



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 02:51 pm BST

PDB ID : 4JKT
Title : Crystal structure of mouse Glutaminase C, BPTES-bound form
Authors : Fornezari, C.; Ferreira, A.P.S.; Dias, S.M.G.; Ambrosio, A.L.B.
Deposited on : 2013-03-11
Resolution : 2.77 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

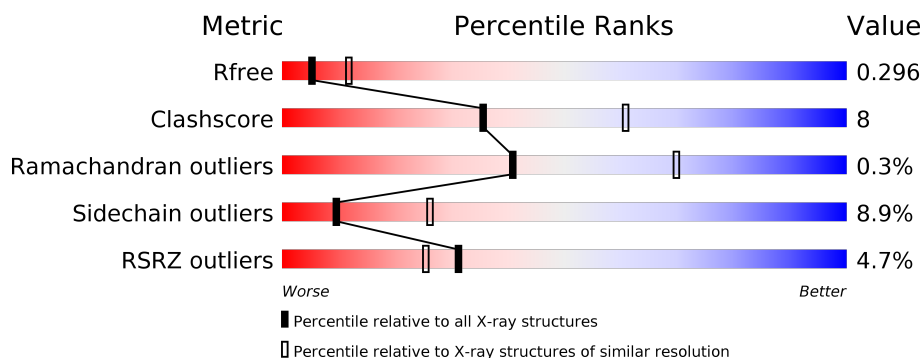
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 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 $\leq 5\%$. 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	479	 6% 63% 18% 18%
1	B	479	 2% 62% 16% 20%
1	C	479	 5% 64% 16% 17%
1	D	479	 3% 61% 18% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12587 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	4	0	0
			3095	1982	523	562	28			
1	B	383	Total	C	N	O	S	6	0	0
			2999	1916	509	546	28			
1	C	397	Total	C	N	O	S	2	0	0
			3115	1993	526	568	28			
1	D	388	Total	C	N	O	S	6	0	0
			3041	1942	516	555	28			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLY	-	EXPRESSION TAG	UNP D3Z7P3
A	126	SER	-	EXPRESSION TAG	UNP D3Z7P3
A	127	HIS	-	EXPRESSION TAG	UNP D3Z7P3
A	556	HIS	-	EXPRESSION TAG	UNP D3Z7P3
A	557	SER	-	EXPRESSION TAG	UNP D3Z7P3
A	558	PHE	-	EXPRESSION TAG	UNP D3Z7P3
A	559	GLY	-	EXPRESSION TAG	UNP D3Z7P3
A	560	PRO	-	EXPRESSION TAG	UNP D3Z7P3
A	561	LEU	-	EXPRESSION TAG	UNP D3Z7P3
A	562	ASP	-	EXPRESSION TAG	UNP D3Z7P3
A	563	TYR	-	EXPRESSION TAG	UNP D3Z7P3
A	564	GLU	-	EXPRESSION TAG	UNP D3Z7P3
A	565	SER	-	EXPRESSION TAG	UNP D3Z7P3
A	566	LEU	-	EXPRESSION TAG	UNP D3Z7P3
A	567	GLN	-	EXPRESSION TAG	UNP D3Z7P3
A	568	GLN	-	EXPRESSION TAG	UNP D3Z7P3
A	569	GLU	-	EXPRESSION TAG	UNP D3Z7P3
A	570	LEU	-	EXPRESSION TAG	UNP D3Z7P3
A	571	ALA	-	EXPRESSION TAG	UNP D3Z7P3
A	572	LEU	-	EXPRESSION TAG	UNP D3Z7P3
A	573	LYS	-	EXPRESSION TAG	UNP D3Z7P3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	574	ASP	-	EXPRESSION TAG	UNP D3Z7P3
A	575	THR	-	EXPRESSION TAG	UNP D3Z7P3
A	576	VAL	-	EXPRESSION TAG	UNP D3Z7P3
A	577	TRP	-	EXPRESSION TAG	UNP D3Z7P3
A	578	LYS	-	EXPRESSION TAG	UNP D3Z7P3
A	579	LYS	-	EXPRESSION TAG	UNP D3Z7P3
A	580	VAL	-	EXPRESSION TAG	UNP D3Z7P3
A	581	SER	-	EXPRESSION TAG	UNP D3Z7P3
A	582	PRO	-	EXPRESSION TAG	UNP D3Z7P3
A	583	GLU	-	EXPRESSION TAG	UNP D3Z7P3
A	584	SER	-	EXPRESSION TAG	UNP D3Z7P3
