



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:46 AM UTC

PDB ID : 4R0Y / pdb_00004r0y
Title : Structure of Maltose-binding Protein Fusion with the C-terminal GH1 domain of Guanylate Kinase-associated Protein from *Rattus norvegicus*
Authors : Im, Y.J.; Tong, J.
Deposited on : 2014-08-03
Resolution : 2.00 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

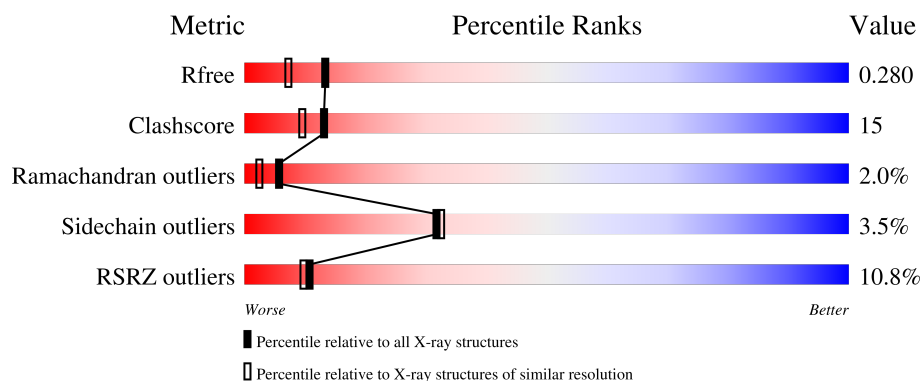
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	501	
1	B	501	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7611 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 Maltose-binding periplasmic protein, Disks large-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3695	2367	613	701	14			
1	B	473	Total	C	N	O	S	0	0	0
			3735	2393	621	707	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	ALA	-	linker	UNP P0AEX9
A	363	MET	-	linker	UNP P0AEX9
A	917	VAL	-	linker	UNP P97836
A	918	ASP	-	linker	UNP P97836
B	362	ALA	-	linker	UNP P0AEX9
B	363	MET	-	linker	UNP P0AEX9
B	917	VAL	-	linker	UNP P97836
B	918	ASP	-	linker	UNP P97836

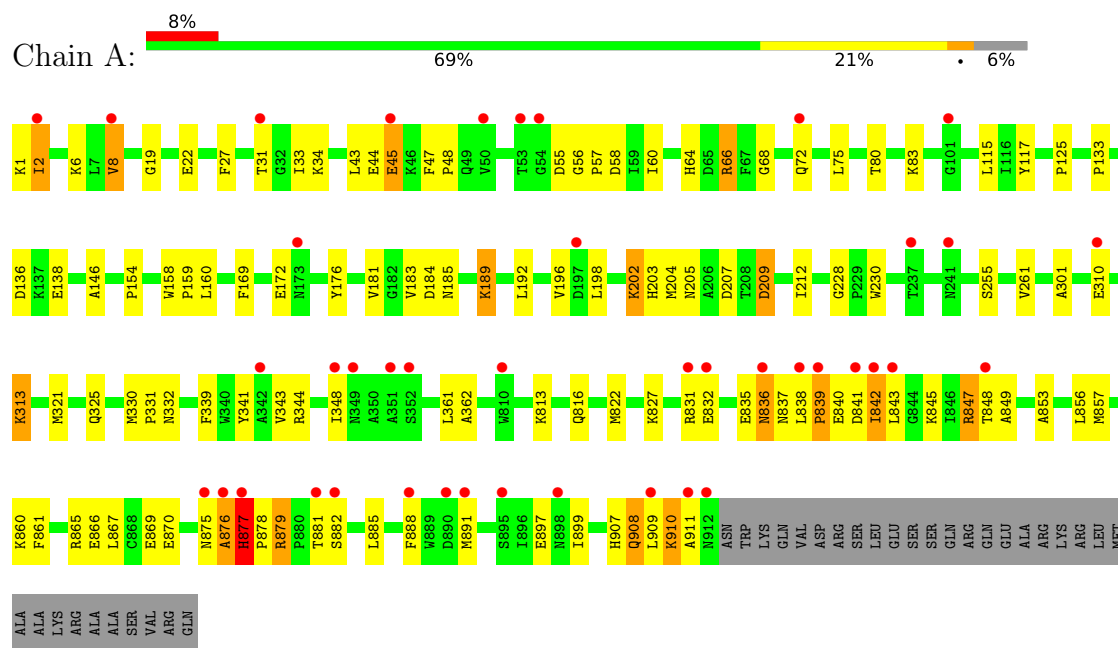
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		
2	B	90	Total	O	0	0
			90	90		

