



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:38 PM GMT

PDB ID : 3UE1
Title : Crystal structure of Acinetobacter baumannii PBP1A in complex with MC-1
Authors : Han, S.
Deposited on : 2011-10-28
Resolution : 2.73 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

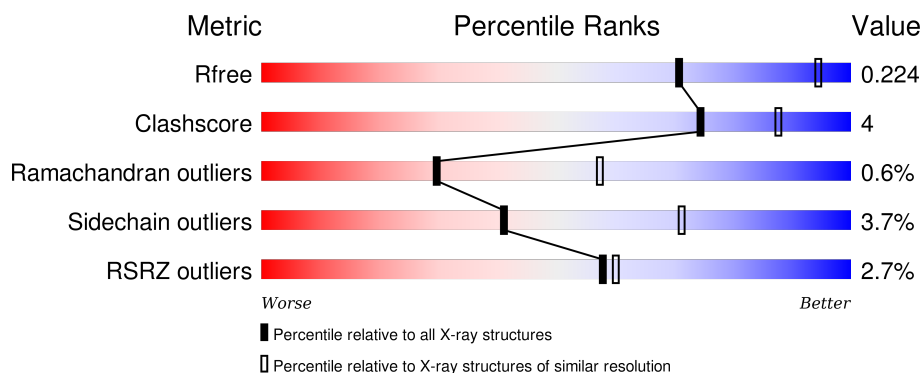
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

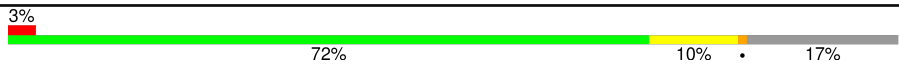

The reported resolution of this entry is 2.73 Å.

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}	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	731	
1	B	731	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9809 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 Penicillin-binding protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	0	0
			4757	3032	842	867	16			
1	B	600	Total	C	N	O	S	0	0	0
			4719	3008	834	861	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	EXPRESSION TAG	UNP G1C794
A	10	HIS	-	EXPRESSION TAG	UNP G1C794
A	11	HIS	-	EXPRESSION TAG	UNP G1C794
A	12	HIS	-	EXPRESSION TAG	UNP G1C794
A	13	HIS	-	EXPRESSION TAG	UNP G1C794
A	14	HIS	-	EXPRESSION TAG	UNP G1C794
A	15	HIS	-	EXPRESSION TAG	UNP G1C794
A	16	GLU	-	EXPRESSION TAG	UNP G1C794
A	17	ASN	-	EXPRESSION TAG	UNP G1C794
A	18	LEU	-	EXPRESSION TAG	UNP G1C794
A	19	TYR	-	EXPRESSION TAG	UNP G1C794
A	20	PHE	-	EXPRESSION TAG	UNP G1C794
A	21	GLN	-	EXPRESSION TAG	UNP G1C794
A	22	SER	-	EXPRESSION TAG	UNP G1C794
A	23	HIS	-	EXPRESSION TAG	UNP G1C794
A	24	MET	-	EXPRESSION TAG	UNP G1C794
B	9	MET	-	EXPRESSION TAG	UNP G1C794
B	10	HIS	-	EXPRESSION TAG	UNP G1C794
B	11	HIS	-	EXPRESSION TAG	UNP G1C794
B	12	HIS	-	EXPRESSION TAG	UNP G1C794
B	13	HIS	-	EXPRESSION TAG	UNP G1C794
B	14	HIS	-	EXPRESSION TAG	UNP G1C794
B	15	HIS	-	EXPRESSION TAG	UNP G1C794
B	16	GLU	-	EXPRESSION TAG	UNP G1C794
B	17	ASN	-	EXPRESSION TAG	UNP G1C794

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Chain	Residue	Modelled	Actual	Comment	Reference
B	18	LEU	-	EXPRESSION TAG	UNP G1C794
B	19	TYR	-	EXPRESSION TAG	UNP G1C794
B	20	PHE	-	EXPRESSION TAG	UNP G1C794
B	21	GLN	-	EXPRESSION TAG	UNP G1C794
B	22	SER	-	EXPRESSION TAG	UNP G1C794
B	23	HIS	-	EXPRESSION TAG	UNP G1C794
B	24	MET	-	EXPRESSION TAG	UNP G1C794

