



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:53 PM UTC

PDB ID : 9RXI / pdb_00009rxi
Title : Schistosoma mansoni Cathepsin D1 bound to Nb10C9
Authors : Parker, K.; Clarke, J.D.; Owens, R.J.
Deposited on : 2025-07-11
Resolution : 2.59 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

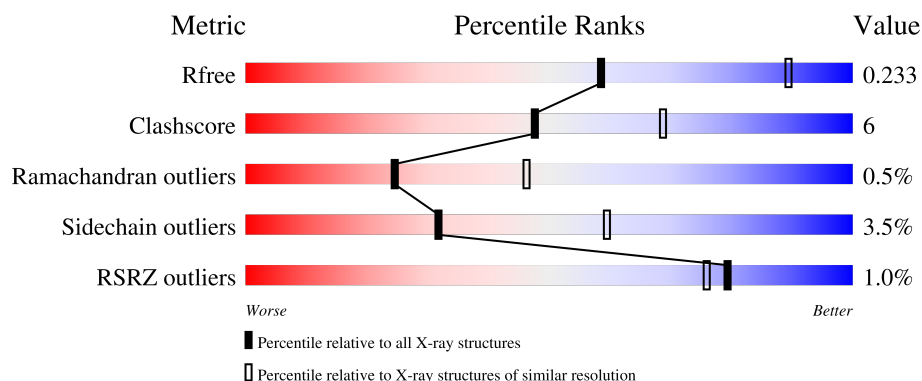
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	381	83% 13% ..
1	B	381	83% 13% ..
1	C	381	79% 15% • 5%
1	D	381	75% 18% • 5%
2	E	152	72% 12% • 14%

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Mol	Chain	Length	Quality of chain
2	H	152	% 72% 13% • 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13335 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 Cathepsin D (A01 family).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2856	1843	452	544	17			
1	B	373	Total	C	N	O	S	0	0	0
			2865	1850	454	544	17			
1	C	363	Total	C	N	O	S	0	0	0
			2787	1803	436	531	17			
1	D	363	Total	C	N	O	S	0	1	0
			2785	1803	439	526	17			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLU	-	expression tag	UNP G4VEV6
A	13	THR	-	expression tag	UNP G4VEV6
A	14	GLY	-	expression tag	UNP G4VEV6
A	386	LYS	-	expression tag	UNP G4VEV6
A	387	HIS	-	expression tag	UNP G4VEV6
A	388	HIS	-	expression tag	UNP G4VEV6
A	389	HIS	-	expression tag	UNP G4VEV6
A	390	HIS	-	expression tag	UNP G4VEV6
A	391	HIS	-	expression tag	UNP G4VEV6
A	392	HIS	-	expression tag	UNP G4VEV6
B	12	GLU	-	expression tag	UNP G4VEV6
B	13	THR	-	expression tag	UNP G4VEV6
B	14	GLY	-	expression tag	UNP G4VEV6
B	386	LYS	-	expression tag	UNP G4VEV6
B	387	HIS	-	expression tag	UNP G4VEV6
B	388	HIS	-	expression tag	UNP G4VEV6
B	389	HIS	-	expression tag	UNP G4VEV6
B	390	HIS	-	expression tag	UNP G4VEV6
B	391	HIS	-	expression tag	UNP G4VEV6
B	392	HIS	-	expression tag	UNP G4VEV6
C	12	GLU	-	expression tag	UNP G4VEV6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	THR	-	expression tag	UNP G4VEV6
C	14	GLY	-	expression tag	UNP G4VEV6
C	386	LYS	-	expression tag	UNP G4VEV6
C	387	HIS	-	expression tag	UNP G4VEV6
C	388	HIS	-	expression tag	UNP G4VEV6
C	389	HIS	-	expression tag	UNP G4VEV6
C	390	HIS	-	expression tag	UNP G4VEV6
C	391	HIS	-	expression tag	UNP G4VEV6
C	392	HIS	-	expression tag	UNP G4VEV6
D	12	GLU	-	expression tag	UNP G4VEV6
D	13	THR	-	expression tag	UNP G4VEV6
D	14	GLY	-	expression tag	UNP G4VEV6
D	386	LYS	-	expression tag	UNP G4VEV6
D	387	HIS	-	expression tag	UNP G4VEV6
D	388	HIS	-	expression tag	UNP G4VEV6
D	389	HIS	-	expression tag	UNP G4VEV6
D	390	HIS	-	expression tag	UNP G4VEV6
D	391	HIS	-	expression tag	UNP G4VEV6
D	392	HIS	-	expression tag	UNP G4VEV6

