



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:15 AM UTC

PDB ID : 3PNY / pdb_00003pny
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

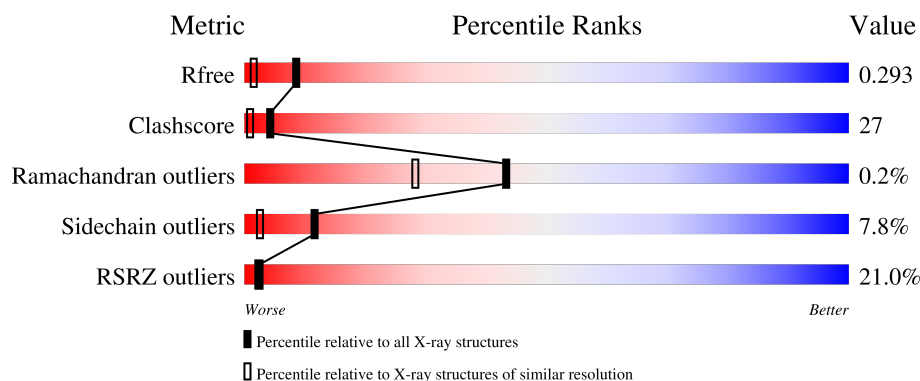
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	505	23% 61% 29% 5% 5%
1	B	505	17% 64% 28% ...

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

Continued on next page...

Continued from previous page...

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

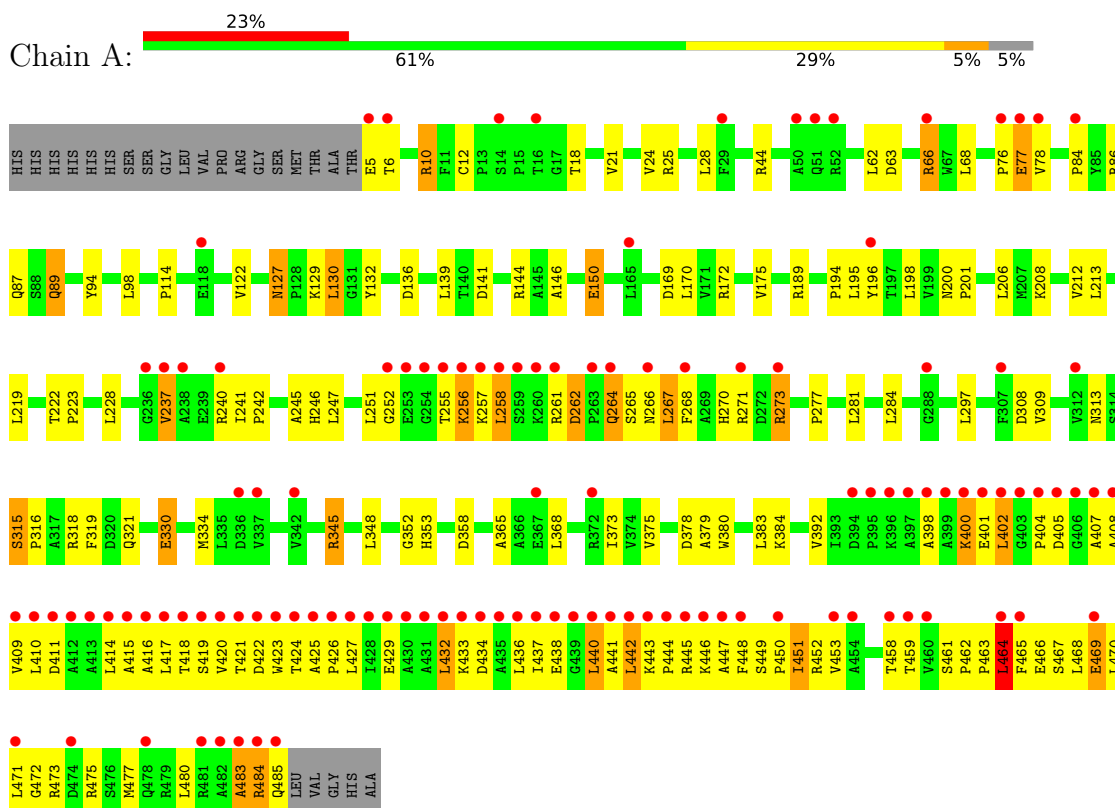
- Molecule 2 is water.

