



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:58 am BST

PDB ID : 3ITM
Title : Catalytic domain of hPDE2A
Authors : Pandit, J.
Deposited on : 2009-08-28
Resolution : 2.49 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

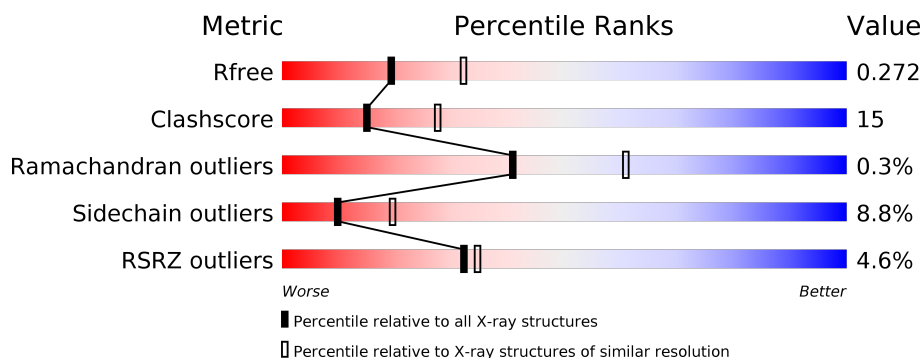
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	345	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>20%</div> <div>• • 11%</div> </div> </div>
1	B	345	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>22%</div> <div>6% 8%</div> </div> </div>
1	C	345	<div> <div>7%</div> <div> <div></div> <div>63%</div> <div>20%</div> <div>6% • 10%</div> </div> </div>
1	D	345	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>26%</div> <div>5% • 8%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10447 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 cGMP-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2514	1605	429	455	25			
1	B	318	Total	C	N	O	S	0	0	0
			2609	1662	446	476	25			
1	C	310	Total	C	N	O	S	0	0	0
			2548	1626	432	465	25			
1	D	318	Total	C	N	O	S	0	0	0
			2609	1662	446	476	25			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	GLY	-	expression tag	UNP O00408
A	576	SER	-	expression tag	UNP O00408
A	577	ALA	-	expression tag	UNP O00408
A	578	MET	-	expression tag	UNP O00408
B	575	GLY	-	expression tag	UNP O00408
B	576	SER	-	expression tag	UNP O00408
B	577	ALA	-	expression tag	UNP O00408
B	578	MET	-	expression tag	UNP O00408
C	575	GLY	-	expression tag	UNP O00408
C	576	SER	-	expression tag	UNP O00408
C	577	ALA	-	expression tag	UNP O00408
C	578	MET	-	expression tag	UNP O00408
D	575	GLY	-	expression tag	UNP O00408
D	576	SER	-	expression tag	UNP O00408
D	577	ALA	-	expression tag	UNP O00408
D	578	MET	-	expression tag	UNP O00408

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

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

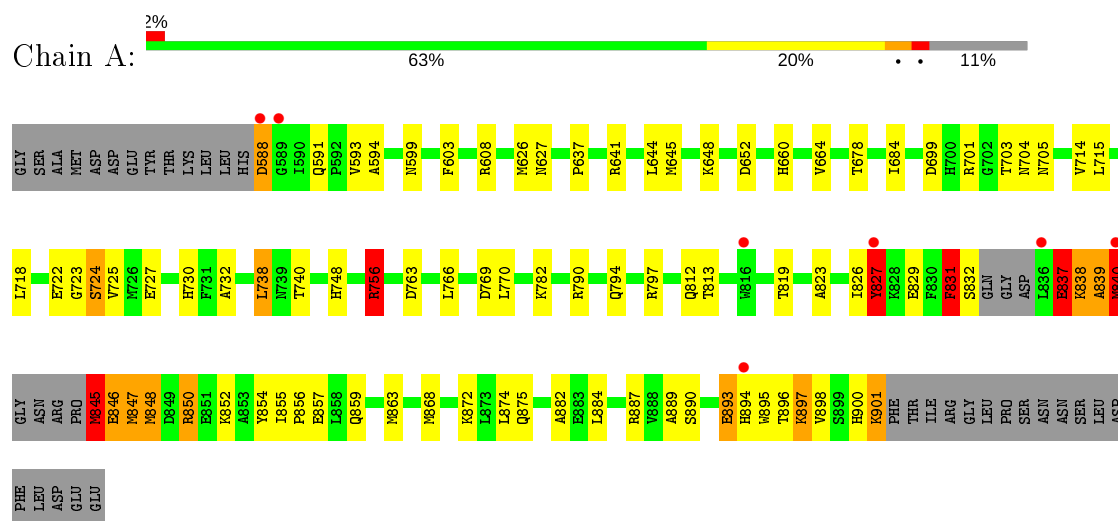
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total 43	O 43	0	0
3	B	65	Total 65	O 65	0	0
3	C	25	Total 25	O 25	0	0
3	D	30	Total 30	O 30	0	0

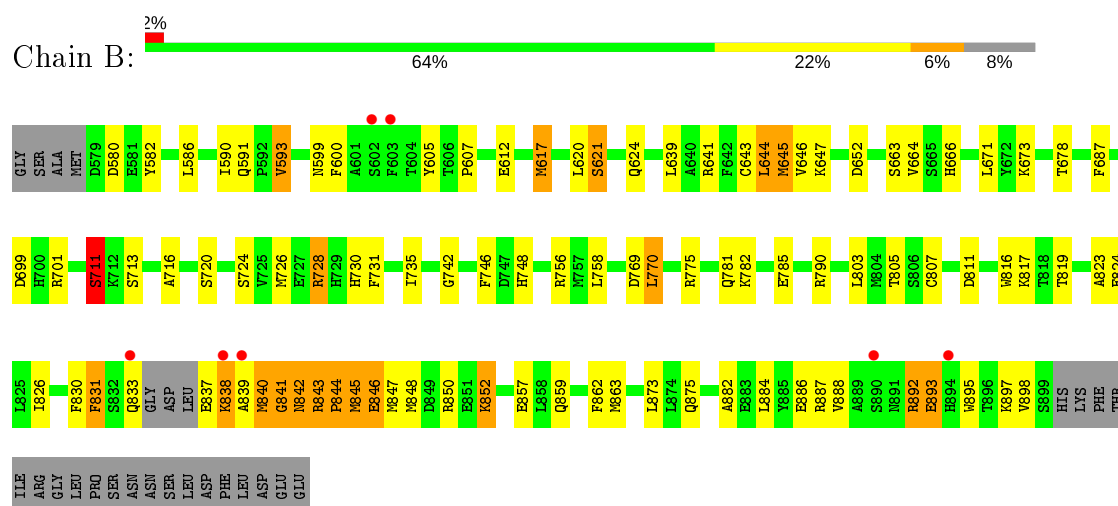
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: cGMP-dependent 3',5'-cyclic phosphodiesterase

