

Full wwPDB X-ray Structure Validation Report (i)

May 1, 2024 – 10:18 am BST

PDB ID	:	8RE0
Title	:	Soluble glucose dehydrogenase from acinetobacter calcoaceticus - double mu-
		tant pH8
Authors	:	Lublin, V.; Chavas, L.; Stines-Chaumeil, C.; Kauffmann, B.; Giraud, M.F.;
		Thompson, A.
Deposited on		
Resolution	:	1.56 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:

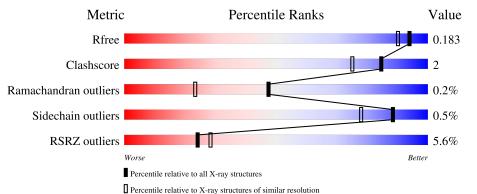
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.56 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1483 (1.56-1.56)
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	А	454	<u>6%</u> 94%	6%				
1	В	454	96%	•				



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15446 atoms, of which 6975 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 Quinoprotein glucose dehydrogenase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	452	Total 7045	C 2260	H 2402	N 602	0 695	S E	0	2	0
			7045	2260		602	685	0 2			
1	В	452	Total	С	Н	Ν	O	\mathbf{S}	0	0	0
-	D	102	7013	2249	3476	600	683	5	0	, , , , , , , , , , , , , , , , , , ,	Ŭ

There are 2 discrepancies between the modelled and reference sequences:

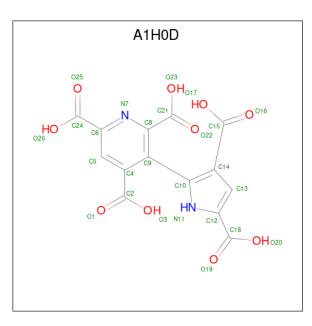
Chain	Residue	Modelled	Actual	Comment	Reference
A	343	PHE	TYR	conflict	UNP P13650
В	343	PHE	TYR	conflict	UNP P13650

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues Atoms		ZeroOcc	AltConf
2	А	3	Total Ca 3 3	0	0
2	В	3	Total Ca 3 3	0	0

• Molecule 3 is 3-(3,5-dicarboxy-1 {H}-pyrrol-2-yl)pyridine-2,4,6-tricarboxylic acid (three-letter code: A1H0D) (formula: $C_{14}H_8N_2O_{10}$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	Λ	1	Total	С	Η	Ν	0	0	0	
5	3 A	1	29	14	3	2	10	0	0	
2	В	1	Total	С	Η	Ν	0	0	0	
5	D	1	29	14	3	2	10	0	0	

• Molecule 4 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Li 1 1	0	0

• Molecule 5 is water.

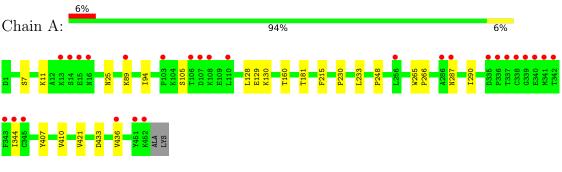
Mol	Chain	Residues Atoms		ZeroOcc	AltConf
5	А	658	Total O 658 658	0	0
5	В	665	Total O 665 665	0	0



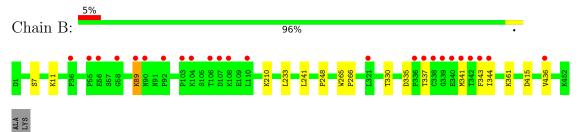
3 Residue-property plots (i)

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: Quinoprotein glucose dehydrogenase B



• Molecule 1: Quinoprotein glucose dehydrogenase B





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	60.73Å 92.61Å 85.34Å	Depositor
a, b, c, α , β , γ	90.00° 105.24° 90.00°	Depositor
Resolution (Å)	42.73 - 1.56	Depositor
Resolution (A)	42.73 - 1.56	EDS
% Data completeness	80.2 (42.73-1.56)	Depositor
(in resolution range)	80.2(42.73-1.56)	EDS
R _{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.43 (at 1.56 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D.	0.160 , 0.183	Depositor
R, R_{free}	0.160 , 0.183	DCC
R_{free} test set	5201 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	16.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , 42.4	EDS
L-test for twinning ²	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15446	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: A1H0D, CA, LI

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.48	0/3642	0.66	0/4962	
1	В	0.49	0/3627	0.65	0/4941	
All	All	0.48	0/7269	0.66	0/9903	

There are no bond length outliers.

There are no bond angle outliers.

