



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:22 AM UTC

PDB ID : 1IE7 / pdb_00001ie7
Title : PHOSPHATE INHIBITED BACILLUS PASTEURII UREASE CRYSTAL STRUCTURE
Authors : Benini, S.; Rypniewski, W.R.; Wilson, K.S.; Ciarli, S.; Mangani, S.
Deposited on : 2001-04-09
Resolution : 1.85 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	:	9.0.010 (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

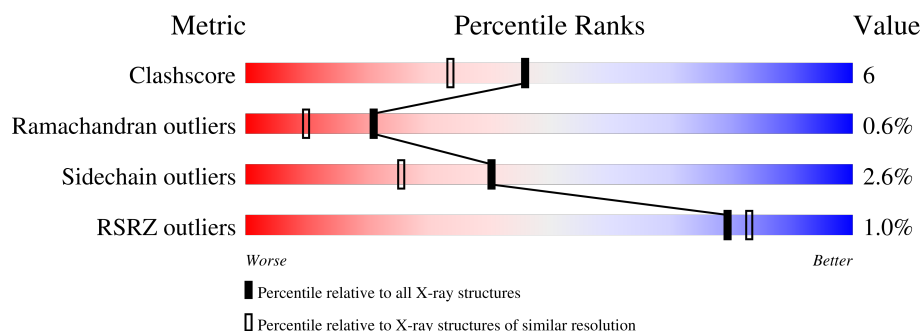
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	100	2% 78% 16% 5%
2	B	126	% 86% 10%
3	C	570	% 78% 17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6964 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 UREASE GAMMA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	5	0	0
			781	493	133	149	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	modified residue	UNP P41022

- Molecule 2 is a protein called UREASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	21	0	0
			951	589	171	190	1			

- Molecule 3 is a protein called UREASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	570	Total	C	N	O	S	57	2	0
			4329	2719	743	843	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	GLU	ARG	conflict	UNP P41020
C	28	TRP	-	insertion	UNP P41020
C	29	ILE	GLY	conflict	UNP P41020
C	36	THR	TYR	conflict	UNP P41020
C	37	THR	TYR	conflict	UNP P41020
C	38	TYR	LEU	conflict	UNP P41020
C	220	KCX	LYS	modified residue	UNP P41020
C	263	LEU	VAL	conflict	UNP P41020
C	327	ASN	GLN	conflict	UNP P41020

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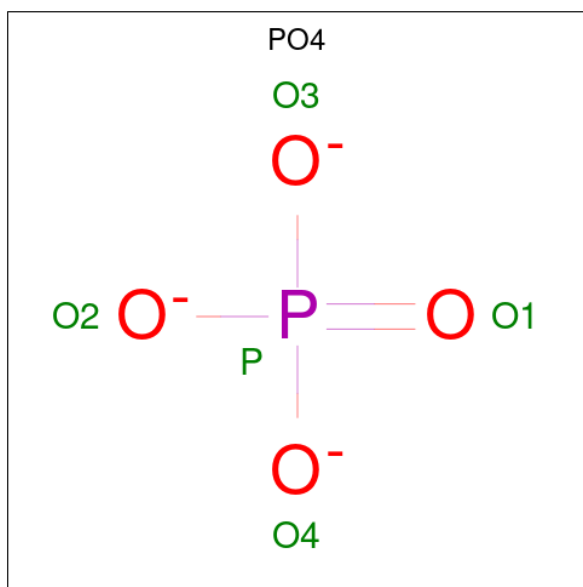
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Chain	Residue	Modelled	Actual	Comment	Reference
C	420	ILE	MET	conflict	UNP P41020

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total Ni 2 2	0	0

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O P 5 4 1	0	0

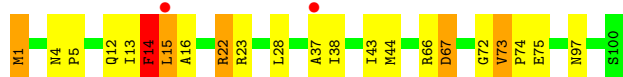
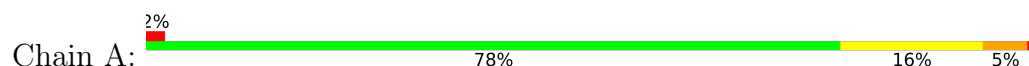
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	130	Total O 130 130	0	0
6	B	186	Total O 186 186	0	0
6	C	580	Total O 580 580	0	0

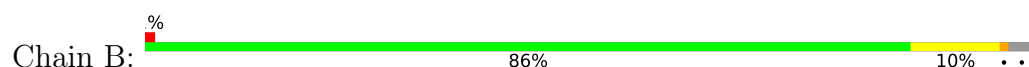
3 Residue-property plots [i](#)

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.

