



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:54 PM UTC

PDB ID : 3ITU / pdb_00003itu
Title : hPDE2A catalytic domain complexed with IBMX
Authors : Pandit, J.
Deposited on : 2009-08-28
Resolution : 1.58 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
Mogul : 2022.3.0, CSD as543be (2022)
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

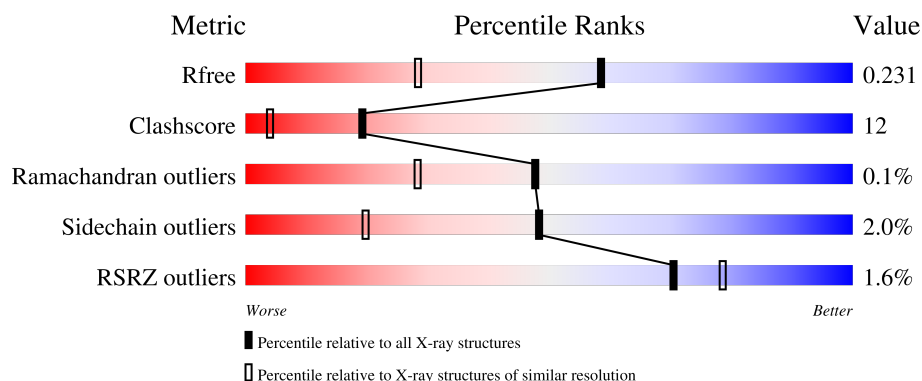
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	
1	B	345	
1	C	345	
1	D	345	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12700 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	338	Total	C	N	O	S	0	0	0
			2767	1763	474	505	25			
1	B	333	Total	C	N	O	S	0	0	0
			2732	1743	469	495	25			
1	C	327	Total	C	N	O	S	0	0	0
			2676	1707	460	484	25			
1	D	327	Total	C	N	O	S	0	0	0
			2676	1707	460	484	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

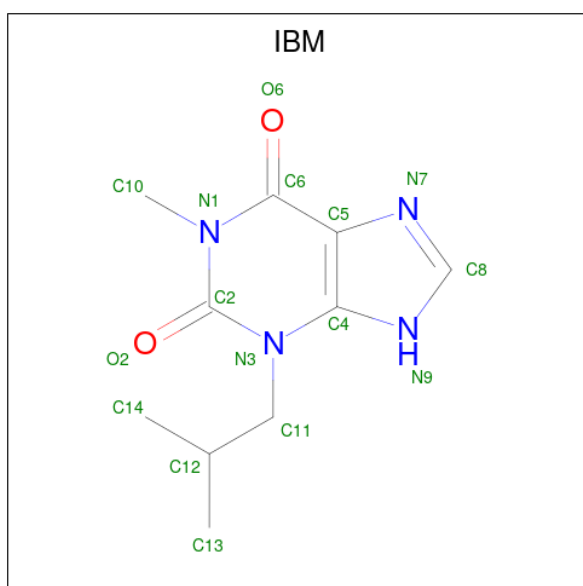
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 3-ISOBUTYL-1-METHYLNANTHINE (CCD ID: IBM) (formula: C₁₀H₁₄N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	10	4	2		
4	B	1	Total	C	N	O	0	0
			16	10	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			16	10	4	2		
4	D	1	Total	C	N	O	0	0
			16	10	4	2		

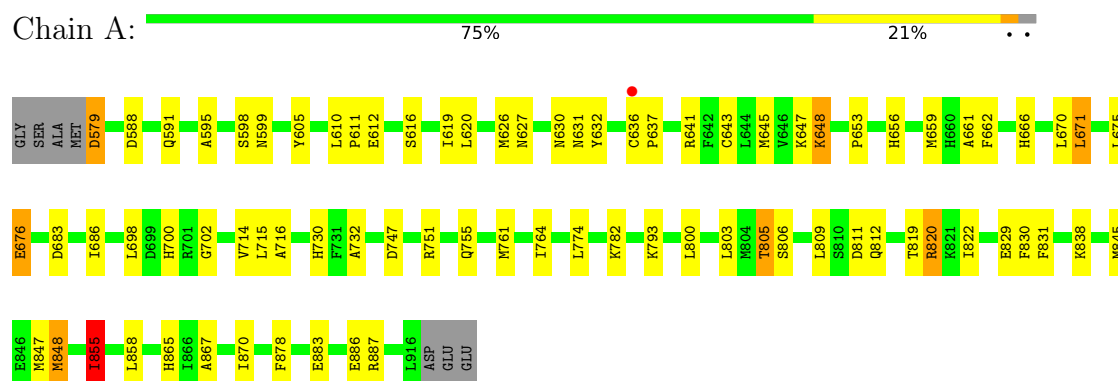
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	514	Total	O	0	0
			514	514		
5	B	447	Total	O	0	0
			447	447		
5	C	397	Total	O	0	0
			397	397		
5	D	419	Total	O	0	0
			419	419		

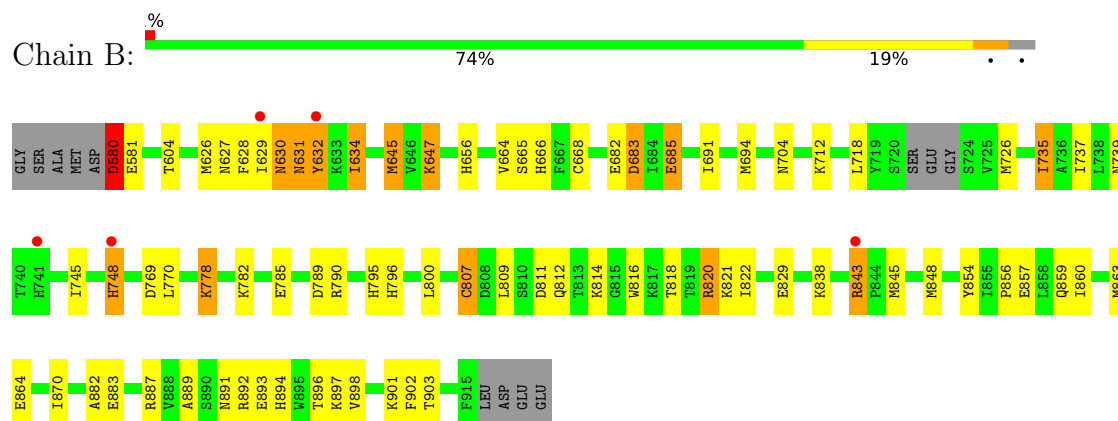
3 Residue-property plots

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.