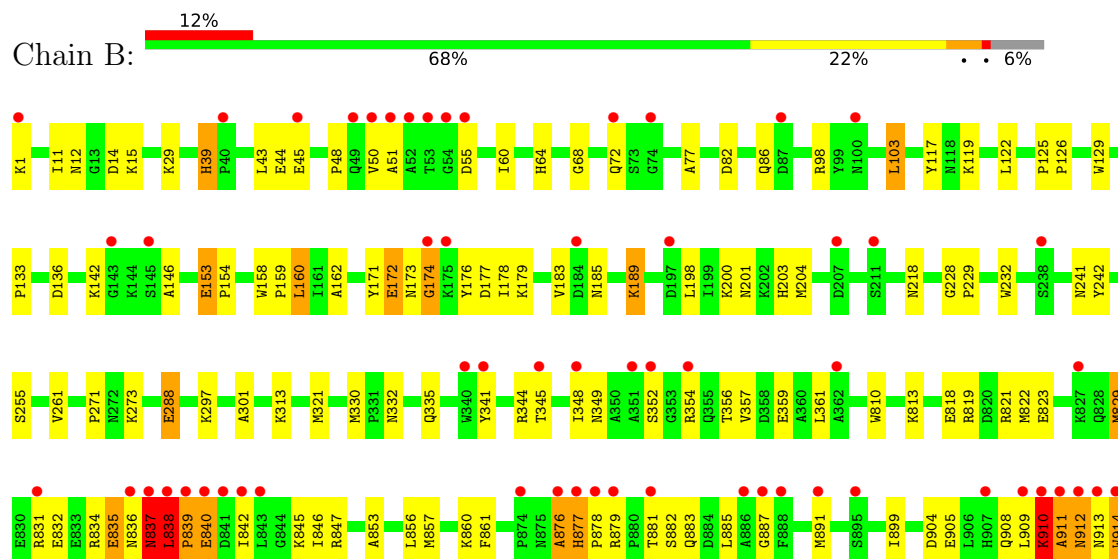
3 Residue-property plots [i](#)

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: Maltose-binding periplasmic protein, Disks large-associated protein 1



- Molecule 1: Maltose-binding periplasmic protein, Disks large-associated protein 1



K915	Q916
VAL	ASP
ARG	ARG
SER	SER
LEU	LEU
GLU	GLU
SER	SER
SER	SER
GLN	GLN
ARG	ARG
GLN	GLN
GLU	GLU
ALA	ALA
ARG	ARG
LYS	LYS
ARG	ARG
LEU	LEU
MET	MET
ALA	ALA
ALA	ALA
LYS	LYS
ARG	ARG
ALA	ALA
ALA	ALA
SER	SER
VAL	VAL
ARG	ARG
GLN	GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.11Å 158.68Å 65.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.52 – 2.00 39.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.52-2.00) 96.8 (39.52-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.91 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.281 0.243 , 0.280	Depositor DCC
R_{free} test set	3452 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7611	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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	0.41	0/3783	0.87	4/5125 (0.1%)
1	B	0.40	0/3825	0.89	15/5182 (0.3%)
All	All	0.41	0/7608	0.88	19/10307 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	SER	N-CA-C	-7.40	100.06	110.50
1	B	255	SER	N-CA-C	-7.01	100.62	110.50
1	B	313	LYS	N-CA-C	-6.10	105.10	112.54
1	A	313	LYS	N-CA-C	-5.95	105.12	112.38
1	B	915	LYS	N-CA-C	-5.85	98.34	110.80
1	B	837	ASN	N-CA-C	5.84	123.23	110.80
1	B	876	ALA	N-CA-C	5.69	118.67	109.86
1	B	914	TRP	N-CA-C	5.57	117.76	108.02
1	B	153	GLU	CA-C-N	5.50	125.85	119.47
1	B	153	GLU	C-N-CA	5.50	125.85	119.47
1	B	271	PRO	N-CA-C	-5.46	107.69	114.68
1	B	838	LEU	CA-C-N	5.36	126.53	119.84
1	B	838	LEU	C-N-CA	5.36	126.53	119.84
1	B	228	GLY	CA-C-N	5.31	124.97	119.56
1	B	228	GLY	C-N-CA	5.31	124.97	119.56
1	A	80	THR	N-CA-C	5.29	118.26	109.79
1	B	174	GLY	N-CA-C	-5.19	107.83	115.30
1	A	841	ASP	N-CA-C	5.18	116.62	110.97
1	B	242	TYR	N-CA-C	5.01	117.50	110.14

