



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:30 AM UTC

PDB ID : 6LB7 / pdb_00006lb7
Title : Crystal structure of the Ca²⁺-free and Ca²⁺-bound MICU1-MICU2 complex
Authors : Wu, W.; Shen, Q.; Zheng, J.; Jia, Z.
Deposited on : 2019-11-13
Resolution : 2.10 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

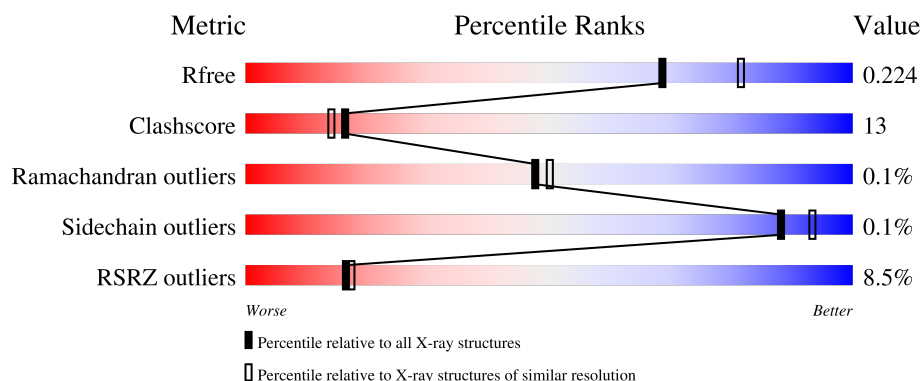
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	377	6% 68% 11% • 19%
1	C	377	6% 64% 14% • 21%
2	B	330	7% 69% 16% •• 12%
2	D	330	11% 74% 18% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10993 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 Calcium uptake protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2468	1576	411	469	12			
1	C	298	Total	C	N	O	S	0	0	0
			2400	1532	400	454	14			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	expression tag	UNP Q9BPX6
A	77	GLY	-	expression tag	UNP Q9BPX6
A	78	SER	-	expression tag	UNP Q9BPX6
A	79	SER	-	expression tag	UNP Q9BPX6
A	80	HIS	-	expression tag	UNP Q9BPX6
A	81	HIS	-	expression tag	UNP Q9BPX6
A	82	HIS	-	expression tag	UNP Q9BPX6
A	83	HIS	-	expression tag	UNP Q9BPX6
A	84	HIS	-	expression tag	UNP Q9BPX6
A	85	HIS	-	expression tag	UNP Q9BPX6
A	86	SER	-	expression tag	UNP Q9BPX6
A	87	SER	-	expression tag	UNP Q9BPX6
A	88	GLY	-	expression tag	UNP Q9BPX6
A	89	LEU	-	expression tag	UNP Q9BPX6
A	90	VAL	-	expression tag	UNP Q9BPX6
A	91	PRO	-	expression tag	UNP Q9BPX6
A	92	ARG	-	expression tag	UNP Q9BPX6
A	93	GLY	-	expression tag	UNP Q9BPX6
A	94	SER	-	expression tag	UNP Q9BPX6
A	95	HIS	-	expression tag	UNP Q9BPX6
A	96	MET	-	expression tag	UNP Q9BPX6
A	445	GLY	-	expression tag	UNP Q9BPX6
A	446	SER	-	expression tag	UNP Q9BPX6
A	447	GLY	-	expression tag	UNP Q9BPX6
A	448	SER	-	expression tag	UNP Q9BPX6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	GLY	-	expression tag	UNP Q9BPX6
A	450	SER	-	expression tag	UNP Q9BPX6
A	451	GLY	-	expression tag	UNP Q9BPX6
A	452	SER	-	expression tag	UNP Q9BPX6
C	76	MET	-	expression tag	UNP Q9BPX6
C	77	GLY	-	expression tag	UNP Q9BPX6
C	78	SER	-	expression tag	UNP Q9BPX6
C	79	SER	-	expression tag	UNP Q9BPX6
C	80	HIS	-	expression tag	UNP Q9BPX6
C	81	HIS	-	expression tag	UNP Q9BPX6
C	82	HIS	-	expression tag	UNP Q9BPX6
C	83	HIS	-	expression tag	UNP Q9BPX6
C	84	HIS	-	expression tag	UNP Q9BPX6
C	85	HIS	-	expression tag	UNP Q9BPX6
C	86	SER	-	expression tag	UNP Q9BPX6
C	87	SER	-	expression tag	UNP Q9BPX6
C	88	GLY	-	expression tag	UNP Q9BPX6
C	89	LEU	-	expression tag	UNP Q9BPX6
C	90	VAL	-	expression tag	UNP Q9BPX6
C	91	PRO	-	expression tag	UNP Q9BPX6
C	92	ARG	-	expression tag	UNP Q9BPX6
C	93	GLY	-	expression tag	UNP Q9BPX6
C	94	SER	-	expression tag	UNP Q9BPX6
C	95	HIS	-	expression tag	UNP Q9BPX6
C	96	MET	-	expression tag	UNP Q9BPX6
C	445	GLY	-	expression tag	UNP Q9BPX6
C	446	SER	-	expression tag	UNP Q9BPX6
C	447	GLY	-	expression tag	UNP Q9BPX6
C	448	SER	-	expression tag	UNP Q9BPX6
C	449	GLY	-	expression tag	UNP Q9BPX6
C	450	SER	-	expression tag	UNP Q9BPX6
C	451	GLY	-	expression tag	UNP Q9BPX6
C	452	SER	-	expression tag	UNP Q9BPX6

- Molecule 2 is a protein called Calcium uptake protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	290	Total	C	N	O	S	0	0	0
			2423	1558	411	438	16			
2	D	313	Total	C	N	O	S	0	0	0
			2602	1669	440	477	16			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	77	GLY	-	expression tag	UNP Q8IYU8
B	78	SER	-	expression tag	UNP Q8IYU8
B	79	GLY	-	expression tag	UNP Q8IYU8
B	80	SER	-	expression tag	UNP Q8IYU8
B	81	GLY	-	expression tag	UNP Q8IYU8
B	82	SER	-	expression tag	UNP Q8IYU8
B	83	GLY	-	expression tag	UNP Q8IYU8
D	77	GLY	-	expression tag	UNP Q8IYU8
D	78	SER	-	expression tag	UNP Q8IYU8
D	79	GLY	-	expression tag	UNP Q8IYU8
D	80	SER	-	expression tag	UNP Q8IYU8
D	81	GLY	-	expression tag	UNP Q8IYU8
D	82	SER	-	expression tag	UNP Q8IYU8
D	83	GLY	-	expression tag	UNP Q8IYU8

