



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 3IH8 / pdb_00003ih8
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

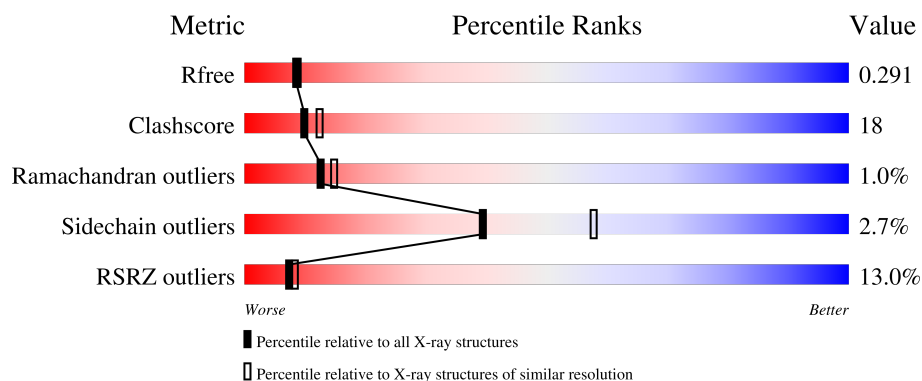
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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	12% 63% 26% 9%
1	B	456	11% 62% 24% 10%

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
1	A	415	Total	C	N	O	S	0	0	0
			3070	1907	561	587	15			
1	B	411	Total	C	N	O	S	0	0	0
			3046	1892	557	582	15			

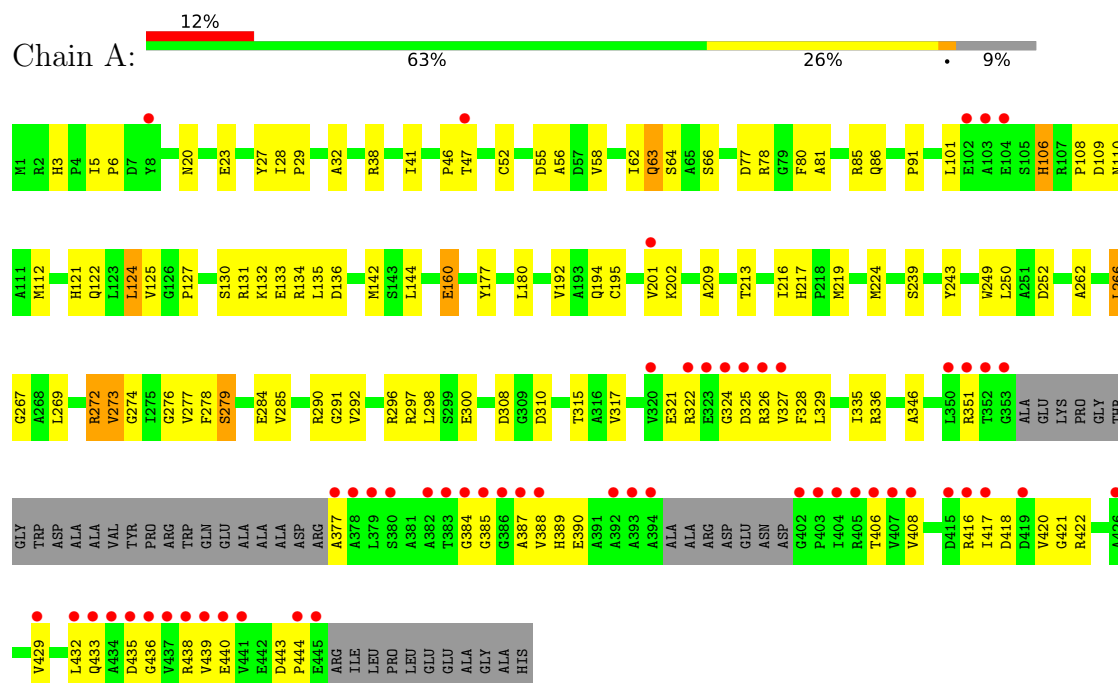
- Molecule 2 is water.

