



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 11:29 PM UTC

PDB ID : 9S60 / pdb_00009s60
Title : Structural and proteomics analysis of the mouse cathepsin B - DARPin 4m3 complex reveals determinants of species - specific binding
Authors : Tusar, L.; Zaric, M.; Usenik, A.; Vasiljeva, O.; Novak, M.; Turk, D.; Turk, B.
Deposited on : 2025-07-30
Resolution : 1.69 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

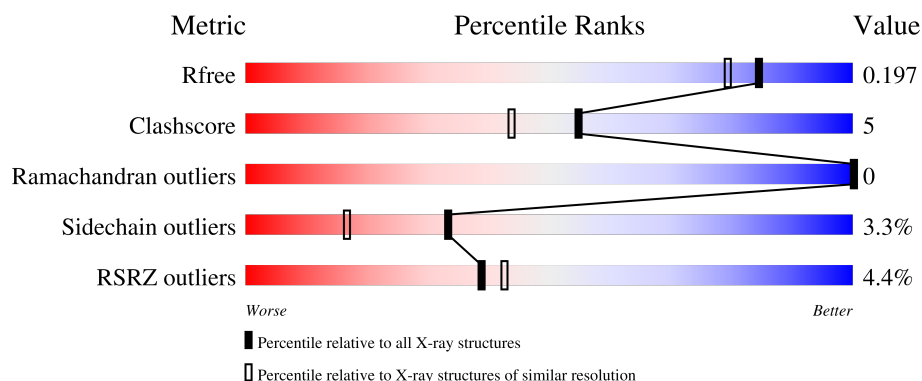
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	254	 6% 75% 24% .
1	A2	254	 6% 76% 22% .
2	B	177	 2% 64% 23% . 10%
2	B2	177	 2% 69% 19% . 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14655 atoms, of which 7583 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 Cathepsin B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	254	Total	C	H	N	O	S	1795	2	0
			3741	1214	1795	334	380	18			
1	A2	254	Total	C	H	N	O	S	1804	3	0
			3750	1217	1798	335	382	18			

- Molecule 2 is a protein called DARPin 4m3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	159	Total	C	H	N	O	S	1115	0	0
			2262	711	1115	202	233	1			
2	B2	159	Total	C	H	N	O	S	1123	0	0
			2262	711	1115	202	233	1			

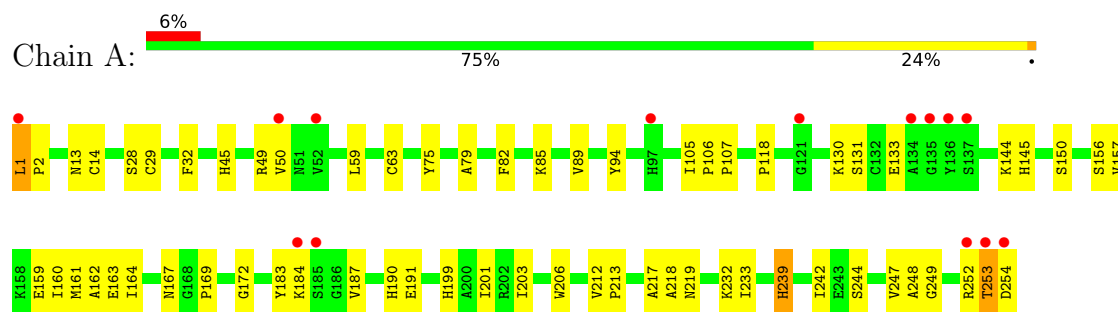
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	298	Total	H	O	596	0
			894	596	298		
3	A2	252	Total	H	O	504	0
			756	504	252		
3	B	174	Total	H	O	348	0
			522	348	174		
3	B2	156	Total	H	O	312	0
			468	312	156		