A	585	SER	-	EXPRESSION TAG	UNP D3Z7P3
A	586	ASP	-	EXPRESSION TAG	UNP D3Z7P3
A	587	ASP	-	EXPRESSION TAG	UNP D3Z7P3
A	588	THR	-	EXPRESSION TAG	UNP D3Z7P3
A	589	SER	-	EXPRESSION TAG	UNP D3Z7P3
A	590	THR	-	EXPRESSION TAG	UNP D3Z7P3
A	591	THR	-	EXPRESSION TAG	UNP D3Z7P3
A	592	VAL	-	EXPRESSION TAG	UNP D3Z7P3
A	593	VAL	-	EXPRESSION TAG	UNP D3Z7P3
A	594	TYR	-	EXPRESSION TAG	UNP D3Z7P3
A	595	ARG	-	EXPRESSION TAG	UNP D3Z7P3
A	596	MET	-	EXPRESSION TAG	UNP D3Z7P3
A	597	GLU	-	EXPRESSION TAG	UNP D3Z7P3
A	598	SER	-	EXPRESSION TAG	UNP D3Z7P3
A	599	LEU	-	EXPRESSION TAG	UNP D3Z7P3
A	600	GLY	-	EXPRESSION TAG	UNP D3Z7P3
A	601	GLU	-	EXPRESSION TAG	UNP D3Z7P3
A	602	ARG	-	EXPRESSION TAG	UNP D3Z7P3
A	603	SER	-	EXPRESSION TAG	UNP D3Z7P3
B	125	GLY	-	EXPRESSION TAG	UNP D3Z7P3
B	126	SER	-	EXPRESSION TAG	UNP D3Z7P3
B	127	HIS	-	EXPRESSION TAG	UNP D3Z7P3
B	556	HIS	-	EXPRESSION TAG	UNP D3Z7P3
B	557	SER	-	EXPRESSION TAG	UNP D3Z7P3
B	558	PHE	-	EXPRESSION TAG	UNP D3Z7P3
B	559	GLY	-	EXPRESSION TAG	UNP D3Z7P3
B	560	PRO	-	EXPRESSION TAG	UNP D3Z7P3
B	561	LEU	-	EXPRESSION TAG	UNP D3Z7P3
B	562	ASP	-	EXPRESSION TAG	UNP D3Z7P3
B	563	TYR	-	EXPRESSION TAG	UNP D3Z7P3
B	564	GLU	-	EXPRESSION TAG	UNP D3Z7P3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	565	SER	-	EXPRESSION TAG	UNP D3Z7P3
B	566	LEU	-	EXPRESSION TAG	UNP D3Z7P3
B	567	GLN	-	EXPRESSION TAG	UNP D3Z7P3
B	568	GLN	-	EXPRESSION TAG	UNP D3Z7P3
B	569	GLU	-	EXPRESSION TAG	UNP D3Z7P3
B	570	LEU	-	EXPRESSION TAG	UNP D3Z7P3
B	571	ALA	-	EXPRESSION TAG	UNP D3Z7P3
B	572	LEU	-	EXPRESSION TAG	UNP D3Z7P3
B	573	LYS	-	EXPRESSION TAG	UNP D3Z7P3
B	574	ASP	-	EXPRESSION TAG	UNP D3Z7P3
B	575	THR	-	EXPRESSION TAG	UNP D3Z7P3
B	576	VAL	-	EXPRESSION TAG	UNP D3Z7P3
B	577	TRP	-	EXPRESSION TAG	UNP D3Z7P3
B	578	LYS	-	EXPRESSION TAG	UNP D3Z7P3
B	579	LYS	-	EXPRESSION TAG	UNP D3Z7P3
B	580	VAL	-	EXPRESSION TAG	UNP D3Z7P3
B	581	SER	-	EXPRESSION TAG	UNP D3Z7P3
B	582	PRO	-	EXPRESSION TAG	UNP D3Z7P3
B	583	GLU	-	EXPRESSION TAG	UNP D3Z7P3
B	584	SER	-	EXPRESSION TAG	UNP D3Z7P3
B	585	SER	-	EXPRESSION TAG	UNP D3Z7P3
B	586	ASP	-	EXPRESSION TAG	UNP D3Z7P3
B	587	ASP	-	EXPRESSION TAG	UNP D3Z7P3
B	588	THR	-	EXPRESSION TAG	UNP D3Z7P3
B	589	SER	-	EXPRESSION TAG	UNP D3Z7P3
B	590	THR	-	EXPRESSION TAG	UNP D3Z7P3
