



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:57 AM UTC

PDB ID : 2WIA / pdb_00002wia
Title : Crystal Structures of the N-terminal Intracellular Domain of FeoB from Klebsiella Pneumoniae in Apo Form
Authors : Hung, K.-W.; Chang, Y.-W.; Chen, J.-H.; Chen, Y.-C.; Sun, Y.-J.; Hsiao, C.-D.; Huang, T.-H.
Deposited on : 2009-05-09
Resolution : 2.45 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

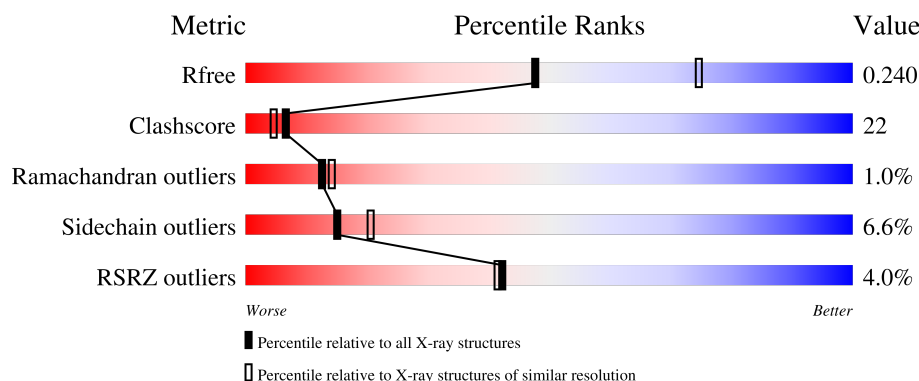
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	267	
1	B	267	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3889 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 FERROUS IRON TRANSPORT PROTEIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1864	1170	331	354	9			
1	B	252	Total	C	N	O	S	0	0	0
			1825	1142	323	351	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	GLN	LYS	conflict	UNP A6TF32
B	129	GLN	LYS	conflict	UNP A6TF32

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

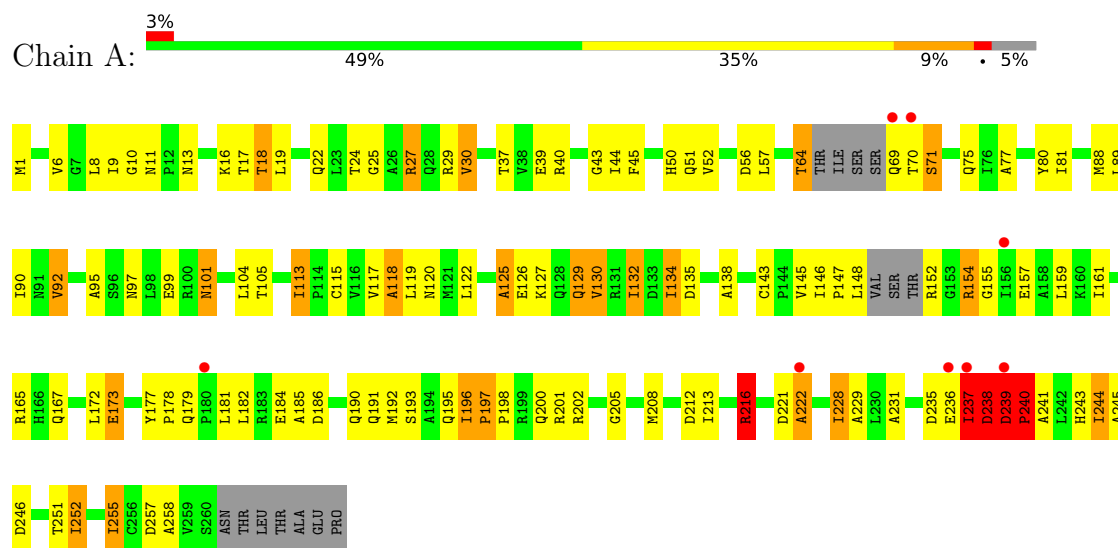
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total	O	0	0
			103	103		
3	B	95	Total	O	0	0
			95	95		