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

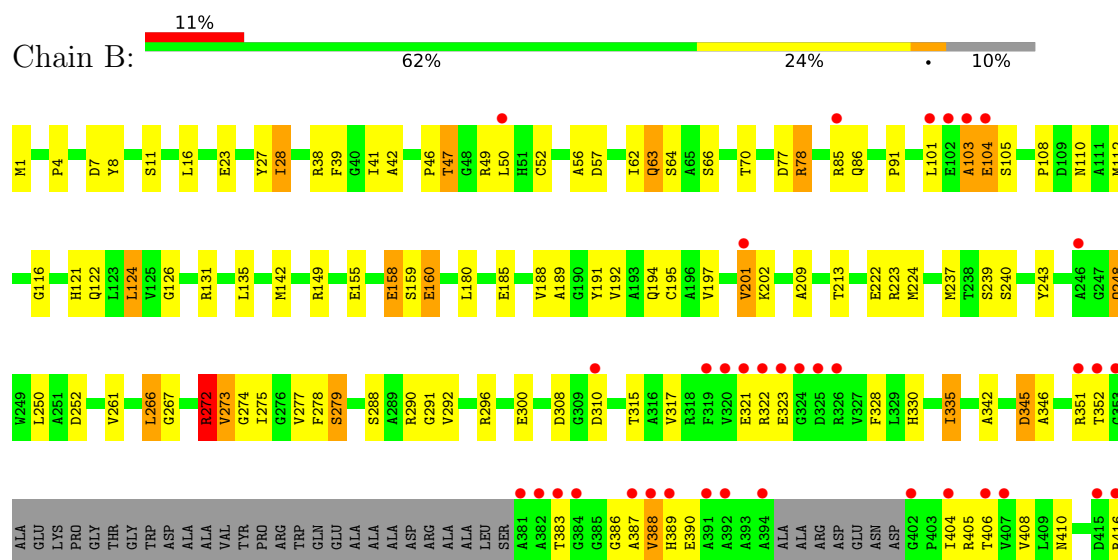
3 Residue-property plots

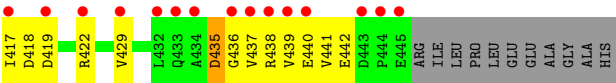
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 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) 99.8 (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)	0.43 , 70.7	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

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	0.43	0/3114	0.98	13/4222 (0.3%)
1	B	0.43	0/3090	1.00	18/4189 (0.4%)
All	All	0.43	0/6204	0.99	31/8411 (0.4%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	LEU	N-CA-C	9.74	127.44	111.37
1	B	124	LEU	N-CA-C	9.51	127.05	111.37
1	A	273	VAL	N-CA-C	7.33	118.16	107.75
1	B	124	LEU	CA-C-N	-7.26	115.14	122.77
1	B	124	LEU	C-N-CA	-7.26	115.14	122.77
1	B	273	VAL	N-CA-C	7.21	117.99	107.75
1	B	346	ALA	N-CA-C	-7.13	103.43	111.14
1	B	435	ASP	N-CA-C	-6.75	104.62	112.92
1	B	390	GLU	N-CA-C	-6.57	105.08	113.23
1	B	28	ILE	CA-C-N	6.32	125.54	118.97
1	B	28	ILE	C-N-CA	6.32	125.54	118.97
1	B	279	SER	CA-C-N	6.00	127.34	119.84
1	B	279	SER	C-N-CA	6.00	127.34	119.84
1	B	335	ILE	N-CA-C	5.98	117.38	108.23
1	B	126	GLY	CA-C-N	5.98	125.45	119.24
1	B	126	GLY	C-N-CA	5.98	125.45	119.24
1	A	335	ILE	N-CA-C	5.69	116.93	108.23
1	A	109	ASP	N-CA-C	5.67	117.92	111.11
1	A	279	SER	CA-C-N	5.66	126.91	119.84
1	A	279	SER	C-N-CA	5.66	126.91	119.84
1	B	252	ASP	N-CA-C	5.61	118.32	111.82
1	B	243	TYR	CB-CA-C	-5.56	110.15	116.54
1	A	272	ARG	N-CA-C	5.48	119.47	112.12
1	A	20	ASN	CA-C-N	5.47	125.44	120.03
1	A	20	ASN	C-N-CA	5.47	125.44	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	GLN	CB-CA-C	-5.43	110.30	116.54
1	A	243	TYR	CB-CA-C	-5.31	110.43	116.54
1	A	63	GLN	CB-CA-C	-5.27	110.48	116.54
1	B	272	ARG	N-CA-C	5.11	121.68	110.80
1	A	80	PHE	N-CA-C	5.05	117.17	111.11
1	A	252	ASP	N-CA-C	5.03	119.13	112.89

There are no chirality outliers.