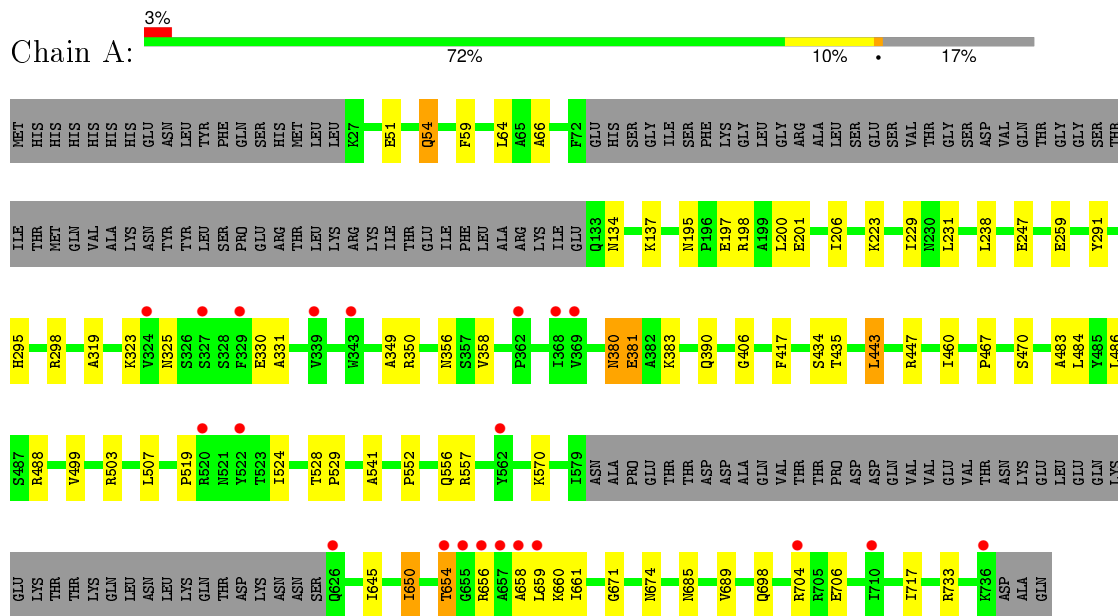
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- Chemical structure of UE1, a complex molecule featuring a pyridine ring, a sulfonamide group, and a sulfonate group. The structure is shown with atom labels (C, N, O, S) and bond types (single, double, triple). The molecule is composed of several interconnected rings and functional groups, including a pyridine ring, a sulfonamide group, and a sulfonate group. The structure is shown in a 3D representation with stereochemistry indicated by wedge and dash bonds.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	104	Total O 104 104	0	0
3	B	133	Total O 133 133	0	0

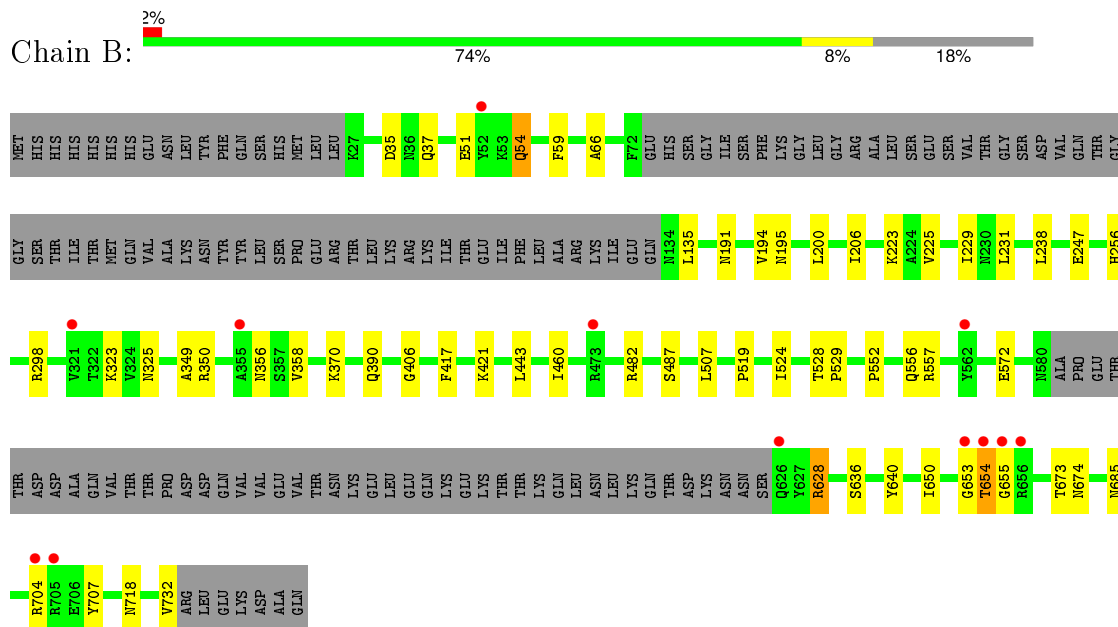
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Penicillin-binding protein 1a