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

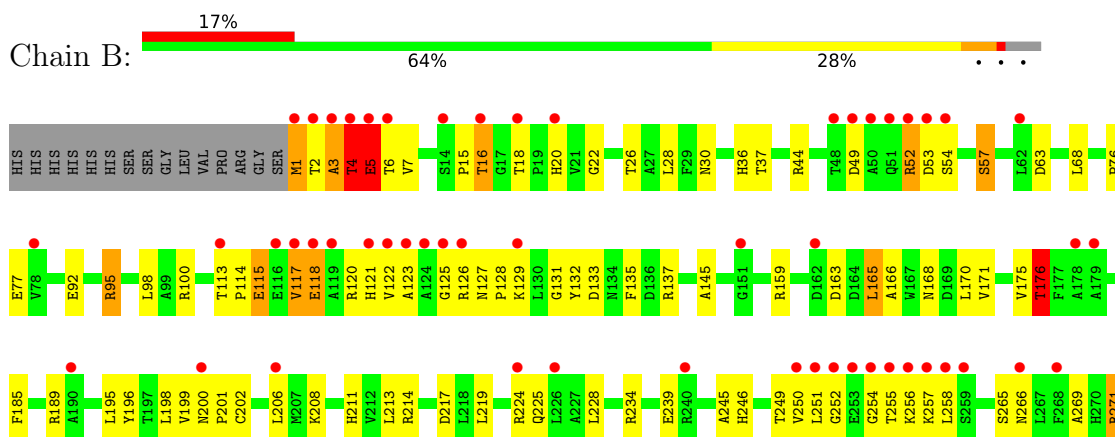
3 Residue-property plots

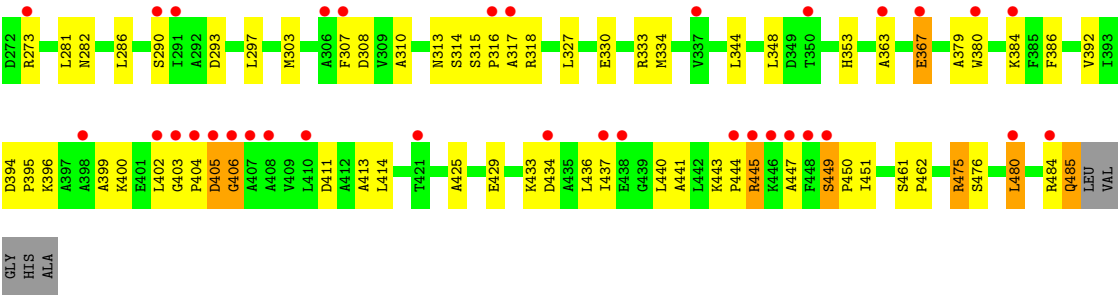
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glutamyl-tRNA synthetase



• Molecule 1: Glutamyl-tRNA synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.16Å 210.55Å 58.15Å 90.00° 99.80° 90.00°	Depositor
Resolution (Å)	10.41 – 1.70 10.41 – 1.70	Depositor EDS
% Data completeness (in resolution range)	90.7 (10.41-1.70) 90.3 (10.41-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.285 0.266 , 0.293	Depositor DCC
R_{free} test set	5179 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.94	2/3923 (0.1%)	1.02	14/5340 (0.3%)
1	B	1.02	4/3944 (0.1%)	1.10	23/5366 (0.4%)
All	All	0.98	6/7867 (0.1%)	1.06	37/10706 (0.3%)

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	95[A]	ARG	CA-C	-9.91	1.40	1.52
1	B	95[B]	ARG	CA-C	-9.91	1.40	1.52
1	A	89[A]	GLN	C-N	8.62	1.45	1.33
1	A	89[B]	GLN	C-N	8.62	1.45	1.33
1	B	176[A]	THR	C-N	-5.39	1.24	1.33
1	B	176[B]	THR	C-N	-5.39	1.24	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	GLU	N-CA-C	12.96	125.13	111.14
1	B	4	THR	CB-CA-C	-9.70	92.47	109.64
1	A	258	LEU	N-CA-C	-8.11	98.13	110.30
1	A	175	VAL	O-C-N	-8.02	114.61	123.03
1	A	345	ARG	N-CA-C	-6.79	103.80	111.07
1	B	115	GLU	CB-CA-C	6.43	118.65	109.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	SER	CA-C-N	6.11	126.47	119.93
1	A	315	SER	C-N-CA	6.11	126.47	119.93
1	A	258	LEU	CB-CA-C	6.02	118.43	110.06
1	B	399	ALA	CA-C-O	5.89	126.78	120.24
1	A	440	LEU	O-C-N	5.88	130.71	122.36
1	B	254	GLY	N-CA-C	-5.79	102.54	111.98
1	B	95[A]	ARG	CA-C-O	-5.77	114.43	120.55
1	B	95[B]	ARG	CA-C-O	-5.77	114.43	120.55
1	B	145	ALA	N-CA-C	-5.76	104.92	111.14
1	B	5	GLU	N-CA-CB	-5.73	101.76	110.07
1	B	44	ARG	CA-C-N	-5.67	115.06	122.37
1	B	44	ARG	C-N-CA	-5.67	115.06	122.37
1	A	352	GLY	N-CA-C	-5.62	105.86	115.08
1	B	176[A]	THR	CA-C-N	5.62	131.09	123.11
1	B	176[A]	THR	C-N-CA	5.62	131.09	123.11
1	B	176[B]	THR	CA-C-N	5.62	131.09	123.11
1	B	176[B]	THR	C-N-CA	5.62	131.09	123.11
1	A	130	LEU	CA-C-N	-5.58	115.38	122.19
1	A	130	LEU	C-N-CA	-5.58	115.38	122.19
1	B	425	ALA	CA-C-N	-5.48	113.38	119.19
1	B	425	ALA	C-N-CA	-5.48	113.38	119.19
1	B	175	VAL	O-C-N	-5.47	117.28	123.18
1	B	57	SER	N-CA-C	5.37	117.13	111.28
1	B	404	PRO	N-CA-C	5.30	120.56	114.20
1	A	122	VAL	N-CA-C	-5.28	105.24	110.62
1	A	256	LYS	N-CA-C	5.13	118.58	109.96
1	B	115	GLU	N-CA-C	-5.12	102.95	110.42
1	B	315	SER	CA-C-N	5.11	126.23	119.84
1	B	315	SER	C-N-CA	5.11	126.23	119.84
1	A	408	ALA	CA-C-N	5.04	127.01	120.56
1	A	408	ALA	C-N-CA	5.04	127.01	120.56