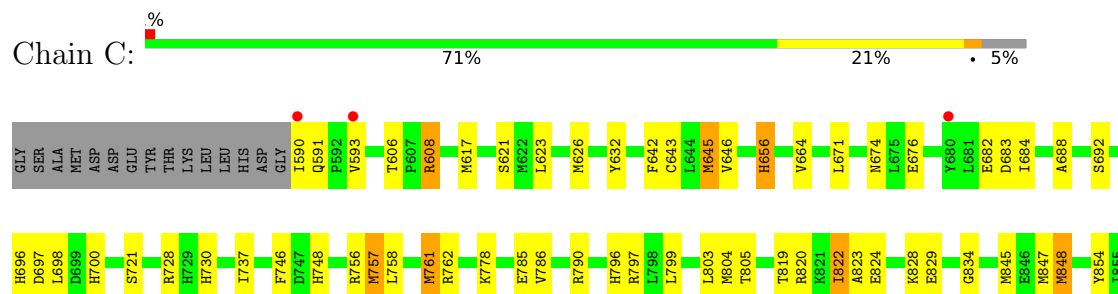
- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

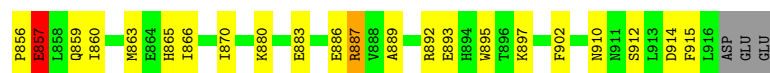


- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase

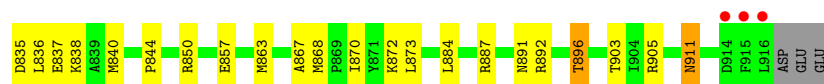


- Molecule 1: cGMP-dependent 3',5'-cyclic phosphodiesterase





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.81Å 73.29Å 91.53Å 109.30° 88.80° 89.00°	Depositor
Resolution (Å)	50.00 – 1.58 50.00 – 1.58	Depositor EDS
% Data completeness (in resolution range)	83.8 (50.00-1.58) 83.8 (50.00-1.58)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.233 0.172 , 0.231	Depositor DCC
R_{free} test set	7854 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12700	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.88% 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: MG, ZN, IBM

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	1.72	33/2834 (1.2%)	1.41	13/3824 (0.3%)
1	B	1.64	22/2798 (0.8%)	1.36	8/3774 (0.2%)
1	C	1.58	15/2741 (0.5%)	1.33	10/3698 (0.3%)
1	D	1.65	26/2741 (0.9%)	1.39	12/3698 (0.3%)
All	All	1.65	96/11114 (0.9%)	1.37	43/14994 (0.3%)