- Molecule 1: Penicillin-binding protein 1a



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.21Å 244.29Å 49.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 2.73 122.14 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.57-2.73) 99.7 (122.14-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.172 , 0.219 0.177 , 0.224	Depositor DCC
R_{free} test set	1970 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 39279 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9809	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: UE1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/4867	0.71	2/6599 (0.0%)
1	B	0.51	0/4829	0.72	0/6550
All	All	0.51	0/9696	0.72	2/13149 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	ARG	N-CA-C	6.26	127.90	111.00
1	A	447	ARG	C-N-CA	5.03	132.87	122.30

There are no chirality outliers.

There are no planarity outliers.

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	4757	0	4755	41	0
1	B	4719	0	4709	33	0
2	A	48	0	26	8	0
2	B	48	0	24	3	0
3	A	104	0	0	0	0
3	B	133	0	0	2	0
All	All	9809	0	9514	75	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 4.

All (75) 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:434:SER:OG	2:A:998:UE1:H11	0.83	1.00
1:A:298:ARG:H	1:A:390:GLN:HE22	1.18	0.90
1:B:298:ARG:H	1:B:390:GLN:HE22	1.15	0.89
1:A:674:ASN:HA	2:A:998:UE1:H24A	1.59	0.84
1:A:434:SER:HG	2:A:998:UE1:C11	1.73	0.79
1:B:191:ASN:HB3	1:B:194:VAL:HG12	1.65	0.76
1:A:434:SER:HG	2:A:998:UE1:H11	0.92	0.74
1:B:718:ASN:ND2	3:B:865:HOH:O	2.22	0.72
1:B:356:ASN:HD21	1:B:704:ARG:H	1.38	0.71
1:A:229:ILE:HG22	1:A:231:LEU:HG	1.72	0.71
1:B:229:ILE:HG22	1:B:231:LEU:HG	1.72	0.70
1:A:443:LEU:HD12	1:A:507:LEU:HD22	1.76	0.68
1:B:654:THR:N	1:B:655:GLY:HA3	2.08	0.68
2:A:998:UE1:H36A	2:A:998:UE1:H46	1.75	0.68
1:B:443:LEU:HB2	1:B:507:LEU:HD22	1.77	0.65
1:A:650:ILE:HG23	1:A:658:ALA:HB2	1.77	0.65
1:A:200:LEU:HD13	1:A:229:ILE:HG13	1.80	0.62
1:B:653:GLY:C	1:B:655:GLY:HA3	2.20	0.62
1:A:556:GLN:HE22	1:A:557:ARG:HH11	1.47	0.60
1:B:556:GLN:HE22	1:B:557:ARG:HH11	1.46	0.60
1:A:656:ARG:HB2	1:A:659:LEU:HB2	1.83	0.59
1:A:443:LEU:HD13	1:A:499:VAL:CG1	2.33	0.59
1:A:350:ARG:HH11	1:A:358:VAL:HG21	1.68	0.56
1:B:66:ALA:HA	1:B:206:ILE:HG12	1.87	0.56
1:A:66:ALA:HA	1:A:206:ILE:HG12	1.86	0.56
1:A:443:LEU:HD11	1:A:503:ARG:HG3	1.89	0.54
1:A:470:SER:HA	2:A:998:UE1:H23B	1.90	0.54
1:B:350:ARG:HH11	1:B:358:VAL:HG21	1.72	0.54
1:A:323:LYS:HE2	1:A:325:ASN:HD21	1.73	0.53
1:A:356:ASN:HD21	1:A:704:ARG:H	1.55	0.53
1:B:406:GLY:O	1:B:552:PRO:HA	2.09	0.52
1:B:732:VAL:HB	3:B:862:HOH:O	2.10	0.52
1:B:674:ASN:HA	2:B:999:UE1:H23A	1.91	0.52
1:B:323:LYS:HE2	1:B:325:ASN:HD21	1.74	0.52
1:B:356:ASN:HD21	1:B:704:ARG:N	2.06	0.51
1:B:650:ILE:O	1:B:655:GLY:HA2	2.11	0.50