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	3695	0	3642	101	0
1	B	3735	0	3679	120	0
2	A	91	0	0	2	0
2	B	90	0	0	0	0
All	All	7611	0	7321	219	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 15.

All (219) 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:876:ALA:HB2	1:B:879:ARG:HB2	1.37	1.06
1:A:64:HIS:HD2	1:A:261:VAL:H	1.09	0.91
1:A:64:HIS:CD2	1:A:261:VAL:H	1.89	0.90
1:A:198:LEU:HD13	1:A:204:MET:HE3	1.57	0.85
1:A:31:THR:HG23	1:A:33:ILE:H	1.41	0.84
1:B:43:LEU:HD13	1:B:60:ILE:HD11	1.61	0.81
1:B:172:GLU:CD	1:B:173:ASN:H	1.89	0.80
1:A:816:GLN:CD	1:B:834:ARG:HH21	1.93	0.76
1:A:837:ASN:C	1:A:838:LEU:HD23	2.12	0.75
1:B:98:ARG:HG2	1:B:103:LEU:HD12	1.68	0.74
1:B:1:LYS:HD2	1:B:1:LYS:N	2.03	0.73
1:A:831:ARG:O	1:A:835:GLU:HG2	1.88	0.73
1:B:876:ALA:HB1	1:B:878:PRO:C	2.14	0.72
1:A:154:PRO:HG3	1:A:344:ARG:HA	1.72	0.71
1:B:829:MET:HE3	1:B:829:MET:HA	1.71	0.71
1:A:44:GLU:HG2	1:A:45:GLU:OE1	1.91	0.70
1:A:877:HIS:H	1:A:878:PRO:HA	1.57	0.69
1:A:66:ARG:HB3	1:A:66:ARG:HH21	1.57	0.69
1:A:66:ARG:HB3	1:A:66:ARG:NH2	2.07	0.69
1:B:876:ALA:CB	1:B:879:ARG:HB2	2.19	0.69
1:B:822:MET:HE2	1:B:853:ALA:HB1	1.74	0.69
1:A:907:HIS:C	1:A:909:LEU:H	2.01	0.68
1:B:64:HIS:HD2	1:B:261:VAL:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:832:GLU:HG2	1:B:911:ALA:HB3	1.75	0.68
1:B:43:LEU:CD1	1:B:60:ILE:HD11	2.24	0.67
1:B:839:PRO:HB2	1:B:842:ILE:HB	1.75	0.67
1:B:154:PRO:HG3	1:B:344:ARG:HA	1.77	0.67
1:A:877:HIS:H	1:A:878:PRO:CA	2.08	0.67
1:A:27:PHE:O	1:A:31:THR:HG22	1.95	0.67
1:B:910:LYS:HD3	1:B:911:ALA:N	2.10	0.65
1:B:185:ASN:O	1:B:189:LYS:HE3	1.96	0.65
1:A:192:LEU:O	1:A:196:VAL:HG23	1.97	0.65
1:A:876:ALA:HA	1:A:879:ARG:HB2	1.77	0.65
1:A:869:GLU:CD	1:B:847:ARG:HH12	2.05	0.64
1:B:846:ILE:HD11	1:B:911:ALA:HB1	1.81	0.63
1:B:877:HIS:H	1:B:878:PRO:CA	2.10	0.63
1:B:344:ARG:O	1:B:348:ILE:HG12	1.99	0.63
1:A:184:ASP:OD2	1:A:362:ALA:HA	1.99	0.62
1:A:6:LYS:HD2	1:A:34:LYS:HE2	1.80	0.62
1:B:178:ILE:HD12	1:B:335:GLN:HG2	1.80	0.62
1:B:877:HIS:H	1:B:878:PRO:C	2.07	0.62
1:B:881:THR:HG22	1:B:883:GLN:H	1.65	0.62
1:A:838:LEU:HD12	1:A:842:ILE:HG21	1.82	0.61
1:A:837:ASN:C	1:A:839:PRO:HD3	2.26	0.61
1:A:875:ASN:O	1:A:876:ALA:O	2.19	0.60
1:B:834:ARG:O	1:B:835:GLU:C	2.45	0.59
1:A:301:ALA:HB1	1:A:321:MET:HE2	1.83	0.59
1:A:341:TYR:CE2	1:A:813:LYS:HE2	2.37	0.59
1:A:822:MET:HE1	1:A:899:ILE:HD13	1.85	0.59
1:B:910:LYS:O	1:B:912:ASN:N	2.36	0.58
1:A:68:GLY:HA3	1:A:332:ASN:O	2.03	0.57
1:A:185:ASN:O	1:A:189:LYS:HE3	2.04	0.57
1:B:839:PRO:O	1:B:840:GLU:CB	2.51	0.57