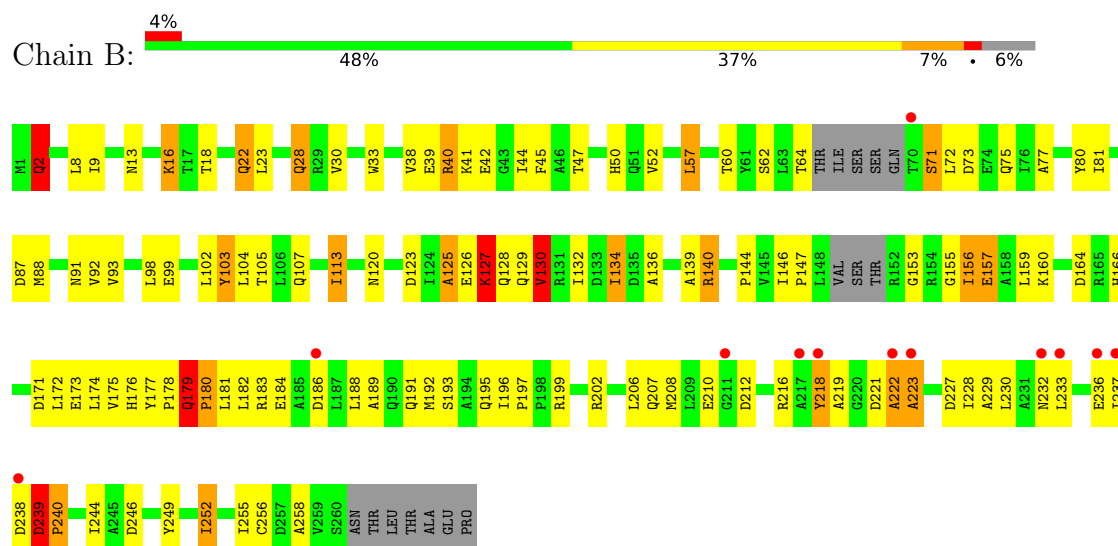
3 Residue-property plots [i](#)

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: FERROUS IRON TRANSPORT PROTEIN B



• Molecule 1: FERROUS IRON TRANSPORT PROTEIN B



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	84.20Å 84.20Å 122.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.13 – 2.45 25.13 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.3 (25.13-2.45) 97.8 (25.13-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.38 (at 2.44Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.209 , 0.230 0.215 , 0.240	Depositor DCC
R_{free} test set	876 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.216 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3889	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 5.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.86	25/1889 (1.3%)	1.80	42/2576 (1.6%)
1	B	1.95	33/1849 (1.8%)	1.88	53/2525 (2.1%)
All	All	1.91	58/3738 (1.6%)	1.84	95/5101 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	3
All	All	0	11