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

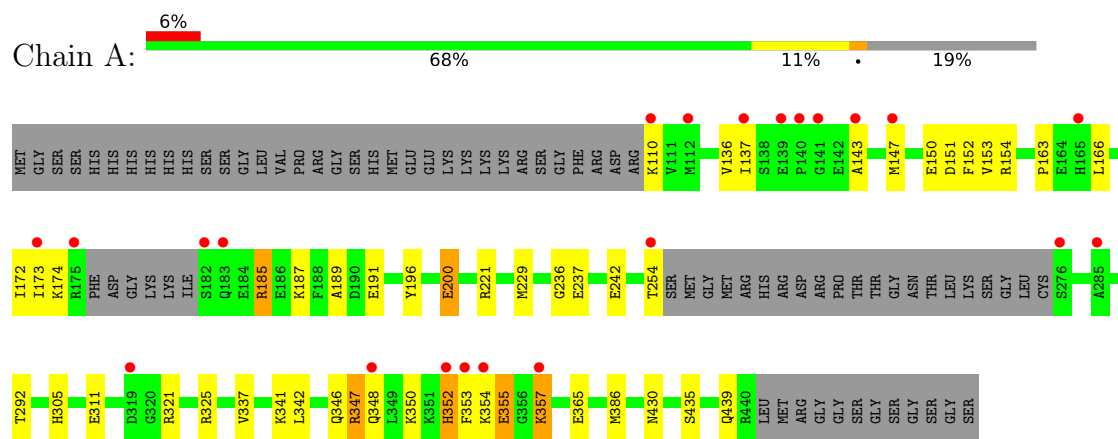
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	278	Total O 278 278	0	0
4	B	305	Total O 305 305	0	0
4	C	240	Total O 240 240	0	0
4	D	275	Total O 275 275	0	0

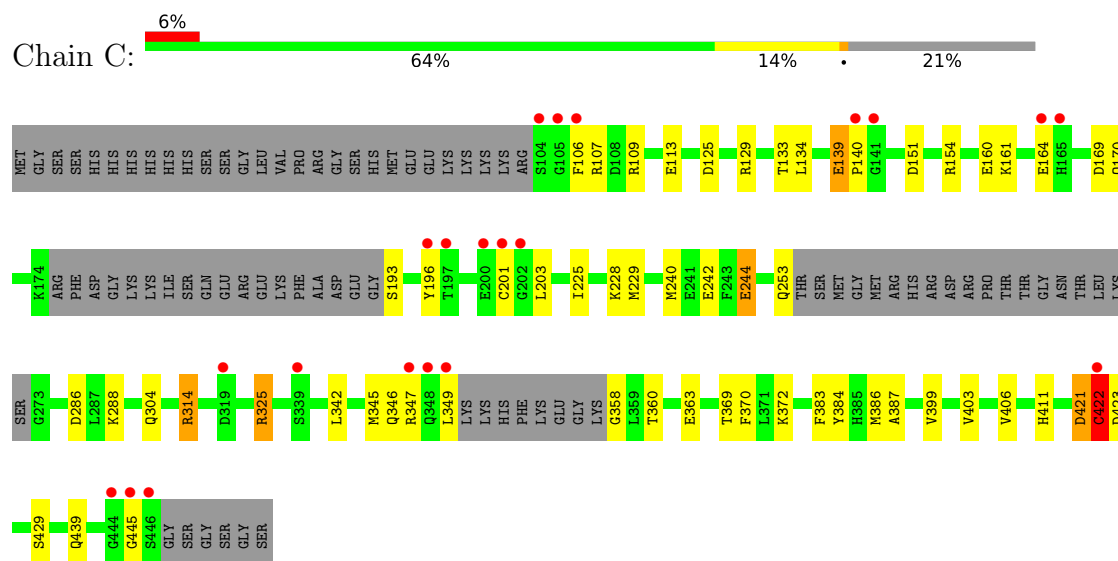
3 Residue-property plots [i](#)

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.

- Molecule 1: Calcium uptake protein 1, mitochondrial

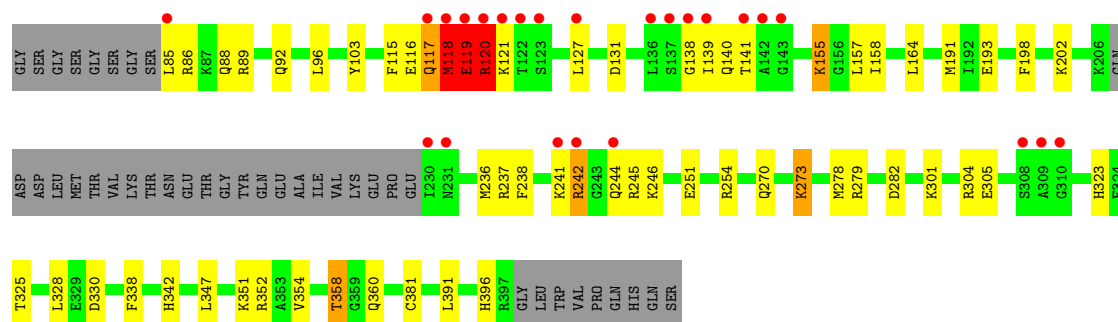


- Molecule 1: Calcium uptake protein 1, mitochondrial

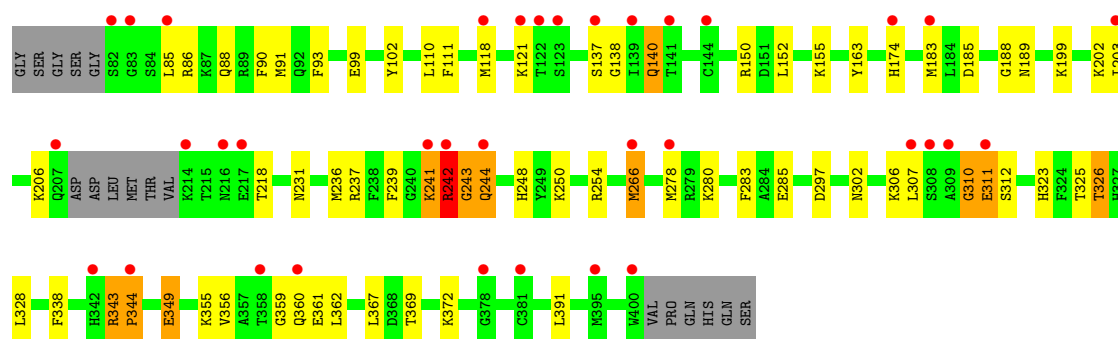
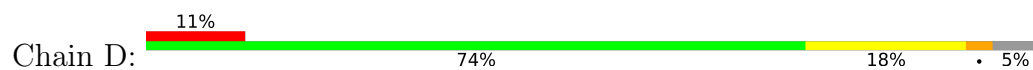


- Molecule 2: Calcium uptake protein 2, mitochondrial





● Molecule 2: Calcium uptake protein 2, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.48Å 107.72Å 170.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 2.10 47.30 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.30-2.10) 98.5 (47.30-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.194 , 0.227 (Not available) , 0.224	Depositor DCC
R_{free} test set	2000 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10993	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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:
CA

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	0.83	17/2514 (0.7%)	0.70	5/3374 (0.1%)
1	C	0.72	11/2443 (0.5%)	0.76	4/3280 (0.1%)
2	B	1.26	26/2474 (1.1%)	0.90	10/3303 (0.3%)
2	D	1.92	22/2657 (0.8%)	0.99	11/3551 (0.3%)
All	All	1.29	76/10088 (0.8%)	0.85	30/13508 (0.2%)

