



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:41 pm BST

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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

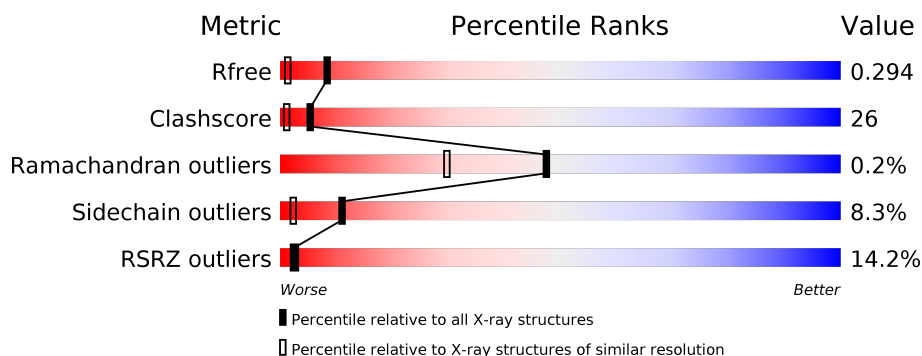
1 Overall quality at a glance

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 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	<div> <div>16%</div> <div>62%</div> <div>29%</div> <div>5%</div> </div>
1	B	505	<div> <div>11%</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

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

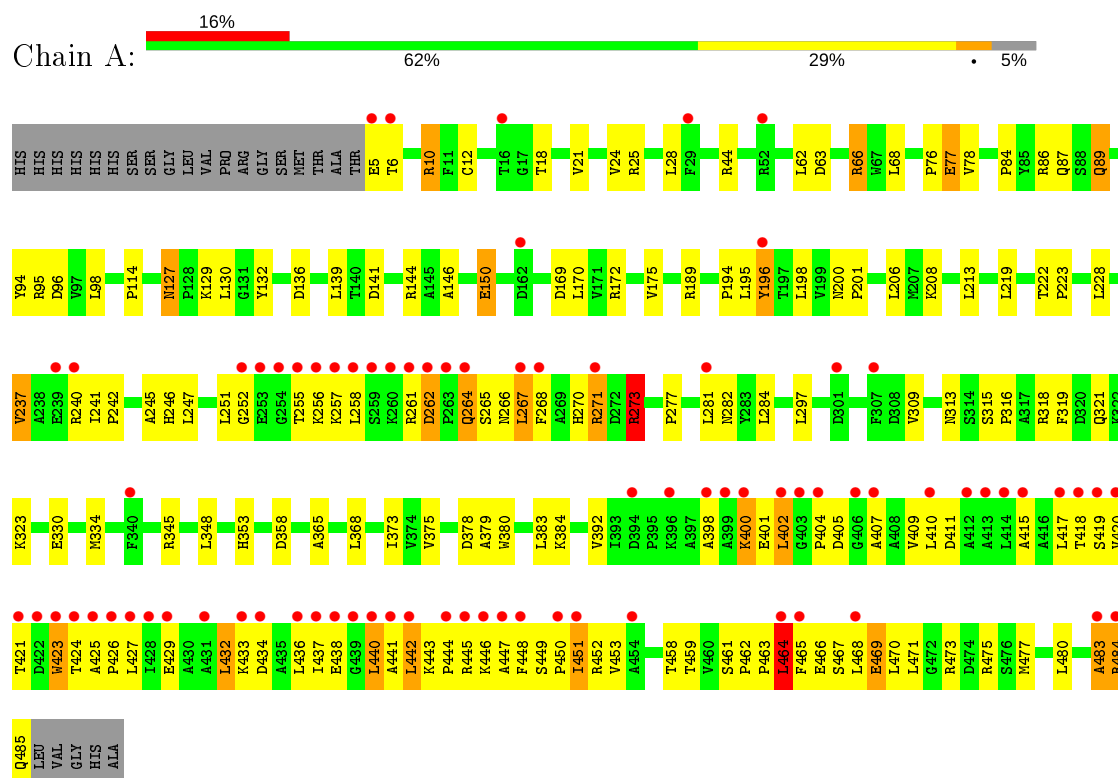
- Molecule 2 is water.

