Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 12:03 PM EST

PDB ID	:	1AOS
Title	:	HUMAN ARGININOSUCCINATE LYASE
Authors	:	Turner, M.A.; Simpson, A.; Mcinnes, R.R.; Howell, P.L.
Deposited on	:	1997-07-10
Resolution	:	4.20 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:

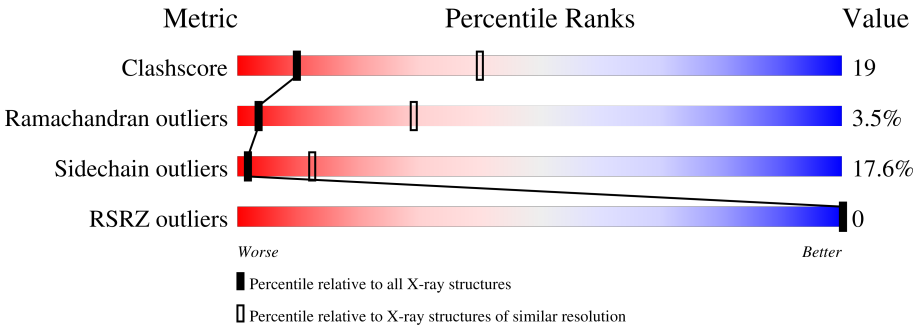
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.20 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))
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 <=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	464	50% 34% 9% 6%
1	B	464	51% 33% 9% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6788 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 ARGININOSUCCINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3394	2134	602	639	19			
1	B	434	Total	C	N	O	S	0	0	0
			3394	2134	602	639	19			

There are 2 discrepancies between the modelled and reference sequences:

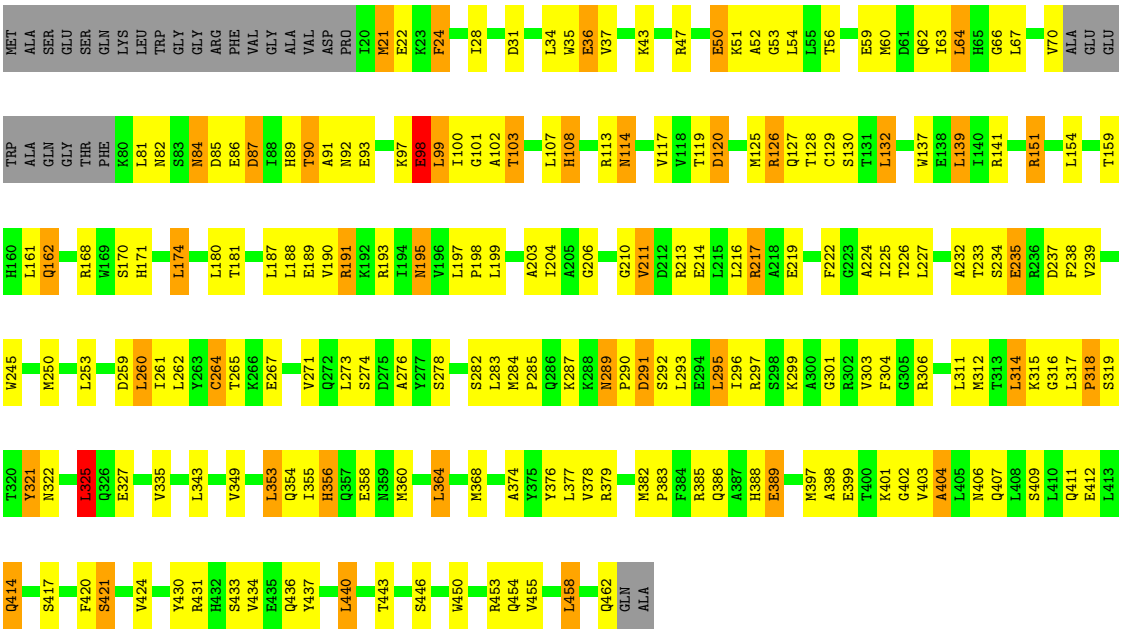
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLN	GLY	conflict	UNP P04424
B	6	GLN	GLY	conflict	UNP P04424

3 Residue-property plots (i)

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.