1:B:822:MET:HE3	1:B:899:ILE:HG21	1.86	0.57
1:A:822:MET:CE	1:A:899:ILE:HG21	2.35	0.57
1:A:64:HIS:HE1	1:A:330:MET:O	1.88	0.57
1:A:310:GLU:O	1:A:313:LYS:HG2	2.04	0.57
1:A:205:ASN:HB3	1:A:207:ASP:OD1	2.05	0.57
1:B:64:HIS:HE1	1:B:330:MET:O	1.87	0.56
1:A:909:LEU:O	1:A:910:LYS:CB	2.53	0.56
1:A:847:ARG:HH11	1:A:847:ARG:HG2	1.71	0.56
1:B:831:ARG:O	1:B:835:GLU:HB2	2.06	0.56
1:B:43:LEU:HD13	1:B:60:ILE:CD1	2.31	0.56
1:B:288:GLU:CD	1:B:288:GLU:H	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:ARG:HG2	1:A:847:ARG:NH1	2.21	0.55
1:B:822:MET:HE2	1:B:853:ALA:CB	2.36	0.55
1:A:838:LEU:HD13	1:A:911:ALA:HB1	1.89	0.55
1:B:832:GLU:HG2	1:B:911:ALA:CB	2.37	0.54
1:A:136:ASP:HA	1:A:146:ALA:HB2	1.90	0.54
1:A:83:LYS:O	1:A:83:LYS:HD3	2.08	0.54
1:A:838:LEU:O	1:A:842:ILE:HG22	2.06	0.54
1:B:43:LEU:HD12	1:B:43:LEU:C	2.33	0.54
1:A:909:LEU:O	1:A:910:LYS:HB3	2.07	0.54
1:A:891:MET:HE3	1:A:891:MET:HA	1.90	0.54
1:B:818:GLU:OE1	1:B:821:ARG:HD3	2.07	0.54
1:B:881:THR:HG22	1:B:882:SER:N	2.23	0.54
1:A:344:ARG:O	1:A:348:ILE:HD13	2.07	0.54
1:B:189:LYS:HD3	1:B:361:LEU:HD12	1.89	0.54
1:B:200:LYS:HE3	1:B:201:ASN:HD21	1.73	0.53
1:B:178:ILE:CD1	1:B:335:GLN:HG2	2.39	0.53
1:B:1:LYS:HD2	1:B:1:LYS:H3	1.74	0.53
1:B:200:LYS:HG3	1:B:201:ASN:ND2	2.23	0.53
1:A:832:GLU:OE1	1:A:911:ALA:HB2	2.10	0.52
1:B:876:ALA:HB1	1:B:879:ARG:N	2.24	0.52
1:A:865:ARG:O	1:A:869:GLU:HG3	2.10	0.52
1:B:119:LYS:HB2	1:B:241:ASN:ND2	2.25	0.52
1:B:912:ASN:C	1:B:914:TRP:H	2.18	0.52
1:B:877:HIS:O	1:B:877:HIS:ND1	2.42	0.52
1:A:133:PRO:HB3	1:A:203:HIS:CE1	2.44	0.52
1:B:178:ILE:HD13	1:B:818:GLU:OE2	2.10	0.52
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.44	0.51
1:B:136:ASP:OD2	1:B:203:HIS:HD2	1.92	0.51
1:B:172:GLU:OE2	1:B:173:ASN:N	2.43	0.51
1:A:822:MET:HE2	1:A:853:ALA:HB1	1.93	0.51
1:A:838:LEU:N	1:A:839:PRO:HD3	2.25	0.51
1:B:189:LYS:HG3	1:B:357:VAL:HG12	1.93	0.51
1:B:341:TYR:CE2	1:B:813:LYS:HE2	2.44	0.51
1:B:877:HIS:N	1:B:878:PRO:CA	2.74	0.51
1:A:845:LYS:O	1:A:848:THR:HG22	2.11	0.51
1:A:857:MET:O	1:A:861:PHE:HB2	2.10	0.51
1:B:12:ASN:ND2	1:B:14:ASP:OD1	2.38	0.51
1:B:172:GLU:CD	1:B:173:ASN:N	2.64	0.51
1:B:218:ASN:N	1:B:218:ASN:HD22	2.09	0.51
1:A:836:ASN:CB	1:A:838:LEU:HD22	2.41	0.50
1:A:907:HIS:C	1:A:909:LEU:N	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:GLN:NE2	2:A:1050:HOH:O	2.44	0.50
1:A:48:PRO:HA	1:A:75:LEU:HD13	1.94	0.50
1:A:83:LYS:HD3	1:A:83:LYS:C	2.36	0.50
1:B:15:LYS:C	1:B:297:LYS:HD2	2.37	0.50
1:A:183:VAL:CG1	1:A:361:LEU:HD22	2.42	0.50
1:A:8:VAL:HG13	1:A:57:PRO:HA	1.93	0.49
