



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:51 PM EDT

PDB ID : 1IN0 / pdb_00001in0
Title : YAJQ PROTEIN (HI1034)
Authors : Teplyakov, A.; Gilliland, G.L.; Structure 2 Function Project (S2F)
Deposited on : 2001-05-11
Resolution : 2.14 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

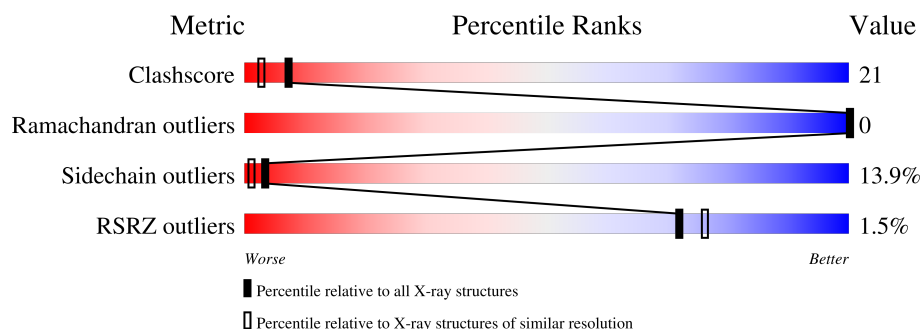
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	163	 51% 37% 10% ..
1	B	163	 3% 45% 34% 19% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2954 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 YAJQ PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1296	811	227	256	2			
1	B	162	Total	C	N	O	S	0	0	0
			1296	811	227	256	2			

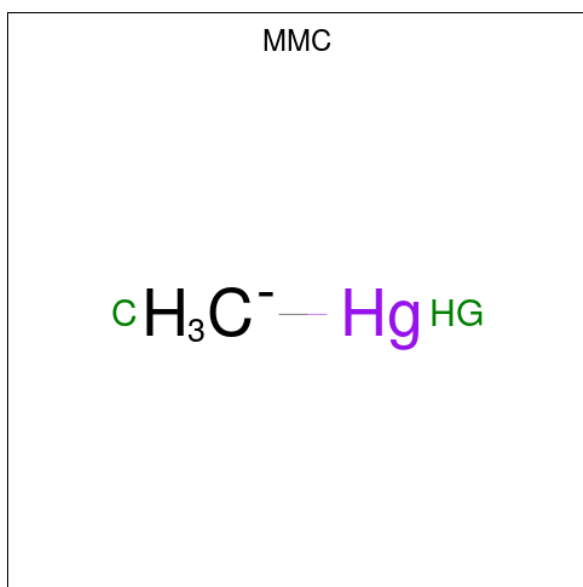
- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Hg	0	0
			1	1		
2	B	2	Total	Hg	0	0
			2	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is METHYL MERCURY ION (CCD ID: MMC) (formula: CH₃Hg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	Hg	0	0
			2	1	1		

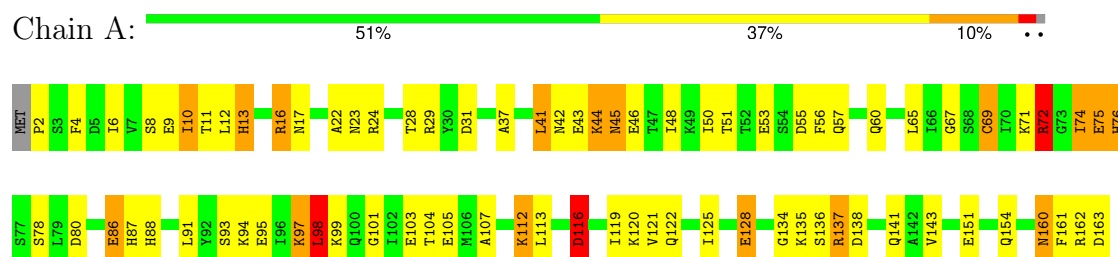
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	212	Total	O	0	0
			212	212		
5	B	143	Total	O	0	0
			143	143		

