Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:49 PM GMT

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 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
http://wwpdb.org/validation/2016/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:

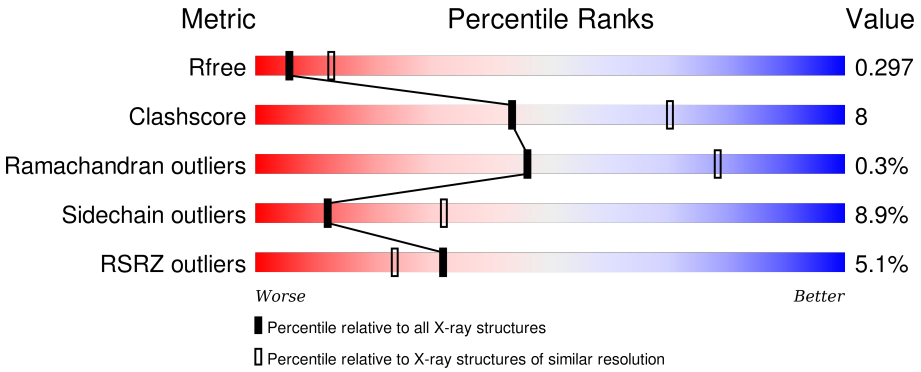
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.77 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}	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (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. 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	479	6% 63% 18% • 18%
1	B	479	2% 62% 16% • 20%
1	C	479	6% 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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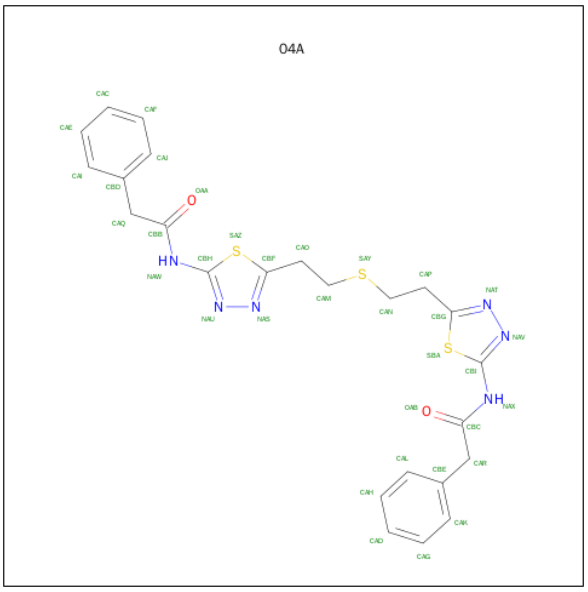
Chain	Residue	Modelled	Actual	Comment	Reference
D	589	SER	-	EXPRESSION TAG	UNP D3Z7P3
D	590	THR	-	EXPRESSION TAG	UNP D3Z7P3
D	591	THR	-	EXPRESSION TAG	UNP D3Z7P3
D	592	VAL	-	EXPRESSION TAG	UNP D3Z7P3
D	593	VAL	-	EXPRESSION TAG	UNP D3Z7P3
D	594	TYR	-	EXPRESSION TAG	UNP D3Z7P3
D	595	ARG	-	EXPRESSION TAG	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: $C_{24}H_{24}N_6O_2S_3$).



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.

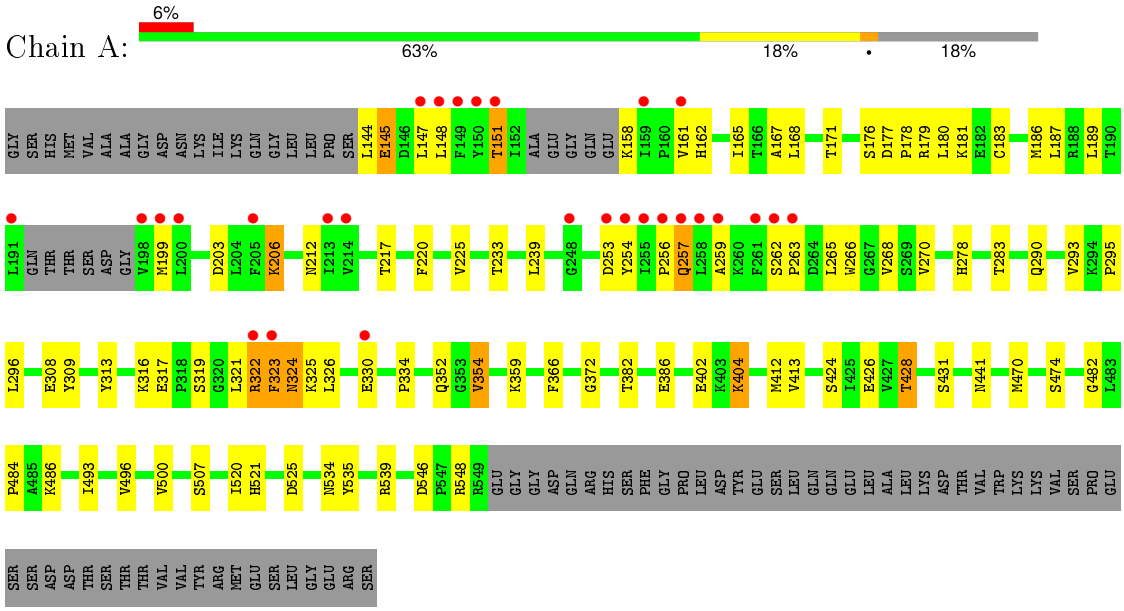
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	73	Total O 73 73	0	0
3	B	67	Total O 67 67	0	0
3	C	57	Total O 57 57	0	0
3	D	70	Total O 70 70	0	0

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 errors 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.

