



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:15 AM UTC

PDB ID : 3AGD / pdb_00003agd
Title : Crystal structure of Mglu in its native form in the presence of 4.3M NaCl
Authors : Yoshimune, K.; Shirakihara, Y.; Yumoto, I.
Deposited on : 2010-03-30
Resolution : 2.20 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	:	4-5-2 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

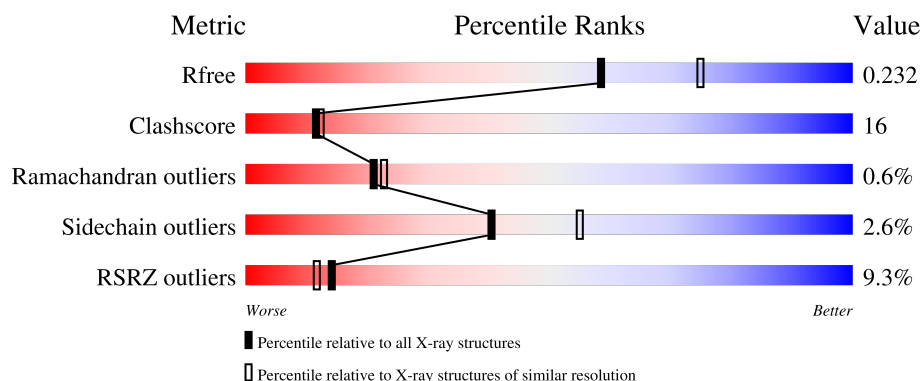
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	8% 71% 23% • •
1	B	456	10% 71% 22% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7283 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	440	Total	C	N	O	S	0	0	0
			3273	2036	599	623	15			
1	B	435	Total	C	N	O	S	0	0	0
			3240	2017	593	615	15			

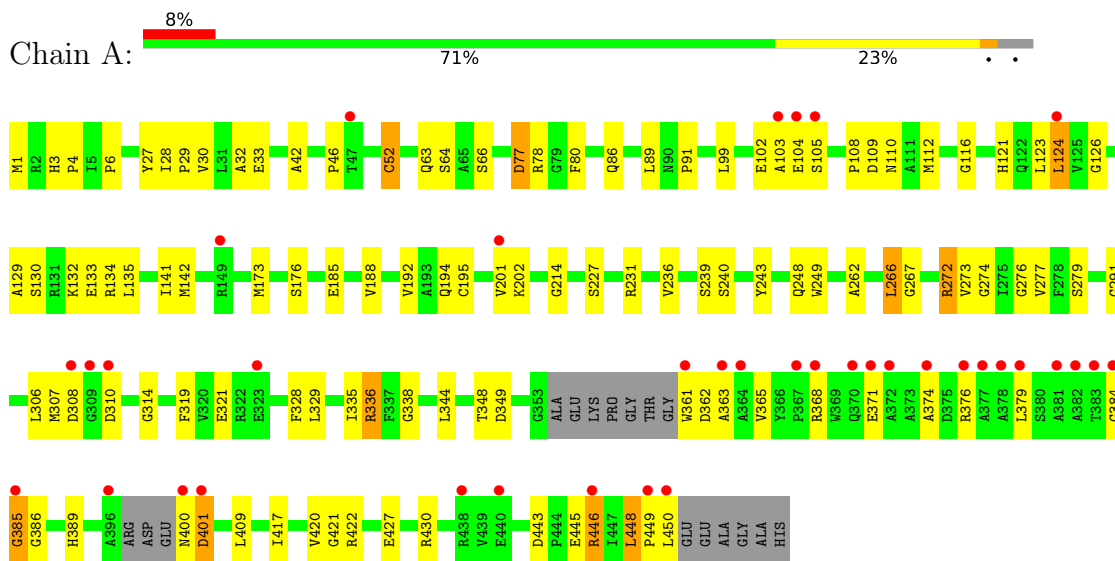
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	415	Total	O	0	0
			415	415		
2	B	355	Total	O	0	0
			355	355		

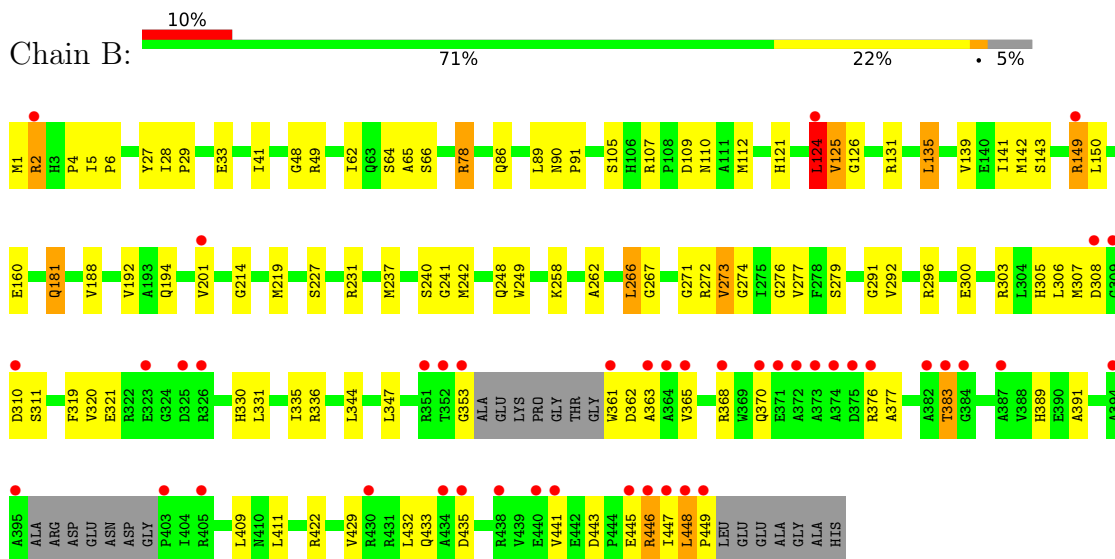
3 Residue-property plots [i](#)

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	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.81Å 131.15Å 73.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.40 – 2.20 59.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.40-2.20) 100.0 (59.40-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.194 , 0.236 0.194 , 0.232	Depositor DCC