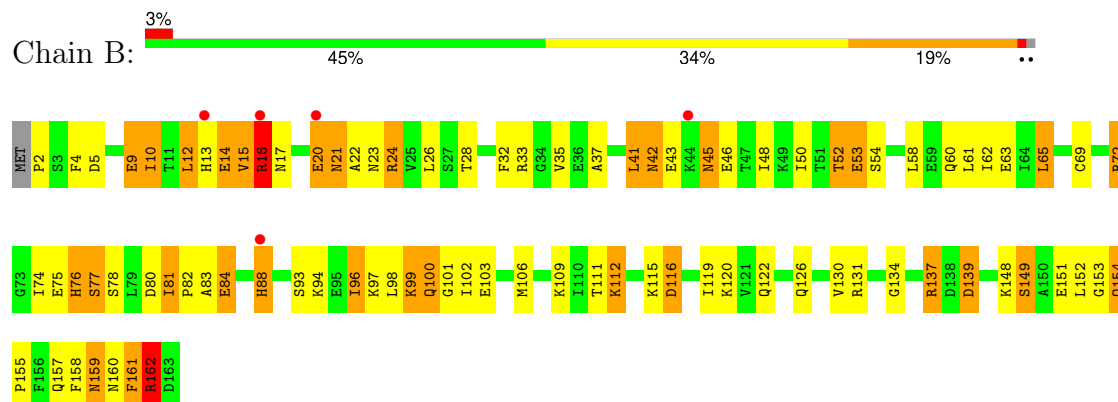
3 Residue-property plots

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: YAJQ PROTEIN



• Molecule 1: YAJQ PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	62.80Å 62.80Å 194.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.14 8.00 – 2.14	Depositor EDS
% Data completeness (in resolution range)	100.0 (8.00-2.14) 97.1 (8.00-2.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.13 (at 2.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , (Not available) 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 101.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2954	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HG, NA, MMC

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	0.96	0/1310	2.21	45/1757 (2.6%)
1	B	0.87	0/1310	2.22	65/1757 (3.7%)
All	All	0.92	0/2620	2.22	110/3514 (3.1%)

There are no bond length outliers.

