



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 10:47 AM EDT

PDB ID : 3IH8
Title : Crystal Structure Analysis of Mglu in its native form
Authors : Yoshimune, K.; Shirakihara, Y.
Deposited on : 2009-07-29
Resolution : 2.30 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

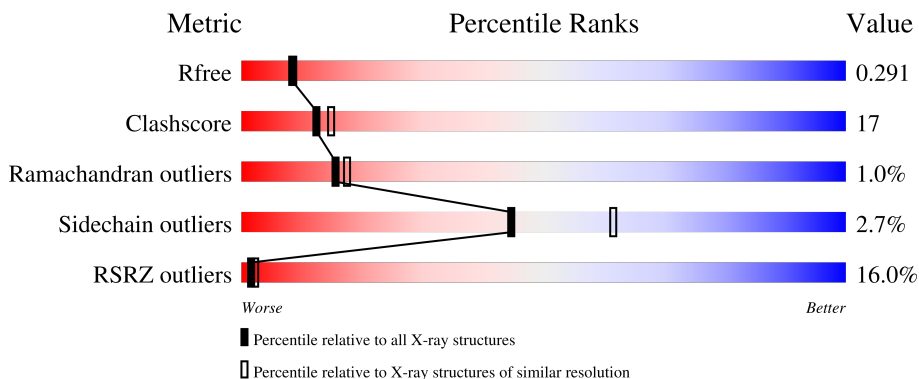
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	456	
1	B	456	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6549 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 Salt-tolerant glutaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	415	3070	1907	561	587	15	0	0	0
1	B	411	3046	1892	557	582	15	0	0	0

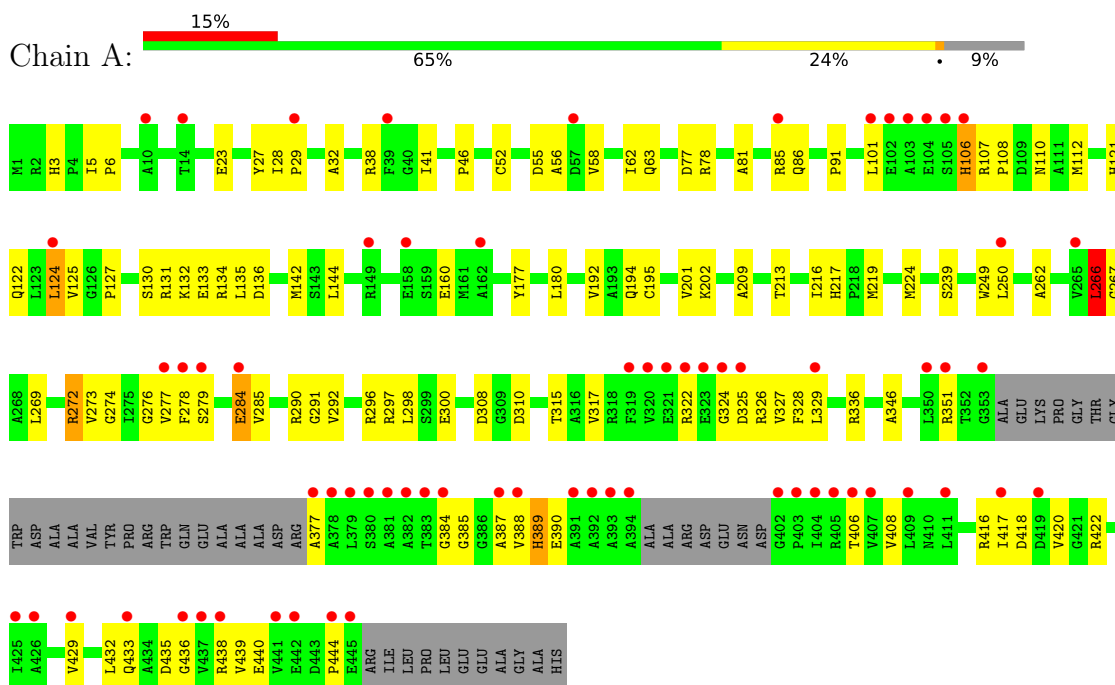
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	226	Total 226	O 226	0	0
2	B	207	Total 207	O 207	0	0

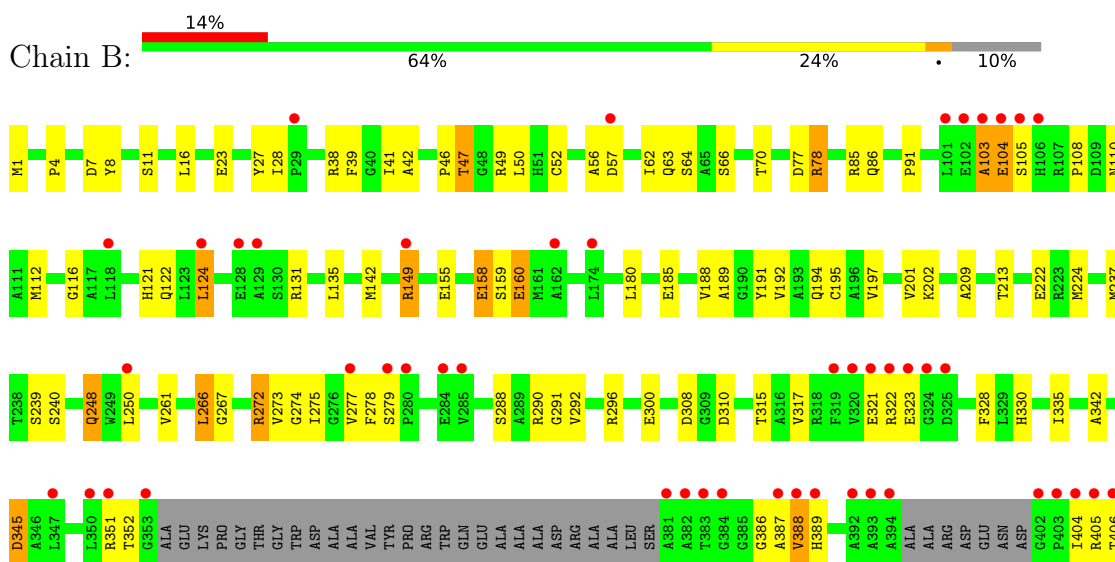
3 Residue-property plots [i](#)

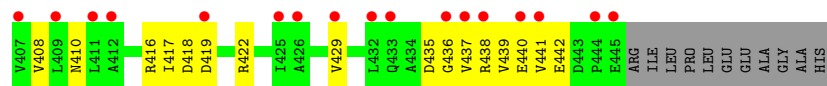
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Salt-tolerant glutaminase



- Molecule 1: Salt-tolerant glutaminase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.08Å 142.25Å 74.25Å 90.00° 104.08° 90.00°	Depositor
Resolution (Å)	19.90 – 2.30 19.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.90-2.30) 100.0 (19.90-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.30Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.247 , 0.291 0.247 , 0.291	Depositor DCC
R_{free} test set	2620 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtrriage
Anisotropy	0.301	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6549	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3606e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/3114	0.61	2/4222 (0.0%)
1	B	0.34	0/3090	0.62	1/4189 (0.0%)
All	All	0.34	0/6204	0.62	3/8411 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	LEU	N-CA-C	6.09	127.44	111.00
1	B	124	LEU	N-CA-C	5.95	127.05	111.00
1	A	266	LEU	CA-CB-CG	5.39	127.71	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3070	0	3070	100	0
1	B	3046	0	3044	107	0
2	A	226	0	0	14	0
2	B	207	0	0	17	0
All	All	6549	0	6114	207	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 17.

