



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:56 PM UTC

PDB ID : 3NX1 / pdb_00003nx1
Title : Crystal structure of Enterobacter sp. Px6-4 Ferulic Acid Decarboxylase
Authors : Gu, W.; Yang, J.K.; Lou, Z.Y.; Meng, Z.H.; Zhang, K.-Q.
Deposited on : 2010-07-12
Resolution : 2.40 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

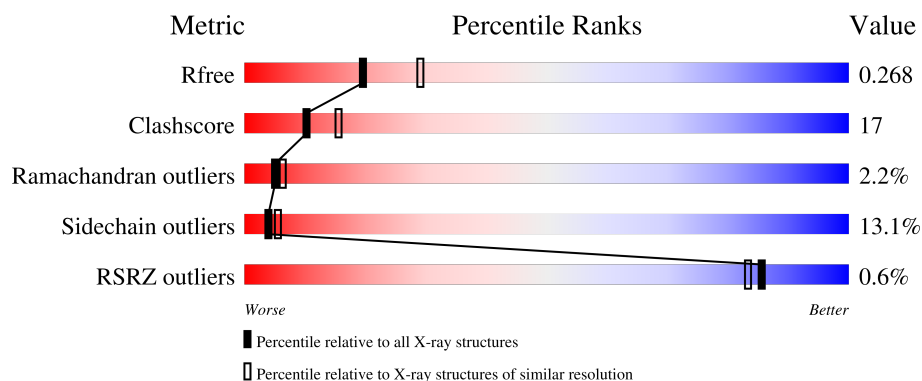
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	168	% 47% 33% 11% 5% .
1	B	168	% 44% 38% 12% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2724 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 Ferulic acid decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1301	830	216	250	5			
1	B	165	Total	C	N	O	S	0	0	0
			1327	849	219	254	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ASN	GLU	SEE REMARK 999	UNP C6F3U5
A	34	ASP	GLU	SEE REMARK 999	UNP C6F3U5
A	37	ILE	LEU	SEE REMARK 999	UNP C6F3U5
A	55	GLU	GLN	SEE REMARK 999	UNP C6F3U5
A	105	PRO	LYS	SEE REMARK 999	UNP C6F3U5
A	122	GLU	ASP	SEE REMARK 999	UNP C6F3U5
B	26	ASN	GLU	SEE REMARK 999	UNP C6F3U5
B	34	ASP	GLU	SEE REMARK 999	UNP C6F3U5
B	37	ILE	LEU	SEE REMARK 999	UNP C6F3U5
B	55	GLU	GLN	SEE REMARK 999	UNP C6F3U5
B	105	PRO	LYS	SEE REMARK 999	UNP C6F3U5
B	122	GLU	ASP	SEE REMARK 999	UNP C6F3U5

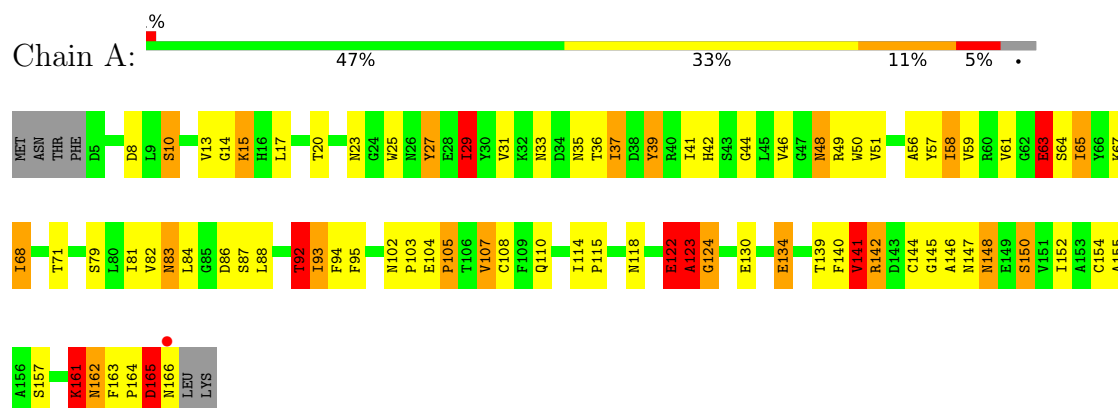
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		
2	B	54	Total	O	0	0
			54	54		

