



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:44 AM GMT

PDB ID : 3PNY
Title : Structure of Glutamyl-tRNA synthetase from Mycobacterium tuberculosis in space group P21
Authors : Kachalova, G.S.; Laurinavichiute, D.; Bartunik, H.D.
Deposited on : 2010-11-20
Resolution : 1.70 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

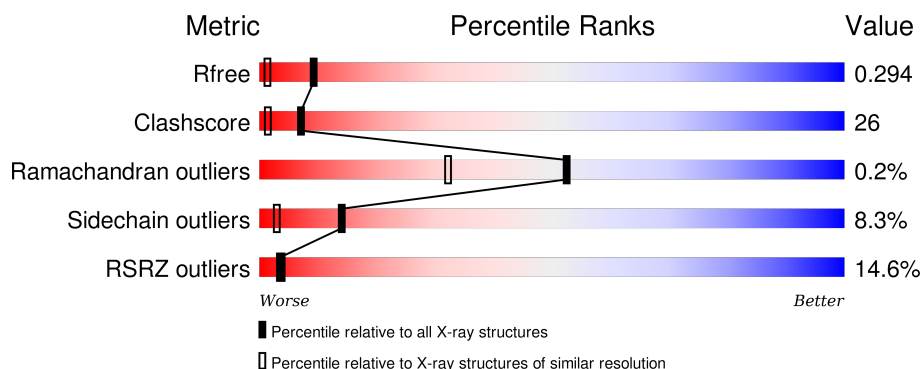
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	505	<div> <div>16%</div> <div>62%</div> <div>29%</div> <div>5%</div> </div>
1	B	505	<div> <div>12%</div> <div>66%</div> <div>26%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7841 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 Glutamyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	10	0
			3822	2419	689	707	7			
1	B	485	Total	C	N	O	S	0	8	0
			3849	2432	699	710	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	EXPRESSION TAG	UNP P0A636
A	-13	HIS	-	EXPRESSION TAG	UNP P0A636
A	-12	HIS	-	EXPRESSION TAG	UNP P0A636
A	-11	HIS	-	EXPRESSION TAG	UNP P0A636
A	-10	HIS	-	EXPRESSION TAG	UNP P0A636
A	-9	HIS	-	EXPRESSION TAG	UNP P0A636
A	-8	SER	-	EXPRESSION TAG	UNP P0A636
A	-7	SER	-	EXPRESSION TAG	UNP P0A636
A	-6	GLY	-	EXPRESSION TAG	UNP P0A636
A	-5	LEU	-	EXPRESSION TAG	UNP P0A636
A	-4	VAL	-	EXPRESSION TAG	UNP P0A636
A	-3	PRO	-	EXPRESSION TAG	UNP P0A636
A	-2	ARG	-	EXPRESSION TAG	UNP P0A636
A	-1	GLY	-	EXPRESSION TAG	UNP P0A636
A	0	SER	-	EXPRESSION TAG	UNP P0A636
B	-14	HIS	-	EXPRESSION TAG	UNP P0A636
B	-13	HIS	-	EXPRESSION TAG	UNP P0A636
B	-12	HIS	-	EXPRESSION TAG	UNP P0A636
B	-11	HIS	-	EXPRESSION TAG	UNP P0A636
B	-10	HIS	-	EXPRESSION TAG	UNP P0A636
B	-9	HIS	-	EXPRESSION TAG	UNP P0A636
B	-8	SER	-	EXPRESSION TAG	UNP P0A636
B	-7	SER	-	EXPRESSION TAG	UNP P0A636
B	-6	GLY	-	EXPRESSION TAG	UNP P0A636
B	-5	LEU	-	EXPRESSION TAG	UNP P0A636

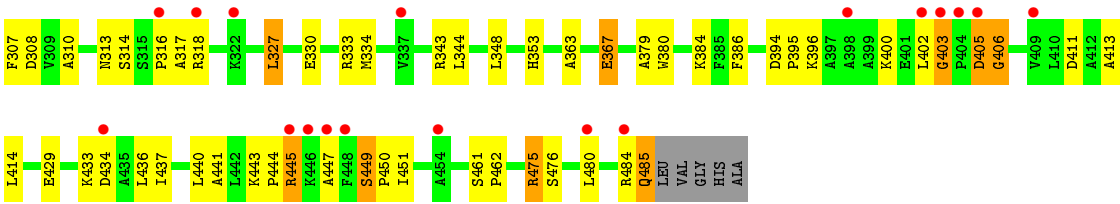
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	VAL	-	EXPRESSION TAG	UNP P0A636
B	-3	PRO	-	EXPRESSION TAG	UNP P0A636
B	-2	ARG	-	EXPRESSION TAG	UNP P0A636
B	-1	GLY	-	EXPRESSION TAG	UNP P0A636
B	0	SER	-	EXPRESSION TAG	UNP P0A636

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	73	Total O 73 73	0	11
2	B	97	Total O 97 97	0	7



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.16 Å 210.55 Å 58.15 Å 90.00° 99.80° 90.00°	Depositor
Resolution (Å)	10.41 – 1.70 19.98 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.7 (10.41-1.70) 90.7 (19.98-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.285 0.264 , 0.294	Depositor DCC
R_{free} test set	5178 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 103653 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7841	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.77	2/3923 (0.1%)	0.82	9/5340 (0.2%)
1	B	0.84	4/3944 (0.1%)	0.85	9/5366 (0.2%)
All	All	0.81	6/7867 (0.1%)	0.83	18/10706 (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	3
1	B	0	3
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	PHE	CE1-CZ	5.75	1.48	1.37
1	B	298	PHE	CE2-CZ	5.30	1.47	1.37
1	A	89[A]	GLN	C-N	5.14	1.45	1.34
1	A	89[B]	GLN	C-N	5.14	1.45	1.34
1	B	95[A]	ARG	CA-C	-5.02	1.40	1.52
1	B	95[B]	ARG	CA-C	-5.02	1.40	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	THR	CB-CA-C	-7.08	92.47	111.60
1	B	43	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	A	25	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	273	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	B	343	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	343	ARG	NE-CZ-NH1	5.58	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	271	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	273	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	403	GLY	C-N-CD	-5.38	108.78	120.60
1	B	267	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	B	273	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	B	327	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	A	25	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	B	5	GLU	N-CA-C	5.23	125.13	111.00
1	A	95	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	175	VAL	O-C-N	-5.06	114.61	122.70
1	A	440	LEU	O-C-N	5.01	130.71	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	LYS	Peptide
1	A	464	LEU	Peptide
1	A	483	ALA	Peptide
1	B	3	ALA	Peptide
1	B	402	LEU	Peptide
1	B	405	ASP	Peptide

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	3822	0	3775	228	0
1	B	3849	0	3804	175	1
2	A	73	0	0	8	0
2	B	97	0	0	9	0
All	All	7841	0	7579	401	1

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 26.