All (207) 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:110:ASN:HD22	1:B:112:MET:H	1.10	0.95
1:A:62:ILE:HG21	1:A:142:MET:HE1	1.50	0.93
1:A:110:ASN:HD22	1:A:112:MET:H	1.26	0.82
1:A:272:ARG:NH2	1:A:308:ASP:HB2	1.95	0.81
1:B:422:ARG:HD3	2:B:560:HOH:O	1.84	0.76
1:A:269:LEU:HD21	1:A:272:ARG:NH1	2.02	0.75
1:B:279:SER:OG	1:B:290:ARG:HD3	1.87	0.74
1:B:272:ARG:NH2	1:B:308:ASP:OD1	2.21	0.73
1:A:201:VAL:HG23	2:A:457:HOH:O	1.87	0.73
1:A:310:ASP:HB3	2:A:477:HOH:O	1.89	0.73
1:A:406:THR:OG1	1:A:438:ARG:HB3	1.89	0.73
1:A:23:GLU:HA	2:A:517:HOH:O	1.88	0.72
1:A:249:TRP:HZ3	1:A:292:VAL:HG13	1.54	0.72
1:B:78:ARG:HH11	1:B:78:ARG:HB3	1.54	0.71
1:B:110:ASN:ND2	1:B:112:MET:H	1.86	0.70
1:B:405:ARG:HH22	1:B:437:VAL:HA	1.56	0.70
1:A:336:ARG:HA	1:A:418:ASP:OD1	1.92	0.69
1:A:272:ARG:NH2	1:A:308:ASP:CB	2.57	0.68
1:B:63:GLN:HA	1:B:195:CYS:HB3	1.76	0.67
1:B:121:HIS:HD2	1:B:194:GLN:OE1	1.78	0.67
1:B:1:MET:HG2	2:B:520:HOH:O	1.93	0.67
1:A:408:VAL:HG22	1:A:440:GLU:HG3	1.78	0.66
1:B:296:ARG:O	1:B:300:GLU:HG3	1.95	0.65
1:B:38:ARG:HD3	2:B:589:HOH:O	1.95	0.65
1:A:201:VAL:HG13	1:A:276:GLY:C	2.17	0.65
1:A:277:VAL:HG11	1:A:291:GLY:HA2	1.79	0.65
1:A:101:LEU:O	1:A:106:HIS:HA	1.96	0.65
1:B:131:ARG:HH11	1:B:131:ARG:HG2	1.60	0.65
1:B:27:TYR:CD1	1:B:28:ILE:HG23	2.31	0.64
1:B:62:ILE:HG21	1:B:142:MET:HE1	1.80	0.64
1:B:310:ASP:HB3	2:B:554:HOH:O	1.97	0.64
1:A:429:VAL:HG13	1:A:439:VAL:HG11	1.78	0.64
1:A:62:ILE:HD13	1:A:142:MET:HE3	1.79	0.64
1:B:160:GLU:HG2	1:B:192:VAL:HG13	1.80	0.64
1:A:296:ARG:O	1:A:300:GLU:HG3	1.98	0.63
1:A:310:ASP:HA	2:A:551:HOH:O	1.97	0.63
1:B:405:ARG:HA	1:B:405:ARG:NE	2.14	0.63
1:A:27:TYR:CD1	1:A:28:ILE:HG23	2.35	0.62
1:A:377:ALA:N	2:A:527:HOH:O	2.32	0.62
1:B:155:GLU:O	1:B:158:GLU:HG3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TRP:CZ3	1:A:292:VAL:HG13	2.36	0.61
1:A:406:THR:HA	1:A:438:ARG:O	2.01	0.60
1:A:420:VAL:HG23	2:A:479:HOH:O	2.02	0.60
1:A:216:ILE:HD12	1:A:416:ARG:NH2	2.17	0.60
1:B:52:CYS:SG	1:B:202:LYS:HE2	2.41	0.60
1:A:326:ARG:HD3	1:A:328:PHE:CZ	2.37	0.60
1:B:62:ILE:CD1	1:B:142:MET:HE3	2.32	0.59
1:A:52:CYS:SG	1:A:202:LYS:HE2	2.43	0.59