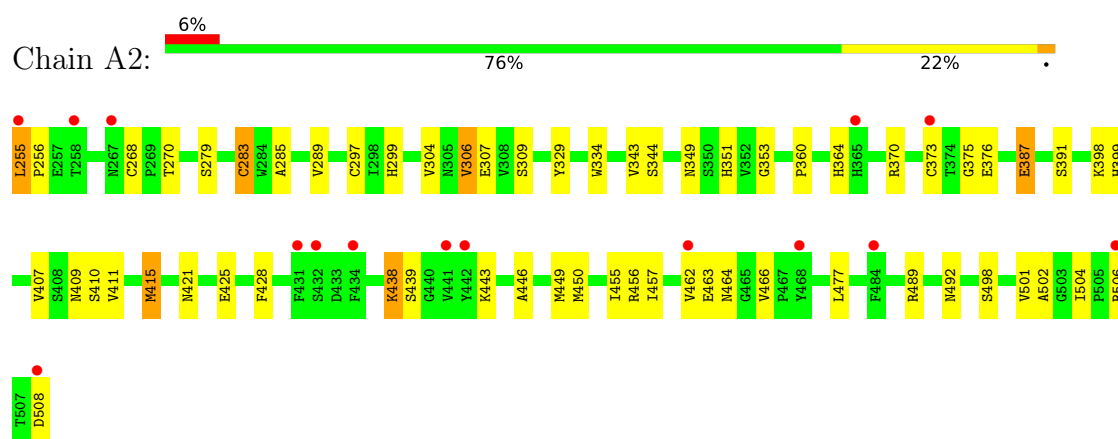
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

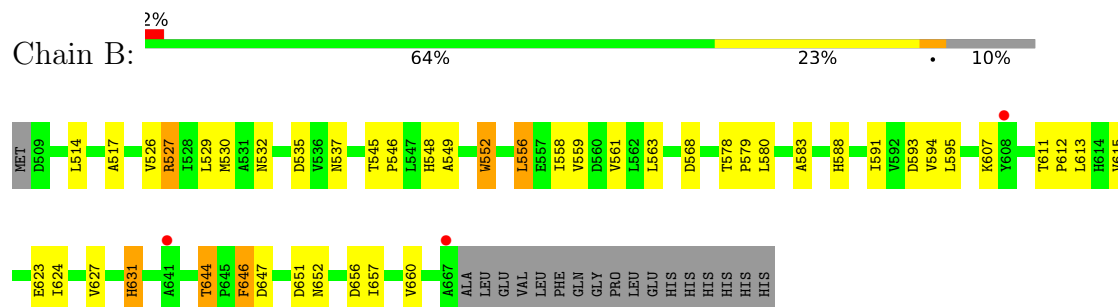
• Molecule 1: Cathepsin B



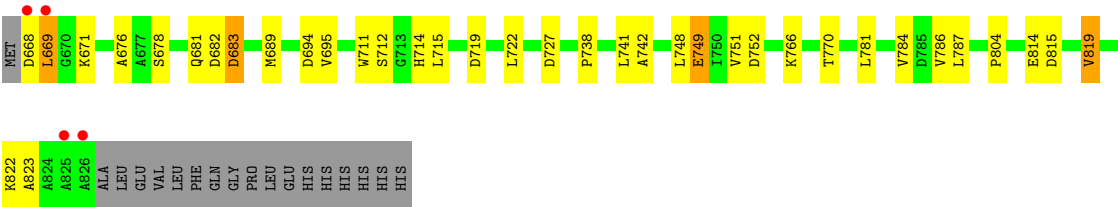
• Molecule 1: Cathepsin B



• Molecule 2: DARPin 4m3



• Molecule 2: DARPin 4m3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.64Å 109.92Å 142.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 1.69 49.39 – 1.69	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.39-1.69) 100.0 (49.39-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.67Å)	Xtriage
Refinement program	MAIN version 2022	Depositor
R, R_{free}	0.193 , 0.216 0.197 , 0.197	Depositor DCC
R_{free} test set	4754 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14655	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: CSO

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	1.94	37/1991 (1.9%)	1.22	10/2702 (0.4%)
1	A2	1.92	36/2001 (1.8%)	1.24	14/2716 (0.5%)
2	B	2.24	34/1166 (2.9%)	1.18	2/1593 (0.1%)
2	B2	2.12	24/1166 (2.1%)	1.13	2/1593 (0.1%)
All	All	2.03	131/6324 (2.1%)	1.20	28/8604 (0.3%)