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	616	SER	N-CA	8.95	1.57	1.46
1	D	689	LEU	N-CA	8.50	1.56	1.46
1	D	835	ASP	N-CA	7.61	1.55	1.46
1	A	626	MET	SD-CE	-7.40	1.61	1.79
1	C	697	ASP	N-CA	7.35	1.54	1.46
1	D	697	ASP	N-CA	7.33	1.54	1.46
1	A	809	LEU	N-CA	7.32	1.55	1.46
1	B	848	MET	CB-CG	7.32	1.74	1.52
1	A	676	GLU	N-CA	7.30	1.57	1.46
1	C	664	VAL	CA-CB	7.25	1.62	1.54
1	B	735	ILE	N-CA	7.21	1.55	1.46
1	D	807	CYS	CA-CB	-7.08	1.42	1.53
1	A	686	ILE	CA-C	7.00	1.61	1.52
1	B	814	LYS	N-CA	7.00	1.53	1.46
1	D	726	MET	C-O	-6.82	1.16	1.24
1	C	786	VAL	CA-CB	6.74	1.63	1.54
1	A	855	ILE	CA-CB	6.70	1.57	1.54
1	B	726	MET	N-CA	6.63	1.54	1.46
1	A	800	LEU	N-CA	6.58	1.54	1.46
1	C	866	ILE	CA-CB	-6.38	1.49	1.55
1	C	646	VAL	CA-CB	-6.37	1.47	1.54
1	D	701	ARG	C-O	6.28	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	737	ILE	N-CA	6.26	1.53	1.46
1	D	868	MET	N-CA	6.26	1.52	1.46
1	C	761	MET	C-O	6.25	1.31	1.24
1	A	715	LEU	N-CA	6.25	1.53	1.46
1	B	769	ASP	N-CA	6.22	1.53	1.46
1	D	643	CYS	C-O	6.17	1.31	1.24
1	A	878	PHE	CA-CB	6.12	1.60	1.53
1	A	747	ASP	N-CA	6.06	1.54	1.46
1	C	848	MET	C-O	-6.04	1.15	1.24
1	B	626	MET	SD-CE	-6.03	1.64	1.79
1	A	662	PHE	C-O	6.02	1.31	1.24
1	B	647	LYS	C-O	6.02	1.31	1.24
1	D	593	VAL	CA-C	5.96	1.60	1.52
1	A	661	ALA	N-CA	5.95	1.53	1.46
1	B	903	THR	N-CA	5.95	1.53	1.46
1	C	804	MET	N-CA	5.94	1.53	1.46
1	A	829	GLU	CA-C	5.82	1.60	1.52
1	D	771	ALA	C-O	5.82	1.30	1.24
1	A	858	LEU	N-CA	5.70	1.53	1.46
1	B	809	LEU	C-O	5.69	1.31	1.24
1	A	732	ALA	CA-CB	-5.69	1.44	1.53
1	A	620	LEU	N-CA	5.69	1.53	1.46
1	C	700	HIS	N-CA	5.69	1.52	1.46
1	B	800	LEU	N-CA	5.68	1.53	1.46
1	D	751	ARG	N-CA	5.65	1.53	1.46
1	D	662	PHE	N-CA	5.61	1.53	1.46
1	A	805	THR	N-CA	5.58	1.53	1.46
1	C	728	ARG	CA-C	5.56	1.60	1.52
1	D	652	ASP	C-O	5.56	1.30	1.23
1	A	716	ALA	C-O	-5.54	1.17	1.24
1	A	648	LYS	N-CA	5.54	1.53	1.46
1	A	627	ASN	CA-CB	5.53	1.61	1.53
1	A	819	THR	C-O	5.52	1.30	1.24
1	C	737	ILE	CA-CB	-5.52	1.47	1.54
1	D	838	LYS	N-CA	5.51	1.53	1.46
1	D	710	ALA	CA-CB	5.49	1.61	1.53
1	B	665	SER	C-O	5.49	1.30	1.24
1	B	882	ALA	CA-CB	5.46	1.62	1.53
1	B	580	ASP	N-CA	5.44	1.56	1.46
1	A	800	LEU	CA-C	5.42	1.59	1.52
1	A	631	ASN	C-O	5.35	1.30	1.24
1	A	666	HIS	N-CA	5.34	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	667	PHE	N-CA	-5.34	1.40	1.46
1	B	694	MET	N-CA	5.28	1.52	1.46
1	D	661	ALA	N-CA	5.27	1.52	1.46
1	D	867	ALA	C-O	5.26	1.30	1.24
1	B	683	ASP	N-CA	5.24	1.52	1.46
1	B	682	GLU	CB-CG	5.23	1.68	1.52
1	D	734	ALA	N-CA	5.22	1.52	1.46
1	B	770	LEU	N-CA	5.21	1.52	1.46
1	D	873	LEU	N-CA	5.21	1.52	1.46
1	D	665	SER	N-CA	5.20	1.52	1.46
1	A	611	PRO	N-CA	5.19	1.53	1.47
1	A	806	SER	CA-C	5.18	1.59	1.52
1	C	823	ALA	CA-CB	5.18	1.61	1.53
1	B	735	ILE	C-O	5.17	1.30	1.24
1	B	668	CYS	N-CA	5.16	1.52	1.46
1	B	685	GLU	N-CA	5.16	1.52	1.46
1	C	626	MET	SD-CE	-5.12	1.66	1.79
1	A	656	HIS	N-CA	5.12	1.52	1.46
1	D	718	LEU	C-O	5.11	1.30	1.24
1	A	805	THR	C-O	5.11	1.30	1.24
1	D	692	SER	N-CA	5.11	1.52	1.46
1	B	870	ILE	CA-CB	5.10	1.60	1.54
1	D	715	LEU	N-CA	5.10	1.52	1.46
1	A	670	LEU	N-CA	5.10	1.52	1.46
1	D	819	THR	CA-CB	5.05	1.61	1.53
1	A	643	CYS	N-CA	5.05	1.52	1.46
1	A	819	THR	N-CA	5.04	1.52	1.46
1	C	757	MET	N-CA	5.03	1.52	1.46
1	C	656	HIS	N-CA	5.02	1.52	1.46
1	D	754	TYR	N-CA	5.01	1.52	1.46
1	A	595	ALA	CA-CB	-5.01	1.44	1.53
1	A	774	LEU	N-CA	5.00	1.52	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	675	LEU	N-CA-C	8.38	126.19	113.61
1	D	617	MET	N-CA-C	-7.34	102.98	112.23
1	D	706	SER	CA-CB-OG	-7.26	96.58	111.10
1	A	610	LEU	CA-C-N	-7.18	112.37	119.76
1	A	610	LEU	C-N-CA	-7.18	112.37	119.76
1	C	608	ARG	NE-CZ-NH2	-6.90	112.99	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	867	ALA	N-CA-C	6.72	118.26	111.07
1	A	671	LEU	N-CA-C	-6.59	104.02	111.14
1	D	658	TRP	N-CA-C	6.47	119.16	111.33
1	D	804	MET	N-CA-C	-6.29	104.35	111.14
1	D	591	GLN	CA-C-N	-6.21	113.36	119.76
1	D	591	GLN	C-N-CA	-6.21	113.36	119.76
1	D	638	THR	N-CA-C	-6.18	104.62	111.36
1	A	662	PHE	N-CA-C	-6.14	104.51	111.14
1	B	889	ALA	N-CA-C	-6.04	104.77	111.36
1	C	606	THR	CA-C-N	-5.86	113.58	119.56
1	C	606	THR	C-N-CA	-5.86	113.58	119.56
1	C	608	ARG	CG-CD-NE	-5.83	99.17	112.00
1	C	799	LEU	N-CA-C	-5.81	105.02	111.36
1	A	619	ILE	N-CA-C	-5.77	104.88	110.42
1	A	855	ILE	N-CA-CB	5.69	114.33	110.52
1	C	796	HIS	N-CA-C	-5.54	105.15	111.07
1	D	754	TYR	N-CA-C	-5.54	105.15	111.07
1	B	668	CYS	N-CA-C	-5.45	105.24	111.07
1	B	630	ASN	N-CA-C	5.44	119.48	111.04
1	A	676	GLU	N-CA-CB	5.42	119.72	111.70
1	B	807	CYS	N-CA-C	5.35	117.11	111.28
1	A	653	PRO	N-CA-C	-5.25	104.30	110.70
1	D	770	LEU	N-CA-C	-5.22	106.17	112.54
1	C	645	MET	CG-SD-CE	-5.21	89.43	100.90
1	D	593	VAL	N-CA-C	5.17	116.52	110.62
1	C	834	GLY	N-CA-C	-5.15	106.55	112.73
1	D	905	ARG	N-CA-C	-5.15	101.31	109.76
1	B	739	ASN	N-CA-C	5.14	119.42	113.20
1	C	857	GLU	N-CA-C	-5.14	105.76	111.36
1	C	642	PHE	N-CA-C	-5.09	105.62	111.07
1	B	632	TYR	N-CA-C	5.08	120.11	112.94
1	A	764	ILE	CA-C-N	-5.04	113.26	120.42
1	A	764	ILE	C-N-CA	-5.04	113.26	120.42
1	B	848	MET	CB-CG-SD	-5.04	97.57	112.70
1	B	645	MET	CB-CG-SD	-5.03	97.60	112.70
1	D	903	THR	N-CA-C	-5.03	100.32	108.52
1	A	588	ASP	N-CA-C	5.03	118.67	112.54

There are no chirality outliers.