1:B:104:GLU:HG2	2:B:514:HOH:O	2.02	0.58
1:B:160:GLU:HG2	1:B:192:VAL:CG1	2.33	0.58
1:B:62:ILE:HD13	1:B:142:MET:HE3	1.85	0.58
1:B:422:ARG:HH11	1:B:422:ARG:HG2	1.67	0.58
1:A:273:VAL:HG22	1:A:274:GLY:N	2.19	0.58
1:B:405:ARG:NH2	1:B:436:GLY:O	2.35	0.58
1:A:417:ILE:HG23	1:A:422:ARG:HG2	1.85	0.58
1:A:160:GLU:HG2	1:A:192:VAL:HG13	1.86	0.57
1:B:322:ARG:NH2	1:B:404:ILE:HG12	2.19	0.57
1:A:144:LEU:HB3	1:A:224:MET:CE	2.35	0.57
1:A:38:ARG:HG2	2:A:667:HOH:O	2.06	0.56
1:B:50:LEU:HD21	1:B:202:LYS:HB3	1.87	0.56
1:B:408:VAL:HG22	1:B:440:GLU:HG3	1.86	0.56
1:B:345:ASP:HB2	2:B:493:HOH:O	2.05	0.55
1:B:419:ASP:HA	1:B:422:ARG:HD2	1.89	0.55
1:A:279:SER:OG	1:A:290:ARG:HD2	2.06	0.55
1:A:262:ALA:HB3	2:A:458:HOH:O	2.07	0.54
1:B:104:GLU:N	2:B:481:HOH:O	2.40	0.54
1:B:273:VAL:HG22	1:B:274:GLY:N	2.21	0.54
1:A:91:PRO:HB3	1:A:239:SER:O	2.07	0.54
1:B:110:ASN:O	1:B:116:GLY:HA3	2.07	0.54
1:B:201:VAL:HG13	2:B:458:HOH:O	2.06	0.54
1:A:62:ILE:CD1	1:A:142:MET:HE3	2.38	0.54
1:B:85:ARG:HD2	1:B:86:GLN:OE1	2.07	0.54
1:A:41:ILE:HA	1:A:201:VAL:HG11	1.90	0.53
1:B:201:VAL:HG12	1:B:278:PHE:HB2	1.90	0.53
1:A:422:ARG:HB3	1:A:422:ARG:NH1	2.24	0.53
1:B:405:ARG:HA	1:B:405:ARG:CZ	2.38	0.53
1:A:41:ILE:HD11	1:A:298:LEU:HD11	1.89	0.53
1:B:185:GLU:H	1:B:185:GLU:CD	2.12	0.53
1:B:222:GLU:O	1:B:224:MET:HE3	2.09	0.53
1:A:272:ARG:HH22	1:A:308:ASP:CB	2.22	0.53
1:B:110:ASN:HD22	1:B:112:MET:N	1.93	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ARG:HG2	1:A:322:ARG:HH21	1.75	0.52
1:B:131:ARG:HG2	1:B:131:ARG:NH1	2.21	0.52
1:B:77:ASP:OD2	1:B:124:LEU:O	2.28	0.52
1:B:47:THR:OG1	1:B:49:ARG:NH1	2.43	0.52
1:B:422:ARG:HG2	1:B:422:ARG:NH1	2.23	0.52
1:B:416:ARG:NH1	2:B:659:HOH:O	2.42	0.52
1:A:417:ILE:CG2	1:A:422:ARG:HG2	2.40	0.51
1:B:158:GLU:HG3	1:B:159:SER:H	1.75	0.51
1:B:272:ARG:NH2	1:B:308:ASP:HB2	2.25	0.51
1:B:330:HIS:CD2	1:B:410:ASN:HB3	2.45	0.51
1:A:124:LEU:HB2	1:A:134:ARG:HG2	1.92	0.51
1:B:209:ALA:O	1:B:213:THR:HG23	2.10	0.51
1:A:135:LEU:HD23	1:A:135:LEU:O	2.10	0.51
1:A:125:VAL:N	2:A:563:HOH:O	2.05	0.51
1:A:110:ASN:ND2	1:A:112:MET:HB2	2.26	0.51
1:A:77:ASP:OD2	1:A:124:LEU:O	2.30	0.50