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	А	3552	3493	3494	21	2
1	В	3537	3476	3476	12	2
2	А	3	0	0	0	0
2	В	3	0	0	0	0
3	А	26	3	0	0	0
3	В	26	3	0	0	0
4	А	1	0	0	0	0
5	А	658	0	0	9	4
5	В	665	0	0	4	6
All	All	8471	6975	6970	33	8

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 2.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:B:415:ASP:OD2	5:B:701:HOH:O	1.94	0.83
1:A:25:ASN:ND2	5:A:704:HOH:O	2.14	0.81
1:A:11:LYS:NZ	5:A:702:HOH:O	2.11	0.81
1:B:361:LYS:HG3	5:B:1019:HOH:O	1.86	0.74
1:A:25:ASN:CG	5:A:704:HOH:O	2.29	0.70
1:A:89:LYS:NZ	5:A:701:HOH:O	1.85	0.70
1:A:129:GLU:OE1	5:A:703:HOH:O	2.13	0.66
1:A:11:LYS:N	1:A:11:LYS:HD3	2.15	0.60
1:B:265:TRP:CD2	1:B:266:PRO:HA	2.39	0.57
1:A:344:ILE:HD13	1:A:436:VAL:HG23	1.88	0.55
1:A:265:TRP:CD2	1:A:266:PRO:HA	2.43	0.53
1:B:344:ILE:HD13	1:B:436:VAL:HG23	1.90	0.53
1:B:341:MET:SD	1:B:436:VAL:HG11	2.49	0.53
1:A:25:ASN:HB3	5:A:704:HOH:O	2.10	0.52
1:B:335:ASP:CG	1:B:337:THR:HG22	2.31	0.50
1:A:94:ILE:HD12	1:A:128:LEU:HD21	1.92	0.50
1:A:25:ASN:CB	5:A:704:HOH:O	2.59	0.49
1:A:160:THR:HG23	1:A:233:LEU:HD22	1.95	0.48
1:A:287:ASN:O	1:A:290[B]:ILE:HG12	2.12	0.48
1:B:335:ASP:OD2	1:B:337:THR:HG22	2.15	0.47
1:A:407:TYR:CD1	1:A:421[B]:VAL:HG11	2.50	0.46
1:A:287:ASN:HB3	1:A:290[B]:ILE:HD11	1.97	0.46
1:B:89:LYS:HD2	1:B:89:LYS:H	1.80	0.46
1:A:130:LYS:HD3	5:A:1010:HOH:O	2.16	0.45
1:A:105:SER:HB2	5:A:710:HOH:O	2.16	0.44
1:A:410:VAL:HG23	1:A:421[A]:VAL:HG12	1.99	0.43
1:B:89:LYS:H	1:B:89:LYS:CD	2.31	0.43
1:B:330:THR:OG1	5:B:702:HOH:O	2.03	0.42
1:B:233:LEU:HG	1:B:241:LEU:HD11	2.00	0.42
1:B:330:THR:HG21	5:B:1162:HOH:O	2.20	0.42
1:A:7:SER:O	1:A:11:LYS:HE2	2.20	0.41
1:A:181:THR:HG21	1:A:215:PHE:HB3	2.02	0.41
1:A:160:THR:HB	1:A:230:PRO:HG2	2.02	0.41

All (8) 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)
5:A:1228:HOH:O	5:B:1210:HOH:O[1_554]	1.80	0.40
5:B:1119:HOH:O	5:B:1284:HOH:O[2_657]	1.93	0.27
5:B:1232:HOH:O	5:B:1284:HOH:O[2_657]	1.96	0.24
5:A:1243:HOH:O	5:B:1324:HOH:O[2_556]	2.09	0.11
1:A:433:ASP:OD2	1:B:210:LYS:NZ[2_656]	2.11	0.09
1:A:433:ASP:OD2	1:B:210:LYS:HZ3[2_656]	1.54	0.06
5:A:1173:HOH:O	5:B:1153:HOH:O[2_646]	2.14	0.06
5:A:1243:HOH:O	5:B:1164:HOH:O[2_556]	2.18	0.02

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	Perce	ntiles
1	А	452/454~(100%)	438 (97%)	13 (3%)	1 (0%)	47	23
1	В	450/454~(99%)	433 (96%)	16 (4%)	1 (0%)	47	23
All	All	902/908~(99%)	871 (97%)	29 (3%)	2~(0%)	47	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	248	PRO
1	В	248	PRO

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	А	392/391~(100%)	392 (100%)	0	100 100
1	В	390/391~(100%)	386~(99%)	4 (1%)	76 57
All	All	782/782~(100%)	778 (100%)	4 (0%)	88 78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	7	SER
1	В	11	LYS
1	В	89	LYS
1	В	343	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	Turne	Chain	Res	Link	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
IVIOI	Type	Unain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	A1H0D	А	604	2	27,27,27	1.23	2 (7%)	29,40,40	1.14	1 (3%)
3	A1H0D	В	604	2	27,27,27	1.29	1 (3%)	29,40,40	1.22	4 (13%)

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.