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	235	0
1	B	3849	0	3804	182	1
2	A	73	0	0	8	0
2	B	97	0	0	9	0
All	All	7841	0	7579	414	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 27.

All (414) 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: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:297:LEU:HD11	1:A:334:MET:HE1	1.18	1.11
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:400:LYS:HB2	1:A:401:GLU:OE2	1.55	1.05
1:A:417:LEU:HD21	1:A:432:LEU:HD21	1.06	1.05
1:B:330:GLU:OE2	1:B:333[A]:ARG:NH1	1.88	1.05
1:A:434:ASP:HA	1:A:438:GLU:CG	1.86	1.05
1:B:249:THR:HG21	1:B:257:LYS:HG2	1.29	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:411:ASP:OD1	1:A:484[B]:ARG:NH1	1.91	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:297:LEU:HD11	1:B:334:MET:HE1	1.45	0.96
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: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:196:TYR:CE1	2:A:509[B]:HOH:O	2.22	0.90
1:A:443:LYS:HG2	1:A:444:PRO:HD2	1.53	0.90
1:A:437:ILE:HD11	1:A:444:PRO:HA	1.52	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: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:A:409:VAL:CG1	1:A:450:PRO:HG2	2.06	0.83
1:B:4:THR:HG21	1:B:7:VAL:N	1.93	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:A:127:ASN:HD22	1:A:129:LYS:H	1.27	0.81
1:B:117:VAL:HG12	1:B:120:ARG:CZ	2.10	0.81
1:A:62:LEU:O	1:A:66[A]:ARG:HG3	1.81	0.80
1:B:297:LEU:HD21	1:B:334:MET:HE2	1.64	0.80
1:B:4:THR:HG23	1:B:5:GLU:N	1.96	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:LEU:HD11	1:A:334:MET:CE	2.06	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:B:166:ALA:HB2	1:B:176[A]:THR:HG22	1.65	0.78
1:B:1:MET:N	1:B:1:MET:HE2	1.98	0.78
1:A:76:PRO:O	1:A:77:GLU:HG3	1.84	0.78
1:A:196:TYR:CE1	1:A:200[B]:ASN:ND2	2.51	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: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
1:A:425:ALA:N	1:A:426:PRO:CD	2.48	0.76
1:A:484[B]:ARG:HG3	1:A:485:GLN:OE1	1.86	0.76
1:B:4:THR:HG22	1:B:4:THR:O	1.84	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:86:ARG:H	1:A:89[B]:GLN:HE21	1.33	0.74
1:A:417:LEU:CD2	1:A:432:LEU:CD2	2.54	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:A:297:LEU:CD1	1:A:334:MET:HE1	2.09	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:N	1:A:451:ILE:CD1	2.51	0.73
1:B:297:LEU:CD1	1:B:334:MET:HE1	2.19	0.73
1:A:461:SER:HB2	1:A:462:PRO:HD2	1.69	0.73
1:B:4:THR:HG21	1:B:7:VAL:HA	1.69	0.73
1:A:315:SER:HB2	1:A:316:PRO:HD2	1.71	0.73
1:A:425:ALA:N	1:A:426:PRO:HD3	2.03	0.72
1:B:117:VAL:CG1	1:B:120:ARG:NE	2.52	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:CYS:O	1:B:206:LEU:CD1	2.38	0.71
1:A:436:LEU:HB3	1:A:447:ALA:HA	1.73	0.71
1:B:4:THR:HB	1:B:7:VAL:HG22	1.71	0.71
1:A:437:ILE:HD11	1:A:444:PRO:CB	2.19	0.71
1:A:170:LEU:HB2	1:A:245:ALA:HB2	1.73	0.70
1:A:421:THR:O	1:A:473:ARG:NH2	2.24	0.70
1:A:266:ASN:OD1	1:A:268[B]:PHE:HB3	1.90	0.70
1:A:84:PRO:HB2	1:A:89[B]:GLN:HG3	1.74	0.69
1:A:443:LYS:CG	1:A:444:PRO:HD2	2.22	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: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
1:A:449:SER:HB3	1:A:450:PRO:CD	2.24	0.68
1:B:363:ALA:O	1:B:367:GLU:HG2	1.93	0.68