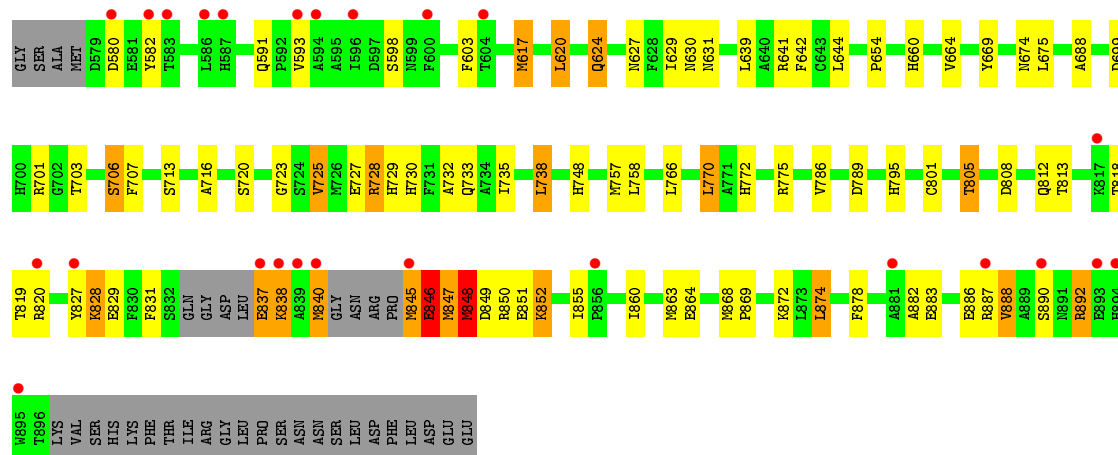


- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

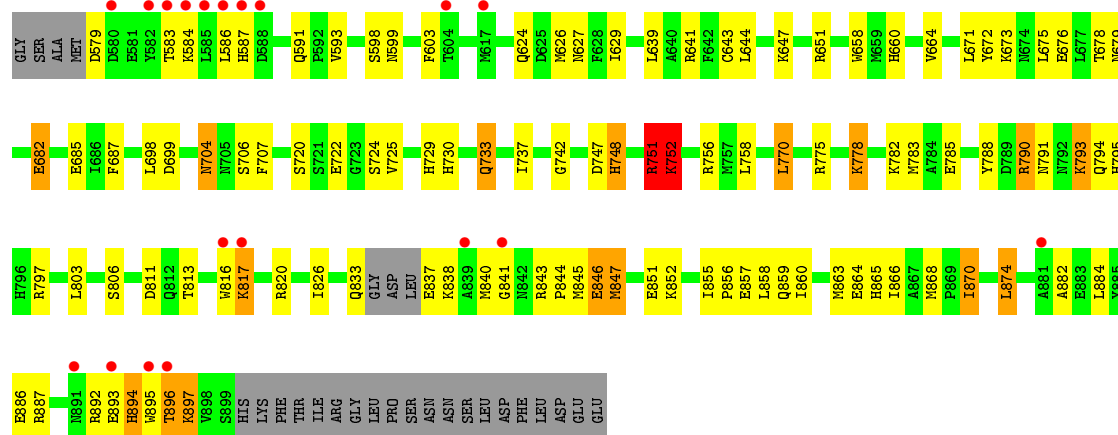


- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase





• Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	108.02Å 108.02Å 515.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.49 49.81 – 2.49	Depositor EDS
% Data completeness (in resolution range)	84.5 (50.00-2.49) 84.6 (49.81-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.227 , 0.286 0.216 , 0.272	Depositor DCC
R_{free} test set	2756 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10447	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.81	30/2573 (1.2%)	1.11	17/3468 (0.5%)
1	B	1.53	26/2671 (1.0%)	1.11	17/3602 (0.5%)
1	C	1.44	24/2608 (0.9%)	1.01	15/3516 (0.4%)
1	D	1.08	13/2671 (0.5%)	0.96	11/3602 (0.3%)
All	All	1.48	93/10523 (0.9%)	1.05	60/14188 (0.4%)