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	450	MET	SD-CE	-10.45	1.53	1.79
1	A	106	PRO	C-O	-8.02	1.18	1.25
1	A	247	VAL	C-O	-8.02	1.16	1.24
1	A2	360	PRO	C-O	-7.89	1.18	1.25
2	B	578	THR	C-O	-7.73	1.17	1.24
1	A2	501	VAL	C-O	-7.18	1.16	1.23
1	A2	428	PHE	C-O	-6.63	1.16	1.23
1	A	79	ALA	C-O	-6.61	1.16	1.24
2	B2	770	THR	C-O	-6.61	1.18	1.24
1	A	75	TYR	C-O	-6.60	1.18	1.24
1	A2	398	LYS	C-O	-6.58	1.16	1.23
1	A	63	CYS	C-O	-6.52	1.16	1.24
1	A2	456	ARG	C-O	-6.52	1.16	1.24
1	A	239	HIS	C-O	-6.41	1.16	1.24
2	B	607	LYS	C-N	-6.41	1.25	1.33
2	B	556	LEU	C-O	-6.39	1.16	1.24
2	B2	751	VAL	C-O	-6.38	1.17	1.24
1	A	164	ILE	C-O	-6.35	1.16	1.24
2	B	530	MET	SD-CE	-6.24	1.64	1.79
2	B	545	THR	C-O	-6.22	1.17	1.24
1	A2	289	VAL	C-O	-6.20	1.16	1.24
2	B	552	TRP	C-O	-6.14	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	449	MET	SD-CE	-6.12	1.64	1.79
1	A	159	GLU	C-O	-6.03	1.17	1.24
1	A2	399	HIS	C-O	-6.02	1.17	1.24
1	A	248	ALA	C-O	-6.00	1.18	1.24
2	B	624	ILE	C-O	-5.99	1.17	1.24
1	A2	415	MET	SD-CE	-5.98	1.64	1.79
1	A	59	LEU	C-O	-5.97	1.17	1.24
1	A	201	ILE	C-O	-5.96	1.17	1.24
1	A2	504	ILE	C-O	-5.92	1.17	1.24
2	B	591	ILE	C-O	-5.92	1.16	1.24
1	A	157	VAL	C-O	-5.91	1.17	1.24
1	A	14	CYS	C-O	-5.90	1.17	1.24
1	A2	455	ILE	C-O	-5.89	1.17	1.24
1	A2	492	ASN	C-O	-5.89	1.16	1.23
2	B	583	ALA	C-O	-5.85	1.17	1.24
2	B2	741	LEU	C-O	-5.83	1.17	1.24
1	A	242	ILE	C-O	-5.79	1.17	1.24
2	B2	683	ASP	C-O	-5.79	1.16	1.24
2	B	558	ILE	C-O	-5.79	1.17	1.24
2	B	559	VAL	C-O	-5.79	1.17	1.24
2	B2	694	ASP	C-N	-5.77	1.27	1.34
1	A	232	LYS	C-O	-5.74	1.16	1.24
2	B	526	VAL	C-O	-5.74	1.17	1.24
2	B	549	ALA	C-O	-5.73	1.17	1.24
2	B	613	LEU	C-O	-5.73	1.16	1.24
2	B	652	ASN	CA-C	-5.71	1.44	1.52
1	A2	270	THR	C-O	-5.71	1.16	1.24
1	A	156	SER	C-O	-5.70	1.17	1.23
1	A2	443	LYS	C-O	-5.70	1.17	1.23
2	B2	712	SER	C-O	-5.66	1.17	1.24
2	B	529	LEU	C-O	-5.66	1.17	1.24
1	A2	329	TYR	C-O	-5.65	1.19	1.24
2	B	612	PRO	C-O	-5.62	1.17	1.24