1:A:217:HIS:HE1	1:A:219:MET:HG2	1.74	0.50
1:A:130:SER:OG	1:A:133:GLU:HG3	2.11	0.50
1:A:121:HIS:HD2	1:A:194:GLN:OE1	1.94	0.50
1:A:317:VAL:O	1:A:387:ALA:HB3	2.12	0.50
1:B:110:ASN:ND2	1:B:112:MET:HB2	2.27	0.50
1:B:41:ILE:HG12	1:B:277:VAL:HG13	1.94	0.50
1:B:248:GLN:NE2	2:B:490:HOH:O	2.45	0.49
1:A:62:ILE:HD13	1:A:142:MET:CE	2.42	0.49
1:B:405:ARG:NH2	1:B:437:VAL:HA	2.27	0.49
1:B:23:GLU:HA	2:B:468:HOH:O	2.12	0.49
1:A:132:LYS:HD3	1:A:136:ASP:OD2	2.13	0.49
1:A:63:GLN:HA	1:A:195:CYS:HB3	1.93	0.49
1:B:322:ARG:HH22	1:B:404:ILE:HG12	1.78	0.49
1:B:441:VAL:HB	2:B:624:HOH:O	2.13	0.49
1:B:158:GLU:HG3	1:B:159:SER:N	2.28	0.48
1:A:440:GLU:OE1	2:A:646:HOH:O	2.20	0.48
1:A:279:SER:OG	1:A:290:ARG:CD	2.62	0.48
1:A:322:ARG:HD3	1:A:327:VAL:HG22	1.95	0.48
1:B:267:GLY:HA3	1:B:275:ILE:HB	1.96	0.48
1:A:417:ILE:HG23	1:A:422:ARG:CG	2.43	0.48
1:B:352:THR:OG1	1:B:435:ASP:OD2	2.31	0.47
1:A:86:GLN:O	1:A:108:PRO:HD2	2.13	0.47
1:A:29:PRO:HA	1:A:32:ALA:HB3	1.95	0.47
1:A:122:GLN:HB2	1:A:180:LEU:HD22	1.96	0.47
1:A:144:LEU:HB3	1:A:224:MET:HE2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:HIS:O	1:A:6:PRO:HD2	2.14	0.47
1:A:269:LEU:HD21	1:A:272:ARG:HH11	1.74	0.47
1:B:103:ALA:O	1:B:105:SER:N	2.47	0.47
1:B:429:VAL:HG13	1:B:439:VAL:HG11	1.96	0.47
1:B:288:SER:O	1:B:292:VAL:HG22	2.15	0.47
1:B:342:ALA:O	1:B:345:ASP:OD2	2.31	0.47
1:A:201:VAL:HG22	1:A:278:PHE:HB2	1.97	0.47
1:A:56:ALA:O	1:A:202:LYS:HG3	2.15	0.46
1:B:131:ARG:HH21	1:B:189:ALA:HB1	1.80	0.46
1:B:387:ALA:HA	1:B:389:HIS:CE1	2.50	0.46
1:A:135:LEU:HD23	1:A:135:LEU:C	2.36	0.46
1:B:86:GLN:O	1:B:108:PRO:HD2	2.16	0.45
1:B:191:TYR:O	1:B:194:GLN:HB3	2.16	0.45
1:A:273:VAL:CG2	1:A:274:GLY:N	2.78	0.45
1:A:422:ARG:NH2	2:A:624:HOH:O	2.47	0.45
1:B:16:LEU:HB2	1:B:39:PHE:HE2	1.82	0.45
1:A:78:ARG:NH2	1:A:127:PRO:HG3	2.31	0.45
1:A:272:ARG:HH21	1:A:308:ASP:HB2	1.75	0.45
1:B:317:VAL:O	1:B:387:ALA:HB3	2.16	0.45
1:B:57:ASP:OD1	1:B:57:ASP:O	2.35	0.44
1:A:351:ARG:HA	1:A:351:ARG:HD3	1.77	0.44
1:B:405:ARG:O	1:B:405:ARG:NH1	2.51	0.44
1:A:5:ILE:HB	1:A:6:PRO:HD3	2.00	0.44
1:A:272:ARG:HH22	1:A:308:ASP:CG	2.18	0.44
1:B:110:ASN:HD21	1:B:112:MET:HB2	1.83	0.44
