Full wwPDB X-ray Structure Validation Report (i)

Sep 15, 2023 – 07:57 AM EDT

PDB ID	:	4UBP
Title	:	STRUCTURE OF BACILLUS PASTEURII UREASE INHIBITED WITH ACETOHYDROXAMIC ACID AT 1.55 A RESOLUTION
Authors	:	Benini, S.; Rypniewski, W.R.; Wilson, K.S.; Ciurli, S.; Mangani, S.
Deposited on	:	1999-02-25
Resolution	:	1.55 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 (i) 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 (i)) were used in the production of this report:

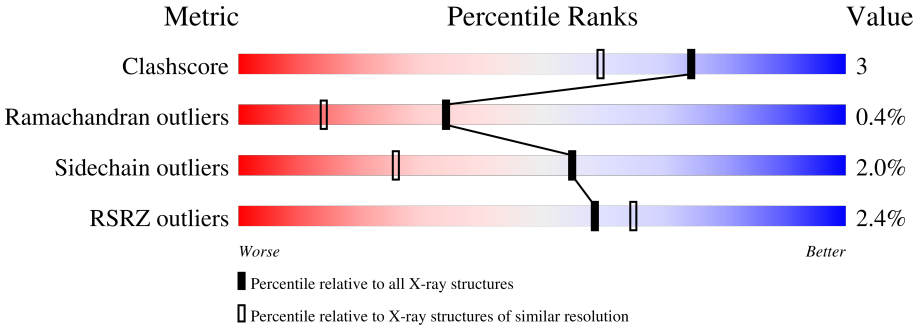
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

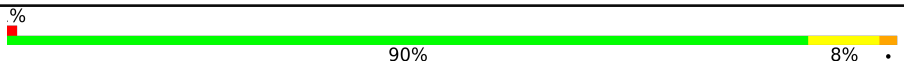
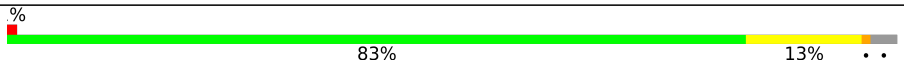
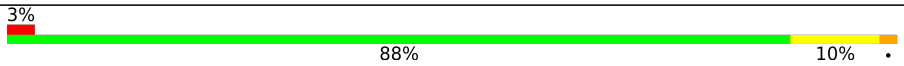
The reported resolution of this entry is 1.55 Å.

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	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 <=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	101	
2	B	126	
3	C	570	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6809 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 PROTEIN (UREASE (CHAIN A)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	101	782	494	133	149	6	7	0	0

- Molecule 2 is a protein called PROTEIN (UREASE (CHAIN B)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	122	951	589	171	190	1	20	0	0

- Molecule 3 is a protein called PROTEIN (UREASE (CHAIN C)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	570	4323	2714	743	843	23	26	0	0

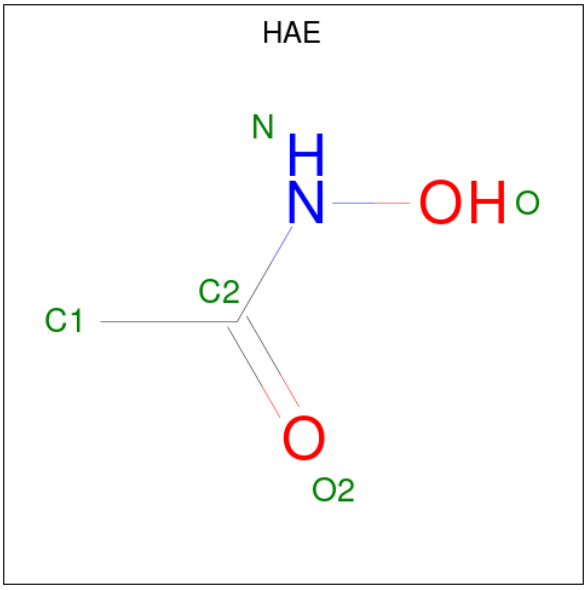
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	GLU	ARG	variant	UNP P41020
C	28	TRP	GLY	variant	UNP P41020
C	29	ILE	-	insertion	UNP P41020
C	36	THR	TYR	variant	UNP P41020
C	37	THR	TYR	variant	UNP P41020
C	38	TYR	LEU	variant	UNP P41020
C	220	KCX	LYS	modified residue	UNP P41020
C	263	LEU	VAL	variant	UNP P41020
C	420	ILE	MET	variant	UNP P41020

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 5 is ACETOHYDROXAMIC ACID (three-letter code: HAE) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	5	2	1	2	0	0

- Molecule 6 is water.