All (401) 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:249:THR:CG2	1:B:257:LYS:HG2	1.63	1.26
1:A:434:ASP:O	1:A:438:GLU:HB2	1.26	1.23
1:A:63:ASP:OD2	1:A:268[A]:PHE:HZ	1.21	1.18
1:B:117:VAL:HG22	1:B:132:TYR:OH	1.41	1.18
1:B:266:ASN:OD1	2:B:571[A]:HOH:O	1.57	1.17
1:B:443:LYS:HG3	1:B:444:PRO:HD2	1.27	1.16
1:A:268[A]:PHE:CZ	1:A:271:ARG:NH1	2.14	1.15
1:A:417:LEU:HD21	1:A:432:LEU:CD2	1.77	1.15
1:B:4:THR:HG22	1:B:7:VAL:HG23	1.27	1.13
1:A:442:LEU:HD13	1:A:446:LYS:HD2	1.26	1.12
1:B:249:THR:HG21	1:B:257:LYS:CG	1.80	1.12
1:A:434:ASP:HA	1:A:438:GLU:HG3	1.12	1.08
1:A:436:LEU:HD23	1:A:440:LEU:HD12	1.34	1.08
1:A:268[A]:PHE:CE1	1:A:271:ARG:NH1	2.24	1.06
1:A:417:LEU:HD21	1:A:432:LEU:HD21	1.06	1.05
1:A:400:LYS:HB2	1:A:401:GLU:OE2	1.55	1.05
1:B:330:GLU:OE2	1:B:333[A]:ARG:NH1	1.88	1.05
1:B:249:THR:HG21	1:B:257:LYS:HG2	1.29	1.05
1:A:434:ASP:HA	1:A:438:GLU:CG	1.86	1.05
1:A:63:ASP:OD2	1:A:268[A]:PHE:CZ	2.10	1.03
1:A:427:LEU:N	2:A:562[B]:HOH:O	1.91	1.03
1:A:417:LEU:CD2	1:A:432:LEU:HD21	1.88	1.02
1:B:4:THR:HG22	1:B:7:VAL:CG2	1.89	1.02
1:A:297:LEU:HD11	1:A:334:MET:HE1	1.39	1.01
1:A:411:ASP:OD1	1:A:484[B]:ARG:NH1	1.91	1.00
1:A:196:TYR:CZ	2:A:509[B]:HOH:O	2.09	0.99
1:A:409:VAL:HG11	1:A:450:PRO:HG2	1.38	0.99
1:A:409:VAL:HG11	1:A:450:PRO:CG	1.91	0.99
1:A:277:PRO:O	1:A:281[B]:LEU:HD13	1.66	0.95
1:B:117:VAL:HG12	1:B:120:ARG:NH1	1.82	0.93
1:A:409:VAL:HG13	1:A:436:LEU:HD22	1.49	0.93
1:B:202:CYS:O	1:B:206:LEU:HD13	1.69	0.92
1:B:297:LEU:HD21	1:B:334:MET:HE1	1.52	0.92
1:B:117:VAL:CG1	1:B:120:ARG:CZ	2.48	0.92
1:B:4:THR:CG2	1:B:7:VAL:CG2	2.48	0.91
1:B:117:VAL:CG2	1:B:132:TYR:OH	2.18	0.91
1:B:133:ASP:OD2	1:B:135:PHE:CZ	2.22	0.91
1:B:433:LYS:HD2	1:B:437:ILE:HD12	1.52	0.90
1:A:443:LYS:HG2	1:A:444:PRO:HD2	1.53	0.90
1:A:196:TYR:CE1	2:A:509[B]:HOH:O	2.22	0.90
1:A:437:ILE:HD11	1:A:444:PRO:HA	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268[A]:PHE:CZ	1:A:271:ARG:CZ	2.55	0.89
1:A:429:GLU:HG3	1:A:465:PHE:CE2	2.06	0.89
1:A:434:ASP:O	1:A:438:GLU:CB	2.19	0.89
1:B:273:ARG:NH1	2:B:572[A]:HOH:O	1.78	0.88
1:B:4:THR:HG21	1:B:7:VAL:CA	2.03	0.88
1:A:297:LEU:HD11	1:A:334:MET:CE	2.06	0.86
1:B:217:ASP:HB2	1:B:257:LYS:HZ1	1.39	0.86
1:A:432:LEU:CD1	1:A:451:ILE:HG12	2.05	0.86
1:A:433:LYS:HG3	1:A:448:PHE:CE2	2.12	0.85
1:B:217:ASP:CB	1:B:257:LYS:NZ	2.39	0.85
1:A:442:LEU:HD13	1:A:446:LYS:CD	2.05	0.84
1:A:437:ILE:HD11	1:A:444:PRO:CA	2.08	0.83
1:B:4:THR:HG21	1:B:7:VAL:N	1.93	0.83
1:A:409:VAL:CG1	1:A:450:PRO:HG2	2.06	0.83
1:B:113:THR:OG1	1:B:114:PRO:HD2	1.77	0.83
1:B:117:VAL:HA	1:B:120:ARG:HD2	1.61	0.82
1:B:433:LYS:HD2	1:B:437:ILE:CD1	2.08	0.82
1:B:63:ASP:OD2	1:B:271:ARG:NH1	2.13	0.82
1:A:433:LYS:HG3	1:A:448:PHE:CZ	2.15	0.82
1:A:449:SER:HB3	1:A:450:PRO:HD3	1.61	0.81
1:A:436:LEU:HD23	1:A:440:LEU:CD1	2.11	0.81
1:B:484[A]:ARG:CZ	2:B:568[A]:HOH:O	2.27	0.81
1:B:117:VAL:HG12	1:B:120:ARG:CZ	2.10	0.81
1:A:127:ASN:HD22	1:A:129:LYS:H	1.27	0.81
1:A:62:LEU:O	1:A:66[A]:ARG:HG3	1.81	0.80
1:B:4:THR:HG23	1:B:5:GLU:N	1.96	0.80
1:B:113:THR:OG1	1:B:114:PRO:CD	2.29	0.80
1:B:249:THR:CG2	1:B:257:LYS:CG	2.46	0.80
1:B:414:LEU:HD12	1:B:484[A]:ARG:HD3	1.65	0.79
1:A:432:LEU:HD12	1:A:451:ILE:HG12	1.64	0.79
1:B:4:THR:CG2	1:B:7:VAL:HG22	2.12	0.79
1:A:297:LEU:HD21	1:A:334:MET:HE1	1.65	0.79
1:B:166:ALA:HB2	1:B:176[A]:THR:HG22	1.65	0.78
1:A:196:TYR:CE1	1:A:200[B]:ASN:ND2	2.51	0.78
1:A:76:PRO:O	1:A:77:GLU:HG3	1.84	0.78
1:B:117:VAL:HG13	1:B:120:ARG:NE	1.99	0.78
1:B:122:VAL:HG12	1:B:123:ALA:O	1.84	0.77