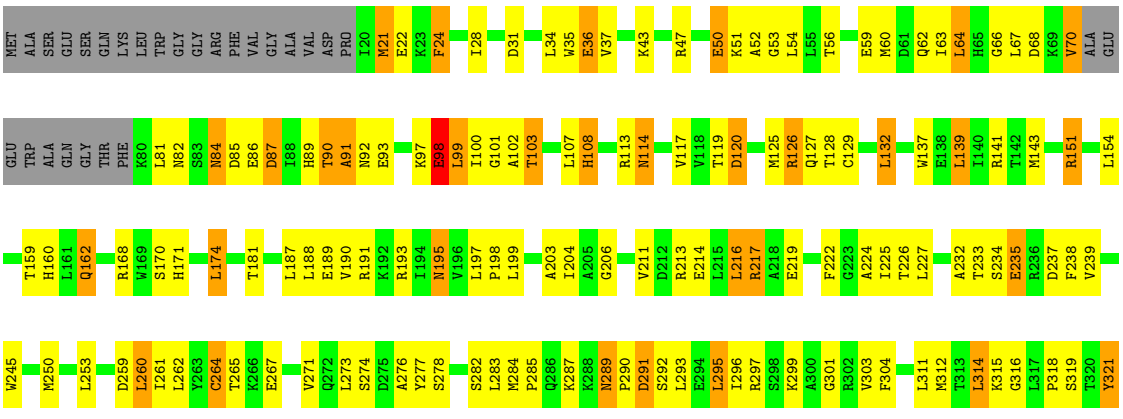
• Molecule 1: ARGININOSUCCINATE LYASE

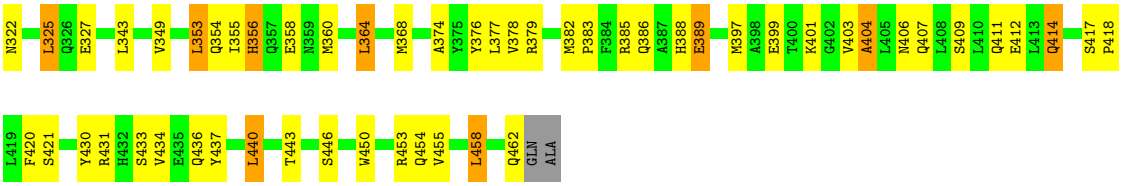
Chain A:



• Molecule 1: ARGININOSUCCINATE LYASE

Chain B:




N322
L325
Q326
E327
L343
V349
L353
Q354
I355
H356
Q357
E358
N359
M360
L364
M368
A374
Y375
Y376
L377
V378
R379
M382
P383
F384
R385
Q386
A387
H388
E389
M397
A398
E399
T400
K401
G402
V403
A404
L405
N406
Q407
L408
S409
L410
Q411
E412
L413
Q414
S417
P418
L419
F420
S421
Y430
R431
H432
S433
V434
E435
Q436
Y437
L440
T443
S446
W450
R453
Q454
V455
L458
Q462
GLN
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	104.60Å 104.60Å 183.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 4.20 45.42 – 4.02	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-4.20) 89.1 (45.42-4.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 4.00Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , 0.298 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	6788	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, 0.333 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	0.74	1/3452 (0.0%)	0.89	3/4665 (0.1%)
1	B	0.73	1/3452 (0.0%)	0.89	4/4665 (0.1%)
All	All	0.74	2/6904 (0.0%)	0.89	7/9330 (0.1%)

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	2
1	B	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLU	CG-CD	5.89	1.60	1.51
1	B	98	GLU	CG-CD	5.41	1.60	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	314	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	314	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	325	LEU	CA-CB-CG	5.32	127.55	115.30
1	B	325	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	289	ASN	N-CA-C	5.14	124.88	111.00
1	A	289	ASN	N-CA-C	5.03	124.58	111.00
1	B	70	VAL	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	TYR	Sidechain
1	A	437	TYR	Sidechain
1	B	277	TYR	Sidechain
1	B	376	TYR	Sidechain
1	B	437	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3394	0	3391	134	0
1	B	3394	0	3391	129	0
All	All	6788	0	6782	260	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 19.