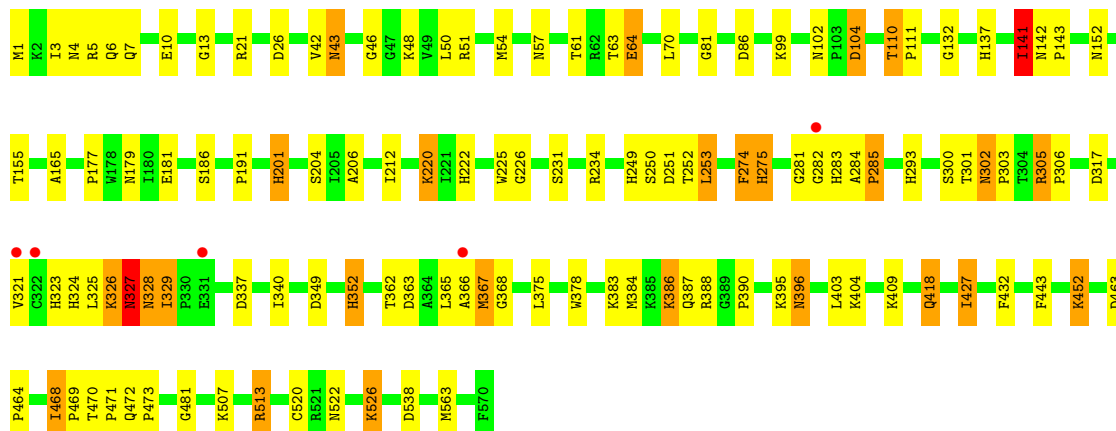
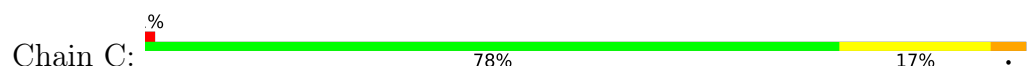
• Molecule 1: UREASE GAMMA SUBUNIT



• Molecule 2: UREASE BETA SUBUNIT



• Molecule 3: UREASE ALPHA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.49Å 131.49Å 189.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	11.99 – 1.85 11.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (11.99-1.85) 97.2 (11.99-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.210 0.168 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 75.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6964	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: NI, CXM, KCX, PO4

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	2.49	2/781 (0.3%)	2.29	24/1053 (2.3%)
2	B	2.81	4/963 (0.4%)	1.83	12/1296 (0.9%)
3	C	0.96	13/4407 (0.3%)	1.74	86/5975 (1.4%)
All	All	1.64	19/6151 (0.3%)	1.83	122/8324 (1.5%)

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	3
3	C	1	6
All	All	1	9

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	126	GLU	CA-C	66.50	2.92	1.52
1	A	22	ARG	CZ-NH2	57.30	2.08	1.33
2	B	126	GLU	CA-CB	50.53	2.54	1.53
1	A	22	ARG	CZ-NH1	-32.83	0.86	1.32
3	C	403	LEU	CB-CG	24.76	2.02	1.53
2	B	5	ASN	CB-CG	11.49	1.80	1.52
3	C	102	ASN	C-O	-11.01	1.16	1.25
3	C	329	ILE	CA-CB	-10.54	1.40	1.54
3	C	326	LYS	C-N	-10.45	1.19	1.33
3	C	102	ASN	C-N	8.32	1.43	1.33
3	C	327	ASN	N-CA	-7.15	1.36	1.46
3	C	324	HIS	CB-CG	-6.67	1.40	1.50
3	C	329	ILE	CA-C	6.67	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	396	ASN	CA-CB	-6.56	1.43	1.53
3	C	325	LEU	CA-CB	-6.21	1.43	1.53
3	C	337	ASP	CG-OD1	-6.07	1.13	1.25
3	C	323	HIS	CB-CG	5.88	1.58	1.50
2	B	115	GLN	CB-CG	-5.38	1.36	1.52
3	C	337	ASP	CG-OD2	5.28	1.35	1.25