R_{free} test set	2950 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7283	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/3324	0.95	13/4512 (0.3%)
1	B	0.36	0/3291	0.92	10/4466 (0.2%)
All	All	0.36	0/6615	0.93	23/8978 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ASP	N-CA-C	7.44	119.03	111.07
1	A	124	LEU	N-CA-C	7.07	125.85	110.80
1	B	125	VAL	N-CA-C	7.01	117.15	110.42
1	B	273	VAL	N-CA-C	6.88	117.38	107.88
1	A	273	VAL	N-CA-C	6.69	117.11	107.88
1	B	249	TRP	N-CA-C	6.63	119.06	111.11
1	A	335	ILE	N-CA-C	6.50	117.48	107.99
1	B	126	GLY	CA-C-N	6.30	126.51	119.32
1	B	126	GLY	C-N-CA	6.30	126.51	119.32
1	A	249	TRP	N-CA-C	6.29	118.66	111.11
1	A	77	ASP	N-CA-C	6.26	118.19	111.36
1	A	279	SER	CA-C-N	5.76	127.04	119.84
1	A	279	SER	C-N-CA	5.76	127.04	119.84
1	B	335	ILE	N-CA-C	5.55	116.72	108.23
1	A	272	ARG	N-CA-C	5.53	120.53	113.18
1	A	80	PHE	N-CA-C	5.46	116.91	111.07
1	A	274	GLY	N-CA-C	-5.35	102.53	110.71
1	A	243	TYR	N-CA-C	5.33	117.78	111.33
1	A	239	SER	N-CA-C	5.32	117.15	111.36
1	B	279	SER	CA-C-N	5.20	126.34	119.84
1	B	279	SER	C-N-CA	5.20	126.34	119.84
1	B	124	LEU	N-CA-C	5.15	121.77	110.80
1	B	109	ASP	N-CA-C	5.01	119.59	111.37

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	3273	0	3261	113	0
1	B	3240	0	3233	116	0
2	A	415	0	0	22	0
2	B	355	0	0	22	0
All	All	7283	0	6494	208	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 16.

