

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 02:10 PM JST

PDB ID : 7YW9

Title : Crystal structure of the triple mutant CmnC-L136Q,S138G,D249Y in complex

with alpha-KG

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Deposited on : 2022-08-22

Resolution : 1.76 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 (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 : 2.35

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)

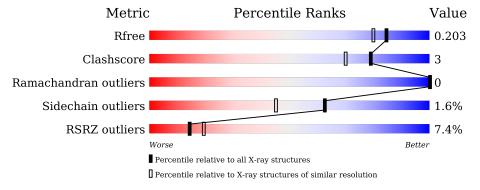
Validation Pipeline (wwPDB-VP) : 2.35

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 1.76 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	358	87%	7%	6%
1	В	358	90%	8	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5771 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 CmnC.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	Δ	338	Total	С	N	О	O S	0	0	0	
1	Λ	33 0	2606	1620	488	495	3	U	U		
1	B	350	Total	С	N	Ο	S	0	0	0	
1	Ъ	330	2695	1673	509	510	3		U	U	

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A6YEH4
A	-18	GLY	_	expression tag	UNP A6YEH4
A	-17	SER	-	expression tag	UNP A6YEH4
A	-16	SER	-	expression tag	UNP A6YEH4
A	-15	HIS	-	expression tag	UNP A6YEH4
A	-14	HIS	-	expression tag	UNP A6YEH4
A	-13	HIS	-	expression tag	UNP A6YEH4
A	-12	HIS	-	expression tag	UNP A6YEH4
A	-11	HIS	-	expression tag	UNP A6YEH4
A	-10	HIS	-	expression tag	UNP A6YEH4
A	-9	SER	-	expression tag	UNP A6YEH4
A	-8	SER	-	expression tag	UNP A6YEH4
A	-7	GLY	-	expression tag	UNP A6YEH4
A	-6	LEU	-	expression tag	UNP A6YEH4
A	-5	VAL	-	expression tag	UNP A6YEH4
A	-4	PRO	-	expression tag	UNP A6YEH4
A	-3	ARG	-	expression tag	UNP A6YEH4
A	-2	GLY	-	expression tag	UNP A6YEH4
A	-1	SER	-	expression tag	UNP A6YEH4
A	0	HIS	-	expression tag	UNP A6YEH4
A	136	GLN	LEU	engineered mutation	UNP A6YEH4
A	138	GLY	SER	engineered mutation	UNP A6YEH4
A	249	TYR	ASP	engineered mutation	UNP A6YEH4
В	-19	MET	_	initiating methionine	UNP A6YEH4
В	-18	GLY	-	expression tag	UNP A6YEH4

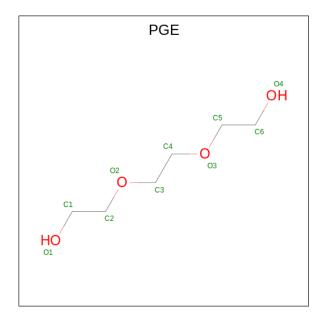
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Chain	Residue	Modelled	Actual	Comment	Reference
В	-17	SER	-	expression tag	UNP A6YEH4
В	-16	SER	-	expression tag	UNP A6YEH4
В	-15	HIS	-	expression tag	UNP A6YEH4
В	-14	HIS	-	expression tag	UNP A6YEH4
В	-13	HIS	-	expression tag	UNP A6YEH4
В	-12	HIS	-	expression tag	UNP A6YEH4
В	-11	HIS	-	expression tag	UNP A6YEH4
В	-10	HIS	-	expression tag	UNP A6YEH4
В	-9	SER	-	expression tag	UNP A6YEH4
В	-8	SER	-	expression tag	UNP A6YEH4
В	-7	GLY	-	expression tag	UNP A6YEH4
В	-6	LEU	=	expression tag	UNP A6YEH4
В	-5	VAL	-	expression tag	UNP A6YEH4
В	-4	PRO	-	expression tag	UNP A6YEH4
В	-3	ARG	-	expression tag	UNP A6YEH4
В	-2	GLY	-	expression tag	UNP A6YEH4
В	-1	SER	-	expression tag	UNP A6YEH4
В	0	HIS	=	expression tag	UNP A6YEH4
В	136	GLN	LEU	engineered mutation	UNP A6YEH4
В	138	GLY	SER	engineered mutation	UNP A6YEH4
В	249	TYR	ASP	engineered mutation	UNP A6YEH4

