wwPDB X-ray Structure Validation Summary Report (i)

Jan 23, 2021 – 02:59 PM EST

PDB ID	:	1RRM
Title	:	Crystal Structure of Lactaldehyde reductase
Authors	:	Kumaran, D.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2003-12-08
Resolution	:	1.60 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:

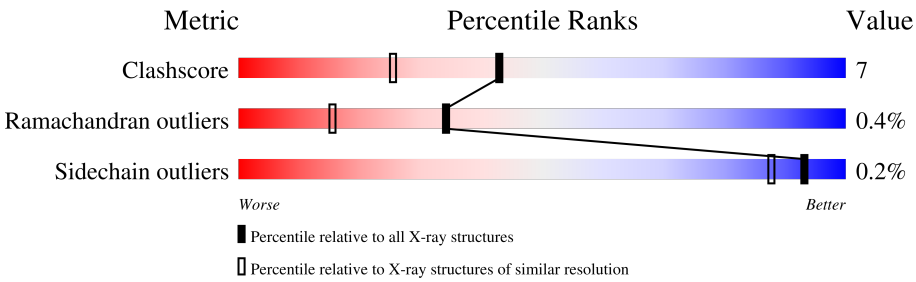
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 1.60 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	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	386	88% 12%
1	B	386	87% 12% ••

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6475 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 Lactaldehyde reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	385	2862	1804	496	546	4	12	0	0	0
1	B	384	2857	1802	495	544	4	12	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P0A9S1
A	2	MSE	MET	modified residue	UNP P0A9S1
A	6	MSE	MET	modified residue	UNP P0A9S1
A	55	MSE	MET	modified residue	UNP P0A9S1
A	181	MSE	MET	modified residue	UNP P0A9S1
A	182	MSE	MET	modified residue	UNP P0A9S1
A	185	MSE	MET	modified residue	UNP P0A9S1
A	243	MSE	MET	modified residue	UNP P0A9S1
A	252	MSE	MET	modified residue	UNP P0A9S1
A	265	MSE	MET	modified residue	UNP P0A9S1
A	289	MSE	MET	modified residue	UNP P0A9S1
A	307	MSE	MET	modified residue	UNP P0A9S1
A	314	MSE	MET	modified residue	UNP P0A9S1
A	384	GLU	-	cloning artifact	UNP P0A9S1
A	385	GLY	-	cloning artifact	UNP P0A9S1
A	386	GLY	-	cloning artifact	UNP P0A9S1
B	1	MSE	MET	modified residue	UNP P0A9S1
B	2	MSE	MET	modified residue	UNP P0A9S1
B	6	MSE	MET	modified residue	UNP P0A9S1
B	55	MSE	MET	modified residue	UNP P0A9S1
B	181	MSE	MET	modified residue	UNP P0A9S1
B	182	MSE	MET	modified residue	UNP P0A9S1
B	185	MSE	MET	modified residue	UNP P0A9S1
B	243	MSE	MET	modified residue	UNP P0A9S1
B	252	MSE	MET	modified residue	UNP P0A9S1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	265	MSE	MET	modified residue	UNP P0A9S1
B	289	MSE	MET	modified residue	UNP P0A9S1
B	307	MSE	MET	modified residue	UNP P0A9S1
B	314	MSE	MET	modified residue	UNP P0A9S1
B	384	GLU	-	cloning artifact	UNP P0A9S1
B	385	GLY	-	cloning artifact	UNP P0A9S1
B	386	GLY	-	cloning artifact	UNP P0A9S1

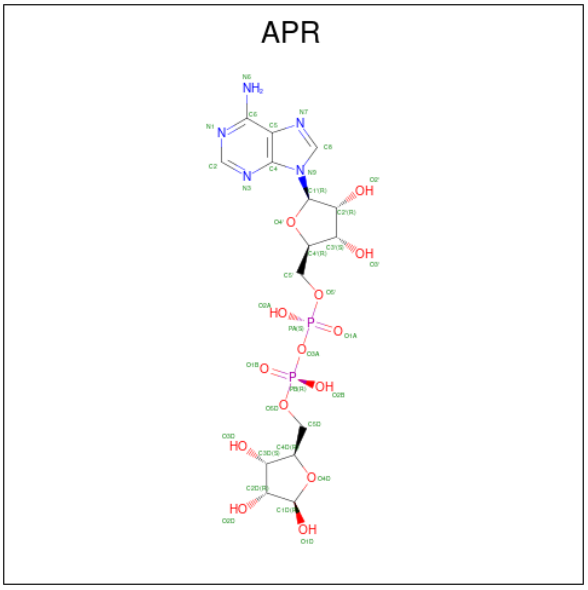
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	B	1	1	1	0	0
2	A	1	1	1	0	0