All (208) 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:112:MET:HE3	1:B:258:LYS:HD3	1.47	0.94
1:A:376:ARG:HG2	1:A:389:HIS:HB2	1.51	0.92
1:B:110:ASN:HD22	1:B:112:MET:H	1.17	0.89
1:A:308:ASP:HB3	2:A:783:HOH:O	1.72	0.89
1:A:129:ALA:HB3	1:A:134:ARG:NH1	1.86	0.89
1:B:376:ARG:HG2	1:B:389:HIS:HB2	1.56	0.87
1:A:110:ASN:HD22	1:A:112:MET:H	1.22	0.84
1:A:231:ARG:HD3	2:A:696:HOH:O	1.77	0.83
1:A:336:ARG:HH11	1:A:336:ARG:HB3	1.42	0.83
1:B:62:ILE:HG21	1:B:142:MET:HE1	1.63	0.79
1:B:347:LEU:HD22	1:B:432:LEU:HD11	1.68	0.76
1:A:134:ARG:NH1	2:A:720:HOH:O	2.21	0.74
1:A:103:ALA:HB2	2:A:718:HOH:O	1.88	0.72
1:A:361:TRP:CZ3	1:A:363:ALA:HA	2.26	0.70
1:B:310:ASP:HB3	2:B:637:HOH:O	1.91	0.70
1:A:185:GLU:HG2	2:A:539:HOH:O	1.92	0.69
1:B:443:ASP:OD2	1:B:446:ARG:HA	1.92	0.69
1:A:384:GLY:O	1:A:386:GLY:N	2.26	0.69
1:A:336:ARG:NH1	2:A:856:HOH:O	2.26	0.68
1:A:306:LEU:HD21	1:B:307:MET:HE1	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:VAL:HG23	2:B:514:HOH:O	1.94	0.67
1:A:443:ASP:OD2	1:A:446:ARG:HA	1.95	0.67
1:B:272:ARG:HH12	1:B:308:ASP:CG	2.01	0.67
1:A:344:LEU:HD13	1:B:4:PRO:HG2	1.75	0.66
1:A:443:ASP:CG	1:A:446:ARG:HA	2.20	0.66
1:A:376:ARG:CG	1:A:389:HIS:HB2	2.25	0.66
1:A:231:ARG:HH12	1:B:303:ARG:NH1	1.93	0.66
1:A:310:ASP:HB3	2:B:795:HOH:O	1.95	0.66
1:A:449:PRO:O	1:A:450:LEU:HB2	1.95	0.66
1:A:307:MET:HE1	1:B:306:LEU:HD21	1.77	0.66
1:A:99:LEU:HD23	1:A:102:GLU:OE1	1.96	0.66
1:A:3:HIS:O	1:A:6:PRO:HD2	1.96	0.65
1:A:336:ARG:HH11	1:A:336:ARG:CB	2.10	0.65
1:B:443:ASP:CG	1:B:446:ARG:HA	2.22	0.65
1:B:241:GLY:O	1:B:242:MET:HE2	1.94	0.65
1:A:201:VAL:HG13	1:A:276:GLY:O	1.97	0.64
1:A:1:MET:HB3	1:B:435:ASP:OD2	1.97	0.64
1:A:86:GLN:HE21	1:A:86:GLN:HA	1.63	0.64
1:B:2:ARG:HD3	2:B:651:HOH:O	1.97	0.64
1:A:129:ALA:HB3	1:A:134:ARG:HH12	1.63	0.63
1:B:78:ARG:NE	2:B:704:HOH:O	2.30	0.63
1:A:308:ASP:HB2	1:B:336:ARG:NH1	2.13	0.63
1:B:62:ILE:HD13	1:B:142:MET:HE3	1.80	0.63
1:A:231:ARG:NH2	2:A:727:HOH:O	2.32	0.63
1:B:362:ASP:HB3	1:B:365:VAL:HG23	1.82	0.62
1:A:29:PRO:O	1:A:33:GLU:HG2	1.99	0.61
1:B:201:VAL:HG13	1:B:276:GLY:C	2.25	0.61
1:A:201:VAL:HG23	2:A:603:HOH:O	1.99	0.61
1:B:242:MET:HE3	1:B:258:LYS:HA	1.83	0.60
1:A:314:GLY:HA3	1:A:385:GLY:HA2	1.82	0.60
1:A:231:ARG:HH12	1:B:303:ARG:HH11	1.47	0.60
1:A:448:LEU:N	1:A:449:PRO:HD2	2.17	0.60
1:A:336:ARG:HB3	1:A:336:ARG:NH1	2.14	0.59
1:A:27:TYR:CD1	1:A:28:ILE:HG23	2.37	0.59