1:B:249:THR:HG21	1:B:257:LYS:HG3	1.67	0.77
1:B:297:LEU:CD2	1:B:334:MET:HE1	2.15	0.77
1:A:427:LEU:CB	2:A:562[B]:HOH:O	2.33	0.76
1:B:217:ASP:HB3	1:B:257:LYS:HE2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ALA:N	1:A:426:PRO:CD	2.48	0.76
1:B:4:THR:O	1:B:4:THR:HG22	1.84	0.76
1:A:484[B]:ARG:HG3	1:A:485:GLN:OE1	1.86	0.76
1:B:414:LEU:CD1	1:B:484[A]:ARG:HD3	2.16	0.76
1:A:196:TYR:CD1	1:A:200[B]:ASN:ND2	2.54	0.75
1:B:3:ALA:HB3	1:B:4:THR:O	1.86	0.75
1:A:24:VAL:HG21	1:A:267:LEU:HD13	1.68	0.75
1:A:429:GLU:HG3	1:A:465:PHE:CZ	2.20	0.75
1:A:417:LEU:CD2	1:A:432:LEU:CD2	2.54	0.74
1:A:86:ARG:H	1:A:89[B]:GLN:HE21	1.33	0.74
1:A:6:THR:HG23	1:A:6:THR:O	1.87	0.74
1:A:86:ARG:O	1:A:89[B]:GLN:HG2	1.88	0.74
1:B:217:ASP:HB2	1:B:257:LYS:NZ	2.01	0.73
1:B:273:ARG:NH2	2:B:572[A]:HOH:O	2.21	0.73
1:A:451:ILE:CD1	1:A:451:ILE:N	2.51	0.73
1:B:4:THR:HG21	1:B:7:VAL:HA	1.69	0.73
1:A:461:SER:HB2	1:A:462:PRO:HD2	1.69	0.73
1:A:297:LEU:CD1	1:A:334:MET:HE1	2.17	0.73
1:A:315:SER:HB2	1:A:316:PRO:HD2	1.71	0.73
1:B:117:VAL:CG1	1:B:120:ARG:NE	2.52	0.72
1:A:425:ALA:N	1:A:426:PRO:HD3	2.03	0.72
1:A:427:LEU:HB2	2:A:562[B]:HOH:O	1.87	0.72
1:A:409:VAL:HG11	1:A:450:PRO:HG3	1.72	0.72
1:B:297:LEU:HD21	1:B:334:MET:CE	2.19	0.72
1:A:437:ILE:HD11	1:A:444:PRO:HB3	1.71	0.71
1:B:202:CYS:O	1:B:206:LEU:CD1	2.38	0.71
1:B:4:THR:HB	1:B:7:VAL:HG22	1.71	0.71
1:A:436:LEU:HB3	1:A:447:ALA:HA	1.73	0.71
1:A:437:ILE:HD11	1:A:444:PRO:CB	2.19	0.71
1:A:421:THR:O	1:A:473:ARG:NH2	2.24	0.70
1:A:170:LEU:HB2	1:A:245:ALA:HB2	1.73	0.70
1:A:266:ASN:OD1	1:A:268[B]:PHE:HB3	1.90	0.70
1:A:443:LYS:CG	1:A:444:PRO:HD2	2.22	0.69
1:A:84:PRO:HB2	1:A:89[B]:GLN:HG3	1.74	0.69
1:A:98:LEU:HG	1:A:198:LEU:HD21	1.73	0.69
1:B:461:SER:HB2	1:B:462:PRO:HD2	1.75	0.69
1:B:4:THR:CG2	1:B:7:VAL:N	2.55	0.69
1:A:432:LEU:HD11	1:A:451:ILE:HG12	1.74	0.68
1:B:297:LEU:HD11	1:B:334:MET:HE1	1.74	0.68
1:B:273:ARG:CZ	2:B:572[A]:HOH:O	2.28	0.68
1:A:432:LEU:HB2	1:A:448:PHE:HE1	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:SER:HB3	1:A:450:PRO:CD	2.24	0.68
1:B:297:LEU:CG	1:B:334:MET:HE1	2.24	0.68
1:B:363:ALA:O	1:B:367:GLU:HG2	1.93	0.68
1:B:117:VAL:CG1	1:B:120:ARG:HD2	2.23	0.67
1:A:379:ALA:O	1:A:383:LEU:HB2	1.94	0.67
1:A:68:LEU:HD22	1:A:281[A]:LEU:CD2	2.25	0.67
1:A:432:LEU:HB2	1:A:448:PHE:CE1	2.30	0.67
1:A:471:LEU:O	1:A:475[A]:ARG:HD3	1.94	0.67
1:A:451:ILE:H	1:A:451:ILE:CD1	2.08	0.67
1:A:432:LEU:HD11	1:A:451:ILE:CG1	2.25	0.67
1:B:484[A]:ARG:NH2	2:B:568[A]:HOH:O	2.27	0.66
1:A:437:ILE:CD1	1:A:444:PRO:HA	2.24	0.66
1:A:68:LEU:CD2	1:A:281[B]:LEU:HD12	2.25	0.66
1:A:451:ILE:HD12	1:A:451:ILE:N	2.08	0.66
1:B:3:ALA:HB2	1:B:37:THR:HG22	1.78	0.66
1:B:15:PRO:O	1:B:53:ASP:HA	1.96	0.65
1:B:3:ALA:CB	1:B:4:THR:O	2.45	0.65
1:A:146:ALA:O	1:A:150:GLU:HG2	1.96	0.65
1:B:217:ASP:HB3	1:B:257:LYS:CE	2.27	0.65
1:B:4:THR:CB	1:B:7:VAL:HG22	2.26	0.65
1:B:443:LYS:HG3	1:B:444:PRO:CD	2.18	0.65
1:A:433:LYS:O	1:A:438:GLU:HG2	1.97	0.65
1:B:117:VAL:CG1	1:B:120:ARG:CD	2.75	0.65
1:B:117:VAL:CA	1:B:120:ARG:HD2	2.27	0.65
1:A:409:VAL:HG13	1:A:436:LEU:CD2	2.25	0.65
1:B:234:ARG:NH2	2:B:504:HOH:O	1.86	0.65
1:A:464:LEU:O	1:A:467:SER:HB2	1.97	0.64
1:B:217:ASP:CB	1:B:257:LYS:HZ3	2.10	0.64
1:A:255:THR:HG22	1:A:318:ARG:HH22	1.61	0.64
1:B:189:ARG:HG3	1:B:195:LEU:HD21	1.78	0.64
1:B:433:LYS:CD	1:B:437:ILE:HD12	2.28	0.64
1:B:1:MET:CE	1:B:1:MET:H1	2.11	0.64
1:A:434:ASP:CA	1:A:438:GLU:HG3	2.07	0.63
1:A:448:PHE:HB3	1:A:464:LEU:HD23	1.79	0.63
1:A:451:ILE:H	1:A:451:ILE:HD13	1.63	0.63