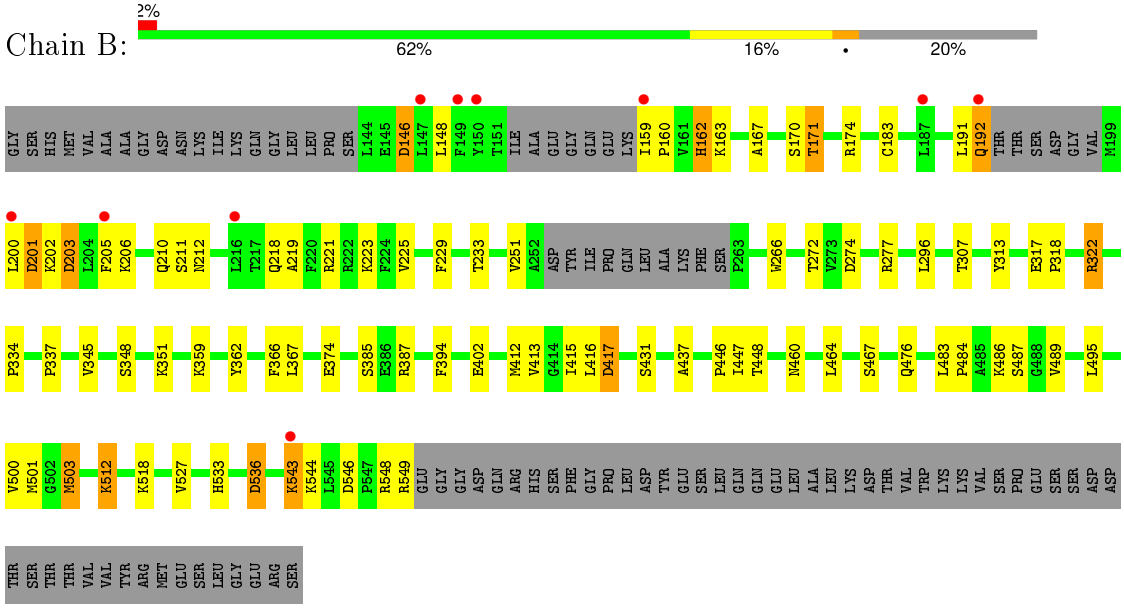
- Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain A:



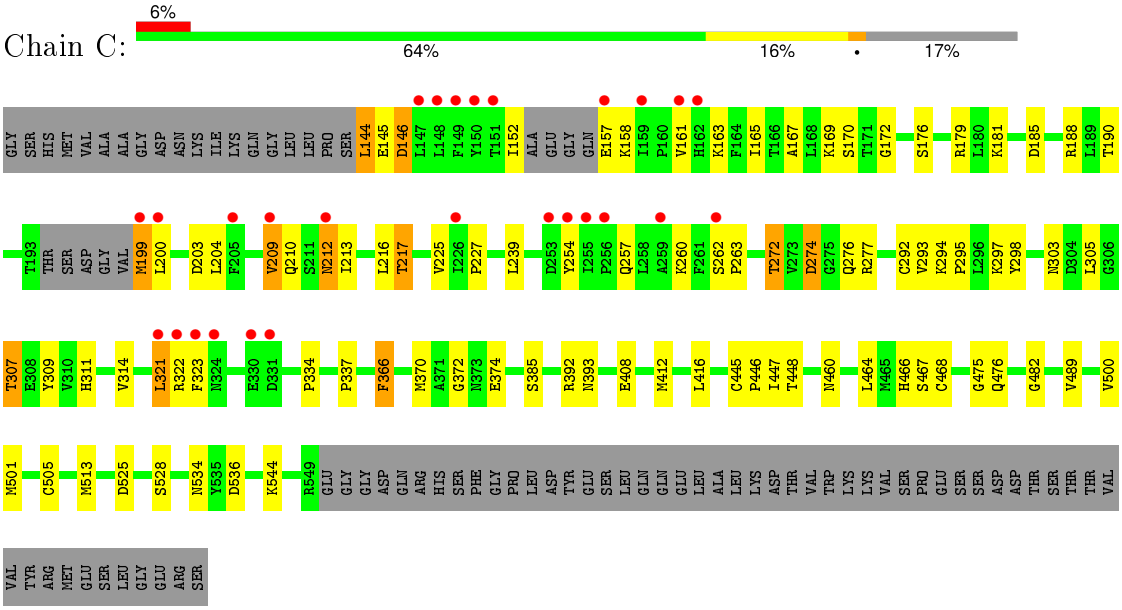
- Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain B:



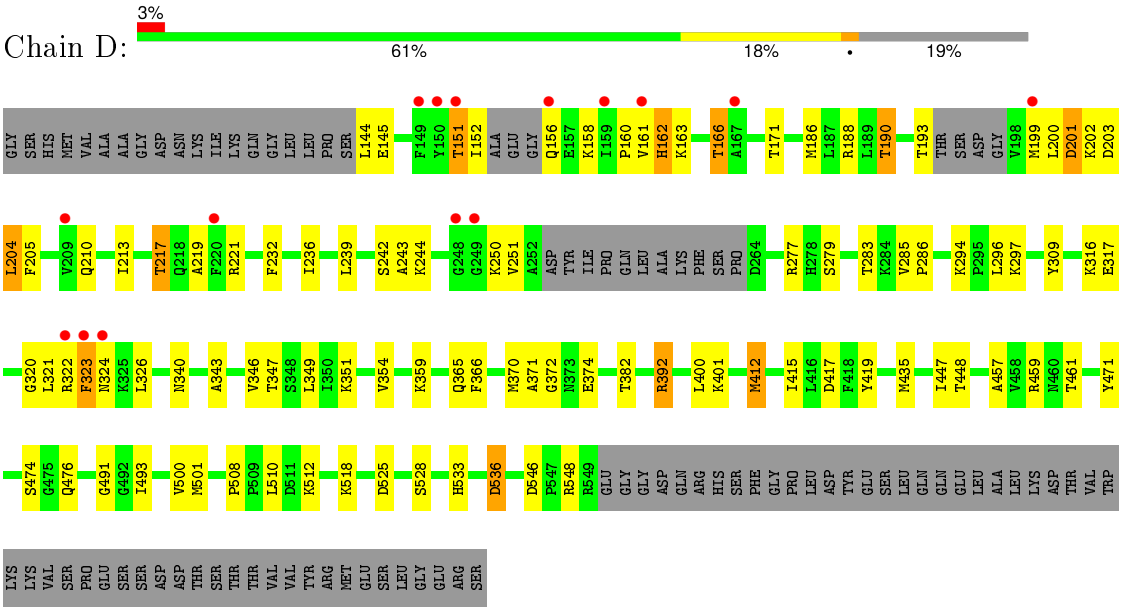
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain C:



• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.75 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.253 , 0.295 0.258 , 0.297	Depositor DCC
R_{free} test set	3226 reflections (5.33%)	DCC
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 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Outliers	6 of 63920 reflections (0.009%)	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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 (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	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.