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	126	GLU	CB-CA-C	-29.46	54.13	110.10
1	A	22	ARG	NE-CZ-NH2	-28.41	93.63	119.20
1	A	22	ARG	NH1-CZ-NH2	-22.02	90.68	119.30
2	B	5	ASN	CA-CB-CG	-21.40	91.20	112.60
1	A	37	ALA	CA-C-O	-17.87	101.78	120.90
1	A	37	ALA	O-C-N	17.14	139.92	122.09
1	A	97	ASN	O-C-N	-12.65	115.71	121.53
3	C	102	ASN	CA-C-O	12.55	132.41	119.49
3	C	326	LYS	CA-C-N	12.03	144.51	121.54
3	C	326	LYS	C-N-CA	12.03	144.51	121.54
3	C	64	GLU	CG-CD-OE2	-11.53	91.89	118.40
3	C	324	HIS	CA-CB-CG	11.40	125.20	113.80
3	C	5	ARG	NE-CZ-NH2	-10.78	109.50	119.20
1	A	37	ALA	CA-C-N	10.31	133.76	120.56
1	A	37	ALA	C-N-CA	10.31	133.76	120.56
3	C	326	LYS	O-C-N	-10.09	110.42	123.13
1	A	97	ASN	CA-C-O	10.08	128.33	120.26
3	C	327	ASN	N-CA-CB	9.48	126.52	110.49
1	A	67	ASP	CA-CB-CG	9.34	121.94	112.60
1	A	72	GLY	CA-C-N	9.04	125.94	120.24
1	A	72	GLY	C-N-CA	9.04	125.94	120.24
3	C	251	ASP	CA-CB-CG	8.93	121.53	112.60
3	C	42	VAL	CA-CB-CG1	8.81	125.37	110.40
3	C	141	ILE	CB-CG1-CD1	-8.57	95.81	113.80
3	C	403	LEU	CA-CB-CG	-8.48	86.60	116.30
3	C	201	HIS	CA-CB-CG	-8.33	105.47	113.80
1	A	14	PHE	CA-C-O	-8.21	108.77	120.51
2	B	5	ASN	CB-CG-ND2	-8.05	104.33	116.40
3	C	468	ILE	CA-C-N	7.77	128.43	120.04
3	C	468	ILE	C-N-CA	7.77	128.43	120.04
3	C	179	ASN	OD1-CG-ND2	7.69	130.29	122.60
3	C	323	HIS	CB-CG-CD2	7.59	141.07	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	ASN	CA-CB-CG	7.36	119.96	112.60
2	B	115	GLN	CA-CB-CG	7.35	128.80	114.10
1	A	14	PHE	O-C-N	-7.22	112.99	122.59
2	B	5	ASN	CB-CG-OD1	7.05	134.91	120.80
3	C	141	ILE	CA-CB-CG2	6.99	122.38	110.50
3	C	396	ASN	N-CA-C	6.97	121.73	113.23
1	A	22	ARG	NE-CZ-NH1	6.97	128.47	121.50
3	C	99	LYS	CA-C-N	6.93	127.60	120.60
3	C	99	LYS	C-N-CA	6.93	127.60	120.60
3	C	64	GLU	OE1-CD-OE2	6.92	139.51	122.90
1	A	38	ILE	N-CA-CB	6.88	119.38	110.57
3	C	110	THR	CA-C-N	6.65	126.59	119.28
3	C	110	THR	C-N-CA	6.65	126.59	119.28
3	C	352	HIS	CA-CB-CG	-6.59	107.21	113.80
1	A	38	ILE	CB-CA-C	-6.48	103.53	112.02
1	A	97	ASN	CA-CB-CG	6.48	119.08	112.60
3	C	329	ILE	CA-CB-CG2	6.41	121.40	110.50
2	B	126	GLU	CA-C-O	6.30	131.50	120.80
3	C	234	ARG	CB-CG-CD	6.28	125.75	111.30
3	C	432	PHE	CA-CB-CG	6.27	120.07	113.80
3	C	64	GLU	CA-CB-CG	-6.23	101.64	114.10
3	C	143	PRO	N-CA-CB	6.20	109.68	103.48
3	C	250	SER	O-C-N	-6.16	115.14	122.65
1	A	73	VAL	N-CA-CB	6.08	114.33	110.50
3	C	538	ASP	CA-CB-CG	-6.07	106.53	112.60
3	C	302	ASN	N-CA-C	6.04	123.15	109.81
3	C	327	ASN	CA-C-N	6.00	134.41	121.64
3	C	327	ASN	C-N-CA	6.00	134.41	121.64
1	A	43	ILE	N-CA-CB	5.99	117.55	110.55
3	C	102	ASN	CA-C-N	-5.97	113.47	119.56
3	C	102	ASN	C-N-CA	-5.97	113.47	119.56
3	C	327	ASN	O-C-N	5.96	130.51	122.59
3	C	3	ILE	CA-C-O	-5.90	114.23	120.48
1	A	66	ARG	CA-CB-CG	5.89	125.89	114.10
2	B	16	GLU	CB-CG-CD	5.87	122.59	112.60
1	A	44	MET	CA-CB-CG	-5.87	102.36	114.10