- Molecule 2 is a protein called Nb_10C9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	130	Total	C	N	O	S	0	0	0
			989	620	170	194	5			
2	E	130	Total	C	N	O	S	0	0	0
			994	622	171	196	5			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Na	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Na 1	0	0
4	D	1	Total 1	Na 1	0	0

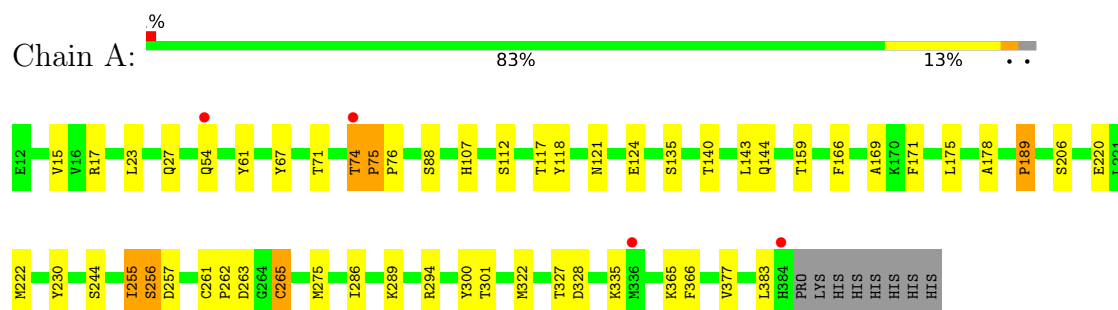
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	13	Total 13	O 13	0	0
5	C	11	Total 11	O 11	0	0
5	D	14	Total 14	O 14	0	0
5	H	2	Total 2	O 2	0	0
5	E	2	Total 2	O 2	0	0

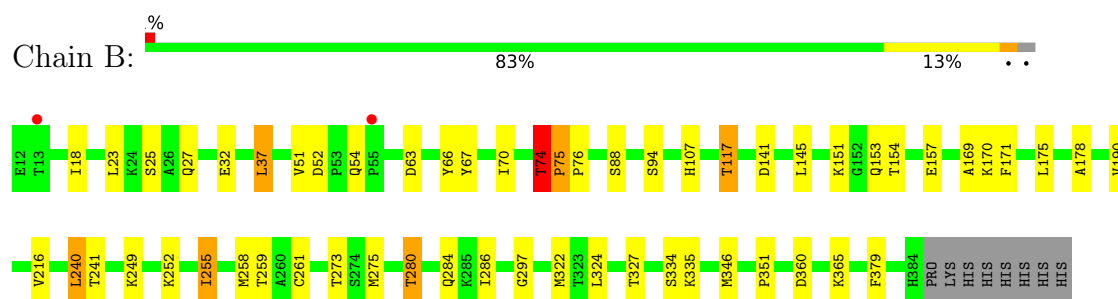
3 Residue-property plots

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.