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ASP	CA-CB-CG	16.10	128.70	112.60
1	B	101	GLY	CA-C-O	-12.29	113.75	122.23
1	A	137	ARG	CD-NE-CZ	11.31	140.24	124.40
1	B	37	ALA	CA-C-O	9.94	130.13	120.09
1	B	21	ASN	CA-CB-CG	9.77	122.37	112.60
1	A	23	ASN	CA-CB-CG	-9.58	103.02	112.60
1	A	137	ARG	NE-CZ-NH2	-8.87	111.22	119.20
1	B	162	ARG	CD-NE-CZ	8.59	136.43	124.40
1	B	21	ASN	O-C-N	8.39	130.71	122.07
1	B	131	ARG	NH1-CZ-NH2	-8.38	108.41	119.30
1	A	160	ASN	CA-C-O	8.33	131.50	121.84
1	A	87	HIS	CA-CB-CG	8.24	122.04	113.80
1	B	131	ARG	NE-CZ-NH2	7.78	126.20	119.20
1	B	82	PRO	CB-CA-C	7.71	121.41	111.46
1	A	48	ILE	CA-C-N	-7.63	112.19	122.72
1	A	48	ILE	C-N-CA	-7.63	112.19	122.72
1	A	74	ILE	CB-CA-C	-7.51	100.92	111.21
1	B	42	ASN	OD1-CG-ND2	7.21	129.81	122.60
1	B	112	LYS	CA-CB-CG	7.20	128.50	114.10
1	A	88	HIS	CA-CB-CG	-7.17	106.63	113.80
1	B	103	GLU	CB-CG-CD	-7.04	100.64	112.60
1	B	37	ALA	O-C-N	-6.93	116.56	123.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	GLN	OE1-CD-NE2	6.68	129.28	122.60
1	B	16	ARG	NE-CZ-NH2	-6.64	113.23	119.20
1	B	9	GLU	CB-CG-CD	6.54	123.72	112.60
1	B	54	SER	CA-C-O	-6.48	114.29	121.23
1	B	35	VAL	CA-C-O	-6.47	113.39	120.71
1	A	60	GLN	OE1-CD-NE2	6.42	129.02	122.60
1	B	139	ASP	O-C-N	6.41	129.72	122.22
1	B	126	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	A	151	GLU	CA-C-O	-6.34	113.72	121.89
1	B	10	ILE	O-C-N	6.33	129.82	123.18
1	B	48	ILE	O-C-N	6.33	129.91	123.20
1	B	5	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	29	ARG	CD-NE-CZ	6.25	133.15	124.40
1	B	22	ALA	CA-C-O	-6.18	113.11	120.10
1	A	69	CYS	CB-CA-C	-6.17	101.19	110.88
1	A	122	GLN	OE1-CD-NE2	6.15	128.75	122.60
1	B	32	PHE	CA-C-N	-6.15	112.14	120.82
1	B	32	PHE	C-N-CA	-6.15	112.14	120.82
1	B	76	HIS	CA-CB-CG	6.12	119.92	113.80
1	B	53	GLU	N-CA-C	6.08	120.40	112.92
1	B	159	ASN	OD1-CG-ND2	6.05	128.65	122.60
1	B	131	ARG	CD-NE-CZ	6.04	132.86	124.40
1	A	56	PHE	CA-C-O	5.99	127.11	120.82
1	A	17	ASN	CA-CB-CG	-5.98	106.62	112.60
1	B	84	GLU	CA-C-O	5.97	127.15	120.70
1	B	48	ILE	CA-C-O	-5.97	114.18	120.39
1	B	157	GLN	OE1-CD-NE2	5.89	128.49	122.60
1	B	15	VAL	CB-CA-C	-5.84	104.49	111.97
1	A	16	ARG	N-CA-C	-5.84	105.00	111.36
1	A	9	GLU	CA-C-N	-5.81	115.53	123.14
1	A	9	GLU	C-N-CA	-5.81	115.53	123.14
1	A	48	ILE	N-CA-CB	5.79	119.20	111.90
1	A	57	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	A	72	ARG	CD-NE-CZ	5.79	132.51	124.40
1	B	126	GLN	CG-CD-NE2	5.73	124.99	116.40
1	B	42	ASN	CA-CB-CG	-5.72	106.88	112.60
1	A	136	SER	N-CA-C	5.70	118.24	109.07
1	A	53	GLU	N-CA-C	5.69	120.22	113.16
1	B	130	VAL	CA-C-N	-5.69	114.17	122.19
1	B	130	VAL	C-N-CA	-5.69	114.17	122.19
1	A	13	HIS	N-CA-C	-5.58	105.10	111.07
1	B	139	ASP	CA-C-O	-5.58	113.79	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	LEU	CA-C-N	5.56	127.67	120.44
1	A	12	LEU	C-N-CA	5.56	127.67	120.44
1	A	57	GLN	CB-CG-CD	5.54	122.03	112.60
1	B	24	ARG	NH1-CZ-NH2	-5.54	112.09	119.30
1	B	100	GLN	O-C-N	5.53	129.57	122.93
1	A	143	VAL	O-C-N	5.53	127.31	121.89
1	B	83	ALA	O-C-N	5.51	128.43	122.15
1	B	41	LEU	CB-CA-C	-5.49	101.75	110.81
1	B	48	ILE	CB-CA-C	-5.49	102.97	110.77
1	B	120	LYS	CA-C-O	-5.45	115.60	122.63
1	A	94	LYS	O-C-N	5.42	129.60	123.42
1	B	63	GLU	CB-CG-CD	-5.41	103.41	112.60
1	B	161	PHE	CA-CB-CG	-5.40	108.40	113.80
1	A	22	ALA	CA-C-O	-5.40	114.83	120.55
1	A	6	ILE	N-CA-C	-5.37	100.69	108.36
1	B	52	THR	N-CA-CB	5.36	118.12	110.51
1	B	23	ASN	N-CA-CB	5.33	118.54	110.28
1	B	28	THR	CA-C-N	-5.32	115.34	122.42
1	B	28	THR	C-N-CA	-5.32	115.34	122.42
1	A	41	LEU	CA-C-O	-5.32	114.64	120.43
1	A	135	LYS	CA-C-O	5.31	126.06	119.79
1	B	76	HIS	O-C-N	5.29	127.59	122.09
1	B	111	THR	O-C-N	-5.29	116.51	122.12
1	B	81	ILE	N-CA-C	5.28	113.09	107.76
1	A	75	GLU	CA-C-N	5.25	127.57	120.38
1	A	75	GLU	C-N-CA	5.25	127.57	120.38
1	B	15	VAL	N-CA-CB	5.25	116.69	110.55
1	B	115	LYS	CB-CA-C	-5.23	102.60	110.92
1	B	99	LYS	CA-C-O	-5.21	115.92	122.63
1	A	128	GLU	N-CA-CB	-5.20	103.73	111.43
1	B	149	SER	CB-CA-C	5.18	120.06	109.55
1	B	81	ILE	CB-CA-C	-5.17	105.17	110.71
1	B	98	LEU	CA-C-N	-5.16	114.41	122.05
1	B	98	LEU	C-N-CA	-5.16	114.41	122.05
1	A	98	LEU	CA-C-O	-5.16	114.50	120.49
1	A	128	GLU	CA-C-O	-5.16	115.25	121.34
1	B	137	ARG	CA-C-O	5.14	125.88	119.97
1	A	55	ASP	N-CA-C	-5.12	105.70	111.28
1	B	60	GLN	CA-C-O	5.11	125.96	120.55
1	B	102	ILE	N-CA-CB	-5.09	105.05	111.41
1	A	60	GLN	CB-CG-CD	-5.05	104.02	112.60
1	A	161	PHE	CA-CB-CG	-5.04	108.76	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	GLU	CA-C-N	5.04	128.38	120.82
1	B	103	GLU	C-N-CA	5.04	128.38	120.82
1	A	91	LEU	N-CA-C	5.02	117.93	109.95
1	B	116	ASP	CB-CA-C	-5.01	99.74	110.32