B	591	THR	-	EXPRESSION TAG	UNP D3Z7P3
B	592	VAL	-	EXPRESSION TAG	UNP D3Z7P3
B	593	VAL	-	EXPRESSION TAG	UNP D3Z7P3
B	594	TYR	-	EXPRESSION TAG	UNP D3Z7P3
B	595	ARG	-	EXPRESSION TAG	UNP D3Z7P3
B	596	MET	-	EXPRESSION TAG	UNP D3Z7P3
B	597	GLU	-	EXPRESSION TAG	UNP D3Z7P3
B	598	SER	-	EXPRESSION TAG	UNP D3Z7P3
B	599	LEU	-	EXPRESSION TAG	UNP D3Z7P3
B	600	GLY	-	EXPRESSION TAG	UNP D3Z7P3
B	601	GLU	-	EXPRESSION TAG	UNP D3Z7P3
B	602	ARG	-	EXPRESSION TAG	UNP D3Z7P3
B	603	SER	-	EXPRESSION TAG	UNP D3Z7P3
C	125	GLY	-	EXPRESSION TAG	UNP D3Z7P3
C	126	SER	-	EXPRESSION TAG	UNP D3Z7P3
C	127	HIS	-	EXPRESSION TAG	UNP D3Z7P3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	556	HIS	-	EXPRESSION TAG	UNP D3Z7P3
C	557	SER	-	EXPRESSION TAG	UNP D3Z7P3
C	558	PHE	-	EXPRESSION TAG	UNP D3Z7P3
C	559	GLY	-	EXPRESSION TAG	UNP D3Z7P3
C	560	PRO	-	EXPRESSION TAG	UNP D3Z7P3
C	561	LEU	-	EXPRESSION TAG	UNP D3Z7P3
C	562	ASP	-	EXPRESSION TAG	UNP D3Z7P3
C	563	TYR	-	EXPRESSION TAG	UNP D3Z7P3
C	564	GLU	-	EXPRESSION TAG	UNP D3Z7P3
C	565	SER	-	EXPRESSION TAG	UNP D3Z7P3
C	566	LEU	-	EXPRESSION TAG	UNP D3Z7P3
C	567	GLN	-	EXPRESSION TAG	UNP D3Z7P3
C	568	GLN	-	EXPRESSION TAG	UNP D3Z7P3
C	569	GLU	-	EXPRESSION TAG	UNP D3Z7P3
C	570	LEU	-	EXPRESSION TAG	UNP D3Z7P3
C	571	ALA	-	EXPRESSION TAG	UNP D3Z7P3
C	572	LEU	-	EXPRESSION TAG	UNP D3Z7P3
C	573	LYS	-	EXPRESSION TAG	UNP D3Z7P3
C	574	ASP	-	EXPRESSION TAG	UNP D3Z7P3
C	575	THR	-	EXPRESSION TAG	UNP D3Z7P3
C	576	VAL	-	EXPRESSION TAG	UNP D3Z7P3
C	577	TRP	-	EXPRESSION TAG	UNP D3Z7P3
C	578	LYS	-	EXPRESSION TAG	UNP D3Z7P3
C	579	LYS	-	EXPRESSION TAG	UNP D3Z7P3
C	580	VAL	-	EXPRESSION TAG	UNP D3Z7P3
C	581	SER	-	EXPRESSION TAG	UNP D3Z7P3
C	582	PRO	-	EXPRESSION TAG	UNP D3Z7P3
C	583	GLU	-	EXPRESSION TAG	UNP D3Z7P3
C	584	SER	-	EXPRESSION TAG	UNP D3Z7P3
C	585	SER	-	EXPRESSION TAG	UNP D3Z7P3
C	586	ASP	-	EXPRESSION TAG	UNP D3Z7P3
C	587	ASP	-	EXPRESSION TAG	UNP D3Z7P3
C	588	THR	-	EXPRESSION TAG	UNP D3Z7P3
C	589	SER	-	EXPRESSION TAG	UNP D3Z7P3
C	590	THR	-	EXPRESSION TAG	UNP D3Z7P3
C	591	THR	-	EXPRESSION TAG	UNP D3Z7P3
C	592	VAL	-	EXPRESSION TAG	UNP D3Z7P3
C	593	VAL	-	EXPRESSION TAG	UNP D3Z7P3
C	594	TYR	-	EXPRESSION TAG	UNP D3Z7P3
C	595	ARG	-	EXPRESSION TAG	UNP D3Z7P3
C	596	MET	-	EXPRESSION TAG	UNP D3Z7P3
C	597	GLU	-	EXPRESSION TAG	UNP D3Z7P3

