

wwPDB X-ray Structure Validation Summary Report (i)

Jun 14, 2020 – 04:42 am BST

PDB ID : 10U6

Title: Biosynthetic thiolase from Zoogloea ramigera in complex with acetyl-O-pante

theine-11-pivalate

Authors: Kursula, P.; Schmitz, W.; Wierenga, R.K.

Deposited on : 2003-03-24

Resolution : 2.07 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) 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 : 2.11

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)

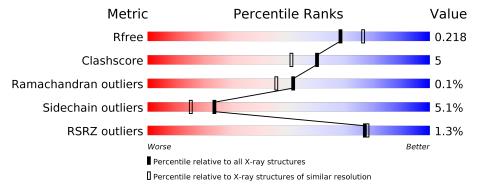
Validation Pipeline (wwPDB-VP) : 2.11

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 2.07 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 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	392	91%	8%	•
1	В	392	86%	12%	•
1	С	392	88%	12%	
1	D	392	86%	14%	



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12967 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 Acetyl-CoA acetyltransferase.

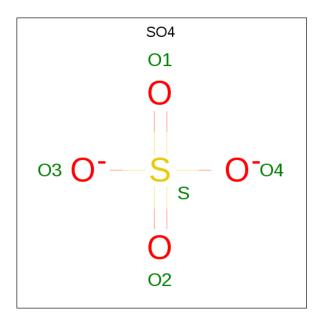
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	392	Total	С	N	О	S	0	0	0
1	A	392	2834	1758	512	543	21	0	0	0
1	В	392	Total	С	N	О	S	0	0	0
1	Б	392	2834	1758	512	543	21	0	U	
1	С	392	Total	С	N	О	S	0	0	0
1		392	2834	1758	512	543	21	0	0	U
1	D	392	Total	С	N	О	S	0	0	0
1	ש	39∠	2834	1758	512	543	21	0	0	U

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	-	SEE REMARK 999	UNP P07097
A	89	CSO	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	SEE REMARK 999	UNP P07097
В	10	ALA	_	SEE REMARK 999	UNP P07097
В	89	CSO	CYS	MODIFIED RESIDUE	UNP P07097
В	129	ARG	ALA	SEE REMARK 999	UNP P07097
С	10	ALA	_	SEE REMARK 999	UNP P07097
С	89	CSO	CYS	MODIFIED RESIDUE	UNP P07097
С	129	ARG	ALA	SEE REMARK 999	UNP P07097
D	10	ALA	-	SEE REMARK 999	UNP P07097
D	89	CSO	CYS	MODIFIED RESIDUE	UNP P07097
D	129	ARG	ALA	SEE REMARK 999	UNP P07097

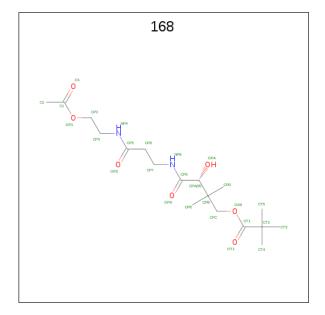
• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0

 \bullet Molecule 3 is PANTOTHENYL-AMINOETHANOL-ACETATE PIVALIC ACID (three-letter code: 168) (formula: $C_{18}H_{32}N_2O_7).$





Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	
3	Λ	1	Total	С	N	О	0	0	
,	Λ	1	27	18	2	7	0		
2	D	1	Total	С	N	О	0	0	
3	D	1	27	18	2	7	0	U	

• Molecule 4 is water.