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

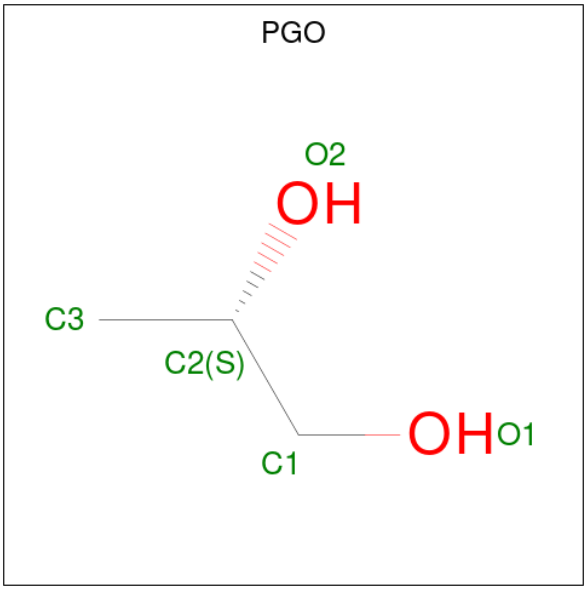
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
3	B	1	1	1	0	0
3	A	1	1	1	0	0

- Molecule 4 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	36	15	5	14	2	0	0
			Total	C	N	O	P		
4	B	1	36	15	5	14	2	0	0

- Molecule 5 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	5	3	2	0	0
			Total	C	O		
5	B	1	5	3	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	323	323	323	0	0
			Total	O		
6	B	347	347	347	0	0

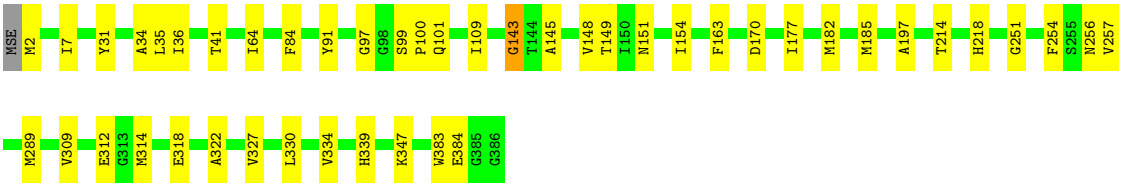
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

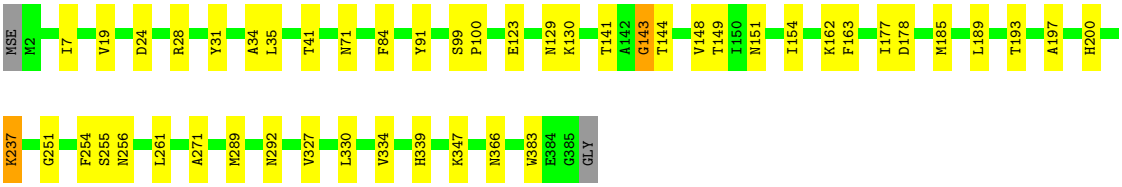
• Molecule 1: Lactaldehyde reductase

Chain A:



• Molecule 1: Lactaldehyde reductase

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.77Å 97.53Å 69.51Å 90.00° 113.63° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60	Depositor
% Data completeness (in resolution range)	90.6 (50.00-1.60)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.211	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6475	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

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: APR, PGO, ZN, FE2

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	0.28	0/2905	0.60	0/3933
1	B	0.28	0/2900	0.60	0/3928
All	All	0.28	0/5805	0.60	0/7861

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	A	2862	0	2851	32	0
1	B	2857	0	2848	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	36	0	21	1	0
4	B	36	0	21	1	0
5	A	5	0	7	1	0
5	B	5	0	7	3	0
6	A	323	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	347	0	0	2	0
All	All	6475	0	5755	79	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 7.

The worst 5 of 79 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:109:ILE:HD11	1:A:170:ASP:HB3	1.51	0.91
1:A:34:ALA:HB2	1:A:91:TYR:CZ	2.14	0.82
1:A:7:ILE:H	1:A:256:ASN:HD21	1.27	0.81
1:B:34:ALA:HB2	1:B:91:TYR:CZ	2.16	0.80
1:A:7:ILE:H	1:A:256:ASN:ND2	1.83	0.77

There are no symmetry-related clashes.

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	383/386 (99%)	371 (97%)	10 (3%)	2 (0%)	29 11
1	B	382/386 (99%)	371 (97%)	10 (3%)	1 (0%)	41 21
All	All	765/772 (99%)	742 (97%)	20 (3%)	3 (0%)	34 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLY
1	B	143	GLY
1	A	312	GLU

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	292/280 (104%)	292 (100%)	0	100	100
1	B	292/280 (104%)	291 (100%)	1 (0%)	92	87
All	All	584/560 (104%)	583 (100%)	1 (0%)	93	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	237	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	9	ASN
1	B	44	GLN
1	B	256	ASN
1	A	256	ASN
1	B	169	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)