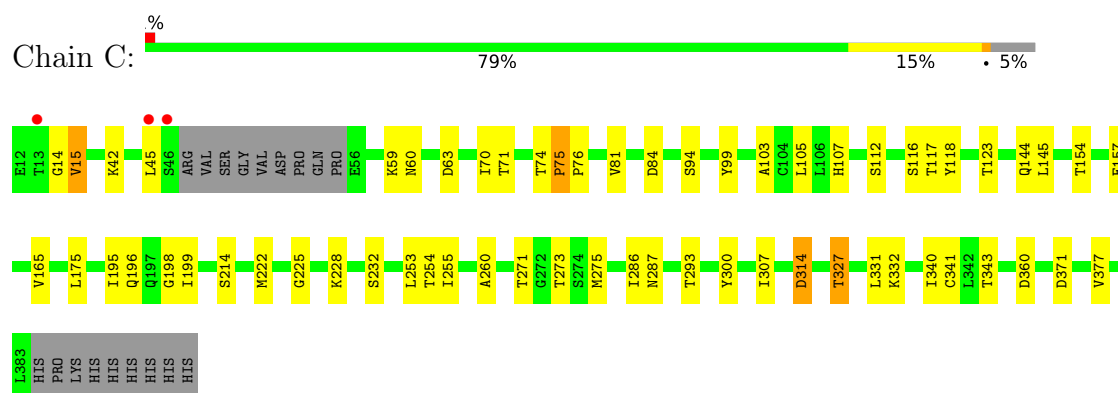
- Molecule 1: Cathepsin D (A01 family)



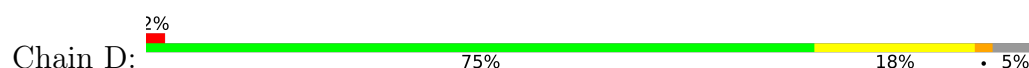
- Molecule 1: Cathepsin D (A01 family)



- Molecule 1: Cathepsin D (A01 family)