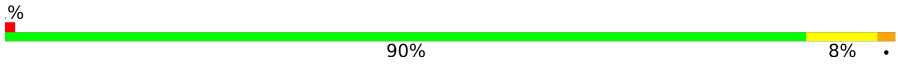
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	99	99	99	0	0
6	B	146	146	146	0	0
6	C	501	501	501	0	0

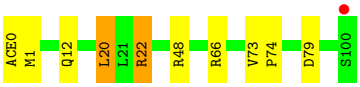
3 Residue-property plots (i)

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: PROTEIN (UREASE (CHAIN A))

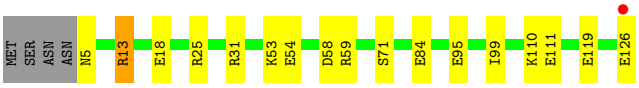
Chain A:





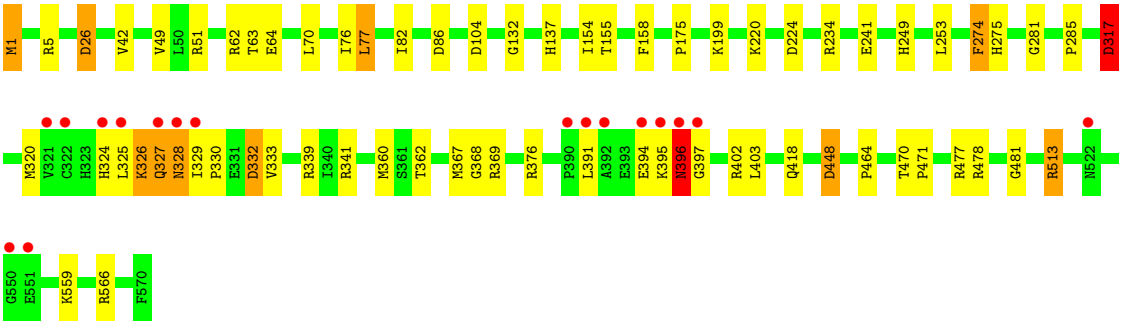
• Molecule 2: PROTEIN (UREASE (CHAIN B))

Chain B:



• Molecule 3: PROTEIN (UREASE (CHAIN C))

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	130.88Å 130.88Å 189.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.73 – 1.55 32.73 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.73-1.55) 99.4 (32.73-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 1.55Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.151 , 0.190 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6809	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NI, ACE, HAE, KCX

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	1.06	2/790 (0.3%)	1.30	9/1063 (0.8%)
2	B	2.95	12/963 (1.2%)	1.76	19/1296 (1.5%)
3	C	1.31	15/4392 (0.3%)	1.53	49/5955 (0.8%)
All	All	1.65	29/6145 (0.5%)	1.54	77/8314 (0.9%)

