



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:55 PM EDT

PDB ID : 3RZU / pdb_00003rzu
Title : The Crystal Structure of the Catalytic Domain of AMSH
Authors : Davies, C.W.; Das, C.
Deposited on : 2011-05-12
Resolution : 2.50 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

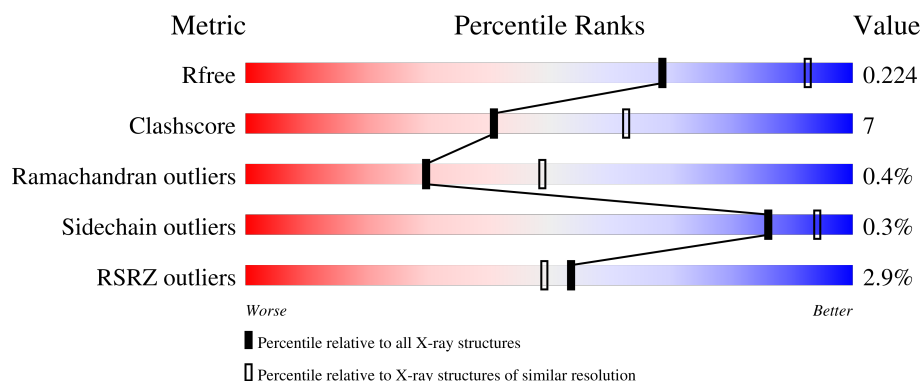
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

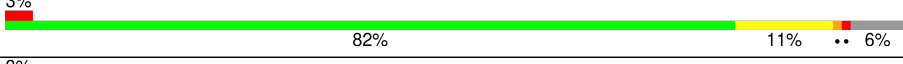
The reported resolution of this entry is 2.50 Å.

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	187	
1	B	187	
1	C	187	
1	D	187	
1	E	187	

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Mol	Chain	Length	Quality of chain
1	F	187	2% 81% 10% • 7%
1	G	187	4% 72% 18% •• 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9740 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 STAM-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	1	0
			1373	864	238	258	13			
1	B	176	Total	C	N	O	S	0	1	0
			1373	864	238	258	13			
1	C	177	Total	C	N	O	S	0	1	0
			1381	870	239	259	13			
1	D	176	Total	C	N	O	S	0	1	0
			1373	864	238	258	13			
1	E	173	Total	C	N	O	S	0	1	0
			1351	849	235	254	13			
1	F	173	Total	C	N	O	S	0	1	0
			1351	849	235	254	13			
1	G	173	Total	C	N	O	S	0	1	0
			1351	849	235	254	13			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLY	-	expression tag	UNP O95630
A	239	PRO	-	expression tag	UNP O95630
A	240	LEU	-	expression tag	UNP O95630
A	241	GLY	-	expression tag	UNP O95630
A	242	SER	-	expression tag	UNP O95630
B	238	GLY	-	expression tag	UNP O95630
B	239	PRO	-	expression tag	UNP O95630
B	240	LEU	-	expression tag	UNP O95630
B	241	GLY	-	expression tag	UNP O95630
B	242	SER	-	expression tag	UNP O95630
C	238	GLY	-	expression tag	UNP O95630
C	239	PRO	-	expression tag	UNP O95630
C	240	LEU	-	expression tag	UNP O95630
C	241	GLY	-	expression tag	UNP O95630
C	242	SER	-	expression tag	UNP O95630

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Chain	Residue	Modelled	Actual	Comment	Reference
D	238	GLY	-	expression tag	UNP O95630
D	239	PRO	-	expression tag	UNP O95630
D	240	LEU	-	expression tag	UNP O95630
D	241	GLY	-	expression tag	UNP O95630
D	242	SER	-	expression tag	UNP O95630
E	238	GLY	-	expression tag	UNP O95630
E	239	PRO	-	expression tag	UNP O95630
E	240	LEU	-	expression tag	UNP O95630
E	241	GLY	-	expression tag	UNP O95630
E	242	SER	-	expression tag	UNP O95630
F	238	GLY	-	expression tag	UNP O95630
F	239	PRO	-	expression tag	UNP O95630
F	240	LEU	-	expression tag	UNP O95630
F	241	GLY	-	expression tag	UNP O95630
F	242	SER	-	expression tag	UNP O95630
G	238	GLY	-	expression tag	UNP O95630
G	239	PRO	-	expression tag	UNP O95630
G	240	LEU	-	expression tag	UNP O95630
G	241	GLY	-	expression tag	UNP O95630
G	242	SER	-	expression tag	UNP O95630