There are no planarity outliers.

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	3070	0	3070	104	0
1	B	3046	0	3044	110	0
2	A	226	0	0	14	0
2	B	207	0	0	18	0
All	All	6549	0	6114	214	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 18.

All (214) 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	1.56	0.88
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:A:62:ILE:HD13	1:A:142:MET:HE3	1.70	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:ILE:HG21	1:B:142:MET:HE1	1.73	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:201:VAL:HG13	1:A:276:GLY:C	2.17	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: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: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: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
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:62:ILE:CD1	1:A:142:MET:HE3	2.31	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: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:422:ARG:HH11	1:B:422:ARG:HG2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:185:GLU:H	1:B:185:GLU:CD	2.12	0.57
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:B:85:ARG:HD2	1:B:86:GLN:OE1	2.07	0.54
1:B:62:ILE:CD1	1:B:142:MET:HE3	2.38	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: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
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:272:ARG:HH22	1:A:308:ASP:CG	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:LEU:HD23	1:A:135:LEU:C	2.36	0.50
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:B:62:ILE:HD13	1:B:142:MET:HE3	1.92	0.50
1:B:142:MET:HE2	1:B:197:VAL:HG11	1.92	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:144:LEU:HB3	1:A:224:MET:HE2	1.94	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: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:B:223:ARG:C	1:B:224:MET:HE2	2.40	0.47
1:A:56:ALA:O	1:A:202:LYS:HG3	2.15	0.46
1:B:64:SER:C	1:B:66:SER:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:202:LYS:NZ	2:B:592:HOH:O	2.48	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:135:LEU:C	1:B:135:LEU:HD13	2.42	0.45
1:B:16:LEU:HB2	1:B:39:PHE:HE2	1.82	0.45
1:A:62:ILE:HD13	1:A:142:MET:CE	2.42	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:B:110:ASN:HD21	1:B:112:MET:HB2	1.83	0.44
1:A:202:LYS:NZ	2:A:559:HOH:O	2.51	0.44
1:A:315:THR:HG22	1:A:315:THR:O	2.18	0.44
1:B:64:SER:C	1:B:66:SER:N	2.76	0.44
1:A:64:SER:C	1:A:66:SER:H	2.25	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:417:ILE:HD11	1:A:421:GLY:C	2.42	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:222:GLU:HB2	1:B:224:MET:HE3	1.99	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
1:B:272:ARG:NH2	1:B:308:ASP:CB	2.82	0.42
1:B:101:LEU:C	1:B:103:ALA:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:443:ASP:OD1	1:A:443:ASP:C	2.62	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: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: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: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:64:SER:C	1:A:66:SER:N	2.78	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
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%)	12	15
1	B	405/456 (89%)	380 (94%)	21 (5%)	4 (1%)	12	15
All	All	814/912 (89%)	769 (94%)	37 (4%)	8 (1%)	12	15

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%)	308 (98%)	5 (2%)	55	73
1	B	311/341 (91%)	299 (96%)	12 (4%)	28	43
All	All	624/682 (92%)	607 (97%)	17 (3%)	39	58

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

Mol	Chain	Res	Type
1	A	47	THR
1	A	160	GLU
1	A	250	LEU
1	A	266	LEU
1	A	321	GLU
1	B	47	THR
1	B	70	THR
1	B	78	ARG
1	B	158	GLU
1	B	160	GLU
1	B	201	VAL
1	B	248	GLN
1	B	250	LEU
1	B	266	LEU
1	B	272	ARG
1	B	345	ASP
1	B	383	THR