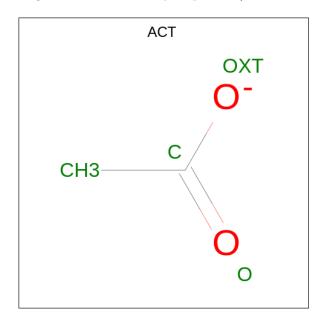
• Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0
2	A	1	Total C O 10 6 4	0	0

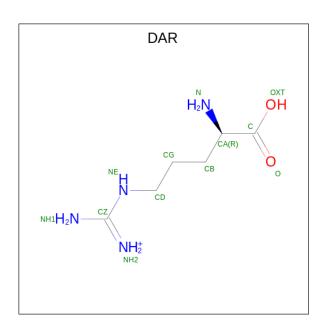
• Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

• Molecule 4 is D-ARGININE (three-letter code: DAR) (formula: $C_6H_{15}N_4O_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
4	A	1	Total 12	C 6	N 4	O 2	0	0

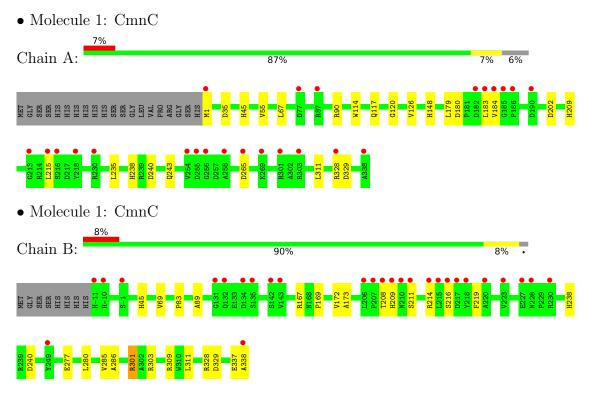
• Molecule 5 is water.

\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	204	Total O 204 204	0	0
5	В	226	Total O 226 226	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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	92.95Å 126.67Å 140.19Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.91 - 1.76	Depositor
resolution (A)	25.90 - 1.76	EDS
% Data completeness	94.8 (25.91-1.76)	Depositor
(in resolution range)	94.8 (25.90-1.76)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.38 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.195	Depositor
it, it free	0.186 , 0.203	DCC
R_{free} test set	3871 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38, 42.2	EDS
L-test for twinning ²	$ < L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5771	wwPDB-VP
Average B, all atoms $(Å^2)$	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.02% 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: ACT, DAR, PGE

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		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.65	0/2659	0.77	0/3620	
1	В	0.66	0/2752	0.76	0/3746	
All	All	0.65	0/5411	0.76	0/7366	

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	2606	0	2545	16	0
1	В	2695	0	2627	14	0
2	A	20	0	28	2	0
3	A	8	0	6	0	0
4	A	12	0	14	2	0
5	A	204	0	0	1	0
5	В	226	0	0	0	1
All	All	5771	0	5220	29	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 3.