There are no planarity outliers.

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	2767	0	2709	61	0
1	B	2732	0	2679	76	0
1	C	2676	0	2630	77	0
1	D	2676	0	2630	39	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	14	3	0
4	B	16	0	14	3	0
4	C	16	0	14	0	0
4	D	16	0	14	1	0
5	A	514	0	0	36	0
5	B	447	0	0	20	2
5	C	397	0	0	31	2
5	D	419	0	0	11	0
All	All	12700	0	10704	252	2

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 12.

All (252) 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:643:CYS:HB3	5:C:1708:HOH:O	1.27	1.29
1:B:892:ARG:HH12	1:B:896:THR:CG2	1.57	1.18
1:D:892:ARG:HH12	1:D:896:THR:HG21	1.14	1.10
1:B:745:ILE:O	1:B:748:HIS:CE1	2.05	1.09
1:B:745:ILE:O	1:B:748:HIS:HE1	1.33	1.09
1:D:892:ARG:HH12	1:D:896:THR:CG2	1.66	1.08
1:A:847:MET:HE1	5:A:1704:HOH:O	1.56	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:ASN:HD21	1:B:845:MET:HE1	1.23	1.03
1:A:820:ARG:HH11	1:A:820:ARG:HG2	1.24	1.02
1:C:845:MET:HE3	1:C:847:MET:CG	1.90	1.02
1:A:847:MET:CE	5:A:1704:HOH:O	2.08	1.01
1:B:748:HIS:HB2	5:B:1518:HOH:O	1.62	0.98
1:B:789:ASP:H	1:B:795:HIS:HD2	1.11	0.97
1:C:591:GLN:H	1:C:617:MET:HE2	1.30	0.96
1:A:676:GLU:HG3	5:A:1038:HOH:O	1.64	0.96
1:D:633:LYS:HE2	5:D:1013:HOH:O	1.66	0.95
1:B:634:ILE:HD12	1:B:748:HIS:CE1	2.01	0.95
1:B:627:ASN:HB3	5:B:1710:HOH:O	1.64	0.95
1:C:897:LYS:HD3	5:C:1724:HOH:O	1.68	0.93
1:B:892:ARG:NH1	1:B:896:THR:CG2	2.31	0.93
1:C:887:ARG:HH11	1:C:887:ARG:HG2	1.35	0.91
1:A:579:ASP:N	5:A:1666:HOH:O	2.05	0.89
1:C:748:HIS:HB3	5:C:1411:HOH:O	1.72	0.89
1:B:704:ASN:ND2	1:B:845:MET:HE1	1.87	0.89
1:C:632:TYR:HE1	5:C:1712:HOH:O	1.56	0.88
1:B:894:HIS:HD2	5:B:1323:HOH:O	1.57	0.87
1:A:636:CYS:SG	5:A:1509:HOH:O	2.32	0.86
1:D:892:ARG:NH1	1:D:896:THR:CG2	2.39	0.85
1:D:593:VAL:HG23	1:D:600:PHE:CD2	2.11	0.85
1:B:892:ARG:HH12	1:B:896:THR:HG23	1.39	0.85
1:A:636:CYS:HB3	5:A:1707:HOH:O	1.77	0.85
1:B:632:TYR:HB3	1:B:748:HIS:CD2	2.11	0.84
1:D:762:ARG:NH2	5:D:1738:HOH:O	2.05	0.84
1:C:914:ASP:HB3	5:C:1454:HOH:O	1.75	0.84
1:A:887:ARG:HD3	5:A:1623:HOH:O	1.78	0.83
1:A:700:HIS:HD2	1:A:702:GLY:H	1.23	0.83
1:B:892:ARG:NH1	1:B:896:THR:HG23	1.95	0.81
1:D:758:LEU:HB3	5:D:1738:HOH:O	1.78	0.81
1:A:845:MET:HB2	1:A:848:MET:HG2	1.64	0.80
1:B:656:HIS:HD2	1:B:829:GLU:OE2	1.66	0.79
1:C:886:GLU:HG2	5:C:975:HOH:O	1.82	0.79
1:C:845:MET:HE3	1:C:847:MET:HG2	1.65	0.78
1:C:897:LYS:CD	5:C:1724:HOH:O	2.26	0.78
1:D:857:GLU:HG3	5:D:1669:HOH:O	1.82	0.78
1:C:656:HIS:HD2	1:C:829:GLU:OE2	1.67	0.78
1:A:883:GLU:OE1	1:A:887:ARG:NH2	2.17	0.78
1:B:685:GLU:OE1	1:B:796:HIS:HD2	1.67	0.78
1:C:617:MET:HG3	5:C:189:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:593:VAL:CG2	1:D:600:PHE:CD2	2.68	0.76
1:C:845:MET:HE3	1:C:847:MET:SD	2.24	0.76
1:D:782:LYS:HE2	5:D:982:HOH:O	1.86	0.75
1:D:857:GLU:CG	5:D:1669:HOH:O	2.35	0.74
1:C:683:ASP:HB3	5:C:1712:HOH:O	1.87	0.74
1:D:627:ASN:HD21	1:D:630:ASN:HD22	1.34	0.74
1:D:892:ARG:NH1	1:D:896:THR:HG21	1.96	0.74
1:B:789:ASP:H	1:B:795:HIS:CD2	2.02	0.73
1:A:865:HIS:CE1	5:A:936:HOH:O	2.41	0.72
1:D:813:THR:O	1:D:887:ARG:HD3	1.90	0.72
1:B:704:ASN:HD21	1:B:845:MET:CE	2.01	0.71
1:C:698:LEU:O	1:C:730:HIS:HD2	1.74	0.70
1:C:887:ARG:HD3	5:C:304:HOH:O	1.91	0.70
1:B:790:ARG:O	1:B:796:HIS:HE1	1.73	0.69
5:A:1560:HOH:O	1:B:712:LYS:HB2	1.92	0.68
1:A:630:ASN:ND2	5:A:1000:HOH:O	2.25	0.68
1:C:676:GLU:HG2	5:C:1364:HOH:O	1.93	0.68
1:B:632:TYR:HB2	1:B:634:ILE:HD11	1.76	0.68
1:B:631:ASN:ND2	1:B:683:ASP:OD2	2.26	0.68
1:A:820:ARG:HG2	1:A:820:ARG:NH1	1.97	0.67
1:C:632:TYR:CE1	5:C:1712:HOH:O	2.37	0.67
1:A:700:HIS:CD2	1:A:702:GLY:H	2.09	0.67
1:C:845:MET:HE2	1:C:848:MET:HG3	1.76	0.67
1:A:830:PHE:CE2	1:A:847:MET:HE2	2.31	0.66
1:A:730:HIS:HE1	5:A:5:HOH:O	1.79	0.66
1:B:812:GLN:HE21	4:B:999:IBM:H103	1.61	0.65
1:C:730:HIS:HE1	5:C:17:HOH:O	1.79	0.65
1:D:751:ARG:HD2	5:D:1022:HOH:O	1.97	0.65
1:B:887:ARG:CD	5:B:1018:HOH:O	2.44	0.65