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

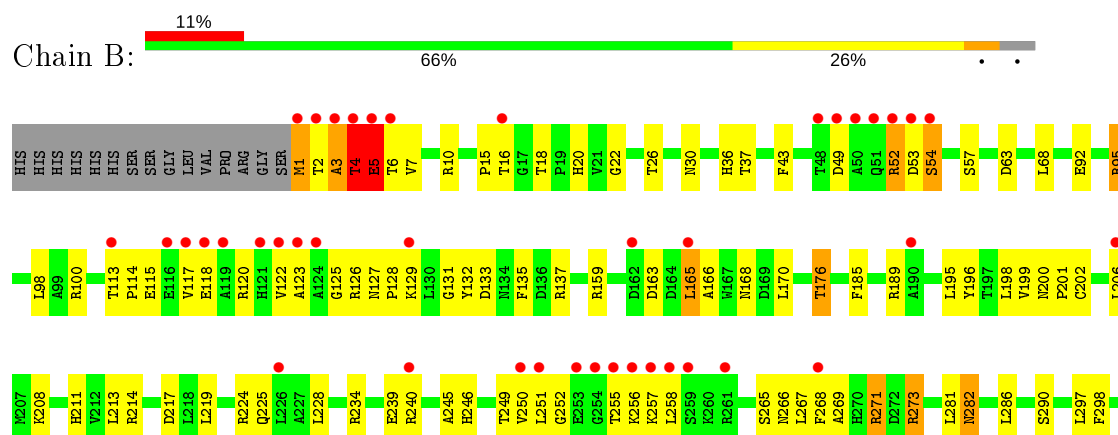
3 Residue-property plots

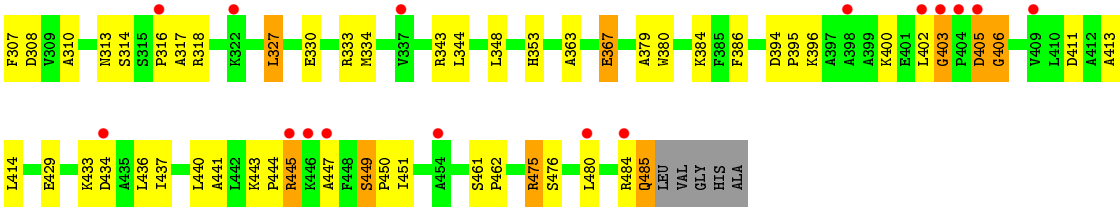
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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	44.16 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 0.266 , 0.294	Depositor DCC
R_{free} test set	5179 reflections (5.00%)	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)	0.35 , 44.6	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	0.77	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

Continued on next page...

Continued from previous page...

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:436:LEU:HD23	1:A:440:LEU:HD12	1.34	1.08
1:A:434:ASP:HA	1:A:438:GLU:HG3	1.12	1.08
1:A:268[A]:PHE:CE1	1:A:271:ARG:NH1	2.24	1.06
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: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: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

Continued on next page...

Continued from previous page...

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: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:4:THR:HG21	1:B:7:VAL:N	1.93	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: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

Continued on next page...

Continued from previous page...

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: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:B:4:THR:O	1:B:4:THR:HG22	1.84	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: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:297:LEU:CD1	1:A:334:MET:HE1	2.17	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
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: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:273:ARG:CZ	2:B:572[A]:HOH:O	2.28	0.68
1:B:297:LEU:HD11	1:B:334:MET:HE1	1.74	0.68
1:A:432:LEU:HB2	1:A:448:PHE:HE1	1.58	0.68

Continued on next page...

Continued from previous page...

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: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:H	1:A:451:ILE:CD1	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: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: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: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: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
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: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: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

Continued on next page...

Continued from previous page...

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:262:ASP:C	1:A:262:ASP:OD1	2.38	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: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:B:297:LEU:CD1	1:B:334:MET:HE1	2.31	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: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:A:237:VAL:HG13	1:A:237:VAL:O	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: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:98:LEU:HD21	1:A:198:LEU:HD22	1.86	0.57
1:A:424:THR:C	1:A:426:PRO:HD2	2.25	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

Continued on next page...

Continued from previous page...

