



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:49 PM UTC

PDB ID : 3ITM / pdb_00003itm
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 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

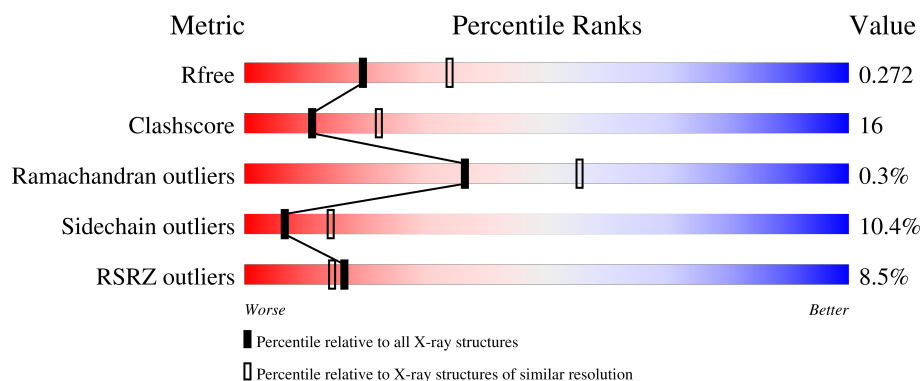
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	345	4% 61% 21% 5% • 11%
1	B	345	4% 62% 23% 6% • 8%
1	C	345	12% 62% 21% 6% • 10%
1	D	345	10% 59% 26% 7% • 8%

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:

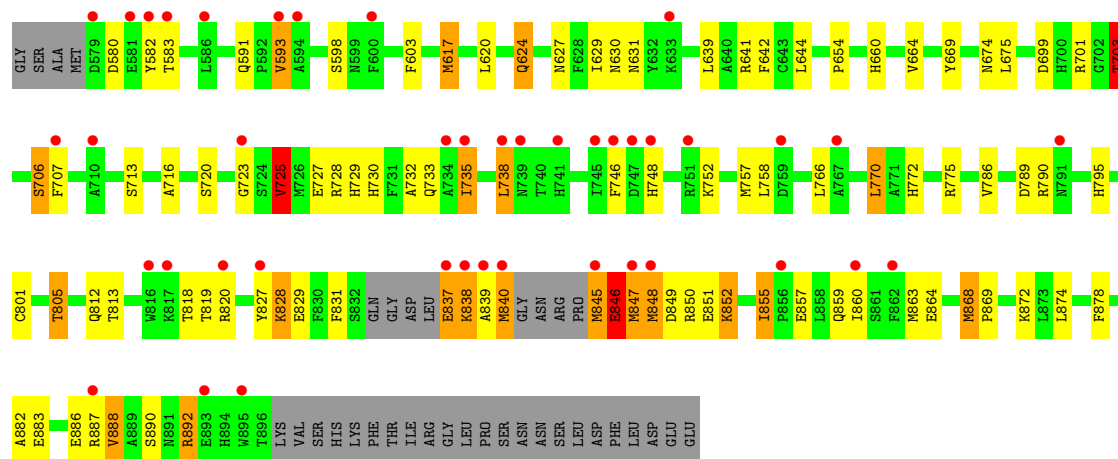
Chain	Residue	Modelled	Actual	Comment	Reference
A	575	GLY	-	expression tag	UNP O00408
A	576	SER	-	expression tag	UNP O00408
A	577	ALA	-	expression tag	UNP O00408
A	578	MET	-	expression tag	UNP O00408
B	575	GLY	-	expression tag	UNP O00408
B	576	SER	-	expression tag	UNP O00408
B	577	ALA	-	expression tag	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 (CCD ID: ZN) (formula: Zn).