1:B:892:ARG:NH1	1:B:896:THR:HG21	2.12	0.64
1:C:915:PHE:HB3	5:C:1750:HOH:O	1.97	0.63
1:C:819:THR:CG2	1:C:895:TRP:HE1	2.12	0.63
1:B:897:LYS:HD2	5:B:1189:HOH:O	1.99	0.63
1:C:590:ILE:HG23	1:C:617:MET:HE1	1.80	0.63
1:C:845:MET:HE2	1:C:848:MET:HE3	1.81	0.63
1:C:845:MET:CE	1:C:847:MET:CG	2.72	0.63
1:B:632:TYR:HB2	1:B:634:ILE:CD1	2.28	0.63
1:A:636:CYS:CB	5:A:1707:HOH:O	2.41	0.62
1:B:887:ARG:HG2	5:B:550:HOH:O	1.98	0.62
1:A:648:LYS:HG3	1:D:790:ARG:HD2	1.82	0.61
1:B:887:ARG:HD3	5:B:1018:HOH:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:ASN:O	1:B:631:ASN:C	2.43	0.61
1:C:591:GLN:H	1:C:617:MET:CE	2.09	0.61
1:D:593:VAL:CG2	1:D:600:PHE:HD2	2.13	0.61
1:A:698:LEU:O	1:A:730:HIS:HD2	1.82	0.60
1:B:893:GLU:CG	5:B:1381:HOH:O	2.49	0.60
1:B:812:GLN:OE1	1:B:863:MET:HE3	2.02	0.60
1:D:892:ARG:HG2	1:D:892:ARG:HH11	1.66	0.60
1:B:893:GLU:HG2	5:B:1381:HOH:O	2.01	0.60
1:C:887:ARG:CD	5:C:304:HOH:O	2.47	0.59
1:C:590:ILE:HA	1:C:617:MET:HE1	1.84	0.59
1:C:683:ASP:CB	5:C:1712:HOH:O	2.47	0.59
1:B:630:ASN:O	1:B:632:TYR:N	2.36	0.58
1:A:591:GLN:HG3	5:A:1584:HOH:O	2.01	0.58
1:A:865:HIS:HE1	5:A:936:HOH:O	1.80	0.57
1:C:865:HIS:HD2	5:C:1269:HOH:O	1.85	0.57
1:A:598:SER:HB2	5:A:1660:HOH:O	2.05	0.57
1:D:682:GLU:OE1	1:D:756:ARG:NH2	2.37	0.57
1:B:859:GLN:OE1	4:B:999:IBM:N7	2.37	0.57
1:A:579:ASP:OD2	5:A:1678:HOH:O	2.17	0.56
1:A:847:MET:HE3	5:A:1704:HOH:O	1.88	0.56
1:C:824:GLU:HG2	1:C:828:LYS:HE3	1.86	0.56
1:D:884:LEU:HA	1:D:887:ARG:HD2	1.87	0.56
1:A:830:PHE:HE2	1:A:847:MET:CE	2.19	0.56
1:B:685:GLU:OE1	1:B:796:HIS:CD2	2.55	0.56
1:B:666:HIS:HD2	5:B:17:HOH:O	1.89	0.56
1:C:845:MET:CE	1:C:848:MET:HE3	2.35	0.55
1:A:630:ASN:HB3	5:A:1499:HOH:O	2.06	0.55
1:A:805:THR:HG22	1:A:870:ILE:HD13	1.88	0.55
1:A:820:ARG:HH11	1:A:820:ARG:CG	2.09	0.55
1:C:887:ARG:HG2	1:C:887:ARG:NH1	2.07	0.55
1:C:674:ASN:O	1:C:880:LYS:CE	2.55	0.55
1:B:785:GLU:HG3	5:B:294:HOH:O	2.07	0.55
1:B:789:ASP:N	1:B:795:HIS:HD2	1.94	0.54
1:C:819:THR:HG21	1:C:895:TRP:HE1	1.71	0.54
1:B:856:PRO:HG3	1:B:902:PHE:CD2	2.43	0.54
1:C:617:MET:HE3	1:C:621:SER:OG	2.08	0.54
5:A:1560:HOH:O	1:B:712:LYS:CB	2.52	0.54
1:B:631:ASN:ND2	5:B:1710:HOH:O	2.41	0.54
1:B:581:GLU:OE2	1:B:647:LYS:NZ	2.36	0.54
1:B:630:ASN:C	1:B:632:TYR:N	2.66	0.54
1:B:634:ILE:CD1	1:B:748:HIS:CE1	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:863:MET:HE1	1:D:891:ASN:HB2	1.91	0.53
1:B:782:LYS:HG2	5:B:1739:HOH:O	2.08	0.53
1:C:887:ARG:CZ	5:C:1632:HOH:O	2.56	0.53
1:C:785:GLU:HB2	5:C:1701:HOH:O	2.09	0.53
1:C:790:ARG:HG2	1:C:790:ARG:O	2.08	0.52
1:B:883:GLU:OE1	1:B:887:ARG:NH1	2.36	0.52
1:A:830:PHE:HE2	1:A:847:MET:HE2	1.71	0.52
1:C:676:GLU:HA	5:C:959:HOH:O	2.10	0.52
1:B:821:LYS:HE2	5:B:1277:HOH:O	2.09	0.51
1:A:831:PHE:HZ	1:A:855:ILE:HD11	1.75	0.51
1:D:627:ASN:ND2	1:D:630:ASN:HD22	2.06	0.51
1:B:656:HIS:HE1	5:B:12:HOH:O	1.92	0.51
1:A:579:ASP:CA	5:A:1666:HOH:O	2.56	0.51
1:B:627:ASN:HA	5:B:1717:HOH:O	2.11	0.51
1:C:845:MET:HE2	1:C:848:MET:CG	2.41	0.50
1:C:797:ARG:HG2	5:C:976:HOH:O	2.11	0.50
1:A:805:THR:CG2	1:A:870:ILE:HD13	2.42	0.50
1:A:630:ASN:CB	5:A:544:HOH:O	2.59	0.50
1:A:636:CYS:HB2	1:A:637:PRO:HD3	1.94	0.50
1:C:910:ASN:ND2	5:C:1620:HOH:O	2.44	0.50
1:A:782:LYS:HD3	5:A:972:HOH:O	2.12	0.50
1:A:714:VAL:HG12	5:A:1092:HOH:O	2.12	0.49
1:D:752:LYS:HG3	5:D:954:HOH:O	2.11	0.49
1:A:838:LYS:HD2	5:A:1718:HOH:O	2.12	0.49
1:A:630:ASN:HB3	5:A:544:HOH:O	2.10	0.49
1:D:781:GLN:HG2	5:D:1089:HOH:O	2.11	0.49
1:B:860:ILE:O	1:B:864:GLU:HG3	2.13	0.49
1:A:641:ARG:HD3	5:A:1743:HOH:O	2.13	0.49
1:B:580:ASP:N	5:B:1716:HOH:O	2.45	0.49
1:C:797:ARG:HB3	5:C:1741:HOH:O	2.12	0.48
1:A:630:ASN:ND2	5:A:475:HOH:O	2.33	0.48
1:C:656:HIS:HE1	5:C:18:HOH:O	1.96	0.48
1:A:886:GLU:OE1	5:A:1559:HOH:O	2.20	0.48
1:B:864:GLU:OE2	1:B:892:ARG:NH2	2.44	0.48
1:C:910:ASN:OD1	1:C:912:SER:HB3	2.14	0.48
1:B:854:TYR:CD2	1:B:857:GLU:HG3	2.49	0.48
1:C:819:THR:HG22	1:C:895:TRP:HE1	1.79	0.47