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	2

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	837	GLU	CD-OE2	40.94	1.70	1.25
1	A	831	PHE	CE1-CZ	29.81	1.94	1.37
1	A	831	PHE	CG-CD2	21.82	1.71	1.38
1	B	831	PHE	CG-CD2	21.14	1.70	1.38
1	C	838	LYS	CE-NZ	21.13	2.01	1.49
1	C	838	LYS	CD-CE	20.67	2.02	1.51
1	B	852	LYS	CD-CE	19.84	2.00	1.51
1	D	752	LYS	CE-NZ	18.50	1.95	1.49
1	B	852	LYS	CG-CD	17.16	2.10	1.52
1	A	847	MET	CG-SD	17.07	2.25	1.81
1	C	851	GLU	CD-OE1	16.55	1.43	1.25
1	B	837	GLU	CD-OE1	16.55	1.43	1.25
1	C	847	MET	CG-SD	16.23	2.23	1.81
1	C	851	GLU	CD-OE2	16.20	1.43	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	831	PHE	CG-CD1	15.69	1.62	1.38
1	C	852	LYS	CE-NZ	15.63	1.88	1.49
1	A	846	GLU	CD-OE2	15.44	1.42	1.25
1	B	838	LYS	CG-CD	15.43	2.04	1.52
1	D	751	ARG	CZ-NH2	15.43	1.53	1.33
1	B	852	LYS	CB-CG	15.42	1.94	1.52
1	A	840	MET	SD-CE	14.88	2.61	1.77
1	C	828	LYS	CG-CD	14.53	2.01	1.52
1	C	852	LYS	CD-CE	14.52	1.87	1.51
1	B	840	MET	C-N	14.33	1.58	1.33
1	A	837	GLU	CB-CG	14.22	1.79	1.52
1	B	838	LYS	CD-CE	13.90	1.85	1.51
1	C	846	GLU	CD-OE2	12.95	1.39	1.25
1	C	828	LYS	CB-CG	12.89	1.87	1.52
1	B	852	LYS	CE-NZ	12.33	1.79	1.49
1	A	838	LYS	CD-CE	12.25	1.81	1.51
1	D	793	LYS	CD-CE	12.10	1.81	1.51
1	B	846	GLU	CD-OE2	11.99	1.38	1.25
1	C	831	PHE	CG-CD1	11.30	1.55	1.38
1	A	837	GLU	CD-OE1	10.86	1.37	1.25
1	A	840	MET	CG-SD	-10.73	1.53	1.81
1	B	846	GLU	CG-CD	10.60	1.67	1.51
1	C	828	LYS	CE-NZ	10.24	1.74	1.49
1	D	846	GLU	CD-OE1	10.17	1.36	1.25
1	A	901	LYS	C-O	10.16	1.42	1.23
1	A	900	HIS	C-N	10.11	1.57	1.34
1	A	848	MET	CG-SD	9.92	2.06	1.81
1	B	831	PHE	CE1-CZ	9.91	1.56	1.37
1	A	901	LYS	CA-CB	9.78	1.75	1.53
1	B	844	PRO	C-N	9.51	1.55	1.34
1	A	897	LYS	CE-NZ	9.32	1.72	1.49
1	A	846	GLU	CD-OE1	9.32	1.35	1.25
1	C	849	ASP	C-O	9.25	1.41	1.23
1	C	840	MET	CG-SD	9.02	2.04	1.81
1	A	898	VAL	C-O	9.00	1.40	1.23
1	D	897	LYS	CE-NZ	8.93	1.71	1.49
1	A	857	GLU	CG-CD	8.65	1.65	1.51
1	B	897	LYS	CD-CE	8.51	1.72	1.51
1	B	841	GLY	CA-C	8.29	1.65	1.51
1	D	778	LYS	CE-NZ	8.26	1.69	1.49
1	C	845	MET	SD-CE	8.04	2.22	1.77
1	B	843	ARG	NE-CZ	7.93	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	831	PHE	CE2-CZ	7.75	1.52	1.37
1	C	849	ASP	CG-OD2	7.56	1.42	1.25
1	D	817	LYS	CE-NZ	7.56	1.68	1.49
1	C	845	MET	CG-SD	7.50	2.00	1.81
1	B	846	GLU	CB-CG	7.42	1.66	1.52
1	C	846	GLU	CD-OE1	7.33	1.33	1.25
1	A	857	GLU	CD-OE1	7.28	1.33	1.25
1	A	850	ARG	CZ-NH1	7.10	1.42	1.33
1	B	842	ASN	C-N	7.06	1.50	1.34
1	D	751	ARG	CD-NE	6.95	1.58	1.46
1	B	845	MET	CG-SD	6.93	1.99	1.81
1	D	790	ARG	CZ-NH1	6.49	1.41	1.33
1	C	849	ASP	CG-OD1	6.44	1.40	1.25
1	B	848	MET	CG-SD	6.34	1.97	1.81
1	A	827	TYR	C-O	6.30	1.35	1.23
1	A	901	LYS	CA-C	6.08	1.68	1.52
1	D	841	GLY	C-N	6.01	1.47	1.34
1	B	841	GLY	C-O	5.99	1.33	1.23
1	A	896	THR	CB-OG1	5.93	1.55	1.43
1	A	850	ARG	NE-CZ	5.93	1.40	1.33
1	C	847	MET	SD-CE	5.92	2.11	1.77
1	C	849	ASP	C-N	5.92	1.47	1.34
1	D	752	LYS	CD-CE	5.89	1.66	1.51
1	D	793	LYS	CG-CD	5.86	1.72	1.52
1	A	857	GLU	CD-OE2	5.84	1.32	1.25
1	B	831	PHE	CG-CD1	5.83	1.47	1.38
1	C	831	PHE	CB-CG	5.75	1.61	1.51
1	D	838	LYS	CE-NZ	5.75	1.63	1.49
1	A	900	HIS	C-O	5.71	1.34	1.23
1	C	846	GLU	CG-CD	5.69	1.60	1.51
1	A	845	MET	SD-CE	5.55	2.08	1.77
1	A	714	VAL	CA-CB	5.28	1.65	1.54
1	B	612	GLU	CD-OE1	5.26	1.31	1.25
1	B	782	LYS	CE-NZ	5.23	1.62	1.49
1	B	841	GLY	C-N	5.22	1.46	1.34
1	C	808	ASP	CB-CG	5.14	1.62	1.51
1	A	845	MET	CA-CB	5.05	1.65	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	751	ARG	NE-CZ-NH2	17.12	128.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	831	PHE	CB-CG-CD1	-14.62	110.56	120.80
1	C	849	ASP	CB-CG-OD1	-12.72	106.86	118.30
1	A	840	MET	CG-SD-CE	-12.61	80.03	100.20
1	B	843	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	D	790	ARG	NE-CZ-NH2	-11.71	114.45	120.30
1	B	852	LYS	CB-CG-CD	-11.17	82.56	111.60
1	C	847	MET	CG-SD-CE	-10.71	83.06	100.20
1	B	852	LYS	CD-CE-NZ	-10.60	87.33	111.70
1	C	852	LYS	CD-CE-NZ	-10.52	87.50	111.70
1	C	831	PHE	CB-CG-CD1	-10.40	113.52	120.80
1	B	848	MET	CG-SD-CE	10.08	116.32	100.20
1	B	838	LYS	CG-CD-CE	-9.95	82.06	111.90
1	B	852	LYS	CG-CD-CE	-9.88	82.27	111.90
1	B	843	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	C	828	LYS	CB-CG-CD	-8.91	88.43	111.60
1	A	831	PHE	CG-CD1-CE1	-8.83	111.09	120.80
1	B	838	LYS	CD-CE-NZ	-8.49	92.18	111.70
1	A	837	GLU	CG-CD-OE1	-8.00	102.29	118.30
1	D	751	ARG	NH1-CZ-NH2	-7.99	110.61	119.40
1	A	738	LEU	CB-CG-CD1	-7.56	98.14	111.00
1	D	793	LYS	CD-CE-NZ	-7.47	94.51	111.70
1	A	846	GLU	OE1-CD-OE2	7.29	132.05	123.30
1	A	850	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	B	838	LYS	CB-CG-CD	-6.87	93.73	111.60
1	B	830	PHE	CB-CG-CD1	-6.85	116.01	120.80
1	B	841	GLY	CA-C-N	-6.72	102.41	117.20
1	C	838	LYS	CD-CE-NZ	-6.66	96.39	111.70
1	A	837	GLU	OE1-CD-OE2	6.65	131.28	123.30
1	D	704	ASN	CB-CA-C	6.63	123.67	110.40
1	A	831	PHE	CD1-CG-CD2	6.46	126.69	118.30
1	D	752	LYS	CD-CE-NZ	-6.38	97.03	111.70
1	D	791	ASN	CB-CA-C	-6.26	97.87	110.40
1	A	840	MET	CA-C-O	6.15	133.02	120.10
1	C	847	MET	CA-CB-CG	-6.14	102.86	113.30
1	C	848	MET	CG-SD-CE	5.89	109.63	100.20
1	C	728	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	838	LYS	CB-CG-CD	5.84	126.77	111.60
1	A	850	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	D	793	LYS	CG-CD-CE	-5.76	94.61	111.90
1	B	850	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	756	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	850	ARG	NE-CZ-NH1	5.56	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	620	LEU	CA-CB-CG	5.56	128.09	115.30
1	C	851	GLU	CG-CD-OE2	-5.53	107.24	118.30
1	A	608	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	837	GLU	CG-CD-OE1	-5.52	107.26	118.30
1	C	849	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	840	MET	CB-CG-SD	-5.50	95.91	112.40
1	C	874	LEU	CA-CB-CG	5.46	127.85	115.30
1	D	790	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	841	GLY	CA-C-O	5.41	130.34	120.60
1	B	845	MET	CA-CB-CG	5.39	122.47	113.30
1	A	874	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	701	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	756	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	808	ASP	CB-CG-OD2	5.32	123.08	118.30
1	D	707	PHE	CB-CA-C	-5.29	99.82	110.40
1	A	901	LYS	CA-C-O	-5.10	109.39	120.10
1	D	852	LYS	CD-CE-NZ	5.01	123.23	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	831	PHE	Sidechain
1	A	837	GLU	Sidechain