1:A:200[A]:ASN:HB3	1:A:201:PRO:HD3	1.81	0.63
1:A:201:PRO:HB2	1:A:228:LEU:HD23	1.80	0.63
1:B:4:THR:CG2	1:B:7:VAL:HG23	2.11	0.62
1:B:249:THR:HG23	1:B:257:LYS:HG2	1.71	0.62
1:A:432:LEU:CD1	1:A:451:ILE:CG1	2.77	0.62
1:A:436:LEU:CB	1:A:447:ALA:HA	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:PRO:HG2	1:B:53:ASP:HB3	1.82	0.61
1:A:425:ALA:N	1:A:469:GLU:HG3	2.15	0.61
1:A:262:ASP:C	1:A:262:ASP:OD1	2.38	0.61
1:B:251:LEU:CD1	1:B:316:PRO:HB3	2.30	0.61
1:B:98:LEU:HG	1:B:198:LEU:HD21	1.82	0.61
1:B:297:LEU:CD1	1:B:334:MET:HE1	2.31	0.61
1:B:133:ASP:OD2	1:B:135:PHE:CE2	2.54	0.61
1:A:461:SER:HB2	1:A:462:PRO:CD	2.31	0.60
1:B:433:LYS:CD	1:B:437:ILE:CD1	2.79	0.60
1:B:249:THR:HG22	1:B:257:LYS:HG2	1.78	0.60
1:A:66[B]:ARG:NH2	2:A:561[B]:HOH:O	2.16	0.60
1:B:433:LYS:HA	1:B:437:ILE:HD12	1.84	0.60
1:A:445:ARG:O	1:A:445:ARG:HG2	2.01	0.60
1:B:117:VAL:HG12	1:B:120:ARG:HH11	1.66	0.59
1:B:297:LEU:HD11	1:B:334:MET:CE	2.32	0.59
1:A:68:LEU:HD22	1:A:281[B]:LEU:HD12	1.82	0.59
1:A:437:ILE:CD1	1:A:444:PRO:HB3	2.33	0.59
1:B:1:MET:CE	1:B:1:MET:N	2.65	0.59
1:A:404:PRO:O	1:A:407:ALA:HB3	2.03	0.59
1:B:98:LEU:HD21	1:B:198:LEU:HD22	1.84	0.59
1:B:1:MET:N	1:B:1:MET:SD	2.74	0.58
1:A:445:ARG:O	1:A:449:SER:HB2	2.03	0.58
1:B:208:LYS:NZ	1:B:239:GLU:OE2	2.27	0.58
1:B:344:LEU:HD11	1:B:379:ALA:CB	2.33	0.58
1:A:237:VAL:O	1:A:237:VAL:HG13	2.02	0.58
1:B:117:VAL:CG1	1:B:120:ARG:NH1	2.58	0.58
1:B:4:THR:HG21	1:B:6:THR:C	2.23	0.58
1:A:421:THR:C	1:A:473:ARG:HH22	2.06	0.58
1:B:117:VAL:HG12	1:B:120:ARG:CD	2.34	0.58
1:B:380:TRP:O	1:B:384:LYS:HB3	2.04	0.57
1:A:400:LYS:CB	1:A:401:GLU:OE2	2.43	0.57
1:B:3:ALA:HB2	1:B:37:THR:CG2	2.34	0.57
1:B:282:ASN:C	1:B:282:ASN:HD22	2.07	0.57
1:A:424:THR:C	1:A:426:PRO:HD2	2.25	0.57
1:A:98:LEU:HD21	1:A:198:LEU:HD22	1.86	0.57
1:B:217:ASP:CG	1:B:257:LYS:HZ3	2.08	0.56
1:B:217:ASP:HB3	1:B:257:LYS:NZ	2.19	0.56
1:A:127:ASN:ND2	1:A:129:LYS:HG2	2.20	0.56
1:B:403:GLY:O	1:B:406:GLY:HA3	2.06	0.56
1:A:189:ARG:HG3	1:A:195:LEU:HD21	1.87	0.56
1:A:297:LEU:CD2	1:A:334:MET:HE1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ALA:HA	1:A:402:LEU:HB2	1.88	0.56
1:B:117:VAL:HG22	1:B:132:TYR:HH	1.63	0.56
1:A:76:PRO:C	1:A:77:GLU:CG	2.73	0.56
1:A:434:ASP:CA	1:A:438:GLU:CG	2.75	0.56
1:A:84:PRO:CB	1:A:89[B]:GLN:HG3	2.36	0.56
1:B:120:ARG:HB3	1:B:131:GLY:O	2.06	0.56
1:B:117:VAL:HG13	1:B:120:ARG:CD	2.35	0.55
1:A:424:THR:C	1:A:426:PRO:CD	2.74	0.55
1:A:127:ASN:ND2	1:A:129:LYS:H	2.01	0.55
1:B:20[A]:HIS:CD2	1:B:265:SER:HB2	2.41	0.55
1:A:255:THR:HA	1:A:318:ARG:HH21	1.70	0.55
1:A:68:LEU:HD23	1:A:281[B]:LEU:CD1	2.37	0.55
1:A:268[A]:PHE:CE2	1:A:271:ARG:CZ	2.90	0.55
1:B:196[A]:TYR:HA	1:B:199:VAL:HG22	1.89	0.54
1:B:133:ASP:CG	1:B:135:PHE:CZ	2.81	0.54
1:A:24:VAL:HG12	1:A:284:LEU:HD13	1.89	0.54
1:A:6:THR:O	1:A:6:THR:CG2	2.56	0.54
1:A:415:ALA:O	1:A:418:THR:HG22	2.08	0.54
1:A:437:ILE:O	1:A:441:ALA:HA	2.07	0.54
1:B:445:ARG:HH11	1:B:445:ARG:HG2	1.72	0.53
1:A:76:PRO:O	1:A:77:GLU:CG	2.55	0.53
1:A:423:TRP:CD1	1:A:473:ARG:N	2.76	0.53
1:A:449:SER:O	1:A:452:ARG:N	2.41	0.53
1:B:273:ARG:HG2	1:B:273:ARG:HH11	1.73	0.53
1:A:86:ARG:H	1:A:89[B]:GLN:NE2	2.04	0.53
1:A:219:LEU:HA	1:A:246:HIS:NE2	2.23	0.53
1:A:411:ASP:CG	1:A:484[B]:ARG:HH12	2.11	0.53
1:B:251:LEU:CD1	1:B:316:PRO:CB	2.87	0.53
1:B:250:VAL:HG13	1:B:317:ALA:O	2.08	0.53
1:A:433:LYS:CG	1:A:448:PHE:CE2	2.90	0.53
1:A:68:LEU:HD23	1:A:281[B]:LEU:HD12	1.91	0.52
1:A:273:ARG:HD2	1:A:375:VAL:HG21	1.91	0.52
1:A:417:LEU:HD21	1:A:432:LEU:HD23	1.84	0.52
1:A:441:ALA:O	1:B:168:ASN:ND2	2.39	0.52