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	236	GLU	C-N	-22.17	1.04	1.33
1	B	103	TYR	C-O	10.58	1.36	1.24
1	B	237	ILE	C-N	10.13	1.41	1.33
1	B	195	GLN	C-N	9.37	1.42	1.33
1	B	239	ASP	C-N	8.89	1.45	1.34
1	A	134	ILE	CA-CB	8.87	1.66	1.54
1	A	237	ILE	C-N	8.73	1.46	1.33
1	B	191	GLN	C-O	8.03	1.34	1.24
1	B	127	LYS	CA-CB	7.84	1.66	1.53
1	B	179	GLN	C-N	7.49	1.44	1.33
1	A	240	PRO	N-CD	7.42	1.58	1.47
1	B	156	ILE	CA-CB	7.25	1.62	1.54
1	A	129	GLN	CA-CB	7.17	1.64	1.53
1	B	258	ALA	CA-C	7.14	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	THR	C-O	-7.11	1.15	1.24
1	B	125	ALA	C-N	7.10	1.42	1.33
1	A	252	ILE	CB-CG2	6.82	1.75	1.52
1	B	228	ILE	CA-CB	6.62	1.62	1.54
1	A	127	LYS	N-CA	6.57	1.53	1.46
1	B	134	ILE	CA-CB	6.55	1.63	1.54
1	A	239	ASP	C-N	6.52	1.43	1.33
1	B	179	GLN	C-O	-6.46	1.18	1.24
1	B	132	ILE	CA-CB	6.40	1.62	1.54
1	B	22	GLN	C-O	-6.35	1.16	1.24
1	B	175	VAL	CA-CB	-6.32	1.46	1.54
1	A	17	THR	N-CA	6.28	1.54	1.46
1	B	139	ALA	CA-C	-6.22	1.44	1.52
1	B	157	GLU	CA-C	-6.16	1.45	1.52
1	A	146	ILE	CA-C	6.16	1.58	1.53
1	B	130	VAL	CA-CB	6.12	1.61	1.53
1	B	140	ARG	N-CA	6.08	1.53	1.46
1	B	180	PRO	N-CD	6.05	1.56	1.47
1	A	258	ALA	CA-C	6.03	1.60	1.52
1	A	138	ALA	CA-CB	5.97	1.62	1.53
1	B	81	ILE	CA-CB	5.96	1.62	1.54
1	A	252	ILE	C-O	-5.88	1.17	1.24
1	B	132	ILE	C-O	5.86	1.30	1.24
1	A	145	VAL	C-O	5.81	1.30	1.24
1	A	159	LEU	C-O	5.68	1.30	1.24
1	A	118	ALA	CA-CB	-5.65	1.45	1.53
1	B	93	VAL	C-O	5.58	1.30	1.24
1	B	189	ALA	CA-C	5.54	1.60	1.52
1	B	113	ILE	N-CA	5.53	1.53	1.47
1	A	241	ALA	N-CA	5.53	1.53	1.46
1	B	16	LYS	N-CA	5.48	1.52	1.46
1	A	119	LEU	C-O	5.48	1.30	1.24
1	B	233	LEU	CA-CB	5.46	1.62	1.53
1	B	87	ASP	C-O	-5.20	1.17	1.24
1	A	246	ASP	C-O	5.18	1.30	1.24
1	A	30	VAL	CA-CB	5.16	1.60	1.54
1	B	60	THR	CA-CB	5.16	1.63	1.53
1	A	190	GLN	CA-C	5.09	1.59	1.52
1	B	258	ALA	C-O	5.09	1.30	1.24
1	A	135	ASP	N-CA	-5.09	1.39	1.46
1	A	45	PHE	N-CA	5.08	1.52	1.45
1	A	51	GLN	CA-CB	-5.07	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	ALA	N-CA	-5.04	1.40	1.46
1	B	93	VAL	CA-CB	5.02	1.60	1.54