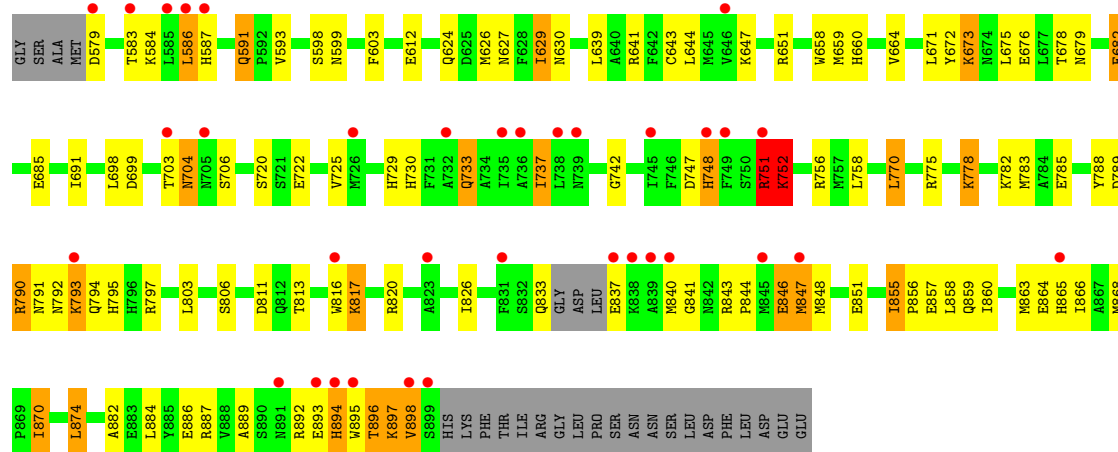
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