Mo	l Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1H0D	A	604	2	-	2/18/24/24	0/2/2/2
3	A1H0D	В	604	2	-	2/18/24/24	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	В	604	A1H0D	C9-C10	-4.63	1.45	1.50
3	А	604	A1H0D	C9-C10	-4.08	1.45	1.50
3	А	604	A1H0D	O20-C18	-2.18	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
3	В	604	A1H0D	C4-C5-C6	-2.36	118.00	119.93
3	А	604	A1H0D	C4-C5-C6	-2.35	118.00	119.93
3	В	604	A1H0D	O25-C24-C6	-2.23	116.71	121.24
3	В	604	A1H0D	O22-C21-C8	-2.16	116.30	120.73
3	В	604	A1H0D	O16-C15-C14	-2.13	116.77	121.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

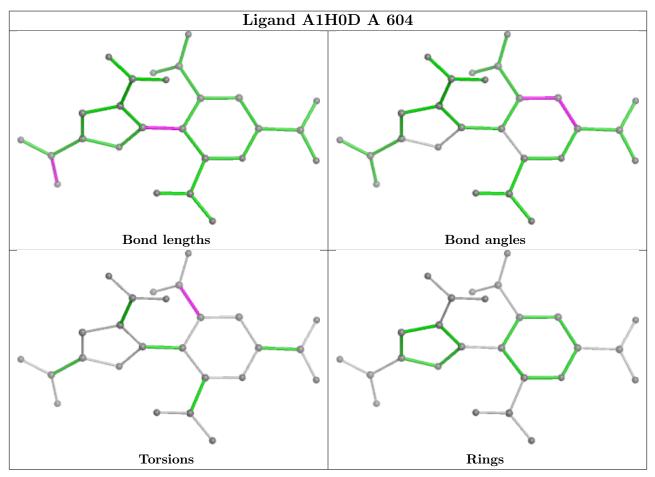
Mol	Chain	Res	Type	Atoms
3	А	604	A1H0D	O3-C2-C4-C5
3	В	604	A1H0D	O3-C2-C4-C5
3	А	604	A1H0D	O1-C2-C4-C5
3	В	604	A1H0D	O1-C2-C4-C5

There are no ring outliers.

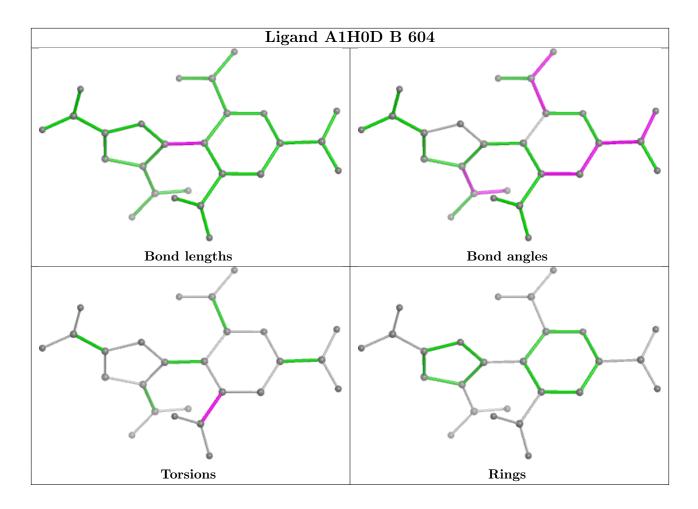
No monomer is involved in short contacts.



The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	А	452/454~(99%)	0.32	27 (5%) 21 25	12, 18, 35, 60	10 (2%)
1	В	452/454~(99%)	0.37	24 (5%) 26 31	11, 18, 34, 69	9 (1%)
All	All	904/908~(99%)	0.35	51 (5%) 24 28	11, 18, 34, 69	19 (2%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	106	THR	13.7
1	А	106	THR	11.9
1	В	339	GLY	10.9
1	А	338	CYS	7.9
1	А	339	GLY	7.0
1	В	338	CYS	7.0
1	В	341	MET	5.7
1	А	337	THR	5.6
1	А	343	PHE	5.0
1	А	451	TYR	4.9
1	В	436	VAL	4.8
1	В	343	PHE	4.6
1	А	336	PRO	4.5
1	В	107	ASP	4.3
1	В	337	THR	4.1
1	А	340	GLU	4.0
1	А	108	LYS	4.0
1	А	341	MET	3.9
1	В	340	GLU	3.9
1	В	336	PRO	3.8
1	А	103	PRO	3.7
1	В	108	LYS	3.7
1	В	55	PRO	3.7
1	А	436	VAL	3.5