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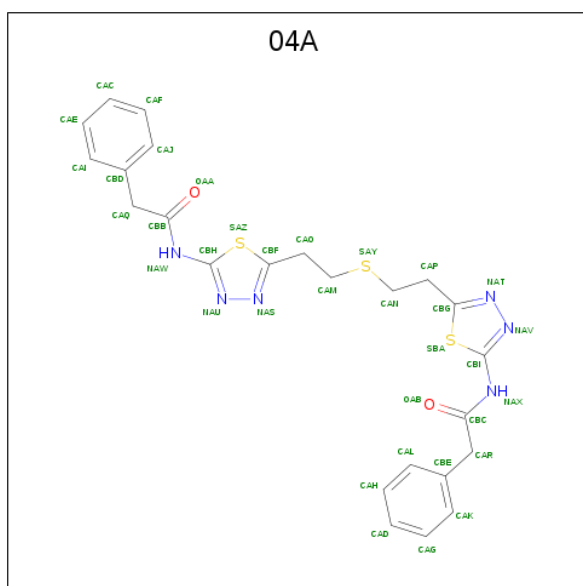
Chain	Residue	Modelled	Actual	Comment	Reference
C	598	SER	-	EXPRESSION TAG	UNP D3Z7P3
C	599	LEU	-	EXPRESSION TAG	UNP D3Z7P3
C	600	GLY	-	EXPRESSION TAG	UNP D3Z7P3
C	601	GLU	-	EXPRESSION TAG	UNP D3Z7P3
C	602	ARG	-	EXPRESSION TAG	UNP D3Z7P3
C	603	SER	-	EXPRESSION TAG	UNP D3Z7P3
D	125	GLY	-	EXPRESSION TAG	UNP D3Z7P3
D	126	SER	-	EXPRESSION TAG	UNP D3Z7P3
D	127	HIS	-	EXPRESSION TAG	UNP D3Z7P3
D	556	HIS	-	EXPRESSION TAG	UNP D3Z7P3
D	557	SER	-	EXPRESSION TAG	UNP D3Z7P3
D	558	PHE	-	EXPRESSION TAG	UNP D3Z7P3
D	559	GLY	-	EXPRESSION TAG	UNP D3Z7P3
D	560	PRO	-	EXPRESSION TAG	UNP D3Z7P3
D	561	LEU	-	EXPRESSION TAG	UNP D3Z7P3
D	562	ASP	-	EXPRESSION TAG	UNP D3Z7P3
D	563	TYR	-	EXPRESSION TAG	UNP D3Z7P3
D	564	GLU	-	EXPRESSION TAG	UNP D3Z7P3
D	565	SER	-	EXPRESSION TAG	UNP D3Z7P3
D	566	LEU	-	EXPRESSION TAG	UNP D3Z7P3
D	567	GLN	-	EXPRESSION TAG	UNP D3Z7P3
D	568	GLN	-	EXPRESSION TAG	UNP D3Z7P3
D	569	GLU	-	EXPRESSION TAG	UNP D3Z7P3
D	570	LEU	-	EXPRESSION TAG	UNP D3Z7P3
D	571	ALA	-	EXPRESSION TAG	UNP D3Z7P3
D	572	LEU	-	EXPRESSION TAG	UNP D3Z7P3
D	573	LYS	-	EXPRESSION TAG	UNP D3Z7P3
D	574	ASP	-	EXPRESSION TAG	UNP D3Z7P3
D	575	THR	-	EXPRESSION TAG	UNP D3Z7P3
D	576	VAL	-	EXPRESSION TAG	UNP D3Z7P3
D	577	TRP	-	EXPRESSION TAG	UNP D3Z7P3
D	578	LYS	-	EXPRESSION TAG	UNP D3Z7P3
D	579	LYS	-	EXPRESSION TAG	UNP D3Z7P3
D	580	VAL	-	EXPRESSION TAG	UNP D3Z7P3
D	581	SER	-	EXPRESSION TAG	UNP D3Z7P3
D	582	PRO	-	EXPRESSION TAG	UNP D3Z7P3
D	583	GLU	-	EXPRESSION TAG	UNP D3Z7P3
D	584	SER	-	EXPRESSION TAG	UNP D3Z7P3
D	585	SER	-	EXPRESSION TAG	UNP D3Z7P3
D	586	ASP	-	EXPRESSION TAG	UNP D3Z7P3
D	587	ASP	-	EXPRESSION TAG	UNP D3Z7P3
D	588	THR	-	EXPRESSION TAG	UNP D3Z7P3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	589	SER	-	EXPRESSION TAG	UNP D3Z7P3
D	590	THR	-	EXPRESSION TAG	UNP D3Z7P3
D	591	THR	-	EXPRESSION TAG	UNP D3Z7P3
D	592	VAL	-	EXPRESSION TAG	UNP D3Z7P3
D	593	VAL	-	EXPRESSION TAG	UNP D3Z7P3
D	594	TYR	-	EXPRESSION TAG	UNP D3Z7P3
D	595	ARG	-	EXPRESSION TAG	UNP D3Z7P3
D	596	MET	-	EXPRESSION TAG	UNP D3Z7P3
D	597	GLU	-	EXPRESSION TAG	UNP D3Z7P3
D	598	SER	-	EXPRESSION TAG	UNP D3Z7P3
D	599	LEU	-	EXPRESSION TAG	UNP D3Z7P3
D	600	GLY	-	EXPRESSION TAG	UNP D3Z7P3
D	601	GLU	-	EXPRESSION TAG	UNP D3Z7P3
D	602	ARG	-	EXPRESSION TAG	UNP D3Z7P3
D	603	SER	-	EXPRESSION TAG	UNP D3Z7P3