- 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



• 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 50.00 – 2.49	Depositor EDS
% Data completeness (in resolution range)	84.5 (50.00-2.49) 84.5 (50.00-2.49)	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 (4.32%)	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)	0.34 , 53.0	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	0.91	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	1.84	40/2573 (1.6%)	1.29	16/3468 (0.5%)
1	B	1.66	35/2671 (1.3%)	1.32	17/3602 (0.5%)
1	C	1.50	28/2608 (1.1%)	1.15	8/3516 (0.2%)
1	D	1.17	14/2671 (0.5%)	1.15	16/3602 (0.4%)
All	All	1.56	117/10523 (1.1%)	1.23	57/14188 (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 (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	840	MET	SD-CE	32.66	2.61	1.79
1	A	837	GLU	CD-OE2	23.86	1.70	1.25
1	B	852	LYS	CG-CD	19.45	2.10	1.52
1	A	831	PHE	CE1-CZ	18.45	1.94	1.38
1	B	844	PRO	C-N	18.36	1.55	1.33
1	A	847	MET	CG-SD	17.91	2.25	1.80
1	C	838	LYS	CE-NZ	17.51	2.01	1.49
1	B	838	LYS	CG-CD	17.49	2.04	1.52
1	B	840	MET	C-N	17.36	1.58	1.33
1	C	845	MET	SD-CE	17.33	2.22	1.79
1	A	900	HIS	C-N	17.10	1.57	1.33
1	C	847	MET	CG-SD	17.04	2.23	1.80
1	C	838	LYS	CD-CE	16.82	2.02	1.52
1	C	828	LYS	CG-CD	16.47	2.01	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	852	LYS	CD-CE	16.13	2.00	1.52
1	A	831	PHE	CG-CD2	15.54	1.71	1.38
1	D	752	LYS	CE-NZ	15.32	1.95	1.49
1	D	751	ARG	CZ-NH2	15.12	1.53	1.33
1	B	831	PHE	CG-CD2	15.05	1.70	1.38
1	B	842	ASN	C-N	14.57	1.50	1.33
1	C	849	ASP	C-O	14.50	1.41	1.24
1	A	898	VAL	C-O	13.92	1.40	1.24
1	B	852	LYS	CB-CG	13.91	1.94	1.52
1	C	852	LYS	CE-NZ	12.92	1.88	1.49
1	C	847	MET	SD-CE	12.59	2.11	1.79
1	A	845	MET	SD-CE	11.75	2.08	1.79
1	C	852	LYS	CD-CE	11.70	1.87	1.52
1	C	828	LYS	CB-CG	11.64	1.87	1.52
1	B	838	LYS	CD-CE	11.18	1.85	1.52
1	A	831	PHE	CG-CD1	11.16	1.62	1.38
1	A	901	LYS	CA-CB	11.01	1.75	1.53
1	A	840	MET	CG-SD	-11.00	1.53	1.80
1	A	848	MET	CG-SD	10.48	2.06	1.80
1	C	849	ASP	C-N	10.37	1.47	1.34
1	B	852	LYS	CE-NZ	10.17	1.79	1.49
1	C	840	MET	SD-CE	9.88	2.04	1.79
1	A	838	LYS	CD-CE	9.81	1.81	1.52
1	A	714	VAL	CA-CB	9.78	1.65	1.54
1	D	841	GLY	C-N	9.76	1.47	1.33
1	A	827	TYR	C-O	9.75	1.35	1.24
1	C	851	GLU	CD-OE1	9.74	1.43	1.25
1	B	837	GLU	CD-OE1	9.74	1.43	1.25
1	D	793	LYS	CD-CE	9.69	1.81	1.52
1	A	848	MET	SD-CE	9.62	2.03	1.79
1	B	841	GLY	C-N	9.58	1.46	1.33
1	A	901	LYS	C-O	9.55	1.42	1.23
1	C	840	MET	CG-SD	9.54	2.04	1.80
1	C	851	GLU	CD-OE2	9.54	1.43	1.25
1	B	841	GLY	CA-C	9.39	1.65	1.51
1	B	843	ARG	NE-CZ	9.38	1.43	1.33
1	A	847	MET	SD-CE	9.29	2.02	1.79
1	C	849	ASP	CG-OD2	9.15	1.42	1.25
1	A	846	GLU	CD-OE2	9.09	1.42	1.25
1	B	846	GLU	CA-C	9.06	1.65	1.52
1	A	837	GLU	CB-CG	8.91	1.79	1.52
1	D	751	ARG	CD-NE	8.59	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	828	LYS	CE-NZ	8.43	1.74	1.49
1	C	831	PHE	CG-CD1	8.03	1.55	1.38
1	C	845	MET	CG-SD	7.96	2.00	1.80
1	C	849	ASP	CG-OD1	7.79	1.40	1.25
1	A	897	LYS	CE-NZ	7.67	1.72	1.49
1	C	846	GLU	CD-OE2	7.65	1.39	1.25
1	A	901	LYS	CA-C	7.53	1.68	1.52
1	B	847	MET	SD-CE	7.41	1.98	1.79
1	B	845	MET	CG-SD	7.37	1.99	1.80
1	D	897	LYS	CE-NZ	7.34	1.71	1.49
1	C	790	ARG	C-N	7.14	1.43	1.33
1	B	848	MET	CA-CB	7.14	1.64	1.53
1	A	846	GLU	CA-C	7.14	1.62	1.52
1	A	896	THR	CB-OG1	7.10	1.55	1.43
1	B	846	GLU	CD-OE2	7.10	1.38	1.25
1	B	842	ASN	CA-CB	7.09	1.64	1.53
1	A	850	ARG	NE-CZ	7.01	1.40	1.33
1	B	842	ASN	CA-C	6.91	1.61	1.53
1	B	841	GLY	C-O	6.89	1.33	1.23
1	A	850	ARG	CZ-NH1	6.81	1.42	1.32
1	B	840	MET	C-O	6.79	1.32	1.23
1	D	778	LYS	CE-NZ	6.79	1.69	1.49
1	B	848	MET	CG-SD	6.75	1.97	1.80
1	B	897	LYS	CD-CE	6.69	1.72	1.52
1	D	793	LYS	CG-CD	6.64	1.72	1.52
1	A	838	LYS	CA-C	6.63	1.61	1.52