All (260) 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:A:312:MET:HG3	1:B:312:MET:HG3	1.45	0.97
1:B:409:SER:O	1:B:412:GLU:HB2	1.80	0.82
1:A:108:HIS:H	1:A:108:HIS:CD2	1.98	0.81
1:A:409:SER:O	1:A:412:GLU:HB2	1.79	0.80
1:B:271:VAL:HG12	1:B:355:ILE:HG22	1.65	0.79
1:A:271:VAL:HG12	1:A:355:ILE:HG22	1.66	0.78
1:B:108:HIS:CD2	1:B:108:HIS:H	2.00	0.78
1:B:89:HIS:CE1	1:B:117:VAL:HG22	2.19	0.77
1:A:89:HIS:CE1	1:A:117:VAL:HG22	2.20	0.76
1:B:265:THR:HG22	1:B:267:GLU:H	1.52	0.75
1:A:108:HIS:H	1:A:108:HIS:HD2	1.33	0.74
1:B:226:THR:HG21	1:B:232:ALA:HB2	1.70	0.73
1:B:99:LEU:HD12	1:B:100:ILE:HG12	1.70	0.73
1:A:226:THR:HG21	1:A:232:ALA:HB2	1.71	0.73
1:B:108:HIS:H	1:B:108:HIS:HD2	1.35	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HD12	1:A:100:ILE:HG12	1.72	0.71
1:A:265:THR:HG22	1:A:267:GLU:H	1.54	0.70
1:A:108:HIS:CD2	1:A:108:HIS:N	2.60	0.69
1:B:443:THR:HG22	1:B:443:THR:O	1.93	0.69
1:A:443:THR:O	1:A:443:THR:HG22	1.94	0.68
1:B:28:ILE:HG13	1:B:86:GLU:O	1.93	0.68
1:B:108:HIS:CD2	1:B:108:HIS:N	2.62	0.68
1:A:187:LEU:HD22	1:A:245:TRP:CZ2	2.29	0.67
1:B:187:LEU:HD22	1:B:245:TRP:CZ2	2.31	0.66
1:A:383:PRO:HG2	1:A:386:GLN:HB2	1.76	0.65
1:A:28:ILE:HG13	1:A:86:GLU:O	1.96	0.65
1:A:154:LEU:HD11	1:A:431:ARG:HG3	1.79	0.64
1:B:404:ALA:HB3	1:B:407:GLN:OE1	1.97	0.64
1:B:113:ARG:O	1:B:117:VAL:HG23	1.98	0.64
1:B:383:PRO:HG2	1:B:386:GLN:HB2	1.79	0.64
1:A:282:SER:C	1:A:284:MET:H	2.01	0.64
1:A:113:ARG:O	1:A:117:VAL:HG23	1.98	0.63
1:B:154:LEU:HD11	1:B:431:ARG:HG3	1.80	0.63
1:B:97:LYS:O	1:B:101:GLY:HA2	1.99	0.63
1:A:168:ARG:H	1:A:443:THR:HG21	1.64	0.62
1:B:197:LEU:HD12	1:B:225:ILE:HG22	1.81	0.62
1:A:404:ALA:HB3	1:A:407:GLN:OE1	1.98	0.62
1:A:454:GLN:O	1:A:458:LEU:HD13	2.00	0.62
1:A:97:LYS:O	1:A:101:GLY:HA2	2.00	0.62
1:B:454:GLN:O	1:B:458:LEU:HD13	1.99	0.62
1:A:203:ALA:O	1:A:204:ILE:HD12	2.00	0.61
1:B:35:TRP:CG	1:B:36:GLU:N	2.68	0.61
1:A:260:LEU:HB3	1:A:293:LEU:HD13	1.83	0.61
1:B:168:ARG:H	1:B:443:THR:HG21	1.65	0.61
1:B:315:LYS:O	1:B:315:LYS:HG2	2.00	0.61
1:B:56:THR:HG23	1:B:59:GLU:OE2	2.01	0.60
1:B:203:ALA:O	1:B:204:ILE:HD12	2.02	0.60
1:A:56:THR:HG23	1:A:59:GLU:OE2	2.00	0.60
1:B:379:ARG:HH22	1:B:436:GLN:HG3	1.67	0.60
1:A:250:MET:HG3	1:A:303:VAL:HG21	1.83	0.59
1:B:282:SER:C	1:B:284:MET:H	2.02	0.59
1:A:197:LEU:HD12	1:A:225:ILE:HG22	1.84	0.59