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	APR	B	389	-	34,39,39	1.11	4 (11%)	40,60,60	0.97	2 (5%)
4	APR	A	389	-	34,39,39	1.09	3 (8%)	40,60,60	1.00	2 (5%)
5	PGO	B	390	2	3,4,4	0.62	0	1,4,4	1.76	0
5	PGO	A	390	2	3,4,4	0.62	0	1,4,4	1.79	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
4	APR	B	389	-	-	1/18/54/54	0/4/4/4
4	APR	A	389	-	-	1/18/54/54	0/4/4/4
5	PGO	B	390	2	-	0/2/2/2	-
5	PGO	A	390	2	-	2/2/2/2	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	389	APR	C2-N1	2.94	1.39	1.33
4	A	389	APR	C2-N1	2.93	1.39	1.33
4	B	389	APR	O4D-C1D	-2.76	1.39	1.43
4	A	389	APR	O4D-C1D	-2.67	1.40	1.43
4	A	389	APR	O1D-C1D	2.45	1.47	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	389	APR	C1'-N9-C4	-2.57	122.12	126.64
4	A	389	APR	C5-C6-N6	2.44	124.06	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	389	APR	C1'-N9-C4	-2.38	122.45	126.64
4	B	389	APR	C5-C6-N6	2.27	123.80	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

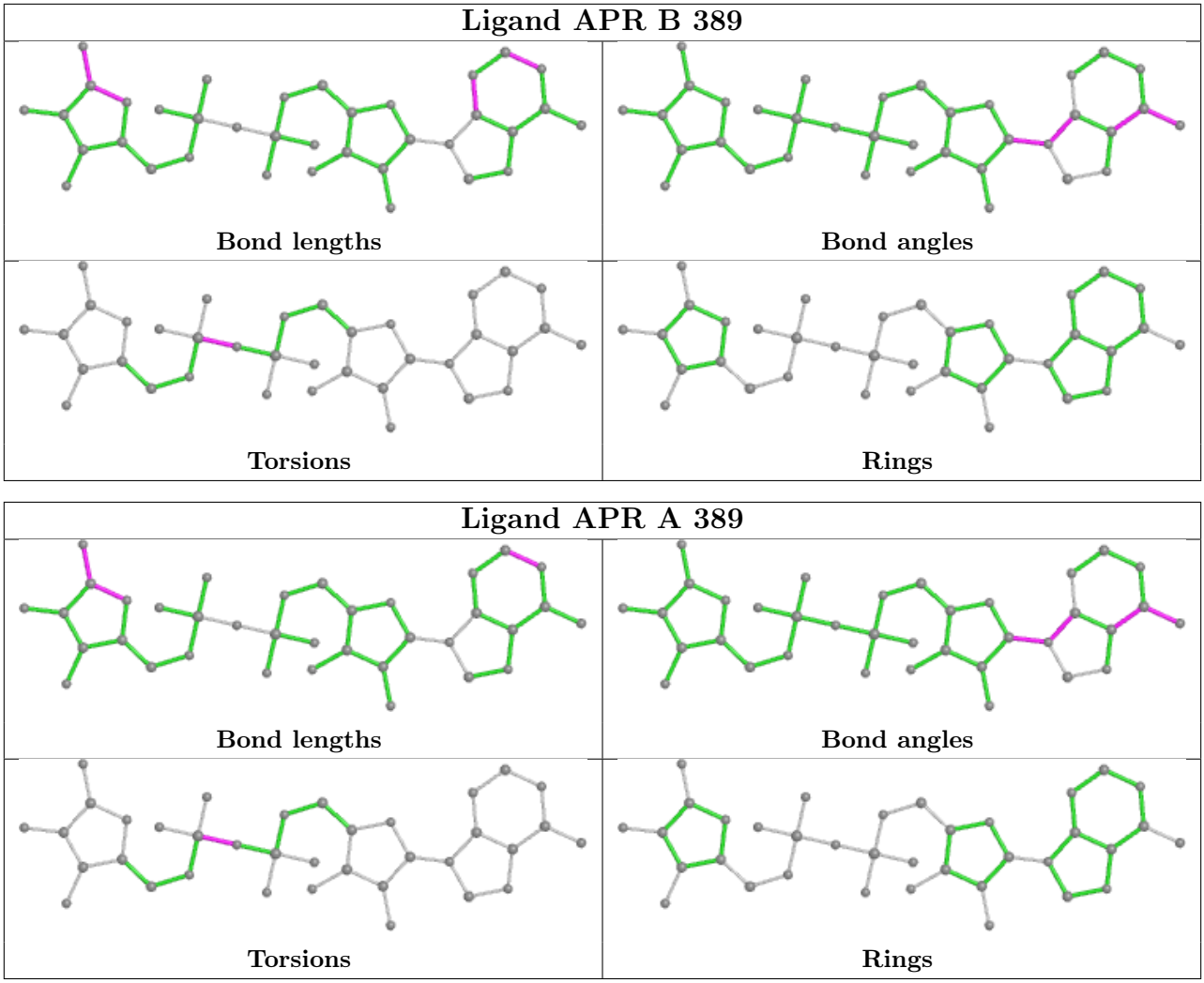
Mol	Chain	Res	Type	Atoms
4	B	389	APR	PA-O3A-PB-O5D
4	A	389	APR	PA-O3A-PB-O5D
5	A	390	PGO	O1-C1-C2-O2
5	A	390	PGO	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	389	APR	1	0
4	A	389	APR	1	0
5	B	390	PGO	3	0
5	A	390	PGO	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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.