1	A	233	ILE	C-O	-5.60	1.18	1.23
2	B2	678	SER	CA-C	-5.58	1.45	1.52
1	A2	407	VAL	C-O	-5.56	1.17	1.24
1	A2	502	ALA	C-O	-5.56	1.19	1.24
1	A2	279	SER	CA-C	-5.55	1.47	1.53
1	A2	457	ILE	C-O	-5.55	1.18	1.24
1	A	187	VAL	C-O	-5.54	1.17	1.24
1	A2	439	SER	C-O	-5.54	1.17	1.23
2	B2	722	LEU	C-O	-5.52	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B2	742	ALA	C-O	-5.51	1.17	1.24
1	A	50	VAL	C-O	-5.49	1.18	1.24
1	A2	439	SER	CA-C	-5.49	1.46	1.52
2	B2	749	GLU	C-O	-5.48	1.17	1.24
2	B	563	LEU	C-O	-5.44	1.17	1.24
1	A	203	ILE	C-O	-5.43	1.18	1.24
1	A2	391	SER	C-O	-5.42	1.18	1.24
2	B	631	HIS	C-O	-5.41	1.16	1.24
2	B	548	HIS	C-O	-5.38	1.17	1.24
2	B	580	LEU	C-O	-5.38	1.17	1.24
1	A	130	LYS	CA-C	-5.37	1.47	1.53
2	B2	748	LEU	C-O	-5.35	1.17	1.24
2	B	611	THR	C-O	-5.34	1.18	1.24
1	A2	387	GLU	C-O	-5.33	1.17	1.23
2	B	546	PRO	C-O	-5.33	1.17	1.24
2	B	595	LEU	C-O	-5.32	1.18	1.24
1	A	172	GLY	C-O	-5.32	1.17	1.23
1	A2	285	ALA	C-O	-5.29	1.17	1.24
1	A2	425	GLU	C-N	-5.26	1.26	1.33
2	B	552	TRP	C-N	-5.26	1.26	1.34
2	B	624	ILE	N-CA	-5.26	1.40	1.46
2	B2	676	ALA	C-O	-5.24	1.17	1.24
1	A2	353	GLY	C-N	-5.22	1.26	1.33
2	B	579	PRO	C-O	-5.22	1.17	1.24
1	A2	297	CYS	C-O	-5.22	1.18	1.24
1	A	82	PHE	C-O	-5.21	1.18	1.24
1	A	218	ALA	C-O	-5.21	1.17	1.24
1	A	131	SER	C-O	-5.20	1.17	1.23
1	A	163	GLU	C-O	-5.20	1.18	1.24
2	B2	786	VAL	CA-C	-5.19	1.46	1.52
1	A2	307	GLU	C-O	-5.19	1.17	1.24
1	A2	344	SER	C-O	-5.19	1.16	1.23
2	B	535	ASP	C-O	-5.19	1.17	1.24
1	A2	304	VAL	C-O	-5.18	1.17	1.24
1	A	160	ILE	C-O	-5.18	1.18	1.24
2	B2	781	LEU	C-O	-5.18	1.18	1.24
2	B2	738	PRO	C-O	-5.17	1.17	1.24
1	A	162	ALA	C-O	-5.16	1.18	1.24
2	B	514	LEU	C-O	-5.16	1.18	1.24
1	A2	343	VAL	C-O	-5.14	1.18	1.24
1	A2	304	VAL	CA-C	-5.14	1.47	1.52
1	A2	334	TRP	C-O	-5.14	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	657	ILE	N-CA	-5.12	1.40	1.46
2	B	646	PHE	C-O	-5.12	1.18	1.24
1	A	105	ILE	C-O	-5.12	1.18	1.24
2	B	517	ALA	C-O	-5.11	1.18	1.24
