Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:57 AM GMT

PDB ID	:	2YYA
Title	:	Crystal structure of GAR synthetase from Aquifex aeolicus
Authors	:	Baba, S.; Kanagawa, M.; Kuramitsu, S.; Yokoyama, S.; Kawai, G.; Sampei, G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-04-27
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

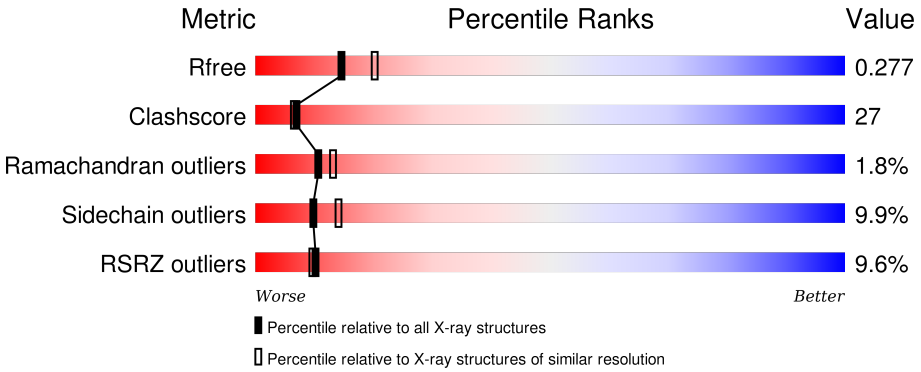
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	424	8% 47% 38% 12%
1	B	424	11% 47% 38% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6553 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 Phosphoribosylamine--glycine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3236	2069	548	608	11			
1	B	423	Total	C	N	O	S	0	0	0
			3228	2065	548	604	11			

- Molecule 2 is water.

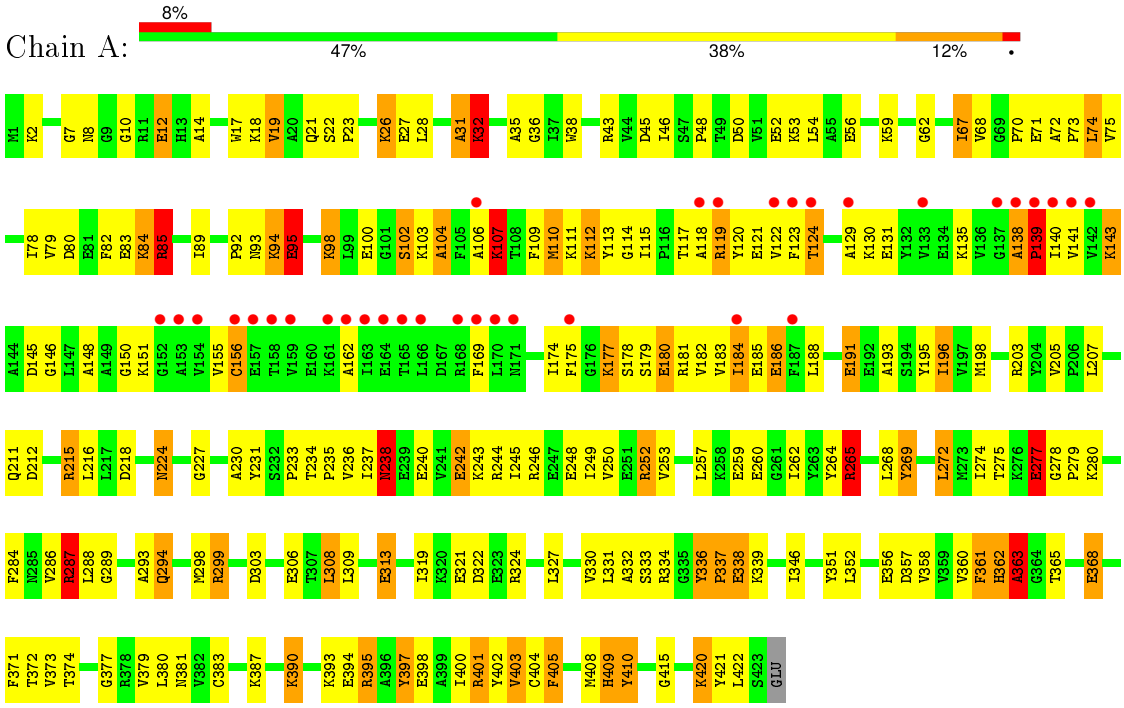
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	51	Total	O	0	0
			51	51		

3 Residue-property plots (i)

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

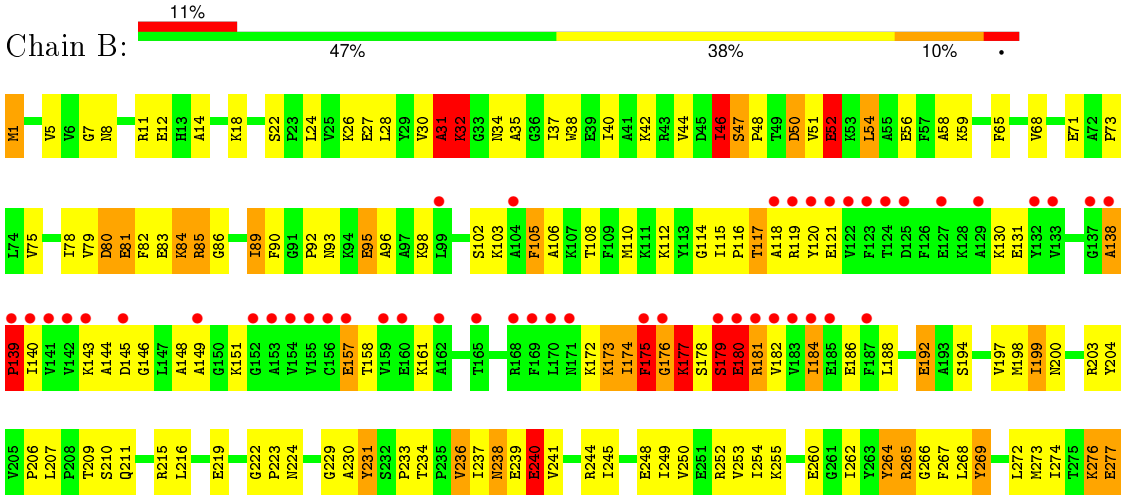
- Molecule 1: Phosphoribosylamine--glycine ligase

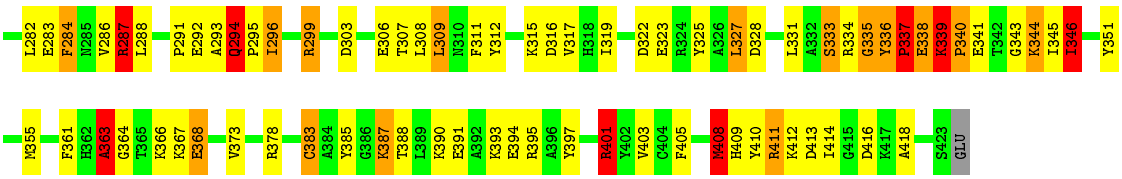
Chain A:



- Molecule 1: Phosphoribosylamine--glycine ligase

Chain B:




L282
E283
F284
N285
V286
R287
L288
P291
E292
A293
Q294
P295
I296
R299
D303
E306
T307
L308
L309
N310
F311
Y312
K315
D316
V317
H318
I319
D322
E323
R324
Y325
A326
L327
D328
L331
A332
S333
R334
G335
Y336
P337
E338
K339
P340
E341
T342
G343
K344
I345
I346
Y351
M355
F361
H362
A363
G364
T365
K366
K367
E368
V373
R378
C383
A384
Y385
G386
K387
T388
L389
K390
E391
A392
K393
E394
R395
A396
Y397
R401
Y402
V403
C404
F405
M408
H409
Y410
R411
K412
D413
I414
G415
D416
K417
A418
S423
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.26Å 45.15Å 103.48Å 90.00° 103.87° 90.00°	Depositor
Resolution (Å)	49.55 – 2.40 49.55 – 2.39	Depositor EDS
% Data completeness (in resolution range)	92.9 (49.55-2.40) 96.2 (49.55-2.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.249 0.228 , 0.277	Depositor DCC
R_{free} test set	1688 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	1.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 33955 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6553	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.78	35/3297 (1.1%)	1.72	76/4447 (1.7%)
1	B	1.74	36/3289 (1.1%)	1.68	64/4436 (1.4%)
All	All	1.76	71/6586 (1.1%)	1.70	140/8883 (1.6%)

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	5
1	B	0	11
All	All	0	16

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	PHE	C-N	6.58	1.44	1.33
1	B	283	GLU	CD-OE1	5.95	1.32	1.25
1	A	321	GLU	CD-OE2	5.95	1.32	1.25
1	B	401	ARG	CG-CD	5.92	1.66	1.51
1	A	401	ARG	C-O	5.88	1.34	1.23
1	A	336	TYR	CD1-CE1	5.87	1.48	1.39
1	B	240	GLU	CB-CG	5.86	1.63	1.52
1	A	405	PHE	CG-CD1	5.85	1.47	1.38
1	A	95	GLU	CB-CG	5.84	1.63	1.52
1	A	398	GLU	CG-CD	5.83	1.60	1.51
1	B	391	GLU	CD-OE2	5.83	1.32	1.25
1	B	56	GLU	CD-OE2	5.76	1.31	1.25
1	A	373	VAL	CB-CG2	-5.72	1.40	1.52
1	A	94	LYS	CD-CE	5.71	1.65	1.51
1	A	2	LYS	C-O	-5.66	1.12	1.23
1	B	37	ILE	C-O	5.62	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	GLU	CD-OE2	5.62	1.31	1.25
1	A	264	TYR	CG-CD2	5.59	1.46	1.39
1	A	403	VAL	CB-CG1	-5.58	1.41	1.52
1	A	250	VAL	CB-CG1	5.55	1.64	1.52
1	A	313	GLU	CB-CG	-5.55	1.41	1.52
1	A	277	GLU	CD-OE1	5.54	1.31	1.25
1	B	42	LYS	CD-CE	5.53	1.65	1.51
1	B	192	GLU	CG-CD	5.50	1.60	1.51
1	B	231	TYR	CD2-CE2	-5.49	1.31	1.39
1	A	332	ALA	C-O	5.47	1.33	1.23
1	B	294	GLN	CB-CG	5.46	1.67	1.52
1	B	351	TYR	CG-CD2	5.44	1.46	1.39
1	B	410	TYR	CG-CD2	5.43	1.46	1.39
1	B	105	PHE	CB-CG	-5.41	1.42	1.51
1	A	62	GLY	C-O	5.41	1.32	1.23
1	A	68	VAL	CB-CG1	5.40	1.64	1.52
1	A	242	GLU	CB-CG	-5.39	1.42	1.52
1	B	269	TYR	CD1-CE1	-5.38	1.31	1.39
1	B	403	VAL	CA-CB	5.35	1.66	1.54
1	B	65	PHE	CE2-CZ	5.33	1.47	1.37
1	B	240	GLU	CD-OE1	5.33	1.31	1.25
1	B	385	TYR	CD2-CE2	5.33	1.47	1.39
1	A	363	ALA	C-O	5.31	1.33	1.23
1	A	193	ALA	CA-CB	-5.31	1.41	1.52
1	A	17	TRP	CE3-CZ3	5.27	1.47	1.38
1	A	98	LYS	CE-NZ	5.26	1.62	1.49
1	B	363	ALA	C-O	5.24	1.33	1.23
1	B	323	GLU	CD-OE2	5.24	1.31	1.25
1	A	119	ARG	CG-CD	5.21	1.65	1.51
1	B	299	ARG	CA-CB	5.21	1.65	1.53
1	A	409	HIS	C-O	-5.20	1.13	1.23
1	B	239	GLU	CD-OE2	5.19	1.31	1.25
1	A	338	GLU	CD-OE1	5.17	1.31	1.25
1	B	327	LEU	CG-CD2	5.17	1.71	1.51
1	B	131	GLU	C-O	5.16	1.33	1.23
1	A	43	ARG	N-CA	-5.16	1.36	1.46
1	A	224	ASN	N-CA	-5.16	1.36	1.46
1	B	383	CYS	CB-SG	-5.15	1.73	1.81
1	A	358	VAL	CB-CG2	5.14	1.63	1.52
1	A	227	GLY	N-CA	5.14	1.53	1.46
1	A	390	LYS	CD-CE	5.14	1.64	1.51
1	B	157	GLU	C-O	5.13	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	ASP	CG-OD1	-5.13	1.13	1.25
1	A	19	VAL	CA-CB	5.12	1.65	1.54
1	A	191	GLU	CD-OE1	5.12	1.31	1.25
1	A	337	PRO	C-N	5.11	1.45	1.34
1	B	343	GLY	C-O	-5.10	1.15	1.23
1	B	284	PHE	CA-C	-5.09	1.39	1.52
1	A	12	GLU	CD-OE1	-5.08	1.20	1.25
1	B	52	GLU	CD-OE1	5.06	1.31	1.25
1	B	267	PHE	CE1-CZ	5.06	1.47	1.37
1	B	367	LYS	CB-CG	5.05	1.66	1.52
1	B	80	ASP	CB-CG	5.03	1.62	1.51
1	B	411	ARG	C-O	5.03	1.32	1.23
1	B	264	TYR	CD1-CE1	5.01	1.46	1.39