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	1
2	B	0	1
3	C	0	1
All	All	0	3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	241	GLU	CD-OE1	-51.68	0.68	1.25
2	B	111	GLU	CD-OE2	44.98	1.75	1.25
2	B	111	GLU	CG-CD	40.13	2.12	1.51
2	B	119	GLU	CG-CD	36.12	2.06	1.51
2	B	13	ARG	NE-CZ	29.66	1.71	1.33
3	C	42	VAL	CB-CG1	-26.85	0.96	1.52
2	B	5	ASN	CG-OD1	-23.70	0.71	1.24
3	C	241	GLU	CD-OE2	23.28	1.51	1.25
1	A	20	LEU	CB-CG	-21.43	0.90	1.52
2	B	5	ASN	CG-ND2	21.36	1.86	1.32
3	C	403	LEU	CB-CG	19.73	2.09	1.52
3	C	326	LYS	CD-CE	18.97	1.98	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	18	GLU	CB-CG	18.27	1.86	1.52
3	C	395	LYS	CA-CB	16.10	1.89	1.53
2	B	5	ASN	CB-CG	13.86	1.82	1.51
2	B	110	LYS	CE-NZ	13.19	1.82	1.49
3	C	320	MET	CG-SD	-13.19	1.46	1.81
1	A	22	ARG	CD-NE	-12.73	1.24	1.46
3	C	332	ASP	CB-CG	-12.51	1.25	1.51
2	B	110	LYS	CG-CD	11.90	1.93	1.52
2	B	18	GLU	CG-CD	11.75	1.69	1.51
3	C	329	ILE	CB-CG2	-9.67	1.22	1.52
3	C	327	GLN	CG-CD	9.59	1.73	1.51
2	B	13	ARG	CG-CD	9.59	1.75	1.51
3	C	317	ASP	CB-CG	-8.66	1.33	1.51
3	C	333	VAL	CB-CG2	-7.15	1.37	1.52
3	C	332	ASP	CG-OD1	6.11	1.39	1.25
3	C	332	ASP	CG-OD2	5.84	1.38	1.25
3	C	317	ASP	CA-CB	5.76	1.66	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	241	GLU	OE1-CD-OE2	34.34	164.51	123.30
3	C	320	MET	CG-SD-CE	27.60	144.37	100.20
2	B	111	GLU	CG-CD-OE2	-21.34	75.62	118.30
3	C	42	VAL	CG1-CB-CG2	20.41	143.56	110.90
3	C	5	ARG	NE-CZ-NH2	-19.93	110.33	120.30
2	B	13	ARG	NE-CZ-NH1	-18.33	111.14	120.30
3	C	241	GLU	CG-CD-OE2	-18.01	82.27	118.30
2	B	54	GLU	OE1-CD-OE2	14.99	141.29	123.30
3	C	317	ASP	CB-CG-OD2	-14.75	105.03	118.30
2	B	5	ASN	CB-CG-OD1	14.56	150.72	121.60
3	C	395	LYS	CB-CA-C	-14.35	81.69	110.40
3	C	448	ASP	CB-CG-OD2	14.21	131.09	118.30
2	B	111	GLU	CG-CD-OE1	14.01	146.31	118.30
1	A	22	ARG	CD-NE-CZ	13.41	142.37	123.60
3	C	395	LYS	N-CA-CB	-13.28	86.70	110.60
3	C	396	ASN	CA-CB-CG	12.35	140.57	113.40
2	B	111	GLU	OE1-CD-OE2	12.16	137.90	123.30
3	C	42	VAL	CA-CB-CG2	-10.99	94.42	110.90
3	C	5	ARG	NH1-CZ-NH2	10.35	130.79	119.40
2	B	111	GLU	CB-CG-CD	-9.99	87.21	114.20
3	C	332	ASP	CB-CG-OD1	9.97	127.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5	ASN	CB-CG-ND2	-9.28	94.44	116.70
3	C	332	ASP	OD1-CG-OD2	-9.25	105.72	123.30
3	C	332	ASP	CB-CG-OD2	8.97	126.37	118.30
3	C	62	ARG	NE-CZ-NH2	-8.92	115.84	120.30
2	B	18	GLU	CA-CB-CG	8.40	131.87	113.40
3	C	234	ARG	NE-CZ-NH2	-8.40	116.10	120.30
2	B	119	GLU	CG-CD-OE1	8.13	134.57	118.30
3	C	51	ARG	NE-CZ-NH2	-7.93	116.34	120.30
2	B	110	LYS	CA-CB-CG	7.74	130.43	113.40
1	A	22	ARG	NE-CZ-NH1	7.72	124.16	120.30
3	C	402	ARG	NE-CZ-NH1	7.61	124.11	120.30
3	C	326	LYS	CG-CD-CE	-7.59	89.14	111.90
1	A	48	ARG	NE-CZ-NH2	-7.54	116.53	120.30
3	C	320	MET	CB-CG-SD	7.50	134.90	112.40
1	A	20	LEU	CB-CG-CD1	7.38	123.55	111.00
2	B	110	LYS	CD-CE-NZ	-7.34	94.83	111.70
3	C	329	ILE	CG1-CB-CG2	7.26	127.38	111.40
2	B	25	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	20	LEU	CA-CB-CG	7.21	131.89	115.30
3	C	77	LEU	CB-CG-CD2	7.17	123.19	111.00
3	C	339	ARG	NE-CZ-NH1	7.16	123.88	120.30
3	C	403	LEU	CA-CB-CG	-7.12	98.93	115.30
3	C	320	MET	CA-CB-CG	-7.12	101.20	113.30
3	C	477	ARG	NE-CZ-NH1	7.08	123.84	120.30
2	B	119	GLU	CG-CD-OE2	-6.79	104.73	118.30
3	C	369	ARG	NE-CZ-NH1	6.59	123.59	120.30
3	C	566	ARG	NE-CZ-NH2	-6.57	117.02	120.30
3	C	327	GLN	CG-CD-OE1	6.54	134.68	121.60
3	C	333	VAL	CA-CB-CG2	6.42	120.53	110.90
3	C	26	ASP	CB-CG-OD1	6.34	124.01	118.30
3	C	327	GLN	CG-CD-NE2	-6.31	101.55	116.70
3	C	339	ARG	NE-CZ-NH2	-6.05	117.27	120.30
3	C	327	GLN	C-N-CA	6.01	136.73	121.70
3	C	478	ARG	NE-CZ-NH2	-5.88	117.36	120.30
3	C	274	PHE	CB-CG-CD2	-5.87	116.69	120.80
3	C	360	MET	CG-SD-CE	-5.84	90.85	100.20
1	A	79	ASP	CB-CG-OD1	-5.82	113.06	118.30
2	B	25	ARG	NE-CZ-NH1	5.80	123.20	120.30
3	C	376	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	79	ASP	CB-CG-OD2	-5.58	113.28	118.30
3	C	234	ARG	NE-CZ-NH1	5.55	123.08	120.30
3	C	513	ARG	NE-CZ-NH2	-5.51	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	119	GLU	CB-CG-CD	-5.47	99.42	114.20
3	C	327	GLN	CB-CG-CD	-5.44	97.46	111.60
1	A	66	ARG	CA-CB-CG	5.39	125.25	113.40
3	C	5	ARG	CD-NE-CZ	-5.36	116.09	123.60
2	B	13	ARG	CD-NE-CZ	5.33	131.07	123.60
3	C	394	GLU	OE1-CD-OE2	5.33	129.69	123.30
2	B	59	ARG	NE-CZ-NH2	-5.26	117.67	120.30
3	C	224	ASP	CB-CG-OD1	5.26	123.04	118.30
3	C	64	GLU	OE1-CD-OE2	5.23	129.58	123.30
3	C	566	ARG	CD-NE-CZ	5.21	130.90	123.60
2	B	58	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	79	ASP	OD1-CG-OD2	5.08	132.96	123.30
3	C	341	ARG	NE-CZ-NH1	5.08	122.84	120.30
3	C	464	PRO	N-CA-CB	5.01	109.31	103.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	ARG	Sidechain
2	B	13	ARG	Sidechain
3	C	317	ASP	Sidechain