All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:A:238:HIS:HD2	1:A:240:ASP:H	1.27	0.82
1:B:238:HIS:HD2	1:B:240:ASP:H	1.26	0.79
1:A:209:HIS:ND1	2:A:401:PGE:H3	2.03	0.73
1:B:328:ARG:NH1	1:B:329:ASP:OD2	2.40	0.55
1:B:301:ARG:O	1:B:301:ARG:HG2	2.08	0.53
1:A:328:ARG:NH2	1:A:329:ASP:OD2	2.44	0.50
1:B:169:PRO:HG2	1:B:303:ARG:HH22	1.77	0.49
1:B:208:THR:HG22	1:B:209:HIS:H	1.78	0.48
1:B:173:ALA:HB1	1:B:277:GLU:HB3	1.96	0.47
1:A:179:LEU:HD23	1:A:235:LEU:HD21	1.97	0.47
1:A:148:HIS:CE1	4:A:405:DAR:HG3	2.50	0.46
1:B:69:VAL:HB	1:B:285:VAL:HG13	1.97	0.46
1:B:309:ARG:CZ	1:B:311:LEU:HD11	2.46	0.46
1:B:337:GLU:O	1:B:338:ALA:HB2	2.16	0.45
1:A:126:VAL:HB	1:A:311:LEU:HB2	1.98	0.45
1:A:55:VAL:HG22	1:A:67:LEU:HD21	1.99	0.43
1:A:238:HIS:CD2	1:A:240:ASP:HB2	2.53	0.43
1:A:45:HIS:CG	1:B:45:HIS:CG	3.07	0.42
1:B:83:PRO:HG2	1:B:89:ALA:HA	2.01	0.42
1:B:211:SER:HB2	1:B:219:PHE:CZ	2.53	0.42
1:A:90:ARG:HB2	5:A:502:HOH:O	2.20	0.42
1:A:180:ASP:OD2	1:A:183:LEU:HD22	2.20	0.42
1:B:172:VAL:HB	1:B:309:ARG:HD2	2.02	0.41
1:A:209:HIS:ND1	2:A:401:PGE:C3	2.80	0.41
1:A:235:LEU:HA	1:A:243:GLN:O	2.21	0.41
1:B:280:LEU:HD21	1:B:286:ALA:HB2	2.03	0.41
1:A:114:TRP:HB2	1:A:117:GLN:HB2	2.03	0.41
1:A:202:ASP:CB	4:A:405:DAR:HD2	2.51	0.41
1:A:114:TRP:O	1:A:120:GLY:HA2	2.21	0.40

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	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	Clash overlap (Å)
5:B:596:HOH:O	5:B:596:HOH:O[2_665]	2.12	0.08



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	A	336/358~(94%)	329 (98%)	7 (2%)	0	100	100
1	В	348/358~(97%)	344 (99%)	4 (1%)	0	100	100
All	All	684/716 (96%)	673 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	$268/285 \ (94\%)$	263 (98%)	5 (2%)	57 37
1	В	278/285 (98%)	274 (99%)	4 (1%)	67 52
All	All	546/570 (96%)	537 (98%)	9 (2%)	62 45

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	35	ASP
1	A	184	VAL
1	A	215	LEU
1	A	265	ASP
1	В	167	ARG
1	В	214	ARG
1	В	216	SER

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Mol	Chain	Res	Type
1	В	301	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	HIS
1	В	26	GLN
1	В	117	GLN
1	В	132	GLN
1	В	210	ASN
1	В	238	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)

5 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	Bo	ond leng	$ ag{ths}$	В	ond ang	les
IVIOI	Туре	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	A	403	-	3,3,3	1.02	0	3,3,3	0.81	0
3	ACT	A	402	-	3,3,3	0.74	0	3,3,3	0.86	0



Mol	Type	Chain	Res	Link	Link Bond lengths				ond ang	les
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DAR	A	405	-	10,11,11	0.68	0	11,13,13	1.25	1 (9%)
2	PGE	A	404	-	9,9,9	0.17	0	8,8,8	0.08	0
2	PGE	A	401	-	9,9,9	0.22	0	8,8,8	0.24	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
2	PGE	A	404	-	-	2/7/7/7	-
2	PGE	A	401	-	-	5/7/7/7	-
4	DAR	A	405	-	-	0/11/11/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	405	DAR	OXT-C-O	-3.21	116.81	124.09

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PGE	O3-C5-C6-O4
2	A	401	PGE	O1-C1-C2-O2
2	A	401	PGE	C6-C5-O3-C4
2	A	404	PGE	C6-C5-O3-C4
2	A	401	PGE	C1-C2-O2-C3
2	A	404	PGE	O1-C1-C2-O2
2	A	401	PGE	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