1:D:837:GLU:OE1	1:D:844:PRO:HB3	2.15	0.47
1:C:805:THR:HG22	1:C:870:ILE:HD13	1.96	0.47
1:D:872:LYS:HD3	5:D:967:HOH:O	2.15	0.47
1:A:793:LYS:HE3	1:A:793:LYS:HB2	1.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:898:VAL:HB	1:B:901:LYS:HD2	1.96	0.47
1:D:688:ALA:HA	1:D:757:MET:HE1	1.95	0.47
1:A:887:ARG:HG2	5:A:1057:HOH:O	2.14	0.47
1:D:827:TYR:HB3	1:D:831:PHE:CE2	2.50	0.47
1:D:805:THR:HG22	1:D:870:ILE:HD13	1.97	0.46
1:C:698:LEU:O	1:C:730:HIS:CD2	2.61	0.46
1:A:811:ASP:HB3	1:A:822:ILE:HG13	1.97	0.46
1:C:854:TYR:HD2	1:C:857:GLU:HB3	1.80	0.46
1:A:730:HIS:CE1	5:A:5:HOH:O	2.61	0.46
1:C:608:ARG:CZ	1:C:822:ILE:HD11	2.45	0.46
1:A:599:ASN:O	1:A:605:TYR:HB2	2.15	0.46
1:B:778:LYS:HB3	1:B:778:LYS:HE3	1.62	0.46
1:C:684:ILE:HD11	1:C:757:MET:SD	2.55	0.46
1:C:860:ILE:HG23	1:C:892:ARG:HH11	1.81	0.46
1:A:782:LYS:HE2	5:A:1504:HOH:O	2.14	0.45
1:C:692:SER:O	1:C:696:HIS:HB3	2.16	0.45
1:D:836:LEU:O	1:D:840:MET:HG3	2.15	0.45
1:C:671:LEU:HD13	1:C:803:LEU:HD22	1.99	0.45
1:A:830:PHE:CE2	1:A:847:MET:CE	2.96	0.45
1:B:735:ILE:HA	1:B:735:ILE:HD13	1.62	0.45
1:C:897:LYS:HD2	5:C:1724:HOH:O	2.05	0.45
1:A:700:HIS:HE1	5:A:143:HOH:O	2.00	0.45
1:B:664:VAL:HG13	1:B:807:CYS:HB3	1.99	0.45
1:C:845:MET:CE	1:C:847:MET:HG2	2.42	0.45
1:A:647:LYS:CD	5:A:968:HOH:O	2.64	0.45
1:C:859:GLN:O	1:C:863:MET:HG3	2.16	0.45
1:B:645:MET:HG2	5:B:388:HOH:O	2.16	0.44
1:A:755:GLN:CG	5:A:1560:HOH:O	2.65	0.44
1:A:761:MET:HE2	1:A:761:MET:HB3	1.87	0.44
1:B:854:TYR:HD2	1:B:857:GLU:HG3	1.82	0.44
1:C:889:ALA:O	1:C:893:GLU:HG2	2.17	0.44
4:A:999:IBM:H8	5:A:1704:HOH:O	2.16	0.44
1:C:645:MET:HG2	5:C:259:HOH:O	2.18	0.44
1:C:688:ALA:HA	1:C:757:MET:HE1	1.98	0.44
1:D:664:VAL:HG13	1:D:807:CYS:HB3	2.00	0.44
1:A:632:TYR:OH	1:A:683:ASP:OD2	2.35	0.44
1:C:762:ARG:NH1	5:C:478:HOH:O	2.50	0.44
1:D:892:ARG:NH1	1:D:892:ARG:HG2	2.33	0.44
1:C:682:GLU:CD	1:C:756:ARG:HH21	2.25	0.44
1:C:758:LEU:HD23	1:C:758:LEU:HA	1.80	0.44
1:A:645:MET:HG2	5:A:1339:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:721:SER:OG	5:C:1671:HOH:O	2.14	0.43
1:C:856:PRO:HG3	1:C:902:PHE:CD2	2.53	0.43
1:A:847:MET:HE1	4:A:999:IBM:H8	1.99	0.43
1:B:893:GLU:OE1	1:B:893:GLU:HA	2.18	0.43
1:C:856:PRO:HG3	1:C:902:PHE:CE2	2.53	0.43
1:C:746:PHE:CZ	1:C:757:MET:HE2	2.53	0.43
1:B:811:ASP:HB3	1:B:822:ILE:HG13	1.99	0.43
1:B:818:THR:O	1:B:822:ILE:HG12	2.18	0.43
1:C:883:GLU:O	1:C:887:ARG:NH1	2.52	0.43
1:A:648:LYS:HG3	1:D:790:ARG:CD	2.48	0.43
1:B:816:TRP:CZ2	1:B:820:ARG:HG3	2.53	0.43
1:C:883:GLU:O	1:C:887:ARG:HG2	2.18	0.43
1:B:892:ARG:HH12	1:B:896:THR:HG22	1.65	0.42
1:D:850:ARG:HH11	1:D:850:ARG:HD3	1.69	0.42
1:B:604:THR:HG22	1:B:887:ARG:NH2	2.35	0.42
1:B:630:ASN:ND2	5:B:235:HOH:O	2.52	0.42
1:D:817:LYS:HD2	1:D:817:LYS:N	2.34	0.42
1:D:812:GLN:HE21	4:D:999:IBM:H101	1.84	0.42
1:B:892:ARG:HH12	1:B:896:THR:HG21	1.59	0.42
1:C:859:GLN:NE2	5:C:1720:HOH:O	2.52	0.42
1:C:845:MET:CE	1:C:847:MET:HG3	2.49	0.42
1:B:628:PHE:O	1:B:629:ILE:C	2.63	0.41
1:B:645:MET:HE3	1:B:645:MET:HB3	1.71	0.41
1:B:893:GLU:HG3	5:B:1381:HOH:O	2.14	0.41
1:D:756:ARG:HD2	5:D:1001:HOH:O	2.20	0.41
1:C:761:MET:HE2	1:C:761:MET:HB3	1.85	0.41
1:A:612:GLU:HG3	1:A:659:MET:SD	2.60	0.41
1:C:886:GLU:CG	5:C:975:HOH:O	2.55	0.41
1:D:911:ASN:HD22	1:D:911:ASN:HA	1.63	0.41
1:B:863:MET:HE1	1:B:891:ASN:HB3	2.02	0.41
1:C:778:LYS:HD3	5:C:979:HOH:O	2.21	0.41
1:B:629:ILE:HA	1:B:634:ILE:HG12	2.03	0.41
1:C:623:LEU:HD23	1:C:623:LEU:HA	1.91	0.41
1:B:812:GLN:NE2	4:B:999:IBM:H103	2.32	0.41
1:B:838:LYS:HE2	1:B:843:ARG:NH2	2.36	0.40
1:A:671:LEU:HD13	1:A:803:LEU:HD22	2.04	0.40
1:A:812:GLN:HE21	4:A:999:IBM:H103	1.87	0.40
1:D:738:LEU:O	1:D:744:ASN:HB2	2.21	0.40
1:B:691:ILE:HD13	1:B:691:ILE:HA	1.94	0.40
1:A:830:PHE:CD2	1:A:847:MET:HE2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:311:HOH:O	5:C:924:HOH:O[1_545]	2.00	0.20
5:B:311:HOH:O	5:C:1618:HOH:O[1_545]	2.19	0.01