1:A:231:ARG:NH1	1:B:303:ARG:HH11	2.01	0.58
1:A:310:ASP:O	1:B:311:SER:HA	2.03	0.58
1:B:422:ARG:NH1	1:B:447:ILE:O	2.36	0.58
1:B:5:ILE:HB	1:B:6:PRO:HD3	1.85	0.58
2:A:851:HOH:O	1:B:303:ARG:HG3	2.04	0.58
1:B:292:VAL:O	1:B:296:ARG:HG3	2.03	0.57
1:A:348:THR:HG22	2:A:824:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:NH1	1:A:123:LEU:O	2.37	0.57
1:A:4:PRO:HG2	1:B:344:LEU:HD13	1.88	0.56
1:B:361:TRP:CH2	1:B:370:GLN:HG2	2.41	0.56
1:B:91:PRO:HA	1:B:240:SER:OG	2.05	0.56
1:A:77:ASP:OD2	1:A:124:LEU:O	2.23	0.55
1:B:78:ARG:CZ	2:B:704:HOH:O	2.54	0.55
1:A:427:GLU:HA	1:A:430:ARG:HE	1.71	0.54
1:B:105:SER:O	1:B:107:ARG:NE	2.36	0.54
1:B:110:ASN:HD22	1:B:112:MET:N	1.98	0.54
1:A:362:ASP:HB3	1:A:365:VAL:CG2	2.38	0.54
1:A:201:VAL:HG13	1:A:276:GLY:C	2.33	0.53
1:B:29:PRO:HG2	2:B:638:HOH:O	2.07	0.53
1:B:361:TRP:CZ3	1:B:363:ALA:HA	2.44	0.53
1:B:331:LEU:HD12	1:B:411:LEU:CD2	2.39	0.53
1:A:427:GLU:HB2	1:A:430:ARG:HH21	1.74	0.53
1:A:46:PRO:O	1:B:383:THR:HG21	2.09	0.53
1:B:62:ILE:CD1	1:B:142:MET:HE3	2.38	0.53
1:B:376:ARG:CG	1:B:389:HIS:HB2	2.35	0.53
1:B:266:LEU:HD22	1:B:267:GLY:N	2.23	0.53
1:A:272:ARG:NH1	1:A:308:ASP:OD1	2.37	0.52
1:B:201:VAL:HG13	1:B:276:GLY:O	2.10	0.52
1:A:277:VAL:HG11	1:A:291:GLY:HA2	1.90	0.52
1:B:41:ILE:HA	1:B:201:VAL:HG11	1.91	0.52
1:B:125:VAL:N	2:B:765:HOH:O	2.43	0.52
1:A:110:ASN:ND2	1:A:112:MET:H	2.02	0.52
1:A:272:ARG:HH12	1:A:308:ASP:CG	2.17	0.52
1:A:78:ARG:HD3	1:A:126:GLY:HA2	1.91	0.51
1:B:242:MET:CE	1:B:258:LYS:HA	2.40	0.51
1:B:448:LEU:N	1:B:449:PRO:HD2	2.24	0.51
1:A:28:ILE:HD12	1:A:30:VAL:CG1	2.40	0.51
1:B:41:ILE:CA	1:B:201:VAL:HG11	2.41	0.51
1:B:319:PHE:HD2	1:B:321:GLU:HG3	1.75	0.51
1:A:420:VAL:CG2	1:B:303:ARG:HG2	2.41	0.51
1:A:319:PHE:CD2	1:A:321:GLU:HG3	2.46	0.50
1:A:379:LEU:C	1:A:379:LEU:HD13	2.36	0.50
1:B:121:HIS:HD2	1:B:194:GLN:OE1	1.94	0.50
1:A:134:ARG:NE	2:A:833:HOH:O	2.44	0.50
1:A:417:ILE:HD11	1:A:421:GLY:C	2.36	0.50
1:A:42:ALA:HB3	1:A:201:VAL:HG12	1.93	0.50
1:B:62:ILE:HG12	1:B:65:ALA:HB3	1.93	0.50
1:A:307:MET:HB2	1:B:231:ARG:CG	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HD22	1:B:139:VAL:HG23	1.94	0.50
1:B:188:VAL:O	1:B:192:VAL:HG23	2.11	0.50
1:A:46:PRO:O	1:B:383:THR:CG2	2.60	0.50
1:B:362:ASP:HB3	1:B:365:VAL:CG2	2.41	0.49
1:A:121:HIS:HD2	1:A:194:GLN:OE1	1.96	0.49
1:B:110:ASN:ND2	1:B:112:MET:H	1.97	0.49
1:A:368:ARG:HG3	2:A:756:HOH:O	2.13	0.49