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	ARG	NE-CZ-NH1	14.95	127.77	120.30
1	A	287	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	B	287	ARG	NE-CZ-NH2	-13.66	113.47	120.30
1	A	395	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	B	139	PRO	O-C-N	-11.88	103.69	122.70
1	A	174	ILE	O-C-N	11.84	141.65	122.70
1	A	395	ARG	NE-CZ-NH1	10.53	125.57	120.30
1	B	175	PHE	O-C-N	10.38	140.84	123.20
1	B	309	LEU	CB-CG-CD1	-9.88	94.20	111.00
1	A	265	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	356	GLU	O-C-N	9.72	138.26	122.70
1	A	107	LYS	O-C-N	-9.63	107.28	122.70
1	B	157	GLU	O-C-N	-9.50	107.49	122.70
1	B	341	GLU	O-C-N	9.49	137.88	122.70
1	B	177	LYS	O-C-N	-9.41	107.65	122.70
1	B	378	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	B	139	PRO	CA-C-N	9.21	137.46	117.20
1	B	175	PHE	CA-C-N	-9.00	98.19	116.20
1	B	157	GLU	CA-C-N	8.72	136.39	117.20
1	A	334	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	397	TYR	CZ-CE2-CD2	8.50	127.45	119.80
1	B	408	MET	CG-SD-CE	-8.48	86.63	100.20
1	A	196	ILE	CG1-CB-CG2	-8.48	92.75	111.40
1	A	85	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	246	ARG	NE-CZ-NH1	-8.40	116.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	395	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	B	85	ARG	NE-CZ-NH1	-8.28	116.16	120.30
1	B	31	ALA	CA-C-N	-8.21	99.14	117.20
1	A	287	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	361	PHE	O-C-N	8.18	135.78	122.70
1	A	31	ALA	C-N-CA	8.12	141.99	121.70
1	B	339	LYS	C-N-CD	-8.06	102.87	120.60
1	A	174	ILE	CA-C-N	-7.95	99.71	117.20
1	A	84	LYS	CD-CE-NZ	7.94	129.97	111.70
1	B	172	LYS	C-N-CA	7.93	141.52	121.70
1	B	26	LYS	CD-CE-NZ	7.88	129.82	111.70
1	A	410	TYR	CZ-CE2-CD2	7.84	126.86	119.80
1	A	357	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	238	ASN	CA-C-O	7.75	136.38	120.10
1	A	356	GLU	CA-C-N	-7.74	100.17	117.20
1	A	299	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	B	299	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	A	84	LYS	O-C-N	7.59	134.85	122.70
1	B	32	LYS	CB-CA-C	7.57	125.54	110.40
1	A	324	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	A	265	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	B	85	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	A	357	ASP	CB-CG-OD1	7.12	124.71	118.30
1	B	50	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	A	309	LEU	CA-CB-CG	-6.99	99.22	115.30
1	B	346	ILE	CG1-CB-CG2	-6.88	96.26	111.40
1	A	237	ILE	CA-C-N	-6.83	102.17	117.20
1	A	410	TYR	CG-CD2-CE2	-6.80	115.86	121.30
1	B	180	GLU	O-C-N	6.72	133.45	122.70
1	A	309	LEU	CB-CG-CD1	-6.66	99.68	111.00
1	A	139	PRO	C-N-CA	6.65	138.32	121.70
1	B	1	MET	CG-SD-CE	-6.58	89.67	100.20
1	A	50	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	B	219	GLU	C-N-CA	6.55	138.07	121.70
1	A	237	ILE	O-C-N	6.49	133.09	122.70
1	A	238	ASN	CA-C-N	-6.42	103.08	117.20
1	A	174	ILE	C-N-CA	-6.37	105.78	121.70
1	B	294	GLN	O-C-N	6.32	133.11	121.10
1	A	422	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	107	LYS	CA-C-N	6.24	130.92	117.20
1	B	31	ALA	O-C-N	6.20	132.62	122.70
1	A	84	LYS	CA-C-N	-6.16	103.64	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	ALA	C-N-CA	6.15	137.07	121.70
1	A	395	ARG	CD-NE-CZ	6.12	132.18	123.60
1	B	401	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	287	ARG	CB-CG-CD	6.08	127.41	111.60
1	B	199	ILE	CG1-CB-CG2	-6.06	98.07	111.40
1	B	395	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	156	CYS	C-N-CA	6.01	136.73	121.70
1	A	246	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	A	351	TYR	CZ-CE2-CD2	-5.99	114.41	119.80
1	A	107	LYS	C-N-CA	5.98	136.65	121.70
1	B	355	MET	CA-C-N	-5.96	104.09	117.20
1	B	355	MET	O-C-N	5.94	132.21	122.70
1	A	401	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	308	LEU	CB-CG-CD1	-5.92	100.94	111.00
1	B	368	GLU	CB-CA-C	5.91	122.22	110.40
1	A	218	ASP	C-N-CA	5.90	136.45	121.70
1	A	244	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	A	31	ALA	N-CA-CB	5.83	118.26	110.10
1	A	2	LYS	CD-CE-NZ	-5.79	98.38	111.70
1	B	229	GLY	N-CA-C	-5.79	98.63	113.10
1	B	344	LYS	CD-CE-NZ	-5.79	98.39	111.70
1	B	336	TYR	O-C-N	5.76	132.05	121.10
1	B	177	LYS	CA-C-N	5.76	129.87	117.20
1	B	336	TYR	C-N-CD	-5.75	107.96	120.60
1	B	346	ILE	N-CA-C	-5.75	95.49	111.00
1	A	361	PHE	CA-C-N	-5.72	104.62	117.20
1	A	224	ASN	N-CA-C	-5.70	95.61	111.00
1	B	31	ALA	C-N-CA	5.69	135.93	121.70