3	C	513	ARG	NE-CZ-NH2	-5.80	113.98	119.20
3	C	152	ASN	OD1-CG-ND2	-5.77	116.83	122.60
3	C	57	ASN	OD1-CG-ND2	5.77	128.37	122.60
3	C	328	ASN	CA-CB-CG	5.74	118.34	112.60
3	C	13	GLY	CA-C-N	5.73	125.70	120.03
3	C	13	GLY	C-N-CA	5.73	125.70	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	165	ALA	CA-C-O	-5.66	114.96	121.47
3	C	513	ARG	CG-CD-NE	-5.63	99.62	112.00
3	C	323	HIS	CB-CG-ND1	-5.61	114.29	122.70
3	C	463	ASP	CA-C-N	5.59	125.68	119.87
3	C	463	ASP	C-N-CA	5.59	125.68	119.87
3	C	507	LYS	CA-C-O	5.58	126.47	120.55
2	B	125	VAL	N-CA-CB	5.58	117.87	111.39
3	C	293	HIS	CA-C-N	5.57	125.10	119.19
3	C	293	HIS	C-N-CA	5.57	125.10	119.19
3	C	54	MET	CA-C-O	-5.54	114.30	119.34
3	C	326	LYS	CA-CB-CG	-5.52	103.06	114.10
3	C	274	PHE	CA-CB-CG	5.52	119.32	113.80
3	C	443	PHE	CA-CB-CG	-5.51	108.29	113.80
3	C	186	SER	CA-C-O	5.51	126.39	120.55
2	B	126	GLU	N-CA-C	-5.48	95.65	111.00
3	C	50	LEU	CA-C-O	5.46	128.30	122.13
3	C	104	ASP	CA-CB-CG	5.45	118.05	112.60
3	C	64	GLU	CB-CA-C	-5.44	103.97	112.12
1	A	43	ILE	CB-CA-C	-5.40	105.06	111.97
1	A	15	LEU	CB-CA-C	5.37	121.11	110.42
3	C	7	GLN	CB-CG-CD	5.37	121.72	112.60
3	C	204	SER	CA-C-O	-5.36	115.06	121.11
3	C	212	ILE	O-C-N	-5.34	116.68	121.91
3	C	206	ALA	CA-C-N	5.30	125.11	119.28
3	C	206	ALA	C-N-CA	5.30	125.11	119.28
2	B	13	ARG	CA-CB-CG	5.27	124.64	114.10
3	C	234	ARG	CG-CD-NE	-5.27	100.41	112.00
3	C	252	THR	CB-CA-C	-5.26	102.05	110.79
3	C	396	ASN	CB-CA-C	-5.26	102.47	111.26
2	B	52	ASN	OD1-CG-ND2	-5.26	117.34	122.60
3	C	251	ASP	CA-C-N	5.26	127.32	120.28
3	C	251	ASP	C-N-CA	5.26	127.32	120.28
2	B	125	VAL	O-C-N	5.21	128.36	122.68
3	C	10	GLU	CA-C-O	-5.20	115.36	120.82
3	C	142	ASN	CA-C-N	5.16	124.82	119.56
3	C	142	ASN	C-N-CA	5.16	124.82	119.56
3	C	418	GLN	N-CA-CB	-5.14	102.38	110.46
3	C	5	ARG	CD-NE-CZ	5.13	131.58	124.40
3	C	403	LEU	CB-CG-CD2	5.13	126.09	110.70
3	C	464	PRO	N-CA-CB	5.13	108.23	103.41
3	C	317	ASP	CA-CB-CG	-5.11	107.49	112.60
3	C	388	ARG	NE-CZ-NH1	5.07	126.57	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ALA	N-CA-CB	5.04	117.46	109.94
3	C	390	PRO	N-CA-CB	5.04	107.69	103.25
3	C	226	GLY	CA-C-O	-5.04	111.81	120.57
3	C	231	SER	O-C-N	-5.03	116.79	122.12
3	C	427	ILE	CA-C-O	-5.02	118.26	122.63
3	C	191	PRO	N-CA-CB	5.01	106.27	102.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	327	ASN	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	CXM	Mainchain
1	A	14	PHE	Mainchain
1	A	22	ARG	Sidechain
3	C	329	ILE	Mainchain
3	C	340	ILE	Mainchain
3	C	366	ALA	Mainchain
3	C	427	ILE	Mainchain
3	C	46	GLY	Mainchain
3	C	522	ASN	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	781	0	801	11	0
2	B	951	0	937	6	0
3	C	4329	0	4297	55	2
4	C	2	0	0	0	0
5	C	5	0	0	0	0
6	A	130	0	0	1	0
6	B	186	0	0	1	0
6	C	580	0	0	10	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6964	0	6035	69	4