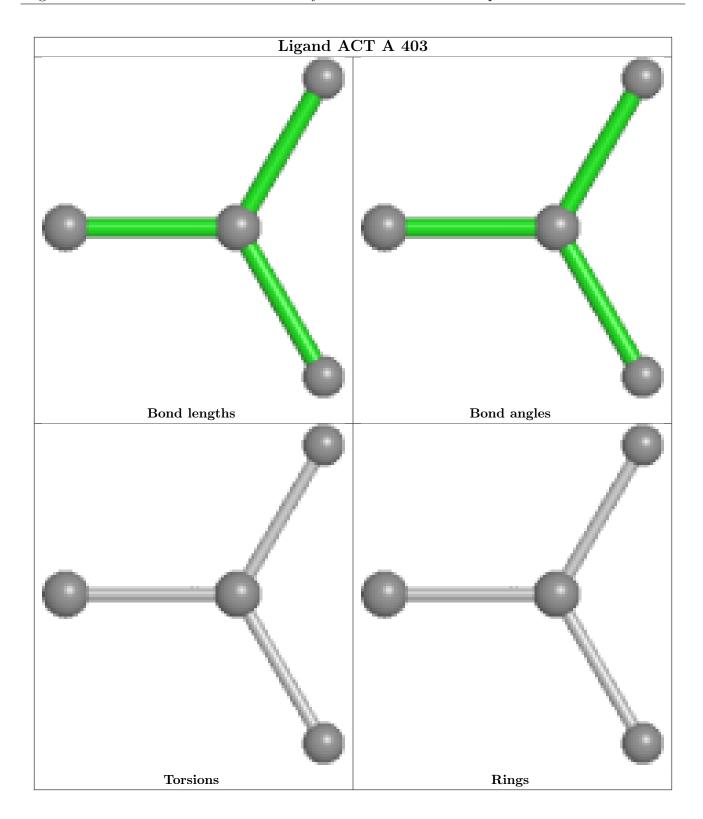
	Mol	Chain	Res	Type	Clashes	Symm-Clashes
	4	A	405	DAR	2	0
ľ	2	A	401	PGE	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

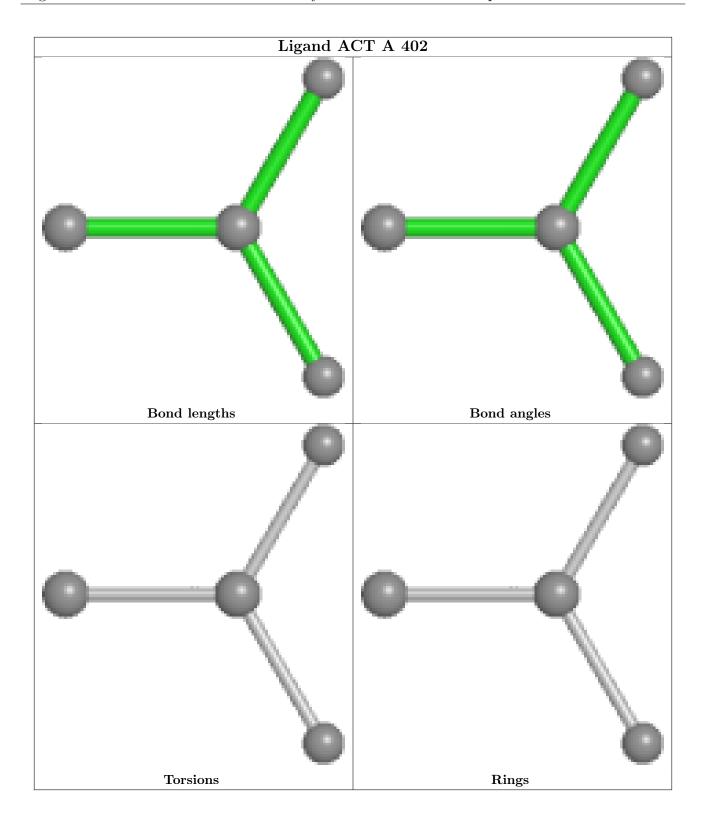


bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 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.