1:B:298:ARG:N	1:B:390:GLN:HE22	1.96	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:GLU:HB2	1:B:54:GLN:HG3	1.93	0.50
1:B:298:ARG:H	1:B:390:GLN:NE2	1.98	0.49
1:A:406:GLY:O	1:A:552:PRO:HA	2.13	0.49
1:A:64:LEU:HG	1:A:134:ASN:HB3	1.94	0.48
1:A:319:ALA:HB1	1:A:331:ALA:HB1	1.97	0.47
1:A:460:ILE:HG23	1:A:467:PRO:HG2	1.97	0.47
2:A:998:UE1:C46	2:A:998:UE1:H36A	2.44	0.46
1:A:247:GLU:HG2	1:A:417:PHE:CE1	2.50	0.46
1:B:650:ILE:HA	1:B:655:GLY:H	1.80	0.46
1:B:356:ASN:ND2	1:B:704:ARG:H	2.08	0.46
1:B:247:GLU:HG2	1:B:417:PHE:CE1	2.50	0.46
1:A:51:GLU:HB2	1:A:54:GLN:HG2	1.97	0.45
1:A:137:LYS:NZ	1:B:256:HIS:HD2	2.15	0.45
1:B:556:GLN:NE2	1:B:557:ARG:HH11	2.13	0.45
1:A:484:LEU:HD23	1:A:645:ILE:HG21	1.98	0.44
1:B:673:THR:O	2:B:999:UE1:H24B	2.16	0.44
1:B:443:LEU:HB2	1:B:507:LEU:CD2	2.47	0.44
1:A:556:GLN:NE2	1:A:557:ARG:HH11	2.14	0.44
1:B:707:TYR:HB2	2:B:999:UE1:H36	2.00	0.44
1:A:483:ALA:HA	1:A:488:ARG:HG2	2.00	0.43
1:A:298:ARG:N	1:A:390:GLN:HE22	2.00	0.43
1:A:323:LYS:HB3	1:A:330:GLU:HB2	1.99	0.43
1:A:519:PRO:HD2	1:A:524:ILE:HG22	2.00	0.43
1:A:661:ILE:HG13	1:A:717:ILE:HG23	2.01	0.43
1:A:541:ALA:HA	1:A:689:VAL:HG21	2.01	0.42
1:B:650:ILE:HA	1:B:655:GLY:N	2.34	0.42
1:A:486:LEU:HB3	1:A:488:ARG:HD3	2.01	0.41
1:A:435:THR:HG23	1:A:671:GLY:HA3	2.03	0.41
1:B:519:PRO:HD2	1:B:524:ILE:HG22	2.02	0.41
1:A:434:SER:CB	2:A:998:UE1:C11	2.88	0.41
1:B:528:THR:N	1:B:529:PRO:CD	2.84	0.41
1:B:572:GLU:HA	1:B:628:ARG:HB3	2.03	0.41
1:A:443:LEU:HD13	1:A:499:VAL:HG13	2.02	0.41
1:A:247:GLU:HG2	1:A:417:PHE:HE1	1.85	0.41
1:A:528:THR:N	1:A:529:PRO:CD	2.84	0.41
1:A:291:TYR:CE1	1:A:295:HIS:CE1	3.09	0.41
1:B:640:TYR:CD1	1:B:732:VAL:HG23	2.57	0.40
1:A:380:ASN:O	1:A:381:GLU:C	2.60	0.40

There are no symmetry-related clashes.

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	598/731 (82%)	576 (96%)	18 (3%)	4 (1%)	26	54
1	B	594/731 (81%)	567 (96%)	24 (4%)	3 (0%)	34	62
All	All	1192/1462 (82%)	1143 (96%)	42 (4%)	7 (1%)	30	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	654	THR
1	B	628	ARG
1	A	381	GLU
1	A	383	LYS
1	A	349	ALA
1	B	135	LEU
1	B	349	ALA

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	493/608 (81%)	474 (96%)	19 (4%)	39	69
1	B	489/608 (80%)	472 (96%)	17 (4%)	43	73
All	All	982/1216 (81%)	946 (96%)	36 (4%)	41	71

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	59	PHE
1	A	195	ASN
1	A	197	GLU
1	A	198	ARG
1	A	201	GLU
1	A	223	LYS
1	A	238	LEU
1	A	259	GLU
1	A	380	ASN
1	A	443	LEU
1	A	570	LYS
1	A	650	ILE
1	A	654	THR
1	A	660	LYS
1	A	685	ASN
1	A	698	GLN
1	A	706	GLU
1	A	733	ARG
1	B	35	ASP
1	B	37	GLN
1	B	54	GLN
1	B	59	PHE
1	B	195	ASN
1	B	200	LEU
1	B	223	LYS
1	B	225	VAL
1	B	238	LEU
1	B	370	LYS
1	B	421	LYS
1	B	460	ILE
1	B	482	ARG
1	B	487	SER
1	B	636	SER
1	B	654	THR
1	B	685	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	ASN
1	A	390	GLN
1	A	556	GLN