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	HIS	CA-C-O	14.20	138.46	120.57
1	B	237	ILE	CA-C-N	-13.40	104.47	122.16
1	B	237	ILE	C-N-CA	-13.40	104.47	122.16
1	B	239	ASP	CA-C-N	-13.32	105.12	118.97
1	B	239	ASP	C-N-CA	-13.32	105.12	118.97
1	A	238	ASP	CA-C-N	13.16	153.91	121.80
1	A	238	ASP	C-N-CA	13.16	153.91	121.80
1	A	239	ASP	O-C-N	-12.50	106.94	121.32
1	A	71	SER	O-C-N	-12.40	110.15	123.42
1	A	240	PRO	CA-N-CD	-10.68	97.04	112.00
1	B	218	TYR	N-CA-C	-10.10	103.11	114.62
1	B	179	GLN	CA-C-O	10.06	127.88	118.63
1	B	239	ASP	O-C-N	-9.22	110.72	121.32
1	B	71	SER	N-CA-C	9.05	122.47	110.53
1	B	57	LEU	CA-C-N	-8.87	110.64	119.78
1	B	57	LEU	C-N-CA	-8.87	110.64	119.78
1	A	237	ILE	O-C-N	-8.54	111.89	122.57
1	A	120	ASN	N-CA-C	8.29	121.89	109.95
1	A	37	THR	N-CA-C	-8.05	102.49	112.88
1	B	73	ASP	CB-CA-C	-7.90	97.25	110.68
1	A	237	ILE	CA-C-O	-7.52	111.38	120.78
1	B	102	LEU	N-CA-C	-7.48	104.16	113.28
1	B	179	GLN	O-C-N	7.29	127.47	120.55
1	A	51	GLN	N-CA-C	-7.26	96.57	108.41
1	A	239	ASP	N-CA-C	7.16	125.63	109.81
1	A	236	GLU	N-CA-C	7.15	120.91	111.75
1	B	240	PRO	CA-N-CD	-7.13	102.02	112.00
1	B	189	ALA	N-CA-C	6.83	119.59	111.33
1	B	239	ASP	C-N-CD	6.78	152.80	125.00
1	A	11	ASN	CA-CB-CG	6.67	119.27	112.60
1	A	240	PRO	N-CA-C	6.62	124.50	113.78
1	B	189	ALA	CA-C-N	6.50	129.87	120.38
1	B	189	ALA	C-N-CA	6.50	129.87	120.38
1	A	236	GLU	CA-C-N	6.41	133.50	121.97
1	A	236	GLU	C-N-CA	6.41	133.50	121.97
1	B	136	ALA	N-CA-C	-6.38	103.84	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ASP	N-CA-C	6.36	117.88	111.07
1	A	240	PRO	O-C-N	-6.18	115.50	122.18
1	B	180	PRO	CA-N-CD	-6.11	103.45	112.00
1	B	221	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	216	ARG	CB-CA-C	-6.05	99.43	110.63
1	A	222	ALA	N-CA-C	6.02	118.65	109.62
1	A	101	ASN	N-CA-C	6.00	118.78	111.82
1	B	156	ILE	CA-C-N	5.96	128.18	120.44
1	B	156	ILE	C-N-CA	5.96	128.18	120.44
1	B	155	GLY	CA-C-O	-5.88	115.04	120.80
1	B	237	ILE	CA-C-O	-5.87	115.56	121.49
1	B	38	VAL	CB-CA-C	-5.86	101.78	111.32
1	B	179	GLN	CA-C-N	-5.81	113.20	119.24
1	B	179	GLN	C-N-CA	-5.81	113.20	119.24
1	B	40	ARG	CB-CG-CD	-5.79	97.97	111.30
1	B	113	ILE	CA-C-N	-5.79	113.97	119.76
1	B	113	ILE	C-N-CA	-5.79	113.97	119.76
1	A	238	ASP	O-C-N	-5.69	115.03	122.59
1	B	174	LEU	N-CA-C	5.68	117.95	111.02
1	B	77	ALA	CA-C-N	5.64	128.09	120.65
1	B	77	ALA	C-N-CA	5.64	128.09	120.65
1	B	103	TYR	CB-CA-C	5.62	120.99	110.70
1	B	103	TYR	O-C-N	-5.56	115.00	122.23
1	A	186	ASP	N-CA-C	5.55	117.41	111.36
1	B	125	ALA	CA-C-O	-5.54	114.97	120.90
1	A	122	LEU	N-CA-C	-5.53	106.38	113.23
1	B	73	ASP	N-CA-C	5.52	118.01	111.33
1	B	223	ALA	O-C-N	5.52	129.93	122.59
1	A	117	VAL	CA-C-N	-5.51	115.29	123.11
1	A	117	VAL	C-N-CA	-5.51	115.29	123.11
1	B	2	GLN	N-CA-C	-5.51	103.26	110.53
1	B	206	LEU	N-CA-C	5.45	117.22	111.28
1	A	246	ASP	N-CA-C	5.44	116.89	111.07
1	B	252	ILE	CB-CA-C	-5.44	104.89	112.02
1	A	11	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	B	222	ALA	CA-C-N	5.34	131.74	121.54
1	B	222	ALA	C-N-CA	5.34	131.74	121.54
1	A	238	ASP	CB-CA-C	5.33	121.02	110.42
1	B	176	HIS	O-C-N	-5.33	114.87	122.96
1	B	193	SER	O-C-N	5.32	129.62	122.82
1	A	92	VAL	CB-CA-C	-5.30	104.25	111.15
1	B	23	LEU	N-CA-C	5.30	117.47	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	THR	N-CA-C	5.27	117.45	111.02
1	B	22	GLN	N-CA-CB	5.25	117.67	110.07
1	A	10	GLY	CA-C-O	-5.23	116.49	121.62
1	A	197	PRO	CA-C-N	5.21	124.65	119.24
1	A	197	PRO	C-N-CA	5.21	124.65	119.24
1	A	113	ILE	CB-CA-C	-5.14	105.33	110.89
1	A	177	TYR	CA-C-N	-5.10	114.32	119.83
1	A	177	TYR	C-N-CA	-5.10	114.32	119.83
1	B	146	ILE	CA-C-N	5.10	126.50	120.23
1	B	146	ILE	C-N-CA	5.10	126.50	120.23
1	A	40	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	A	228	ILE	CA-C-N	5.05	127.31	120.44
1	A	228	ILE	C-N-CA	5.05	127.31	120.44
1	A	25	GLY	CA-C-N	5.03	129.22	120.68
1	A	25	GLY	C-N-CA	5.03	129.22	120.68
1	A	240	PRO	CB-CA-C	5.02	121.68	113.20
1	B	164	ASP	CB-CG-OD2	-5.02	106.86	118.40