1:A:433:SER:O	1:A:436:GLN:HB3	2.02	0.59
1:A:379:ARG:HH22	1:A:436:GLN:HG3	1.67	0.59
1:B:250:MET:HG3	1:B:303:VAL:HG21	1.84	0.59
1:A:35:TRP:CG	1:A:36:GLU:N	2.70	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LYS:O	1:A:315:LYS:HG2	2.03	0.59
1:B:114:ASN:HD21	1:B:203:ALA:HA	1.68	0.59
1:B:195:ASN:OD1	1:B:222:PHE:HD1	1.86	0.59
1:A:114:ASN:HD21	1:A:203:ALA:HA	1.67	0.59
1:A:195:ASN:OD1	1:A:222:PHE:HD1	1.86	0.58
1:B:35:TRP:CD1	1:B:36:GLU:N	2.71	0.58
1:B:260:LEU:HB3	1:B:293:LEU:HD13	1.85	0.58
1:A:35:TRP:CD1	1:A:36:GLU:N	2.72	0.58
1:B:433:SER:O	1:B:436:GLN:HB3	2.03	0.57
1:A:431:ARG:O	1:A:434:VAL:HG22	2.03	0.57
1:B:401:LYS:HE3	1:B:403:VAL:HG23	1.85	0.57
1:B:114:ASN:ND2	1:B:203:ALA:HA	2.20	0.57
1:B:197:LEU:HD23	1:B:222:PHE:CD2	2.40	0.57
1:A:22:GLU:C	1:A:24:PHE:H	2.08	0.57
1:B:89:HIS:NE2	1:B:117:VAL:HG22	2.19	0.56
1:A:401:LYS:HE3	1:A:403:VAL:HG23	1.87	0.56
1:A:114:ASN:ND2	1:A:203:ALA:HA	2.19	0.56
1:B:431:ARG:O	1:B:434:VAL:HG22	2.05	0.56
1:B:213:ARG:HH22	1:B:226:THR:HG22	1.69	0.56
1:A:197:LEU:HD23	1:A:222:PHE:CD2	2.41	0.56
1:A:213:ARG:HH22	1:A:226:THR:HG22	1.71	0.55
1:B:22:GLU:C	1:B:24:PHE:H	2.09	0.55
1:A:89:HIS:NE2	1:A:117:VAL:HG22	2.21	0.55
1:A:98:GLU:HG3	1:A:99:LEU:N	2.21	0.55
1:A:284:MET:N	1:A:285:PRO:HD3	2.21	0.54
1:B:98:GLU:HG3	1:B:99:LEU:N	2.22	0.54
1:B:21:MET:O	1:B:24:PHE:HB2	2.07	0.54
1:B:126:ARG:O	1:B:126:ARG:HG2	2.07	0.54
1:B:284:MET:N	1:B:285:PRO:HD3	2.22	0.53
1:B:282:SER:O	1:B:284:MET:N	2.42	0.53
1:A:282:SER:O	1:A:284:MET:N	2.41	0.53
1:A:126:ARG:O	1:A:126:ARG:HG2	2.08	0.52
1:A:287:LYS:HG2	1:B:162:GLN:HB3	1.90	0.52
1:B:301:GLY:HA2	1:B:304:PHE:HB3	1.90	0.52
1:A:52:ALA:HB3	1:A:54:LEU:HD23	1.93	0.51
1:A:43:LYS:HD2	1:A:67:LEU:O	2.11	0.51
1:A:301:GLY:HA2	1:A:304:PHE:HB3	1.92	0.51
1:A:21:MET:O	1:A:24:PHE:HB2	2.10	0.51
1:B:52:ALA:HB3	1:B:54:LEU:HD23	1.93	0.51
1:B:273:LEU:HD11	1:B:293:LEU:HD12	1.93	0.51
1:A:187:LEU:HD12	1:A:190:VAL:CG1	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:SER:O	1:A:322:ASN:ND2	2.43	0.50
1:B:108:HIS:HD2	1:B:108:HIS:N	2.06	0.50
1:B:430:TYR:O	1:B:434:VAL:HG13	2.11	0.50
1:A:411:GLN:HA	1:A:414:GLN:HB2	1.92	0.50
1:B:450:TRP:HD1	1:B:453:ARG:HH12	1.60	0.50
1:A:139:LEU:HD12	1:A:343:LEU:HD22	1.94	0.50
1:A:430:TYR:O	1:A:434:VAL:HG13	2.11	0.50