2	B	588	HIS	C-O	-5.11	1.17	1.23
2	B2	719	ASP	C-O	-5.11	1.18	1.24
2	B2	752	ASP	C-O	-5.11	1.18	1.24
1	A	249	GLY	C-O	-5.09	1.18	1.24
1	A	150	SER	C-O	-5.09	1.17	1.23
1	A	32	PHE	C-N	-5.08	1.27	1.33
1	A2	268	CYS	CA-C	-5.08	1.47	1.52
1	A	145	HIS	C-O	-5.07	1.18	1.24
1	A	217	ALA	C-O	-5.06	1.17	1.23
1	A	191	GLU	C-O	-5.06	1.18	1.24
2	B2	727	ASP	C-O	-5.05	1.18	1.24
2	B2	787	LEU	C-O	-5.05	1.18	1.24
2	B2	689	MET	SD-CE	-5.04	1.67	1.79
1	A2	306	VAL	C-O	-5.04	1.17	1.23
1	A	213	PRO	C-O	-5.04	1.17	1.23
2	B2	715	LEU	C-O	-5.04	1.17	1.24
2	B2	784	VAL	C-O	-5.02	1.18	1.24
1	A	169	PRO	C-O	-5.02	1.17	1.23
2	B2	814	GLU	CA-C	-5.01	1.45	1.52
2	B	615	VAL	C-O	-5.00	1.17	1.24
2	B2	804	PRO	C-O	-5.00	1.18	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	PRO	N-CA-C	8.81	118.93	110.47
1	A2	360	PRO	N-CA-C	8.18	118.33	110.47
1	A	14	CYS	CA-C-N	7.10	127.09	119.28
1	A	14	CYS	C-N-CA	7.10	127.09	119.28
1	A	244	SER	N-CA-C	6.84	121.62	113.28
1	A2	466	VAL	N-CA-C	6.50	114.55	107.60
1	A2	498	SER	N-CA-C	6.19	120.97	113.17
1	A2	446	ALA	N-CA-C	6.11	117.51	108.60
1	A2	409	ASN	CA-C-N	6.10	131.50	121.86
1	A2	409	ASN	C-N-CA	6.10	131.50	121.86
1	A	252	ARG	CA-C-N	-6.04	114.39	122.72
1	A	252	ARG	C-N-CA	-6.04	114.39	122.72
1	A2	370	ARG	CA-C-N	5.90	123.97	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	370	ARG	C-N-CA	5.90	123.97	119.66
2	B2	669	LEU	N-CA-C	-5.79	105.10	111.82
1	A2	268	CYS	CA-C-N	5.77	125.62	119.28
1	A2	268	CYS	C-N-CA	5.77	125.62	119.28
1	A2	309	SER	N-CA-C	5.70	117.96	109.25
2	B	651	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	212	VAL	N-CA-C	5.53	114.04	107.73
2	B	593	ASP	CA-CB-CG	5.43	118.03	112.60
2	B2	781	LEU	N-CA-C	5.42	117.19	111.28
1	A	253	THR	CA-C-N	5.36	131.35	121.70
1	A	253	THR	C-N-CA	5.36	131.35	121.70
1	A2	477	LEU	N-CA-C	5.19	118.87	112.54
1	A	118	PRO	CA-C-O	-5.12	115.63	121.56
1	A2	360	PRO	CA-C-N	5.04	125.02	120.03
1	A2	360	PRO	C-N-CA	5.04	125.02	120.03

