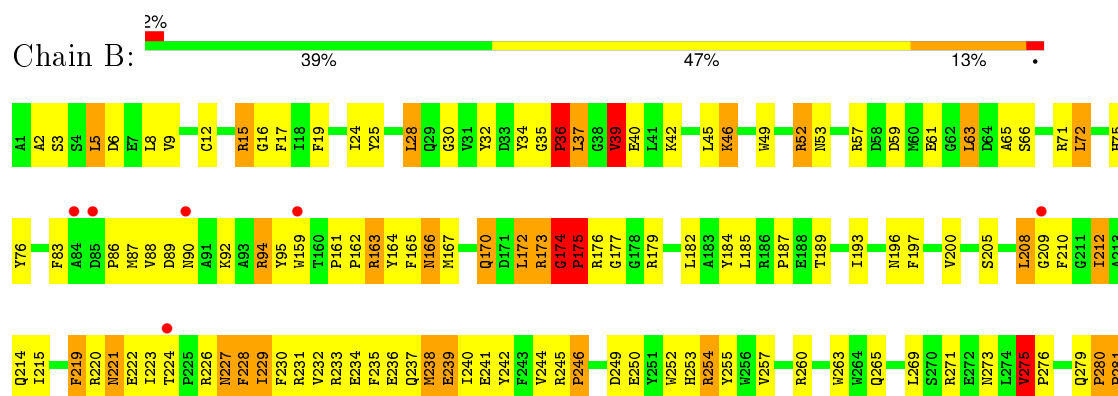
3 Residue-property plots

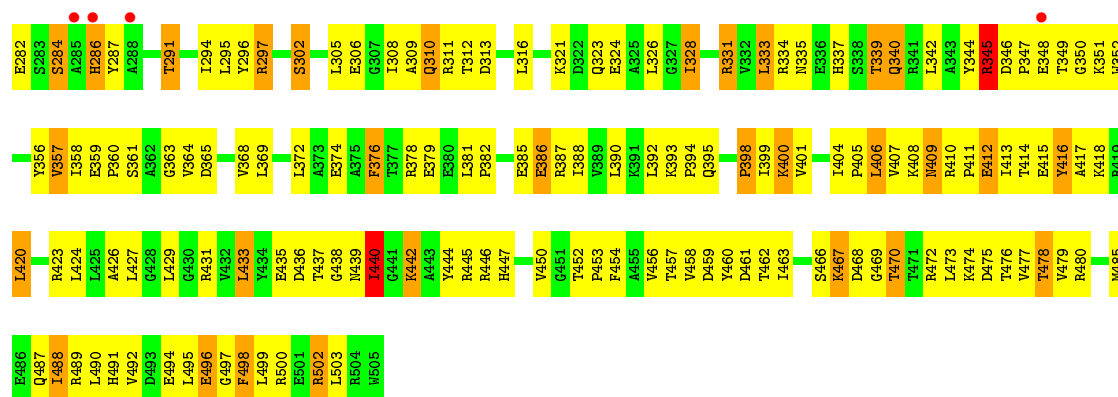
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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)



• Molecule 1: PROTEIN (GLYCYL-TRNA SYNTHETASE)