- Molecule 1: Cathepsin D (A01 family)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.14Å 181.80Å 78.85Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	90.90 – 2.59 90.90 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (90.90-2.59) 99.7 (90.90-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.173 , 0.234 0.178 , 0.233	Depositor DCC
R_{free} test set	1900 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13335	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: CA, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	0/2922	1.20	8/3968 (0.2%)
1	B	0.62	0/2931	1.20	18/3977 (0.5%)
1	C	0.58	0/2849	1.16	12/3863 (0.3%)
1	D	0.56	0/2847	1.16	14/3860 (0.4%)
2	E	0.63	0/1014	1.17	9/1374 (0.7%)
2	H	0.63	0/1009	1.13	4/1366 (0.3%)
All	All	0.60	0/13572	1.18	65/18408 (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	1
1	B	0	1
1	D	0	1
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	THR	CA-CB-OG1	-12.23	91.25	109.60
1	B	75	PRO	CB-CA-C	11.85	125.38	110.92
1	A	265	CYS	CB-CA-C	-10.65	88.74	111.11
1	A	75	PRO	CB-CA-C	9.76	122.83	110.92
1	C	75	PRO	CB-CA-C	9.74	122.80	110.92
1	B	75	PRO	N-CA-C	-9.38	99.25	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	THR	CA-CB-OG1	-8.04	97.55	109.60
1	B	74	THR	CA-CB-OG1	-7.78	97.92	109.60
1	D	327	THR	CA-CB-OG1	-7.76	97.96	109.60
1	A	327	THR	CA-CB-OG1	-7.45	98.43	109.60
1	D	78	THR	CA-CB-OG1	-7.21	98.79	109.60
1	B	74	THR	CA-C-N	-6.71	113.47	120.38
1	B	74	THR	C-N-CA	-6.71	113.47	120.38
1	D	167	VAL	N-CA-CB	6.66	122.22	111.23
2	E	69	THR	CA-CB-OG1	-6.56	99.76	109.60
2	E	91	THR	CA-CB-OG1	-6.52	99.82	109.60
1	B	249	LYS	N-CA-CB	6.45	119.94	109.95
1	B	280	THR	CA-CB-OG1	-6.38	100.02	109.60
1	B	74	THR	OG1-CB-CG2	6.38	122.06	109.30
1	D	129	TYR	CB-CA-C	6.35	121.43	110.45
1	B	141	ASP	CA-CB-CG	6.34	118.94	112.60
1	D	285	LYS	CB-CA-C	-6.24	100.82	110.81
1	C	271	THR	CA-CB-OG1	-6.20	100.31	109.60
1	D	117	THR	CA-CB-OG1	-6.16	100.36	109.60
1	C	123	THR	CA-CB-OG1	-6.15	100.38	109.60
1	D	75	PRO	CB-CA-C	6.11	118.38	110.92
1	B	52	ASP	CB-CA-C	6.07	117.43	108.87
1	D	280	THR	CA-CB-OG1	-5.91	100.74	109.60
1	C	154	THR	CA-CB-OG1	-5.81	100.88	109.60
1	A	244	SER	O-C-N	5.77	125.10	120.83
2	E	78	THR	CA-CB-OG1	-5.75	100.98	109.60
1	B	249	LYS	CB-CA-C	-5.70	100.56	109.84
2	H	37	PHE	CA-CB-CG	5.68	119.48	113.80
2	H	29	PHE	CA-CB-CG	-5.64	108.16	113.80
1	B	335	LYS	CB-CA-C	-5.63	101.77	110.78
2	E	113	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	154	THR	CA-CB-OG1	-5.57	101.25	109.60
1	C	75	PRO	N-CA-C	-5.57	103.90	110.70
1	D	228	LYS	CB-CA-C	5.55	119.65	109.99
2	E	31	THR	CA-CB-OG1	-5.55	101.28	109.60
2	H	46	GLU	N-CA-CB	-5.54	102.01	110.65
1	C	228	LYS	CB-CA-C	5.52	120.61	110.11
1	C	371	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	189	PRO	CB-CA-C	5.46	118.14	110.60
1	A	75	PRO	N-CA-C	-5.45	104.05	110.70
1	A	140	THR	CA-CB-OG1	-5.45	101.43	109.60
1	B	18	ILE	CA-C-O	5.43	122.36	119.15
1	D	343	THR	CA-CB-OG1	-5.40	101.50	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	THR	CA-CB-OG1	-5.38	101.53	109.60
2	E	46	GLU	CB-CA-C	5.35	118.98	109.72
1	C	360	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	117	THR	CA-CB-OG1	-5.30	101.65	109.60
1	D	261	CYS	CB-CA-C	5.28	115.67	110.71
1	B	252	LYS	N-CA-CB	-5.27	103.55	111.56
1	D	185	ASP	CA-CB-CG	5.26	117.86	112.60
2	H	77	ASN	CB-CA-C	-5.25	104.07	111.95
1	D	129	TYR	N-CA-CB	-5.25	102.33	110.46
2	E	108	GLU	CB-CG-CD	5.24	121.51	112.60
2	E	46	GLU	N-CA-CB	-5.20	102.41	110.57
1	C	327	THR	CA-CB-OG1	-5.14	101.89	109.60
1	C	314	ASP	CA-CB-CG	5.08	117.67	112.60
2	E	118	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	159	THR	CA-CB-OG1	-5.02	102.06	109.60
1	D	241	THR	CA-CB-OG1	-5.01	102.09	109.60
1	B	360	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	GLN	Peptide
1	B	54	GLN	Peptide
1	D	162	PRO	Peptide
2	H	106	ARG	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	2856	0	2827	34	0
1	B	2865	0	2854	32	0
1	C	2787	0	2776	29	0
1	D	2785	0	2771	41	0
2	E	994	0	954	5	0
2	H	989	0	952	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	11	0	0	1	0
5	B	13	0	0	0	0
5	C	11	0	0	0	0
5	D	14	0	0	0	0
5	E	2	0	0	0	0
5	H	2	0	0	1	0
All	All	13335	0	13134	147	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 6.