1	A	830	PHE	CA-C	6.56	1.61	1.52
1	A	900	HIS	C-O	6.56	1.34	1.23
1	A	831	PHE	CA-CB	6.48	1.64	1.53
1	A	853	ALA	C-N	6.47	1.43	1.33
1	A	837	GLU	CA-C	6.46	1.61	1.52
1	A	837	GLU	CD-OE1	6.44	1.37	1.25
1	C	847	MET	CA-CB	6.43	1.64	1.53
1	B	846	GLU	CG-CD	6.32	1.67	1.52
1	D	790	ARG	CZ-NH1	6.24	1.41	1.32
1	D	817	LYS	CE-NZ	6.20	1.68	1.49
1	B	830	PHE	CA-C	6.18	1.60	1.52
1	A	636	CYS	C-O	-6.13	1.18	1.24
1	D	846	GLU	CD-OE1	6.04	1.36	1.25
1	A	898	VAL	C-N	5.97	1.42	1.33
1	B	831	PHE	CA-CB	5.88	1.63	1.53
1	B	831	PHE	CE1-CZ	5.84	1.56	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	845	MET	CA-CB	5.81	1.65	1.53
1	C	839	ALA	CA-C	5.72	1.60	1.53
1	A	846	GLU	CD-OE1	5.55	1.35	1.25
1	B	661	ALA	CA-CB	-5.53	1.44	1.53
1	B	672	TYR	C-O	-5.48	1.17	1.24
1	C	839	ALA	CA-CB	5.44	1.61	1.53
1	C	725	VAL	CA-CB	5.30	1.60	1.55
1	B	635	ASP	CA-C	5.27	1.59	1.52
1	D	791	ASN	CA-C	-5.26	1.45	1.52
1	C	703	THR	C-O	5.26	1.30	1.23
1	B	878	PHE	C-O	-5.23	1.19	1.24
1	D	691	ILE	CA-CB	5.21	1.61	1.54
1	B	830	PHE	CA-CB	5.17	1.61	1.53
1	A	857	GLU	CG-CD	5.15	1.65	1.52
1	C	852	LYS	CG-CD	5.12	1.67	1.52
1	A	732	ALA	CA-CB	-5.04	1.45	1.53
1	B	734	ALA	CA-CB	-5.02	1.45	1.53
1	D	789	ASP	C-O	5.01	1.29	1.24
1	A	827	TYR	N-CA	-5.00	1.40	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	838	LYS	CG-CD-CE	-12.71	82.06	111.30
1	B	852	LYS	CG-CD-CE	-12.62	82.27	111.30
1	B	852	LYS	CB-CG-CD	-12.50	82.56	111.30
1	D	751	ARG	NE-CZ-NH2	10.73	128.86	119.20
1	B	842	ASN	CA-C-N	-10.51	109.50	122.42
1	B	842	ASN	C-N-CA	-10.51	109.50	122.42
1	C	828	LYS	CB-CG-CD	-9.95	88.43	111.30
1	A	840	MET	CG-SD-CE	-9.48	80.03	100.90
1	D	898	VAL	N-CA-C	8.75	120.77	107.99
1	B	898	VAL	N-CA-C	8.39	119.96	107.80
1	C	847	MET	CG-SD-CE	-8.11	83.06	100.90
1	D	704	ASN	CB-CA-C	7.90	123.67	110.79
1	B	852	LYS	CD-CE-NZ	-7.68	87.33	111.90
1	C	849	ASP	O-C-N	7.66	130.36	122.09
1	B	838	LYS	CB-CG-CD	-7.64	93.73	111.30
1	C	852	LYS	CD-CE-NZ	-7.62	87.50	111.90
1	D	793	LYS	CG-CD-CE	-7.25	94.61	111.30
1	A	840	MET	CA-C-O	7.19	133.02	120.80
1	A	831	PHE	N-CA-C	7.17	121.72	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	735	ILE	CB-CA-C	-7.07	102.60	112.14
1	B	848	MET	CG-SD-CE	7.01	116.32	100.90
1	A	837	GLU	CG-CD-OE1	-7.00	102.29	118.40
1	A	646	VAL	N-CA-CB	6.92	119.95	110.54
1	C	838	LYS	CB-CG-CD	6.73	126.77	111.30
1	A	901	LYS	CA-C-O	-6.71	109.39	120.80
1	D	751	ARG	NH1-CZ-NH2	-6.68	110.61	119.30
1	D	703	THR	CA-C-N	-6.47	113.92	123.11
1	D	703	THR	C-N-CA	-6.47	113.92	123.11
1	B	689	LEU	N-CA-C	-6.37	104.26	111.14
1	A	827	TYR	O-C-N	6.26	128.52	122.07
1	C	852	LYS	CG-CD-CE	-6.21	97.02	111.30
1	B	838	LYS	CD-CE-NZ	-6.16	92.18	111.90
1	D	591	GLN	CB-CA-C	6.06	117.89	108.61
1	B	838	LYS	N-CA-C	6.01	118.91	109.96
1	A	831	PHE	CB-CG-CD1	-5.96	110.56	120.70
1	D	848	MET	N-CA-C	-5.93	105.54	112.89
1	A	859	GLN	N-CA-C	-5.81	105.02	111.36
1	A	828	LYS	N-CA-C	-5.77	105.12	111.82
1	D	791	ASN	CB-CA-C	-5.75	97.87	109.55
1	D	792	ASN	OD1-CG-ND2	5.67	128.28	122.60
1	A	831	PHE	CG-CD1-CE1	-5.66	111.09	120.70
1	C	847	MET	CA-CB-CG	-5.62	102.86	114.10
1	B	841	GLY	CA-C-O	5.62	130.34	120.57
1	D	737	ILE	CB-CA-C	-5.61	104.80	111.81
1	A	840	MET	CB-CG-SD	-5.60	95.91	112.70
1	A	610	LEU	CA-C-N	-5.56	114.05	119.78
1	A	610	LEU	C-N-CA	-5.56	114.05	119.78
1	B	852	LYS	CA-CB-CG	-5.50	103.10	114.10
1	D	793	LYS	CD-CE-NZ	-5.43	94.51	111.90
1	A	831	PHE	CD1-CG-CD2	5.40	126.69	118.60
1	B	843	ARG	NE-CZ-NH2	-5.34	114.40	119.20
1	A	631	ASN	N-CA-C	5.33	117.09	111.28
1	B	839	ALA	N-CA-C	-5.29	103.16	110.35
1	D	790	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	D	791	ASN	CA-CB-CG	-5.17	107.43	112.60
1	D	855	ILE	CB-CA-C	-5.09	108.86	113.70
1	C	849	ASP	CB-CG-OD1	-5.02	106.86	118.40