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Mol	Chain	Res	Type
1	A	626	GLN
1	B	170	ASN
1	B	256	HIS
1	B	325	ASN
1	B	356	ASN
1	B	390	GLN
1	B	469	ASN
1	B	556	GLN
1	B	674	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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	$\# Z > 2$
2	UE1	A	998	1	36,50,50	1.68	6 (16%)	32,73,73	1.33	4 (12%)
2	UE1	B	999	1	36,50,50	1.69	7 (19%)	32,73,73	2.04	7 (21%)

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
2	UE1	A	998	1	-	0/28/52/52	0/3/3/3
2	UE1	B	999	1	-	0/28/52/52	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	UE1	O47-C45	-6.44	1.23	1.36
2	A	998	UE1	O47-C45	-6.23	1.23	1.36
2	B	999	UE1	C29-N31	-2.95	1.34	1.39
2	A	998	UE1	C29-N31	-2.93	1.34	1.39
2	A	998	UE1	C43-C44	-2.36	1.37	1.39
2	B	999	UE1	C43-C44	-2.33	1.37	1.39
2	B	999	UE1	C18-C16	-2.10	1.46	1.50
2	B	999	UE1	C45-C44	2.12	1.43	1.40
2	A	998	UE1	C45-C44	2.43	1.44	1.40
2	B	999	UE1	C46-C45	2.67	1.42	1.38
2	A	998	UE1	C46-C45	2.97	1.43	1.38
2	B	999	UE1	C9-S8	3.23	1.75	1.70
2	A	998	UE1	C9-S8	3.27	1.75	1.70

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	UE1	N31-C29-N12	-7.98	105.71	114.41
2	A	998	UE1	C24-C21-C23	-3.50	104.36	110.27
2	A	998	UE1	N31-C29-N12	-2.33	111.87	114.41
2	A	998	UE1	C27-C9-S8	-2.25	109.03	111.79
2	B	999	UE1	C27-C9-S8	-2.13	109.17	111.79
2	B	999	UE1	O30-C29-N12	2.14	126.73	122.75
2	B	999	UE1	O17-C16-C18	2.37	123.17	120.53
2	B	999	UE1	O30-C29-N31	2.95	127.53	121.62
2	B	999	UE1	C43-N42-C41	3.21	122.41	117.84
2	A	998	UE1	C43-N42-C41	3.26	122.47	117.84
2	B	999	UE1	C13-N12-C29	3.82	130.91	121.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	998	UE1	8	0
2	B	999	UE1	3	0

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 ⓘ

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	604/731 (82%)	0.25	21 (3%)	48 50	35, 60, 104, 136	0
1	B	600/731 (82%)	0.19	12 (2%)	68 71	26, 56, 93, 120	0
All	All	1204/1462 (82%)	0.22	33 (2%)	58 60	26, 57, 99, 136	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	626	GLN	6.6
1	B	656	ARG	6.6
1	B	653	GLY	5.4
1	B	705	ARG	4.7
1	B	655	GLY	4.3
1	B	473	ARG	4.2
1	A	362	PRO	4.1
1	A	626	GLN	3.5
1	B	654	THR	3.0
1	A	343	TRP	2.9
1	B	321	VAL	2.7
1	A	657	ALA	2.6
1	A	324	VAL	2.5
1	A	655	GLY	2.5
1	A	704	ARG	2.4
1	A	520	ARG	2.4
1	A	659	LEU	2.3
1	A	327	SER	2.3
1	A	339	VAL	2.3
1	A	329	PHE	2.3
1	A	368	ILE	2.2
1	A	654	THR	2.2
1	A	522	TYR	2.1
1	A	656	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	658	ALA	2.1
1	A	736	LYS	2.1
1	B	562	TYR	2.1
1	A	562	TYR	2.1
1	A	710	ILE	2.0
1	B	704	ARG	2.0
1	B	52	TYR	2.0
1	B	355	ALA	2.0
1	A	369	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	UE1	A	998	48/48	0.91	0.26	1.18	69,90,106,108	0
2	UE1	B	999	48/48	0.95	0.23	0.01	35,77,101,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.