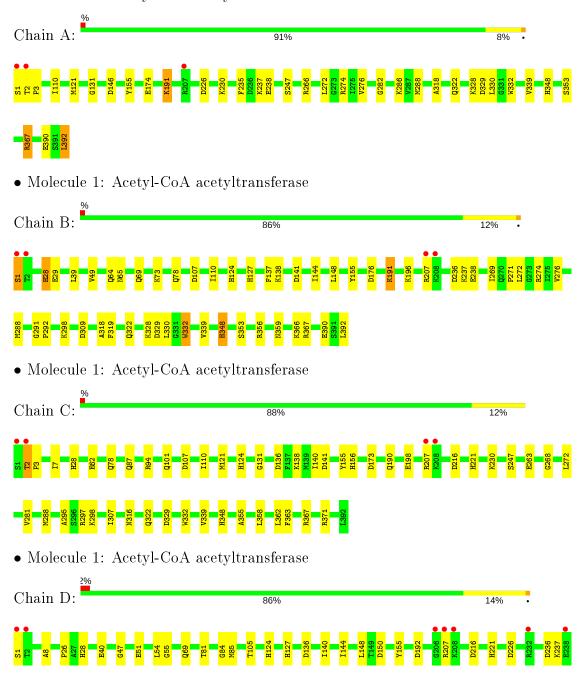
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
4	A	455	Total O 455 455	0	0
4	В	508	Total O 508 508	0	0
4	С	337	Total O 337 337	0	0
4	D	257	Total O 257 257	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Acetyl-CoA acetyltransferase







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	84.38Å 78.95Å 148.82Å	Depositor
a, b, c, α , β , γ	90.00° 92.96° 90.00°	Depositor
Resolution (Å)	20.00 - 2.07	Depositor
rtesolution (A)	19.39 - 2.07	EDS
% Data completeness	94.3 (20.00-2.07)	Depositor
(in resolution range)	81.4 (19.39-2.07)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$2.74~({\rm at}~2.07{\rm \AA})$	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.212	Depositor
II, II free	0.171 , 0.218	DCC
R_{free} test set	4876 reflections $(4.36%)$	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.936	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 36.3	EDS
L-test for twinning ²	$< L >=0.41, < L^2>=0.23$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12967	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: CSO, 168, SO4

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	Bo	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.72	0/2868	0.88	7/3872 (0.2%)	
1	В	0.73	0/2868	0.85	$6/3872 \ (0.2\%)$	
1	С	0.58	$1/2868 \; (0.0\%)$	0.79	5/3872 (0.1%)	
1	D	0.52	0/2868	0.78	$9/3872 \ (0.2\%)$	
All	All	0.64	$1/11472 \ (0.0\%)$	0.83	$27/15488 \ (0.2\%)$	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(ext{\AA})$
1	С	136	ASP	CB-CG	5.67	1.63	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	В	309	ASP	CB-CG-OD2	8.25	125.72	118.30
1	A	266	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	266	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	D	136	ASP	CB-CG-OD2	7.22	124.80	118.30
1	С	107	ASP	CB-CG-OD2	6.96	124.56	118.30

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	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	Α	2834	0	2841	17	0
1	В	2834	0	2841	40	0
1	С	2834	0	2841	31	0
1	D	2834	0	2841	24	0
2	A	10	0	0	0	0
2	В	10	0	0	1	0
3	A	27	0	32	3	0
3	В	27	0	32	2	0
4	A	455	0	0	5	0
4	В	508	0	0	14	0
4	С	337	0	0	12	1
4	D	257	0	0	5	1
All	All	12967	0	11428	105	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 105 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:B:191:LYS:HB3	1:B:191:LYS:HZ2	1.34	0.92
1:B:191:LYS:HB3	1:B:191:LYS:NZ	1.82	0.91
1:C:156:HIS:ND1	4:C:436:HOH:O	2.09	0.86
1:C:156:HIS:CE1	4:C:436:HOH:O	2.31	0.82
1:C:358:LEU:HD23	4:C:495:HOH:O	1.82	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{\AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
4:C:553:HOH:O	4:D:481:HOH:O[2_646]	2.16	0.04

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	$389/392 \ (99\%)$	374 (96%)	15 (4%)	0	100	100	
1	В	$389/392 \ (99\%)$	378 (97%)	11 (3%)	0	100	100	
1	С	389/392 (99%)	376 (97%)	12 (3%)	1 (0%)	41	32	
1	D	$389/392 \ (99\%)$	377 (97%)	12 (3%)	0	100	100	
All	All	1556/1568~(99%)	1505 (97%)	50 (3%)	1 (0%)	51	45	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	247	SER

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	${f Analysed}$	Rotameric Outliers		Percentiles		
1	A	278/278 (100%)	263 (95%)	15 (5%)	22	14	
1	В	278/278 (100%)	262 (94%)	16 (6%)	20	11	
1	С	278/278 (100%)	266 (96%)	12 (4%)	29	22	
1	D	$278/278 \; (100\%)$	264 (95%)	14 (5%)	24	16	
All	All	1112/1112 (100%)	1055 (95%)	57 (5%)	24	15	