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	1296	0	1323	36	1
1	B	1296	0	1323	71	1
2	A	1	0	0	0	0
2	B	2	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	1	0
5	A	212	0	0	8	0
5	B	143	0	0	3	0
All	All	2954	0	2646	108	1

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 21.

All (108) 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)
4:A:201:MMC:HG	4:A:201:MMC:C	1.44	1.26
1:A:160:ASN:HD21	1:A:162:ARG:NH2	1.65	0.94
1:B:2:PRO:HD2	1:B:134:GLY:O	1.70	0.89
1:B:16:ARG:NE	1:B:41:LEU:HD23	1.89	0.88
1:B:14:GLU:HG2	1:B:72:ARG:NH2	1.89	0.87
1:B:14:GLU:HB3	1:B:72:ARG:NE	1.89	0.86
1:B:50:ILE:HD13	1:B:62:ILE:HG13	1.56	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:MET:HE1	1:B:152:LEU:O	1.80	0.82
1:B:69:CYS:SG	2:B:202:HG:HG	1.98	0.82
1:B:14:GLU:HA	1:B:72:ARG:HE	1.46	0.80
1:B:14:GLU:HB3	1:B:72:ARG:CZ	2.14	0.77
1:B:17:ASN:HB2	1:B:72:ARG:HD3	1.67	0.77
1:B:65:LEU:HD21	1:B:96:ILE:HD13	1.71	0.73
1:A:76:HIS:CD2	1:A:76:HIS:C	2.67	0.73
1:B:50:ILE:CD1	1:B:62:ILE:HG13	2.19	0.72
1:B:148:LYS:HE3	1:B:158:PHE:CE2	2.25	0.71
1:A:119:ILE:HG22	1:A:121:VAL:HG13	1.73	0.71
1:B:50:ILE:HD12	1:B:58:LEU:HD12	1.74	0.68
1:B:77:SER:HB2	1:B:155:PRO:HD3	1.76	0.68
1:A:44:LYS:HD3	5:A:383:HOH:O	1.92	0.68
1:B:45:ASN:N	1:B:45:ASN:OD1	2.27	0.68
1:B:72:ARG:O	1:B:72:ARG:HG3	1.94	0.67
1:A:128:GLU:HA	5:A:361:HOH:O	1.95	0.67
1:B:21:ASN:HB2	5:B:283:HOH:O	1.94	0.67
1:A:107:ALA:HB1	1:A:125:ILE:HG12	1.78	0.66
1:B:16:ARG:HE	1:B:41:LEU:HD23	1.58	0.66
1:B:81:ILE:HG12	1:B:96:ILE:HG12	1.80	0.63
1:B:75:GLU:HG3	1:B:76:HIS:N	2.15	0.62
1:B:160:ASN:HD21	1:B:162:ARG:HH11	1.48	0.62
1:B:65:LEU:HD12	1:B:65:LEU:C	2.25	0.61
1:B:42:ASN:OD1	1:B:42:ASN:C	2.43	0.59
1:B:80:ASP:HB3	1:B:97:LYS:HB2	1.84	0.59
1:B:4:PHE:HB3	1:B:161:PHE:CD1	2.38	0.58
1:B:75:GLU:HG3	1:B:76:HIS:H	1.69	0.58
1:A:160:ASN:HD21	1:A:162:ARG:CZ	2.16	0.58
1:B:16:ARG:HD3	1:B:41:LEU:HD22	1.86	0.58
1:B:109:LYS:HE3	5:B:240:HOH:O	2.04	0.58
1:B:65:LEU:CD2	1:B:96:ILE:HD13	2.34	0.57
1:B:50:ILE:HD13	1:B:62:ILE:CG1	2.32	0.57
1:B:9:GLU:HG3	5:B:264:HOH:O	2.05	0.56
1:B:50:ILE:HD12	1:B:58:LEU:CD1	2.35	0.56
1:B:50:ILE:O	1:B:50:ILE:HG13	2.05	0.56
1:B:77:SER:O	1:B:99:LYS:NZ	2.39	0.56
1:B:26:LEU:HD13	1:B:61:LEU:CD2	2.37	0.55
1:B:15:VAL:HA	1:B:74:ILE:CD1	2.37	0.55
1:B:99:LYS:HD3	1:B:154:GLN:HB2	1.89	0.55
1:A:112:LYS:HD2	5:A:275:HOH:O	2.06	0.54
1:B:14:GLU:HA	1:B:72:ARG:NE	2.19	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:PRO:CD	1:B:134:GLY:O	2.51	0.54