1:A:822:MET:HE2	1:A:853:ALA:CB	2.41	0.49
1:B:177:ASP:OD1	1:B:179:LYS:HB2	2.12	0.49
1:B:172:GLU:OE2	1:B:173:ASN:ND2	2.45	0.49
1:B:904:ASP:O	1:B:908:GLN:HG3	2.12	0.49
1:A:64:HIS:HD2	1:A:261:VAL:N	1.93	0.49
1:A:842:ILE:HD13	1:A:842:ILE:O	2.12	0.49
1:B:356:THR:OG1	1:B:359:GLU:HG3	2.13	0.49
1:A:881:THR:O	1:A:885:LEU:HD13	2.12	0.49
1:B:158:TRP:CE2	1:B:162:ALA:HB2	2.47	0.49
1:B:117:TYR:CE2	1:B:125:PRO:HD3	2.48	0.48
1:B:838:LEU:HA	1:B:839:PRO:HD3	1.63	0.48
1:B:1:LYS:HD2	1:B:1:LYS:H1	1.74	0.48
1:B:183:VAL:HG21	1:B:810:TRP:CH2	2.48	0.48
1:A:341:TYR:CD2	1:A:813:LYS:HE2	2.49	0.48
1:A:2:ILE:HG12	1:A:56:GLY:O	2.13	0.47
1:B:68:GLY:HA3	1:B:332:ASN:O	2.13	0.47
1:B:133:PRO:HB3	1:B:203:HIS:CE1	2.49	0.47
1:B:842:ILE:HG21	1:B:911:ALA:HA	1.96	0.47
1:A:136:ASP:OD2	1:A:203:HIS:HD2	1.97	0.47
1:B:857:MET:O	1:B:861:PHE:HB2	2.15	0.47
1:A:908:GLN:O	1:A:909:LEU:HD23	2.15	0.47
1:A:43:LEU:C	1:A:43:LEU:HD12	2.40	0.46
1:B:39:HIS:CD2	1:B:39:HIS:N	2.83	0.46
1:B:171:TYR:CE1	1:B:174:GLY:HA2	2.50	0.46
1:A:198:LEU:HD13	1:A:204:MET:CE	2.37	0.46
1:A:867:LEU:HD13	1:A:888:PHE:CE2	2.51	0.46
1:A:877:HIS:H	1:A:878:PRO:C	2.24	0.46
1:A:907:HIS:O	1:A:909:LEU:N	2.48	0.46
1:B:910:LYS:HD3	1:B:910:LYS:C	2.41	0.46
1:A:1:LYS:HA	1:A:55:ASP:OD1	2.15	0.45
1:A:202:LYS:HZ2	1:A:202:LYS:HB3	1.81	0.45
1:B:45:GLU:O	1:B:48:PRO:HG2	2.17	0.45
1:A:209:ASP:OD1	1:A:212:ILE:HG13	2.16	0.45
1:A:881:THR:HG22	1:A:882:SER:N	2.32	0.45
1:A:910:LYS:HG3	1:A:911:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:838:LEU:N	1:B:838:LEU:HD23	2.31	0.45
1:B:909:LEU:C	1:B:909:LEU:HD12	2.41	0.45
1:A:66:ARG:NH2	2:A:1072:HOH:O	2.49	0.45
1:A:19:GLY:O	1:A:22:GLU:HB2	2.16	0.45
1:A:47:PHE:CG	1:A:60:ILE:HD12	2.52	0.45
1:A:158:TRP:N	1:A:159:PRO:CD	2.80	0.45
1:A:837:ASN:O	1:A:838:LEU:C	2.60	0.44
1:B:829:MET:HE2	1:B:911:ALA:HB2	1.99	0.44
1:B:887:GLY:O	1:B:891:MET:HG2	2.17	0.44
1:A:6:LYS:CE	1:A:34:LYS:HE2	2.47	0.44
1:A:848:THR:HG23	1:A:849:ALA:N	2.31	0.44
1:A:154:PRO:HG3	1:A:344:ARG:CA	2.45	0.44
1:A:866:GLU:O	1:A:870:GLU:HG3	2.17	0.44
1:B:178:ILE:HG12	1:B:178:ILE:O	2.18	0.44
1:B:345:THR:HG22	1:B:349:ASN:ND2	2.32	0.44
1:A:176:TYR:CZ	1:A:331:PRO:HA	2.52	0.44
1:A:836:ASN:HB2	1:A:838:LEU:HD22	2.00	0.44
1:B:82:ASP:O	1:B:86:GLN:HG3	2.18	0.44
1:B:98:ARG:HG2	1:B:103:LEU:CD1	2.44	0.44
1:B:136:ASP:HA	1:B:146:ALA:HB2	1.98	0.44
1:B:837:ASN:C	1:B:838:LEU:HD23	2.42	0.44
1:B:856:LEU:HD12	1:B:860:LYS:CG	2.47	0.44
1:B:43:LEU:HD12	1:B:44:GLU:N	2.33	0.44
1:B:122:LEU:HD21	1:B:126:PRO:HD3	2.00	0.44
1:A:856:LEU:CD1	1:A:860:LYS:HD2	2.47	0.44