All (147) 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:D:117:THR:HG23	1:D:141:ASP:OD1	1.79	0.81
1:B:74:THR:O	1:B:76:PRO:N	2.19	0.75
1:D:94:SER:HB2	1:D:157:GLU:OE2	1.86	0.74
1:A:74:THR:HG23	1:A:117:THR:OG1	1.90	0.70
1:B:275:MET:HG3	1:B:346:MET:HE2	1.75	0.69
1:B:74:THR:O	1:B:76:PRO:CD	2.43	0.67
1:C:287:ASN:OD1	1:C:343:THR:HG21	1.96	0.66
1:A:74:THR:OG1	1:A:75:PRO:HD3	1.95	0.66
1:D:58:LEU:HD12	1:D:58:LEU:O	1.97	0.65
1:A:74:THR:CG2	1:A:117:THR:HG23	2.27	0.65
1:B:74:THR:O	1:B:75:PRO:C	2.36	0.64
1:D:74:THR:HG23	1:D:117:THR:CG2	2.27	0.63
1:D:331:LEU:O	1:D:341:CYS:HA	1.98	0.63
1:A:255:ILE:HD11	1:A:286:ILE:HG12	1.81	0.63
1:C:195:ILE:O	1:C:198:GLY:N	2.26	0.63
1:D:287:ASN:OD1	1:D:343:THR:HG21	1.98	0.62
1:A:74:THR:OG1	1:A:75:PRO:CD	2.48	0.62
1:B:74:THR:OG1	1:B:75:PRO:CD	2.48	0.61
1:D:17:ARG:NH2	1:D:227:ASP:OD2	2.34	0.61
1:D:335:LYS:O	1:D:337:GLY:N	2.33	0.59
1:A:88:SER:OG	1:A:178:ALA:HB3	2.02	0.58
1:A:322:MET:HE3	1:A:366:PHE:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:THR:HG23	1:D:117:THR:HB	1.86	0.57
1:B:74:THR:OG1	1:B:75:PRO:HD3	2.03	0.57
1:A:74:THR:HG23	1:A:117:THR:CG2	2.35	0.57
1:B:74:THR:O	1:B:76:PRO:HD3	2.05	0.57
1:A:15:VAL:HG11	1:A:222:MET:HE3	1.87	0.56
1:C:332:LYS:HD3	1:C:341:CYS:SG	2.45	0.56
1:C:275:MET:HE1	1:C:331:LEU:HD21	1.87	0.56
1:A:23:LEU:HD21	1:A:67:TYR:CD2	2.41	0.55
1:B:258:MET:HE1	1:B:286:ILE:HA	1.90	0.54
1:B:255:ILE:HD11	1:B:286:ILE:HG23	1.90	0.54
1:C:175:LEU:HD23	1:C:175:LEU:C	2.32	0.54
1:D:25:SER:HB2	1:D:63:ASP:HA	1.89	0.54
2:E:68:PHE:HA	2:E:82:GLN:O	2.08	0.53
1:C:59:LYS:NZ	1:C:84:ASP:OD1	2.42	0.53
1:B:153:GLN:OE1	1:B:190:VAL:HA	2.09	0.53
1:B:258:MET:HG2	1:B:259:THR:N	2.23	0.53
1:D:17:ARG:HH11	1:D:17:ARG:HG3	1.73	0.53
1:C:112:SER:HB2	1:C:118:TYR:CG	2.44	0.53
1:D:71:THR:OG1	1:D:144:GLN:HB2	2.09	0.53
1:D:119:ILE:O	1:D:120:PRO:C	2.52	0.53
1:A:206:SER:HB2	1:A:222:MET:HB3	1.91	0.52
1:B:74:THR:HG23	1:B:117:THR:OG1	2.10	0.52
2:E:30:SER:O	2:E:53:TRP:HB2	2.09	0.52
1:C:112:SER:HB2	1:C:118:TYR:CD2	2.45	0.52
1:A:74:THR:HG23	1:A:117:THR:HG23	1.92	0.51
1:C:254:THR:OG1	1:C:314:ASP:HB2	2.09	0.51
1:C:255:ILE:CD1	1:C:286:ILE:HG12	2.40	0.51
1:C:71:THR:OG1	1:C:144:GLN:HB2	2.10	0.50
1:B:37:LEU:HB3	1:B:297:GLY:HA3	1.94	0.50
1:D:308:ASN:OD1	1:D:308:ASN:N	2.37	0.50
1:B:94:SER:HB2	1:B:157:GLU:HB3	1.93	0.49
1:A:15:VAL:CG1	1:A:222:MET:HE3	2.43	0.49
1:B:27:GLN:OE1	1:B:346:MET:HE1	2.12	0.49
1:A:261:CYS:SG	1:A:265:CYS:N	2.86	0.49
1:C:70:ILE:HG22	1:C:145:LEU:HD23	1.94	0.49
1:C:222:MET:HE2	1:C:225:GLY:CA	2.43	0.49
1:B:32:GLU:HG2	1:B:334:SER:O	2.12	0.49
1:D:166:PHE:O	1:D:167:VAL:HB	2.12	0.48
1:A:261:CYS:N	1:A:262:PRO:CD	2.76	0.48
1:D:74:THR:HG23	1:D:117:THR:HG21	1.96	0.48
1:C:222:MET:HE2	1:C:225:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:THR:OG1	1:A:144:GLN:HB2	2.14	0.48
1:A:255:ILE:O	1:A:256:SER:C	2.56	0.48
1:B:255:ILE:CD1	1:B:286:ILE:HG23	2.44	0.47
1:C:253:LEU:HD22	1:C:260:ALA:HB3	1.97	0.47
1:D:57:TYR:CE1	1:D:357:ILE:HD13	2.49	0.47
1:A:294:ARG:HB2	1:A:300:TYR:CE1	2.50	0.47
2:E:83:MET:HE1	2:E:94:TYR:CE2	2.50	0.47
1:B:322:MET:HE2	1:B:379:PHE:HB2	1.95	0.46
1:A:328:ASP:CG	1:A:365:LYS:HD3	2.41	0.46
1:D:252:LYS:HA	1:D:261:CYS:O	2.15	0.46