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 6.

All (69) 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)
3:C:201:HIS:HE1	3:C:222:HIS:H	1.24	0.85
1:A:14:PHE:O	1:A:15:LEU:C	2.18	0.85
1:A:13:ILE:O	1:A:14:PHE:O	2.05	0.74
3:C:201:HIS:CE1	3:C:222:HIS:H	2.06	0.73
3:C:43:ASN:HD22	3:C:48:LYS:HB3	1.58	0.69
3:C:383:LYS:NZ	3:C:387:GLN:HE22	1.92	0.67
3:C:383:LYS:HZ1	3:C:387:GLN:HE22	1.46	0.64
1:A:14:PHE:O	1:A:16:ALA:N	2.31	0.63
3:C:26:ASP:HB3	6:C:1366:HOH:O	1.99	0.60
2:B:25:ARG:NH2	6:B:233:HOH:O	2.37	0.57
3:C:352:HIS:HD2	3:C:409:LYS:NZ	2.03	0.56
2:B:22:ASN:HD21	2:B:66:ARG:HH22	1.52	0.56
3:C:418:GLN:NE2	6:C:1239:HOH:O	2.38	0.56
3:C:321:VAL:HA	6:C:1389:HOH:O	2.06	0.56
3:C:274:PHE:O	3:C:275:HIS:C	2.49	0.55
3:C:375:LEU:HD12	3:C:563:MET:HE2	1.89	0.55
1:A:13:ILE:C	1:A:14:PHE:O	2.51	0.54
3:C:470:THR:N	3:C:471:PRO:CD	2.71	0.54
3:C:81:GLY:HA2	3:C:404:LYS:HE2	1.89	0.54
1:A:12:GLN:HG3	6:A:198:HOH:O	2.08	0.53
3:C:6:GLN:NE2	6:C:1302:HOH:O	2.41	0.53
3:C:300:SER:OG	3:C:352:HIS:HE1	1.93	0.51
2:B:95:GLU:O	3:C:104:ASP:HB3	2.11	0.51
3:C:249:HIS:CE1	3:C:281:GLY:HA3	2.45	0.51
1:A:4:ASN:HB2	1:A:5:PRO:HD2	1.92	0.50
3:C:220:KCX:HE2	3:C:274:PHE:CD2	2.47	0.50
3:C:253:LEU:HD23	6:C:1274:HOH:O	2.11	0.50
3:C:141:ILE:O	3:C:141:ILE:HD12	2.12	0.49
3:C:302:ASN:N	3:C:303:PRO:CD	2.76	0.48
3:C:386:LYS:HG3	6:C:1236:HOH:O	2.14	0.48
3:C:26:ASP:HB2	6:C:1236:HOH:O	2.13	0.48
3:C:468:ILE:HB	3:C:469:PRO:HD2	1.95	0.47
3:C:481:GLY:HA3	6:C:1333:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:383:LYS:NZ	3:C:387:GLN:NE2	2.60	0.46