1:B:364:LEU:HB3	1:B:430:TYR:CE1	2.47	0.49
1:A:171:HIS:HB2	1:A:443:THR:HG23	1.94	0.49
1:A:253:LEU:HD11	1:A:343:LEU:HD23	1.93	0.49
1:B:137:TRP:CZ2	1:B:462:GLN:HB3	2.47	0.49
1:B:43:LYS:HD2	1:B:67:LEU:O	2.12	0.49
1:A:233:THR:HG22	1:A:321:TYR:HB2	1.94	0.49
1:A:382:MET:CG	1:A:383:PRO:HD2	2.42	0.49
1:B:187:LEU:HD12	1:B:190:VAL:CG1	2.43	0.49
1:B:319:SER:O	1:B:322:ASN:ND2	2.46	0.49
1:B:411:GLN:HA	1:B:414:GLN:HB2	1.95	0.49
1:A:213:ARG:HB3	1:A:225:ILE:HG21	1.95	0.49
1:B:21:MET:O	1:B:24:PHE:CB	2.61	0.49
1:B:90:THR:O	1:B:92:ASN:N	2.46	0.48
1:A:364:LEU:HB3	1:A:430:TYR:CE1	2.48	0.48
1:B:171:HIS:HB2	1:B:443:THR:HG23	1.95	0.48
1:B:213:ARG:NH2	1:B:226:THR:HG22	2.27	0.48
1:B:253:LEU:HD11	1:B:343:LEU:HD23	1.94	0.48
1:B:377:LEU:HD13	1:B:382:MET:SD	2.53	0.48
1:A:86:GLU:HB3	1:A:87:ASP:OD1	2.14	0.48
1:B:197:LEU:HD23	1:B:222:PHE:HD2	1.78	0.48
1:B:356:HIS:O	1:B:360:MET:HG3	2.14	0.48
1:A:197:LEU:HD23	1:A:222:PHE:HD2	1.78	0.48
1:A:377:LEU:HD13	1:A:382:MET:SD	2.53	0.48
1:B:233:THR:HG22	1:B:321:TYR:HB2	1.95	0.48
1:A:93:GLU:HG2	1:A:108:HIS:CE1	2.48	0.48
1:A:213:ARG:NH2	1:A:226:THR:HG22	2.29	0.48
1:B:299:LYS:O	1:B:303:VAL:HG23	2.14	0.48
1:B:139:LEU:HD12	1:B:343:LEU:HD22	1.95	0.48
1:A:21:MET:O	1:A:24:PHE:CB	2.62	0.48
1:A:137:TRP:CZ2	1:A:462:GLN:HB3	2.49	0.47
1:B:238:PHE:CE2	1:B:239:VAL:HG13	2.49	0.47
1:B:274:SER:C	1:B:276:ALA:H	2.18	0.47
1:A:238:PHE:CE2	1:A:239:VAL:HG13	2.50	0.47
1:A:450:TRP:O	1:A:454:GLN:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:THR:HG21	1:B:199:LEU:HD22	1.96	0.47
1:B:455:VAL:HA	1:B:458:LEU:HD22	1.96	0.47
1:A:162:GLN:HB3	1:B:287:LYS:HG2	1.96	0.47
1:A:56:THR:H	1:A:59:GLU:HG2	1.79	0.47
1:B:382:MET:CG	1:B:383:PRO:HD2	2.44	0.47
1:A:90:THR:O	1:A:92:ASN:N	2.48	0.47
1:A:273:LEU:HD11	1:A:293:LEU:HD12	1.96	0.47
1:A:450:TRP:HD1	1:A:453:ARG:HH12	1.61	0.47
1:A:455:VAL:HA	1:A:458:LEU:HD22	1.96	0.47
1:B:397:MET:O	1:B:401:LYS:HB2	2.15	0.47
1:A:137:TRP:HE1	1:A:462:GLN:NE2	2.13	0.47
1:B:93:GLU:HG2	1:B:108:HIS:CE1	2.49	0.47
1:B:450:TRP:O	1:B:454:GLN:HG2	2.14	0.47
1:A:129:CYS:HA	1:A:132:LEU:HB2	1.97	0.46
1:B:261:ILE:HD11	1:B:297:ARG:NH1	2.30	0.46
1:A:119:THR:HG21	1:A:199:LEU:HD22	1.98	0.46
1:A:132:LEU:HB3	1:A:187:LEU:HD21	1.96	0.46
1:A:261:ILE:HD11	1:A:297:ARG:NH1	2.31	0.46
1:A:299:LYS:O	1:A:303:VAL:HG23	2.16	0.46