All (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
1:A:323:PHE:O	1:A:324:ASN:HB2	1.84	0.77
1:A:322:ARG:HG3	1:A:323:PHE:N	2.03	0.74
1:A:309:TYR:OH	1:A:352:GLN:NE2	2.21	0.73
1:A:322:ARG:O	1:A:323:PHE:HB2	1.88	0.72
1:B:495:LEU:HB3	1:B:503:MET:HB3	1.71	0.70
1:A:158:LYS:HD2	1:A:199:MET:HG2	1.71	0.70
1:B:536:ASP:OD2	1:B:544:LYS:NZ	2.21	0.70
1:C:209:VAL:HG22	1:C:216:LEU:HD13	1.73	0.69
1:A:322:ARG:CG	1:A:323:PHE:N	2.57	0.68
1:A:322:ARG:HH21	2:D:701:04A:HAJ	1.59	0.68
1:A:317:GLU:OE1	1:C:476:GLN:NE2	2.26	0.68
1:A:322:ARG:HD3	1:A:325:LYS:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ARG:C	1:A:323:PHE:O	2.29	0.66
1:D:320:GLY:O	1:D:324:ASN:ND2	2.29	0.66
1:C:460:ASN:ND2	3:C:754:HOH:O	2.29	0.66
1:D:239:LEU:HD22	1:D:525:ASP:HB3	1.77	0.65
1:A:158:LYS:N	3:A:742:HOH:O	2.28	0.65
1:D:158:LYS:HE3	1:D:199:MET:HG2	1.77	0.65
1:A:239:LEU:HD22	1:A:525:ASP:HB3	1.79	0.64
1:D:546:ASP:OD1	1:D:548:ARG:NH1	2.29	0.64
1:B:171:THR:HG21	1:B:219:ALA:HB1	1.79	0.64
1:D:188:ARG:NH1	3:D:849:HOH:O	2.31	0.64
1:B:191:LEU:HD22	1:B:192:GLN:H	1.64	0.62
1:C:169:LYS:NZ	3:C:711:HOH:O	2.31	0.62
1:A:316:LYS:NZ	3:A:750:HOH:O	2.26	0.62
1:D:340:ASN:ND2	1:D:419:TYR:OH	2.33	0.61
1:A:253:ASP:HA	1:A:259:ALA:HB2	1.82	0.61
1:C:225:VAL:HG21	1:C:500:VAL:HA	1.80	0.61
1:A:539:ARG:NH2	1:C:274:ASP:OD2	2.34	0.60
1:A:283:THR:O	1:A:428:THR:OG1	2.18	0.60
1:A:330:GLU:OE1	1:C:322:ARG:NH1	2.34	0.60
1:D:151:THR:OG1	1:D:221:ARG:NH2	2.35	0.60
1:B:546:ASP:OD1	1:B:548:ARG:NH1	2.35	0.60
1:B:277:ARG:NH2	1:B:374:GLU:OE2	2.31	0.59
1:D:277:ARG:NH2	1:D:374:GLU:OE2	2.36	0.59
1:A:181:LYS:NZ	3:A:736:HOH:O	2.34	0.59
1:C:144:LEU:N	1:C:146:ASP:OD1	2.36	0.58
1:D:244:LYS:NZ	3:D:853:HOH:O	2.36	0.58
1:C:212:ASN:OD1	1:C:212:ASN:N	2.37	0.58
1:D:243:ALA:HB1	1:D:518:LYS:HG2	1.85	0.58
1:B:148:LEU:HD22	1:B:205:PHE:HZ	1.67	0.57
1:D:201:ASP:OD1	1:D:201:ASP:N	2.34	0.57
1:A:322:ARG:CG	1:A:323:PHE:H	2.16	0.57
1:A:539:ARG:NH1	3:A:706:HOH:O	2.38	0.56
1:A:317:GLU:HG2	1:C:475:GLY:HA3	1.87	0.56
1:C:181:LYS:NZ	1:C:185:ASP:OD2	2.38	0.56
1:C:257:GLN:HA	1:C:260:LYS:HE2	1.87	0.56
1:A:546:ASP:OD1	1:A:548:ARG:NH1	2.39	0.56
1:B:387:ARG:NH1	1:B:417:ASP:OD2	2.37	0.56
1:A:225:VAL:HG21	1:A:500:VAL:HA	1.87	0.55
1:D:200:LEU:HD23	1:D:205:PHE:HD1	1.71	0.55
1:C:185:ASP:OD1	1:C:188:ARG:NH2	2.39	0.55
1:B:500:VAL:HG12	1:B:501:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:N	1:B:274:ASP:OD2	2.37	0.55
1:D:412:MET:HA	1:D:415:ILE:HB	1.89	0.54
1:D:371:ALA:HB2	1:D:435:MET:HE2	1.88	0.54
1:C:294:LYS:HA	1:C:297:LYS:HE2	1.90	0.54
1:B:160:PRO:HG2	1:B:163:LYS:HB2	1.90	0.54
1:A:535:TYR:OH	1:C:466:HIS:ND1	2.40	0.53
1:D:370:MET:HB3	1:D:435:MET:HG3	1.90	0.53
1:A:147:LEU:HD12	1:A:147:LEU:H	1.73	0.53
1:A:326:LEU:HD13	2:D:701:04A:HAL	1.90	0.53
1:C:254:TYR:HE2	1:C:489:VAL:HG11	1.74	0.53