1:A:379:ALA:O	1:A:383:LEU:HB2	1.94	0.67
1:B:117:VAL:CG1	1:B:120:ARG:HD2	2.23	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:432:LEU:HD11	1:A:451:ILE:CG1	2.25	0.67
1:A:451:ILE:CD1	1:A:451:ILE:H	2.08	0.67
1:B:484[A]:ARG:NH2	2:B:568[A]:HOH:O	2.27	0.66
1:A:68:LEU:CD2	1:A:281[B]:LEU:HD12	2.25	0.66
1:A:437:ILE:CD1	1:A:444:PRO:HA	2.24	0.66
1:A:451:ILE:N	1:A:451:ILE:HD12	2.08	0.66
1:B:3:ALA:HB2	1:B:37:THR:HG22	1.78	0.66
1:A:262:ASP:OD1	1:A:262:ASP:C	2.38	0.66
1:B:15:PRO:O	1:B:53:ASP:HA	1.96	0.65
1:A:146:ALA:O	1:A:150:GLU:HG2	1.96	0.65
1:B:3:ALA:CB	1:B:4:THR:O	2.45	0.65
1:B:1:MET:HE2	1:B:1:MET:H3	1.60	0.65
1:B:4:THR:CB	1:B:7:VAL:HG22	2.26	0.65
1:B:217:ASP:HB3	1:B:257:LYS:CE	2.27	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:A:409:VAL:HG13	1:A:436:LEU:CD2	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:217:ASP:CB	1:B:257:LYS:HZ3	2.10	0.64
1:B:1:MET:CE	1:B:1:MET:H1	2.11	0.64
1:B:433:LYS:CD	1:B:437:ILE:HD12	2.28	0.64
1:B:330:GLU:C	1:B:334:MET:HE3	2.22	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:200[A]:ASN:HB3	1:A:201:PRO:HD3	1.81	0.63
1:A:451:ILE:H	1:A:451:ILE:HD13	1.63	0.63
1:A:201:PRO:HB2	1:A:228:LEU:HD23	1.80	0.63
1:A:421:THR:C	1:A:473:ARG:HH22	2.06	0.63
1:B:4:THR:HG21	1:B:6:THR:C	2.23	0.63
1:B:4:THR:CG2	1:B:7:VAL:HG23	2.11	0.62
1:B:282:ASN:C	1:B:282:ASN:HD22	2.07	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
1:A:424:THR:C	1:A:426:PRO:HD2	2.25	0.61
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:B:251:LEU:CD1	1:B:316:PRO:HB3	2.30	0.61
1:B:217:ASP:CG	1:B:257:LYS:HZ3	2.08	0.61
1:A:76:PRO:C	1:A:77:GLU:CG	2.73	0.61
1:B:98:LEU:HG	1:B:198:LEU:HD21	1.82	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:A:66[B]:ARG:NH2	2:A:561[B]:HOH:O	2.16	0.60
1:B:249:THR:HG22	1:B:257:LYS:HG2	1.78	0.60
1:A:424:THR:C	1:A:426:PRO:CD	2.74	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: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:A:404:PRO:O	1:A:407:ALA:HB3	2.03	0.59
1:B:133:ASP:CG	1:B:135:PHE:CZ	2.81	0.59
1:B:98:LEU:HD21	1:B:198:LEU:HD22	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:237:VAL:O	1:A:237:VAL:HG13	2.02	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:B:117:VAL:CG1	1:B:120:ARG:NH1	2.58	0.58
1:A:411:ASP:CG	1:A:484[B]:ARG:HH12	2.11	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:114:PRO:O	1:B:115:GLU:C	2.47	0.57
1:B:3:ALA:HB2	1:B:37:THR:CG2	2.34	0.57
1:B:1:MET:N	1:B:1:MET:CE	2.65	0.57
1:A:98:LEU:HD21	1:A:198:LEU:HD22	1.86	0.57
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:1:MET:HE2	1:B:1:MET:H1	1.67	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:398:ALA:HA	1:A:402:LEU:HB2	1.88	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:A:257:LYS:O	1:A:258:LEU:C	2.48	0.56
1:B:120:ARG:HB3	1:B:131:GLY:O	2.06	0.56
1:B:4:THR:CG2	1:B:6:THR:C	2.79	0.55
1:B:117:VAL:HG13	1:B:120:ARG:CD	2.35	0.55
1:A:297:LEU:HD21	1:A:334:MET:HE2	1.86	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:256:LYS:O	1:A:257:LYS:C	2.50	0.54
1:B:196[A]:TYR:HA	1:B:199:VAL:HG22	1.89	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:HG2	1:B:445:ARG:HH11	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:86:ARG:H	1:A:89[B]:GLN:NE2	2.04	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:SER:O	1:A:452:ARG:N	2.41	0.53