1	A	401	ARG	CD-NE-CZ	5.64	131.49	123.60
1	B	174	ILE	O-C-N	-5.62	113.71	122.70
1	A	212	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	B	31	ALA	N-CA-CB	5.61	117.96	110.10
1	A	357	ASP	C-N-CA	5.59	135.68	121.70
1	B	337	PRO	C-N-CA	5.54	135.55	121.70
1	A	143	LYS	C-N-CA	-5.52	107.89	121.70
1	A	334	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	335	GLY	O-C-N	-5.51	113.88	122.70
1	A	308	LEU	CA-CB-CG	-5.50	102.64	115.30
1	A	306	GLU	OE1-CD-OE2	5.49	129.88	123.30
1	A	243	LYS	CB-CG-CD	5.48	125.85	111.60
1	A	67	ILE	CA-CB-CG1	5.47	121.40	111.00
1	A	32	LYS	N-CA-C	-5.47	96.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	50	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	110	MET	O-C-N	-5.44	113.99	122.70
1	A	106	ALA	O-C-N	5.41	131.36	122.70
1	B	11	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	A	26	LYS	CD-CE-NZ	5.39	124.09	111.70
1	A	387	LYS	CD-CE-NZ	5.35	124.00	111.70
1	B	181	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	299	ARG	CG-CD-NE	-5.32	100.64	111.80
1	A	32	LYS	CB-CA-C	5.30	120.99	110.40
1	A	397	TYR	CE1-CZ-CE2	-5.30	111.33	119.80
1	A	287	ARG	CB-CG-CD	5.29	125.35	111.60
1	B	315	LYS	CA-C-N	-5.26	105.63	117.20
1	A	143	LYS	O-C-N	5.24	131.08	122.70
1	B	222	GLY	N-CA-C	-5.22	100.05	113.10
1	B	363	ALA	C-N-CA	5.21	133.25	122.30
1	B	299	ARG	NH1-CZ-NH2	5.20	125.11	119.40
1	B	32	LYS	CD-CE-NZ	5.17	123.59	111.70
1	A	357	ASP	O-C-N	-5.17	114.44	122.70
1	A	272	LEU	CB-CG-CD2	-5.14	102.25	111.00
1	B	84	LYS	CD-CE-NZ	5.14	123.53	111.70
1	A	74	LEU	CA-CB-CG	-5.14	103.48	115.30
1	B	413	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	47	SER	C-N-CD	5.11	139.13	128.40
1	B	236	VAL	CB-CA-C	-5.11	101.69	111.40
1	B	385	TYR	CD1-CE1-CZ	5.10	124.39	119.80
1	B	32	LYS	N-CA-C	-5.09	97.24	111.00
1	A	362	HIS	C-N-CA	5.06	134.35	121.70
1	A	129	ALA	C-N-CA	5.05	134.34	121.70
1	B	46	ILE	CB-CA-C	-5.04	101.51	111.60
1	A	72	ALA	C-N-CD	5.04	138.98	128.40
1	A	368	GLU	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ALA	Peptide
1	A	139	PRO	Peptide
1	A	238	ASN	Peptide
1	A	31	ALA	Peptide
1	A	371	PHE	Peptide
1	B	138	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	B	139	PRO	Peptide
1	B	173	LYS	Peptide
1	B	174	ILE	Peptide
1	B	179	SER	Peptide
1	B	31	ALA	Peptide
1	B	337	PRO	Peptide
1	B	338	GLU	Peptide
1	B	339	LYS	Peptide
1	B	340	PRO	Peptide
1	B	50	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3236	0	3194	173	0
1	B	3228	0	3180	171	0
2	A	38	0	0	4	0
2	B	51	0	0	1	0
All	All	6553	0	6374	342	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (342) 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:337:PRO:HD2	1:B:338:GLU:CD	1.49	1.32
1:B:337:PRO:HD2	1:B:338:GLU:OE2	1.38	1.18
1:A:103:LYS:HD2	1:A:143:LYS:HE2	1.27	1.11
1:B:265:ARG:HG2	1:B:265:ARG:HH11	0.94	1.09
1:A:103:LYS:CD	1:A:143:LYS:HE2	1.85	1.05
1:A:46:ILE:HD13	1:A:53:LYS:HG2	1.51	0.93
1:B:194:SER:HB3	1:B:269:TYR:HE1	1.30	0.93
1:A:71:GLU:HB3	1:A:287:ARG:HD2	1.50	0.92
1:B:265:ARG:NH1	1:B:265:ARG:HG2	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LEU:HD23	1:B:319:ILE:CD1	2.00	0.91
1:B:103:LYS:CD	1:B:143:LYS:HE2	2.01	0.91
1:B:337:PRO:CD	1:B:338:GLU:OE2	2.19	0.90
1:B:265:ARG:CG	1:B:265:ARG:HH11	1.84	0.88
1:A:184:ILE:HD12	1:A:184:ILE:N	1.90	0.86
1:A:215:ARG:NH1	1:A:224:ASN:HD22	1.73	0.86
1:A:124:THR:HG21	1:A:181:ARG:NH1	1.90	0.86
1:B:90:PHE:CE2	1:B:266:GLY:HA2	2.10	0.86
1:B:103:LYS:HD3	1:B:143:LYS:HE2	1.57	0.85
1:B:110:MET:HG2	1:B:115:ILE:HB	1.60	0.83
1:B:116:PRO:HG2	1:B:249:ILE:HD11	1.58	0.83
1:B:177:LYS:HE2	1:B:180:GLU:OE2	1.78	0.82
1:A:59:LYS:HE2	1:A:85:ARG:HH21	1.44	0.82
1:A:207:LEU:HD23	1:A:319:ILE:HD12	1.60	0.82
1:A:140:ILE:HG23	1:A:141:VAL:H	1.45	0.81
1:B:138:ALA:HB1	1:B:157:GLU:O	1.80	0.81
1:B:120:TYR:O	1:B:121:GLU:HG2	1.80	0.81
1:A:103:LYS:HE3	1:A:143:LYS:HE3	1.63	0.80
1:B:294:GLN:HE21	1:B:294:GLN:N	1.79	0.80
1:B:79:VAL:HG22	1:B:89:ILE:HD12	1.63	0.80
1:B:210:SER:HB3	1:B:296:ILE:HD11	1.63	0.78
1:B:51:VAL:HG23	1:B:81:GLU:OE2	1.84	0.78
1:A:115:ILE:O	1:A:117:THR:HG22	1.86	0.76
1:A:140:ILE:HG23	1:A:141:VAL:N	2.02	0.75
1:B:336:TYR:CD1	1:B:337:PRO:HA	2.20	0.75
1:B:194:SER:HB3	1:B:269:TYR:CE1	2.18	0.75
1:A:260:GLU:HB2	1:A:262:ILE:HG13	1.67	0.75
1:B:337:PRO:CD	1:B:338:GLU:CD	2.44	0.75
1:B:176:GLY:O	1:B:180:GLU:HG2	1.87	0.74
1:A:207:LEU:HD23	1:A:319:ILE:CD1	2.18	0.74
1:B:390:LYS:HE2	1:B:394:GLU:OE2	1.88	0.73
1:A:216:LEU:O	1:A:409:HIS:HE1	1.71	0.73