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
1	C	0	4
2	B	0	3
2	D	0	1
All	All	0	9

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	344	PRO	N-CD	84.88	2.66	1.47
2	B	242	ARG	NE-CZ	-23.13	1.07	1.33
2	B	242	ARG	CD-NE	-18.71	1.20	1.46
2	B	242	ARG	CZ-NH2	-17.94	1.10	1.33
2	B	242	ARG	CZ-NH1	-16.38	1.09	1.32
2	D	242	ARG	NE-CZ	-13.82	1.17	1.33
2	D	242	ARG	CZ-NH2	-12.19	1.17	1.33
2	D	237	ARG	NE-CZ	-12.14	1.19	1.33
2	D	244	GLN	CD-OE1	-12.00	1.00	1.23
2	B	237	ARG	NE-CZ	-11.90	1.20	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	GLU	CD-OE1	-10.79	1.04	1.25
2	B	140	GLN	CD-OE1	-10.79	1.03	1.23
2	B	352	ARG	NE-CZ	-10.59	1.21	1.33
2	B	237	ARG	CZ-NH2	-10.08	1.20	1.33
2	B	352	ARG	CZ-NH2	-9.93	1.20	1.33
2	B	237	ARG	CD-NE	-9.92	1.32	1.46
2	B	254	ARG	NE-CZ	-9.85	1.22	1.33
2	B	352	ARG	CD-NE	-9.79	1.32	1.46
1	C	109	ARG	NE-CZ	-9.77	1.22	1.33
2	D	242	ARG	CD-NE	-9.74	1.32	1.46
2	D	244	GLN	CD-NE2	-9.61	1.13	1.33
2	D	266	MET	SD-CE	-9.53	1.55	1.79
2	B	140	GLN	CD-NE2	-9.37	1.13	1.33
1	C	347	ARG	NE-CZ	-9.00	1.23	1.33
1	A	355	GLU	CD-OE1	-8.94	1.08	1.25
2	D	237	ARG	CD-NE	-8.94	1.33	1.46
2	B	155	LYS	CD-CE	-8.92	1.25	1.52
2	D	311	GLU	CD-OE1	-8.83	1.08	1.25
1	A	150	GLU	CD-OE2	-8.75	1.08	1.25
2	D	237	ARG	CZ-NH1	-8.63	1.20	1.32
1	A	355	GLU	CD-OE2	-8.45	1.09	1.25
1	A	185	ARG	NE-CZ	-8.31	1.24	1.33
2	D	237	ARG	CZ-NH2	-8.27	1.22	1.33
1	A	347	ARG	NE-CZ	-8.27	1.24	1.33
2	D	361	GLU	CD-OE1	-8.22	1.09	1.25
2	B	237	ARG	CZ-NH1	-8.20	1.21	1.32
1	A	439	GLN	CD-OE1	-8.01	1.08	1.23
2	B	254	ARG	CZ-NH2	-7.87	1.23	1.33
2	B	254	ARG	CD-NE	-7.63	1.35	1.46
2	B	254	ARG	CZ-NH1	-7.61	1.22	1.32
2	D	242	ARG	CZ-NH1	-7.61	1.22	1.32
1	A	185	ARG	CZ-NH2	-7.61	1.23	1.33
1	C	244	GLU	CD-OE1	-7.38	1.11	1.25
2	D	311	GLU	CD-OE2	-7.35	1.11	1.25
1	C	109	ARG	CZ-NH1	-7.31	1.22	1.32
1	A	439	GLN	CD-NE2	-7.14	1.18	1.33
1	A	185	ARG	CD-NE	-6.87	1.36	1.46
2	B	352	ARG	CZ-NH1	-6.86	1.23	1.32
2	B	273	LYS	CD-CE	-6.80	1.32	1.52
2	B	155	LYS	CE-NZ	-6.74	1.29	1.49
1	C	347	ARG	CZ-NH1	-6.62	1.23	1.32
1	C	109	ARG	CZ-NH2	-6.60	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	ARG	CD-NE	-6.48	1.37	1.46
1	A	352	HIS	CG-ND1	-6.46	1.31	1.38
1	A	352	HIS	CE1-NE2	-6.24	1.26	1.32
2	D	140	GLN	CD-OE1	-6.22	1.11	1.23
2	D	121	LYS	CD-CE	-6.13	1.34	1.52
1	A	347	ARG	CD-NE	-6.11	1.37	1.46
1	A	347	ARG	CZ-NH1	-6.09	1.24	1.32
1	A	347	ARG	CZ-NH2	-6.08	1.25	1.33
2	D	361	GLU	CD-OE2	-6.05	1.13	1.25
2	D	241	LYS	CD-CE	-5.99	1.34	1.52
2	D	244	GLN	CG-CD	-5.88	1.37	1.52
1	A	350	LYS	CD-CE	-5.83	1.34	1.52
1	A	352	HIS	CD2-NE2	-5.68	1.31	1.37
2	B	251	GLU	CD-OE1	-5.59	1.14	1.25
1	C	244	GLU	CD-OE2	-5.56	1.14	1.25
2	B	119	GLU	CD-OE2	-5.50	1.14	1.25
2	B	396	HIS	CE1-NE2	-5.43	1.27	1.32
2	D	140	GLN	CD-NE2	-5.42	1.21	1.33
2	B	270	GLN	CD-OE1	-5.39	1.13	1.23
1	C	242	GLU	CD-OE1	-5.31	1.15	1.25
2	D	349	GLU	CD-OE1	-5.18	1.15	1.25
2	B	119	GLU	CD-OE1	-5.14	1.15	1.25
1	C	242	GLU	CD-OE2	-5.03	1.15	1.25
1	C	347	ARG	CZ-NH2	-5.01	1.26	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	344	PRO	N-CD-CG	-29.33	59.20	103.20
2	D	344	PRO	CA-N-CD	-26.52	74.87	112.00
1	C	422	CYS	O-C-N	-20.20	95.72	122.59
2	B	358	THR	N-CA-C	18.88	138.13	113.97
1	C	421	ASP	CA-C-N	-11.78	99.03	121.54
1	C	421	ASP	C-N-CA	-11.78	99.03	121.54
2	B	117	GLN	CA-C-N	10.00	140.64	121.54
2	B	117	GLN	C-N-CA	10.00	140.64	121.54
2	B	121	LYS	N-CA-C	-9.84	94.33	110.17
2	B	140	GLN	OE1-CD-NE2	-7.73	114.87	122.60
2	B	120	ARG	N-CA-C	-7.11	95.67	110.80
1	A	236	GLY	CA-C-N	6.91	132.45	122.44
1	A	236	GLY	C-N-CA	6.91	132.45	122.44
2	D	343	ARG	CA-C-N	6.79	128.33	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	343	ARG	C-N-CA	6.79	128.33	119.84
2	D	310	GLY	CA-C-N	6.42	129.94	120.95
2	D	310	GLY	C-N-CA	6.42	129.94	120.95
2	D	243	GLY	CA-C-N	-6.08	113.07	122.49
2	D	243	GLY	C-N-CA	-6.08	113.07	122.49
1	C	139	GLU	O-C-N	6.04	126.06	121.65
2	D	244	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	200	GLU	CB-CG-CD	5.76	122.39	112.60
2	D	344	PRO	O-C-N	-5.71	114.93	122.64
1	A	439	GLN	OE1-CD-NE2	-5.57	117.03	122.60
2	B	118	MET	CA-C-N	-5.36	115.74	125.66
2	B	118	MET	C-N-CA	-5.36	115.74	125.66
2	D	311	GLU	O-C-N	-5.33	116.38	122.93
2	B	119	GLU	CA-C-N	5.24	131.54	121.54
2	B	119	GLU	C-N-CA	5.24	131.54	121.54
1	A	357	LYS	CD-CE-NZ	-5.01	95.86	111.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ARG	Sidechain
2	B	118	MET	Mainchain
2	B	119	GLU	Mainchain
2	B	120	ARG	Sidechain
1	C	107	ARG	Sidechain
1	C	314	ARG	Sidechain
1	C	325	ARG	Sidechain
1	C	422	CYS	Mainchain
2	D	242	ARG	Sidechain