1:B:429:VAL:O	1:B:433:GLN:HG3	2.12	0.49
1:A:89:LEU:O	1:B:248:GLN:HG3	2.13	0.49
1:B:272:ARG:NH1	1:B:308:ASP:OD2	2.45	0.49
1:B:2:ARG:NH1	2:B:651:HOH:O	2.43	0.48
1:A:134:ARG:NH2	2:A:833:HOH:O	2.46	0.48
1:B:29:PRO:O	1:B:33:GLU:HG2	2.13	0.48
1:B:112:MET:HE2	1:B:237:MET:HA	1.95	0.48
1:A:130:SER:OG	1:A:133:GLU:HG3	2.14	0.48
1:A:104:GLU:CD	1:A:105:SER:N	2.72	0.47
1:A:173:MET:O	1:A:176:SER:HB3	2.14	0.47
1:B:121:HIS:HE1	2:B:481:HOH:O	1.95	0.47
1:B:1:MET:HA	2:B:651:HOH:O	2.15	0.47
1:A:262:ALA:HB3	2:A:583:HOH:O	2.13	0.47
1:A:307:MET:HB2	1:B:231:ARG:HG2	1.95	0.47
1:B:149:ARG:HD2	1:B:150:LEU:O	2.14	0.47
1:B:330:HIS:HD2	2:B:793:HOH:O	1.97	0.47
1:B:143:SER:CB	1:B:149:ARG:HH11	2.28	0.47
1:A:63:GLN:HA	1:A:195:CYS:HB3	1.96	0.47
1:A:319:PHE:CD2	1:A:319:PHE:C	2.92	0.47
1:B:48:GLY:C	1:B:219:MET:HE1	2.40	0.47
1:A:103:ALA:HB3	2:A:606:HOH:O	2.16	0.46
1:B:300:GLU:O	1:B:303:ARG:HD2	2.16	0.46
1:B:361:TRP:HH2	1:B:370:GLN:HG2	1.80	0.46
1:A:308:ASP:CB	1:B:336:ARG:NH1	2.78	0.46
1:B:27:TYR:CD1	1:B:28:ILE:HG23	2.51	0.46
1:B:277:VAL:HG11	1:B:291:GLY:HA2	1.97	0.46
1:A:427:GLU:CB	1:A:430:ARG:HH21	2.29	0.46
1:B:303:ARG:NH1	2:B:726:HOH:O	2.47	0.46
1:A:52:CYS:SG	1:A:202:LYS:HE2	2.56	0.45
1:A:266:LEU:HD22	1:A:267:GLY:N	2.31	0.45
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.80	0.45
1:A:121:HIS:HE1	2:A:541:HOH:O	1.99	0.45
1:B:242:MET:HE3	1:B:258:LYS:CA	2.46	0.45
1:B:377:ALA:HB3	2:B:635:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HD3	2:A:720:HOH:O	2.16	0.45
1:A:308:ASP:CG	2:A:783:HOH:O	2.60	0.45
1:A:112:MET:HG2	1:A:236:VAL:HG12	1.99	0.45
1:A:308:ASP:CB	2:A:783:HOH:O	2.46	0.45
1:A:338:GLY:HA3	2:B:546:HOH:O	2.17	0.44
1:B:273:VAL:HG22	1:B:274:GLY:N	2.32	0.44
1:A:400:ASN:O	1:A:401:ASP:HB3	2.18	0.44
1:B:319:PHE:CD2	1:B:321:GLU:HG3	2.53	0.44
1:B:201:VAL:CG1	1:B:276:GLY:O	2.66	0.44
1:B:271:GLY:C	1:B:272:ARG:HG3	2.43	0.44
1:B:149:ARG:NH2	2:B:701:HOH:O	2.50	0.44
1:B:242:MET:CE	2:B:642:HOH:O	2.66	0.44
1:A:420:VAL:HG21	1:B:303:ARG:HG2	2.00	0.44
1:B:149:ARG:HA	1:B:149:ARG:HD3	1.79	0.43
1:B:305:HIS:CE1	1:B:307:MET:HG2	2.53	0.43
1:A:110:ASN:HD22	1:A:112:MET:N	2.03	0.43
1:B:363:ALA:HB1	1:B:370:GLN:HG3	2.00	0.43
1:B:445:GLU:O	1:B:446:ARG:C	2.60	0.43
1:A:4:PRO:CG	1:B:344:LEU:HD13	2.49	0.43
1:B:62:ILE:HD13	1:B:142:MET:CE	2.48	0.43
1:B:62:ILE:CG1	1:B:65:ALA:HB3	2.49	0.43