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	322	GLN
1	С	2	THR
1	D	288	MET
1	В	328	LYS
1	В	339	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:



Mol	Chain	Res	Type
1	С	169	GLN
1	С	175	GLN
1	D	28	HIS
1	С	124	HIS
1	С	348	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	Tuno	e Chain	Res	Link	Bond lengths				Bond angles		
MIGI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
1	CSO	A	89	1	3,6,7	0.63	0	0,6,8	0.00	-	
1	CSO	С	89	1	3,6,7	0.44	0	0,6,8	0.00	-	
1	CSO	В	89	1	3,6,7	0.81	0	0,6,8	0.00	-	
1	CSO	D	89	1	3,6,7	0.68	0	0,6,8	0.00	-	

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.

\mathbf{Mol}	\mathbf{Type}	Chain	${ m Res}$	Link	Chirals	Torsions	Rings
1	CSO	Α	89	1	-	0/1/5/7	-
1	CSO	С	89	1	-	0/1/5/7	-
1	CSO	В	89	1	-	0/1/5/7	-
1	CSO	D	89	1	-	0/1/5/7	-

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.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	Tuno	Chain	Res	Link	Во	ond leng	$ ag{ths}$	Bond angles		
MIGI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	$\mid \# Z > 2$
3	168	В	6001	-	23,26,26	1.32	2 (8%)	34,36,36	1.61	6 (17%)
2	SO4	В	2001	-	4,4,4	0.17	0	6,6,6	0.15	0
3	168	A	5001	-	23,26,26	1.35	2 (8%)	34,36,36	1.92	9 (26%)
2	SO4	A	2004	-	4,4,4	0.17	0	6,6,6	0.21	0
2	SO4	В	2003	-	4,4,4	0.19	0	6,6,6	0.47	0
2	SO4	A	2002	-	4,4,4	0.14	0	6,6,6	0.36	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	${f Torsions}$	Rings
3	168	A	5001	-	-	17/35/35/35	_
3	168	В	6001	_	-	15/35/35/35	_

All (4) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\mathring{A}})$
3	В	6001	168	OA6-CT1	5.24	1.45	1.33
3	A	5001	168	OA6-CT1	5.13	1.44	1.33
3	A	5001	168	OP1-C1	2.39	1.45	1.33
3	В	6001	168	OP1-C1	2.27	1.44	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
3	A	5001	168	OA6-CT1-CT2	5.78	124.10	112.56
3	В	6001	168	OA6-CT1-CT2	4.33	121.20	112.56
3	A	5001	168	OA6-CT1-OT1	-4.29	115.72	124.54
3	A	5001	168	CP6-CP7-NP8	-3.50	104.83	111.90
3	A	5001	168	CPC-OA6-CT1	-3.31	112.13	116.81

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	6001	168	CP3-CP2-OP1-C1
3	В	6001	168	CP9-CPA-CPB-CPE
3	В	6001	168	CT2-CT1-OA6-CPC
3	A	5001	168	CP9-CPA-CPB-CPD
3	A	5001	168	CP9-CPA-CPB-CPE

There are no ring outliers.

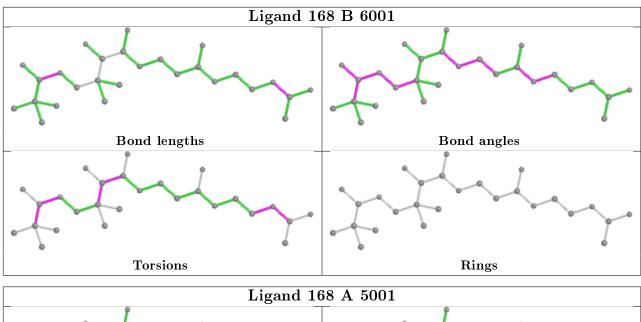
3 monomers are involved in 6 short contacts:

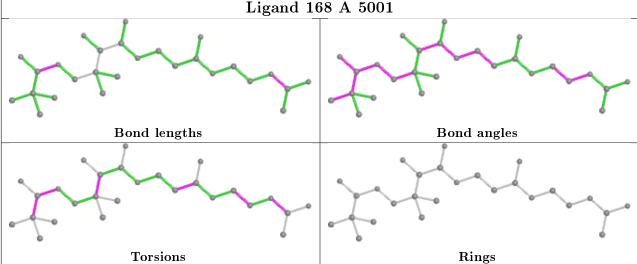
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	6001	168	2	0
3	A	5001	168	3	0
2	В	2003	SO4	1	0

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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. 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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	$391/392 \ (99\%)$	-0.67	3 (0%) 86 87	2, 7, 21, 52	0
1	В	$391/392 \ (99\%)$	-0.67	4 (1%) 82 83	2, 7, 20, 46	0
1	С	$391/392 \ (99\%)$	-0.46	4 (1%) 82 83	3, 8, 18, 42	0
1	D	$391/392 \ (99\%)$	-0.20	9 (2%) 60 63	3, 9, 19, 39	0
All	All	1564/1568~(99%)	-0.50	20 (1%) 77 78	2, 8, 20, 52	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	6.7
1	D	1	SER	5.4
1	С	2	THR	5.0
1	D	2	THR	4.0
1	В	1	SER	4.0

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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	CSO	D	89	7/8	0.97	0.09	5,8,10,12	0
1	CSO	С	89	7/8	0.98	0.08	5,7,16,17	0
1	CSO	В	89	7/8	0.98	0.08	5,7,12,19	0
1	CSO	A	89	7/8	0.98	0.08	6,6,13,21	0



6.3 Carbohydrates (i)

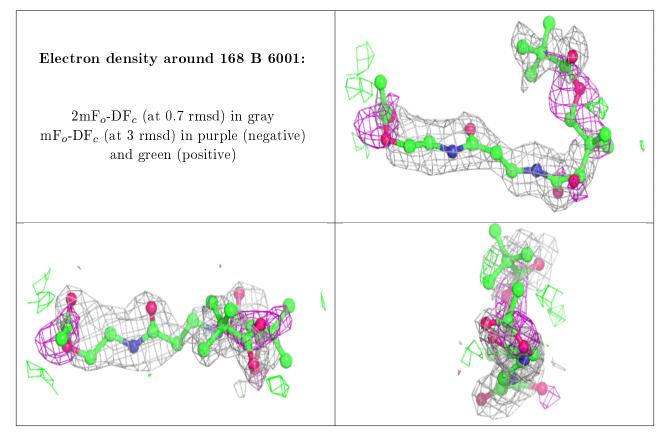
There are no carbohydrates in this entry.

6.4 Ligands (i)

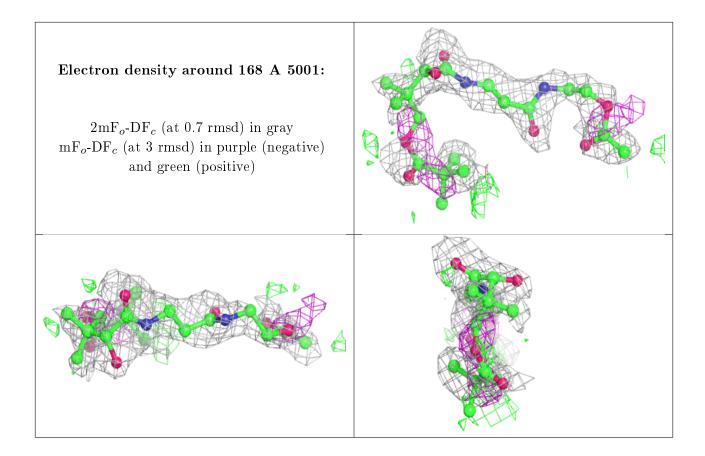
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
3	168	В	6001	27/27	0.71	0.33	40,49,55,57	0
3	168	A	5001	27/27	0.73	0.26	35,44,46,52	0
2	SO4	A	2004	5/5	0.95	0.18	67,68,69,71	0
2	SO4	A	2002	5/5	0.96	0.16	52,56,57,60	0
2	SO4	В	2001	5/5	0.97	0.12	66,66,68,69	0
2	SO4	В	2003	5/5	0.99	0.10	41,41,45,46	0

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.