1:A:428:THR:HG23	1:A:431:SER:H	1.73	0.53
1:D:162:HIS:O	1:D:166:THR:OG1	2.20	0.52
1:B:351:LYS:HE2	1:B:362:TYR:CD1	2.44	0.52
1:C:321:LEU:HD12	1:C:322:ARG:H	1.74	0.52
1:D:171:THR:HG21	1:D:219:ALA:HB1	1.92	0.52
1:D:186:MET:O	1:D:190:THR:OG1	2.28	0.51
1:D:201:ASP:H	1:D:204:LEU:HD11	1.75	0.51
1:D:491:GLY:HA3	1:D:508:PRO:HA	1.92	0.51
1:B:167:ALA:O	1:B:170:SER:OG	2.27	0.51
1:A:179:ARG:O	1:A:212:ASN:ND2	2.43	0.51
1:A:203:ASP:HA	1:A:206:LYS:HB2	1.93	0.51
1:C:157:GLU:HG3	1:C:158:LYS:HG3	1.93	0.51
1:C:145:GLU:HG3	1:C:213:ILE:HG12	1.93	0.50
1:D:476:GLN:NE2	3:D:815:HOH:O	2.42	0.50
1:C:210:GLN:HA	1:C:213:ILE:HB	1.93	0.50
1:A:145:GLU:HB2	1:A:206:LYS:HG2	1.94	0.49
1:B:394:PHE:HD1	1:B:416:LEU:HD13	1.77	0.49
1:C:314:VAL:HG23	1:C:334:PRO:HG2	1.95	0.49
1:D:447:ILE:HG13	1:D:448:THR:HG23	1.94	0.49
1:D:392:ARG:HG3	1:D:392:ARG:HH21	1.77	0.49
1:D:217:THR:O	1:D:221:ARG:N	2.39	0.49
1:A:262:SER:HB3	1:A:265:LEU:HG	1.94	0.49
1:B:200:LEU:HD23	1:B:205:PHE:HA	1.95	0.49
1:D:401:LYS:HD2	1:D:412:MET:HG2	1.94	0.49
1:B:337:PRO:HD2	1:B:464:LEU:HD13	1.95	0.48
1:B:160:PRO:HB2	1:B:162:HIS:CD2	2.49	0.48
1:D:351:LYS:O	1:D:359:LYS:HE2	2.13	0.48
1:B:437:ALA:HB1	1:B:446:PRO:HG2	1.95	0.48
1:C:277:ARG:NH2	1:C:374:GLU:OE2	2.46	0.48
1:D:533:HIS:HB3	1:D:536:ASP:HB2	1.95	0.48
1:A:167:ALA:HB1	1:A:220:PHE:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:LYS:HE3	1:B:543:LYS:HB3	1.76	0.47
1:C:298:TYR:OH	1:C:311:HIS:NE2	2.33	0.47
1:C:179:ARG:O	1:C:212:ASN:ND2	2.43	0.47
1:C:314:VAL:HG11	1:C:337:PRO:HG3	1.97	0.47
1:D:144:LEU:HG	1:D:213:ILE:HG12	1.95	0.47
1:D:471:TYR:O	1:D:474:SER:OG	2.30	0.47
1:B:512:LYS:HG3	1:B:512:LYS:H	1.43	0.47
1:B:527:VAL:O	1:B:544:LYS:HE2	2.14	0.47
1:A:534:ASN:OD1	1:C:534:ASN:ND2	2.41	0.47
1:C:337:PRO:HD2	1:C:464:LEU:HD13	1.97	0.47
1:B:202:LYS:HE2	1:B:202:LYS:HB3	1.65	0.46
1:D:251:VAL:HG22	1:D:508:PRO:HB2	1.97	0.46
1:B:402:GLU:HG2	1:C:392:ARG:HB2	1.97	0.46
1:D:323:PHE:HA	1:D:326:LEU:HD13	1.98	0.46
1:A:295:PRO:CG	1:A:486:LYS:HG3	2.46	0.46
1:B:322:ARG:CZ	1:B:322:ARG:HB3	2.44	0.46
1:B:318:PRO:HG3	1:B:467:SER:HB2	1.98	0.46
1:D:285:VAL:HA	1:D:286:PRO:HD3	1.83	0.46
1:B:447:ILE:HG13	1:B:448:THR:HG23	1.98	0.45
1:B:272:THR:HA	1:B:501:MET:HA	1.99	0.45
1:B:322:ARG:NH1	2:B:701:04A:HAD	2.32	0.45
1:D:343:ALA:O	1:D:347:THR:OG1	2.23	0.45
1:A:426:GLU:OE2	3:A:765:HOH:O	2.21	0.45
1:C:536:ASP:OD2	1:C:544:LYS:NZ	2.43	0.45
1:C:445:CYS:HA	1:C:446:PRO:HD2	1.82	0.45
1:C:239:LEU:HD22	1:C:525:ASP:HB3	1.98	0.45
1:A:319:SER:O	3:A:770:HOH:O	2.21	0.45
1:C:272:THR:HA	1:C:501:MET:HA	1.99	0.45
1:A:257:GLN:HG3	1:A:382:THR:HA	1.99	0.45
1:A:168:LEU:HD21	1:A:180:LEU:HD13	1.98	0.45
1:B:394:PHE:CD1	1:B:416:LEU:HD13	2.53	0.44
1:A:256:PRO:HA	1:A:259:ALA:HB3	1.98	0.44
1:C:321:LEU:H	1:C:321:LEU:HG	1.73	0.44
1:B:148:LEU:HD22	1:B:205:PHE:CZ	2.51	0.44