1:B:236:VAL:HG12	1:B:274:ILE:HG13	1.70	0.72
1:B:71:GLU:HB3	1:B:287:ARG:HD2	1.71	0.72
1:A:403:VAL:O	1:A:404:CYS:HB2	1.89	0.72
1:B:405:PHE:O	1:B:408:MET:HG2	1.90	0.72
1:A:215:ARG:HH12	1:A:224:ASN:HD22	1.38	0.71
1:A:207:LEU:CD2	1:A:319:ILE:CD1	2.69	0.71
1:A:95:GLU:HA	1:A:95:GLU:OE1	1.90	0.71
1:B:238:ASN:C	1:B:238:ASN:HD22	1.94	0.70
1:A:124:THR:HG22	1:A:181:ARG:HG3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LYS:O	1:B:397:TYR:HD2	1.75	0.69
1:A:215:ARG:HH12	1:A:224:ASN:HB2	1.56	0.69
1:A:265:ARG:HG2	1:A:265:ARG:HH11	1.57	0.69
1:A:177:LYS:HE2	1:A:180:GLU:OE2	1.92	0.68
1:A:95:GLU:OE1	1:A:98:LYS:HE2	1.92	0.68
1:A:112:LYS:O	1:A:112:LYS:HG2	1.95	0.67
1:A:124:THR:CG2	1:A:181:ARG:NH1	2.58	0.67
1:B:114:GLY:O	1:B:252:ARG:NH1	2.27	0.67
1:A:245:ILE:HA	1:A:249:ILE:HD13	1.75	0.67
1:B:116:PRO:HG2	1:B:249:ILE:CD1	2.25	0.67
1:A:103:LYS:CD	1:A:143:LYS:CE	2.70	0.66
1:B:276:LYS:HG3	1:B:277:GLU:OE2	1.95	0.66
1:A:14:ALA:HA	1:A:361:PHE:CE1	2.31	0.66
1:A:103:LYS:HD2	1:A:143:LYS:CE	2.15	0.66
1:B:294:GLN:NE2	1:B:294:GLN:H	1.95	0.65
1:B:68:VAL:HG23	1:B:89:ILE:HD11	1.79	0.65
1:A:277:GLU:H	1:A:277:GLU:CD	2.00	0.65
1:B:175:PHE:CD1	1:B:175:PHE:N	2.59	0.65
1:A:114:GLY:O	1:A:252:ARG:NH1	2.29	0.65
1:B:175:PHE:H	1:B:175:PHE:HD1	1.42	0.65
1:B:199:ILE:CD1	1:B:254:ILE:HD11	2.26	0.64
1:B:59:LYS:HD3	1:B:85:ARG:HB3	1.78	0.64
1:A:146:GLY:HA3	1:A:178:SER:HB2	1.79	0.64
1:A:119:ARG:O	1:A:185:GLU:HA	1.96	0.64
1:A:111:LYS:O	1:A:113:TYR:N	2.30	0.64
1:A:8:ASN:OD1	1:A:32:LYS:HB2	1.97	0.64
1:B:210:SER:HB3	1:B:296:ILE:CD1	2.27	0.64
1:B:8:ASN:OD1	1:B:32:LYS:HB2	1.98	0.64
1:A:103:LYS:HE3	1:A:143:LYS:CE	2.27	0.63
1:A:207:LEU:CD2	1:A:319:ILE:HD12	2.27	0.63
1:B:393:LYS:NZ	1:B:416:ASP:OD1	2.31	0.63
1:A:195:TYR:C	1:A:196:ILE:HD12	2.19	0.63
1:A:109:PHE:O	1:A:113:TYR:HB2	1.98	0.63
1:A:115:ILE:HD13	1:A:253:VAL:HG23	1.80	0.63
1:B:294:GLN:NE2	1:B:294:GLN:N	2.46	0.63
1:A:191:GLU:HG3	1:A:421:TYR:OH	1.99	0.63
1:A:140:ILE:CG2	1:A:141:VAL:N	2.61	0.63
1:A:184:ILE:N	1:A:184:ILE:CD1	2.59	0.62
1:A:333:SER:HB2	2:A:428:HOH:O	2.00	0.62
1:A:215:ARG:NH1	1:A:224:ASN:HB2	2.15	0.61
1:B:116:PRO:HD2	1:B:249:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLY:O	1:B:180:GLU:CG	2.49	0.61
1:B:199:ILE:HD12	1:B:254:ILE:HD11	1.82	0.61
1:A:84:LYS:O	1:B:86:GLY:HA2	2.00	0.61
1:A:7:GLY:HA3	1:A:12:GLU:HG2	1.84	0.60
1:A:139:PRO:HB2	1:A:140:ILE:HG13	1.84	0.60
1:B:51:VAL:CG2	1:B:81:GLU:OE2	2.49	0.60
1:A:183:VAL:C	1:A:184:ILE:HD12	2.23	0.59
1:B:95:GLU:OE2	1:B:262:ILE:HD12	2.02	0.59
1:A:288:LEU:HB3	1:A:293:ALA:HB2	1.82	0.59
1:B:95:GLU:OE1	1:B:98:LYS:HE2	2.02	0.59
1:B:117:THR:HG23	1:B:118:ALA:O	2.03	0.59
1:B:92:PRO:HG3	1:B:286:VAL:HB	1.83	0.59
1:A:115:ILE:CD1	1:A:253:VAL:HG23	2.32	0.59
1:A:111:LYS:C	1:A:113:TYR:H	2.06	0.59
1:B:216:LEU:O	1:B:409:HIS:HE1	1.85	0.59
1:A:156:CYS:SG	1:A:162:ALA:HA	2.43	0.59
1:A:330:VAL:HG22	1:A:381:ASN:OD1	2.02	0.59
1:A:120:TYR:CE1	1:A:122:VAL:HG23	2.37	0.58
1:A:253:VAL:HG21	1:A:284:PHE:CZ	2.38	0.58
1:A:113:TYR:OH	1:A:259:GLU:HB2	2.03	0.58
1:A:131:GLU:O	1:A:135:LYS:N	2.36	0.58
1:A:46:ILE:CD1	1:A:53:LYS:HG2	2.32	0.57
1:A:59:LYS:HD3	1:A:85:ARG:HE	1.67	0.57
1:B:277:GLU:N	1:B:277:GLU:CD	2.56	0.57
1:A:238:ASN:O	1:A:242:GLU:HB3	2.03	0.57
1:A:36:GLY:HA3	1:A:362:HIS:CG	2.40	0.57
1:A:119:ARG:HB2	1:A:186:GLU:HG2	1.87	0.57
1:B:288:LEU:HB3	1:B:293:ALA:HB2	1.86	0.57
1:A:224:ASN:ND2	2:A:449:HOH:O	2.38	0.56
1:B:337:PRO:HD2	1:B:338:GLU:OE1	2.03	0.56
1:A:141:VAL:HG22	1:A:155:VAL:HA	1.87	0.56
1:A:393:LYS:O	1:A:397:TYR:HD2	1.89	0.56
1:B:22:SER:HB2	1:B:303:ASP:OD1	2.05	0.56
1:B:210:SER:HA	1:B:231:TYR:O	2.06	0.56
1:A:294:GLN:N	1:A:294:GLN:HE21	2.03	0.56
1:A:83:GLU:HB3	1:B:84:LYS:HA	1.88	0.56
1:B:79:VAL:HB	1:B:93:ASN:HA	1.88	0.56
1:B:309:LEU:O	1:B:312:TYR:HB3	2.05	0.56
1:A:123:PHE:CD2	1:A:184:ILE:HD11	2.41	0.56
1:B:31:ALA:O	1:B:48:PRO:HG3	2.06	0.55
1:B:103:LYS:CE	1:B:143:LYS:HE2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:HE2	1:A:117:THR:OG1	2.07	0.55
1:B:89:ILE:HD13	1:B:90:PHE:C	2.27	0.55
1:A:207:LEU:CD2	1:A:319:ILE:HD11	2.37	0.55
1:A:35:ALA:HA	1:A:38:TRP:CE3	2.42	0.55
1:A:403:VAL:O	1:A:404:CYS:CB	2.49	0.55
1:A:110:MET:HB3	1:A:117:THR:HG21	1.89	0.54
1:A:73:PRO:O	1:A:78:ILE:HG22	2.07	0.54
1:A:123:PHE:CD2	1:A:184:ILE:CD1	2.90	0.54
1:A:233:PRO:HB3	1:A:299:ARG:NH2	2.23	0.54
1:A:175:PHE:HB2	1:A:179:SER:HB3	1.88	0.54
1:B:215:ARG:HH11	1:B:224:ASN:HD22	1.54	0.54