1:B:28:ILE:HA	1:B:31:ASP:OD1	2.15	0.46
1:B:137:TRP:HE1	1:B:462:GLN:NE2	2.13	0.46
1:A:168:ARG:H	1:A:443:THR:CG2	2.29	0.46
1:A:170:SER:O	1:A:174:LEU:HB2	2.16	0.46
1:A:289:ASN:HA	1:A:290:PRO:HD3	1.69	0.46
1:B:132:LEU:HB3	1:B:187:LEU:HD21	1.97	0.46
1:A:397:MET:O	1:A:401:LYS:HB2	2.16	0.46
1:B:213:ARG:HB3	1:B:225:ILE:HG21	1.97	0.46
1:A:235:GLU:HG2	1:A:237:ASP:H	1.81	0.45
1:B:66:GLY:O	1:B:70:VAL:N	2.48	0.45
1:B:235:GLU:HG2	1:B:237:ASP:H	1.82	0.45
1:A:50:GLU:O	1:A:53:GLY:N	2.49	0.45
1:B:56:THR:H	1:B:59:GLU:HG2	1.82	0.45
1:A:274:SER:C	1:A:276:ALA:H	2.19	0.45
1:A:66:GLY:O	1:A:70:VAL:N	2.49	0.45
1:B:86:GLU:HB3	1:B:87:ASP:OD1	2.17	0.45
1:B:374:ALA:O	1:B:378:VAL:HG23	2.17	0.45
1:A:28:ILE:HA	1:A:31:ASP:OD1	2.17	0.45
1:B:170:SER:O	1:B:174:LEU:HB2	2.17	0.45
1:A:260:LEU:O	1:A:264:CYS:HB2	2.17	0.45
1:A:292:SER:O	1:A:296:ILE:HG13	2.16	0.44
1:B:117:VAL:HA	1:B:120:ASP:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HD22	1:B:143:MET:SD	2.58	0.44
1:B:292:SER:O	1:B:296:ILE:HG13	2.17	0.44
1:B:260:LEU:O	1:B:264:CYS:HB2	2.17	0.44
1:A:282:SER:C	1:A:284:MET:N	2.69	0.44
1:B:129:CYS:HA	1:B:132:LEU:HB2	1.98	0.44
1:A:22:GLU:C	1:A:24:PHE:N	2.70	0.44
1:A:117:VAL:HA	1:A:120:ASP:HB2	2.00	0.44
1:B:151:ARG:HA	1:B:170:SER:OG	2.17	0.44
1:B:295:LEU:O	1:B:299:LYS:HG2	2.18	0.44
1:B:385:ARG:O	1:B:389:GLU:HB2	2.18	0.44
1:A:417:SER:HB3	1:A:420:PHE:CD2	2.53	0.44
1:A:217:ARG:HD2	1:A:224:ALA:HA	2.00	0.44
1:B:50:GLU:O	1:B:53:GLY:N	2.51	0.44
1:A:87:ASP:OD1	1:A:87:ASP:N	2.51	0.43
1:A:431:ARG:HA	1:A:434:VAL:HG22	2.00	0.43
1:B:282:SER:C	1:B:284:MET:N	2.70	0.43
1:B:417:SER:HA	1:B:418:PRO:HD3	1.91	0.43
1:A:214:GLU:O	1:A:217:ARG:HG3	2.17	0.43
1:A:317:LEU:HA	1:A:318:PRO:HD2	1.83	0.43
1:A:82:ASN:HB3	1:A:85:ASP:OD2	2.19	0.43
1:A:35:TRP:C	1:A:37:VAL:H	2.22	0.43
1:B:349:VAL:O	1:B:353:LEU:HB2	2.19	0.43
1:A:151:ARG:HA	1:A:170:SER:OG	2.18	0.43
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.75	0.43
1:A:353:LEU:HA	1:A:353:LEU:HD12	1.77	0.43
1:A:374:ALA:O	1:A:378:VAL:HG23	2.19	0.43
1:B:60:MET:O	1:B:64:LEU:HB2	2.19	0.43
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.78	0.43
1:B:214:GLU:O	1:B:217:ARG:HG3	2.19	0.43
1:B:417:SER:HB3	1:B:420:PHE:CD2	2.53	0.43
1:A:125:MET:SD	1:A:239:VAL:HG12	2.58	0.42
1:A:385:ARG:O	1:A:389:GLU:HB2	2.19	0.42