1:A:315:THR:HG22	1:A:315:THR:O	2.18	0.44
1:A:433:GLN:O	1:A:436:GLY:N	2.41	0.44
1:B:149:ARG:HD2	1:B:149:ARG:N	2.33	0.44
1:A:46:PRO:HD3	1:A:272:ARG:O	2.18	0.43
1:B:8:TYR:O	1:B:11:SER:HB3	2.18	0.43
1:A:81:ALA:O	1:A:85:ARG:HG3	2.18	0.43
1:A:55:ASP:HB3	1:A:58:VAL:HG21	1.99	0.43
1:A:106:HIS:ND1	1:A:177:TYR:HD2	2.17	0.43
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.79	0.43
1:A:325:ASP:HB2	2:A:679:HOH:O	2.19	0.43
1:B:46:PRO:HD3	1:B:272:ARG:O	2.18	0.43
1:A:209:ALA:O	1:A:213:THR:HG23	2.18	0.43
1:B:240:SER:HB3	2:B:475:HOH:O	2.18	0.43
1:B:277:VAL:HG11	1:B:291:GLY:HA2	2.00	0.43
1:A:385:GLY:O	1:A:388:VAL:HG23	2.19	0.43
1:A:131:ARG:HD3	2:A:675:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ARG:NH2	1:B:308:ASP:CB	2.82	0.42
1:B:386:GLY:HA2	2:B:608:HOH:O	2.19	0.42
1:A:297:ARG:HH11	1:A:297:ARG:HG3	1.85	0.42
1:A:322:ARG:HG2	1:A:322:ARG:NH2	2.34	0.42
1:B:142:MET:HE2	1:B:197:VAL:HG11	2.00	0.42
1:B:237:MET:CE	1:B:266:LEU:HD13	2.49	0.42
1:B:290:ARG:HD2	2:B:480:HOH:O	2.18	0.42
1:B:202:LYS:HD2	2:B:592:HOH:O	2.20	0.42
1:A:217:HIS:CE1	1:A:219:MET:HG2	2.54	0.42
1:B:4:PRO:O	1:B:7:ASP:HB2	2.20	0.42
1:B:321:GLU:HB2	1:B:328:PHE:HB2	2.02	0.42
1:A:266:LEU:HD22	1:A:267:GLY:N	2.35	0.42
1:B:149:ARG:CD	1:B:149:ARG:H	2.32	0.42
1:A:422:ARG:HB3	1:A:422:ARG:HH11	1.84	0.42
1:B:64:SER:C	1:B:66:SER:H	2.23	0.42
1:A:432:LEU:O	1:A:435:ASP:HB2	2.19	0.41
1:B:188:VAL:O	1:B:192:VAL:HG23	2.21	0.41
1:B:388:VAL:HG12	1:B:388:VAL:O	2.21	0.41
1:A:41:ILE:CA	1:A:201:VAL:HG11	2.49	0.41
1:A:389:HIS:HD2	1:A:390:GLU:H	1.69	0.41
1:A:429:VAL:HA	1:A:432:LEU:HD12	2.02	0.41
1:B:63:GLN:HG3	1:B:261:VAL:HG22	2.02	0.41
1:B:122:GLN:HB2	1:B:180:LEU:HD22	2.02	0.41
1:B:42:ALA:HB2	1:B:201:VAL:HG23	2.03	0.41
1:A:284:GLU:HG2	1:A:285:VAL:HG13	2.03	0.41
1:B:62:ILE:HD12	1:B:142:MET:HE3	2.03	0.41
1:B:323:GLU:HA	1:B:323:GLU:OE1	2.20	0.41
1:A:389:HIS:CD2	1:A:390:GLU:N	2.89	0.41
1:B:91:PRO:HB3	1:B:239:SER:O	2.20	0.41
1:B:410:ASN:HA	1:B:442:GLU:HB2	2.01	0.41
1:B:422:ARG:HB2	2:B:639:HOH:O	2.21	0.41
1:B:135:LEU:HD13	1:B:135:LEU:C	2.42	0.40
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.82	0.40