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	2468	0	2430	40	0
1	C	2400	0	2364	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2423	0	2405	83	0
2	D	2602	0	2572	89	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	278	0	0	6	0
4	B	305	0	0	11	1
4	C	240	0	0	17	0
4	D	275	0	0	12	1
All	All	10993	0	9771	256	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 13.

All (256) 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:C:325:ARG:HD3	1:C:346:GLN:NE2	1.30	1.45
1:C:325:ARG:CD	1:C:346:GLN:NE2	1.80	1.44
1:C:421:ASP:O	1:C:422:CYS:CB	1.69	1.30
1:C:325:ARG:NE	1:C:346:GLN:HE22	1.29	1.27
1:C:325:ARG:CD	1:C:346:GLN:HE21	1.42	1.24
2:B:236:MET:HE1	2:B:241:LYS:CD	1.70	1.21
2:D:236:MET:CE	2:D:241:LYS:HE2	1.69	1.21
2:B:85:LEU:CD2	2:B:88:GLN:OE1	1.89	1.21
1:A:353:PHE:HA	1:A:355:GLU:OE2	1.37	1.20
2:B:85:LEU:HD22	2:B:88:GLN:OE1	1.46	1.12
1:C:325:ARG:NE	1:C:346:GLN:NE2	1.91	1.11
2:D:110:LEU:HD13	2:D:266:MET:HE1	1.14	1.10
1:A:147:MET:HE2	1:A:152:PHE:HA	1.25	1.09
1:C:421:ASP:O	1:C:422:CYS:HB3	1.28	1.08
2:B:118:MET:HB2	2:B:120:ARG:O	1.53	1.07
2:B:241:LYS:HE2	2:B:241:LYS:H	1.11	1.06
1:A:353:PHE:CA	1:A:355:GLU:OE2	2.04	1.04
2:D:236:MET:HE1	2:D:241:LYS:CE	1.86	1.04
2:B:103:TYR:CD2	2:B:157:LEU:HD21	1.93	1.04
2:B:236:MET:HE1	2:B:241:LYS:HD2	1.39	1.02
2:B:236:MET:HE1	2:B:241:LYS:HD3	1.38	1.02
1:A:147:MET:CE	1:A:152:PHE:HA	1.92	0.99
1:C:421:ASP:O	1:C:422:CYS:HB2	1.64	0.96
2:D:236:MET:HE1	2:D:241:LYS:HE2	0.98	0.96
2:B:342:HIS:O	4:B:601:HOH:O	1.83	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:231:ASN:HD21	2:D:236:MET:HE3	1.31	0.95
1:A:147:MET:HE2	1:A:152:PHE:CA	1.95	0.95
1:A:355:GLU:CD	1:A:355:GLU:H	1.77	0.93
2:B:236:MET:CE	2:B:241:LYS:HD3	1.98	0.93
2:D:110:LEU:CD1	2:D:266:MET:HE1	1.99	0.92
2:D:206:LYS:HD3	2:D:206:LYS:O	1.68	0.92
2:D:236:MET:HE1	2:D:241:LYS:HA	1.52	0.90
2:B:85:LEU:HD23	2:B:88:GLN:OE1	1.70	0.90
2:D:344:PRO:O	2:D:344:PRO:CD	2.19	0.90
2:B:85:LEU:O	2:B:88:GLN:NE2	2.04	0.90
2:D:188:GLY:O	4:D:501:HOH:O	1.88	0.89
2:B:241:LYS:HE2	2:B:241:LYS:N	1.85	0.89
1:C:325:ARG:HE	1:C:346:GLN:HE22	1.19	0.88
1:C:386:MET:HE1	2:D:206:LYS:HE3	1.55	0.88
2:B:155:LYS:O	2:B:155:LYS:HG3	1.72	0.87
1:C:325:ARG:HD3	1:C:346:GLN:HE21	0.74	0.87
1:A:353:PHE:C	1:A:355:GLU:OE2	2.20	0.84
1:A:321:ARG:NH1	4:A:602:HOH:O	2.10	0.84
2:B:241:LYS:H	2:B:241:LYS:CE	1.90	0.83
2:D:344:PRO:O	2:D:344:PRO:HD2	1.79	0.82
2:B:85:LEU:C	2:B:88:GLN:HE22	1.87	0.82
2:B:92:GLN:HE21	2:B:118:MET:HE2	1.44	0.82
1:C:201:CYS:SG	4:C:657:HOH:O	2.37	0.81
1:A:354:LYS:HG2	1:A:355:GLU:OE1	1.81	0.81
2:D:99:GLU:OE2	4:D:502:HOH:O	2.01	0.78
2:D:343:ARG:NH2	2:D:349:GLU:OE2	2.16	0.77
2:B:198:PHE:HD2	2:B:202:LYS:HE3	1.48	0.77
2:B:236:MET:CE	2:B:241:LYS:CD	2.56	0.76
2:B:191:MET:CE	2:B:246:LYS:HD2	2.15	0.75
2:D:202:LYS:NZ	4:D:506:HOH:O	2.20	0.75
2:D:343:ARG:O	4:D:503:HOH:O	2.03	0.75
2:B:198:PHE:CD2	2:B:202:LYS:HE3	2.22	0.73
1:A:348:GLN:HG2	1:A:352:HIS:NE2	2.03	0.73
2:D:110:LEU:HD22	2:D:266:MET:CE	2.18	0.73
1:C:170:GLN:NE2	4:C:511:HOH:O	2.21	0.73
1:A:200:GLU:CD	1:A:200:GLU:H	1.96	0.72
2:D:199:LYS:O	2:D:203:ILE:HG12	1.88	0.72
2:D:236:MET:SD	2:D:241:LYS:CE	2.78	0.71
2:D:206:LYS:NZ	4:D:508:HOH:O	2.23	0.71
2:D:236:MET:SD	2:D:241:LYS:HE2	2.30	0.71
2:D:150:ARG:HD3	2:D:266:MET:SD	2.31	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:THR:O	4:A:601:HOH:O	2.08	0.70
2:D:236:MET:CE	2:D:241:LYS:CE	2.59	0.70
1:C:349:LEU:O	4:C:502:HOH:O	2.09	0.70
1:C:113:GLU:OE1	4:C:503:HOH:O	2.10	0.69
1:A:237:GLU:HG3	1:A:292:THR:HG22	1.75	0.69
2:D:236:MET:CE	2:D:241:LYS:HA	2.22	0.68
1:C:360:THR:HG23	1:C:363:GLU:H	1.58	0.68
1:A:242:GLU:OE2	4:A:603:HOH:O	2.11	0.68
2:D:278:MET:HE3	2:D:283:PHE:HB2	1.74	0.68
2:B:358:THR:HG22	2:B:360:GLN:H	1.58	0.67
2:B:198:PHE:HE2	2:B:202:LYS:HE2	1.59	0.67
1:C:125:ASP:OD1	4:C:505:HOH:O	2.13	0.67
2:D:152:LEU:O	2:D:155:LYS:HG2	1.94	0.67