1:B:114:PRO:O	1:B:115:GLU:C	2.47	0.52
1:A:5:GLU:HG2	1:A:6:THR:HA	1.91	0.52
1:B:273:ARG:NH1	1:B:273:ARG:HG2	2.24	0.52
1:B:117:VAL:HG13	1:B:120:ARG:HD2	1.91	0.52
1:A:255:THR:CG2	1:A:318:ARG:HH22	2.23	0.52
1:B:251:LEU:HD12	1:B:316:PRO:CB	2.40	0.52
1:B:68:LEU:HD13	1:B:281:LEU:CD2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ALA:O	1:A:402:LEU:HB3	2.09	0.52
1:B:30:ASN:OD1	1:B:213:LEU:HB2	2.10	0.52
1:A:10:ARG:O	1:A:10:ARG:HG2	2.09	0.52
1:A:206:LEU:O	1:A:208:LYS:HE2	2.10	0.51
1:A:409:VAL:CG1	1:A:450:PRO:CG	2.74	0.51
1:B:16:THR:HG23	1:B:52:ARG:O	2.10	0.51
1:A:257:LYS:O	1:A:258:LEU:C	2.48	0.51
1:A:258:LEU:HG	1:A:265:SER:HB3	1.92	0.51
1:B:4:THR:CG2	1:B:6:THR:C	2.79	0.51
1:A:213:LEU:HG	1:A:245:ALA:HB3	1.92	0.51
1:B:1:MET:HE1	1:B:1:MET:H1	1.75	0.51
1:B:413:ALA:CB	1:B:451:ILE:HD11	2.40	0.51
1:B:201:PRO:HG2	1:B:228:LEU:HD23	1.93	0.50
1:A:405:ASP:O	1:A:409:VAL:HG23	2.11	0.50
1:A:424:THR:OG1	1:A:426:PRO:HD2	2.11	0.50
1:A:213:LEU:N	1:A:213:LEU:HD12	2.27	0.50
1:B:443:LYS:CG	1:B:444:PRO:HD2	2.20	0.50
1:B:484[A]:ARG:HB3	2:B:568[A]:HOH:O	2.11	0.50
1:B:363:ALA:O	1:B:367:GLU:CG	2.58	0.50
1:A:297:LEU:HD21	1:A:334:MET:CE	2.39	0.50
1:A:256:LYS:O	1:A:257:LYS:C	2.50	0.50
1:A:5:GLU:HG2	1:A:6:THR:CA	2.42	0.49
1:A:452:ARG:HG2	1:A:458:THR:O	2.13	0.49
1:A:368:LEU:HD11	1:A:466:GLU:HB2	1.94	0.49
1:A:200[B]:ASN:HB2	1:A:201:PRO:HD3	1.93	0.49
1:B:68:LEU:HD13	1:B:281:LEU:HD23	1.93	0.49
1:A:437:ILE:CD1	1:A:444:PRO:CA	2.85	0.49
1:A:485:GLN:N	1:A:485:GLN:OE1	2.46	0.49
1:B:49:ASP:OD2	1:B:52:ARG:HB2	2.12	0.49
1:A:194:PRO:HB3	1:A:198:LEU:HD23	1.95	0.49
1:B:170:LEU:HB2	1:B:245:ALA:HB2	1.94	0.49
1:A:237:VAL:O	1:A:237:VAL:CG1	2.60	0.48
1:B:200:ASN:HB3	1:B:201:PRO:HD3	1.94	0.48
1:B:405:ASP:C	1:B:405:ASP:OD2	2.51	0.48
1:B:436:LEU:HD13	1:B:447:ALA:O	2.12	0.48
1:A:315:SER:CB	1:A:316:PRO:HD2	2.35	0.48
1:B:92:GLU:HA	1:B:95[B]:ARG:HG3	1.94	0.48
1:A:420:VAL:O	1:A:473:ARG:NH1	2.38	0.48
1:A:483:ALA:O	1:A:485:GLN:N	2.47	0.48
1:B:68:LEU:O	1:B:281:LEU:HD11	2.14	0.48
1:A:268[A]:PHE:CZ	1:A:271:ARG:NH2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HA	1:A:442:LEU:HD23	1.77	0.47
1:B:461:SER:HB2	1:B:462:PRO:CD	2.44	0.47
1:B:54:SER:OG	1:B:57:SER:N	2.31	0.47
1:A:28:LEU:HD22	1:A:281[A]:LEU:HD22	1.95	0.47
1:B:414:LEU:HD13	1:B:484[A]:ARG:HE	1.79	0.47
1:B:165:LEU:HD12	1:B:165:LEU:H	1.79	0.47
1:A:277:PRO:C	1:A:281[B]:LEU:HD13	2.31	0.47
1:A:68:LEU:HD22	1:A:281[A]:LEU:HD21	1.95	0.47
1:A:222:THR:N	1:A:223:PRO:HD2	2.28	0.47
1:A:417:LEU:CG	1:A:432:LEU:HD21	2.44	0.47
1:B:4:THR:OG1	1:B:211:HIS:HE1	1.97	0.47
1:A:213:LEU:HD23	1:A:309:VAL:HG21	1.96	0.47
1:A:466:GLU:O	1:A:470:LEU:HG	2.15	0.47
1:B:217:ASP:CB	1:B:257:LYS:HZ1	2.07	0.47
1:B:137:ARG:HD3	1:B:159[B]:ARG:HE	1.80	0.47
1:B:445:ARG:HH11	1:B:445:ARG:CG	2.28	0.46
1:A:172:ARG:CD	1:A:219:LEU:CD1	2.93	0.46
1:B:414:LEU:CD1	1:B:484[A]:ARG:CD	2.91	0.46
1:B:166:ALA:HB2	1:B:176[A]:THR:CG2	2.39	0.46
1:B:214:ARG:HH12	1:B:225:GLN:HE22	1.62	0.46
1:A:373:ILE:HB	1:A:378:ASP:HB2	1.96	0.46
1:B:251:LEU:HD11	1:B:316:PRO:HA	1.97	0.46
1:A:258:LEU:HD21	1:A:265:SER:HA	1.98	0.46
1:A:132:TYR:OH	1:A:136:ASP:HB2	2.16	0.46
1:A:418:THR:HG23	1:A:419:SER:N	2.31	0.45
1:A:410:LEU:HA	1:A:410:LEU:HD23	1.62	0.45
1:A:255:THR:HG22	1:A:318:ARG:NH2	2.30	0.45
1:A:12:CYS:HA	1:A:44:ARG:O	2.17	0.45
1:A:380:TRP:O	1:A:384:LYS:HB3	2.15	0.45
1:A:427:LEU:HG	2:A:562[B]:HOH:O	2.17	0.45
1:A:252:GLY:O	1:A:318:ARG:HG3	2.16	0.45
1:A:76:PRO:O	1:A:78:VAL:N	2.47	0.45