There are no chirality outliers.

There are no planarity outliers.

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	1946	1795	1794	18	0
1	A2	1952	1798	1792	20	0
2	B	1147	1115	1105	12	0
2	B2	1147	1115	1105	7	0
3	A	298	596	0	2	0
3	A2	252	504	0	6	0
3	B	174	348	0	4	0
3	B2	156	312	0	3	0
All	All	7072	7583	5796	56	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 5.

All (56) 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)
2:B:644:THR:HG22	2:B:647:ASP:H	1.39	0.84
1:A2:415:MET:HE1	1:A2:489:ARG:NH1	1.94	0.82
1:A2:411:VAL:CG1	1:A2:415:MET:HE3	2.09	0.82
2:B2:683:ASP:HB3	3:B2:1026:HOH:O	1.82	0.78
1:A:190:HIS:H	1:A:239:HIS:HE1	1.36	0.71
1:A2:415:MET:HE1	1:A2:489:ARG:HH11	1.55	0.71
1:A2:464:ASN:O	1:A2:464:ASN:OD1	2.08	0.71
2:B2:681:GLN:HG2	3:B2:1034:HOH:O	1.90	0.70
1:A2:411:VAL:HG13	1:A2:415:MET:HE3	1.74	0.70
1:A2:415:MET:CE	1:A2:489:ARG:NH1	2.55	0.69
1:A2:283[B]:CSO:SG	3:A2:605:HOH:O	2.48	0.67
2:B:623:GLU:OE2	3:B:701:HOH:O	2.13	0.66
1:A2:415:MET:CE	1:A2:489:ARG:HH11	2.09	0.66
1:A2:283[A]:CSO:SG	3:A2:605:HOH:O	2.53	0.65
1:A:190:HIS:H	1:A:239:HIS:CE1	2.15	0.65
1:A:161:MET:HE3	1:A:206:TRP:CE2	2.33	0.64
1:A:1:LEU:N	1:A:2:PRO:HD3	2.14	0.63
1:A:49:ARG:HE	1:A:254:ASP:CG	2.07	0.62
1:A2:306:VAL:HG12	3:A2:805:HOH:O	2.00	0.61
2:B:644:THR:HG22	2:B:647:ASP:N	2.13	0.60
1:A2:506:ARG:HD2	3:A2:796:HOH:O	2.01	0.60
2:B:527:ARG:HH22	2:B:561:VAL:HG11	1.67	0.60
1:A2:438:LYS:HE3	3:A2:615:HOH:O	2.01	0.60
1:A:253:THR:O	1:A:254:ASP:OXT	2.22	0.57
2:B2:749:GLU:H	2:B2:749:GLU:CD	2.13	0.56
2:B:537:ASN:HD21	2:B:568:ASP:H	1.54	0.56
1:A:49:ARG:NH2	1:A:254:ASP:OD2	2.39	0.56
2:B:627:VAL:O	2:B:631:HIS:HD2	1.88	0.55
2:B:532:ASN:ND2	3:B:706:HOH:O	2.40	0.55
1:A2:351:HIS:HD2	1:A2:387:GLU:OE2	1.91	0.52
1:A:49:ARG:NE	1:A:254:ASP:OD2	2.42	0.52
1:A:1:LEU:H2	1:A:2:PRO:HD3	1.72	0.52
2:B:644:THR:CG2	2:B:646:PHE:HB3	2.40	0.51
1:A2:411:VAL:HG12	1:A2:415:MET:HE3	1.92	0.51
1:A:254:ASP:HB2	2:B2:766:LYS:NZ	2.25	0.51
2:B2:815:ASP:O	2:B2:819:VAL:HG13	2.13	0.49
1:A2:306:VAL:CG1	3:A2:805:HOH:O	2.58	0.49
2:B:644:THR:HG23	2:B:646:PHE:H	1.79	0.46
1:A2:255:LEU:HB3	1:A2:256:PRO:CD	2.45	0.46
2:B2:682:ASP:OD1	2:B2:714:HIS:HD2	1.98	0.46
1:A:94:TYR:CD1	1:A:107:PRO:HD3	2.51	0.45
1:A:45:HIS:HE1	1:A:167:ASN:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:644:THR:HG21	3:B:830:HOH:O	2.17	0.45
1:A2:299:HIS:HE1	1:A2:421:ASN:O	2.00	0.43
2:B:656:ASP:HB2	3:B:805:HOH:O	2.18	0.43
1:A2:375:GLY:O	1:A2:376:GLU:C	2.62	0.43
1:A2:411:VAL:CG1	1:A2:415:MET:CE	2.88	0.42
1:A:183:TYR:CD2	1:A:183:TYR:C	2.97	0.42
2:B:556:LEU:HD11	2:B:594:VAL:HG21	2.02	0.42
1:A:89:VAL:HG13	1:A:144:LYS:HD3	2.02	0.42
1:A:199:HIS:HE1	1:A:219:ASN:OD1	2.02	0.42
1:A:85:LYS:NZ	3:A:301:HOH:O	2.25	0.41
1:A:13:ASN:HA	3:A:496:HOH:O	2.21	0.41
1:A2:364:HIS:CE1	1:A2:373:CYS:SG	3.14	0.40
2:B2:823:ALA:HB1	3:B2:1025:HOH:O	2.20	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	252/254 (99%)	241 (96%)	11 (4%)	0	100	100
1	A2	253/254 (100%)	242 (96%)	11 (4%)	0	100	100
2	B	157/177 (89%)	156 (99%)	1 (1%)	0	100	100
2	B2	157/177 (89%)	157 (100%)	0	0	100	100
All	All	819/862 (95%)	796 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	206/205 (100%)	203 (98%)	3 (2%)	57	43
1	A2	207/205 (101%)	200 (97%)	7 (3%)	32	16
2	B	114/130 (88%)	110 (96%)	4 (4%)	32	15
2	B2	114/130 (88%)	107 (94%)	7 (6%)	17	5
All	All	641/670 (96%)	620 (97%)	21 (3%)	33	17