- Molecule 2 is N,N'-[sulfanediylbis(ethane-2,1-diyl-1,3,4-thiadiazole-5,2-diyl)]bis(2-phenylacetamide) (three-letter code: 04A) (formula: C₂₄H₂₄N₆O₂S₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			35	24	6	2	3		
2	D	1	Total	C	N	O	S	0	0
			35	24	6	2	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total 73	O 73	0	0
3	B	67	Total 67	O 67	0	0
3	C	57	Total 57	O 57	0	0
3	D	70	Total 70	O 70	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.67Å 140.24Å 180.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.77 38.39 – 2.77	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.77) 97.5 (38.39-2.77)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.253 , 0.295 0.254 , 0.296	Depositor DCC
R_{free} test set	3232 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	1.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12587	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6817e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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.

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: 04A

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	0.26	0/3164	0.44	1/4267 (0.0%)
1	B	0.24	0/3064	0.42	0/4129
1	C	0.24	0/3184	0.42	0/4294
1	D	0.24	0/3105	0.44	0/4184
All	All	0.24	0/12517	0.43	1/16874 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	PHE	N-CA-C	-7.01	92.07	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	ASN	Peptide

5.2 Too-close contacts ⓘ

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	3095	0	3087	64	0
1	B	2999	0	2987	48	0
1	C	3115	0	3106	49	0
1	D	3041	0	3033	45	0
2	B	35	0	24	1	0
2	D	35	0	24	3	0
3	A	73	0	0	7	0
3	B	67	0	0	0	0
3	C	57	0	0	2	0
3	D	70	0	0	3	0
All	All	12587	0	12261	198	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 8.

The worst 5 of 198 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:319:SER:OG	1:A:324:ASN:ND2	2.10	0.84
1:A:323:PHE:O	1:A:324:ASN:CB	2.26	0.83
1:A:322:ARG:HD2	1:A:323:PHE:H	1.43	0.82
1:A:322:ARG:CD	1:A:323:PHE:H	1.94	0.81
1:A:322:ARG:O	1:A:323:PHE:CB	2.31	0.78

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	389/479 (81%)	370 (95%)	17 (4%)	2 (0%)	29	58
1	B	375/479 (78%)	358 (96%)	17 (4%)	0	100	100
1	C	391/479 (82%)	373 (95%)	17 (4%)	1 (0%)	41	70
1	D	380/479 (79%)	368 (97%)	11 (3%)	1 (0%)	41	70
All	All	1535/1916 (80%)	1469 (96%)	62 (4%)	4 (0%)	41	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	323	PHE
1	A	290	GLN
1	A	354	VAL
1	C	227	PRO