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ILE	Mainchain,Peptide
1	A	238	ASP	Mainchain,Peptide
1	A	239	ASP	Mainchain
1	A	240	PRO	Mainchain
1	A	69	GLN	Mainchain
1	A	70	THR	Mainchain
1	B	103	TYR	Mainchain
1	B	223	ALA	Mainchain
1	B	239	ASP	Mainchain

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	1864	0	1823	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1825	0	1750	67	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	103	0	0	8	0
3	B	95	0	0	8	0
All	All	3889	0	3573	157	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 22.

All (157) 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:A:252:ILE:CG2	1:A:252:ILE:CB	1.75	1.57
1:A:228:ILE:O	1:A:231:ALA:HB3	1.62	0.99
1:B:64:THR:HG21	1:B:207:GLN:HE21	1.28	0.98
1:A:192:MET:HE2	1:A:208:MET:HE1	1.46	0.97
1:B:140:ARG:HD2	1:B:255:ILE:HD13	1.49	0.93
1:A:216:ARG:HH21	1:A:216:ARG:CG	1.85	0.90
1:B:184:GLU:OE1	1:B:232:ASN:HB2	1.72	0.89
1:A:237:ILE:HB	1:A:238:ASP:HA	1.54	0.88
1:A:192:MET:CE	1:A:208:MET:HE1	2.04	0.88
1:A:216:ARG:NH2	1:A:216:ARG:HB2	1.88	0.88
1:B:64:THR:HG21	1:B:207:GLN:NE2	1.89	0.87
1:B:47:THR:HG22	1:B:160:LYS:HB3	1.58	0.86
1:B:178:PRO:HD2	1:B:181:LEU:HD12	1.58	0.84
1:A:251:THR:O	1:A:255:ILE:HD13	1.77	0.82
1:A:157:GLU:O	1:A:161:ILE:HD13	1.80	0.82
1:A:216:ARG:HH21	1:A:216:ARG:CB	1.94	0.80
1:B:30:VAL:CG1	1:B:39:GLU:HG3	2.12	0.79
1:A:216:ARG:HH21	1:A:216:ARG:HG2	1.47	0.79
1:A:216:ARG:HH21	1:A:216:ARG:HB2	1.46	0.79
1:B:140:ARG:HB3	1:B:255:ILE:HD12	1.64	0.79
1:A:134:ILE:HD13	1:A:147:PRO:HG3	1.65	0.78
1:A:252:ILE:CG2	1:A:252:ILE:HB	2.12	0.78
1:A:192:MET:HE2	1:A:208:MET:CE	2.15	0.77
1:B:239:ASP:O	1:B:240:PRO:C	2.25	0.77
1:A:237:ILE:HG13	1:A:238:ASP:HB3	1.68	0.75
1:A:27:ARG:HH11	1:A:27:ARG:HG3	1.50	0.73
1:A:178:PRO:HD2	1:A:181:LEU:HD12	1.69	0.73
1:A:30:VAL:HG13	1:A:39:GLU:HG3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:MET:CE	1:A:208:MET:CE	2.68	0.72
1:A:196:ILE:O	1:A:201:ARG:NH1	2.22	0.71
1:B:179:GLN:HG2	3:B:2078:HOH:O	1.91	0.70
1:B:210:GLU:HG3	1:B:244:ILE:HB	1.75	0.67
1:A:252:ILE:CG2	1:A:252:ILE:CA	2.71	0.66
1:B:199:ARG:HB2	3:B:2081:HOH:O	1.95	0.66
1:B:40:ARG:NH1	1:B:42:GLU:OE2	2.29	0.66
1:A:228:ILE:O	1:A:231:ALA:CB	2.41	0.65
1:A:64:THR:HB	1:A:212:ASP:OD2	1.97	0.65
1:B:126:GLU:O	1:B:129:GLN:N	2.30	0.64
1:B:64:THR:HB	1:B:212:ASP:OD2	1.97	0.64
1:B:171:ASP:HB2	3:B:2074:HOH:O	1.95	0.64
1:B:181:LEU:CD2	1:B:240:PRO:HB3	2.28	0.64
1:A:191:GLN:O	1:A:221:ASP:HB3	1.97	0.63
1:A:237:ILE:HG13	1:A:238:ASP:CB	2.29	0.63
1:A:29:ARG:HB3	3:A:2021:HOH:O	1.98	0.63