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.80 Å 250.90 Å 105.70 Å 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 3.28 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.227 , 0.318 0.292 , 0.361	Depositor DCC
R_{free} test set	751 reflections (3.94%)	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 , 108.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3610	841	3565	308	0
1	B	3601	839	3547	319	0
2	A	31	3	12	5	0
2	B	31	3	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	7275	1686	7136	599	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (599) 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: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:HH22	1:B:347:PRO:HA	1.35	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG21	1:A:252:TRP:CD1	2.09	0.86
1:A:387:ARG:HD2	1:A:445:ARG:HH22	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:HH21	1.44	0.83
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:B:245:ARG:HH12	1:B:347:PRO:HB3	1.48	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: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:A:323:GLN:NE2	1:A:335:ASN:H	1.84	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:174:GLY:H	1:B:221:ASN:HD21	1.36	0.72
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:323:GLN:HE22	1:A:334:ARG:HA	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:189:THR:HG23	1:A:237:GLN:HE21	1.59	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:B:323:GLN:HE22	1:B:334:ARG:HA	1.57	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:423:ARG:HH12	1:B:496:GLU:HG3	1.59	0.67
1:B:440:ILE:HD11	1:B:444:TYR:CE2	2.29	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:480:ARG:HG2	1:A:480:ARG:HH11	1.59	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:B:454:PHE:HE1	1:B:503:LEU:HD21	1.59	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: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:480:ARG:NH1	1:A:480:ARG:HG2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:65:ALA:H	1:B:214:GLN:NE2	1.95	0.65
1:B:83:PHE:CG	1:B:166:ASN:HA	2.31	0.65
1:B:323:GLN:NE2	1:B:334:ARG:HA	2.12	0.65
1:B:323:GLN:NE2	1:B:335:ASN:H	1.95	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	1.45	0.65
1:B:308:ILE:H	1:B:308:ILE:HD12	1.61	0.64
1:B:394:PRO:HB2	1:B:395:GLN:OE1	1.98	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: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:HH21	1.46	0.63
1:A:323:GLN:NE2	1:A:334:ARG:HA	2.13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:52:ARG:HH11	1:B:52:ARG:HG3	1.66	0.60
1:A:387:ARG:HB2	1:A:445:ARG:NH1	2.17	0.60
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:71:ARG:HE	1:B:182:LEU:HD23	1.66	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: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:412:GLU:H	1:A:412:GLU:CD	2.06	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:36:PRO:O	1:B:39:VAL:HG23	2.02	0.59
1:B:57:ARG:HH21	1:B:242:TYR:HE1	1.50	0.59
1:B:363:GLY:HA3	2:B:2552:ATP:H1'	1.85	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: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:B:245:ARG:HH12	1:B:347:PRO:CB	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:333:LEU:H	1:B:333:LEU:CD2	2.17	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: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:A:221:ASN:HD21	1:B:174:GLY:HA3	1.68	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: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:A:319:HIS:HA	1:A:335:ASN:HD21	1.71	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:71:ARG:HH21	1:B:179:ARG:HE	1.53	0.56
1:A:71:ARG:HE	1:A:179:ARG:HE	1.52	0.56
1:B:454:PHE:CE2	1:B:498:PHE:HE1	2.23	0.56
1:A:480:ARG:HD2	1:A:487:GLN:HE21	1.70	0.56
1:B:390:LEU:HD13	1:B:392:LEU:HD11	1.88	0.56
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: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:378:ARG:HH21	1:B:388:ILE:HD11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:CZ	1:B:302:SER:HB2	2.37	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:165:PHE:HZ	1:A:221:ASN:HD22	1.54	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:B:52:ARG:CG	1:B:52:ARG:HH11	2.19	0.55
1:A:504:ARG:HB3	1:A:504:ARG:HH11	1.72	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
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: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: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:476:THR:OG1	1:A:489:ARG:NH1	2.37	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:A:221:ASN:HD21	1:B:174:GLY:CA	2.21	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: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:490:LEU:HD11	1:A:495:LEU:HD13	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LEU:H	1:B:333:LEU:HD23	1.73	0.53
1:B:406:LEU:CB	1:B:459:ASP:HB3	2.39	0.53
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:B:381:LEU:HD21	1:B:387:ARG:HG2	1.92	0.52
1:B:226:ARG:HG3	1:B:231:ARG:HH21	1.73	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
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:B:63:LEU:HD21	1:B:196:ASN:HD22	1.74	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:HH21	1.75	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: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: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:174:GLY:N	1:B:221:ASN:HD21	2.05	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: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:A:305:LEU:HD11	1:A:367:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:331:ARG:HH11	1:B:331:ARG:CB	2.14	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:A:165:PHE:HZ	1:A:221:ASN:ND2	2.11	0.49
1:B:189:THR:HG21	1:B:214:GLN:HG2	1.95	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:A:406:LEU:HD23	1:A:459:ASP:HB2	1.94	0.48
1:B:473:LEU:HD22	1:B:489:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:87:MET:HB3	1:B:94:ARG:HH22	1.77	0.48
1:B:454:PHE:CE2	1:B:498:PHE:CE1	3.01	0.48
1:B:476:THR:HB	1:B:489:ARG:HH11	1.78	0.48
1:A:326:LEU:HD22	1:A:343:ALA:HB2	1.95	0.48
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:B:407:VAL:HG12	1:B:409:ASN:H	1.79	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:319:HIS:HA	1:A:335:ASN:ND2	2.28	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:176:ARG:NE	1:B:163:ARG:HH22	2.13	0.47
1:A:454:PHE:CE1	1:A:498:PHE:HE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:238:MET:SD	1:A:364:VAL:HG22	2.55	0.46
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:286:HIS:CG	1:A:287:TYR:H	2.34	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:A:231:ARG:O	1:A:231:ARG:HG2	2.16	0.46
1:A:310:GLN:HE21	1:A:310:GLN:CA	2.29	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:HH21	1:B:179:ARG:HH21	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:245:ARG:NH2	1:A:347:PRO:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASP:HB3	1:B:356:TYR:CD1	2.52	0.45
1:A:323:GLN:HE22	1:A:334:ARG:CA	2.27	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
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:A:92:LYS:HG3	1:A:92:LYS:H	1.70	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:15:ARG:HH21	1:A:449:GLU:HG3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:467:LYS:C	1:A:469:GLY:H	2.22	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:470:THR:HG22	1:A:471:THR:H	1.82	0.43
1:A:230:PHE:HZ	1:A:303:LEU:HB3	1.82	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:B:221:ASN:O	1:B:221:ASN:OD1	2.37	0.43
1:A:223:ILE:HA	1:A:223:ILE:HD13	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:89:ASP:H	1:A:160:THR:HG1	1.67	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: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:467:LYS:C	1:B:469:GLY:H	2.22	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:53:ASN:N	1:B:53:ASN:HD22	2.18	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:326:LEU:HG	1:A:326:LEU:H	1.50	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:B:328:ILE:H	1:B:328:ILE:HG12	1.51	0.42
1:A:410:ARG:HE	1:A:460:TYR:HE1	1.55	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:HD12	1:A:308:ILE:N	2.34	0.42
1:A:344:TYR:HD2	1:A:353:PHE:CZ	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:321:LYS:H	1:A:341:ARG:HA	1.84	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:A:321:LYS:NZ	1:A:321:LYS:HB3	2.35	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:198:LYS:HD2	1:A:202:ASP:OD1	2.20	0.41
1:B:63:LEU:HD23	1:B:214:GLN:NE2	2.35	0.41
1:A:287:TYR:HD1	1:A:287:TYR:H	1.68	0.41
1:A:310:GLN:O	1:A:310:GLN:CG	2.69	0.41
1:B:40:GLU:HB2	1:B:398:PRO:HB3	2.02	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:323:GLN:HE22	1:B:335:ASN:H	1.65	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:B:461:ASP:O	1:B:474:LYS:HA	2.20	0.41
1:B:163:ARG:HB3	1:B:163:ARG:HE	1.62	0.41
1:A:1:ALA:H3	1:A:377:THR:HG22	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:176:ARG:HE	1:B:163:ARG:NH1	2.14	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: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:200:VAL:O	1:A:204:THR:HG23	2.21	0.40
1:A:306:GLU:HG3	1:A:361:SER:O	2.22	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 [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	438/442 (99%)	355 (81%)	65 (15%)	18 (4%)	3	30
1	B	438/442 (99%)	354 (81%)	63 (14%)	21 (5%)	3	25
All	All	876/884 (99%)	709 (81%)	128 (15%)	39 (4%)	3	27