1:B:7:GLY:HA3	1:B:12:GLU:HG2	1.90	0.54
1:B:199:ILE:HD13	1:B:204:TYR:HB2	1.89	0.54
1:B:179:SER:C	1:B:181:ARG:H	2.10	0.54
1:B:238:ASN:HD21	1:B:240:GLU:HG3	1.73	0.54
1:B:34:ASN:ND2	1:B:363:ALA:O	2.41	0.54
1:B:138:ALA:CB	1:B:157:GLU:O	2.53	0.53
1:A:95:GLU:OE1	1:A:95:GLU:CA	2.56	0.53
1:B:245:ILE:HD13	1:B:272:LEU:HD11	1.91	0.53
1:B:215:ARG:NH1	1:B:224:ASN:HD22	2.07	0.53
1:A:420:LYS:HG2	2:A:439:HOH:O	2.08	0.53
1:A:26:LYS:O	1:A:27:GLU:HG3	2.08	0.53
1:A:346:ILE:HD12	1:A:372:THR:HG22	1.91	0.52
1:B:335:GLY:O	1:B:338:GLU:OE1	2.26	0.52
1:B:387:LYS:HG2	1:B:388:THR:HG23	1.91	0.52
1:A:140:ILE:HG21	1:A:184:ILE:HG22	1.91	0.52
1:A:215:ARG:HH11	1:A:215:ARG:HG2	1.74	0.52
1:B:345:ILE:HG22	1:B:346:ILE:N	2.23	0.52
1:B:238:ASN:ND2	1:B:241:VAL:H	2.08	0.52
1:A:148:ALA:O	1:A:151:LYS:HB2	2.10	0.52
1:A:115:ILE:HG12	1:A:252:ARG:HB2	1.91	0.51
1:A:299:ARG:NH1	1:A:322:ASP:O	2.40	0.51
1:B:144:ALA:CB	1:B:179:SER:OG	2.58	0.51
1:A:103:LYS:CE	1:A:143:LYS:CE	2.89	0.51
1:A:110:MET:HG2	1:A:115:ILE:HB	1.91	0.51
1:A:249:ILE:HD12	1:A:249:ILE:N	2.26	0.51
1:B:197:VAL:HG12	1:B:206:PRO:HB3	1.91	0.51
1:B:83:GLU:O	1:B:86:GLY:N	2.42	0.51
1:A:120:TYR:HE1	1:A:122:VAL:HG23	1.75	0.51
1:B:291:PRO:O	1:B:295:PRO:HD2	2.10	0.51
1:A:277:GLU:N	1:A:277:GLU:CD	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:VAL:HG12	1:B:75:VAL:O	2.10	0.51
1:B:277:GLU:H	1:B:277:GLU:CD	2.14	0.51
1:B:207:LEU:HD23	1:B:319:ILE:HD13	1.90	0.50
1:A:215:ARG:NH1	1:A:224:ASN:ND2	2.52	0.50
1:A:177:LYS:CE	1:A:180:GLU:OE2	2.58	0.50
1:A:182:VAL:HG23	1:A:184:ILE:HD11	1.93	0.50
1:B:260:GLU:HA	1:B:260:GLU:OE1	2.12	0.50
1:A:405:PHE:CE1	1:A:408:MET:HA	2.47	0.50
1:A:287:ARG:NH2	1:A:289:GLY:HA2	2.26	0.50
1:A:245:ILE:HD13	1:A:279:PRO:HB2	1.92	0.50
1:A:104:ALA:HB1	1:A:122:VAL:HG21	1.93	0.50
1:B:276:LYS:HG3	1:B:277:GLU:CD	2.32	0.50
1:A:118:ALA:HB2	1:A:188:LEU:HD11	1.94	0.50
1:B:207:LEU:HD23	1:B:319:ILE:HD12	1.92	0.49
1:A:56:GLU:HG2	1:A:85:ARG:CZ	2.41	0.49
1:B:345:ILE:CG2	1:B:346:ILE:N	2.74	0.49
1:A:102:SER:HA	1:A:145:ASP:O	2.11	0.49
1:B:46:ILE:O	1:B:47:SER:C	2.47	0.49
1:A:124:THR:HG21	1:A:181:ARG:HH12	1.74	0.49
1:A:327:LEU:O	1:A:383:CYS:HA	2.11	0.49
1:B:103:LYS:HE3	1:B:143:LYS:HE2	1.94	0.49
1:B:192:GLU:HA	1:B:272:LEU:O	2.12	0.49
1:B:148:ALA:CB	1:B:175:PHE:CD2	2.95	0.49
1:B:244:ARG:O	1:B:248:GLU:HG3	2.13	0.49
1:A:110:MET:SD	1:A:117:THR:HB	2.53	0.49
1:B:105:PHE:HD2	1:B:106:ALA:N	2.09	0.49
1:B:89:ILE:HD13	1:B:90:PHE:O	2.13	0.49
1:A:111:LYS:C	1:A:113:TYR:N	2.66	0.49
1:B:366:LYS:NZ	2:B:452:HOH:O	2.42	0.49
1:B:73:PRO:O	1:B:78:ILE:HG22	2.12	0.49
1:B:238:ASN:C	1:B:238:ASN:ND2	2.66	0.48
1:A:245:ILE:HD12	1:A:272:LEU:HD13	1.95	0.48
1:B:105:PHE:O	1:B:108:THR:HB	2.13	0.48
1:B:146:GLY:HA3	1:B:178:SER:HB3	1.95	0.48
1:B:115:ILE:HD13	1:B:253:VAL:HG23	1.96	0.48
1:B:90:PHE:CE2	1:B:266:GLY:CA	2.90	0.48
1:A:18:LYS:O	1:A:21:GLN:HB2	2.14	0.48
1:B:265:ARG:NH1	1:B:265:ARG:CG	2.49	0.48
1:A:82:PHE:HB2	1:A:89:ILE:HG21	1.95	0.48
1:A:248:GLU:HB2	1:A:249:ILE:HD12	1.96	0.48
1:A:333:SER:N	1:A:377:GLY:O	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:TYR:OH	1:B:418:ALA:HB2	2.14	0.47
1:B:408:MET:HE3	1:B:408:MET:HB3	1.21	0.47
1:B:144:ALA:HB1	1:B:179:SER:OG	2.14	0.47
1:B:268:LEU:HD11	1:B:284:PHE:CD1	2.49	0.47
1:A:80:ASP:OD2	1:A:94:LYS:HB2	2.15	0.47
1:A:48:PRO:HA	1:A:54:LEU:HD11	1.96	0.47
1:A:275:THR:HG21	1:A:280:LYS:HD2	1.97	0.47
1:A:95:GLU:OE1	1:A:98:LYS:CE	2.61	0.47
1:A:124:THR:CG2	1:A:181:ARG:HH11	2.27	0.47
1:B:299:ARG:NH1	1:B:322:ASP:O	2.45	0.47
1:A:257:LEU:HD23	1:A:262:ILE:HD12	1.96	0.47
1:A:362:HIS:ND1	1:A:365:THR:HG21	2.30	0.47
1:B:14:ALA:HA	1:B:361:PHE:CE1	2.50	0.47
1:B:241:VAL:O	1:B:245:ILE:HG13	2.14	0.47
1:B:105:PHE:CD2	1:B:106:ALA:N	2.83	0.47
1:A:92:PRO:HG3	1:A:286:VAL:HB	1.96	0.47
1:B:35:ALA:HA	1:B:38:TRP:CE3	2.50	0.46
1:B:68:VAL:CG2	1:B:89:ILE:HD11	2.42	0.46
1:B:207:LEU:HD23	1:B:319:ILE:HD11	1.92	0.46
1:B:393:LYS:HD2	1:B:414:ILE:O	2.15	0.46
1:A:336:TYR:CD1	1:A:337:PRO:HA	2.51	0.46
1:B:96:ALA:HB1	1:B:264:TYR:CD1	2.51	0.46
1:B:34:ASN:OD1	1:B:34:ASN:C	2.53	0.46
1:B:112:LYS:O	1:B:112:LYS:HG2	2.16	0.46
1:B:209:THR:HG21	1:B:237:ILE:HG21	1.97	0.46
1:A:32:LYS:HE2	1:A:45:ASP:HA	1.96	0.46
1:B:344:LYS:O	1:B:373:VAL:HA	2.16	0.46
1:B:307:THR:HG23	1:B:317:VAL:HB	1.97	0.46
1:B:327:LEU:O	1:B:383:CYS:HA	2.15	0.46
1:A:374:THR:HG22	1:A:379:VAL:HG11	1.97	0.46
1:A:245:ILE:HD13	1:A:279:PRO:CB	2.45	0.46