1:B:168:ARG:HH22	1:B:431:ARG:CZ	2.31	0.42
1:B:289:ASN:HA	1:B:290:PRO:HD3	1.69	0.42
1:A:63:ILE:HG23	1:A:103:THR:HB	2.01	0.42
1:B:87:ASP:OD1	1:B:87:ASP:N	2.51	0.42
1:A:60:MET:O	1:A:64:LEU:HB2	2.19	0.42
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.85	0.42
1:A:28:ILE:HG13	1:A:28:ILE:H	1.71	0.42
1:B:217:ARG:HD2	1:B:224:ALA:HA	2.01	0.42
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ARG:HD3	1:A:306:ARG:HA	1.92	0.42
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.70	0.42
1:A:168:ARG:HH22	1:A:431:ARG:CZ	2.32	0.41
1:A:356:HIS:O	1:A:360:MET:HG3	2.20	0.41
1:B:168:ARG:H	1:B:443:THR:CG2	2.29	0.41
1:A:52:ALA:CB	1:A:54:LEU:HD23	2.50	0.41
1:A:213:ARG:HH22	1:A:226:THR:CG2	2.33	0.41
1:B:125:MET:SD	1:B:239:VAL:HG12	2.61	0.41
1:B:431:ARG:HA	1:B:434:VAL:HG22	2.02	0.41
1:A:137:TRP:HE1	1:A:462:GLN:HE21	1.67	0.41
1:A:322:ASN:O	1:A:325:LEU:HD13	2.21	0.41
1:B:22:GLU:C	1:B:24:PHE:N	2.71	0.41
1:B:261:ILE:HD11	1:B:297:ARG:HH12	1.85	0.41
1:A:210:GLY:O	1:A:211:VAL:C	2.59	0.41
1:A:265:THR:HG22	1:A:267:GLU:HB2	2.03	0.41
1:A:295:LEU:O	1:A:299:LYS:HG2	2.20	0.41
1:A:82:ASN:ND2	1:A:84:ASN:OD1	2.53	0.41
1:A:398:ALA:O	1:A:402:GLY:N	2.54	0.41
1:A:421:SER:O	1:A:424:VAL:HG13	2.20	0.41
1:B:66:GLY:C	1:B:68:ASP:H	2.24	0.41
1:B:82:ASN:HB3	1:B:85:ASP:OD2	2.21	0.41
1:B:160:HIS:CD2	1:B:160:HIS:N	2.88	0.41
1:B:250:MET:HE1	1:B:253:LEU:HD12	2.02	0.41
1:B:287:LYS:HE2	1:B:287:LYS:HB3	1.87	0.41
1:A:56:THR:O	1:A:60:MET:N	2.49	0.41
1:A:303:VAL:HG13	1:A:335:VAL:HG13	2.02	0.41
1:B:187:LEU:HD12	1:B:190:VAL:HG11	2.03	0.41
1:B:35:TRP:C	1:B:37:VAL:H	2.25	0.40
1:B:82:ASN:ND2	1:B:84:ASN:OD1	2.54	0.40
1:B:90:THR:O	1:B:91:ALA:C	2.59	0.40
1:B:137:TRP:HZ2	1:B:462:GLN:HB3	1.86	0.40
1:A:130:SER:HA	1:A:191:ARG:CZ	2.51	0.40
1:A:287:LYS:HE2	1:A:287:LYS:HB3	1.86	0.40
1:A:349:VAL:O	1:A:353:LEU:HB2	2.21	0.40
1:B:52:ALA:CB	1:B:54:LEU:HD23	2.51	0.40
1:B:54:LEU:N	1:B:54:LEU:HD22	2.36	0.40
1:A:443:THR:O	1:A:443:THR:CG2	2.64	0.40
1:B:63:ILE:HG23	1:B:103:THR:HB	2.02	0.40
1:A:139:LEU:HD13	1:A:180:LEU:HD13	2.03	0.40
1:B:265:THR:HG22	1:B:267:GLU:N	2.29	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	430/464 (93%)	383 (89%)	32 (7%)	15 (4%)	3 29
1	B	430/464 (93%)	384 (89%)	31 (7%)	15 (4%)	3 29
All	All	860/928 (93%)	767 (89%)	63 (7%)	30 (4%)	3 29