2:B:10:GLY:HA2	3:C:21:ARG:O	2.16	0.46
3:C:362:THR:O	3:C:368:GLY:HA3	2.16	0.45
2:B:22:ASN:ND2	2:B:66:ARG:HH22	2.15	0.45
3:C:282:GLY:O	3:C:283:HIS:C	2.60	0.45
3:C:220:KCX:HE2	3:C:274:PHE:HD2	1.82	0.45
1:A:23:ARG:HB3	1:A:28:LEU:HD12	1.99	0.44
3:C:61:THR:OG1	3:C:64:GLU:HG3	2.17	0.44
3:C:201:HIS:CE1	3:C:225:TRP:HB2	2.52	0.44
3:C:70:LEU:HD11	3:C:86:ASP:HB3	1.99	0.44
3:C:470:THR:N	3:C:471:PRO:HD3	2.33	0.44
3:C:110:THR:HA	3:C:111:PRO:HD3	1.85	0.43
3:C:177:PRO:O	3:C:181:GLU:HG3	2.19	0.43
3:C:305:ARG:HA	3:C:306:PRO:HA	1.75	0.43
3:C:284:ALA:HA	3:C:285:PRO:HA	1.78	0.43
1:A:73:VAL:N	1:A:74:PRO:CD	2.81	0.43
3:C:303:PRO:HG2	3:C:367:MET:O	2.19	0.43
3:C:452:LYS:HG3	6:C:1045:HOH:O	2.19	0.43
3:C:220:KCX:OX	3:C:222:HIS:HD2	2.32	0.43
3:C:51:ARG:HH11	3:C:51:ARG:HD2	1.63	0.42
3:C:43:ASN:ND2	3:C:48:LYS:HB3	2.30	0.42
3:C:301:THR:CG2	3:C:363:ASP:HB2	2.50	0.42
3:C:349:ASP:HB3	3:C:384:MET:HE3	2.02	0.42
3:C:386:LYS:HB2	3:C:386:LYS:HE3	1.84	0.42
3:C:526:LYS:HD3	6:C:1293:HOH:O	2.19	0.42
3:C:378:TRP:HB2	3:C:563:MET:HE1	2.02	0.42
1:A:75:GLU:HG2	2:B:8:VAL:HG22	2.01	0.41
3:C:468:ILE:HB	3:C:469:PRO:CD	2.50	0.41
3:C:472:GLN:HB3	3:C:473:PRO:HA	2.02	0.41
3:C:513:ARG:HE	3:C:513:ARG:HB3	1.71	0.41
1:A:15:LEU:HD12	1:A:15:LEU:O	2.20	0.41
3:C:132:GLY:HA3	3:C:155:THR:OG1	2.21	0.41
3:C:141:ILE:HG13	3:C:365:LEU:HD13	2.02	0.41
1:A:4:ASN:HB2	1:A:5:PRO:CD	2.51	0.40
3:C:137:HIS:CE1	3:C:274:PHE:CD2	3.09	0.40
3:C:383:LYS:HZ3	3:C:387:GLN:NE2	2.19	0.40