1:B:56:ALA:CA	1:B:201:VAL:HG22	2.51	0.40
1:B:273:VAL:CG2	1:B:274:GLY:N	2.84	0.40
1:B:315:THR:O	1:B:315:THR:HG22	2.21	0.40
1:A:202:LYS:NZ	2:A:559:HOH:O	2.51	0.40
1:A:269:LEU:CD2	1:A:272:ARG:HH11	2.33	0.40
1:B:335:ILE:O	1:B:417:ILE:HA	2.21	0.40
1:A:110:ASN:HD22	1:A:112:MET:N	2.06	0.40
1:A:329:LEU:HD11	1:A:346:ALA:HB1	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ALA:HA	1:B:201:VAL:HG22	2.04	0.40
1:B:406:THR:HG23	1:B:438:ARG:O	2.21	0.40
1:B:418:ASP:O	1:B:422:ARG:HG3	2.21	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	409/456 (90%)	389 (95%)	16 (4%)	4 (1%)	15	17
1	B	405/456 (89%)	380 (94%)	21 (5%)	4 (1%)	15	17
All	All	814/912 (89%)	769 (94%)	37 (4%)	8 (1%)	15	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	ALA
1	B	104	GLU
1	A	106	HIS
1	A	384	GLY
1	B	351	ARG
1	A	324	GLY
1	A	444	PRO
1	B	388	VAL

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	313/341 (92%)	307 (98%)	6 (2%)	57	73
1	B	311/341 (91%)	300 (96%)	11 (4%)	36	50
All	All	624/682 (92%)	607 (97%)	17 (3%)	44	61

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	250	LEU
1	A	266	LEU
1	A	272	ARG
1	A	284	GLU
1	A	389	HIS
1	B	47	THR
1	B	70	THR
1	B	78	ARG
1	B	149	ARG
1	B	158	GLU
1	B	160	GLU
1	B	248	GLN
1	B	250	LEU
1	B	266	LEU
1	B	272	ARG
1	B	345	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	110	ASN
1	A	121	HIS
1	A	181	GLN
1	A	248	GLN
1	A	389	HIS
1	B	26	GLN
1	B	90	ASN
1	B	110	ASN
1	B	121	HIS
1	B	248	GLN

5.3.3 RNA [i](#)

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 monosaccharides 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	415/456 (91%)	0.94	68 (16%) 1 2	19, 33, 75, 110	0
1	B	411/456 (90%)	0.88	64 (15%) 2 2	19, 34, 75, 109	0
All	All	826/912 (90%)	0.91	132 (15%) 1 2	19, 34, 75, 110	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	GLU	9.3
1	B	323	GLU	8.1
1	A	392	ALA	7.9
1	B	392	ALA	7.5
1	A	402	GLY	6.6
1	B	402	GLY	6.5
1	A	379	LEU	6.0
1	B	324	GLY	6.0
1	B	387	ALA	5.9
1	A	382	ALA	5.8
1	B	444	PRO	5.7
1	A	324	GLY	5.7
1	A	406	THR	5.4
1	A	104	GLU	5.3
1	A	380	SER	5.3
1	A	103	ALA	5.3
1	B	103	ALA	5.2
1	A	351	ARG	5.0