1:A:177:ASP:HA	1:A:178:PRO:HD2	1.84	0.44
1:D:160:PRO:HD2	1:D:163:LYS:HD3	1.98	0.44
1:D:309:TYR:HE2	1:D:349:LEU:HD22	1.82	0.44
1:B:313:TYR:O	1:B:334:PRO:HD2	2.18	0.44
1:D:500:VAL:HG12	1:D:501:MET:HG2	2.00	0.43
1:C:307:THR:OG1	1:C:460:ASN:OD1	2.20	0.43
1:C:213:ILE:O	1:C:217:THR:OG1	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ALA:O	1:C:170:SER:OG	2.29	0.43
1:A:233:THR:HB	1:A:278:HIS:CE1	2.53	0.43
1:A:266:TRP:CE3	1:A:507:SER:HB2	2.54	0.43
1:C:158:LYS:HB3	1:C:200:LEU:O	2.19	0.43
1:B:277:ARG:HH22	1:B:374:GLU:CD	2.21	0.43
1:A:168:LEU:O	1:A:171:THR:OG1	2.28	0.43
1:C:372:GLY:HA3	1:C:447:ILE:HD11	2.00	0.43
1:A:323:PHE:C	1:A:325:LYS:H	2.21	0.43
1:B:159:ILE:O	1:B:200:LEU:N	2.37	0.43
1:B:206:LYS:O	1:B:210:GLN:HB2	2.18	0.43
1:C:292:CYS:O	1:C:295:PRO:HD2	2.19	0.43
1:B:191:LEU:O	1:B:192:GLN:HG3	2.19	0.42
1:C:447:ILE:HG13	1:C:448:THR:HG23	2.00	0.42
1:A:520:ILE:HG13	1:A:521:HIS:N	2.34	0.42
1:B:201:ASP:OD1	1:B:203:ASP:N	2.48	0.42
1:B:160:PRO:HB2	1:B:162:HIS:HD2	1.84	0.42
1:A:183:CYS:O	1:A:187:LEU:HB2	2.19	0.42
1:A:313:TYR:O	1:A:334:PRO:HD2	2.20	0.42
1:D:372:GLY:HA3	1:D:447:ILE:HD11	2.00	0.42
1:C:190:THR:HG21	1:C:204:LEU:HD21	2.02	0.42
1:B:533:HIS:CG	1:D:459:ARG:HD2	2.54	0.42
1:A:322:ARG:O	1:A:323:PHE:HB3	2.18	0.42
1:A:254:TYR:OH	1:A:386:GLU:OE2	2.23	0.42
1:B:146:ASP:OD2	1:B:146:ASP:N	2.52	0.42
1:B:351:LYS:O	1:B:359:LYS:HE2	2.20	0.42
1:B:486:LYS:NZ	1:B:487:SER:O	2.51	0.42
1:C:482:GLY:O	1:C:534:ASN:HB2	2.20	0.42
1:B:415:ILE:HD13	1:B:415:ILE:HA	1.89	0.42
1:A:295:PRO:HG2	1:A:486:LYS:HG3	2.02	0.41
1:D:145:GLU:OE1	1:D:145:GLU:N	2.48	0.41
1:A:372:GLY:O	3:A:713:HOH:O	2.21	0.41
1:A:262:SER:HA	1:A:263:PRO:HD3	1.82	0.41
1:C:366:PHE:O	1:C:370:MET:HG3	2.20	0.41
1:B:334:PRO:HG2	1:B:345:VAL:HG21	2.02	0.41
1:D:279:SER:HB3	1:D:283:THR:HG21	2.02	0.41
1:B:266:TRP:CG	1:B:518:LYS:HD3	2.55	0.41
1:A:486:LYS:O	1:A:493:ILE:HA	2.21	0.41
1:C:305:LEU:HD13	1:C:309:TYR:CE2	2.55	0.41
1:D:201:ASP:H	1:D:204:LEU:CD1	2.33	0.41
1:A:482:GLY:O	1:A:534:ASN:HB2	2.20	0.41
1:C:272:THR:HG1	1:C:276:GLN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:LYS:HA	1:D:297:LYS:HE2	2.01	0.41
1:C:393:ASN:HB3	1:C:416:LEU:HD21	2.02	0.41
1:A:470:MET:HB2	1:A:474:SER:HA	2.03	0.41
1:B:307:THR:OG1	1:B:460:ASN:OD1	2.35	0.41
1:D:457:ALA:O	1:D:461:THR:OG1	2.32	0.41
1:B:483:LEU:HA	1:B:484:PRO:HD3	1.98	0.41
1:C:262:SER:HA	1:C:263:PRO:HD3	1.90	0.40
1:A:484:PRO:HG2	1:A:496:VAL:HB	2.04	0.40
1:A:354:VAL:HG23	1:A:359:LYS:HG3	2.03	0.40
1:A:404:LYS:HB2	1:A:404:LYS:HE3	1.91	0.40
1:C:158:LYS:HD2	1:C:199:MET:HE1	2.03	0.40
1:D:322:ARG:HH11	2:D:701:04A:CAG	2.34	0.40
1:A:147:LEU:O	1:A:151:THR:OG1	2.40	0.40
1:C:172:GLY:HA3	1:C:276:GLN:HB3	2.04	0.40
1:B:476:GLN:OE1	1:B:476:GLN:N	2.49	0.40
1:B:229:PHE:O	1:B:233:THR:HG23	2.21	0.40
1:D:232:PHE:CZ	1:D:236:ILE:HD11	2.57	0.40