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:A:24:VAL:HG12	1:A:284:LEU:HD13	1.89	0.54
1:B:133:ASP:CG	1:B:135:PHE:CZ	2.81	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:423:TRP:CD1	1:A:473:ARG:N	2.76	0.53
1:A:76:PRO:O	1:A:77:GLU:CG	2.55	0.53
1:A:449:SER:O	1:A:452:ARG:N	2.41	0.53
1:A:86:ARG:H	1:A:89[B]:GLN:NE2	2.04	0.53
1:B:273:ARG:HG2	1:B:273:ARG:HH11	1.73	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:5:GLU:HG2	1:A:6:THR:HA	1.91	0.52
1:B:114:PRO:O	1:B:115:GLU:C	2.47	0.52
1:A:441:ALA:O	1:B:168:ASN:ND2	2.39	0.52
1:B:273:ARG:NH1	1:B:273:ARG:HG2	2.24	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: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

Continued on next page...

Continued from previous page...

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:A:213:LEU:HG	1:A:245:ALA:HB3	1.92	0.51
1:B:4:THR:CG2	1:B:6:THR:C	2.79	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:256:LYS:O	1:A:257:LYS:C	2.50	0.50
1:A:297:LEU:HD21	1:A:334:MET:CE	2.39	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:CG1	1:A:237:VAL:O	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

Continued on next page...

Continued from previous page...

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: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:222:THR:N	1:A:223:PRO:HD2	2.28	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:466:GLU:O	1:A:470:LEU:HG	2.15	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: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:172:ARG:CD	1:A:219:LEU:CD1	2.93	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
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:HA	1:A:410:LEU:HD23	1.62	0.45
1:A:380:TRP:O	1:A:384:LYS:HB3	2.15	0.45
1:A:12:CYS:HA	1:A:44:ARG:O	2.17	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:264:GLN:CG	1:A:264:GLN:O	2.64	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: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: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:141:ASP:OD1	1:A:144:ARG:NH1	2.49	0.44
1:A:297:LEU:CG	1:A:334:MET:HE1	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:THR:O	1:B:30:ASN:ND2	2.37	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: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: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:86:ARG:HB2	1:A:89[B]:GLN:NE2	2.33	0.44
1:A:451:ILE:CG2	1:A:468:LEU:HD11	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:B:98:LEU:HG	1:B:198:LEU:CD2	2.48	0.43
1:A:196:TYR:CD2	1:A:196:TYR:C	2.91	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: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:127:ASN:HA	1:B:128:PRO:HD2	1.84	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:A:368:LEU:HD22	1:A:463:PRO:HG2	2.00	0.43
1:B:266:ASN:ND2	1:B:269:ALA:H	2.16	0.43
1:A:433:LYS:HZ2	1:A:448:PHE:HE2	1.66	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: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: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:358:ASP:OD1	1:A:358:ASP:C	2.58	0.42
1:A:432:LEU:HD11	1:A:451:ILE:HG13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ASP:OD1	1:B:308:ASP:C	2.58	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:B:258:LEU:HD21	1:B:265:SER:CA	2.51	0.41
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.80	0.41
1:B:4:THR:CB	1:B:211:HIS:HE1	2.33	0.41
1:A:264:GLN:HG3	1:A:319:PHE:CD1	2.56	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:417:LEU:HD12	1:A:480:LEU:HD23	2.01	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: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:429:GLU:OE2	1:A:465:PHE:HE2	2.04	0.40
1:A:417:LEU:CD1	1:A:480:LEU:CD2	2.99	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%)	34	18
All	All	980/1010 (97%)	950 (97%)	28 (3%)	2 (0%)	47	30

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%)	8	1
1	B	394/402 (98%)	363 (92%)	31 (8%)	12	2
All	All	787/804 (98%)	719 (91%)	68 (9%)	11	2