1:B:14:GLU:CB	1:B:72:ARG:NE	2.68	0.54
1:A:41:LEU:HD12	1:A:42:ASN:N	2.22	0.54
1:A:76:HIS:CD2	1:A:76:HIS:O	2.61	0.54
1:A:69:CYS:HB3	1:A:74:ILE:O	2.08	0.54
1:A:10:ILE:HG21	1:A:98:LEU:HD13	1.91	0.52
1:B:78:SER:HA	1:B:99:LYS:HD2	1.92	0.52
1:B:99:LYS:NZ	1:B:153:GLY:O	2.44	0.51
1:B:75:GLU:CG	1:B:76:HIS:H	2.24	0.51
1:B:160:ASN:HD21	1:B:162:ARG:NH1	2.09	0.50
1:A:42:ASN:OD1	1:A:45:ASN:N	2.39	0.50
1:B:14:GLU:C	1:B:74:ILE:HD11	2.36	0.49
1:A:13:HIS:HB2	5:A:328:HOH:O	2.12	0.49
1:B:78:SER:C	1:B:99:LYS:HD2	2.37	0.49
1:B:12:LEU:HD11	1:B:43:GLU:HG2	1.94	0.48
1:A:24:ARG:O	1:A:28:THR:HG23	2.14	0.48
1:A:160:ASN:HD21	1:A:162:ARG:HH21	1.55	0.48
1:A:10:ILE:HD12	1:A:99:LYS:C	2.38	0.48
1:A:72:ARG:HA	1:A:72:ARG:HD3	1.63	0.48
1:A:4:PHE:C	1:A:4:PHE:CD1	2.91	0.48
1:A:24:ARG:NH2	5:A:273:HOH:O	2.46	0.47
1:B:88:HIS:CE1	1:B:93:SER:OG	2.67	0.47
1:B:159:ASN:C	1:B:159:ASN:OD1	2.58	0.47
1:A:2:PRO:HD2	1:A:134:GLY:O	2.14	0.47
1:A:105:GLU:HB3	5:A:277:HOH:O	2.15	0.46
1:A:37:ALA:HA	1:A:51:THR:O	2.15	0.46
1:B:75:GLU:CG	1:B:76:HIS:N	2.77	0.46
1:B:12:LEU:HA	1:B:15:VAL:HG23	1.97	0.46
1:B:14:GLU:CB	1:B:72:ARG:CZ	2.91	0.45
1:B:16:ARG:O	1:B:20:GLU:CD	2.59	0.45
1:B:15:VAL:N	1:B:74:ILE:HD11	2.31	0.45
1:B:119:ILE:CG2	1:B:139:ASP:HB3	2.46	0.45
1:B:13:HIS:N	1:B:13:HIS:CD2	2.84	0.45
1:B:16:ARG:HD3	1:B:41:LEU:CD2	2.46	0.44
1:A:43:GLU:HG2	5:A:384:HOH:O	2.17	0.44
1:A:50:ILE:HD13	1:A:50:ILE:HG21	1.74	0.44
1:A:103:GLU:O	1:A:104:THR:C	2.59	0.44
1:A:67:GLY:O	1:A:71:LYS:HD3	2.17	0.44
1:B:81:ILE:CG1	1:B:96:ILE:HG12	2.47	0.44
1:B:17:ASN:HB2	1:B:72:ARG:CD	2.44	0.44
1:A:16:ARG:NH2	1:A:43:GLU:CD	2.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:NE	1:B:41:LEU:CD2	2.71	0.43
1:B:41:LEU:HD21	1:B:43:GLU:CG	2.49	0.43
1:B:77:SER:O	1:B:99:LYS:CE	2.66	0.43
1:B:50:ILE:CD1	1:B:58:LEU:CD1	2.97	0.43
1:A:101:GLY:HA2	5:A:232:HOH:O	2.18	0.43
1:A:137:ARG:NH2	1:A:163:ASP:OD1	2.38	0.43
1:B:52:THR:OG1	1:B:53:GLU:N	2.49	0.42
1:A:80:ASP:HB3	1:A:97:LYS:HB2	2.00	0.42
1:B:77:SER:O	1:B:99:LYS:CD	2.68	0.42
1:A:86:GLU:H	1:A:86:GLU:HG3	1.60	0.42
1:B:41:LEU:CD2	1:B:43:GLU:HG3	2.50	0.42
1:A:50:ILE:O	1:A:93:SER:HB2	2.20	0.42
1:B:78:SER:CA	1:B:99:LYS:HD2	2.49	0.42
1:B:62:ILE:HD11	1:B:94:LYS:HD2	2.00	0.42
1:B:10:ILE:HD13	1:B:10:ILE:HA	1.65	0.41
1:B:14:GLU:CG	1:B:72:ARG:NH2	2.72	0.41
1:A:8:SER:CB	1:A:154:GLN:HE21	2.34	0.41
1:A:31:ASP:OD1	1:A:31:ASP:N	2.53	0.40
1:A:16:ARG:HH21	1:A:43:GLU:CD	2.29	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:OD2	1:B:116:ASP:OD2[8_664]	1.38	0.82