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8 RE0

Mol	Chain	Res	Type	RSRZ
1	А	342	THR	3.5
1	В	110	LEU	3.5
1	В	36	PRO	3.5
1	В	90	ASN	3.4
1	А	287	ASN	3.2
1	А	344	ILE	3.1
1	В	56	GLU	3.0
1	А	16	ASN	3.0
1	В	103	PRO	2.9
1	А	110	LEU	2.9
1	А	286	ALA	2.9
1	В	104	LYS	2.7
1	В	321	LEU	2.7
1	А	335	ASP	2.6
1	В	89	LYS	2.6
1	В	344	ILE	2.5
1	А	89	LYS	2.4
1	А	15	GLU	2.4
1	А	256	LEU	2.3
1	В	92	PRO	2.2
1	А	14	SER	2.2
1	А	452	LYS	2.2
1	А	107	ASP	2.2
1	В	58	GLY	2.2
1	В	342	THR	2.1
1	А	13	LYS	2.1
1	А	345	CYS	2.1

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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 monosaccharides in this entry.

6.4 Ligands (i)

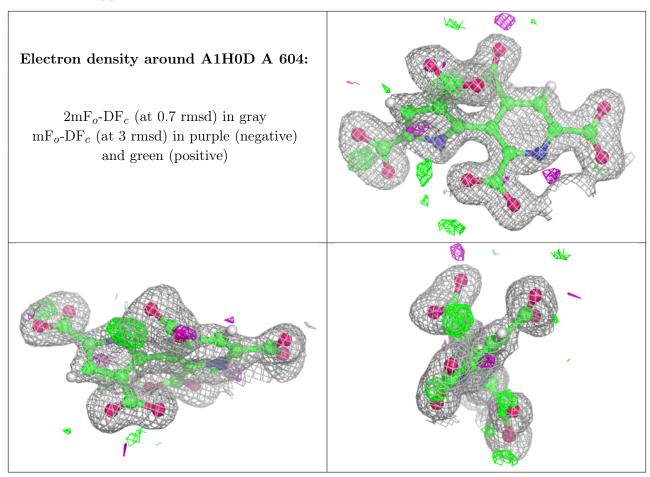
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



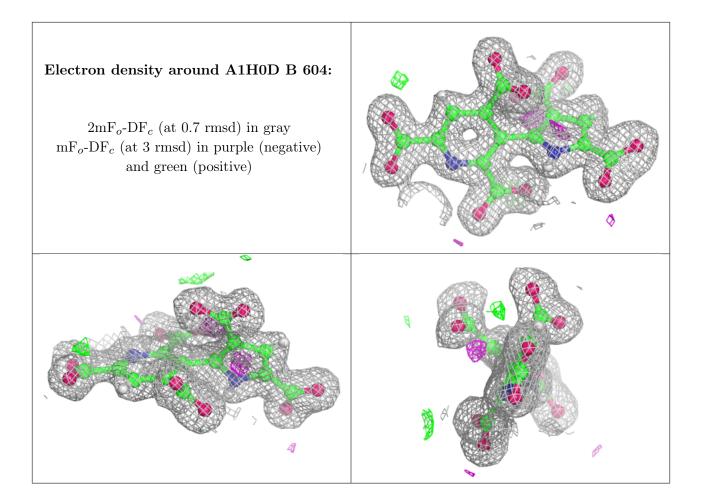
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
3	A1H0D	А	604	26/26	0.87	0.15	19,27,33,39	0
3	A1H0D	В	604	26/26	0.93	0.10	13,20,26,28	0
4	LI	А	605	1/1	0.97	0.75	10,10,10,10	0
2	CA	А	601	1/1	0.99	0.06	$19,\!19,\!19,\!19$	0
2	CA	В	602	1/1	1.00	0.12	12,12,12,12	0
2	CA	В	603	1/1	1.00	0.12	12,12,12,12	0
2	CA	А	602	1/1	1.00	0.12	13,13,13,13	0
2	CA	А	603	1/1	1.00	0.12	12,12,12,12	0
2	CA	В	601	1/1	1.00	0.07	$15,\!15,\!15,\!15$	0

median, 95^{th} 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.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