1:B:405:ASP:OD2	1:B:405:ASP:C	2.51	0.53
1:A:219:LEU:HA	1:A:246:HIS:NE2	2.23	0.53
1:B:251:LEU:CD1	1:B:316:PRO:CB	2.87	0.53
1:A:297:LEU:HD21	1:A:334:MET:CE	2.39	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:277:PRO:C	1:A:281[B]:LEU:HD13	2.31	0.52
1:A:5:GLU:HG2	1:A:6:THR:HA	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:A:255:THR:CG2	1:A:318:ARG:HH22	2.23	0.52
1:B:117:VAL:HG13	1:B:120:ARG:HD2	1.91	0.52
1:B:68:LEU:HD13	1:B:281:LEU:CD2	2.38	0.52
1:B:251:LEU:HD12	1:B:316:PRO:CB	2.40	0.52
1:A:398:ALA:O	1:A:402:LEU:HB3	2.09	0.52
1:A:411:ASP:CG	1:A:484[B]:ARG:NH1	2.68	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:330:GLU:C	1:A:334:MET:HE3	2.35	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:297:LEU:CG	1:B:334:MET:HE1	2.40	0.51
1:B:16:THR:HG23	1:B:52:ARG:O	2.10	0.51
1:A:258:LEU:HG	1:A:265:SER:HB3	1.92	0.51
1:A:213:LEU:HG	1:A:245:ALA:HB3	1.92	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:HD12	1:A:213:LEU:N	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: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:76:PRO:C	1:A:77:GLU:HG3	2.37	0.49
1:A:200[B]:ASN:HB2	1:A:201:PRO:HD3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:A:485:GLN:N	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: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:196:TYR:CD2	1:A:196:TYR:C	2.91	0.48
1:A:76:PRO:C	1:A:78:VAL:H	2.22	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:442:LEU:HD23	1:A:442:LEU:HA	1.77	0.47
1:B:54:SER:OG	1:B:57:SER:N	2.31	0.47
1:B:461:SER:HB2	1:B:462:PRO:CD	2.44	0.47
1:A:28:LEU:HD22	1:A:281[A]:LEU:HD22	1.95	0.47
1:B:165:LEU:HD12	1:B:165:LEU:H	1.79	0.47
1:B:414:LEU:HD13	1:B:484[A]:ARG:HE	1.79	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:213:LEU:HD23	1:A:309:VAL:HG21	1.96	0.47
1:A:417:LEU:CG	1:A:432:LEU:HD21	2.44	0.47
1:A:466:GLU:O	1:A:470:LEU:HG	2.15	0.47
1:B:4:THR:OG1	1:B:211:HIS:HE1	1.97	0.47
1:B:137:ARG:HD3	1:B:159[B]:ARG:HE	1.80	0.47
1:B:217:ASP:CB	1:B:257:LYS:HZ1	2.07	0.47
1:B:445:ARG:HH11	1:B:445:ARG:CG	2.28	0.46
1:A:358:ASP:C	1:A:358:ASP:OD1	2.58	0.46
1:B:308:ASP:OD1	1:B:308:ASP:C	2.58	0.46
1:A:172:ARG:CD	1:A:219:LEU:CD1	2.93	0.46
1:B:330:GLU:O	1:B:334:MET:HE3	2.15	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:B:414:LEU:CD1	1:B:484[A]:ARG:CD	2.91	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:132:TYR:OH	1:A:136:ASP:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD21	1:A:265:SER:HA	1.98	0.46
1:A:418:THR:HG23	1:A:419:SER:N	2.31	0.45
1:A:255:THR:HG22	1:A:318:ARG:NH2	2.30	0.45
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.62	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:252:GLY:O	1:A:318:ARG:HG3	2.16	0.45
1:A:427:LEU:HG	2:A:562[B]:HOH:O	2.17	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:A:264:GLN:O	1:A:264:GLN:CG	2.64	0.45
1:B:185:PHE:CD1	1:B:224[A]:ARG:HG2	2.52	0.45
1:B:476:SER:O	1:B:480:LEU:HB2	2.17	0.45
1:A:127:ASN:HD22	1:A:127:ASN:C	2.24	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:A:25:ARG:HD2	1:A:25:ARG:C	2.41	0.45