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	78	0
1	B	2609	0	2552	91	0
1	C	2548	0	2487	92	0
1	D	2609	0	2552	91	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
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	331	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 16.

All (331) 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:CE	1:D:817:LYS:NZ	1.68	1.57
1:A:831:PHE:CZ	1:A:831:PHE:CE1	1.94	1.56
1:A:837:GLU:CB	1:A:837:GLU:CG	1.79	1.55
1:A:838:LYS:CE	1:A:838:LYS:CD	1.81	1.54
1:D:778:LYS:CE	1:D:778:LYS:NZ	1.69	1.54
1:D:793:LYS:CE	1:D:793:LYS:CD	1.81	1.53
1:C:852:LYS:CE	1:C:852:LYS:CD	1.87	1.53
1:B:838:LYS:CD	1:B:838:LYS:CE	1.86	1.50
1:C:828:LYS:CE	1:C:828:LYS:NZ	1.74	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:897:LYS:NZ	1:D:897:LYS:CE	1.71	1.49
1:C:828:LYS:CG	1:C:828:LYS:CB	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:SD	1:C:840:MET:CE	2.04	1.46
1:A:847:MET:CE	1:A:847:MET:SD	2.02	1.45
1:C:840:MET:SD	1:C:840:MET:CG	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:CE	1:B:852:LYS:NZ	1.79	1.42
1:A:845:MET:SD	1:A:845:MET:CE	2.08	1.40
1:B:852:LYS:CE	1:B:852:LYS:CD	2.00	1.39
1:C:847:MET:SD	1:C:847:MET:CE	2.11	1.39
1:C:852:LYS:CE	1:C:852:LYS:NZ	1.88	1.37
1:C:838:LYS:CE	1:C:838:LYS:CD	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:A:837:GLU:CD	1:A:837:GLU:OE2	1.70	1.34
1:D:752:LYS:NZ	1:D:752:LYS:CE	1.95	1.29
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:CE	1:C:838:LYS:NZ	2.01	1.22
1:C:837:GLU:OE1	1:C:837:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:725:VAL:HA	1:B:847:MET:HE2	1.57	0.85
1:D:751:ARG:HG2	1:D:751:ARG:HH11	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:CD	1:B:838:LYS:NZ	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:CE	1:D:793:LYS:CG	2.60	0.79
1:B:819:THR:CG2	1:B:895:TRP:HE1	1.96	0.79
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:CE	1:C:852:LYS:CG	2.66	0.73
1:B:852:LYS:CB	1:B:852:LYS:CD	2.67	0.73
1:A:723:GLY:O	1:B:840:MET:HG3	1.88	0.73
1:C:746:PHE:CZ	1:C:757:MET:HE2	2.24	0.73
1:A:837:GLU:CG	1:A:837:GLU:CA	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:A:868:MET:HE3	1:A:889:ALA:HA	1.71	0.71
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:SD	1:C:840:MET:CB	2.81	0.68
1:D:897:LYS:NZ	1:D:897:LYS:CD	2.54	0.68
1:B:852:LYS:CG	1:B:852:LYS:CA	2.72	0.68
1:C:838:LYS:CE	1:C:838:LYS:CG	2.71	0.68
1:A:893:GLU:OE1	1:A:893:GLU:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:893:GLU:OE2	1:B:893:GLU:HA	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:D:868:MET:HE1	1:D:892:ARG:HB2	1.76	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:C:837:GLU:N	1:C:837:GLU:CD	2.57	0.63
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
1:B:852:LYS:NZ	1:B:852:LYS:CD	2.63	0.62
1:C:868:MET:HE2	1:C:888:VAL:HG23	1.82	0.62
1:D:863:MET:HE3	1:D:892:ARG:HA	1.81	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: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: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:C:848:MET:HA	1:C:848:MET:HE3	1.84	0.58
1:B:701:ARG:HB2	1:B:728:ARG:HH11	1.66	0.58
1:A:868:MET:HE2	1:A:889:ALA:HA	1.79	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:863:MET:HE2	1:D:895:TRP:CD1	2.41	0.55
1:A:837:GLU:CB	1:A:837:GLU:CD	2.75	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:B:645:MET:HE2	1:B:645:MET:HA	1.90	0.54
1:A:901:LYS:CB	1:A:901:LYS:N	2.63	0.54
1:B:646:VAL:HG21	1:B:694:MET:HE2	1.88	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:CG	1:C:828:LYS:CA	2.80	0.54
1:D:751:ARG:HH11	1:D:751:ARG:CG	2.17	0.53
1:C:859:GLN:OE1	1:C:863:MET:HE3	2.09	0.53
1:D:752:LYS:NZ	1:D:752:LYS:CD	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:O	1:C:703:THR:HG22	2.09	0.52