1:A:98:LEU:HG	1:A:198:LEU:CD2	2.45	0.45
1:B:476:SER:O	1:B:480:LEU:HB2	2.17	0.45
1:B:185:PHE:CD1	1:B:224[A]:ARG:HG2	2.52	0.45
1:A:264:GLN:CG	1:A:264:GLN:O	2.64	0.45
1:A:241:ILE:HG23	1:A:242:PRO:HD2	1.99	0.45
1:A:5:GLU:HA	1:A:6:THR:HA	1.67	0.45
1:B:36:HIS:CG	1:B:307:PHE:O	2.70	0.45
1:A:297:LEU:CG	1:A:334:MET:HE1	2.46	0.44
1:B:26:THR:O	1:B:30:ASN:ND2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:OD1	1:A:144:ARG:NH1	2.49	0.44
1:A:87:GLN:HG2	1:A:94:TYR:OH	2.18	0.44
1:B:449:SER:N	1:B:450:PRO:CD	2.80	0.44
1:A:444:PRO:HD3	1:B:310:ALA:HB1	1.99	0.44
1:A:442:LEU:CD1	1:A:446:LYS:CD	2.88	0.44
1:B:414:LEU:HD13	1:B:484[A]:ARG:NE	2.33	0.44
1:B:165:LEU:HD12	1:B:165:LEU:N	2.33	0.44
1:A:401:GLU:HB2	1:A:453:VAL:HG21	2.00	0.44
1:A:86:ARG:HB2	1:A:89[B]:GLN:NE2	2.33	0.44
1:A:255:THR:CG2	1:A:318:ARG:NH2	2.81	0.44
1:A:451:ILE:CG2	1:A:468:LEU:HD11	2.48	0.43
1:B:429:GLU:O	1:B:433:LYS:HG2	2.18	0.43
1:B:98:LEU:HG	1:B:198:LEU:CD2	2.48	0.43
1:B:214:ARG:HH12	1:B:225:GLN:NE2	2.16	0.43
1:A:451:ILE:HG21	1:A:468:LEU:HD11	2.01	0.43
1:A:196:TYR:CD2	1:A:196:TYR:C	2.91	0.43
1:B:49:ASP:O	1:B:53:ASP:OD2	2.36	0.43
1:A:76:PRO:C	1:A:78:VAL:H	2.22	0.43
1:B:123:ALA:N	1:B:129:LYS:O	2.52	0.43
1:B:20[A]:HIS:CE1	1:B:22:GLY:H	2.36	0.43
1:B:68:LEU:HD22	1:B:281:LEU:HG	2.01	0.43
1:B:127:ASN:HA	1:B:128:PRO:HD2	1.84	0.43
1:B:266:ASN:ND2	1:B:269:ALA:H	2.16	0.43
1:A:368:LEU:HD22	1:A:463:PRO:HG2	2.00	0.43
1:A:448:PHE:HB3	1:A:464:LEU:CD2	2.48	0.43
1:A:433:LYS:HZ2	1:A:448:PHE:HE2	1.66	0.43
1:B:286:LEU:HD12	1:B:327:LEU:HD11	2.01	0.43
1:A:437:ILE:CG1	1:A:444:PRO:HA	2.49	0.43
1:B:485:GLN:OE1	2:B:568[A]:HOH:O	2.21	0.43
1:B:440:LEU:O	1:B:441:ALA:HB3	2.18	0.43
1:B:348:LEU:HB3	1:B:353:HIS:O	2.19	0.43
1:A:241:ILE:CG2	1:A:242:PRO:HD2	2.49	0.42
1:B:4:THR:HB	1:B:211:HIS:CE1	2.55	0.42
1:A:473:ARG:O	1:A:477:MET:HG2	2.20	0.42
1:A:365:ALA:O	1:A:368:LEU:HB2	2.19	0.42
1:A:270:HIS:HE1	1:A:321:GLN:OE1	2.02	0.42
1:A:66[B]:ARG:NH1	2:A:561[B]:HOH:O	2.51	0.42
1:B:129:LYS:HB3	1:B:129:LYS:HZ2	1.85	0.42
1:A:429:GLU:CG	1:A:465:PHE:CE2	2.90	0.42
1:A:432:LEU:HD11	1:A:451:ILE:HG13	2.01	0.42
1:B:449:SER:CB	1:B:450:PRO:HD3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ASP:OD1	1:A:358:ASP:C	2.58	0.42
1:B:386:PHE:O	1:B:475:ARG:NH2	2.53	0.42
1:B:308:ASP:OD1	1:B:308:ASP:C	2.58	0.42
1:B:266:ASN:ND2	1:B:269:ALA:N	2.68	0.41
1:A:21:VAL:HG22	1:A:258:LEU:HD21	2.01	0.41
1:B:219:LEU:HA	1:B:246:HIS:NE2	2.35	0.41
1:B:394:ASP:HA	1:B:395:PRO:HD2	1.83	0.41
1:A:432:LEU:CB	1:A:448:PHE:CE1	3.00	0.41
1:A:437:ILE:HG13	1:A:447:ALA:HB2	2.02	0.41
1:A:213:LEU:CD2	1:A:309:VAL:HG21	2.49	0.41
1:B:54:SER:OG	1:B:57:SER:CB	2.68	0.41
1:A:172:ARG:HD3	1:A:219:LEU:CD1	2.51	0.41
1:B:258:LEU:HD21	1:B:265:SER:CA	2.51	0.41
1:B:4:THR:CB	1:B:211:HIS:HE1	2.33	0.41
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.80	0.41
1:A:417:LEU:HD12	1:A:480:LEU:HD23	2.01	0.41
1:A:66[A]:ARG:HH11	1:A:66[A]:ARG:HD2	1.71	0.41
1:A:423:TRP:O	1:A:469:GLU:HG2	2.21	0.41
1:A:264:GLN:HG3	1:A:319:PHE:CD1	2.56	0.41
1:A:169:ASP:HB3	1:A:172:ARG:HB2	2.03	0.41
1:A:255:THR:HA	1:A:318:ARG:NH2	2.34	0.40
1:B:251:LEU:O	1:B:318:ARG:HA	2.21	0.40
1:A:348:LEU:HB3	1:A:353:HIS:O	2.21	0.40
1:A:410:LEU:HB3	1:A:484[B]:ARG:HB3	2.03	0.40
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.86	0.40
1:A:417:LEU:CD1	1:A:480:LEU:CD2	2.99	0.40
1:A:429:GLU:OE2	1:A:465:PHE:HE2	2.04	0.40
1:A:127:ASN:HD22	1:A:127:ASN:C	2.24	0.40
1:A:150:GLU:HG2	1:A:150:GLU:H	1.54	0.40
1:A:443:LYS:CB	1:A:444:PRO:HD2	2.52	0.40