All (4) 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)
3:C:64:GLU:OE2	6:C:1432:HOH:O[11_555]	1.60	0.60
6:C:1032:HOH:O	6:C:1473:HOH:O[12_565]	1.91	0.29
6:C:1032:HOH:O	6:C:1480:HOH:O[12_565]	2.01	0.19
3:C:63:THR:OG1	6:C:1470:HOH:O[11_555]	2.13	0.07

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	98/100 (98%)	93 (95%)	4 (4%)	1 (1%)	12	4
2	B	120/126 (95%)	116 (97%)	3 (2%)	1 (1%)	16	6
3	C	569/570 (100%)	544 (96%)	22 (4%)	3 (0%)	24	13
All	All	787/796 (99%)	753 (96%)	29 (4%)	5 (1%)	21	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	327	ASN
1	A	14	PHE
2	B	99	ILE
3	C	275	HIS
3	C	367	MET

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	84/84 (100%)	83 (99%)	1 (1%)	63	55
2	B	101/105 (96%)	100 (99%)	1 (1%)	68	60
3	C	462/460 (100%)	447 (97%)	15 (3%)	34	19
All	All	647/649 (100%)	630 (97%)	17 (3%)	40	25

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

Mol	Chain	Res	Type
1	A	67	ASP
2	B	126	GLU
3	C	1	MET
3	C	43	ASN
3	C	141	ILE
3	C	253	LEU
3	C	285	PRO
3	C	305	ARG
3	C	326	LYS
3	C	327	ASN
3	C	328	ASN
3	C	386	LYS
3	C	395	LYS
3	C	396	ASN
3	C	452	LYS
3	C	520	CYS
3	C	526	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	22	ASN
3	C	43	ASN
3	C	65	ASN
3	C	201	HIS
3	C	254	ASN
3	C	267	ASN
3	C	352	HIS
3	C	387	GLN
3	C	472	GLN
3	C	491	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	CXM	A	1	1	9,10,11	1.63	3 (33%)	9,11,13	6.73	6 (66%)
3	KCX	C	220	3,4	10,11,12	2.80	2 (20%)	6,12,14	2.70	3 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	A	1	1	-	3/9/10/12	-
3	KCX	C	220	3,4	-	0/9/10/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	220	KCX	CX-NZ	7.99	1.49	1.35
3	C	220	KCX	OQ1-CX	2.97	1.27	1.21
1	A	1	CXM	CB-CA	-2.58	1.47	1.53
1	A	1	CXM	CA-N	-2.29	1.43	1.46
1	A	1	CXM	O-C	2.11	1.28	1.20

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	CXM	CB-CA-N	-16.95	79.64	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	CXM	CA-N-CN	-6.52	110.15	122.11
1	A	1	CXM	ON1-CN-N	5.49	133.86	124.86
3	C	220	KCX	CE-NZ-CX	-4.97	113.54	121.98
1	A	1	CXM	O-C-CA	-4.08	114.27	124.77
1	A	1	CXM	C-CA-N	-4.08	101.63	109.50
3	C	220	KCX	OQ1-CX-NZ	-3.16	120.12	124.92
1	A	1	CXM	CB-CG-SD	3.08	134.12	113.82
3	C	220	KCX	CD-CE-NZ	-2.09	106.32	112.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CXM	C-CA-CB-CG
1	A	1	CXM	N-CA-CB-CG
1	A	1	CXM	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	220	KCX	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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	$\# Z > 2$
5	PO4	C	901	4	4,4,4	1.16	0	6,6,6	0.57	0

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
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	326:LYS	C	327:ASN	N	1.19

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	99/100 (99%)	-0.45	2 (2%) 65 68	13, 26, 36, 43	2 (2%)
2	B	122/126 (96%)	-0.41	1 (0%) 82 86	11, 28, 38, 50	5 (4%)
3	C	567/570 (99%)	-0.41	5 (0%) 81 84	14, 25, 44, 58	14 (2%)
All	All	788/796 (98%)	-0.41	8 (1%) 79 83	11, 26, 42, 58	21 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	126	GLU	4.1
3	C	366	ALA	4.0
1	A	37	ALA	3.2
1	A	15	LEU	2.5
3	C	322	CYS	2.4
3	C	282	GLY	2.3
3	C	331	GLU	2.1
3	C	321	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CXM	A	1	11/12	0.95	0.07	21,27,34,34	0
3	KCX	C	220	12/13	0.95	0.08	19,22,35,40	0

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
5	PO4	C	901	5/5	0.94	0.10	33,35,39,41	5
4	NI	C	601	1/1	0.99	0.05	34,34,34,34	0
4	NI	C	600	1/1	1.00	0.06	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.