1:A:32:LYS:HE2	1:A:45:ASP:OD1	2.15	0.45
1:B:408:MET:HE2	1:B:408:MET:HB2	1.76	0.45
1:B:105:PHE:C	1:B:105:PHE:CD2	2.90	0.45
1:B:188:LEU:HD12	1:B:282:LEU:CD2	2.46	0.45
1:A:253:VAL:HG21	1:A:284:PHE:HZ	1.79	0.45
1:B:188:LEU:HB2	1:B:273:MET:HG2	1.99	0.45
1:B:234:THR:OG1	1:B:236:VAL:HG23	2.17	0.45
1:A:107:LYS:HD3	1:A:107:LYS:HA	1.70	0.45
1:B:44:VAL:HG12	1:B:46:ILE:HG12	1.99	0.45
1:B:250:VAL:O	1:B:253:VAL:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ILE:CD1	1:A:272:LEU:HD13	2.47	0.44
1:A:363:ALA:HB3	1:A:379:VAL:C	2.37	0.44
1:B:198:MET:O	1:B:204:TYR:HA	2.18	0.44
1:B:92:PRO:HB2	1:B:96:ALA:HB3	1.98	0.44
1:B:58:ALA:CB	1:B:82:PHE:CE2	3.00	0.44
1:B:333:SER:O	1:B:334:ARG:C	2.54	0.44
1:A:253:VAL:HG11	1:A:268:LEU:HD21	1.99	0.44
1:A:245:ILE:HD12	1:A:272:LEU:CD1	2.47	0.44
1:B:237:ILE:O	1:B:237:ILE:HG22	2.16	0.44
1:A:70:PRO:HB2	2:A:454:HOH:O	2.17	0.44
1:B:146:GLY:CA	1:B:178:SER:HB3	2.46	0.44
1:B:139:PRO:HB2	1:B:140:ILE:HD12	2.00	0.44
1:A:238:ASN:O	1:A:242:GLU:CB	2.65	0.44
1:B:89:ILE:C	1:B:89:ILE:HD13	2.38	0.44
1:B:236:VAL:CG1	1:B:274:ILE:HG13	2.43	0.44
1:B:119:ARG:NE	1:B:186:GLU:OE2	2.48	0.44
1:B:401:ARG:HE	1:B:401:ARG:HB3	1.47	0.44
1:A:275:THR:OG1	1:A:278:GLY:O	2.33	0.44
1:B:148:ALA:HB2	1:B:175:PHE:CD2	2.52	0.43
1:B:54:LEU:HA	1:B:54:LEU:HD23	1.81	0.43
1:A:393:LYS:O	1:A:397:TYR:CD2	2.69	0.43
1:B:387:LYS:HE3	1:B:387:LYS:HB3	1.87	0.43
1:A:360:VAL:CG1	1:A:380:LEU:HD22	2.48	0.43
1:A:28:LEU:HD12	1:A:28:LEU:HA	1.76	0.43
1:B:90:PHE:CD2	1:B:266:GLY:HA2	2.52	0.43
1:B:148:ALA:HB1	1:B:175:PHE:CD2	2.52	0.43
1:A:75:VAL:O	1:A:94:LYS:HG3	2.17	0.43
1:B:18:LYS:HD2	1:B:18:LYS:HA	1.81	0.43
1:A:80:ASP:O	1:A:84:LYS:HG3	2.19	0.43
1:A:215:ARG:HH12	1:A:224:ASN:ND2	2.10	0.43
1:A:352:LEU:HD11	1:A:402:TYR:HB2	2.00	0.43
1:A:121:GLU:O	1:A:184:ILE:HD13	2.19	0.43
1:B:52:GLU:HB2	1:B:85:ARG:HH22	1.82	0.43
1:A:196:ILE:HG13	1:A:269:TYR:HA	2.01	0.43
1:A:401:ARG:HB3	1:A:401:ARG:HE	1.54	0.43
1:B:139:PRO:HB2	1:B:140:ILE:CD1	2.49	0.43
1:A:294:GLN:O	1:A:298:MET:HG3	2.19	0.42
1:B:158:THR:O	1:B:161:LYS:N	2.51	0.42
1:B:252:ARG:HH11	1:B:252:ARG:HD2	1.65	0.42
1:B:102:SER:OG	1:B:145:ASP:OD1	2.27	0.42
1:A:74:LEU:HA	1:A:74:LEU:HD23	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HA	1:B:28:LEU:HD12	1.81	0.42
1:A:100:GLU:OE1	1:A:287:ARG:HD3	2.19	0.42
1:B:216:LEU:HB3	1:B:223:PRO:HD2	2.00	0.42
1:B:24:LEU:HD11	1:B:306:GLU:HB2	2.00	0.42
1:B:233:PRO:HD2	1:B:325:TYR:CD1	2.54	0.42
1:A:211:GLN:O	1:A:230:ALA:HA	2.19	0.42
1:A:59:LYS:HE2	1:A:85:ARG:NH2	2.24	0.42
1:A:260:GLU:HB2	1:A:262:ILE:CG1	2.43	0.42
1:B:95:GLU:OE2	1:B:262:ILE:CD1	2.67	0.42
1:A:138:ALA:HA	1:A:139:PRO:C	2.41	0.41
1:A:216:LEU:O	1:A:409:HIS:CE1	2.61	0.41
1:A:269:TYR:CD1	1:A:269:TYR:C	2.94	0.41
1:A:7:GLY:CA	1:A:12:GLU:HG2	2.49	0.41
1:A:79:VAL:HB	1:A:93:ASN:HA	2.02	0.41
1:A:400:ILE:HG21	1:A:410:TYR:CZ	2.55	0.41
1:B:276:LYS:CG	1:B:277:GLU:OE2	2.65	0.41
1:B:200:ASN:HB2	1:B:311:PHE:CE2	2.55	0.41
1:A:22:SER:HA	1:A:23:PRO:HD3	1.72	0.41
1:A:390:LYS:HE2	1:A:394:GLU:OE2	2.20	0.41
1:A:196:ILE:HG13	1:A:269:TYR:HB2	2.03	0.41
1:A:236:VAL:CG1	1:A:274:ILE:HD13	2.51	0.41
1:B:199:ILE:CD1	1:B:204:TYR:HB2	2.50	0.41
1:A:119:ARG:H	1:A:186:GLU:CG	2.33	0.41
1:B:197:VAL:HA	1:B:206:PRO:HA	2.02	0.41
1:B:211:GLN:O	1:B:230:ALA:HA	2.21	0.41
1:B:84:LYS:HE2	1:B:84:LYS:HB3	1.65	0.41
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.74	0.41
1:A:234:THR:HA	1:A:235:PRO:HD2	1.91	0.41
1:B:149:ALA:C	1:B:151:LYS:H	2.23	0.41
1:A:120:TYR:CD1	1:A:122:VAL:HG23	2.55	0.41
1:A:231:TYR:CE2	1:A:415:GLY:HA2	2.56	0.41
1:B:339:LYS:HA	1:B:340:PRO:HD2	1.71	0.41
1:B:144:ALA:HB2	1:B:179:SER:OG	2.21	0.41
1:A:19:VAL:C	1:A:21:GLN:H	2.24	0.41
1:A:393:LYS:HG3	1:A:397:TYR:HE2	1.86	0.40
1:B:188:LEU:HD12	1:B:282:LEU:HD23	2.03	0.40
1:B:5:VAL:O	1:B:30:VAL:HA	2.21	0.40
1:A:198:MET:N	1:A:205:VAL:O	2.52	0.40
1:A:395:ARG:HE	1:A:395:ARG:HB2	1.65	0.40
1:B:269:TYR:OH	1:B:292:GLU:OE2	2.26	0.40
1:A:253:VAL:CG2	1:A:284:PHE:CZ	3.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:SER:HG	1:B:24:LEU:HG	1.86	0.40
1:B:140:ILE:HG21	1:B:184:ILE:CG2	2.52	0.40
1:B:294:GLN:N	1:B:295:PRO:HD2	2.36	0.40
1:A:10:GLY:HA2	1:A:362:HIS:O	2.21	0.40
1:A:169:PHE:O	1:A:179:SER:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	421/424 (99%)	383 (91%)	30 (7%)	8 (2%)	10	12
1	B	421/424 (99%)	366 (87%)	48 (11%)	7 (2%)	11	14
All	All	842/848 (99%)	749 (89%)	78 (9%)	15 (2%)	11	13