1:B:51:ALA:HA	1:B:55:ASP:O	2.17	0.44
1:B:352:SER:OG	1:B:354:ARG:NH1	2.51	0.44
1:A:202:LYS:HB3	1:A:202:LYS:NZ	2.33	0.43
1:A:31:THR:HG23	1:A:33:ILE:N	2.21	0.43
1:B:912:ASN:O	1:B:914:TRP:N	2.45	0.43
1:A:66:ARG:HH21	1:A:66:ARG:CB	2.27	0.43
1:B:153:GLU:HA	1:B:154:PRO:HD3	1.82	0.43
1:B:50:VAL:HG23	1:B:51:ALA:N	2.33	0.43
1:B:876:ALA:O	1:B:877:HIS:HB2	2.16	0.43
1:B:877:HIS:N	1:B:878:PRO:HA	2.32	0.43
1:B:173:ASN:O	1:B:173:ASN:OD1	2.37	0.43
1:B:909:LEU:O	1:B:910:LYS:O	2.37	0.43
1:B:835:GLU:HB3	1:B:836:ASN:H	1.64	0.43
1:B:171:TYR:HB2	1:B:176:TYR:CE1	2.53	0.43
1:A:339:PHE:CZ	1:A:343:VAL:HG21	2.54	0.43
1:B:64:HIS:CD2	1:B:261:VAL:H	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ALA:HB1	1:B:321:MET:HE2	2.01	0.42
1:B:356:THR:HG23	1:B:359:GLU:OE1	2.19	0.42
1:A:8:VAL:HG12	1:A:58:ASP:OD2	2.19	0.42
1:B:829:MET:HA	1:B:829:MET:CE	2.45	0.42
1:B:198:LEU:CD1	1:B:204:MET:HE2	2.50	0.42
1:B:64:HIS:CE1	1:B:330:MET:O	2.69	0.42
1:B:914:TRP:CZ3	1:B:916:GLN:HB3	2.55	0.42
1:A:877:HIS:N	1:A:878:PRO:C	2.78	0.42
1:A:836:ASN:HB3	1:A:838:LEU:HD22	2.00	0.42
1:A:228:GLY:HA3	1:A:230:TRP:CH2	2.55	0.41
1:A:845:LYS:C	1:A:848:THR:HG22	2.45	0.41
1:B:842:ILE:HG22	1:B:846:ILE:HG13	2.01	0.41
1:B:829:MET:HE2	1:B:911:ALA:CB	2.50	0.41
1:B:185:ASN:C	1:B:189:LYS:HE3	2.45	0.41
1:B:15:LYS:O	1:B:297:LYS:HD2	2.21	0.41
1:B:77:ALA:HB2	1:B:273:LYS:HE3	2.02	0.41
1:B:819:ARG:O	1:B:823:GLU:HG3	2.20	0.41
1:A:6:LYS:CD	1:A:34:LYS:HE2	2.46	0.41
1:A:839:PRO:O	1:A:840:GLU:HB2	2.21	0.41
1:A:877:HIS:N	1:A:878:PRO:CA	2.78	0.41
1:B:129:TRP:CE2	1:B:160:LEU:HG	2.55	0.41
1:B:845:LYS:HD3	1:B:905:GLU:OE2	2.21	0.41
1:B:857:MET:HA	1:B:861:PHE:HB2	2.03	0.41
1:A:117:TYR:CE2	1:A:125:PRO:HD3	2.56	0.41
1:B:11:ILE:O	1:B:39:HIS:HA	2.21	0.41
1:B:158:TRP:N	1:B:159:PRO:CD	2.84	0.40
1:B:914:TRP:CE3	1:B:914:TRP:HA	2.55	0.40
1:A:839:PRO:HA	1:A:843:LEU:CD1	2.51	0.40
1:B:142:LYS:O	1:B:142:LYS:HG2	2.21	0.40
1:B:881:THR:CG2	1:B:882:SER:N	2.83	0.40
1:B:136:ASP:OD2	1:B:203:HIS:CD2	2.73	0.40
1:A:169:PHE:CE1	1:A:181:VAL:HG22	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	467/501 (93%)	440 (94%)	20 (4%)	7 (2%)	8	4
1	B	471/501 (94%)	445 (94%)	14 (3%)	12 (2%)	4	1
All	All	938/1002 (94%)	885 (94%)	34 (4%)	19 (2%)	6	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	876	ALA
1	A	877	HIS
1	A	910	LYS
1	B	835	GLU
1	B	837	ASN
1	B	838	LEU
1	B	840	GLU
1	B	877	HIS
1	B	910	LYS
1	B	915	LYS
1	A	2	ILE
1	A	836	ASN
1	B	172	GLU
1	B	911	ALA
1	B	912	ASN
1	A	908	GLN
1	B	839	PRO
1	B	913	ASN
1	A	839	PRO