1:A:705:ASN:O	1:B:831:PHE:HE2	1.92	0.52
1:B:646:VAL:HG23	1:B:647:LYS:N	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:A:893:GLU:CA	2.58	0.52
1:D:612:GLU:HB2	1:D:659:MET:HE1	1.92	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:D:863:MET:HE3	1:D:892:ARG:N	2.24	0.51
1:C:642:PHE:CD2	1:C:642:PHE:C	2.89	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:OD1	1:A:588:ASP:N	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:847:MET:HE3	1:B:725:VAL:HA	1.93	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:C:827:TYR:CZ	1:C:852:LYS:CG	2.92	0.50
1:D:863:MET:HE3	1:D:892:ARG:CA	2.40	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:626:MET:HE3	1:D:672:TYR:CG	2.48	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:A:901:LYS:CB	1:A:901:LYS:C	2.78	0.49
1:C:703:THR:HG21	1:D:837:GLU:OE2	2.13	0.49
1:C:827:TYR:OH	1:C:848:MET:HE2	2.12	0.49
1:D:863:MET:HE2	1:D:895:TRP:HD1	1.77	0.49
1:B:863:MET:HE2	1:B:895:TRP:CD1	2.48	0.48
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:645:MET:HE2	1:A:743:CYS:SG	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:THR:CG2	1:A:705:ASN:ND2	2.77	0.48
1:D:868:MET:HE1	1:D:892:ARG:CB	2.42	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:C:729:HIS:O	1:C:733:GLN:HB2	2.15	0.47
1:D:626:MET:HE3	1:D:672:TYR:CB	2.44	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:D:584:LYS:C	1:D:586:LEU:H	2.23	0.46
1:A:840:MET:HE2	1:B:766:LEU:HD11	1.96	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:CG	1:B:838:LYS:HE3	2.44	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:C:725:VAL:HG23	1:D:847:MET:HE3	1.98	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:C:703:THR:HG21	1:D:837:GLU:CD	2.42	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:D:659:MET:HB2	1:D:659:MET:HE2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:840:MET:CE	1:C:840:MET:CG	2.95	0.44
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: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:A:838:LYS:C	1:A:839:ALA:O	2.57	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:HG2	1:D:682:GLU:H	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:HE3	1:B:673:LYS:HB3	1.75	0.44
1:B:852:LYS:CD	1:B:852:LYS:HB2	2.47	0.44
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: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:HD12	1:B:644:LEU:HA	1.71	0.42
1:C:789:ASP:H	1:C:795:HIS:CD2	2.30	0.42
1:A:832:SER:C	1:A:836:LEU:HD23	2.43	0.42
1:D:855:ILE:HB	1:D:856:PRO:HD3	2.00	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
1:A:740:THR:O	1:A:741:HIS:C	2.62	0.42
1:A:840:MET:HE2	1:B:766:LEU:CD1	2.50	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:OD1	1:B:652:ASP:N	2.47	0.42
1:D:682:GLU:HG2	1:D:685:GLU:CD	2.45	0.42
1:B:843:ARG:HA	1:B:844:PRO:HD2	1.85	0.41
1:B:816:TRP:CZ3	1:B:895:TRP:CE2	3.09	0.41
1:C:868:MET:HE1	1:C:892:ARG:CB	2.50	0.41
1:D:794:GLN:OE1	1:D:794:GLN:HA	2.19	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:HA	1:B:785:GLU:OE1	2.20	0.41
1:C:582:TYR:O	1:C:583:THR:C	2.63	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:A:847:MET:SD	1:A:847:MET:CB	2.99	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:C:713:SER:HB3	1:C:716:ALA:CB	2.50	0.41
1:D:840:MET:HE3	1:D:840:MET:HB3	1.82	0.41
1:B:687:PHE:CE1	1:B:746:PHE:HE1	2.40	0.40
1:B:840:MET:C	1:B:842:ASN:H	2.28	0.40
1:D:865:HIS:O	1:D:866:ILE:HD13	2.21	0.40
1:D:868:MET:HE2	1:D:889:ALA:HA	2.02	0.40
1:B:643:CYS:O	1:B:646:VAL:HG22	2.21	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%)	18	34
1	B	314/345 (91%)	305 (97%)	8 (2%)	1 (0%)	36	55
1	C	304/345 (88%)	292 (96%)	11 (4%)	1 (0%)	36	55
1	D	314/345 (91%)	301 (96%)	13 (4%)	0	100	100
All	All	1233/1380 (89%)	1183 (96%)	46 (4%)	4 (0%)	36	55