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	336/345 (97%)	332 (99%)	4 (1%)	0	100	100
1	B	329/345 (95%)	318 (97%)	10 (3%)	1 (0%)	36	20
1	C	325/345 (94%)	320 (98%)	5 (2%)	0	100	100
1	D	325/345 (94%)	320 (98%)	5 (2%)	0	100	100
All	All	1315/1380 (95%)	1290 (98%)	24 (2%)	1 (0%)	48	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	631	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/310 (98%)	300 (98%)	5 (2%)	55	28
1	B	301/310 (97%)	294 (98%)	7 (2%)	44	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	295/310 (95%)	290 (98%)	5 (2%)	53	25
1	D	295/310 (95%)	288 (98%)	7 (2%)	43	13
All	All	1196/1240 (96%)	1172 (98%)	24 (2%)	48	20

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	579	ASP
1	A	751	ARG
1	A	820	ARG
1	A	848	MET
1	A	855	ILE
1	B	580	ASP
1	B	634	ILE
1	B	718	LEU
1	B	748	HIS
1	B	778	LYS
1	B	820	ARG
1	B	843	ARG
1	C	593	VAL
1	C	820	ARG
1	C	822	ILE
1	C	857	GLU
1	C	887	ARG
1	D	599	ASN
1	D	611	PRO
1	D	684	ILE
1	D	819	THR
1	D	820	ARG
1	D	896	THR
1	D	911	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	700	HIS
1	A	708	GLN
1	A	730	HIS
1	A	781	GLN
1	A	812	GLN