2:D:174:HIS:CE1	2:D:326:THR:HG23	2.29	0.67
2:B:103:TYR:CG	2:B:157:LEU:HD21	2.30	0.67
1:C:288:LYS:O	4:C:504:HOH:O	2.12	0.67
2:D:138:GLY:O	2:D:155:LYS:NZ	2.27	0.66
2:B:323:HIS:NE2	4:B:605:HOH:O	2.22	0.66
1:C:304:GLN:OE1	4:C:507:HOH:O	2.15	0.65
2:B:118:MET:HG3	2:B:119:GLU:H	1.60	0.65
1:A:348:GLN:CG	1:A:352:HIS:NE2	2.60	0.65
2:D:110:LEU:HD22	2:D:266:MET:HE1	1.79	0.65
1:C:422:CYS:O	1:C:423:ASP:C	2.38	0.64
2:B:191:MET:HE2	2:B:246:LYS:HD2	1.80	0.63
2:B:118:MET:CG	2:B:119:GLU:H	2.12	0.63
2:D:236:MET:SD	2:D:241:LYS:HE3	2.39	0.63
2:B:118:MET:HG3	2:B:119:GLU:N	2.14	0.63
2:D:110:LEU:HD22	2:D:266:MET:HE2	1.81	0.62
2:B:92:GLN:HE21	2:B:118:MET:CE	2.13	0.62
2:D:110:LEU:HD13	2:D:266:MET:CE	2.08	0.62
1:A:221:ARG:HD3	2:B:330:ASP:OD1	1.98	0.62
1:C:386:MET:SD	2:D:206:LYS:HG3	2.40	0.62
2:B:354:VAL:O	2:B:358:THR:HB	2.00	0.62
2:B:241:LYS:N	2:B:241:LYS:CE	2.56	0.62
2:B:103:TYR:CD2	2:B:157:LEU:CD2	2.79	0.61
2:B:198:PHE:CE2	2:B:202:LYS:HE2	2.36	0.61
1:C:325:ARG:HH22	1:C:342:LEU:HB3	1.64	0.61
2:B:89:ARG:NH2	2:B:115:PHE:O	2.33	0.60
1:A:430:ASN:OD1	1:A:435:SER:OG	2.17	0.60
2:D:285:GLU:OE2	4:D:505:HOH:O	2.16	0.60
1:A:137:ILE:HG12	1:A:143:ALA:HB2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:GLU:H	1:C:164:GLU:CD	2.10	0.59
1:C:358:GLY:N	4:C:516:HOH:O	2.35	0.59
2:B:138:GLY:HA3	2:B:155:LYS:HZ3	1.68	0.59
1:C:429:SER:OG	4:C:506:HOH:O	2.13	0.59
1:A:337:VAL:HG11	1:A:342:LEU:HD12	1.84	0.59
2:B:85:LEU:HB3	2:B:88:GLN:OE1	2.02	0.59
2:B:238:PHE:O	2:B:245:ARG:NH1	2.35	0.58
2:D:241:LYS:HE2	2:D:241:LYS:HA	1.86	0.58
2:B:118:MET:CG	2:B:119:GLU:N	2.67	0.58
2:B:273:LYS:NZ	4:B:612:HOH:O	2.36	0.58
2:B:116:GLU:OE2	4:B:603:HOH:O	2.17	0.58
2:B:236:MET:SD	2:B:241:LYS:HG3	2.43	0.58
2:D:231:ASN:ND2	2:D:236:MET:HE3	2.13	0.57
2:B:88:GLN:H	2:B:88:GLN:CD	2.12	0.57
1:C:193:SER:N	4:C:518:HOH:O	2.37	0.57
2:B:85:LEU:HD23	2:B:88:GLN:H	1.68	0.57
2:D:111:PHE:CD2	2:D:118:MET:HE2	2.39	0.57
1:C:383:PHE:HB3	2:D:183:MET:SD	2.44	0.57
2:D:91:MET:HE2	2:D:91:MET:HA	1.85	0.57
2:D:174:HIS:NE2	2:D:326:THR:HG23	2.19	0.57
2:D:93:PHE:HE1	2:D:118:MET:HG2	1.69	0.57
2:D:206:LYS:O	2:D:206:LYS:CD	2.49	0.56
1:C:399:VAL:O	1:C:403:VAL:HG22	2.04	0.56
2:B:347:LEU:C	2:B:347:LEU:HD13	2.31	0.56
1:A:348:GLN:HG2	1:A:352:HIS:CD2	2.40	0.56
4:C:525:HOH:O	2:D:202:LYS:HE3	2.04	0.56
2:D:218:THR:HA	4:D:726:HOH:O	2.06	0.55
2:B:325:THR:O	2:B:328:LEU:HG	2.05	0.55
2:D:355:LYS:NZ	2:D:359:GLY:O	2.33	0.55
1:A:229:MET:HE1	2:B:338:PHE:CE2	2.41	0.55
1:A:137:ILE:HD12	1:A:173:ILE:HD11	1.88	0.54
2:B:279:ARG:NH1	4:B:617:HOH:O	2.39	0.54
1:C:151:ASP:OD1	1:C:154:ARG:NH2	2.40	0.54
2:D:355:LYS:HE3	2:D:359:GLY:C	2.33	0.54
1:A:354:LYS:CG	1:A:355:GLU:OE1	2.53	0.54
2:B:198:PHE:CD2	2:B:202:LYS:CE	2.91	0.54
2:D:140:GLN:H	2:D:140:GLN:CD	2.17	0.53
2:B:138:GLY:HA3	2:B:155:LYS:NZ	2.23	0.53
1:C:225:ILE:O	1:C:229:MET:HG2	2.08	0.53
2:D:254:ARG:NH2	4:D:504:HOH:O	2.12	0.53
2:D:307:LEU:HD21	2:D:369:THR:HA	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:HIS:HB3	4:C:514:HOH:O	2.09	0.53
2:B:301:LYS:HZ2	2:B:305:GLU:CD	2.17	0.53
2:D:203:ILE:O	2:D:206:LYS:HD2	2.09	0.52
2:B:198:PHE:CE2	2:B:202:LYS:CE	2.92	0.52
2:B:157:LEU:HD23	2:B:158:ILE:N	2.23	0.52
2:D:90:PHE:CD2	2:D:91:MET:HE3	2.44	0.52
2:D:280:LYS:HZ2	2:D:310:GLY:H	1.58	0.51
2:D:311:GLU:OE1	2:D:312:SER:O	2.27	0.51
2:D:231:ASN:HD21	2:D:236:MET:CE	2.13	0.51
2:B:117:GLN:HG3	1:C:106:PHE:CD1	2.45	0.51
2:B:85:LEU:HD23	2:B:88:GLN:CD	2.35	0.51
1:C:161:LYS:NZ	4:C:515:HOH:O	2.33	0.51
1:C:325:ARG:NH2	1:C:342:LEU:HB3	2.26	0.50
2:D:338:PHE:CE2	2:D:349:GLU:HB3	2.47	0.50
2:D:344:PRO:CD	2:D:344:PRO:C	2.76	0.50
1:C:325:ARG:CD	1:C:346:GLN:HE22	1.73	0.49
2:D:110:LEU:CG	2:D:266:MET:HE1	2.40	0.49
2:D:110:LEU:CD2	2:D:266:MET:HE1	2.42	0.49
1:C:129:ARG:HD2	1:C:169:ASP:OD1	2.12	0.49
2:D:86:ARG:HD3	4:D:713:HOH:O	2.12	0.49
2:D:155:LYS:HE2	4:D:632:HOH:O	2.12	0.49
2:D:355:LYS:HA	2:D:360:GLN:O	2.12	0.49