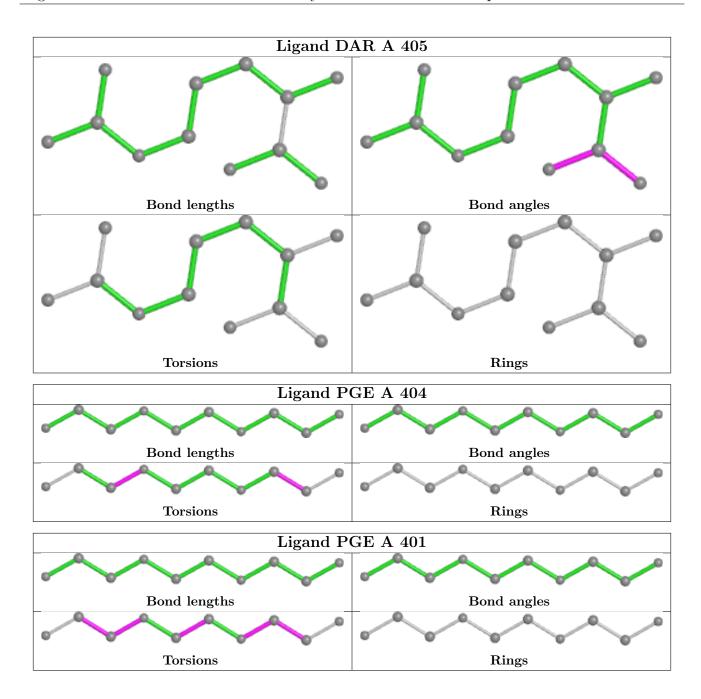












5.7 Other polymers (i)

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	338/358 (94%)	0.21	24 (7%) 16 21	12, 21, 44, 64	0
1	В	350/358 (97%)	0.28	27 (7%) 13 18	11, 20, 42, 58	0
All	All	688/716 (96%)	0.25	51 (7%) 14 19	11, 21, 43, 64	0

All (51) RSRZ outliers are listed below:

Mol	Mol Chain		Type	RSRZ	
1			ALA	8.7	
1	В	209	HIS	6.3	
1	В	-11	HIS	6.1	
1	A	215	LEU	4.8	
1	В	223	VAL	4.6	
1	В	216	SER	4.2	
1	В	208	THR	4.2	
1	В	220	ALA	4.2	
1	A	258	ALA	4.0	
1	A	338	ALA	4.0	
1	A	269	LYS	4.0	
1	A	183	LEU	4.0	
1	A	256	GLY	4.0	
1	A	1	MET	3.9	
1	A	213	GLY	3.9	
1	В	134	ASP	3.7	
1	В	217	ASP	3.5	
1	A	218	TYR	3.4	
1	В	230	ARG	2.9	
1	В	214	ARG	2.9	
1	В	-1	SER	2.8	
1	В	215	LEU	2.8	
1	В	206	LEU	2.8	
1	В	218	TYR	2.7	

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Mol	Mol Chain		Type	RSRZ	
1			VAL	2.7	
1	A	255	ASP	2.6	
1	A	265	ASP	2.6	
1	В	132	GLN	2.6	
1	A	186	PRO	2.6	
1	В	227	GLU	2.5	
1	A	87	ARG	2.5	
1	В	207	PRO	2.5	
1	В	143	VAL	2.5	
1	В	131	GLY	2.5	
1	В	249	TYR	2.4	
1	В	228	ASN	2.4	
1	A	216	SER	2.4	
1	A	303	ARG	2.3	
1	A	182	ASP	2.3	
1	A	185	GLY	2.2	
1	В	-10	HIS	2.2	
1	A	230	ARG	2.2	
1	В	135	SER	2.1	
1	В	142	SER	2.1	
1	В	211	SER	2.1	
1	A	77	ASP	2.1	
1	В	210	ASN	2.1	
1	A	301	ARG	2.1	
1	A	328	ARG	2.0	
1	A	190	ASP	2.0	
1	A	184	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 monosaccharides in this entry.

6.4 Ligands (i)

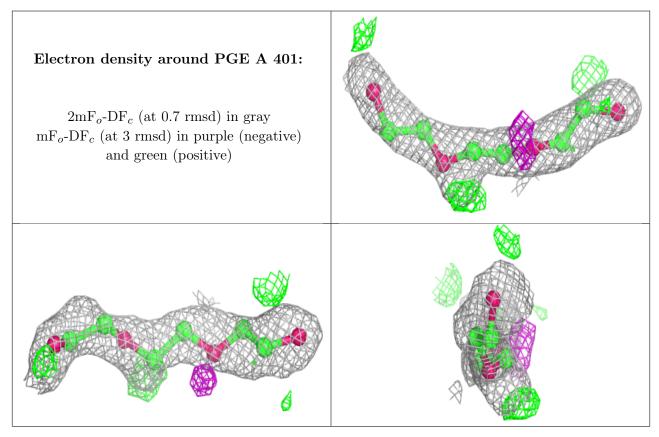
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



median, 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
2	PGE	A	401	10/10	0.82	0.17	33,40,47,48	0
4	DAR	A	405	12/12	0.86	0.14	38,40,41,42	0
2	PGE	A	404	10/10	0.90	0.12	49,50,51,55	0
3	ACT	A	403	4/4	0.94	0.13	29,32,32,36	0
3	ACT	A	402	4/4	0.97	0.09	17,18,19,19	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.