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	389/479 (81%)	370 (95%)	17 (4%)	2 (0%)	34 68
1	B	375/479 (78%)	358 (96%)	17 (4%)	0	100 100
1	C	391/479 (82%)	373 (95%)	17 (4%)	1 (0%)	46 78
1	D	380/479 (79%)	368 (97%)	11 (3%)	1 (0%)	46 78
All	All	1535/1916 (80%)	1469 (96%)	62 (4%)	4 (0%)	46 78

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 (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	343/415 (83%)	315 (92%)	28 (8%)	14 36
1	B	333/415 (80%)	302 (91%)	31 (9%)	11 30
1	C	346/415 (83%)	318 (92%)	28 (8%)	15 37
1	D	338/415 (81%)	304 (90%)	34 (10%)	9 25
All	All	1360/1660 (82%)	1239 (91%)	121 (9%)	12 32

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	A	145	GLU
1	A	148	LEU
1	A	151	THR
1	A	161	VAL
1	A	162	HIS
1	A	165	ILE
1	A	176	SER
1	A	186	MET
1	A	189	LEU
1	A	206	LYS
1	A	217	THR
1	A	257	GLN
1	A	268	VAL
1	A	270	VAL
1	A	293	VAL
1	A	296	LEU
1	A	308	GLU

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Mol	Chain	Res	Type
1	A	321	LEU
1	A	322	ARG
1	A	366	PHE
1	A	402	GLU
1	A	404	LYS
1	A	412	MET
1	A	413	VAL
1	A	424	SER
1	A	428	THR
1	A	441	ASN
1	B	146	ASP
1	B	162	HIS
1	B	171	THR
1	B	174	ARG
1	B	183	CYS
1	B	192	GLN
1	B	201	ASP
1	B	203	ASP
1	B	211	SER
1	B	212	ASN
1	B	218	GLN
1	B	221	ARG
1	B	223	LYS
1	B	251	VAL
1	B	296	LEU
1	B	317	GLU
1	B	322	ARG
1	B	348	SER
1	B	366	PHE
1	B	367	LEU
1	B	385	SER
1	B	412	MET
1	B	413	VAL
1	B	417	ASP
1	B	431	SER
1	B	489	VAL
1	B	503	MET
1	B	512	LYS
1	B	536	ASP
1	B	543	LYS
1	B	549	ARG
1	C	144	LEU

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Mol	Chain	Res	Type
1	C	146	ASP
1	C	152	ILE
1	C	161	VAL
1	C	163	LYS
1	C	165	ILE
1	C	176	SER
1	C	199	MET
1	C	203	ASP
1	C	209	VAL
1	C	212	ASN
1	C	217	THR
1	C	272	THR
1	C	274	ASP
1	C	293	VAL
1	C	303	ASN
1	C	307	THR
1	C	321	LEU
1	C	323	PHE
1	C	366	PHE
1	C	385	SER
1	C	408	GLU
1	C	412	MET
1	C	467	SER
1	C	468	CYS
1	C	505	CYS
1	C	513	MET
1	C	528	SER
1	D	151	THR
1	D	152	ILE
1	D	156	GLN
1	D	161	VAL
1	D	162	HIS
1	D	166	THR
1	D	190	THR
1	D	193	THR
1	D	201	ASP
1	D	202	LYS
1	D	203	ASP
1	D	204	LEU
1	D	210	GLN
1	D	217	THR
1	D	242	SER

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Mol	Chain	Res	Type
1	D	250	LYS
1	D	296	LEU
1	D	316	LYS
1	D	317	GLU
1	D	321	LEU
1	D	346	VAL
1	D	354	VAL
1	D	365	GLN
1	D	366	PHE
1	D	382	THR
1	D	392	ARG
1	D	400	LEU
1	D	412	MET
1	D	417	ASP
1	D	493	ILE
1	D	510	LEU
1	D	512	LYS
1	D	528	SER
1	D	536	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	ASN
1	A	352	GLN
1	A	380	ASN
1	A	460	ASN
1	B	162	HIS
1	B	335	HIS
1	B	534	ASN
1	D	340	ASN
1	D	476	GLN
1	D	480	HIS