1:C:133:THR:O	1:C:134:LEU:HD23	2.13	0.49
2:D:302:ASN:OD1	2:D:306:LYS:HE3	2.13	0.48
2:B:193:GLU:HG3	4:B:638:HOH:O	2.13	0.48
2:D:91:MET:HE1	2:D:102:TYR:HB2	1.95	0.48
2:B:358:THR:HG22	2:B:360:GLN:N	2.28	0.48
1:C:325:ARG:HA	1:C:345:MET:HE1	1.94	0.48
2:D:239:PHE:O	2:D:243:GLY:HA2	2.14	0.48
1:A:191:GLU:OE2	4:A:606:HOH:O	2.20	0.48
2:B:323:HIS:CD2	4:B:605:HOH:O	2.64	0.48
2:D:90:PHE:HD2	2:D:91:MET:HE3	1.79	0.47
2:D:254:ARG:NH1	4:D:521:HOH:O	2.43	0.47
2:B:347:LEU:HD11	2:B:351:LYS:HE3	1.96	0.47
1:C:201:CYS:HB2	1:C:203:LEU:HG	1.97	0.47
2:D:278:MET:HE1	2:D:283:PHE:HD1	1.80	0.47
1:C:286:ASP:OD2	4:C:509:HOH:O	2.20	0.47
1:C:384:TYR:HA	2:D:183:MET:HE1	1.96	0.47
2:B:241:LYS:HE2	2:B:244:GLN:HE22	1.80	0.47
1:C:228:LYS:HB3	2:D:356:VAL:HG22	1.97	0.47
1:C:240:MET:O	1:C:244:GLU:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:LYS:CD	2:B:241:LYS:N	2.78	0.46
2:D:323:HIS:O	2:D:326:THR:HB	2.15	0.46
1:A:187:LYS:O	4:A:607:HOH:O	2.20	0.46
2:D:93:PHE:CE1	2:D:118:MET:HG2	2.49	0.46
2:D:152:LEU:HA	2:D:155:LYS:HE3	1.97	0.46
2:D:344:PRO:CD	2:D:344:PRO:N	2.66	0.46
2:B:242:ARG:HH11	2:B:242:ARG:HD3	1.31	0.46
2:B:127:LEU:HD22	2:B:131:ASP:HB3	1.97	0.46
2:B:86:ARG:CA	2:B:88:GLN:HE22	2.29	0.46
2:D:248:HIS:HE1	2:D:250:LYS:HG3	1.81	0.46
2:D:248:HIS:CE1	2:D:250:LYS:HG3	2.50	0.46
2:B:328:LEU:HD21	2:B:391:LEU:HD13	1.97	0.46
1:C:423:ASP:N	4:C:501:HOH:O	2.03	0.45
1:A:153:VAL:HG13	1:A:311:GLU:HG2	1.98	0.45
2:D:90:PHE:HB2	2:D:163:TYR:CE2	2.51	0.45
2:D:362:LEU:HB2	2:D:367:LEU:HD21	1.98	0.45
2:B:157:LEU:HD23	2:B:157:LEU:C	2.41	0.45
2:D:297:ASP:OD1	4:D:507:HOH:O	2.21	0.45
2:B:155:LYS:O	2:B:155:LYS:CG	2.53	0.45
2:D:242:ARG:HB3	2:D:244:GLN:HE21	1.82	0.44
2:B:118:MET:O	2:B:119:GLU:HB2	2.16	0.44
2:D:325:THR:HG22	2:D:391:LEU:HD11	2.00	0.44
1:A:166:LEU:HD21	1:A:172:ILE:HG13	1.99	0.44
1:A:325:ARG:O	1:A:346:GLN:NE2	2.45	0.44
2:B:138:GLY:O	2:B:141:THR:HG22	2.18	0.44
1:A:200:GLU:CD	1:A:200:GLU:N	2.73	0.44
1:C:387:ALA:HB1	2:D:199:LYS:HD3	1.98	0.44
2:B:139:ILE:HB	4:B:609:HOH:O	2.17	0.43
2:B:351:LYS:HE2	4:B:787:HOH:O	2.17	0.43
1:A:163:PRO:HB2	1:A:166:LEU:HD12	2.00	0.43
1:C:253:GLN:O	4:C:510:HOH:O	2.20	0.43
1:A:305:HIS:HD2	1:A:365:GLU:OE1	2.00	0.43
1:C:439:GLN:HG2	1:C:445:GLY:HA2	1.99	0.43
1:A:151:ASP:OD2	1:A:154:ARG:NH2	2.50	0.43
2:B:381:CYS:HB2	4:B:831:HOH:O	2.18	0.43
1:C:139:GLU:HB2	1:C:140:PRO:HD2	2.00	0.43
2:B:96:LEU:HD13	2:B:127:LEU:HD11	2.00	0.43
1:C:369:THR:O	1:C:372:LYS:HG2	2.19	0.43
1:A:341:LYS:HB3	1:A:341:LYS:HE2	1.54	0.43
2:B:127:LEU:HD22	2:B:131:ASP:CB	2.49	0.43
2:D:85:LEU:HB2	2:D:88:GLN:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:LEU:HB3	2:D:266:MET:CE	2.50	0.42
1:C:370:PHE:HB2	1:C:406:VAL:HG21	2.02	0.42
1:A:110:LYS:N	4:A:636:HOH:O	2.52	0.42
2:B:358:THR:O	2:B:358:THR:CG2	2.67	0.42
1:A:136:VAL:HA	1:A:174:LYS:O	2.19	0.41
2:B:118:MET:CB	2:B:120:ARG:O	2.43	0.41
2:D:174:HIS:CE1	2:D:326:THR:CG2	3.02	0.41
1:A:386:MET:HE3	2:B:164:LEU:HD22	2.02	0.41
2:D:137:SER:O	2:D:140:GLN:NE2	2.25	0.41
1:A:357:LYS:HE3	1:A:357:LYS:HB2	1.71	0.41
2:B:278:MET:HG2	2:B:282:ASP:HB2	2.03	0.41
1:A:353:PHE:C	1:A:355:GLU:N	2.77	0.41
1:A:347:ARG:HH11	1:A:347:ARG:HD2	1.64	0.41
1:C:240:MET:HE1	4:C:714:HOH:O	2.21	0.41
2:D:236:MET:HE2	2:D:236:MET:HA	2.02	0.41
1:C:160:GLU:HB3	1:C:314:ARG:HE	1.85	0.41
1:A:189:ALA:HB3	1:A:196:TYR:CE1	2.56	0.41
2:B:191:MET:HE3	2:B:246:LYS:HB2	2.02	0.41
2:B:304:ARG:HD3	4:B:637:HOH:O	2.21	0.40
1:C:372:LYS:HB3	1:C:372:LYS:HE3	1.81	0.40
2:D:185:ASP:HB2	2:D:189:ASN:OD1	2.21	0.40
2:B:193:GLU:CD	2:B:246:LYS:HD3	2.46	0.40
2:D:328:LEU:HD23	2:D:328:LEU:HA	1.83	0.40
1:C:193:SER:HB3	1:C:196:TYR:CD2	2.56	0.40
2:D:306:LYS:HB3	2:D:372:LYS:HD2	2.02	0.40
2:B:86:ARG:HA	2:B:88:GLN:HE22	1.87	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	Interatomic distance (Å)	Clash overlap (Å)
4:B:754:HOH:O	4:D:759:HOH:O[2_594]	1.95	0.25