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	343/415 (83%)	315 (92%)	28 (8%)	11	30
1	B	333/415 (80%)	302 (91%)	31 (9%)	9	24
1	C	346/415 (83%)	318 (92%)	28 (8%)	11	30
1	D	338/415 (81%)	304 (90%)	34 (10%)	7	20
All	All	1360/1660 (82%)	1239 (91%)	121 (9%)	9	26

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	503	MET
1	C	203	ASP
1	D	382	THR
1	B	536	ASP
1	C	152	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	162	HIS
1	B	335	HIS
1	D	340	ASN
1	A	460	ASN
1	B	534	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	04A	B	701	-	32,38,38	2.65	11 (34%)	29,49,49	1.47	6 (20%)
2	04A	D	701	-	32,38,38	2.64	11 (34%)	29,49,49	1.47	6 (20%)

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	04A	B	701	-	-	3/18/24/24	0/4/4/4
2	04A	D	701	-	-	2/18/24/24	0/4/4/4

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	04A	CAE-CAI	5.09	1.49	1.38
2	D	701	04A	CAH-CAL	5.07	1.49	1.38
2	B	701	04A	CAE-CAI	5.06	1.49	1.38
2	B	701	04A	CAH-CAL	5.04	1.49	1.38
2	B	701	04A	CAJ-CBD	5.02	1.49	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	04A	CAQ-CBB-NAW	3.83	122.68	114.77
2	B	701	04A	CAQ-CBB-NAW	3.62	122.25	114.77
2	D	701	04A	CBI-NAX-CBC	-2.74	122.13	129.54
2	B	701	04A	CBI-NAX-CBC	-2.58	122.58	129.54
2	D	701	04A	CAP-CAN-SAY	-2.38	107.62	113.84

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	04A	CAQ-CBB-NAW-CBH
2	D	701	04A	CAQ-CBB-NAW-CBH
2	B	701	04A	OAA-CBB-NAW-CBH
2	D	701	04A	OAA-CBB-NAW-CBH
2	B	701	04A	SAY-CAM-CAO-CBF

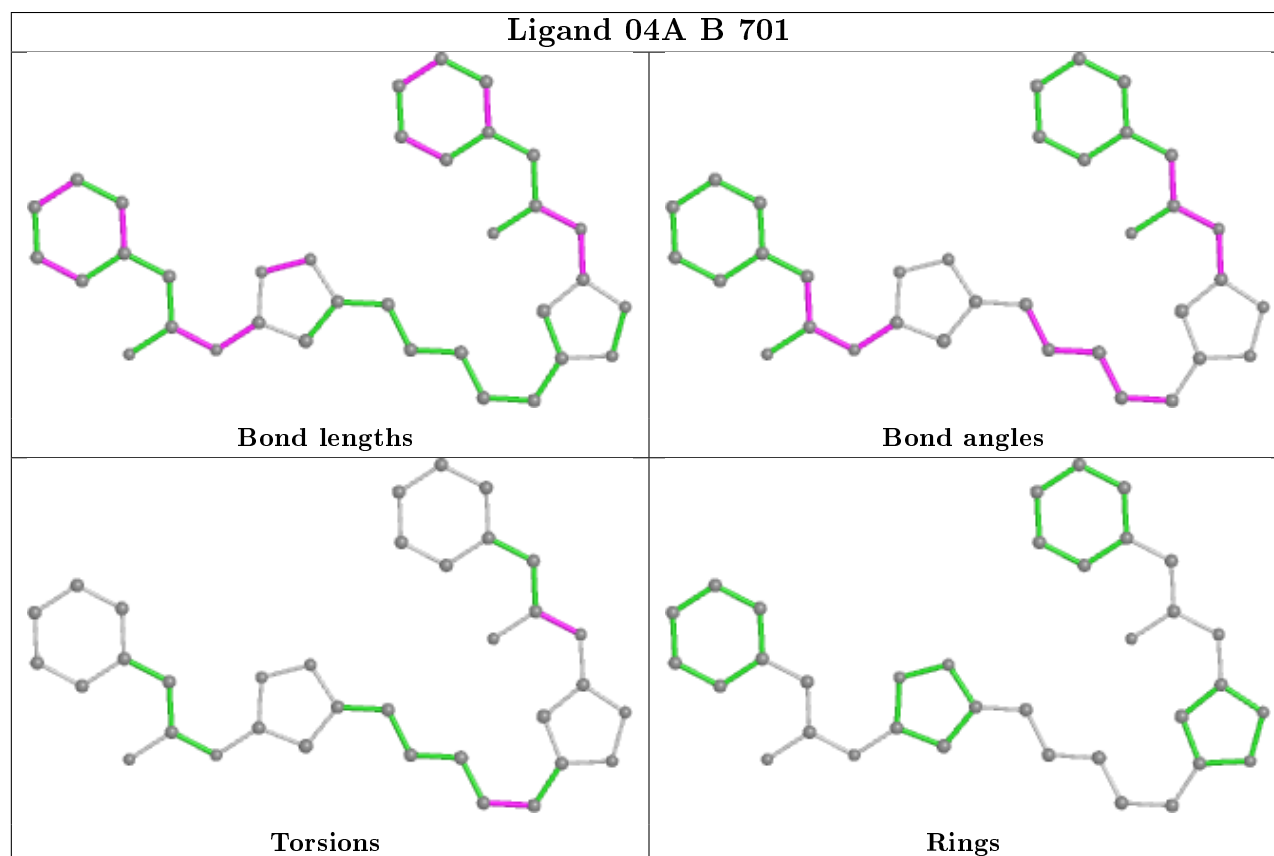
There are no ring outliers.