5.3.3 RNA

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	-	34,38,38	2.63	12 (35%)	27,49,49	1.20	4 (14%)
2	04A	D	701	-	34,38,38	2.62	12 (35%)	27,49,49	1.20	3 (11%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	04A	CBG-NAT	2.21	1.36	1.33
2	B	701	04A	CBG-NAT	2.28	1.36	1.33
2	B	701	04A	CBF-NAS	2.32	1.36	1.33
2	D	701	04A	CBF-NAS	2.33	1.36	1.33
2	B	701	04A	CBC-NAX	3.40	1.43	1.35
2	D	701	04A	CBB-NAW	3.45	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	04A	CBC-NAX	3.47	1.44	1.35
2	B	701	04A	CBB-NAW	3.54	1.44	1.35
2	D	701	04A	CBH-NAW	3.91	1.43	1.36
2	D	701	04A	CBI-NAX	4.00	1.43	1.36
2	B	701	04A	CBI-NAX	4.01	1.43	1.36
2	B	701	04A	CBH-NAW	4.08	1.43	1.36
2	D	701	04A	CAD-CAG	4.45	1.49	1.38
2	B	701	04A	CAC-CAF	4.46	1.49	1.38
2	D	701	04A	CAC-CAF	4.48	1.49	1.38
2	B	701	04A	CAD-CAG	4.49	1.49	1.38
2	D	701	04A	CAK-CBE	5.04	1.49	1.38
2	B	701	04A	CAK-CBE	5.08	1.49	1.38
2	D	701	04A	CAJ-CBD	5.10	1.49	1.38
2	B	701	04A	CAJ-CBD	5.11	1.49	1.38
2	B	701	04A	CAH-CAL	5.17	1.49	1.38
2	B	701	04A	CAE-CAI	5.19	1.49	1.38
2	D	701	04A	CAH-CAL	5.20	1.49	1.38
2	D	701	04A	CAE-CAI	5.22	1.49	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	04A	OAA-CBB-NAW	-2.35	119.52	123.72
2	D	701	04A	CAP-CAN-SAY	-2.30	107.62	113.96
2	B	701	04A	CAP-CAN-SAY	-2.09	108.21	113.96
2	B	701	04A	CAO-CAM-SAY	-2.07	108.27	113.96
2	B	701	04A	OAA-CBB-NAW	-2.06	120.05	123.72
2	B	701	04A	CAQ-CBB-NAW	2.47	122.25	114.81
2	D	701	04A	CAQ-CBB-NAW	2.62	122.68	114.81

There are no chirality outliers.

There are no torsion outliers.

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	395/479 (82%)	0.30	28 (7%)	19	12	20, 35, 62, 79	3 (0%)
1	B	383/479 (79%)	0.17	10 (2%)	59	52	19, 34, 53, 75	5 (1%)
1	C	397/479 (82%)	0.32	27 (6%)	20	14	19, 34, 64, 87	1 (0%)
1	D	388/479 (81%)	0.29	15 (3%)	43	35	24, 34, 57, 74	4 (1%)
All	All	1563/1916 (81%)	0.27	80 (5%)	32	23	19, 34, 60, 87	13 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	PHE	6.5
1	A	256	PRO	5.7
1	D	324	ASN	4.5
1	C	323	PHE	4.4
1	A	149	PHE	4.2
1	C	147	LEU	4.1
1	C	209	VAL	4.0
1	D	149	PHE	4.0
1	C	205	PHE	4.0
1	A	257	GLN	4.0
1	A	259	ALA	3.8
1	A	161	VAL	3.7
1	C	162	HIS	3.6
1	C	150	TYR	3.5
1	C	324	ASN	3.4
1	A	255	ILE	3.3
1	B	187	LEU	3.3
1	D	199	MET	3.2
1	A	258	LEU	3.2
1	B	149	PHE	3.1
1	D	150	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	262	SER	3.1
1	B	150	TYR	3.0
1	D	323	PHE	3.0
1	D	159	ILE	3.0
1	C	151	THR	2.9
1	B	200	LEU	2.9
1	C	157	GLU	2.9
1	A	200	LEU	2.9
1	D	249	GLY	2.9
1	A	148	LEU	2.9
1	C	200	LEU	2.8
1	C	262	SER	2.8
1	C	256	PRO	2.8
1	C	255	ILE	2.7
1	B	147	LEU	2.7
1	A	198	VAL	2.7
1	A	150	TYR	2.7
1	A	159	ILE	2.7
1	C	330	GLU	2.7
1	A	253	ASP	2.6
1	C	253	ASP	2.6
1	C	254	TYR	2.6
1	A	151	THR	2.6
1	A	205	PHE	2.5
1	A	263	PRO	2.5
1	A	261	PHE	2.5
1	A	147	LEU	2.5
1	A	199	MET	2.5
1	D	248	GLY	2.4
1	A	254	TYR	2.4
1	D	151	THR	2.4
1	A	323	PHE	2.4
1	D	156	GLN	2.4
1	C	148	LEU	2.4
1	D	209	VAL	2.4
1	B	159	ILE	2.3
1	B	192	GLN	2.3
1	C	322	ARG	2.2
1	C	212	ASN	2.2
1	A	214	VAL	2.2
1	C	226	ILE	2.2
1	C	199	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	167	ALA	2.1
1	B	543	LYS	2.1
1	C	259	ALA	2.1
1	A	191	LEU	2.1
1	A	322	ARG	2.1
1	C	321	LEU	2.1
1	C	161	VAL	2.1
1	D	220	PHE	2.1
1	A	330	GLU	2.1
1	C	331	ASP	2.1
1	B	205	PHE	2.0
1	D	322	ARG	2.0
1	A	248	GLY	2.0
1	B	216	LEU	2.0
1	C	159	ILE	2.0
1	D	161	VAL	2.0
1	A	213	ILE	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	04A	D	701	35/35	0.92	0.24	-0.12	37,45,61,62	0
2	04A	B	701	35/35	0.88	0.23	-0.38	38,48,60,64	0

6.5 Other polymers (i)

There are no such residues in this entry.