1:A:143:LEU:HD23	1:A:143:LEU:C	2.41	0.46
1:C:15:VAL:CG1	1:C:222:MET:HE3	2.45	0.46
1:D:60:ASN:O	1:D:165:VAL:HG21	2.15	0.46
1:D:141:ASP:OD1	1:D:142:SER:N	2.42	0.46
1:C:103:ALA:O	1:C:107:HIS:HD2	1.99	0.46
1:B:66:TYR:CZ	1:B:216:VAL:HG13	2.52	0.45
1:A:61:TYR:HA	5:A:504:HOH:O	2.16	0.45
1:C:255:ILE:HD11	1:C:286:ILE:HG12	1.98	0.45
1:C:15:VAL:HG11	1:C:222:MET:HE3	1.99	0.45
1:D:110:TYR:OH	1:D:141:ASP:OD2	2.29	0.45
1:B:25:SER:HB2	1:B:63:ASP:HA	1.98	0.45
1:D:108:ARG:NH1	1:D:172:ASP:OD2	2.50	0.45
1:A:27:GLN:HE22	1:A:275:MET:HE2	1.82	0.45
1:A:112:SER:HB2	1:A:118:TYR:CD2	2.52	0.45
1:D:179:TYR:CD2	1:D:243:GLN:HB3	2.52	0.45
2:H:17:SER:HA	2:H:83:MET:O	2.17	0.45
1:A:71:THR:HB	1:A:76:PRO:HB2	1.99	0.45
1:D:166:PHE:O	1:D:167:VAL:CB	2.65	0.45
1:A:175:LEU:C	1:A:175:LEU:HD23	2.41	0.44
1:B:324:LEU:HD23	1:B:365:LYS:HG2	1.99	0.44
1:D:235:ILE:CG2	1:D:237:TYR:CE2	3.00	0.44
1:D:204:VAL:HG12	1:D:371:ASP:HA	1.99	0.44
2:H:6:GLU:HA	2:H:21:SER:O	2.17	0.44
1:D:235:ILE:HG22	1:D:237:TYR:CE2	2.53	0.44
1:C:14:GLY:HA2	1:C:199:ILE:O	2.18	0.44
1:B:169:ALA:HB1	1:B:171:PHE:CE2	2.53	0.44
2:E:83:MET:HE1	2:E:94:TYR:CZ	2.53	0.44
1:A:88:SER:O	1:A:189:PRO:HB3	2.18	0.43
2:H:22:CYS:O	2:H:78:THR:HA	2.18	0.43
1:D:74:THR:HG23	1:D:117:THR:CB	2.49	0.43
1:D:255:ILE:HD11	1:D:286:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:C	1:B:175:LEU:HD23	2.43	0.43
1:A:220:GLU:CD	1:A:230:TYR:OH	2.62	0.43
2:E:12:VAL:HG11	2:E:18:LEU:HD13	2.01	0.43
1:C:99:TYR:HA	1:C:105:LEU:HD21	2.01	0.43
1:B:261:CYS:SG	1:B:261:CYS:O	2.77	0.43
1:C:60:ASN:O	1:C:165:VAL:HG21	2.19	0.43
1:C:94:SER:HB2	1:C:157:GLU:HB3	2.01	0.43
1:D:17:ARG:HG3	1:D:17:ARG:NH1	2.34	0.42
1:D:60:ASN:O	1:D:61:TYR:HB2	2.19	0.42
1:D:81:VAL:HA	1:D:173:GLY:O	2.19	0.42
1:D:334:SER:HA	1:D:338:SER:O	2.20	0.42
1:D:89:ASN:HD21	1:D:184:VAL:HG23	1.83	0.42
1:C:63:ASP:OD1	1:C:273:THR:HA	2.20	0.42
1:A:263:ASP:OD2	1:A:263:ASP:N	2.52	0.42
1:B:280:THR:O	1:B:284:GLN:HG3	2.19	0.42
1:B:74:THR:HG23	1:B:117:THR:CG2	2.50	0.42
1:C:75:PRO:HA	1:C:76:PRO:HD3	1.84	0.42
1:C:222:MET:HE2	1:C:225:GLY:C	2.46	0.41
2:H:24:ALA:HB1	2:H:29:PHE:CD2	2.55	0.41
1:A:74:THR:HG23	1:A:117:THR:CB	2.50	0.41
1:D:97:CYS:HA	1:D:159:THR:HA	2.02	0.41
1:A:112:SER:HB2	1:A:118:TYR:CG	2.56	0.41
1:D:200:VAL:HG22	1:D:224:GLY:HA3	2.03	0.41
1:A:107:HIS:HE1	1:A:166:PHE:O	2.03	0.41
1:D:322:MET:HE2	1:D:322:MET:HA	2.03	0.41
1:C:293:THR:O	1:C:300:TYR:HA	2.21	0.41
1:D:261:CYS:N	1:D:262:PRO:HD3	2.36	0.41
1:A:121:ASN:OD1	1:A:121:ASN:C	2.64	0.41
1:B:23:LEU:HD21	1:B:67:TYR:CD2	2.56	0.41
1:B:70:ILE:HG22	1:B:145:LEU:HD13	2.02	0.41
1:B:107:HIS:HE1	1:B:169:ALA:O	2.04	0.41
1:B:240:LEU:HD12	1:B:240:LEU:HA	1.91	0.41
1:B:66:TYR:CZ	1:B:216:VAL:CG1	3.04	0.41
2:H:22:CYS:HB3	2:H:79:VAL:CG1	2.51	0.41
1:B:88:SER:OG	1:B:178:ALA:HB3	2.21	0.40
2:H:56:GLU:CG	5:H:202:HOH:O	2.69	0.40
1:A:257:ASP:OD1	1:A:289:LYS:NZ	2.51	0.40
1:C:81:VAL:HG21	1:C:175:LEU:HB2	2.03	0.40
1:C:195:ILE:O	1:C:196:GLN:C	2.65	0.40
1:D:200:VAL:CG2	1:D:224:GLY:HA3	2.51	0.40
1:A:169:ALA:HB1	1:A:171:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:CYS:N	1:D:262:PRO:CD	2.85	0.40
1:D:326:PRO:HA	1:D:329:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