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	2514	0	2462	73	0
1	B	2609	0	2552	87	0
1	C	2548	0	2487	87	0
1	D	2609	0	2552	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	43	0	0	6	0
3	B	65	0	0	9	0
3	C	25	0	0	3	0
3	D	30	0	0	6	0
All	All	10447	0	10053	307	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 15.

All (307) 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:901:LYS:CB	1:A:901:LYS:CA	1.75	1.62
1:D:817:LYS:NZ	1:D:817:LYS:CE	1.68	1.57
1:A:831:PHE:CE1	1:A:831:PHE:CZ	1.94	1.56
1:A:837:GLU:CB	1:A:837:GLU:CG	1.79	1.55
1:D:778:LYS:NZ	1:D:778:LYS:CE	1.69	1.54
1:A:838:LYS:CE	1:A:838:LYS:CD	1.81	1.54
1:D:793:LYS:CD	1:D:793:LYS:CE	1.81	1.53
1:C:852:LYS:CD	1:C:852:LYS:CE	1.87	1.53
1:B:838:LYS:CE	1:B:838:LYS:CD	1.86	1.50
1:C:828:LYS:CE	1:C:828:LYS:NZ	1.74	1.50
1:D:897:LYS:CE	1:D:897:LYS:NZ	1.71	1.49
1:C:828:LYS:CB	1:C:828:LYS:CG	1.87	1.48
1:A:897:LYS:NZ	1:A:897:LYS:CE	1.72	1.47
1:A:848:MET:SD	1:A:848:MET:CE	2.03	1.47
1:C:840:MET:CE	1:C:840:MET:SD	2.04	1.46
1:A:847:MET:SD	1:A:847:MET:CE	2.02	1.45
1:C:840:MET:CG	1:C:840:MET:SD	2.04	1.45
1:B:852:LYS:CG	1:B:852:LYS:CB	1.94	1.44
1:A:848:MET:SD	1:A:848:MET:CG	2.06	1.44
1:B:852:LYS:NZ	1:B:852:LYS:CE	1.79	1.42
1:A:845:MET:SD	1:A:845:MET:CE	2.08	1.40
1:B:852:LYS:CD	1:B:852:LYS:CE	2.00	1.39
1:C:847:MET:CE	1:C:847:MET:SD	2.11	1.39
1:C:852:LYS:NZ	1:C:852:LYS:CE	1.88	1.37
1:C:838:LYS:CD	1:C:838:LYS:CE	2.02	1.36
1:C:828:LYS:CG	1:C:828:LYS:CD	2.01	1.34
1:B:838:LYS:CD	1:B:838:LYS:CG	2.04	1.34
1:D:752:LYS:CE	1:D:752:LYS:NZ	1.95	1.29
1:A:837:GLU:CD	1:A:837:GLU:OE2	1.70	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:852:LYS:CG	1:B:852:LYS:CD	2.10	1.28
1:C:847:MET:SD	1:C:847:MET:CG	2.23	1.25
1:C:845:MET:CE	1:C:845:MET:SD	2.22	1.25
1:A:847:MET:SD	1:A:847:MET:CG	2.25	1.23
1:C:838:LYS:NZ	1:C:838:LYS:CE	2.01	1.22
1:C:837:GLU:N	1:C:837:GLU:OE1	1.82	1.12
1:A:845:MET:HG2	1:A:846:GLU:H	0.96	1.09
1:A:704:ASN:HB2	3:A:77:HOH:O	1.54	1.05
1:B:824:GLU:HB3	3:B:153:HOH:O	1.57	1.04
1:A:845:MET:CG	1:A:846:GLU:H	1.73	1.02
1:A:868:MET:CE	1:A:889:ALA:HA	1.91	0.99
1:A:837:GLU:OE2	1:B:726:MET:HG3	1.64	0.97
1:A:845:MET:HG2	1:A:846:GLU:N	1.79	0.97
1:B:846:GLU:HB3	3:B:123:HOH:O	1.65	0.96
1:A:748:HIS:HB2	3:A:4:HOH:O	1.67	0.95
1:D:699:ASP:H	1:D:730:HIS:HD2	1.08	0.94
1:D:699:ASP:H	1:D:730:HIS:CD2	1.85	0.92
1:B:699:ASP:H	1:B:730:HIS:CD2	1.89	0.91
1:D:846:GLU:HG2	3:D:131:HOH:O	1.71	0.89
1:B:699:ASP:H	1:B:730:HIS:HD2	1.10	0.89
1:A:840:MET:CE	1:A:840:MET:SD	2.61	0.89
1:C:699:ASP:H	1:C:730:HIS:CD2	1.91	0.89
1:D:748:HIS:ND1	1:D:748:HIS:N	2.21	0.88
1:B:748:HIS:HB2	3:B:920:HOH:O	1.73	0.87
1:D:751:ARG:HH11	1:D:751:ARG:HG2	1.38	0.85
1:C:699:ASP:H	1:C:730:HIS:HD2	1.24	0.85
1:A:875:GLN:HE21	1:A:882:ALA:HA	1.42	0.84
1:B:819:THR:HG21	1:B:895:TRP:HE1	1.42	0.83
1:B:838:LYS:CE	1:B:838:LYS:CG	2.56	0.82
1:B:838:LYS:NZ	1:B:838:LYS:CD	2.42	0.82
1:B:838:LYS:HE2	1:B:842:ASN:HB2	1.62	0.80
1:C:827:TYR:CZ	1:C:852:LYS:HG3	2.17	0.80
1:D:793:LYS:CG	1:D:793:LYS:CE	2.60	0.79
1:B:819:THR:CG2	1:B:895:TRP:HE1	1.96	0.79
1:A:868:MET:HE2	1:A:889:ALA:HA	1.65	0.78
1:D:882:ALA:O	1:D:886:GLU:HG2	1.83	0.78
1:B:838:LYS:CD	1:B:838:LYS:CB	2.64	0.76
1:B:701:ARG:HB2	1:B:728:ARG:NH1	2.00	0.75
1:C:852:LYS:HA	1:C:855:ILE:HD13	1.69	0.74
1:C:863:MET:O	1:C:868:MET:HB2	1.87	0.74
1:C:852:LYS:CG	1:C:852:LYS:CE	2.66	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:852:LYS:CD	1:B:852:LYS:CB	2.67	0.73