1:A:86:GLN:NE2	2:A:666:HOH:O	2.50	0.43
1:A:214:GLY:O	1:A:227:SER:HA	2.19	0.43
1:A:427:GLU:CA	1:A:430:ARG:HH21	2.30	0.43
1:B:78:ARG:NH2	2:B:704:HOH:O	2.52	0.43
1:B:266:LEU:CD2	1:B:267:GLY:N	2.82	0.42
1:A:427:GLU:HA	1:A:430:ARG:HH21	1.83	0.42
1:B:131:ARG:HB2	2:B:755:HOH:O	2.18	0.42
1:B:141:ILE:HG23	1:B:142:MET:N	2.34	0.42
1:A:86:GLN:HA	1:A:86:GLN:NE2	2.33	0.42
1:A:445:GLU:O	1:A:446:ARG:C	2.61	0.42
1:A:248:GLN:HG3	1:B:89:LEU:O	2.20	0.42
1:B:160:GLU:HG2	1:B:192:VAL:HG13	2.01	0.42
1:A:86:GLN:O	1:A:108:PRO:HD2	2.20	0.42
1:A:328:PHE:CD1	1:A:328:PHE:N	2.88	0.42
1:B:33:GLU:OE2	1:B:33:GLU:HA	2.19	0.42
1:A:110:ASN:O	1:A:116:GLY:HA3	2.20	0.41
1:A:64:SER:C	1:A:66:SER:H	2.27	0.41
1:A:201:VAL:CG1	1:A:276:GLY:O	2.65	0.41
1:A:362:ASP:HB3	1:A:365:VAL:HG23	2.01	0.41
1:A:379:LEU:HA	2:B:757:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ARG:HE	1:B:368:ARG:HB3	1.71	0.41
1:A:110:ASN:ND2	1:A:112:MET:HB2	2.35	0.41
1:B:441:VAL:HG11	1:B:448:LEU:HD12	2.03	0.41
1:A:29:PRO:HA	1:A:32:ALA:HB3	2.02	0.41
1:B:214:GLY:O	1:B:227:SER:HA	2.20	0.41
1:B:353:GLY:HA2	1:B:435:ASP:OD1	2.21	0.41
1:A:141:ILE:HG23	1:A:142:MET:N	2.36	0.41
1:A:188:VAL:O	1:A:192:VAL:HG23	2.20	0.41
1:A:91:PRO:HA	1:A:240:SER:OG	2.20	0.41
1:A:134:ARG:CZ	2:A:833:HOH:O	2.68	0.41
1:B:64:SER:C	1:B:66:SER:H	2.28	0.41
1:B:368:ARG:HG2	2:B:693:HOH:O	2.21	0.41
1:B:432:LEU:O	1:B:435:ASP:HB2	2.21	0.41
1:A:371:GLU:O	1:A:374:ALA:HB3	2.20	0.41
1:B:160:GLU:HG2	1:B:192:VAL:CG1	2.51	0.41
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.81	0.40
1:B:262:ALA:HB3	2:B:521:HOH:O	2.21	0.40
1:B:320:VAL:HG11	1:B:391:ALA:HA	2.03	0.40
1:A:368:ARG:NH1	2:A:755:HOH:O	2.55	0.40
1:A:422:ARG:HG3	1:A:448:LEU:O	2.21	0.40
1:B:90:ASN:HA	1:B:91:PRO:HD2	1.98	0.40
1:B:181:GLN:N	1:B:181:GLN:HE21	2.19	0.40
1:A:349:ASP:OD1	1:B:49:ARG:NH2	2.51	0.40
1:B:86:GLN:HA	1:B:86:GLN:HE21	1.87	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	434/456 (95%)	418 (96%)	13 (3%)	3 (1%)	18 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	429/456 (94%)	414 (96%)	13 (3%)	2 (0%)	24	27
All	All	863/912 (95%)	832 (96%)	26 (3%)	5 (1%)	21	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	GLY
1	B	124	LEU
1	A	446	ARG
1	B	446	ARG
1	A	401	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/341 (97%)	323 (98%)	8 (2%)	43	58
1	B	328/341 (96%)	319 (97%)	9 (3%)	39	53