1:B:36:HIS:CG	1:B:307:PHE:O	2.70	0.45
1:A:141:ASP:OD1	1:A:144:ARG:NH1	2.49	0.44
1:B:26:THR:O	1:B:30:ASN:ND2	2.37	0.44
1:A:86:ARG:HB2	1:A:89[B]:GLN:CD	2.42	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:414:LEU:O	1:A:415:ALA:C	2.61	0.44
1:A:442:LEU:CD1	1:A:446:LYS:CD	2.88	0.44
1:B:165:LEU:HD12	1:B:165:LEU:N	2.33	0.44
1:B:414:LEU:HD13	1:B:484[A]:ARG:NE	2.33	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:401:GLU:HB2	1:A:453:VAL:HG21	2.00	0.44
1:A:451:ILE:CG2	1:A:468:LEU:HD11	2.48	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:B:429:GLU:O	1:B:433:LYS:HG2	2.18	0.43
1:A:63:ASP:CG	1:A:271:ARG:HH22	2.26	0.43
1:A:451:ILE:HG21	1:A:468:LEU:HD11	2.01	0.43
1:B:49:ASP:O	1:B:53:ASP:OD2	2.36	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:121:HIS:O	1:B:122:VAL:C	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ALA:N	1:B:129:LYS:O	2.52	0.43
1:B:127:ASN:HA	1:B:128:PRO:HD2	1.84	0.43
1:A:308:ASP:C	1:A:308:ASP:OD1	2.60	0.43
1:A:368:LEU:HD22	1:A:463:PRO:HG2	2.00	0.43
1:A:415:ALA:O	1:A:416:ALA:C	2.60	0.43
1:B:266:ASN:ND2	1:B:269:ALA:H	2.16	0.43
1:A:422:ASP:CG	1:A:424:THR:HG22	2.44	0.43
1:A:448:PHE:HB3	1:A:464:LEU:CD2	2.48	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:348:LEU:HB3	1:B:353:HIS:O	2.19	0.43
1:B:440:LEU:O	1:B:441:ALA:HB3	2.18	0.43
1:B:485:GLN:OE1	2:B:568[A]:HOH:O	2.21	0.43
1:A:241:ILE:CG2	1:A:242:PRO:HD2	2.49	0.42
1:B:297:LEU:HD11	1:B:334:MET:CE	2.32	0.42
1:A:212:VAL:C	1:A:213:LEU:HD12	2.44	0.42
1:A:365:ALA:O	1:A:368:LEU:HB2	2.19	0.42
1:A:473:ARG:O	1:A:477:MET:HG2	2.20	0.42
1:B:4:THR:HB	1:B:211:HIS:CE1	2.55	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:HZ2	1:B:129:LYS:HB3	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:386:PHE:O	1:B:475:ARG:NH2	2.53	0.42
1:B:449:SER:CB	1:B:450:PRO:HD3	2.50	0.42
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:266:ASN:ND2	1:B:269:ALA:N	2.68	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:A:423:TRP:CD1	1:A:472:GLY:C	2.99	0.41
1:B:117:VAL:O	1:B:118:GLU:C	2.64	0.41
1:B:258:LEU:HD21	1:B:265:SER:CA	2.51	0.41
1:A:471:LEU:HA	1:A:471:LEU:HD23	1.80	0.41
1:B:4:THR:CB	1:B:211:HIS:HE1	2.33	0.41
1:A:66[A]:ARG:HH11	1:A:66[A]:ARG:HD2	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLN:HG3	1:A:319:PHE:CD1	2.56	0.41
1:A:417:LEU:HD12	1:A:480:LEU:HD23	2.01	0.41
1:A:423:TRP:O	1:A:469:GLU:HG2	2.21	0.41
1:A:443:LYS:NZ	1:B:171:VAL:O	2.35	0.41
1:B:76:PRO:C	1:B:77:GLU:HG3	2.45	0.41
1:B:444:PRO:O	1:B:445:ARG:C	2.63	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:A:348:LEU:HB3	1:A:353:HIS:O	2.21	0.40
1:B:28:LEU:HG	1:B:303:MET:HE1	2.03	0.40
1:B:251:LEU:O	1:B:318:ARG:HA	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:150:GLU:HG2	1:A:150:GLU:H	1.54	0.40
1:A:266:ASN:OD1	1:A:266:ASN:C	2.64	0.40
1:A:443:LYS:CB	1:A:444:PRO:HD2	2.52	0.40
1:B:293:ASP:OD1	1:B:293:ASP:C	2.64	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 [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	489/505 (97%)	475 (97%)	14 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	491/505 (97%)	475 (97%)	14 (3%)	2 (0%)	30	16
All	All	980/1010 (97%)	950 (97%)	28 (3%)	2 (0%)	43	28