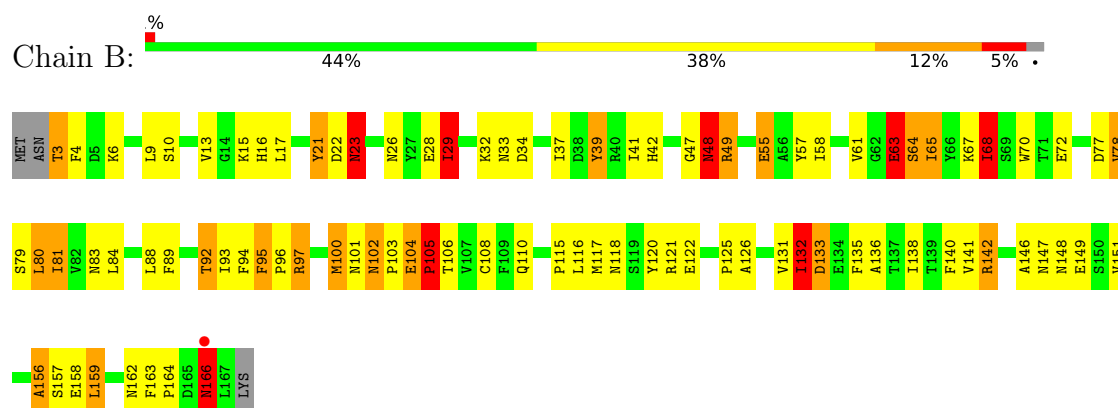
3 Residue-property plots [i](#)

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: Ferulic acid decarboxylase



• Molecule 1: Ferulic acid decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.48Å 88.72Å 49.26Å 90.00° 102.25° 90.00°	Depositor
Resolution (Å)	36.87 – 2.40 36.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.2 (36.87-2.40) 93.2 (36.87-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.40 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.162 , 0.262 0.168 , 0.268	Depositor DCC
R_{free} test set	625 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	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	0.96	EDS
Total number of atoms	2724	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% 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	2.14	41/1339 (3.1%)	1.85	28/1829 (1.5%)
1	B	1.98	33/1366 (2.4%)	1.81	32/1866 (1.7%)
All	All	2.06	74/2705 (2.7%)	1.83	60/3695 (1.6%)