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	26	GLN
1	A	86	GLN
1	A	110	ASN
1	A	121	HIS
1	A	248	GLN
1	A	389	HIS
1	B	26	GLN
1	B	110	ASN
1	B	121	HIS
1	B	181	GLN
1	B	248	GLN
1	B	433	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 [i](#)

There are no oligosaccharides 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%)	0.58	56 (13%) 7 8	19, 33, 75, 110	0
1	B	411/456 (90%)	0.47	51 (12%) 8 9	19, 34, 75, 109	0
All	All	826/912 (90%)	0.52	107 (12%) 7 8	19, 34, 75, 110	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	GLY	6.4
1	B	388	VAL	6.2
1	A	324	GLY	5.8
1	B	445	GLU	5.4
1	A	387	ALA	4.7
1	A	379	LEU	4.7
1	B	353	GLY	4.7
1	B	444	PRO	4.6
1	A	351	ARG	4.6
1	A	388	VAL	4.6
1	B	324	GLY	4.5
1	A	382	ALA	4.5
1	A	445	GLU	4.4
1	B	437	VAL	4.4
1	B	387	ALA	4.2
1	A	437	VAL	3.8
1	A	406	THR	3.8
1	A	383	THR	3.7
1	A	103	ALA	3.6
1	A	380	SER	3.6
1	A	393	ALA	3.6
1	A	377	ALA	3.6
1	A	325	ASP	3.5
1	B	429	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	432	LEU	3.5
1	B	432	LEU	3.4
1	B	320	VAL	3.4
1	A	378	ALA	3.4
1	A	322	ARG	3.3
1	A	402	GLY	3.3
1	A	323	GLU	3.3
1	B	381	ALA	3.2
1	B	382	ALA	3.2
1	A	350	LEU	3.2
1	A	320	VAL	3.1
1	A	404	ILE	3.1
1	A	403	PRO	3.1
1	A	444	PRO	3.1
1	B	389	HIS	3.0
1	B	440	GLU	3.0
1	A	417	ILE	3.0
1	A	201	VAL	3.0
1	A	439	VAL	3.0
1	B	404	ILE	3.0
1	B	384	GLY	3.0
1	A	394	ALA	2.9
1	A	429	VAL	2.9
1	B	394	ALA	2.9
1	B	416	ARG	2.9
1	B	434	ALA	2.9
1	B	325	ASP	2.9
1	B	102	GLU	2.8
1	A	352	THR	2.8
1	A	384	GLY	2.8
1	B	201	VAL	2.8
1	B	443	ASP	2.8
1	B	323	GLU	2.8
1	A	327	VAL	2.8
1	A	102	GLU	2.7
1	A	426	ALA	2.7
1	A	419	ASP	2.7
1	B	417	ILE	2.7
1	A	415	ASP	2.6
1	B	322	ARG	2.6
1	B	351	ARG	2.6
1	A	433	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	103	ALA	2.6
1	A	405	ARG	2.6
1	B	383	THR	2.6
1	A	416	ARG	2.6
1	B	433	GLN	2.6
1	A	438	ARG	2.6
1	B	438	ARG	2.5
1	A	392	ALA	2.5
1	B	392	ALA	2.5
1	B	422	ARG	2.5
1	B	419	ASP	2.5
1	B	101	LEU	2.4
1	B	85	ARG	2.4
1	A	434	ALA	2.4
1	A	436	GLY	2.4
1	A	385	GLY	2.4
1	B	436	GLY	2.4
1	B	104	GLU	2.4
1	A	8	TYR	2.3
1	A	47	THR	2.3
1	A	440	GLU	2.3
1	A	441	VAL	2.3
1	A	386	GLY	2.3
1	B	246	ALA	2.3
1	B	391	ALA	2.3
1	B	321	GLU	2.3
1	A	326	ARG	2.2
1	B	326	ARG	2.2
1	B	439	VAL	2.2
1	B	310	ASP	2.2
1	A	435	ASP	2.2
1	A	407	VAL	2.1
1	B	407	VAL	2.1
1	B	406	THR	2.1
1	B	319	PHE	2.1
1	B	402	GLY	2.1
1	B	352	THR	2.1
1	A	104	GLU	2.1
1	A	408	VAL	2.1
1	B	50	LEU	2.0
1	B	415	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.