1:A:723:GLY:O	1:B:840:MET:HG3	1.88	0.73
1:A:837:GLU:CA	1:A:837:GLU:CG	2.66	0.72
1:A:699:ASP:H	1:A:730:HIS:HD2	1.34	0.72
1:D:793:LYS:CD	1:D:793:LYS:NZ	2.51	0.71
1:A:838:LYS:CE	1:A:838:LYS:CG	2.66	0.71
1:C:848:MET:HA	1:C:848:MET:HE2	1.73	0.70
1:C:723:GLY:O	1:D:840:MET:HG3	1.91	0.70
1:D:817:LYS:NZ	1:D:817:LYS:CD	2.55	0.69
1:B:852:LYS:CG	1:B:852:LYS:CE	2.70	0.69
1:A:699:ASP:H	1:A:730:HIS:CD2	2.10	0.69
1:C:827:TYR:CE1	1:C:852:LYS:HG3	2.28	0.69
3:A:126:HOH:O	1:B:833:GLN:HB2	1.93	0.69
1:D:866:ILE:O	1:D:870:ILE:HG23	1.94	0.68
1:C:766:LEU:HB3	3:C:164:HOH:O	1.93	0.68
1:C:828:LYS:CB	1:C:828:LYS:CD	2.71	0.68
1:C:840:MET:CB	1:C:840:MET:SD	2.81	0.68
1:D:897:LYS:CD	1:D:897:LYS:NZ	2.54	0.68
1:B:852:LYS:CG	1:B:852:LYS:CA	2.72	0.68
1:C:838:LYS:CG	1:C:838:LYS:CE	2.71	0.68
1:A:893:GLU:OE1	1:A:893:GLU:HA	1.94	0.67
1:B:893:GLU:HA	1:B:893:GLU:OE2	1.93	0.67
1:C:627:ASN:HB3	1:C:631:ASN:ND2	2.09	0.67
1:D:778:LYS:NZ	1:D:778:LYS:CD	2.55	0.67
1:B:724:SER:HB3	1:B:769:ASP:OD1	1.96	0.66
1:D:816:TRP:CD1	1:D:894:HIS:HB3	2.31	0.66
1:A:859:GLN:HG2	1:A:895:TRP:CE2	2.31	0.66
1:C:789:ASP:H	1:C:795:HIS:HD2	1.43	0.66
1:A:727:GLU:HB2	1:B:839:ALA:O	1.96	0.65
1:C:812:GLN:OE1	1:C:819:THR:HG22	1.95	0.65
1:C:852:LYS:CD	1:C:852:LYS:NZ	2.59	0.65
1:B:781:GLN:OE1	3:B:9:HOH:O	2.14	0.65
1:A:897:LYS:NZ	1:A:897:LYS:CD	2.58	0.64
1:C:748:HIS:HB2	3:C:15:HOH:O	1.97	0.64
1:A:893:GLU:O	1:A:897:LYS:HG3	1.98	0.64
3:A:126:HOH:O	1:B:833:GLN:CB	2.45	0.64
1:D:863:MET:O	1:D:868:MET:HB2	1.98	0.63
1:A:845:MET:CG	1:A:846:GLU:N	2.45	0.63
1:C:860:ILE:HG23	1:C:892:ARG:HE	1.64	0.63
1:C:772:HIS:CD2	3:C:164:HOH:O	2.52	0.63
1:C:827:TYR:CE2	1:C:852:LYS:HE3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:852:LYS:CD	1:B:852:LYS:NZ	2.63	0.62
1:C:850:ARG:HH12	1:D:775:ARG:HD2	1.65	0.61
1:D:860:ILE:HD11	1:D:896:THR:HA	1.81	0.61
1:B:859:GLN:HG2	1:B:895:TRP:CE2	2.36	0.61
1:A:722:GLU:O	1:A:730:HIS:HE1	1.83	0.61
1:A:840:MET:CE	1:A:840:MET:CG	2.78	0.60
1:A:854:TYR:HD2	1:B:711:SER:HG	1.48	0.60
1:B:664:VAL:HG13	1:B:807:CYS:HB3	1.83	0.60
1:B:840:MET:SD	1:B:841:GLY:N	2.74	0.60
1:C:827:TYR:CZ	1:C:852:LYS:HE3	2.36	0.59
1:D:720:SER:HB2	1:D:770:LEU:HD22	1.83	0.59
1:A:660:HIS:O	1:A:664:VAL:HG23	2.03	0.59
1:C:837:GLU:CD	1:C:837:GLU:N	2.57	0.59
1:B:591:GLN:O	1:B:621:SER:OG	2.20	0.58
1:A:812:GLN:OE1	1:A:819:THR:HG22	2.03	0.58
1:C:848:MET:HA	1:C:848:MET:CE	2.33	0.58
1:B:701:ARG:HB2	1:B:728:ARG:HH11	1.66	0.58
1:A:840:MET:CE	1:A:840:MET:HG2	2.34	0.57
1:C:706:SER:HB2	1:C:725:VAL:HG21	1.86	0.57
1:D:671:LEU:HD13	1:D:803:LEU:HD22	1.85	0.57
1:C:827:TYR:OH	1:C:852:LYS:HE3	2.04	0.57
1:D:641:ARG:HD2	1:D:742:GLY:O	2.04	0.56
1:A:848:MET:SD	1:A:848:MET:HA	2.46	0.56
1:B:593:VAL:HG22	1:B:600:PHE:CD2	2.41	0.56
1:A:859:GLN:O	1:A:863:MET:HG2	2.05	0.56
1:A:724:SER:HB3	1:A:769:ASP:OD1	2.05	0.56
1:C:852:LYS:HA	1:C:855:ILE:CD1	2.33	0.56
1:C:660:HIS:O	1:C:664:VAL:HG23	2.06	0.55
1:C:813:THR:O	1:C:887:ARG:HD2	2.06	0.55
1:B:875:GLN:HE21	1:B:882:ALA:HA	1.71	0.55
1:C:868:MET:HB3	1:C:869:PRO:HD3	1.87	0.55
1:D:698:LEU:HD13	1:D:733:GLN:HG2	1.89	0.55
1:D:813:THR:O	1:D:887:ARG:HG2	2.06	0.55
1:D:733:GLN:O	1:D:737:ILE:HG12	2.07	0.55
1:B:731:PHE:CZ	1:B:735:ILE:HD11	2.42	0.55
1:C:828:LYS:CE	1:C:828:LYS:CG	2.85	0.55
1:A:901:LYS:CB	1:A:901:LYS:N	2.63	0.54
1:A:838:LYS:HB2	1:D:651:ARG:HD3	1.90	0.54
1:C:603:PHE:HD2	1:C:883:GLU:OE1	1.91	0.54