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	2
1	B	0	2
All	All	0	4

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	SER	N-CA	14.27	1.62	1.46
1	B	132	ILE	CA-CB	9.57	1.65	1.53
1	A	152	ILE	CA-CB	9.39	1.63	1.53
1	B	42	HIS	C-O	-8.91	1.12	1.24
1	B	131	VAL	C-O	-8.87	1.14	1.24
1	A	64	SER	CA-C	8.81	1.65	1.52
1	B	64	SER	N-CA	8.18	1.56	1.46
1	B	41	ILE	C-O	8.12	1.33	1.24
1	A	13	VAL	CA-CB	8.01	1.63	1.54
1	A	93	ILE	CA-CB	7.87	1.64	1.54
1	A	107	VAL	CA-CB	7.87	1.62	1.53
1	B	78	VAL	CA-CB	7.77	1.64	1.54
1	A	44	GLY	C-O	-7.71	1.18	1.24
1	B	70	TRP	N-CA	7.63	1.54	1.46
1	B	138	ILE	CA-CB	-7.35	1.45	1.54
1	B	65	ILE	C-O	-7.11	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	VAL	C-O	-7.05	1.16	1.23
1	A	155	ALA	CA-CB	6.92	1.64	1.53
1	B	29	ILE	CA-CB	6.80	1.67	1.55
1	B	16	HIS	CA-C	6.74	1.60	1.52
1	B	115	PRO	CA-C	6.72	1.62	1.52
1	A	115	PRO	CA-C	6.72	1.61	1.52
1	A	146	ALA	CA-CB	6.68	1.64	1.53
1	A	92	THR	CA-CB	6.58	1.63	1.53
1	B	13	VAL	CA-CB	6.41	1.61	1.54
1	B	121	ARG	C-O	6.41	1.31	1.24
1	B	108	CYS	C-O	6.39	1.30	1.24
1	A	58	ILE	CA-CB	6.31	1.62	1.54
1	B	61	VAL	CA-CB	6.20	1.61	1.54
1	A	36	THR	CA-CB	6.19	1.64	1.53
1	A	27	TYR	C-O	-6.18	1.16	1.23
1	A	29	ILE	CA-C	6.17	1.60	1.52
1	B	118	ASN	N-CA	6.16	1.53	1.46
1	A	154	CYS	C-O	6.14	1.30	1.23
1	A	124	GLY	N-CA	6.06	1.53	1.44
1	A	164	PRO	CA-C	5.92	1.64	1.52
1	B	68	ILE	N-CA	5.86	1.53	1.46
1	A	110	GLN	C-O	5.84	1.31	1.24
1	A	79	SER	CA-C	-5.84	1.46	1.52
1	B	105	PRO	CG-CD	5.81	1.70	1.50
1	A	23	ASN	CA-C	5.79	1.62	1.52
1	B	57	TYR	C-O	-5.78	1.17	1.24
1	A	61	VAL	CA-CB	5.76	1.61	1.54
1	A	87	SER	C-O	5.75	1.31	1.23
1	A	148	ASN	N-CA	-5.75	1.39	1.46
1	B	146	ALA	N-CA	5.73	1.53	1.45
1	A	139	THR	CA-C	5.69	1.60	1.52
1	A	141	VAL	CA-CB	5.69	1.65	1.55
1	B	105	PRO	CA-C	-5.67	1.44	1.52
1	A	25	TRP	CA-C	5.66	1.60	1.52
1	B	156	ALA	CA-CB	-5.62	1.44	1.53
1	A	130	GLU	N-CA	5.61	1.53	1.46
1	A	27	TYR	CA-C	-5.54	1.45	1.52
1	A	27	TYR	N-CA	5.49	1.52	1.45
1	B	126	ALA	CA-CB	5.37	1.61	1.53
1	B	151	VAL	CA-CB	5.36	1.60	1.54
1	B	80	LEU	CG-CD2	5.34	1.70	1.52
1	B	93	ILE	CA-CB	5.31	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	SER	N-CA	-5.30	1.39	1.46
1	A	134	GLU	CA-C	5.30	1.59	1.52
1	B	102	ASN	CA-CB	5.27	1.59	1.53
1	A	123	ALA	CA-CB	-5.26	1.44	1.53
1	A	59	VAL	C-O	5.23	1.29	1.23
1	B	49	ARG	N-CA	-5.21	1.39	1.46
1	A	148	ASN	C-O	-5.19	1.18	1.24
1	B	94	PHE	CA-C	5.18	1.59	1.53
1	A	31	VAL	C-O	5.12	1.29	1.23
1	B	6	LYS	N-CA	5.10	1.52	1.46
1	A	15	LYS	CA-C	-5.07	1.46	1.52
1	A	56	ALA	CA-C	5.07	1.58	1.52
1	B	117	MET	C-O	5.06	1.30	1.24
1	A	114	ILE	N-CA	5.04	1.52	1.46
1	A	20	THR	CA-CB	5.02	1.61	1.53
1	B	133	ASP	C-O	-5.01	1.18	1.24