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%)	247 (90%)	29 (10%)	6	14
1	B	287/310 (93%)	263 (92%)	24 (8%)	10	22
1	C	280/310 (90%)	251 (90%)	29 (10%)	7	14
1	D	287/310 (93%)	252 (88%)	35 (12%)	5	10
All	All	1130/1240 (91%)	1013 (90%)	117 (10%)	7	14

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	588	ASP
1	A	591	GLN
1	A	593	VAL
1	A	599	ASN
1	A	610	LEU
1	A	624	GLN
1	A	644	LEU
1	A	646	VAL
1	A	652	ASP
1	A	724	SER
1	A	725	VAL
1	A	733	GLN
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	826	ILE
1	A	827	TYR
1	A	838	LYS
1	A	845	MET
1	A	863	MET
1	A	870	ILE
1	A	872	LYS
1	A	890	SER
1	A	893	GLU
1	A	894	HIS
1	B	583	THR
1	B	586	LEU
1	B	593	VAL
1	B	599	ASN
1	B	624	GLN
1	B	644	LEU
1	B	645	MET
1	B	648	LYS
1	B	711	SER
1	B	715	LEU
1	B	758	LEU
1	B	770	LEU
1	B	775	ARG

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Mol	Chain	Res	Type
1	B	805	THR
1	B	822	ILE
1	B	826	ILE
1	B	843	ARG
1	B	852	LYS
1	B	857	GLU
1	B	886	GLU
1	B	887	ARG
1	B	892	ARG
1	B	893	GLU
1	B	898	VAL
1	C	593	VAL
1	C	598	SER
1	C	617	MET
1	C	624	GLN
1	C	630	ASN
1	C	703	THR
1	C	706	SER
1	C	725	VAL
1	C	735	ILE
1	C	738	LEU
1	C	752	LYS
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	855	ILE
1	C	857	GLU
1	C	864	GLU
1	C	868	MET
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	586	LEU

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Mol	Chain	Res	Type
1	D	587	HIS
1	D	591	GLN
1	D	593	VAL
1	D	598	SER
1	D	599	ASN
1	D	629	ILE
1	D	630	ASN
1	D	644	LEU
1	D	673	LYS
1	D	678	THR
1	D	682	GLU
1	D	722	GLU
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
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	847	MET
1	D	870	ILE
1	D	874	LEU
1	D	893	GLU
1	D	894	HIS
1	D	896	THR
1	D	898	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	599	ASN
1	A	627	ASN
1	A	630	ASN
1	A	656	HIS
1	A	704	ASN