1:B:123:ASP:N	1:B:123:ASP:OD1	2.31	0.62
1:A:238:ASP:HB2	1:A:240:PRO:HG3	1.80	0.61
1:B:140:ARG:HB3	1:B:255:ILE:CD1	2.31	0.60
1:B:153:GLY:O	1:B:157:GLU:HG2	2.00	0.60
1:A:8:LEU:HD21	1:A:16:LYS:HG3	1.83	0.60
1:B:210:GLU:HA	1:B:244:ILE:HD12	1.83	0.60
1:B:9:ILE:HA	3:B:2002:HOH:O	2.02	0.60
1:B:140:ARG:CD	1:B:255:ILE:HD13	2.27	0.60
1:A:6:VAL:HG11	1:A:90:ILE:HG13	1.84	0.59
1:A:237:ILE:HB	1:A:238:ASP:CA	2.31	0.59
1:B:188:LEU:HD13	1:B:208:MET:HE3	1.84	0.59
1:A:44:ILE:HA	1:A:52:VAL:O	2.03	0.58
1:A:50:HIS:CE1	3:A:2027:HOH:O	2.56	0.58
1:A:71:SER:O	1:A:75:GLN:HG3	2.04	0.57
1:A:81:ILE:HG23	1:A:113:ILE:HD11	1.86	0.57
1:A:77:ALA:O	1:A:81:ILE:HG12	2.05	0.56
1:A:181:LEU:HD13	1:A:244:ILE:HG13	1.88	0.56
1:B:30:VAL:HG12	1:B:39:GLU:HG3	1.88	0.56
1:B:99:GLU:HG3	1:B:252:ILE:HG22	1.86	0.56
1:A:216:ARG:NH2	1:A:216:ARG:CB	2.59	0.56
1:A:6:VAL:CG1	1:A:90:ILE:HG13	2.36	0.56
1:A:50:HIS:HE1	3:A:2027:HOH:O	1.89	0.55
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.22	0.55
1:B:210:GLU:CA	1:B:244:ILE:HD12	2.37	0.55
1:B:126:GLU:O	1:B:127:LYS:C	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLY:HA2	1:A:208:MET:HE3	1.90	0.54
1:A:229:ALA:HA	3:A:2097:HOH:O	2.07	0.54
1:A:81:ILE:HG23	1:A:113:ILE:CD1	2.37	0.54
1:A:134:ILE:CD1	1:A:147:PRO:HG3	2.35	0.54
1:A:64:THR:HG21	3:A:2091:HOH:O	2.08	0.54
1:B:57:LEU:HD21	1:B:80:TYR:CD2	2.44	0.54
1:B:153:GLY:O	1:B:157:GLU:CG	2.57	0.53
1:A:182:LEU:HD22	1:A:202:ARG:HH21	1.73	0.53
1:B:30:VAL:CG1	1:B:39:GLU:CG	2.85	0.53
1:B:104:LEU:O	1:B:107:GLN:HB2	2.08	0.53
1:A:18:THR:O	1:A:22:GLN:HG3	2.10	0.52
1:B:182:LEU:O	1:B:183:ARG:C	2.52	0.51
1:A:8:LEU:CD2	1:A:16:LYS:HG3	2.40	0.51
1:A:132:ILE:HD12	1:A:132:ILE:N	2.25	0.51
1:B:44:ILE:HD12	1:B:44:ILE:N	2.25	0.51
1:B:8:LEU:HG	1:B:16:LYS:HG3	1.93	0.50
1:B:9:ILE:HG13	1:B:104:LEU:HD21	1.94	0.50
1:A:81:ILE:HD12	1:A:89:LEU:HD11	1.93	0.50
1:A:24:THR:HG21	1:A:43:GLY:HA3	1.94	0.50
1:A:197:PRO:O	1:A:201:ARG:HG3	2.11	0.49
1:A:244:ILE:HG22	1:A:245:ALA:N	2.28	0.49
1:A:89:LEU:HD11	1:A:113:ILE:HD13	1.93	0.49
1:B:18:THR:O	1:B:22:GLN:HG3	2.12	0.49
1:B:238:ASP:CB	3:B:2087:HOH:O	2.60	0.48
1:B:219:ALA:HB1	1:B:222:ALA:O	2.13	0.48
1:A:154:ARG:O	1:A:155:GLY:C	2.55	0.48
1:A:152:ARG:C	1:A:154:ARG:H	2.20	0.48
1:A:115:CYS:O	1:A:143:CYS:HB2	2.14	0.47
1:B:156:ILE:O	1:B:159:LEU:HB3	2.14	0.47
1:A:118:ALA:HB1	1:A:148:LEU:HD11	1.96	0.47
1:A:197:PRO:HG2	1:A:200:GLN:HG3	1.97	0.47
1:A:8:LEU:HD11	1:A:92:VAL:CG2	2.45	0.47
1:B:186:ASP:OD2	1:B:202:ARG:NH2	2.48	0.47
1:B:8:LEU:HD11	1:B:92:VAL:CG2	2.45	0.47
1:A:30:VAL:CG1	1:A:39:GLU:HG3	2.44	0.46