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	SER	N-CA-C	13.03	128.62	113.38
1	B	166	ASN	CA-C-N	-11.41	101.17	121.70
1	B	166	ASN	C-N-CA	-11.41	101.17	121.70
1	A	165	ASP	N-CA-C	-10.69	97.38	111.71
1	B	72	GLU	CA-C-N	10.07	131.16	119.47
1	B	72	GLU	C-N-CA	10.07	131.16	119.47
1	A	63	GLU	CA-C-N	-9.39	108.33	123.91
1	A	63	GLU	C-N-CA	-9.39	108.33	123.91
1	A	162	ASN	N-CA-C	9.08	130.15	110.80
1	A	35	ASN	N-CA-C	9.06	124.06	111.56
1	A	124	GLY	N-CA-C	-8.98	94.03	112.34
1	A	164	PRO	N-CA-C	8.45	134.08	112.10
1	B	95	PHE	CA-C-N	8.14	128.07	119.85
1	B	95	PHE	C-N-CA	8.14	128.07	119.85
1	B	120	TYR	CA-C-N	7.99	130.99	120.28
1	B	120	TYR	C-N-CA	7.99	130.99	120.28
1	B	64	SER	N-CA-C	7.84	125.59	113.28
1	A	164	PRO	CA-C-N	7.38	136.13	121.81
1	A	164	PRO	C-N-CA	7.38	136.13	121.81
1	B	63	GLU	CA-C-N	-6.95	114.15	126.45
1	B	63	GLU	C-N-CA	-6.95	114.15	126.45
1	A	122	GLU	N-CA-C	6.86	121.39	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	GLY	N-CA-C	-6.61	104.89	111.56
1	B	39	TYR	N-CA-C	6.36	119.38	109.52
1	B	166	ASN	O-C-N	-6.34	114.16	122.59
1	B	142	ARG	NE-CZ-NH1	-6.32	115.18	121.50
1	B	116	LEU	CA-C-N	6.32	128.75	120.28
1	B	116	LEU	C-N-CA	6.32	128.75	120.28
1	A	23	ASN	N-CA-C	6.20	120.56	113.19
1	A	142	ARG	N-CA-C	-6.14	98.96	108.42
1	B	55	GLU	N-CA-C	-6.13	101.34	110.23
1	B	162	ASN	N-CA-C	6.08	120.39	113.15
1	A	68	ILE	CB-CA-C	-6.04	101.62	110.62
1	A	150	SER	CB-CA-C	5.90	120.79	110.64
1	B	26	ASN	CB-CA-C	5.89	119.86	110.19
1	A	63	GLU	N-CA-CB	-5.87	100.57	110.49
1	A	124	GLY	O-C-N	5.75	127.52	121.77
1	B	10	SER	N-CA-C	5.74	120.00	112.89
1	A	87	SER	N-CA-C	5.70	119.25	111.39
1	A	37	ILE	CB-CG1-CD1	-5.69	101.85	113.80
1	B	106	THR	N-CA-C	-5.52	106.54	113.72
1	A	39	TYR	N-CA-C	5.38	117.16	109.14
1	B	159	LEU	N-CA-C	-5.36	102.90	110.29
1	B	63	GLU	N-CA-CB	-5.35	101.87	109.85
1	B	21	TYR	N-CA-C	5.27	117.33	110.43
1	A	145	GLY	CA-C-N	5.23	130.08	121.39
1	A	145	GLY	C-N-CA	5.23	130.08	121.39
1	B	100	MET	N-CA-C	5.23	116.67	111.07
1	A	61	VAL	N-CA-C	-5.23	108.19	113.47
1	B	84	LEU	N-CA-C	5.22	116.66	110.97
1	B	142	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A	42	HIS	N-CA-C	5.17	119.64	113.23
1	B	29	ILE	CA-CB-CG2	5.09	119.16	110.50
1	B	101	ASN	CA-C-N	-5.06	117.29	122.85
1	B	101	ASN	C-N-CA	-5.06	117.29	122.85
1	A	163	PHE	CA-C-O	-5.05	115.00	119.75
1	B	15	LYS	N-CA-C	5.03	117.60	110.10
1	B	97	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	A	114	ILE	CA-C-N	-5.00	113.50	119.05
1	A	114	ILE	C-N-CA	-5.00	113.50	119.05

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	LYS	Peptide
1	A	165	ASP	Peptide
1	B	166	ASN	Peptide
1	B	22	ASP	Peptide

5.2 Too-close contacts [i](#)

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	1301	0	1221	48	1
1	B	1327	0	1248	45	1
2	A	42	0	0	0	0
2	B	54	0	0	1	0
All	All	2724	0	2469	87	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 17.