All (1) 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:B:100:ARG:NH2	1:B:125:GLY:O[1_655]	2.00	0.20

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	489/505 (97%)	475 (97%)	14 (3%)	0	100	100
1	B	491/505 (97%)	475 (97%)	14 (3%)	2 (0%)	39	20
All	All	980/1010 (97%)	950 (97%)	28 (3%)	2 (0%)	52	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	406	GLY
1	B	252	GLY

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	393/402 (98%)	356 (91%)	37 (9%)	11	2
1	B	394/402 (98%)	363 (92%)	31 (8%)	15	3
All	All	787/804 (98%)	719 (91%)	68 (9%)	14	3

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	18	THR
1	A	66[A]	ARG
1	A	66[B]	ARG

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Mol	Chain	Res	Type
1	A	77	GLU
1	A	114	PRO
1	A	127	ASN
1	A	130	LEU
1	A	139	LEU
1	A	150	GLU
1	A	196	TYR
1	A	237	VAL
1	A	240	ARG
1	A	247	LEU
1	A	251	LEU
1	A	261	ARG
1	A	262	ASP
1	A	264	GLN
1	A	267	LEU
1	A	273	ARG
1	A	282	ASN
1	A	313	ASN
1	A	323	LYS
1	A	330	GLU
1	A	345	ARG
1	A	392[A]	VAL
1	A	392[B]	VAL
1	A	402	LEU
1	A	423	TRP
1	A	432	LEU
1	A	442	LEU
1	A	451	ILE
1	A	459	THR
1	A	464	LEU
1	A	469	GLU
1	A	484[A]	ARG
1	A	484[B]	ARG
1	B	1	MET
1	B	2	THR
1	B	4	THR
1	B	5	GLU
1	B	10	ARG
1	B	18	THR
1	B	52	ARG
1	B	54	SER
1	B	118	GLU