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total 2 Zn 2	0	0
2	B	2	Total 2 Zn 2	0	0
2	C	2	Total 2 Zn 2	0	0
2	D	2	Total 2 Zn 2	0	0
2	E	2	Total 2 Zn 2	0	0
2	F	2	Total 2 Zn 2	0	0
2	G	2	Total 2 Zn 2	0	0

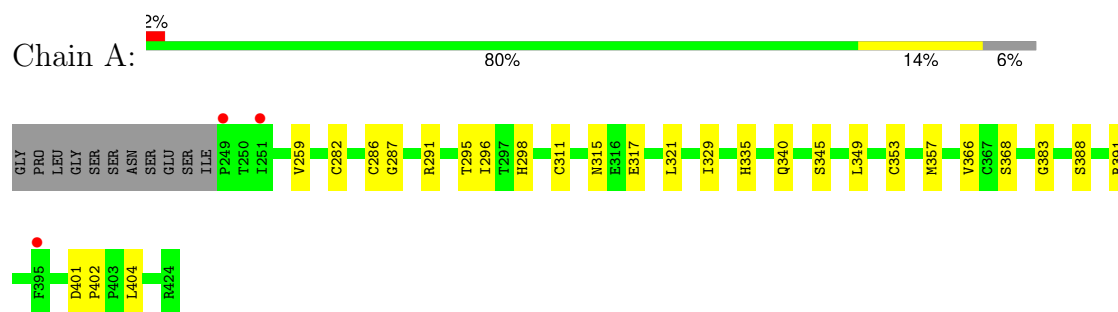
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	25	Total 25	O 25	0	0
3	C	34	Total 34	O 34	0	0
3	D	29	Total 29	O 29	0	0
3	E	17	Total 17	O 17	0	0
3	F	14	Total 14	O 14	0	0
3	G	24	Total 24	O 24	0	0

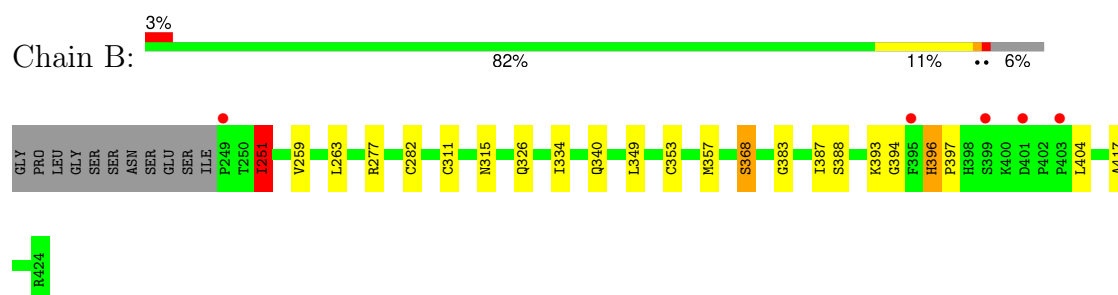
3 Residue-property plots [i](#)

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.