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	782	0	806	12	0
2	B	951	0	937	4	0
3	C	4323	0	4290	23	1
4	C	2	0	0	0	0
5	C	5	0	4	0	0
6	A	99	0	0	1	0
6	B	146	0	0	1	0
6	C	501	0	0	8	2
All	All	6809	0	6037	37	3

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 3.

All (37) 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:0:ACE:CH3	1:A:0:ACE:O	1.86	1.20
1:A:0:ACE:O	1:A:0:ACE:H3	1.46	1.14
1:A:0:ACE:C	1:A:1:MET:H2	1.50	1.12
1:A:0:ACE:C	1:A:0:ACE:H1	1.50	1.10
1:A:0:ACE:C	1:A:0:ACE:H2	1.50	1.08
1:A:0:ACE:H3	1:A:0:ACE:C	1.50	1.07
1:A:0:ACE:CH3	1:A:0:ACE:C	0.87	0.96
3:C:26:ASP:HB2	6:C:1260:HOH:O	1.84	0.77
1:A:0:ACE:CH3	1:A:1:MET:H2	2.04	0.68
1:A:0:ACE:O	1:A:1:MET:N	2.27	0.65
3:C:63:THR:OG1	6:C:1191:HOH:O	2.14	0.64
1:A:0:ACE:CH3	1:A:1:MET:N	2.63	0.62
3:C:418:GLN:NE2	6:C:1037:HOH:O	2.40	0.54
3:C:513:ARG:NH1	6:C:1077:HOH:O	2.40	0.54
3:C:325:LEU:HB3	3:C:332:ASP:HB3	1.91	0.53
2:B:31:ARG:HG2	2:B:84:GLU:HG2	1.91	0.52
2:B:53:LYS:HD2	6:B:214:HOH:O	2.10	0.51
3:C:559:LYS:HE2	6:C:1290:HOH:O	2.12	0.49
2:B:71:SER:OG	3:C:49:VAL:HG21	2.13	0.49
3:C:470:THR:N	3:C:471:PRO:CD	2.76	0.49
3:C:70:LEU:HD11	3:C:86:ASP:HB3	1.94	0.48
3:C:391:LEU:HA	6:C:1241:HOH:O	2.14	0.48
3:C:175:PRO:HB3	3:C:199:LYS:HE3	1.96	0.48
2:B:95:GLU:O	3:C:104:ASP:HB3	2.14	0.47
3:C:132:GLY:HA3	3:C:155:THR:OG1	2.14	0.47
3:C:249:HIS:CE1	3:C:281:GLY:HA3	2.51	0.46
1:A:12:GLN:NE2	6:A:146:HOH:O	2.43	0.45
3:C:481:GLY:HA3	6:C:1025:HOH:O	2.15	0.45
3:C:274:PHE:O	3:C:275:HIS:C	2.55	0.44
3:C:137:HIS:CE1	3:C:274:PHE:CD2	3.07	0.43
3:C:362:THR:O	3:C:368:GLY:HA3	2.19	0.43
3:C:328:ASN:O	3:C:330:PRO:HD3	2.19	0.42
3:C:396:ASN:HB3	3:C:397:GLY:H	1.67	0.41
3:C:154:ILE:HD11	6:C:1082:HOH:O	2.20	0.41
1:A:73:VAL:N	1:A:74:PRO:CD	2.84	0.40
3:C:1:MET:HE2	3:C:1:MET:HB3	1.97	0.40
3:C:76:ILE:O	3:C:82:ILE:HA	2.22	0.40