1:A:155:GLY:N	3:A:2074:HOH:O	2.46	0.46
1:B:240:PRO:O	1:B:244:ILE:HG13	2.15	0.46
1:A:239:ASP:HB2	1:A:243:HIS:HE1	1.80	0.46
1:A:161:ILE:O	1:A:165:ARG:HG3	2.16	0.46
1:A:125:ALA:HB1	1:A:130:VAL:HG13	1.97	0.46
1:A:197:PRO:HG2	1:A:200:GLN:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:O	1:A:173:GLU:C	2.59	0.45
1:A:255:ILE:CD1	1:A:255:ILE:N	2.80	0.45
1:B:144:PRO:HD3	1:B:166:HIS:CE1	2.52	0.45
1:B:140:ARG:HD2	1:B:255:ILE:CD1	2.32	0.45
1:B:256:CYS:HB3	3:B:2093:HOH:O	2.17	0.45
1:A:57:LEU:HD21	1:A:80:TYR:CD2	2.52	0.45
1:A:216:ARG:NH2	1:A:216:ARG:HG2	2.23	0.45
1:B:177:TYR:HB2	1:B:182:LEU:HD11	1.99	0.45
1:A:192:MET:HE1	1:A:208:MET:CE	2.46	0.44
1:A:193:SER:OG	1:A:195:GLN:HB2	2.17	0.44
1:B:28:GLN:HA	1:B:42:GLU:O	2.17	0.44
1:B:45:PHE:CZ	1:B:52:VAL:HG11	2.53	0.44
1:A:13:ASN:OD1	1:B:71:SER:HB2	2.17	0.44
1:A:126:GLU:O	1:A:129:GLN:N	2.47	0.44
1:A:184:GLU:O	1:A:185:ALA:C	2.60	0.44
1:A:64:THR:CB	1:A:212:ASP:OD2	2.65	0.44
1:A:252:ILE:CG2	1:A:252:ILE:C	2.90	0.44
1:A:81:ILE:CG2	1:A:113:ILE:HD11	2.48	0.44
1:B:9:ILE:HD12	3:B:2002:HOH:O	2.16	0.44
1:B:134:ILE:HG12	1:B:147:PRO:HG3	1.99	0.44
1:A:6:VAL:HG23	1:A:52:VAL:HG13	2.00	0.43
1:B:33:TRP:HA	3:B:2015:HOH:O	2.19	0.43
1:B:120:ASN:OD1	1:B:120:ASN:C	2.61	0.43
1:A:257:ASP:HA	3:A:2101:HOH:O	2.19	0.43
1:B:2:GLN:HB2	1:B:50:HIS:CD2	2.54	0.43
1:B:88:MET:HE2	1:B:88:MET:HB3	1.77	0.43
1:B:196:ILE:HA	1:B:197:PRO:HD2	1.84	0.42
1:A:167:GLN:OE1	1:A:167:GLN:HA	2.19	0.42
1:A:6:VAL:HA	1:A:88:MET:O	2.19	0.42
1:A:19:LEU:HD23	1:A:92:VAL:HG22	2.01	0.42
1:A:56:ASP:OD2	3:A:2034:HOH:O	2.22	0.42
1:A:95:ALA:HB1	1:A:132:ILE:HD11	2.03	0.41
1:B:125:ALA:O	1:B:130:VAL:HG13	2.20	0.41
1:B:91:ASN:HD22	1:B:105:THR:HG23	1.85	0.41
1:A:191:GLN:HB2	1:A:222:ALA:HB2	2.03	0.41
1:B:126:GLU:O	1:B:128:GLN:N	2.54	0.41
1:A:99:GLU:HG3	1:A:252:ILE:HG22	2.02	0.41
1:A:9:ILE:HG12	1:A:104:LEU:HD21	2.02	0.41
1:A:197:PRO:HG2	1:A:200:GLN:CG	2.50	0.41
1:B:98:LEU:HD12	1:B:98:LEU:HA	1.73	0.41
1:A:97:ASN:O	1:A:101:ASN:ND2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:C	1:B:218:TYR:H	2.28	0.40
1:B:184:GLU:OE1	1:B:229:ALA:HA	2.21	0.40
1:B:249:TYR:CD2	1:B:249:TYR:C	2.99	0.40
1:B:30:VAL:HG11	1:B:39:GLU:CD	2.46	0.40
1:B:72:LEU:O	1:B:75:GLN:HB2	2.21	0.40
1:B:172:LEU:O	1:B:173:GLU:C	2.64	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	247/267 (92%)	226 (92%)	18 (7%)	3 (1%)	10	11
1	B	246/267 (92%)	228 (93%)	16 (6%)	2 (1%)	16	20
All	All	493/534 (92%)	454 (92%)	34 (7%)	5 (1%)	12	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	227	ASP
1	A	154	ARG
1	A	235	ASP
1	B	127	LYS
1	A	173	GLU