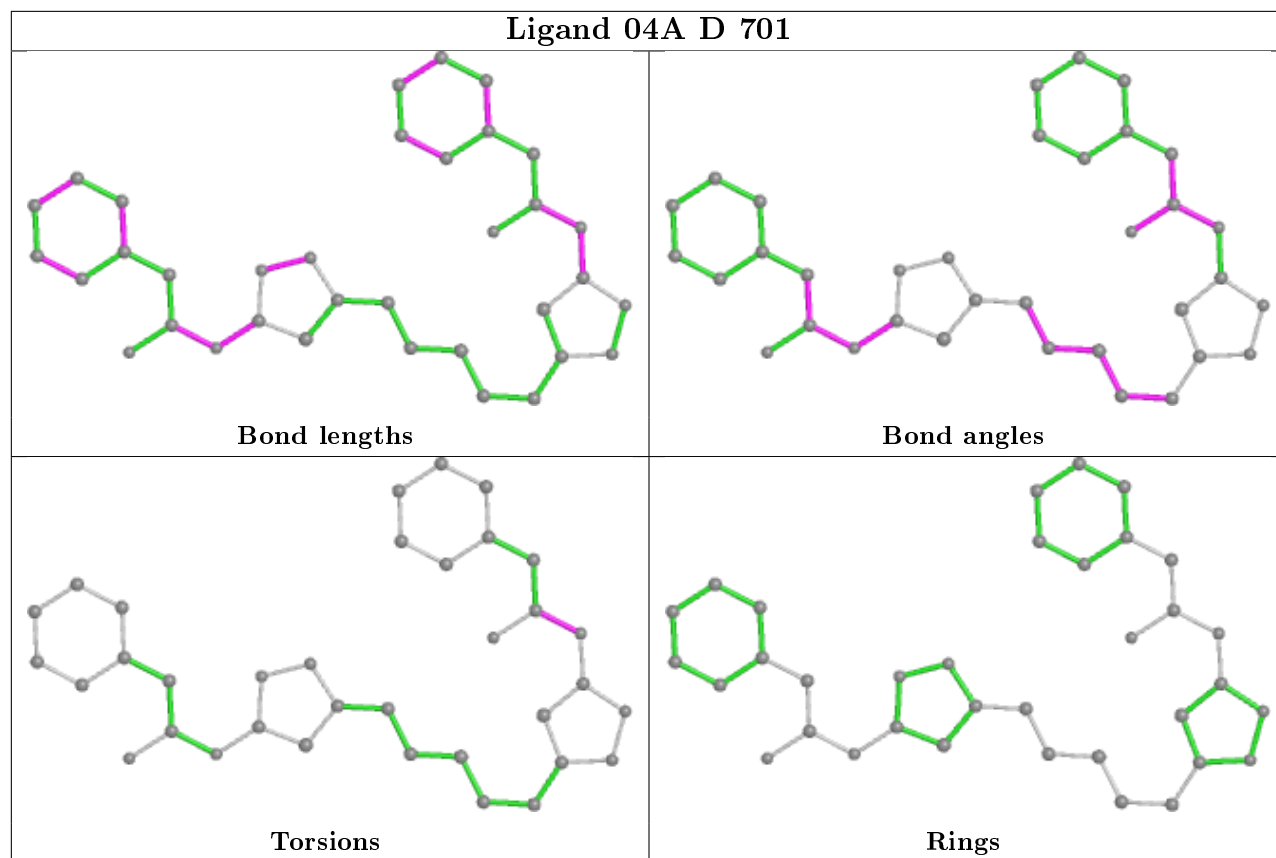
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	04A	1	0
2	D	701	04A	3	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 than 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, 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	395/479 (82%)	0.27	27 (6%) 17 12	20, 35, 62, 79	3 (0%)
1	B	383/479 (79%)	0.13	8 (2%) 63 59	19, 34, 53, 75	5 (1%)
1	C	397/479 (82%)	0.29	25 (6%) 20 15	19, 34, 64, 87	1 (0%)
1	D	388/479 (81%)	0.26	14 (3%) 42 37	24, 34, 57, 74	4 (1%)
All	All	1563/1916 (81%)	0.24	74 (4%) 31 25	19, 34, 60, 87	13 (0%)