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	112	LYS
1	A	139	PRO
1	B	32	LYS
1	B	130	LYS
1	B	364	GLY
1	A	130	LYS
1	A	277	GLU
1	B	173	LYS
1	B	176	GLY
1	B	363	ALA
1	A	303	ASP
1	A	363	ALA

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Mol	Chain	Res	Type
1	B	139	PRO
1	A	150	GLY

5.3.2 Protein sidechains (i)

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	324/351 (92%)	299 (92%)	25 (8%)	16 24
1	B	321/351 (92%)	282 (88%)	39 (12%)	6 8
All	All	645/702 (92%)	581 (90%)	64 (10%)	10 14

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	A	85	ARG
1	A	95	GLU
1	A	102	SER
1	A	107	LYS
1	A	124	THR
1	A	139	PRO
1	A	177	LYS
1	A	180	GLU
1	A	184	ILE
1	A	186	GLU
1	A	203	ARG
1	A	215	ARG
1	A	240	GLU
1	A	252	ARG
1	A	265	ARG
1	A	269	TYR
1	A	287	ARG
1	A	294	GLN
1	A	313	GLU
1	A	331	LEU

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Mol	Chain	Res	Type
1	A	338	GLU
1	A	339	LYS
1	A	368	GLU
1	A	420	LYS
1	B	1	MET
1	B	27	GLU
1	B	40	ILE
1	B	46	ILE
1	B	52	GLU
1	B	54	LEU
1	B	80	ASP
1	B	81	GLU
1	B	89	ILE
1	B	95	GLU
1	B	117	THR
1	B	139	PRO
1	B	175	PHE
1	B	177	LYS
1	B	179	SER
1	B	180	GLU
1	B	182	VAL
1	B	184	ILE
1	B	203	ARG
1	B	238	ASN
1	B	240	GLU
1	B	255	LYS
1	B	265	ARG
1	B	276	LYS
1	B	277	GLU
1	B	287	ARG
1	B	294	GLN
1	B	296	ILE
1	B	316	ASP
1	B	331	LEU
1	B	333	SER
1	B	339	LYS
1	B	346	ILE
1	B	368	GLU
1	B	387	LYS
1	B	401	ARG
1	B	408	MET
1	B	411	ARG

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Mol	Chain	Res	Type
1	B	412	LYS

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

Mol	Chain	Res	Type
1	A	224	ASN
1	A	285	ASN
1	A	294	GLN
1	A	310	ASN
1	A	370	ASN
1	A	409	HIS
1	B	224	ASN
1	B	238	ASN
1	B	294	GLN
1	B	310	ASN
1	B	318	HIS
1	B	370	ASN
1	B	409	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 carbohydrates 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, 95^{th} 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	423/424 (99%)	0.24	34 (8%) 15 15	21, 43, 103, 125	0
1	B	423/424 (99%)	0.51	47 (11%) 7 7	21, 46, 114, 137	0
All	All	846/848 (99%)	0.37	81 (9%) 10 10	21, 44, 109, 137	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	ALA	8.3
1	B	179	SER	7.9
1	B	184	ILE	7.7
1	B	142	VAL	7.4
1	B	182	VAL	7.1
1	B	153	ALA	7.0
1	B	123	PHE	6.9
1	B	140	ILE	6.6
1	B	154	VAL	6.4
1	B	118	ALA	6.0
1	A	165	THR	5.9
1	B	141	VAL	5.7
1	B	143	LYS	5.3
1	B	129	ALA	5.2
1	B	149	ALA	5.1
1	A	140	ILE	5.0
1	B	124	THR	4.8
1	A	162	ALA	4.7
1	B	183	VAL	4.6
1	A	154	VAL	4.5
1	B	139	PRO	4.5
1	A	170	LEU	4.5
1	B	170	LEU	4.5
1	B	119	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	169	PHE	4.4
1	B	122	VAL	4.4
1	B	156	CYS	4.4
1	B	175	PHE	4.2
1	B	137	GLY	4.2
1	B	152	GLY	4.2
1	A	141	VAL	4.1
1	B	133	VAL	4.0
1	A	159	VAL	4.0
1	B	155	VAL	3.9
1	A	164	GLU	3.8
1	B	125	ASP	3.7
1	B	120	TYR	3.7
1	A	124	THR	3.6
1	A	161	LYS	3.5
1	B	138	ALA	3.4
1	A	184	ILE	3.4
1	A	156	CYS	3.4
1	A	158	THR	3.4
1	B	165	THR	3.2
1	A	175	PHE	3.2
1	B	169	PHE	3.2
1	B	187	PHE	3.1
1	B	160	GLU	3.1
1	A	123	PHE	3.0
1	B	159	VAL	3.0
1	B	176	GLY	3.0
1	A	153	ALA	3.0
1	A	171	ASN	3.0
1	B	132	TYR	3.0
1	A	122	VAL	2.9
1	A	168	ARG	2.9
1	B	121	GLU	2.9
1	A	133	VAL	2.9
1	B	181	ARG	2.8
1	A	163	ILE	2.8
1	A	129	ALA	2.6
1	A	137	GLY	2.6
1	A	119	ARG	2.5
1	B	99	LEU	2.5
1	A	157	GLU	2.5
1	A	118	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	138	ALA	2.5
1	A	152	GLY	2.5
1	A	139	PRO	2.4
1	A	142	VAL	2.4
1	B	171	ASN	2.3
1	A	187	PHE	2.3
1	A	166	LEU	2.2
1	B	104	ALA	2.2
1	B	168	ARG	2.2
1	B	157	GLU	2.1
1	B	145	ASP	2.1
1	A	106	ALA	2.1
1	B	127	GLU	2.0
1	B	185	GLU	2.0
1	B	180	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.