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	374/411 (91%)	357 (96%)	17 (4%)	24	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	388/411 (94%)	378 (97%)	10 (3%)	40	44
All	All	762/822 (93%)	735 (96%)	27 (4%)	32	32

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	45	GLU
1	A	66	ARG
1	A	72	GLN
1	A	115	LEU
1	A	138	GLU
1	A	160	LEU
1	A	172	GLU
1	A	189	LYS
1	A	202	LYS
1	A	209	ASP
1	A	827	LYS
1	A	842	ILE
1	A	847	ARG
1	A	877	HIS
1	A	879	ARG
1	A	897	GLU
1	B	29	LYS
1	B	39	HIS
1	B	72	GLN
1	B	103	LEU
1	B	160	LEU
1	B	189	LYS
1	B	288	GLU
1	B	829	MET
1	B	885	LEU
1	B	910	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	86	GLN
1	A	201	ASN
1	A	203	HIS

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Mol	Chain	Res	Type
1	A	218	ASN
1	A	325	GLN
1	A	837	ASN
1	A	907	HIS
1	B	39	HIS
1	B	64	HIS
1	B	86	GLN
1	B	124	ASN
1	B	201	ASN
1	B	203	HIS
1	B	205	ASN
1	B	218	ASN
1	B	241	ASN
1	B	325	GLN
1	B	809	HIS
1	B	828	GLN
1	B	883	GLN
1	B	908	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 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 ⓘ