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	160/163 (98%)	158 (99%)	2 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
All	All	320/326 (98%)	311 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	147/148 (99%)	128 (87%)	19 (13%)	4	1
1	B	147/148 (99%)	125 (85%)	22 (15%)	3	1
All	All	294/296 (99%)	253 (86%)	41 (14%)	3	1

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	11	THR
1	A	44	LYS
1	A	45	ASN
1	A	46	GLU
1	A	65	LEU
1	A	72	ARG
1	A	75	GLU
1	A	76	HIS
1	A	78	SER
1	A	86	GLU
1	A	95	GLU
1	A	97	LYS
1	A	98	LEU
1	A	112	LYS
1	A	113	LEU
1	A	116	ASP
1	A	120	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	138	ASP
1	B	12	LEU
1	B	14	GLU
1	B	16	ARG
1	B	20	GLU
1	B	24	ARG
1	B	33	ARG
1	B	45	ASN
1	B	46	GLU
1	B	65	LEU
1	B	72	ARG
1	B	77	SER
1	B	84	GLU
1	B	88	HIS
1	B	96	ILE
1	B	100	GLN
1	B	112	LYS
1	B	122	GLN
1	B	137	ARG
1	B	149	SER
1	B	151	GLU
1	B	154	GLN
1	B	162	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	88	HIS
1	A	154	GLN
1	A	160	ASN
1	B	13	HIS
1	B	88	HIS
1	B	126	GLN
1	B	160	ASN

5.3.3 RNA ⓘ

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](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MMC	A	201	1	0,1,1	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	201	MMC	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	162/163 (99%)	-0.53	0 100 100	23, 39, 66, 86	0
1	B	162/163 (99%)	-0.27	5 (3%) 51 55	27, 43, 76, 87	0
All	All	324/326 (99%)	-0.40	5 (1%) 72 76	23, 41, 72, 87	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	HIS	4.5
1	B	44	LYS	3.7
1	B	88	HIS	2.9
1	B	16	ARG	2.4
1	B	20	GLU	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	203	1/1	0.91	0.09	34,34,34,34	0
2	HG	A	202	1/1	0.96	0.10	61,61,61,61	1
2	HG	B	202	1/1	0.97	0.03	67,67,67,67	1
3	NA	B	203	1/1	0.98	0.03	31,31,31,31	0
4	MMC	A	201	2/2	0.99	0.06	24,24,24,37	2
2	HG	B	201	1/1	1.00	0.02	49,49,49,49	1

6.5 Other polymers [i](#)

There are no such residues in this entry.