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	1.16	80 (16%)  	13, 26, 52, 68	9 (1%)
1	B	485/505 (96%)	0.94	57 (11%)  	12, 23, 46, 66	2 (0%)
All	All	966/1010 (95%)	1.05	137 (14%)  	12, 25, 49, 68	11 (1%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	THR	13.3
1	B	4	THR	13.0
1	A	257	LYS	11.9
1	B	3	ALA	11.1
1	B	51	GLN	11.0
1	A	419	SER	11.0
1	A	254	GLY	10.9
1	A	421	THR	10.1
1	A	253	GLU	9.6
1	A	427	LEU	9.4
1	B	118	GLU	8.7
1	B	119	ALA	8.7
1	B	257	LYS	8.6
1	A	418	THR	8.5
1	A	256	LYS	8.3
1	B	50	ALA	7.9
1	A	260	LYS	7.5
1	B	117	VAL	7.5
1	A	258	LEU	7.2
1	A	442	LEU	7.1
1	B	5	GLU	7.1
1	A	422	ASP	6.9
1	A	439	GLY	6.9
1	A	259	SER	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	52	ARG	6.9
1	B	1	MET	6.0
1	A	423	TRP	5.9
1	A	402	LEU	5.8
1	A	426	PRO	5.6
1	B	251	LEU	5.6
1	B	2	THR	5.6
1	A	403	GLY	5.3
1	B	116	GLU	5.0
1	B	255	THR	5.0
1	A	440	LEU	4.9
1	A	424	THR	4.8
1	A	5	GLU	4.7
1	B	403	GLY	4.7
1	B	402	LEU	4.7
1	B	124	ALA	4.6
1	A	261	ARG	4.5
1	A	268[A]	PHE	4.4
1	A	404	PRO	4.4
1	A	431	ALA	4.3
1	A	420	VAL	4.3
1	A	447	ALA	4.2
1	B	254	GLY	4.0
1	A	417	LEU	4.0
1	A	415	ALA	3.9
1	B	268	PHE	3.9
1	B	6	THR	3.8
1	A	398	ALA	3.8
1	A	6	THR	3.8
1	B	447	ALA	3.8
1	A	436	LEU	3.8
1	A	428	ILE	3.7
1	A	307	PHE	3.7
1	A	425	ALA	3.7
1	A	450	PRO	3.7
1	A	240	ARG	3.7
1	A	396	LYS	3.6
1	A	438	GLU	3.5
1	A	196	TYR	3.4
1	A	399	ALA	3.4
1	A	264	GLN	3.4
1	A	429	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	253	GLU	3.4
1	B	162	ASP	3.3
1	B	446	LYS	3.3
1	A	263	PRO	3.3
1	A	262	ASP	3.2
1	B	53	ASP	3.2
1	B	121	HIS	3.2
1	B	54	SER	3.2
1	A	445	ARG	3.1
1	A	406	GLY	3.1
1	A	454	ALA	3.1
1	B	404	PRO	3.0
1	A	252	GLY	3.0
1	B	49	ASP	3.0
1	B	256	LYS	2.9
1	B	240	ARG	2.9
1	A	437	ILE	2.9
1	A	16	THR	2.9
1	B	261	ARG	2.9
1	A	446	LYS	2.9
1	A	444	PRO	2.9
1	B	398	ALA	2.8
1	A	271	ARG	2.8
1	B	409	VAL	2.8
1	B	250	VAL	2.8
1	A	410	LEU	2.7
1	A	448	PHE	2.7
1	A	483	ALA	2.6
1	B	454	ALA	2.6
1	A	465	PHE	2.6
1	A	52	ARG	2.6
1	B	122	VAL	2.6
1	B	48	THR	2.5
1	A	434	ASP	2.5
1	A	413	ALA	2.5
1	A	464	LEU	2.5
1	A	484[A]	ARG	2.5
1	B	258	LEU	2.5
1	A	29	PHE	2.5
1	A	162	ASP	2.5
1	B	322	LYS	2.4
1	A	451	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	414	LEU	2.4
1	B	259	SER	2.4
1	B	405	ASP	2.4
1	B	123	ALA	2.4
1	A	400	LYS	2.3
1	B	480	LEU	2.3
1	A	407	ALA	2.3
1	A	433	LYS	2.3
1	B	226	LEU	2.3
1	A	412	ALA	2.3
1	A	441	ALA	2.3
1	B	113	THR	2.3
1	B	337	VAL	2.2
1	A	340	PHE	2.2
1	B	206	LEU	2.2
1	A	239	GLU	2.1
1	B	16	THR	2.1
1	B	316	PRO	2.1
1	A	394	ASP	2.1
1	B	445	ARG	2.1
1	A	281[A]	LEU	2.1
1	B	165	LEU	2.1
1	A	468	LEU	2.0
1	B	484[A]	ARG	2.0
1	B	434	ASP	2.0
1	B	190	ALA	2.0
1	B	129	LYS	2.0
1	A	267	LEU	2.0
1	A	301	ASP	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.