1:C:727:GLU:HB2	1:D:840:MET:HA	1.90	0.54
1:C:828:LYS:CA	1:C:828:LYS:CG	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:751:ARG:HH11	1:D:751:ARG:CG	2.17	0.53
1:D:752:LYS:CD	1:D:752:LYS:NZ	2.71	0.53
1:C:701:ARG:HG3	1:C:728:ARG:CZ	2.37	0.53
1:D:660:HIS:O	1:D:664:VAL:HG23	2.09	0.53
1:B:781:GLN:HG3	3:B:9:HOH:O	2.09	0.53
1:D:626:MET:HG2	1:D:672:TYR:CD2	2.43	0.53
1:B:641:ARG:HD2	1:B:742:GLY:O	2.08	0.53
1:C:703:THR:HG22	1:C:703:THR:O	2.09	0.52
1:B:646:VAL:HG23	1:B:647:LYS:N	2.23	0.52
1:A:705:ASN:O	1:B:831:PHE:HE2	1.92	0.52
1:C:725:VAL:HG23	1:D:847:MET:CE	2.40	0.52
1:D:843:ARG:HD2	3:D:131:HOH:O	2.09	0.52
1:A:684:ILE:HD13	1:A:756:ARG:HG2	1.91	0.52
1:C:591:GLN:HG3	1:C:617:MET:CE	2.40	0.52
1:C:847:MET:CE	1:C:847:MET:CG	2.88	0.52
1:C:789:ASP:N	1:C:795:HIS:HD2	2.08	0.52
1:C:624:GLN:HB2	1:C:629:ILE:HD12	1.91	0.52
1:A:893:GLU:CA	1:A:893:GLU:OE1	2.58	0.52
1:A:848:MET:O	1:A:852:LYS:HG2	2.10	0.51
1:B:580:ASP:HB3	3:B:27:HOH:O	2.10	0.51
1:B:731:PHE:CE1	1:B:735:ILE:HD11	2.45	0.51
1:B:811:ASP:HB2	3:B:14:HOH:O	2.10	0.51
1:A:823:ALA:O	1:A:826:ILE:HG22	2.10	0.51
1:A:855:ILE:HB	1:A:856:PRO:HD3	1.91	0.51
1:C:620:LEU:HD22	1:C:639:LEU:HG	1.92	0.51
1:C:850:ARG:HH12	1:D:775:ARG:CD	2.23	0.51
1:C:707:PHE:N	1:D:851:GLU:OE2	2.28	0.51
1:D:859:GLN:O	1:D:863:MET:HG2	2.11	0.51
1:A:588:ASP:N	1:A:588:ASP:OD1	2.44	0.51
1:B:671:LEU:HD13	1:B:803:LEU:HD22	1.93	0.51
1:A:812:GLN:OE1	1:A:819:THR:CG2	2.59	0.50
1:A:637:PRO:HB2	1:A:641:ARG:NH2	2.27	0.50
1:C:846:GLU:HG3	1:C:847:MET:N	2.26	0.50
1:B:645:MET:HA	1:B:645:MET:HE2	1.94	0.50
1:C:827:TYR:CZ	1:C:852:LYS:CG	2.92	0.50
1:B:620:LEU:HD22	1:B:639:LEU:HG	1.93	0.50
1:B:823:ALA:O	1:B:826:ILE:HG22	2.12	0.49
1:C:713:SER:HB3	1:C:716:ALA:HB3	1.93	0.49
1:D:788:TYR:CE1	1:D:795:HIS:HB3	2.47	0.49
1:B:838:LYS:CD	1:B:838:LYS:HB3	2.42	0.49
1:C:703:THR:HG21	1:D:837:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:MET:HG3	1:B:892:ARG:HB2	1.95	0.48
1:B:716:ALA:HB2	1:B:862:PHE:HD1	1.76	0.48
1:A:703:THR:CG2	1:A:705:ASN:ND2	2.77	0.48
1:D:682:GLU:HG2	1:D:685:GLU:OE1	2.14	0.48
1:A:813:THR:O	1:A:887:ARG:HD2	2.14	0.48
1:D:783:MET:HG3	1:D:795:HIS:CE1	2.48	0.48
1:C:735:ILE:HA	1:C:738:LEU:HB2	1.96	0.47
1:D:671:LEU:HD22	1:D:675:LEU:HD11	1.96	0.47
1:D:826:ILE:HD12	1:D:826:ILE:HA	1.77	0.47
1:D:859:GLN:HG2	1:D:895:TRP:CE2	2.49	0.47
1:B:617:MET:HG2	1:B:617:MET:O	2.12	0.47
1:C:729:HIS:O	1:C:733:GLN:HB2	2.15	0.47
1:D:811:ASP:HB2	3:D:21:HOH:O	2.15	0.47
1:A:827:TYR:CZ	1:A:855:ILE:HD11	2.50	0.47
1:C:582:TYR:OH	1:C:641:ARG:NH2	2.48	0.47
1:B:845:MET:HB2	1:B:846:GLU:OE2	2.15	0.47
1:D:706:SER:HB2	1:D:725:VAL:HG11	1.96	0.47
1:C:642:PHE:CD2	1:C:642:PHE:C	2.89	0.46
1:B:645:MET:HA	1:B:645:MET:CE	2.45	0.46
1:C:654:PRO:HD2	1:C:829:GLU:HB2	1.98	0.46
1:B:720:SER:HB2	1:B:770:LEU:HB2	1.98	0.46
1:B:859:GLN:O	1:B:863:MET:HG2	2.16	0.46
1:B:590:ILE:HD13	1:B:620:LEU:HB3	1.98	0.46
1:B:781:GLN:HE21	1:B:873:LEU:HD21	1.81	0.46
1:B:790:ARG:NE	3:B:154:HOH:O	2.47	0.46
1:C:868:MET:CE	1:C:888:VAL:HG23	2.46	0.46
1:A:715:LEU:HD12	1:A:718:LEU:HD12	1.98	0.46
1:B:838:LYS:HE3	1:B:838:LYS:CG	2.44	0.45
1:C:688:ALA:HA	1:C:757:MET:HE1	1.98	0.45
1:A:732:ALA:HB1	1:C:732:ALA:HB1	1.98	0.45
1:B:620:LEU:CD2	1:B:639:LEU:HG	2.46	0.45
1:B:838:LYS:NZ	1:C:733:GLN:HE22	2.13	0.45
1:A:763:ASP:OD2	1:A:797:ARG:NH2	2.49	0.45
1:D:647:LYS:HG3	1:D:658:TRP:CD1	2.52	0.45
1:C:801:CYS:O	1:C:805:THR:HG22	2.16	0.45