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%)	360 (92%)	33 (8%)	10	2
1	B	394/402 (98%)	363 (92%)	31 (8%)	11	2
All	All	787/804 (98%)	723 (92%)	64 (8%)	11	2

All (64) 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
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	237	VAL
1	A	240	ARG
1	A	247	LEU
1	A	251	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	261	ARG
1	A	262	ASP
1	A	264	GLN
1	A	267	LEU
1	A	273	ARG
1	A	313	ASN
1	A	330	GLU
1	A	345	ARG
1	A	392[A]	VAL
1	A	392[B]	VAL
1	A	402	LEU
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	16	THR
1	B	18	THR
1	B	52	ARG
1	B	117	VAL
1	B	118	GLU
1	B	126	ARG
1	B	163	ASP
1	B	165	LEU
1	B	176[A]	THR
1	B	176[B]	THR
1	B	255	THR
1	B	256	LYS
1	B	271	ARG
1	B	290	SER
1	B	313	ASN
1	B	314	SER
1	B	367	GLU
1	B	392	VAL
1	B	396	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	480	LEU
1	B	485	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	51	GLN
1	A	127	ASN
1	A	264	GLN
1	A	270	HIS
1	A	313	ASN
1	A	347	HIS
1	B	121	HIS
1	B	225	GLN
1	B	264	GLN
1	B	266	ASN
1	B	347	HIS
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	481/505 (95%)	1.42	116 (24%) 2 2	8, 26, 52, 68	19 (3%)
1	B	485/505 (96%)	1.16	87 (17%) 3 3	11, 23, 46, 66	10 (2%)
All	All	966/1010 (95%)	1.29	203 (21%) 2 2	8, 24, 49, 68	29 (3%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	THR	9.4
1	B	50	ALA	8.5
1	A	439	GLY	8.4
1	A	254	GLY	8.0
1	B	119	ALA	7.7
1	A	427	LEU	7.3
1	A	419	SER	7.3
1	A	423	TRP	7.2
1	A	431	ALA	7.2
1	A	253	GLU	7.0
1	B	3	ALA	6.9
1	B	257	LYS	6.9
1	B	54	SER	6.6
1	A	255	THR	6.4
1	A	438	GLU	6.3
1	A	257	LYS	6.3
1	A	421	THR	6.2
1	A	425	ALA	6.1
1	B	117	VAL	6.1
1	A	442	LEU	6.1
1	B	403	GLY	6.1
1	B	2	THR	6.0
1	B	251	LEU	6.0
1	B	254	GLY	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	447	ALA	5.9
1	B	5	GLU	5.9
1	A	418	THR	5.8
1	A	429	GLU	5.8
1	B	118	GLU	5.7
1	A	260	LYS	5.6
1	B	51	GLN	5.6
1	B	53	ASP	5.5
1	B	52	ARG	5.5
1	A	437	ILE	5.5
1	A	422	ASP	5.4
1	A	307	PHE	5.3
1	A	256	LYS	5.3
1	B	255	THR	5.3
1	A	426	PRO	5.2
1	A	258	LEU	5.2
1	A	440	LEU	5.0
1	A	403	GLY	5.0
1	A	399	ALA	4.9
1	A	420	VAL	4.9
1	A	436	LEU	4.7
1	A	450	PRO	4.6
1	A	252	GLY	4.6
1	A	406	GLY	4.6
1	A	415	ALA	4.6
1	A	264	GLN	4.5
1	B	337	VAL	4.5
1	A	404	PRO	4.5
1	A	77	GLU	4.5
1	A	444	PRO	4.4
1	A	271	ARG	4.4
1	B	408	ALA	4.3
1	B	116	GLU	4.3
1	A	395	PRO	4.3
1	A	424	THR	4.3
1	A	447	ALA	4.3
1	A	337	VAL	4.3
1	A	402	LEU	4.2
1	A	5	GLU	4.2
1	A	414	LEU	4.1
1	B	6	THR	4.1
1	B	124	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	258	LEU	4.1