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	371/381 (97%)	351 (95%)	18 (5%)	2 (0%)	24	46
1	B	371/381 (97%)	360 (97%)	9 (2%)	2 (0%)	24	46
1	C	359/381 (94%)	335 (93%)	24 (7%)	0	100	100
1	D	360/381 (94%)	333 (92%)	22 (6%)	5 (1%)	9	19
2	E	128/152 (84%)	121 (94%)	7 (6%)	0	100	100
2	H	128/152 (84%)	124 (97%)	4 (3%)	0	100	100
All	All	1717/1828 (94%)	1624 (95%)	84 (5%)	9 (0%)	24	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	167	VAL
1	D	340	ILE
1	A	256	SER
1	D	146	GLY
1	D	336	MET
1	A	335	LYS
1	B	74	THR
1	B	351	PRO
1	D	162	PRO

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	315/328 (96%)	307 (98%)	8 (2%)	42	69
1	B	318/328 (97%)	309 (97%)	9 (3%)	38	66
1	C	309/328 (94%)	299 (97%)	10 (3%)	34	62
1	D	306/328 (93%)	294 (96%)	12 (4%)	28	55
2	E	103/122 (84%)	98 (95%)	5 (5%)	22	47
2	H	102/122 (84%)	95 (93%)	7 (7%)	14	32
All	All	1453/1556 (93%)	1402 (96%)	51 (4%)	32	59