1:B:678:THR:O	1:B:790:ARG:NH2	2.50	0.45
1:D:624:GLN:HB2	1:D:629:ILE:HD13	1.99	0.45
1:B:816:TRP:HZ3	1:B:895:TRP:CE2	2.35	0.45
1:A:727:GLU:OE1	1:B:838:LYS:HD3	2.17	0.45
1:A:868:MET:HE3	1:A:889:ALA:HA	1.89	0.44
1:C:840:MET:CE	1:C:840:MET:CG	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:GLU:O	1:A:832:SER:HB3	2.17	0.44
1:C:882:ALA:HB1	1:C:886:GLU:OE2	2.17	0.44
1:D:673:LYS:HA	1:D:673:LYS:HD2	1.81	0.44
1:A:901:LYS:C	1:A:901:LYS:CB	2.78	0.44
1:B:875:GLN:NE2	1:B:882:ALA:HA	2.31	0.44
1:D:626:MET:O	1:D:627:ASN:HB2	2.17	0.44
1:D:676:GLU:HA	3:D:122:HOH:O	2.18	0.44
1:B:605:TYR:HD2	1:B:666:HIS:CE1	2.36	0.44
1:C:593:VAL:HG21	1:C:669:TYR:OH	2.18	0.44
1:D:579:ASP:N	1:D:579:ASP:OD1	2.51	0.44
1:D:682:GLU:H	1:D:682:GLU:HG2	1.64	0.44
1:D:729:HIS:O	1:D:733:GLN:HB2	2.18	0.44
1:D:816:TRP:NE1	1:D:894:HIS:HB3	2.32	0.44
1:B:673:LYS:HB3	1:B:673:LYS:HE3	1.75	0.44
1:B:852:LYS:HB2	1:B:852:LYS:CD	2.47	0.44
1:A:645:MET:HE1	1:A:740:THR:HG21	1.99	0.43
1:B:699:ASP:N	1:B:730:HIS:CD2	2.73	0.43
1:D:639:LEU:O	1:D:643:CYS:HB2	2.17	0.43
1:D:844:PRO:O	1:D:847:MET:HG3	2.18	0.43
1:C:827:TYR:CE2	1:C:852:LYS:CE	3.01	0.43
1:D:704:ASN:HD22	1:D:704:ASN:HA	1.67	0.43
1:A:725:VAL:HA	1:B:847:MET:CE	2.49	0.43
1:C:603:PHE:CZ	1:C:674:ASN:HB2	2.54	0.43
1:A:603:PHE:CD1	1:A:884:LEU:HD21	2.54	0.43
1:B:646:VAL:CG2	1:B:647:LYS:N	2.81	0.43
1:C:827:TYR:OH	1:C:852:LYS:HG3	2.18	0.43
1:D:671:LEU:HD13	1:D:803:LEU:CD2	2.49	0.43
1:C:675:LEU:HD22	1:C:878:PHE:HB3	2.01	0.43
1:D:603:PHE:CD1	1:D:884:LEU:HD21	2.53	0.43
1:B:582:TYR:HB2	1:B:644:LEU:HD23	2.00	0.42
1:C:582:TYR:HB2	1:C:644:LEU:CD1	2.49	0.42
1:D:858:LEU:HD23	1:D:858:LEU:HA	1.71	0.42
1:D:864:GLU:HG3	1:D:892:ARG:HD2	2.01	0.42
1:B:644:LEU:HA	1:B:644:LEU:HD12	1.71	0.42
1:C:789:ASP:H	1:C:795:HIS:CD2	2.30	0.42
1:D:794:GLN:OE1	1:D:794:GLN:HA	2.19	0.42
1:D:855:ILE:HB	1:D:856:PRO:HD3	2.00	0.42
1:A:838:LYS:C	1:A:839:ALA:O	2.57	0.42
1:B:884:LEU:O	1:B:888:VAL:HG23	2.20	0.42
1:D:699:ASP:N	1:D:730:HIS:CD2	2.69	0.42
1:D:857:GLU:HB2	3:D:43:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:PRO:HG2	1:B:663:SER:HB2	2.02	0.42
1:C:627:ASN:HB3	1:C:631:ASN:HD21	1.82	0.42
1:B:652:ASP:N	1:B:652:ASP:OD1	2.47	0.42
1:D:584:LYS:C	1:D:586:LEU:H	2.23	0.42
1:B:843:ARG:HA	1:B:844:PRO:HD2	1.85	0.41
1:D:840:MET:HB3	1:D:840:MET:HE3	1.98	0.41
1:B:816:TRP:CZ3	1:B:895:TRP:CE2	3.09	0.41
1:D:806:SER:HA	1:D:870:ILE:HD11	2.02	0.41
1:A:826:ILE:O	1:A:829:GLU:HB3	2.21	0.41
1:C:720:SER:HB2	1:C:770:LEU:HD23	2.01	0.41
1:D:725:VAL:HB	3:D:163:HOH:O	2.20	0.41
1:A:594:ALA:CB	3:A:65:HOH:O	2.68	0.41
1:A:703:THR:CG2	1:A:705:ASN:HD22	2.33	0.41
1:A:678:THR:HB	3:A:40:HOH:O	2.19	0.41
1:B:785:GLU:OE1	1:B:785:GLU:HA	2.20	0.41
1:D:874:LEU:HD23	1:D:874:LEU:HA	1.71	0.41
1:B:701:ARG:HB2	1:B:728:ARG:HH12	1.83	0.41
1:B:852:LYS:CG	1:B:852:LYS:HA	2.48	0.41
1:D:676:GLU:HG3	1:D:679:ASN:HD22	1.85	0.41
1:C:758:LEU:HD12	1:C:758:LEU:N	2.35	0.41
1:D:647:LYS:HG3	1:D:658:TRP:CG	2.56	0.41
1:A:847:MET:SD	1:A:847:MET:CB	2.99	0.41
1:D:863:MET:HE2	1:D:892:ARG:HA	2.03	0.41
1:C:713:SER:HB3	1:C:716:ALA:CB	2.50	0.41
1:C:827:TYR:HH	1:C:852:LYS:HG3	1.85	0.41
1:B:687:PHE:CE1	1:B:746:PHE:HE1	2.40	0.40
1:D:865:HIS:O	1:D:866:ILE:HD13	2.21	0.40
1:B:643:CYS:O	1:B:646:VAL:HG22	2.21	0.40
1:C:703:THR:HG21	1:D:837:GLU:CD	2.42	0.40
1:A:626:MET:O	1:A:627:ASN:HB3	2.21	0.40
1:A:893:GLU:O	1:A:897:LYS:CG	2.66	0.40
1:B:824:GLU:CB	3:B:153:HOH:O	2.38	0.40