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	PRO
1	A	281	PRO

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Mol	Chain	Res	Type
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
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	16
1	B	374/376 (100%)	310 (83%)	64 (17%)	2	14
All	All	749/752 (100%)	625 (83%)	124 (17%)	3	15

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	ATP	A	1552	-	24,33,33	0.64	0	31,52,52	0.64	0
2	ATP	B	2552	-	24,33,33	0.68	0	31,52,52	0.63	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	-	-	0/18/38/38	0/3/3/3
2	ATP	B	2552	-	-	0/18/38/38	0/3/3/3

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.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1552	ATP	5	0
2	B	2552	ATP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/442 (100%)	-0.05	7 (1%) 74 69	14, 38, 78, 95	0
1	B	442/442 (100%)	0.11	10 (2%) 64 58	13, 41, 79, 96	0
All	All	884/884 (100%)	0.03	17 (1%) 70 64	13, 40, 79, 96	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	HIS	3.7
1	B	159	TRP	3.0
1	B	90	ASN	2.9
1	A	349	THR	2.8
1	B	286	HIS	2.8
1	B	85	ASP	2.7
1	B	285	ALA	2.5
1	B	84	ALA	2.4
1	B	288	ALA	2.4
1	B	224	THR	2.3
1	B	209	GLY	2.2
1	B	348	GLU	2.2
1	A	470	THR	2.2
1	A	159	TRP	2.2
1	A	334	ARG	2.1
1	A	180	GLY	2.0
1	A	471	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ATP	B	2552	31/31	0.82	0.31	1.28	0,67,102,102	0
2	ATP	A	1552	31/31	0.89	0.25	1.00	0,42,82,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.