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Mol	Chain	Res	Type
1	A	705	ASN
1	A	730	HIS
1	A	733	GLN
1	A	739	ASN
1	A	859	GLN
1	A	875	GLN
1	B	587	HIS
1	B	599	ASN
1	B	624	GLN
1	B	700	HIS
1	B	730	HIS
1	B	733	GLN
1	B	739	ASN
1	B	781	GLN
1	B	833	GLN
1	B	875	GLN
1	C	630	ASN
1	C	631	ASN
1	C	656	HIS
1	C	666	HIS
1	C	729	HIS
1	C	730	HIS
1	C	733	GLN
1	C	739	ASN
1	C	773	HIS
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
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.57	15 (4%)	35 31	37, 42, 48, 56	0
1	B	318/345 (92%)	0.44	14 (4%)	39 34	36, 43, 49, 71	0
1	C	310/345 (89%)	1.11	42 (13%)	7 5	38, 43, 47, 71	0
1	D	318/345 (92%)	0.91	35 (11%)	10 8	37, 42, 49, 74	0
All	All	1253/1380 (90%)	0.76	106 (8%)	16 14	36, 43, 49, 74	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	839	ALA	7.6
1	A	588	ASP	4.6
1	C	827	TYR	4.4
1	C	838	LYS	4.3
1	A	827	TYR	4.2
1	C	845	MET	4.0
1	A	901	LYS	4.0
1	D	739	ASN	3.9
1	A	589	GLY	3.8
1	D	838	LYS	3.8
1	C	895	TRP	3.7
1	C	837	GLU	3.7
1	C	856	PRO	3.6
1	A	836	LEU	3.5
1	D	839	ALA	3.4
1	B	838	LYS	3.4
1	D	579	ASP	3.3
1	C	840	MET	3.3
1	D	837	GLU	3.3
1	C	579	ASP	3.3
1	D	586	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	839	ALA	3.2
1	D	891	ASN	3.2
1	D	587	HIS	3.1
1	C	593	VAL	3.1
1	D	745	ILE	3.1
1	B	846	GLU	3.0
1	B	890	SER	3.0
1	D	732	ALA	3.0
1	A	845	MET	2.9
1	D	895	TRP	2.9
1	C	707	PHE	2.9
1	D	845	MET	2.9
1	C	745	ILE	2.7
1	C	586	LEU	2.7
1	C	817	LYS	2.7
1	D	585	LEU	2.7
1	C	816	TRP	2.7
1	D	703	THR	2.7
1	C	751	ARG	2.6
1	B	847	MET	2.6
1	C	738	LEU	2.6
1	D	893	GLU	2.6
1	D	899	SER	2.6
1	C	820	ARG	2.6
1	D	738	LEU	2.6
1	D	736	ALA	2.6
1	C	893	GLU	2.5
1	C	791	ASN	2.5
1	C	847	MET	2.5
1	C	748	HIS	2.5
1	D	894	HIS	2.5
1	B	893	GLU	2.5
1	D	748	HIS	2.5
1	C	600	PHE	2.4
1	B	845	MET	2.4
1	C	583	THR	2.4
1	D	749	PHE	2.4
1	C	759	ASP	2.4
1	D	735	ILE	2.4
1	A	840	MET	2.4
1	B	703	THR	2.4
1	C	734	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	847	MET	2.3
1	B	589	GLY	2.3
1	C	723	GLY	2.3
1	A	707	PHE	2.3
1	D	816	TRP	2.3
1	A	848	MET	2.3
1	D	840	MET	2.3
1	C	710	ALA	2.3
1	A	900	HIS	2.3
1	C	735	ILE	2.3
1	D	831	PHE	2.3
1	D	751	ARG	2.3
1	A	652	ASP	2.2
1	B	704	ASN	2.2
1	D	823	ALA	2.2
1	B	579	ASP	2.2
1	C	767	ALA	2.2
1	C	633	LYS	2.2
1	C	848	MET	2.2
1	D	793	LYS	2.2
1	C	582	TYR	2.2
1	C	739	ASN	2.1
1	D	583	THR	2.1
1	C	860	ILE	2.1
1	C	747	ASP	2.1
1	D	898	VAL	2.1
1	D	726	MET	2.1
1	C	594	ALA	2.1
1	C	581	GLU	2.1
1	C	862	PHE	2.1
1	D	646	VAL	2.1
1	A	816	TRP	2.1
1	B	651	ARG	2.1
1	A	887	ARG	2.1
1	C	887	ARG	2.1
1	A	750	SER	2.1
1	B	840	MET	2.1
1	C	741	HIS	2.1
1	D	865	HIS	2.1
1	B	844	PRO	2.0
1	C	746	PHE	2.0
1	A	766	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	705	ASN	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
2	ZN	C	3	1/1	0.98	0.12	42,42,42,42	0
2	ZN	B	2	1/1	0.99	0.14	30,30,30,30	0
2	ZN	A	1	1/1	0.99	0.14	33,33,33,33	0
2	ZN	D	4	1/1	0.99	0.13	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.