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	469/501 (93%)	0.78	42 (8%) 15 14	27, 45, 69, 95	0
1	B	473/501 (94%)	0.81	60 (12%) 8 7	30, 45, 78, 103	0
All	All	942/1002 (94%)	0.80	102 (10%) 11 10	27, 45, 74, 103	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	876	ALA	6.1
1	B	914	TRP	5.7
1	A	877	HIS	5.4
1	A	839	PRO	5.0
1	B	174	GLY	4.6
1	B	345	THR	4.2
1	A	881	THR	4.2
1	A	838	LEU	4.2
1	A	8	VAL	4.1
1	B	907	HIS	3.9
1	A	310	GLU	3.8
1	A	72	GLN	3.8
1	B	876	ALA	3.7
1	B	838	LEU	3.6
1	B	839	PRO	3.6
1	A	909	LEU	3.6
1	A	348	ILE	3.4
1	B	52	ALA	3.4
1	B	341	TYR	3.3
1	A	912	ASN	3.3
1	B	877	HIS	3.2
1	A	842	ILE	3.2
1	B	842	ILE	3.2
1	A	101	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	910	LYS	3.1
1	B	886	ALA	3.1
1	A	911	ALA	3.0
1	B	49	GLN	2.9
1	B	175	LYS	2.9
1	B	895	SER	2.9
1	B	831	ARG	2.8
1	A	31	THR	2.8
1	A	836	ASN	2.8
1	A	898	ASN	2.8
1	A	888	PHE	2.8
1	B	881	THR	2.8
1	A	351	ALA	2.8
1	B	362	ALA	2.8
1	A	891	MET	2.7
1	B	911	ALA	2.7
1	A	810	TRP	2.7
1	B	354	ARG	2.7
1	A	895	SER	2.6
1	B	55	ASP	2.6
1	B	145	SER	2.6
1	B	211	SER	2.6
1	B	51	ALA	2.6
1	A	241	ASN	2.6
1	A	2	ILE	2.5
1	B	841	ASP	2.5
1	B	351	ALA	2.5
1	B	72	GLN	2.5
1	B	891	MET	2.5
1	A	50	VAL	2.5
1	B	53	THR	2.5
1	B	184	ASP	2.4
1	B	340	TRP	2.4
1	A	237	THR	2.4
1	B	913	ASN	2.4
1	B	888	PHE	2.4
1	B	1	LYS	2.4
1	B	50	VAL	2.3
1	B	74	GLY	2.3
1	A	197	ASP	2.3
1	B	909	LEU	2.3
1	B	238	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	349	ASN	2.3
1	A	875	ASN	2.3
1	B	912	ASN	2.3
1	B	879	ARG	2.3
1	B	87	ASP	2.3
1	B	197	ASP	2.3
1	B	207	ASP	2.3
1	A	843	LEU	2.2
1	B	45	GLU	2.2
1	A	173	ASN	2.2
1	B	54	GLY	2.2
1	B	878	PRO	2.2
1	B	837	ASN	2.2
1	A	848	THR	2.2
1	A	54	GLY	2.1
1	B	827	LYS	2.1
1	B	836	ASN	2.1
1	A	832	GLU	2.1
1	B	874	PRO	2.1
1	A	342	ALA	2.1
1	A	352	SER	2.1
1	A	882	SER	2.1
1	A	890	ASP	2.1
1	B	40	PRO	2.1
1	B	143	GLY	2.1
1	B	348	ILE	2.1
1	B	100	ASN	2.1
1	B	916	GLN	2.1
1	A	45	GLU	2.0
1	B	843	LEU	2.0
1	A	831	ARG	2.0
1	A	53	THR	2.0
1	B	887	GLY	2.0
1	B	840	GLU	2.0
1	B	352	SER	2.0
1	A	841	ASP	2.0

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 [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.