All	All	659/682 (97%)	642 (97%)	17 (3%)	40	55

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

Mol	Chain	Res	Type
1	A	52	CYS
1	A	132	LYS
1	A	135	LEU
1	A	266	LEU
1	A	329	LEU
1	A	336	ARG
1	A	409	LEU
1	A	448	LEU
1	B	2	ARG
1	B	78	ARG
1	B	135	LEU

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Mol	Chain	Res	Type
1	B	149	ARG
1	B	181	GLN
1	B	266	LEU
1	B	383	THR
1	B	409	LEU
1	B	448	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	26	GLN
1	A	86	GLN
1	A	110	ASN
1	A	121	HIS
1	A	330	HIS
1	B	26	GLN
1	B	86	GLN
1	B	110	ASN
1	B	121	HIS
1	B	181	GLN
1	B	330	HIS
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	440/456 (96%)	-0.01	37 (8%) 17 14	13, 24, 56, 80	0
1	B	435/456 (95%)	0.03	44 (10%) 12 10	10, 24, 61, 76	0
All	All	875/912 (95%)	0.01	81 (9%) 14 12	10, 24, 60, 80	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	450	LEU	7.7
1	B	361	TRP	5.4
1	A	384	GLY	4.9
1	B	384	GLY	4.9
1	A	361	TRP	4.8
1	A	372	ALA	4.2
1	A	382	ALA	4.0
1	B	353	GLY	3.9
1	B	449	PRO	3.8
1	A	383	THR	3.6
1	A	401	ASP	3.6
1	A	385	GLY	3.5
1	A	400	ASN	3.5
1	B	310	ASP	3.4
1	B	395	ALA	3.3
1	A	374	ALA	3.3
1	B	383	THR	3.2
1	B	352	THR	3.2
1	B	149	ARG	3.2
1	B	374	ALA	3.2
1	A	310	ASP	3.1
1	A	309	GLY	3.1
1	A	377	ALA	3.0
1	B	309	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	308	ASP	3.0
1	B	201	VAL	2.9
1	B	447	ILE	2.9
1	A	378	ALA	2.9
1	B	364	ALA	2.9
1	B	403	PRO	2.9
1	A	396	ALA	2.8
1	B	308	ASP	2.8
1	A	103	ALA	2.8
1	B	351	ARG	2.8
1	A	201	VAL	2.7
1	B	435	ASP	2.7
1	A	381	ALA	2.6
1	B	375	ASP	2.6
1	B	430	ARG	2.6
1	B	363	ALA	2.6
1	B	325	ASP	2.6
1	A	367	PRO	2.6
1	A	363	ALA	2.5
1	A	438	ARG	2.5
1	A	124	LEU	2.5
1	B	441	VAL	2.5
1	B	445	GLU	2.5
1	B	434	ALA	2.5
1	B	371	GLU	2.4
1	A	368	ARG	2.4
1	B	372	ALA	2.4
1	B	440	GLU	2.4
1	A	364	ALA	2.3
1	B	394	ALA	2.3
1	B	326	ARG	2.3
1	B	438	ARG	2.3
1	A	446	ARG	2.3
1	A	104	GLU	2.3
1	A	371	GLU	2.3
1	A	323	GLU	2.3
1	B	448	LEU	2.3
1	A	376	ARG	2.3
1	B	124	LEU	2.2
1	A	149	ARG	2.2
1	B	405	ARG	2.2
1	B	446	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	449	PRO	2.2
1	B	382	ALA	2.2
1	A	105	SER	2.2
1	B	387	ALA	2.2
1	B	376	ARG	2.1
1	B	323	GLU	2.1
1	B	368	ARG	2.1
1	A	440	GLU	2.1
1	B	370	GLN	2.1
1	A	47	THR	2.1
1	B	2	ARG	2.1
1	A	370	GLN	2.1
1	A	379	LEU	2.1
1	B	365	VAL	2.0
1	B	373	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 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.