All (87) 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:8:ASP:OD1	1:A:10:SER:HB2	1.62	0.97
1:B:166:ASN:ND2	1:B:166:ASN:H	1.61	0.93
1:A:102:ASN:O	1:A:105:PRO:HD2	1.67	0.92
1:A:102:ASN:O	1:A:105:PRO:CD	2.21	0.89
1:B:95:PHE:CD2	1:B:100:MET:HE1	2.08	0.88
1:A:33:ASN:HD22	1:A:147:ASN:HD21	1.23	0.85
1:B:166:ASN:ND2	1:B:166:ASN:N	2.29	0.81
1:B:95:PHE:HB2	1:B:100:MET:HE3	1.65	0.79
1:A:17:LEU:HD23	1:A:141:VAL:HG13	1.64	0.78
1:A:123:ALA:C	1:A:124:GLY:O	2.28	0.72
1:A:123:ALA:O	1:A:124:GLY:O	2.08	0.72
1:B:95:PHE:CB	1:B:100:MET:CE	2.69	0.71
1:A:103:PRO:C	1:A:105:PRO:HD2	2.15	0.70
1:B:58:ILE:HG12	1:B:68:ILE:HG23	1.73	0.69
1:A:27:TYR:CE2	1:A:41:ILE:HG12	2.27	0.69
1:B:95:PHE:CD2	1:B:100:MET:CE	2.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASN:N	1:B:166:ASN:HD22	1.91	0.67
1:B:95:PHE:CB	1:B:100:MET:HE3	2.26	0.65
1:A:92:THR:HG23	1:B:67:LYS:HZ1	1.63	0.63
1:A:33:ASN:HD22	1:A:147:ASN:ND2	1.94	0.63
1:B:3:THR:N	2:B:192:HOH:O	2.32	0.62
1:B:88:LEU:HD21	1:B:135:PHE:HE1	1.67	0.59
1:A:29:ILE:HD11	1:A:37:ILE:CD1	2.33	0.59
1:B:95:PHE:CG	1:B:100:MET:CE	2.87	0.58
1:B:102:ASN:O	1:B:105:PRO:HD2	2.04	0.57
1:A:17:LEU:CD2	1:A:141:VAL:HG13	2.32	0.57
1:A:83:ASN:ND2	1:A:86:ASP:H	2.03	0.56
1:B:33:ASN:HD22	1:B:147:ASN:HD21	1.54	0.56
1:B:3:THR:HG22	1:B:4:PHE:HD1	1.70	0.55
1:A:83:ASN:C	1:A:83:ASN:HD22	2.15	0.55
1:A:29:ILE:HD11	1:A:37:ILE:HD12	1.88	0.54
1:A:58:ILE:HG12	1:A:68:ILE:HG23	1.89	0.54
1:A:140:PHE:CE2	1:A:142:ARG:HD3	2.43	0.53
1:B:140:PHE:CE2	1:B:142:ARG:HG2	2.43	0.53
1:B:63:GLU:O	1:B:64:SER:HB2	2.09	0.53
1:A:118:ASN:O	1:A:122:GLU:HG2	2.09	0.52
1:A:48:ASN:HD21	1:A:157:SER:H	1.57	0.52
1:A:41:ILE:HD13	1:A:46:VAL:HG23	1.91	0.52
1:B:21:TYR:HB3	1:B:23:ASN:HB2	1.92	0.51
1:B:3:THR:HG22	1:B:4:PHE:CD1	2.45	0.51
1:B:49:ARG:NH2	1:B:110:GLN:OE1	2.40	0.50
1:A:39:TYR:CD1	1:A:39:TYR:C	2.90	0.50
1:B:97:ARG:HB3	1:B:125:PRO:O	2.12	0.49
1:A:140:PHE:CZ	1:A:142:ARG:HD3	2.48	0.48
1:A:63:GLU:O	1:A:63:GLU:HG3	2.12	0.48
1:B:92:THR:HB	1:B:133:ASP:OD2	2.14	0.48
1:A:107:VAL:O	1:A:108:CYS:HB3	2.14	0.47
1:B:29:ILE:HD12	1:B:39:TYR:HB2	1.96	0.47
1:B:48:ASN:ND2	1:B:156:ALA:HB3	2.29	0.47
1:B:63:GLU:O	1:B:64:SER:CB	2.62	0.47
1:A:67:LYS:NZ	1:B:92:THR:HG22	2.30	0.47
1:A:37:ILE:HG21	1:A:37:ILE:HD13	1.51	0.46
1:B:32:LYS:NZ	1:B:149:GLU:OE1	2.47	0.46
1:A:104:GLU:N	1:A:105:PRO:CD	2.79	0.46
1:A:48:ASN:HD21	1:A:157:SER:N	2.13	0.46
1:B:78:VAL:CG1	1:B:80:LEU:HD21	2.46	0.46
1:A:94:PHE:CD1	1:A:94:PHE:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:HB3	1:B:100:MET:CE	2.47	0.45
1:A:93:ILE:HG21	1:A:95:PHE:CZ	2.52	0.45
1:A:15:LYS:HE2	1:A:84:LEU:HD13	1.98	0.44
1:A:57:TYR:N	1:A:57:TYR:CD2	2.85	0.44
1:B:163:PHE:HA	1:B:164:PRO:HA	1.70	0.44
1:A:65:ILE:HD13	1:A:83:ASN:CG	2.43	0.44
1:B:48:ASN:HD21	1:B:157:SER:N	2.16	0.44
1:B:95:PHE:HA	1:B:96:PRO:HD3	1.84	0.44
1:A:94:PHE:CE2	1:B:77:ASP:HB3	2.54	0.43
1:B:95:PHE:HB3	1:B:100:MET:HE2	2.00	0.42
1:B:17:LEU:O	1:B:28:GLU:HA	2.19	0.42
1:B:103:PRO:HD2	1:B:104:GLU:OE1	2.19	0.42
1:B:83:ASN:HB3	1:B:88:LEU:HB3	2.00	0.42
1:B:88:LEU:HD21	1:B:135:PHE:CE1	2.51	0.42
1:A:161:LYS:HB3	1:A:161:LYS:HE2	1.77	0.42
1:A:104:GLU:N	1:A:105:PRO:HD2	2.34	0.41
1:B:89:PHE:CD2	1:B:136:ALA:HB3	2.54	0.41
1:A:81:ILE:HD11	1:B:81:ILE:HD11	2.03	0.41
1:A:123:ALA:O	1:A:124:GLY:C	2.63	0.41
1:A:14:GLY:O	1:A:144:CYS:N	2.47	0.41
1:A:81:ILE:CD1	1:B:81:ILE:HD11	2.51	0.41
1:B:132:ILE:O	1:B:132:ILE:HG22	2.19	0.41
1:A:50:TRP:C	1:A:51:VAL:HG23	2.45	0.41
1:B:156:ALA:HA	1:B:159:LEU:HD12	2.03	0.41
1:A:27:TYR:CD2	1:A:41:ILE:HG12	2.56	0.41
1:A:41:ILE:HD12	1:A:49:ARG:HB3	2.02	0.41
1:A:148:ASN:OD1	1:A:148:ASN:C	2.63	0.41
1:A:67:LYS:HZ1	1:B:92:THR:HG22	1.86	0.40
1:A:29:ILE:CD1	1:A:37:ILE:HG21	2.51	0.40
1:A:81:ILE:HD12	1:A:81:ILE:HG23	1.79	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:166:ASN:ND2	1:B:148:ASN:ND2[2_556]	2.11	0.09