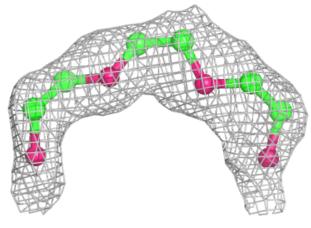


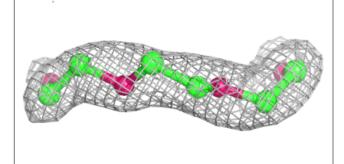


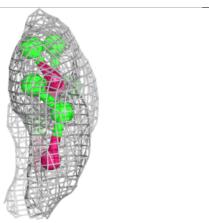
Electron density around DAR A 405: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around PGE A 404:

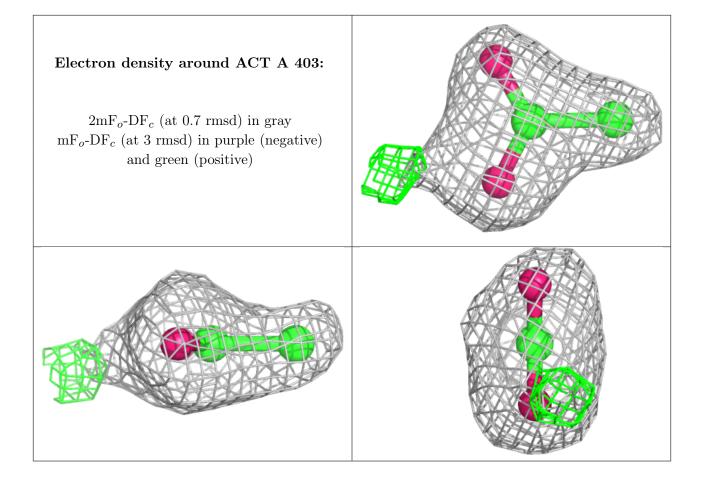
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



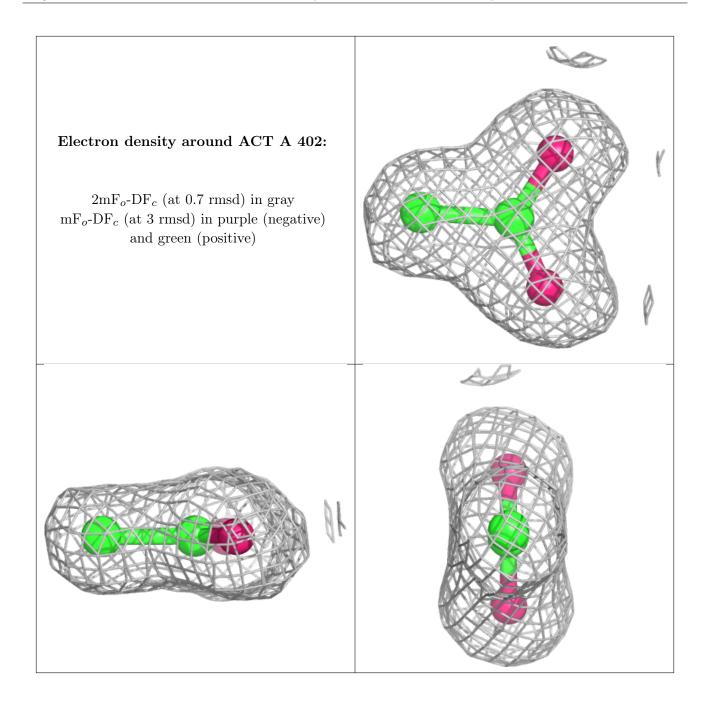












6.5 Other polymers (i)

There are no such residues in this entry.