1	B	383	THR	4.9
1	B	438	ARG	4.8
1	A	378	ALA	4.8
1	A	377	ALA	4.8
1	A	277	VAL	4.6
1	B	388	VAL	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	444	PRO	4.6
1	B	382	ALA	4.5
1	B	102	GLU	4.5
1	A	438	ARG	4.5
1	B	433	GLN	4.4
1	B	437	VAL	4.4
1	B	350	LEU	4.3
1	B	104	GLU	4.3
1	A	433	GLN	4.3
1	B	403	PRO	4.3
1	A	437	VAL	4.3
1	A	353	GLY	4.3
1	A	29	PRO	4.2
1	A	350	LEU	3.9
1	B	321	GLU	3.9
1	A	393	ALA	3.9
1	A	441	VAL	3.8
1	B	384	GLY	3.7
1	A	102	GLU	3.6
1	B	29	PRO	3.6
1	B	277	VAL	3.6
1	A	403	PRO	3.6
1	B	351	ARG	3.6
1	A	105	SER	3.5
1	A	321	GLU	3.5
1	B	429	VAL	3.5
1	B	381	ALA	3.5
1	B	393	ALA	3.5
1	A	322	ARG	3.5
1	A	388	VAL	3.4
1	B	406	THR	3.4
1	A	394	ALA	3.4
1	A	407	VAL	3.4
1	B	441	VAL	3.4
1	B	405	ARG	3.4
1	B	325	ASP	3.3
1	A	442	GLU	3.3
1	B	57	ASP	3.3
1	A	284	GLU	3.3
1	A	383	THR	3.2
1	A	387	ALA	3.2
1	B	319	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	426	ALA	3.1
1	A	279	SER	3.1
1	B	322	ARG	3.1
1	A	404	ILE	3.0
1	A	419	ASP	3.0
1	A	101	LEU	3.0
1	B	389	HIS	2.9
1	A	319	PHE	2.9
1	A	391	ALA	2.9
1	B	407	VAL	2.8
1	B	353	GLY	2.8
1	A	320	VAL	2.7
1	B	105	SER	2.7
1	B	118	LEU	2.7
1	A	265	VAL	2.7
1	B	425	ILE	2.7
1	B	124	LEU	2.7
1	B	404	ILE	2.7
1	B	320	VAL	2.7
1	B	445	GLU	2.7
1	A	325	ASP	2.6
1	B	128	GLU	2.6
1	B	432	LEU	2.6
1	A	381	ALA	2.6
1	B	394	ALA	2.6
1	B	347	LEU	2.5
1	B	279	SER	2.5
1	B	409	LEU	2.5
1	B	284	GLU	2.5
1	B	101	LEU	2.5
1	A	162	ALA	2.4
1	B	436	GLY	2.4
1	B	162	ALA	2.4
1	A	384	GLY	2.4
1	A	409	LEU	2.4
1	A	429	VAL	2.4
1	A	149	ARG	2.4
1	A	426	ALA	2.4
1	B	149	ARG	2.4
1	A	106	HIS	2.4
1	B	250	LEU	2.4
1	B	411	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	417	ILE	2.3
1	B	280	PRO	2.3
1	B	440	GLU	2.3
1	A	39	PHE	2.3
1	B	419	ASP	2.3
1	A	425	ILE	2.3
1	B	106	HIS	2.2
1	A	250	LEU	2.2
1	B	174	LEU	2.2
1	A	411	LEU	2.2
1	A	445	GLU	2.2
1	A	436	GLY	2.2
1	A	85	ARG	2.1
1	A	405	ARG	2.1
1	B	285	VAL	2.1
1	A	278	PHE	2.1
1	A	329	LEU	2.1
1	A	158	GLU	2.1
1	A	57	ASP	2.1
1	A	124	LEU	2.1
1	A	14	THR	2.1
1	B	129	ALA	2.1
1	A	10	ALA	2.0
1	B	412	ALA	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 monosaccharides 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.