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	160/168 (95%)	146 (91%)	12 (8%)	2 (1%)	9	14
1	B	163/168 (97%)	145 (89%)	13 (8%)	5 (3%)	3	3
All	All	323/336 (96%)	291 (90%)	25 (8%)	7 (2%)	5	6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	B	23	ASN
1	B	47	GLY
1	B	166	ASN
1	A	123	ALA
1	B	48	ASN
1	B	105	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	143/149 (96%)	126 (88%)	17 (12%)	5	7
1	B	146/149 (98%)	125 (86%)	21 (14%)	3	4
All	All	289/298 (97%)	251 (87%)	38 (13%)	4	5

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	29	ILE
1	A	48	ASN
1	A	63	GLU
1	A	65	ILE
1	A	71	THR
1	A	82	VAL
1	A	83	ASN
1	A	88	LEU
1	A	92	THR
1	A	105	PRO
1	A	122	GLU
1	A	134	GLU
1	A	141	VAL
1	A	150	SER
1	A	161	LYS
1	A	165	ASP
1	B	3	THR
1	B	9	LEU
1	B	23	ASN
1	B	29	ILE
1	B	34	ASP
1	B	37	ILE
1	B	48	ASN
1	B	55	GLU
1	B	63	GLU
1	B	65	ILE
1	B	68	ILE
1	B	79	SER
1	B	81	ILE
1	B	92	THR
1	B	104	GLU
1	B	105	PRO
1	B	122	GLU
1	B	132	ILE
1	B	141	VAL
1	B	158	GLU
1	B	166	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS

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Mol	Chain	Res	Type
1	A	23	ASN
1	A	26	ASN
1	A	48	ASN
1	A	83	ASN
1	A	102	ASN
1	A	113	HIS
1	A	118	ASN
1	A	147	ASN
1	B	23	ASN
1	B	26	ASN
1	B	48	ASN
1	B	118	ASN
1	B	147	ASN
1	B	166	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](#)

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 [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	162/168 (96%)	-0.65	1 (0%) 85 83	8, 26, 38, 52	2 (1%)
1	B	165/168 (98%)	-0.62	1 (0%) 85 83	13, 26, 38, 52	2 (1%)
All	All	327/336 (97%)	-0.63	2 (0%) 85 83	8, 26, 38, 52	4 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	ASN	2.6
1	B	166	ASN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.