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	133	GLU
1	A	184	LYS
1	A2	255	LEU
1	A2	349	ASN
1	A2	410	SER
1	A2	438	LYS
1	A2	462	VAL
1	A2	463	GLU
1	A2	508	ASP
2	B	527	ARG
2	B	552	TRP
2	B	644	THR
2	B	660	VAL
2	B2	668	ASP
2	B2	669	LEU
2	B2	671	LYS
2	B2	695	VAL
2	B2	711	TRP
2	B2	819	VAL
2	B2	822	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	45	HIS
1	A	47	ASN
1	A	72	ASN
1	A	95	ASN
1	A	111	HIS
1	A	199	HIS
1	A	210	ASN
1	A	239	HIS
1	A2	264	GLN
1	A2	273	GLN
1	A2	299	HIS
1	A2	351	HIS
1	A2	464	ASN
2	B	537	ASN
2	B	631	HIS
2	B	638	ASN
2	B	652	ASN
2	B	654	ASN
2	B2	681	GLN
2	B2	714	HIS
2	B2	780	HIS
2	B2	797	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CSO	A	29[A]	-	3,6,7	0.75	0	1,6,8	2.57	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSO	A2	283[A]	-	3,6,7	0.74	0	1,6,8	2.58	1 (100%)
1	CSO	A2	283[B]	-	3,6,7	0.76	0	1,6,8	1.12	0
1	CSO	A	29[B]	-	3,6,7	0.79	0	1,6,8	1.01	0

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
1	CSO	A	29[A]	-	-	1/1/5/7	-
1	CSO	A2	283[A]	-	-	1/1/5/7	-
1	CSO	A2	283[B]	-	-	1/1/5/7	-
1	CSO	A	29[B]	-	-	1/1/5/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	283[A]	CSO	CB-CA-C	-2.58	103.80	110.80
1	A	29[A]	CSO	CB-CA-C	-2.57	103.83	110.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	29[A]	CSO	N-CA-CB-SG
1	A	29[B]	CSO	N-CA-CB-SG
1	A2	283[B]	CSO	N-CA-CB-SG
1	A2	283[A]	CSO	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A2	283[A]	CSO	1	0
1	A2	283[B]	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	253/254 (99%)	0.30	14 (5%)	30 34	8, 16, 35, 76	1 (0%)
1	A2	253/254 (99%)	0.61	15 (5%)	28 31	9, 18, 35, 51	5 (1%)
2	B	159/177 (89%)	0.17	3 (1%)	66 71	9, 16, 36, 52	0
2	B2	159/177 (89%)	0.20	4 (2%)	58 62	9, 16, 30, 51	5 (3%)
All	All	824/862 (95%)	0.35	36 (4%)	39 42	8, 17, 35, 76	11 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	LEU	6.6
1	A2	255	LEU	6.1
2	B2	669	LEU	4.4
2	B2	826	ALA	3.4
2	B2	825	ALA	3.4
1	A	135	GLY	3.3
1	A	254	ASP	3.0
1	A	134	ALA	2.9
1	A	253	THR	2.9
1	A2	258	THR	2.9
2	B	608	TYR	2.9
1	A2	373	CYS	2.9
2	B	667	ALA	2.8
1	A	136	TYR	2.6
1	A	252	ARG	2.6
1	A	184	LYS	2.5
1	A	121	GLY	2.5
1	A2	462	VAL	2.4
2	B2	668	ASP	2.4
2	B	641	ALA	2.4
1	A	50	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A2	365	HIS	2.2
1	A2	508	ASP	2.2
1	A2	434	PHE	2.2
1	A	97	HIS	2.2
1	A2	506	ARG	2.2
1	A2	442	TYR	2.2
1	A	185[A]	SER	2.2
1	A2	431	PHE	2.1
1	A2	484	PHE	2.1
1	A	52	VAL	2.1
1	A	137	SER	2.1
1	A2	468	TYR	2.1
1	A2	267[A]	ASN	2.1
1	A2	441	VAL	2.0
1	A2	432	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSO	A2	283[A]	7/8	0.96	0.06	20,25,33,34	8
1	CSO	A2	283[B]	7/8	0.96	0.06	20,25,41,43	8
1	CSO	A	29[A]	7/8	0.97	0.07	20,20,27,27	7
1	CSO	A	29[B]	7/8	0.97	0.07	20,20,29,36	7

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.