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	298/377 (79%)	294 (99%)	4 (1%)	0	100	100
1	C	290/377 (77%)	284 (98%)	5 (2%)	1 (0%)	36	36
2	B	286/330 (87%)	278 (97%)	8 (3%)	0	100	100
2	D	309/330 (94%)	299 (97%)	10 (3%)	0	100	100
All	All	1183/1414 (84%)	1155 (98%)	27 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	422	CYS

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	271/331 (82%)	271 (100%)	0	100	100
1	C	264/331 (80%)	264 (100%)	0	100	100
2	B	265/298 (89%)	265 (100%)	0	100	100
2	D	284/298 (95%)	283 (100%)	1 (0%)	84	89
All	All	1084/1258 (86%)	1083 (100%)	1 (0%)	88	93

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

Mol	Chain	Res	Type
2	D	326	THR

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

Mol	Chain	Res	Type
1	A	362	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	397	GLN
2	B	92	GLN
2	B	201	GLN
2	B	393	ASN
1	C	170	GLN
1	C	346	GLN
1	C	385	HIS
1	C	397	GLN
2	D	231	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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, 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	304/377 (80%)	0.35	22 (7%) 21 23	13, 34, 65, 123	0
1	C	298/377 (79%)	0.35	21 (7%) 22 24	20, 36, 66, 81	0
2	B	290/330 (87%)	0.13	24 (8%) 17 18	12, 27, 68, 104	0
2	D	313/330 (94%)	0.31	35 (11%) 10 10	12, 29, 65, 84	0
All	All	1205/1414 (85%)	0.28	102 (8%) 16 17	12, 32, 66, 123	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	309	ALA	7.8
2	B	309	ALA	5.1
2	D	83	GLY	4.9
2	B	139	ILE	4.8
1	A	140	PRO	4.6
2	B	85	LEU	4.4
2	D	400	TRP	4.3
2	B	138	GLY	4.3
2	B	118	MET	4.2
2	D	82	SER	4.1
2	D	122	THR	4.0
2	B	142	ALA	3.9
2	B	308	SER	3.9
1	C	200	GLU	3.9
2	D	381	CYS	3.8
2	D	344	PRO	3.6
1	C	197	THR	3.5
1	C	196	TYR	3.4
1	A	137	ILE	3.4
2	B	230	ILE	3.4
1	A	141	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	311	GLU	3.1
2	D	217	GLU	3.1
1	A	173	ILE	3.1
1	A	352	HIS	3.1
1	C	349	LEU	3.1
1	A	182	SER	3.0
2	B	310	GLY	3.0
1	C	445	GLY	3.0
2	B	123	SER	2.9
2	D	214	LYS	2.9
1	C	422	CYS	2.9
2	B	141	THR	2.8
2	D	266	MET	2.7
2	B	122	THR	2.7
1	C	201	CYS	2.7
1	C	141	GLY	2.7
2	D	123	SER	2.6
2	D	118	MET	2.6
1	C	104	SER	2.6
2	B	242	ARG	2.6
1	C	106	PHE	2.5
1	C	319	ASP	2.5
1	A	285	ALA	2.5
2	D	244	GLN	2.5
2	D	308	SER	2.5
1	A	354	LYS	2.5
1	A	139	GLU	2.5
1	A	143	ALA	2.5
2	D	242	ARG	2.5
1	A	319	ASP	2.4
2	B	244	GLN	2.4
1	C	140	PRO	2.4
1	A	175	ARG	2.4
2	D	360	GLN	2.4
2	D	137	SER	2.4
2	B	119	GLU	2.4
1	A	348	GLN	2.4
2	B	120	ARG	2.4
2	B	121	LYS	2.4
2	D	307	LEU	2.3
1	A	147	MET	2.3
1	C	165	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	110	LYS	2.3
2	D	139	ILE	2.3
2	D	174	HIS	2.3
2	D	144	CYS	2.3
1	C	105	GLY	2.3
2	D	378	GLY	2.3
2	D	207	GLN	2.3
1	A	254	THR	2.3
2	D	216	ASN	2.3
2	B	136	LEU	2.3
1	C	164	GLU	2.2
1	C	202	GLY	2.2
1	C	348	GLN	2.2
1	A	183	GLN	2.2
1	A	276	SER	2.2
1	A	357	LYS	2.2
2	D	183	MET	2.2
2	D	278	MET	2.2
1	A	353	PHE	2.1
2	B	117	GLN	2.1
2	D	342	HIS	2.1
2	D	121	LYS	2.1
2	D	141	THR	2.1
1	A	165	HIS	2.1
1	A	112	MET	2.1
2	D	358	THR	2.1
1	C	444	GLY	2.1
1	C	339	SER	2.1
1	C	446	SER	2.1
2	B	127	LEU	2.1
2	D	85	LEU	2.1
2	D	395	MET	2.1
2	B	241	LYS	2.1
2	B	137	SER	2.1
2	D	203	ILE	2.0
2	B	231	ASN	2.0
1	C	347	ARG	2.0
2	D	241	LYS	2.0
2	B	143	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