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	PHE	6.4
1	A	256	PRO	5.7
1	D	324	ASN	4.4
1	C	323	PHE	4.3
1	A	149	PHE	4.2

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](#)

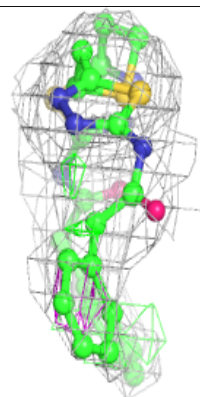
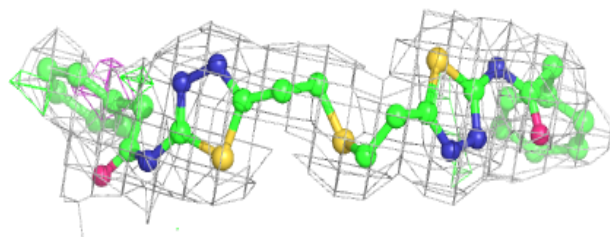
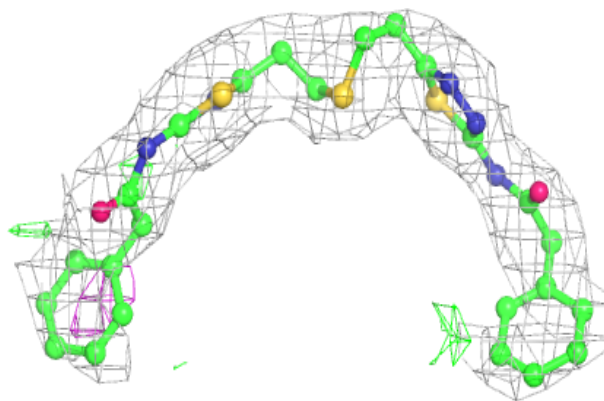
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	04A	B	701	35/35	0.88	0.23	38,48,60,64	0
2	04A	D	701	35/35	0.91	0.24	37,45,61,62	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.

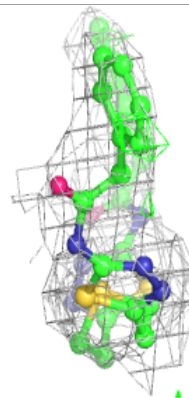
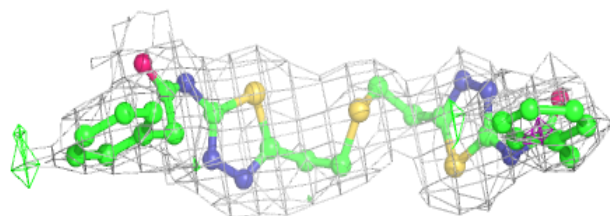
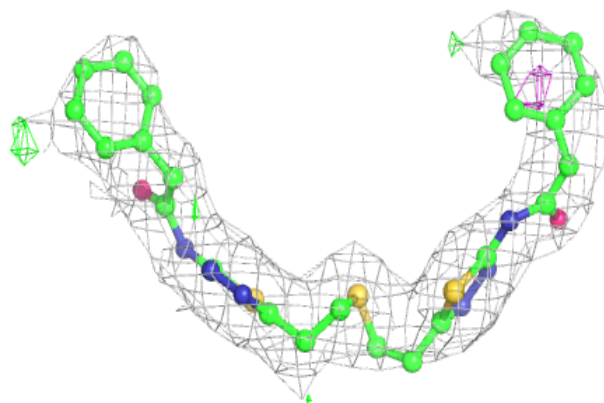
Electron density around 04A B 701:

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 04A D 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.