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	74	THR
1	A	124	GLU
1	A	135	SER
1	A	255	ILE
1	A	301	THR
1	A	377	VAL
1	A	383	LEU
1	B	37	LEU
1	B	51	VAL
1	B	74	THR
1	B	117	THR
1	B	151	LYS
1	B	170	LYS
1	B	240	LEU
1	B	241	THR
1	B	255	ILE
1	C	15	VAL
1	C	42	LYS
1	C	45	LEU
1	C	116	SER
1	C	214	SER

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Mol	Chain	Res	Type
1	C	232	SER
1	C	307	ILE
1	C	327	THR
1	C	340	ILE
1	C	377	VAL
1	D	18	ILE
1	D	74	THR
1	D	145	LEU
1	D	164	LEU
1	D	199	ILE
1	D	202	SER
1	D	210	SER
1	D	240	LEU
1	D	284	GLN
1	D	308	ASN
1	D	322	MET
1	D	327	THR
2	H	1	GLN
2	H	11	LEU
2	H	12	VAL
2	H	45	ARG
2	H	87	LYS
2	H	114	LEU
2	H	127	THR
2	E	13	GLN
2	E	30	SER
2	E	56	GLU
2	E	86	LEU
2	E	112	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	65	GLN
1	A	375	ASN
1	B	65	GLN
1	B	107	HIS
1	B	144	GLN
1	B	287	ASN
1	B	306	ASN
1	B	309	ASN

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Mol	Chain	Res	Type
1	C	21	HIS
1	C	161	GLN
1	C	375	ASN
1	D	27	GLN
1	D	107	HIS
1	D	144	GLN
1	D	284	GLN
2	H	82	GLN
2	E	82	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	373/381 (97%)	-0.48	4 (1%) 78 74	23, 40, 78, 129	0
1	B	373/381 (97%)	-0.47	2 (0%) 87 85	24, 41, 75, 126	0
1	C	363/381 (95%)	-0.31	3 (0%) 82 80	27, 48, 84, 114	0
1	D	363/381 (95%)	0.04	6 (1%) 69 64	33, 59, 95, 124	1 (0%)
2	E	130/152 (85%)	-0.54	1 (0%) 82 80	28, 40, 64, 77	0
2	H	130/152 (85%)	-0.58	1 (0%) 82 80	27, 37, 62, 84	0
All	All	1732/1828 (94%)	-0.35	17 (0%) 79 76	23, 45, 84, 129	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	46	SER	5.5
1	C	45	LEU	4.2
2	H	130	SER	3.6
1	D	13	THR	3.3
1	D	46	SER	3.2
1	D	74	THR	3.1
2	E	130	SER	3.1
1	A	384	HIS	2.9
1	A	74	THR	2.9
1	A	336	MET	2.7
1	A	54	GLN	2.7
1	C	13	THR	2.5
1	D	351	PRO	2.5
1	B	13	THR	2.3
1	D	213	ILE	2.3
1	B	55	PRO	2.1
1	D	350	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
3	CA	A	401	1/1	0.60	0.20	71,71,71,71	0
4	NA	D	401	1/1	0.79	0.20	79,79,79,79	0
3	CA	C	401	1/1	0.84	0.11	70,70,70,70	0
4	NA	C	402	1/1	0.91	0.10	60,60,60,60	0
4	NA	B	402	1/1	0.92	0.08	45,45,45,45	0
4	NA	B	401	1/1	0.93	0.09	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.