All (3) 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:327:GLN:O	3:C:327:GLN:OE1[7_556]	1.76	0.44
6:C:1191:HOH:O	6:C:1191:HOH:O[11_555]	1.81	0.39
6:C:1198:HOH:O	6:C:1198:HOH:O[10_665]	1.92	0.28

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	98/101 (97%)	98 (100%)	0	0	100	100
2	B	120/126 (95%)	115 (96%)	4 (3%)	1 (1%)	19	4
3	C	567/570 (100%)	544 (96%)	21 (4%)	2 (0%)	34	14
All	All	785/797 (98%)	757 (96%)	25 (3%)	3 (0%)	34	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	396	ASN
2	B	99	ILE
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	85/85 (100%)	84 (99%)	1 (1%)	71	49
2	B	101/105 (96%)	100 (99%)	1 (1%)	76	57
3	C	460/460 (100%)	449 (98%)	11 (2%)	49	20
All	All	646/650 (99%)	633 (98%)	13 (2%)	55	26

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
2	B	126	GLU
3	C	1	MET
3	C	77	LEU
3	C	158	PHE
3	C	253	LEU
3	C	285	PRO
3	C	317	ASP
3	C	324	HIS
3	C	326	LYS
3	C	328	ASN
3	C	396	ASN
3	C	448	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
3	C	328	ASN
3	C	418	GLN
3	C	519	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
3	KCX	C	220	3,4	9,11,12	2.53	2 (22%)	5,12,14	3.71	3 (60%)

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
3	KCX	C	220	3,4	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	220	KCX	CX-NZ	5.76	1.45	1.35
3	C	220	KCX	OQ1-CX	4.33	1.29	1.21

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	220	KCX	OQ1-CX-NZ	-6.96	114.17	124.96
3	C	220	KCX	CE-NZ-CX	-3.89	115.64	121.89
3	C	220	KCX	CD-CE-NZ	-2.16	106.03	112.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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	HAE	C	800	4	4,4,4	0.46	0	2,4,4	1.32	0

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
5	HAE	C	800	4	-	0/1/2/2	-

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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	0:ACE	C	1:MET	N	2.20

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	100/101 (99%)	-0.72	1 (1%)	82	86	18, 22, 30, 42	2 (2%)
2	B	122/126 (96%)	-0.34	1 (0%)	86	89	19, 25, 35, 61	6 (4%)
3	C	569/570 (99%)	-0.49	17 (2%)	50	58	17, 21, 42, 106	12 (2%)
All	All	791/797 (99%)	-0.50	19 (2%)	59	65	17, 22, 38, 106	20 (2%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	391	LEU	7.3
3	C	390	PRO	5.5
3	C	328	ASN	4.9
3	C	397	GLY	4.8
3	C	329	ILE	4.5
2	B	126	GLU	4.2
3	C	392	ALA	3.6
3	C	396	ASN	3.3
1	A	100	SER	3.1
3	C	395	LYS	2.8
3	C	321	VAL	2.8
3	C	550	GLY	2.7
3	C	322	CYS	2.5
3	C	551	GLU	2.5
3	C	394	GLU	2.3
3	C	327	GLN	2.1
3	C	522	ASN	2.1
3	C	325	LEU	2.0
3	C	324	HIS	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
3	KCX	C	220	12/13	0.98	0.05	16,18,19,21	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
5	HAE	C	800	5/5	0.97	0.05	23,24,28,30	0
4	NI	C	799	1/1	1.00	0.02	20,20,20,20	0
4	NI	C	798	1/1	1.00	0.01	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.