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Mol	Chain	Res	Type
1	A	865	HIS
1	A	911	ASN
1	B	624	GLN
1	B	656	HIS
1	B	666	HIS
1	B	674	ASN
1	B	733	GLN
1	B	748	HIS
1	B	781	GLN
1	B	795	HIS
1	B	796	HIS
1	B	859	GLN
1	B	875	GLN
1	B	894	HIS
1	B	900	HIS
1	B	911	ASN
1	C	656	HIS
1	C	730	HIS
1	C	781	GLN
1	C	865	HIS
1	C	875	GLN
1	D	627	ASN
1	D	791	ASN
1	D	859	GLN
1	D	875	GLN
1	D	894	HIS
1	D	900	HIS
1	D	911	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IBM	B	999	-	17,17,17	1.57	4 (23%)	19,25,25	2.51	6 (31%)
4	IBM	C	999	-	17,17,17	1.57	3 (17%)	19,25,25	2.16	5 (26%)
4	IBM	D	999	-	17,17,17	2.29	9 (52%)	19,25,25	3.03	8 (42%)
4	IBM	A	999	-	17,17,17	2.02	6 (35%)	19,25,25	2.08	7 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IBM	B	999	-	-	0/4/4/4	0/2/2/2
4	IBM	C	999	-	-	0/4/4/4	0/2/2/2
4	IBM	D	999	-	-	0/4/4/4	0/2/2/2
4	IBM	A	999	-	-	0/4/4/4	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	IBM	C8-N9	4.93	1.43	1.35
4	D	999	IBM	C8-N9	3.91	1.41	1.35
4	A	999	IBM	C2-N3	-3.51	1.32	1.38
4	D	999	IBM	O6-C6	3.49	1.30	1.23
4	B	999	IBM	O2-C2	3.23	1.28	1.22
4	D	999	IBM	C2-N3	-3.17	1.33	1.38
4	D	999	IBM	C2-N1	-3.10	1.32	1.39
4	D	999	IBM	C4-N9	-3.00	1.31	1.36
4	B	999	IBM	C5-C6	-2.98	1.38	1.45
4	D	999	IBM	C8-N7	2.82	1.39	1.33
4	D	999	IBM	C5-C6	-2.71	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	IBM	C5-C6	-2.70	1.38	1.45
4	C	999	IBM	C5-C6	-2.69	1.39	1.45
4	A	999	IBM	C2-N1	-2.66	1.33	1.39
4	D	999	IBM	O2-C2	2.60	1.27	1.22
4	B	999	IBM	O6-C6	2.56	1.28	1.23
4	D	999	IBM	C4-N3	-2.50	1.34	1.38
4	C	999	IBM	C8-N9	2.38	1.38	1.35
4	A	999	IBM	C8-N7	2.36	1.38	1.33
4	A	999	IBM	C4-N9	-2.31	1.32	1.36
4	B	999	IBM	C8-N9	2.15	1.38	1.35
4	C	999	IBM	C11-N3	-2.10	1.42	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	999	IBM	N3-C2-N1	6.48	124.71	116.72
4	D	999	IBM	O2-C2-N1	-6.22	112.73	121.33
4	B	999	IBM	N3-C2-N1	6.21	124.37	116.72
4	C	999	IBM	O2-C2-N1	-5.11	114.26	121.33
4	C	999	IBM	N3-C2-N1	5.03	122.93	116.72
4	D	999	IBM	C10-N1-C6	4.74	124.99	117.64
4	A	999	IBM	O2-C2-N3	-4.42	116.02	121.98
4	B	999	IBM	C6-N1-C2	-4.37	118.56	125.66
4	B	999	IBM	C10-N1-C6	4.34	124.37	117.64
4	D	999	IBM	C6-N1-C2	-4.32	118.64	125.66
4	D	999	IBM	N9-C4-N3	-3.77	122.33	127.81
4	C	999	IBM	C6-N1-C2	-3.47	120.02	125.66
4	D	999	IBM	C11-N3-C2	3.38	124.55	117.67
4	A	999	IBM	N3-C2-N1	3.29	120.78	116.72
4	A	999	IBM	N9-C4-N3	-3.11	123.30	127.81
4	A	999	IBM	C6-N1-C2	-3.08	120.65	125.66
4	B	999	IBM	O2-C2-N1	-3.02	117.16	121.33
4	D	999	IBM	C4-C5-N7	-2.87	105.53	109.26
4	B	999	IBM	C11-N3-C2	2.83	123.42	117.67
4	A	999	IBM	C6-C5-N7	2.79	135.55	129.36
4	A	999	IBM	C10-N1-C6	2.72	121.86	117.64
4	B	999	IBM	O2-C2-N3	-2.61	118.47	121.98
4	A	999	IBM	C5-C6-N1	2.57	119.77	115.02
4	C	999	IBM	C5-C6-N1	2.54	119.72	115.02
4	D	999	IBM	C6-C5-N7	2.52	134.97	129.36
4	C	999	IBM	C12-C11-N3	-2.29	109.05	112.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	999	IBM	3	0
4	D	999	IBM	1	0
4	A	999	IBM	3	0

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	338/345 (97%)	-0.15	1 (0%) 90 91	8, 17, 31, 43	0
1	B	333/345 (96%)	-0.01	5 (1%) 72 80	10, 20, 32, 44	0
1	C	327/345 (94%)	0.07	3 (0%) 81 86	11, 21, 36, 44	0
1	D	327/345 (94%)	0.14	12 (3%) 45 56	9, 20, 35, 47	0
All	All	1325/1380 (96%)	0.01	21 (1%) 70 78	8, 19, 34, 47	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	590	ILE	3.4
1	D	593	VAL	3.4
1	D	599	ASN	3.4
1	D	595	ALA	2.9
1	D	594	ALA	2.8
1	D	596	ILE	2.8
1	B	748	HIS	2.7
1	C	680	TYR	2.5
1	D	636	CYS	2.4
1	D	592	PRO	2.4
1	C	593	VAL	2.4
1	C	590	ILE	2.4
1	D	632	TYR	2.4
1	B	741	HIS	2.3
1	B	632	TYR	2.2
1	D	915	PHE	2.2
1	B	629	ILE	2.1
1	D	914	ASP	2.1
1	B	843	ARG	2.0
1	A	636	CYS	2.0
1	D	916	LEU	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
4	IBM	C	999	16/16	0.90	0.10	25,28,30,31	0
4	IBM	B	999	16/16	0.91	0.09	23,25,28,30	0
4	IBM	A	999	16/16	0.94	0.06	17,21,22,24	0
4	IBM	D	999	16/16	0.94	0.07	18,22,25,29	0
3	MG	C	920	1/1	0.98	0.03	12,12,12,12	0
3	MG	A	920	1/1	0.99	0.01	10,10,10,10	0
3	MG	D	920	1/1	0.99	0.04	12,12,12,12	0
2	ZN	C	3	1/1	1.00	0.01	14,14,14,14	0
2	ZN	D	4	1/1	1.00	0.02	14,14,14,14	0
2	ZN	A	1	1/1	1.00	0.01	13,13,13,13	0
3	MG	B	920	1/1	1.00	0.03	10,10,10,10	0
2	ZN	B	2	1/1	1.00	0.01	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.