1	A	6	THR	4.1
1	B	49	ASP	4.1
1	B	1	MET	4.0
1	B	404	PRO	4.0
1	A	259	SER	4.0
1	B	434	ASP	4.0
1	B	402	LEU	3.9
1	B	122	VAL	3.8
1	A	433	LYS	3.8
1	A	435	ALA	3.8
1	A	16	THR	3.8
1	A	428	ILE	3.8
1	A	464	LEU	3.7
1	A	441	ALA	3.7
1	B	268	PHE	3.7
1	A	410	LEU	3.7
1	A	408	ALA	3.7
1	A	372	ARG	3.7
1	A	263	PRO	3.6
1	A	413	ALA	3.6
1	B	113	THR	3.6
1	B	252	GLY	3.5
1	A	417	LEU	3.5
1	A	398	ALA	3.4
1	A	458	THR	3.4
1	B	256	LYS	3.4
1	A	50	ALA	3.3
1	A	397	ALA	3.3
1	A	196	TYR	3.3
1	B	121	HIS	3.3
1	B	444	PRO	3.3
1	A	465	PHE	3.3
1	A	412	ALA	3.3
1	A	416	ALA	3.3
1	A	367	GLU	3.2
1	A	78	VAL	3.2
1	A	407	ALA	3.2
1	A	236	GLY	3.1
1	A	268[A]	PHE	3.1
1	B	306	ALA	3.0
1	B	407	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	484[A]	ARG	3.0
1	B	380	TRP	3.0
1	A	430	ALA	3.0
1	B	123	ALA	3.0
1	B	259	SER	2.9
1	B	48	THR	2.9
1	B	446	LYS	2.8
1	A	240	ARG	2.8
1	A	396	LYS	2.8
1	B	438	GLU	2.8
1	A	411	ASP	2.7
1	B	405	ASP	2.7
1	B	178	ALA	2.7
1	B	62	LEU	2.7
1	A	445	ARG	2.7
1	B	250	VAL	2.7
1	B	410	LEU	2.7
1	B	406	GLY	2.7
1	A	446	LYS	2.7
1	B	200	ASN	2.6
1	B	125	GLY	2.6
1	B	206	LEU	2.6
1	A	14	SER	2.6
1	B	384	LYS	2.6
1	A	434	ASP	2.6
1	A	84	PRO	2.6
1	B	484[A]	ARG	2.6
1	A	400	LYS	2.6
1	A	394	ASP	2.5
1	A	165	LEU	2.5
1	A	460	VAL	2.5
1	B	363	ALA	2.5
1	A	288	GLY	2.5
1	A	443	LYS	2.5
1	B	253	GLU	2.5
1	B	273	ARG	2.5
1	B	266	ASN	2.5
1	B	16	THR	2.5
1	B	449	SER	2.5
1	A	482	ALA	2.4
1	B	398	ALA	2.4
1	B	290	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	291	ILE	2.4
1	A	266	ASN	2.4
1	A	474	ASP	2.4
1	B	162	ASP	2.4
1	B	20[A]	HIS	2.4
1	A	76	PRO	2.4
1	A	459	THR	2.4
1	A	312	VAL	2.4
1	A	481	ARG	2.4
1	B	126	ARG	2.4
1	A	52	ARG	2.3
1	B	179	ALA	2.3
1	B	14	SER	2.3
1	B	18	THR	2.3
1	A	483	ALA	2.3
1	B	480	LEU	2.3
1	A	405	ASP	2.3
1	A	454	ALA	2.2
1	A	66[A]	ARG	2.2
1	A	261	ARG	2.2
1	B	78	VAL	2.2
1	A	273	ARG	2.2
1	B	129	LYS	2.2
1	A	336[A]	ASP	2.2
1	A	432	LEU	2.2
1	A	401	GLU	2.2
1	B	448	PHE	2.2
1	B	437	ILE	2.2
1	B	445	ARG	2.2
1	B	350	THR	2.2
1	A	342	VAL	2.2
1	A	409	VAL	2.2
1	A	485	GLN	2.2
1	A	448	PHE	2.2
1	A	51	GLN	2.1
1	B	367	GLU	2.1
1	B	226	LEU	2.1
1	B	307	PHE	2.1
1	A	118	GLU	2.1
1	A	469	GLU	2.1
1	B	224[A]	ARG	2.1
1	A	237	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	317	ALA	2.1
1	B	316	PRO	2.1
1	A	478	GLN	2.1
1	B	240	ARG	2.1
1	A	29	PHE	2.1
1	B	151	GLY	2.0
1	A	238	ALA	2.0
1	B	190	ALA	2.0
1	A	471	LEU	2.0
1	B	421	THR	2.0
1	A	453	VAL	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 oligosaccharides 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.