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	ALA
1	A	440	LEU
1	B	404	ALA
1	B	440	LEU
1	A	102	ALA
1	A	206	GLY
1	A	283	LEU
1	A	321	TYR
1	B	102	ALA
1	B	206	GLY
1	B	283	LEU
1	B	321	TYR
1	A	91	ALA
1	A	195	ASN
1	A	291	ASP
1	A	318	PRO
1	A	325	LEU
1	B	91	ALA
1	B	195	ASN
1	B	291	ASP
1	B	318	PRO
1	B	325	LEU
1	B	353	LEU
1	A	353	LEU
1	B	198	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	151	ARG
1	A	198	PRO
1	B	151	ARG
1	A	316	GLY
1	B	316	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	364/389 (94%)	300 (82%)	64 (18%)	2 12
1	B	364/389 (94%)	300 (82%)	64 (18%)	2 12
All	All	728/778 (94%)	600 (82%)	128 (18%)	2 12

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	24	PHE
1	A	34	LEU
1	A	36	GLU
1	A	47	ARG
1	A	50	GLU
1	A	51	LYS
1	A	62	GLN
1	A	64	LEU
1	A	81	LEU
1	A	84	ASN
1	A	87	ASP
1	A	90	THR
1	A	98	GLU
1	A	99	LEU
1	A	103	THR
1	A	107	LEU
1	A	108	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	114	ASN
1	A	120	ASP
1	A	126	ARG
1	A	127	GLN
1	A	128	THR
1	A	132	LEU
1	A	139	LEU
1	A	141	ARG
1	A	159	THR
1	A	162	GLN
1	A	174	LEU
1	A	181	THR
1	A	189	GLU
1	A	191	ARG
1	A	193	ARG
1	A	211	VAL
1	A	216	LEU
1	A	217	ARG
1	A	219	GLU
1	A	227	LEU
1	A	234	SER
1	A	235	GLU
1	A	259	ASP
1	A	260	LEU
1	A	262	LEU
1	A	264	CYS
1	A	278	SER
1	A	291	ASP
1	A	295	LEU
1	A	311	LEU
1	A	314	LEU
1	A	327	GLU
1	A	354	GLN
1	A	356	HIS
1	A	358	GLU
1	A	364	LEU
1	A	368	MET
1	A	388	HIS
1	A	389	GLU
1	A	399	GLU
1	A	406	ASN
1	A	414	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	421	SER
1	A	440	LEU
1	A	446	SER
1	A	458	LEU
1	B	21	MET
1	B	24	PHE
1	B	34	LEU
1	B	36	GLU
1	B	47	ARG
1	B	50	GLU
1	B	51	LYS
1	B	62	GLN
1	B	64	LEU
1	B	81	LEU
1	B	84	ASN
1	B	87	ASP
1	B	90	THR
1	B	98	GLU
1	B	99	LEU
1	B	103	THR
1	B	107	LEU
1	B	108	HIS
1	B	114	ASN
1	B	120	ASP
1	B	126	ARG
1	B	127	GLN
1	B	128	THR
1	B	132	LEU
1	B	139	LEU
1	B	141	ARG
1	B	159	THR
1	B	162	GLN
1	B	174	LEU
1	B	181	THR
1	B	189	GLU
1	B	191	ARG
1	B	193	ARG
1	B	211	VAL
1	B	216	LEU
1	B	217	ARG
1	B	219	GLU
1	B	227	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	234	SER
1	B	235	GLU
1	B	259	ASP
1	B	260	LEU
1	B	262	LEU
1	B	264	CYS
1	B	278	SER
1	B	291	ASP
1	B	295	LEU
1	B	311	LEU
1	B	314	LEU
1	B	327	GLU
1	B	354	GLN
1	B	356	HIS
1	B	358	GLU
1	B	364	LEU
1	B	368	MET
1	B	388	HIS
1	B	389	GLU
1	B	399	GLU
1	B	406	ASN
1	B	414	GLN
1	B	421	SER
1	B	440	LEU
1	B	446	SER
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	108	HIS
1	A	114	ASN
1	A	386	GLN
1	A	454	GLN
1	A	462	GLN
1	B	65	HIS
1	B	108	HIS
1	B	114	ASN
1	B	386	GLN
1	B	454	GLN
1	B	462	GLN

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 monosaccharides 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	434/464 (93%)	-0.45	0	100	100	20, 20, 20, 20	0
1	B	434/464 (93%)	-0.44	0	100	100	20, 20, 20, 20	0
All	All	868/928 (93%)	-0.44	0	100	100	20, 20, 20, 20	0

There are no RSRZ outliers to report.

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.