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	186/221 (84%)	174 (94%)	12 (6%)	15	21
1	B	178/221 (80%)	166 (93%)	12 (7%)	15	20
All	All	364/442 (82%)	340 (93%)	24 (7%)	15	20

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	27	ARG
1	A	64	THR
1	A	130	VAL
1	A	132	ILE
1	A	179	GLN
1	A	196	ILE
1	A	198	PRO
1	A	213	ILE
1	A	216	ARG
1	A	244	ILE
1	A	255	ILE
1	B	2	GLN
1	B	13	ASN
1	B	28	GLN
1	B	41	LYS
1	B	62	SER
1	B	113	ILE
1	B	130	VAL
1	B	179	GLN
1	B	180	PRO
1	B	192	MET
1	B	230	LEU
1	B	239	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	28	GLN
1	A	32	ASN

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Mol	Chain	Res	Type
1	A	179	GLN
1	B	11	ASN
1	B	22	GLN
1	B	91	ASN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	236:GLU	C	237:ILE	N	1.04

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	253/267 (94%)	0.28	8 (3%) 50 51	11, 27, 53, 64	0
1	B	252/267 (94%)	0.34	12 (4%) 35 34	12, 27, 56, 63	0
All	All	505/534 (94%)	0.31	20 (3%) 42 41	11, 27, 55, 64	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	ALA	6.4
1	B	238	ASP	4.2
1	A	222	ALA	3.4
1	B	233	LEU	3.1
1	B	223	ALA	3.1
1	B	217	ALA	2.9
1	B	186	ASP	2.7
1	B	211	GLY	2.6
1	B	237	ILE	2.6
1	B	232	ASN	2.6
1	A	70	THR	2.6
1	A	237	ILE	2.6
1	A	236	GLU	2.5
1	A	239	ASP	2.4
1	B	218	TYR	2.2
1	B	236	GLU	2.2
1	B	70	THR	2.1
1	A	180	PRO	2.1
1	A	156	ILE	2.0
1	A	69	GLN	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](#)

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
2	MG	A	1262	1/1	0.81	0.06	19,19,19,19	1
2	MG	B	1262	1/1	0.91	0.23	34,34,34,34	1

6.5 Other polymers [i](#)

There are no such residues in this entry.