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	301/345 (87%)	285 (95%)	14 (5%)	2 (1%)	22	39
1	B	314/345 (91%)	305 (97%)	8 (2%)	1 (0%)	41	61
1	C	304/345 (88%)	292 (96%)	11 (4%)	1 (0%)	41	61
1	D	314/345 (91%)	301 (96%)	13 (4%)	0	100	100
All	All	1233/1380 (89%)	1183 (96%)	46 (4%)	4 (0%)	41	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	837	GLU
1	A	839	ALA
1	B	711	SER
1	C	580	ASP

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	276/310 (89%)	253 (92%)	23 (8%)	11	22
1	B	287/310 (93%)	265 (92%)	22 (8%)	13	25
1	C	280/310 (90%)	258 (92%)	22 (8%)	12	24
1	D	287/310 (93%)	254 (88%)	33 (12%)	5	11
All	All	1130/1240 (91%)	1030 (91%)	100 (9%)	10	19

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	588	ASP
1	A	591	GLN

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Mol	Chain	Res	Type
1	A	593	VAL
1	A	599	ASN
1	A	644	LEU
1	A	648	LYS
1	A	652	ASP
1	A	724	SER
1	A	738	LEU
1	A	756	ARG
1	A	766	LEU
1	A	770	LEU
1	A	782	LYS
1	A	790	ARG
1	A	794	GLN
1	A	827	TYR
1	A	840	MET
1	A	845	MET
1	A	850	ARG
1	A	872	LYS
1	A	890	SER
1	A	893	GLU
1	A	894	HIS
1	B	586	LEU
1	B	593	VAL
1	B	599	ASN
1	B	617	MET
1	B	621	SER
1	B	624	GLN
1	B	644	LEU
1	B	645	MET
1	B	711	SER
1	B	713	SER
1	B	728	ARG
1	B	758	LEU
1	B	770	LEU
1	B	775	ARG
1	B	805	THR
1	B	817	LYS
1	B	857	GLU
1	B	886	GLU
1	B	887	ARG
1	B	892	ARG
1	B	893	GLU

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Mol	Chain	Res	Type
1	B	898	VAL
1	C	598	SER
1	C	617	MET
1	C	624	GLN
1	C	630	ASN
1	C	706	SER
1	C	725	VAL
1	C	738	LEU
1	C	770	LEU
1	C	775	ARG
1	C	786	VAL
1	C	805	THR
1	C	818	THR
1	C	820	ARG
1	C	837	GLU
1	C	846	GLU
1	C	848	MET
1	C	864	GLU
1	C	872	LYS
1	C	874	LEU
1	C	888	VAL
1	C	890	SER
1	C	892	ARG
1	D	583	THR
1	D	587	HIS
1	D	591	GLN
1	D	593	VAL
1	D	598	SER
1	D	599	ASN
1	D	644	LEU
1	D	678	THR
1	D	682	GLU
1	D	687	PHE
1	D	722	GLU
1	D	724	SER
1	D	733	GLN
1	D	747	ASP
1	D	748	HIS
1	D	751	ARG
1	D	752	LYS
1	D	756	ARG
1	D	758	LEU

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Mol	Chain	Res	Type
1	D	770	LEU
1	D	782	LYS
1	D	785	GLU
1	D	790	ARG
1	D	797	ARG
1	D	820	ARG
1	D	833	GLN
1	D	845	MET
1	D	847	MET
1	D	870	ILE
1	D	874	LEU
1	D	893	GLU
1	D	894	HIS
1	D	896	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	656	HIS
1	A	705	ASN
1	A	730	HIS
1	A	733	GLN
1	A	859	GLN
1	A	875	GLN
1	B	587	HIS
1	B	730	HIS
1	B	733	GLN
1	B	739	ASN
1	B	781	GLN
1	B	875	GLN
1	C	630	ASN
1	C	631	ASN
1	C	656	HIS
1	C	730	HIS
1	C	733	GLN
1	C	795	HIS
1	C	875	GLN
1	D	599	ASN
1	D	679	ASN
1	D	704	ASN
1	D	730	HIS
1	D	733	GLN

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Mol	Chain	Res	Type
1	D	755	GLN
1	D	859	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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 ⓘ

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	307/345 (88%)	0.31	7 (2%) 60 63	37, 42, 48, 56	0
1	B	318/345 (92%)	0.23	7 (2%) 62 65	36, 43, 49, 71	0
1	C	310/345 (89%)	0.45	25 (8%) 12 12	38, 43, 47, 71	0
1	D	318/345 (92%)	0.48	19 (5%) 21 22	37, 42, 49, 74	0
All	All	1253/1380 (90%)	0.37	58 (4%) 32 34	36, 43, 49, 74	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	839	ALA	7.6
1	C	586	LEU	5.1
1	D	586	LEU	5.0
1	C	827	TYR	4.9
1	A	588	ASP	4.9
1	C	593	VAL	4.5
1	D	587	HIS	4.4
1	C	582	TYR	4.3
1	C	594	ALA	4.1
1	C	840	MET	4.0
1	A	589	GLY	4.0
1	C	837	GLU	3.7
1	D	841	GLY	3.6
1	C	845	MET	3.6
1	C	838	LYS	3.6
1	C	587	HIS	3.5
1	D	895	TRP	3.5
1	C	856	PRO	3.5
1	B	890	SER	3.4
1	D	588	ASP	3.3
1	D	585	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	596	ILE	3.3
1	D	816	TRP	3.3
1	B	603	PHE	3.2
1	D	893	GLU	3.2
1	D	583	THR	3.2
1	D	580	ASP	3.0
1	B	839	ALA	3.0
1	A	894	HIS	2.9
1	A	827	TYR	2.9
1	D	881	ALA	2.9
1	C	817	LYS	2.8
1	C	604	THR	2.8
1	D	582	TYR	2.7
1	D	584	LYS	2.7
1	C	580	ASP	2.7
1	D	891	ASN	2.7
1	D	896	THR	2.6
1	D	817	LYS	2.6
1	C	820	ARG	2.6
1	B	894	HIS	2.5
1	B	602	SER	2.5
1	C	881	ALA	2.5
1	A	836	LEU	2.5
1	C	893	GLU	2.4
1	A	840	MET	2.3
1	C	887	ARG	2.3
1	D	617	MET	2.3
1	D	839	ALA	2.3
1	B	838	LYS	2.3
1	A	816	TRP	2.2
1	C	895	TRP	2.2
1	C	600	PHE	2.1
1	B	833	GLN	2.1
1	C	890	SER	2.1
1	C	583	THR	2.1
1	C	894	HIS	2.0
1	D	604	THR	2.0

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

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	ZN	D	4	1/1	0.99	0.02	38,38,38,38	0
2	ZN	C	3	1/1	0.99	0.03	42,42,42,42	0
2	ZN	B	2	1/1	0.99	0.02	30,30,30,30	0
2	ZN	A	1	1/1	1.00	0.01	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.