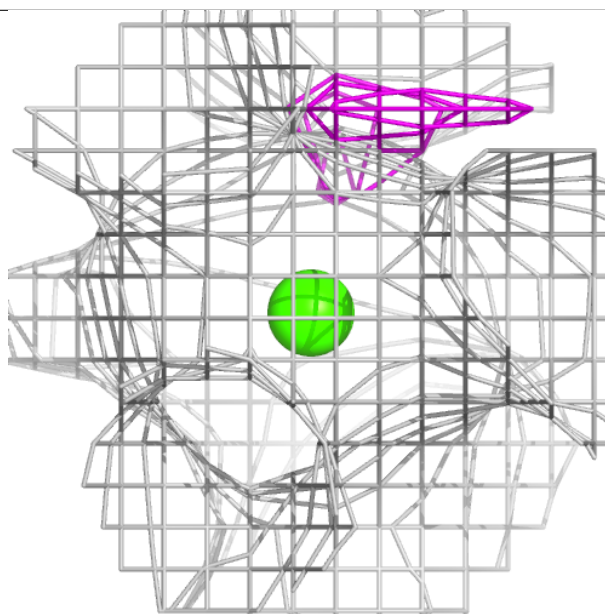
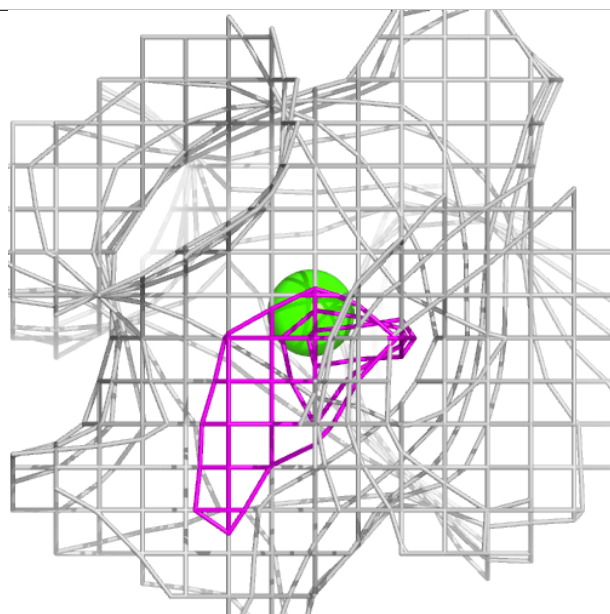
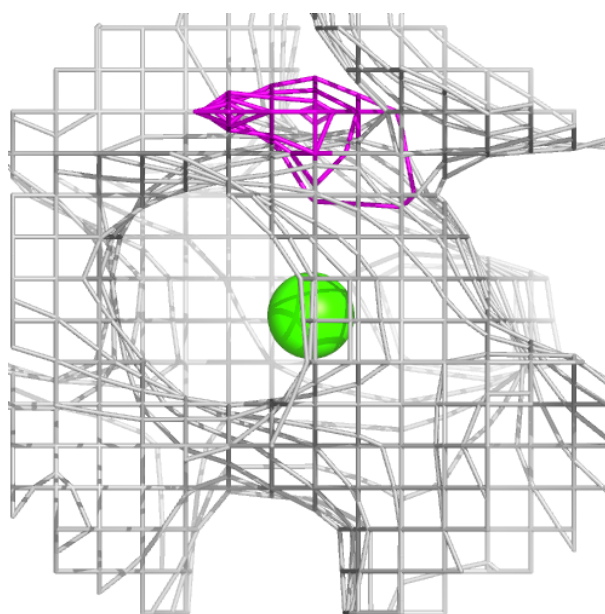
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	501	1/1	0.97	0.04	34,34,34,34	0
3	CA	B	501	1/1	0.98	0.03	22,22,22,22	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.

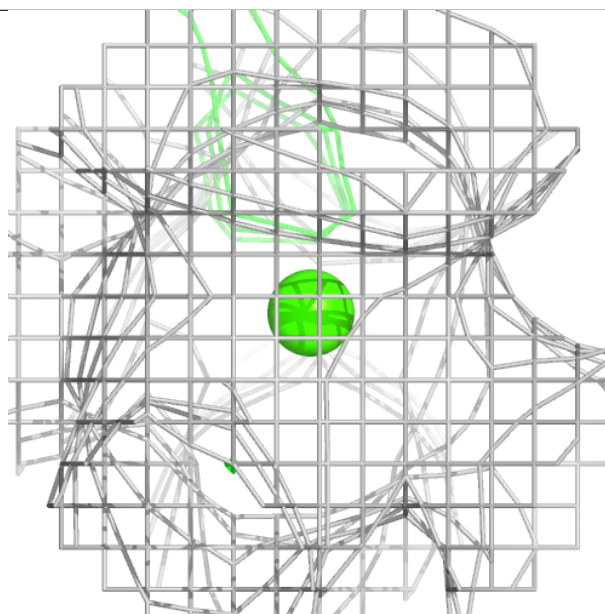
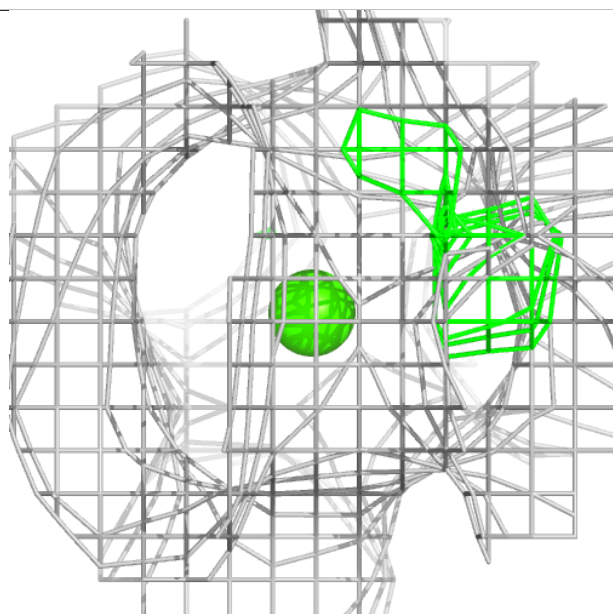
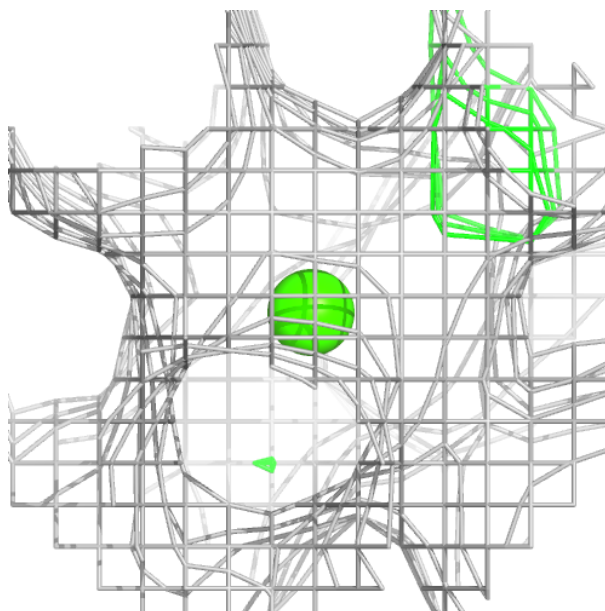
Electron density around CA A 501:

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



Electron density around CA B 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.