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Mol	Chain	Res	Type
1	B	126	ARG
1	B	163	ASP
1	B	165	LEU
1	B	176[A]	THR
1	B	176[B]	THR
1	B	240	ARG
1	B	255	THR
1	B	256	LYS
1	B	271	ARG
1	B	282	ASN
1	B	290	SER
1	B	313	ASN
1	B	314	SER
1	B	367	GLU
1	B	396	LYS
1	B	400	LYS
1	B	411	ASP
1	B	434	ASP
1	B	445	ARG
1	B	449	SER
1	B	475	ARG
1	B	485	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	127	ASN
1	A	270	HIS
1	A	313	ASN
1	B	225	GLN
1	B	264	GLN
1	B	266	ASN
1	B	313	ASN
1	B	353	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	481/505 (95%)	1.19	81 (16%) 2 2	13, 26, 52, 68	9 (1%)
1	B	485/505 (96%)	0.96	60 (12%) 5 6	12, 23, 46, 66	2 (0%)
All	All	966/1010 (95%)	1.07	141 (14%) 3 4	12, 25, 49, 68	11 (1%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	THR	13.4
1	B	4	THR	13.0
1	A	257	LYS	11.8
1	B	3	ALA	11.2
1	A	419	SER	11.1
1	B	51	GLN	11.0
1	A	254	GLY	11.0
1	A	421	THR	10.2
1	A	253	GLU	9.6
1	A	427	LEU	9.5
1	B	119	ALA	8.8
1	B	118	GLU	8.7
1	B	257	LYS	8.6
1	A	418	THR	8.6
1	A	256	LYS	8.2
1	B	50	ALA	8.0
1	B	117	VAL	7.5
1	A	260	LYS	7.5
1	A	258	LEU	7.3
1	A	442	LEU	7.2
1	B	5	GLU	7.1
1	A	422	ASP	7.0
1	A	439	GLY	6.9
1	A	259	SER	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	52	ARG	6.9
1	A	423	TRP	6.0
1	B	1	MET	6.0
1	A	402	LEU	5.8
1	B	251	LEU	5.7
1	A	426	PRO	5.7
1	B	2	THR	5.6
1	A	403	GLY	5.4
1	B	116	GLU	5.0
1	B	255	THR	5.0
1	A	440	LEU	5.0
1	A	424	THR	4.8
1	B	402	LEU	4.7
1	B	403	GLY	4.7
1	A	5	GLU	4.7
1	B	124	ALA	4.7
1	A	261	ARG	4.5
1	A	404	PRO	4.5
1	A	268[A]	PHE	4.5
1	A	431	ALA	4.4
1	A	447	ALA	4.3
1	A	420	VAL	4.3
1	A	417	LEU	4.0
1	B	254	GLY	4.0
1	A	415	ALA	3.9
1	B	268	PHE	3.9
1	A	398	ALA	3.9
1	B	6	THR	3.9
1	B	447	ALA	3.8
1	A	6	THR	3.8
1	A	436	LEU	3.8
1	A	428	ILE	3.8
1	A	425	ALA	3.7
1	A	450	PRO	3.7
1	A	307	PHE	3.7
1	A	240	ARG	3.7
1	A	396	LYS	3.6
1	A	438	GLU	3.5
1	A	399	ALA	3.5
1	A	196	TYR	3.5
1	A	429	GLU	3.4
1	B	253	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	264	GLN	3.4
1	B	162	ASP	3.3
1	A	263	PRO	3.3
1	B	446	LYS	3.3
1	A	262	ASP	3.3
1	B	53	ASP	3.2
1	B	54	SER	3.2
1	B	121	HIS	3.2
1	A	406	GLY	3.2
1	A	454	ALA	3.2
1	A	445	ARG	3.2
1	B	404	PRO	3.1
1	A	252	GLY	3.0
1	B	49	ASP	3.0
1	A	437	ILE	3.0
1	B	240	ARG	2.9
1	B	256	LYS	2.9
1	A	16	THR	2.9
1	B	261	ARG	2.9
1	B	398	ALA	2.9
1	A	444	PRO	2.9
1	A	446	LYS	2.9
1	B	409	VAL	2.8
1	A	271	ARG	2.8
1	B	250	VAL	2.8
1	A	410	LEU	2.8
1	A	448	PHE	2.7
1	A	483	ALA	2.7
1	B	454	ALA	2.7
1	B	122	VAL	2.6
1	A	413	ALA	2.6
1	A	465	PHE	2.6
1	A	52	ARG	2.6
1	A	464	LEU	2.6
1	A	434	ASP	2.6
1	B	48	THR	2.6
1	B	258	LEU	2.6
1	A	484[A]	ARG	2.5
1	A	29	PHE	2.5
1	A	414	LEU	2.5
1	A	451	ILE	2.5
1	A	162	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	259	SER	2.5
1	B	322	LYS	2.4
1	B	405	ASP	2.4
1	B	123	ALA	2.4
1	A	407	ALA	2.4
1	B	480	LEU	2.4
1	A	441	ALA	2.4
1	B	226	LEU	2.3
1	A	400	LYS	2.3
1	B	113	THR	2.3
1	A	412	ALA	2.3
1	A	433	LYS	2.3
1	A	340	PHE	2.3
1	B	337	VAL	2.3
1	B	206	LEU	2.2
1	B	16	THR	2.2
1	B	316	PRO	2.2
1	A	239	GLU	2.2
1	A	281[A]	LEU	2.1
1	B	165	LEU	2.1
1	A	394	ASP	2.1
1	B	445	ARG	2.1
1	A	468	LEU	2.1
1	A	267	LEU	2.1
1	B	190	ALA	2.0
1	B	484[A]	ARG	2.0
1	B	434	ASP	2.0
1	B	129	LYS	2.0
1	A	301	ASP	2.0
1	B	196[A]	TYR	2.0
1	A	367	GLU	2.0
1	B	318	ARG	2.0
1	B	448	PHE	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.