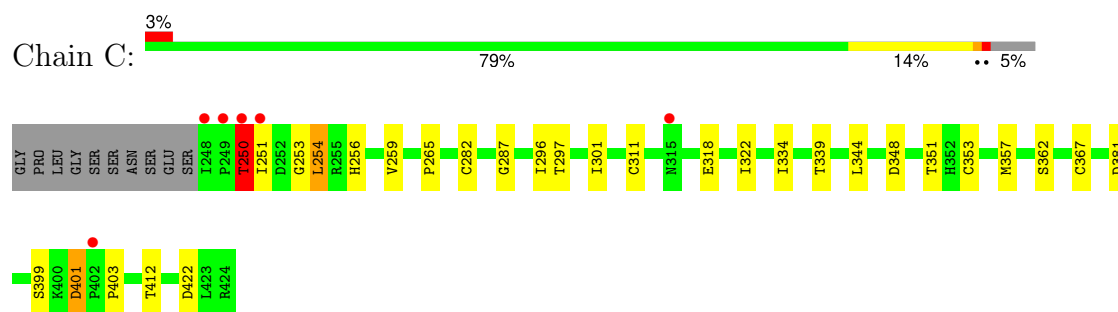
- Molecule 1: STAM-binding protein



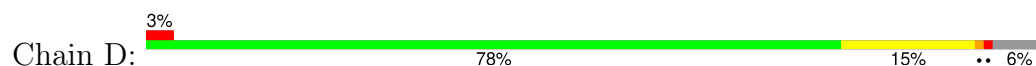
- Molecule 1: STAM-binding protein

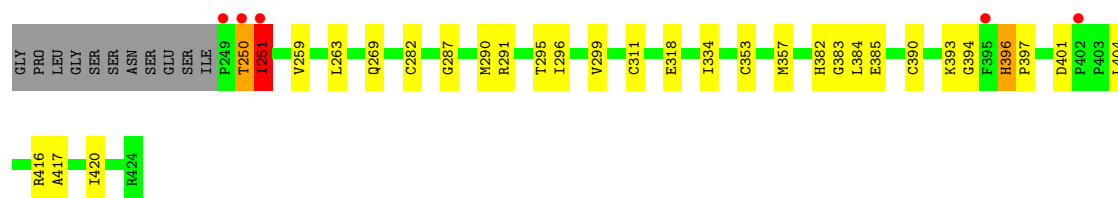


- Molecule 1: STAM-binding protein

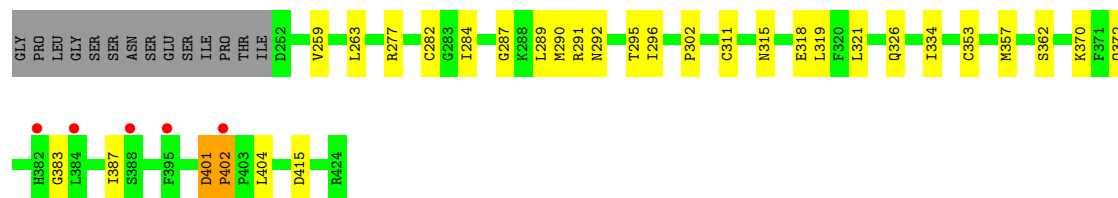
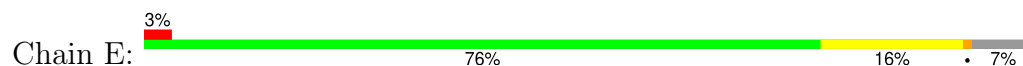


- Molecule 1: STAM-binding protein

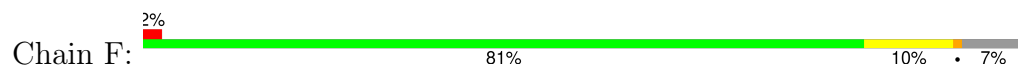




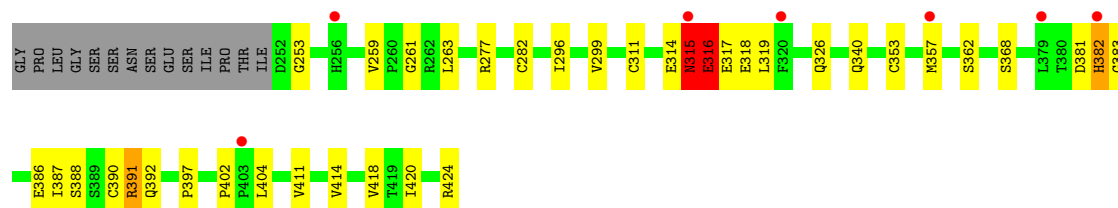
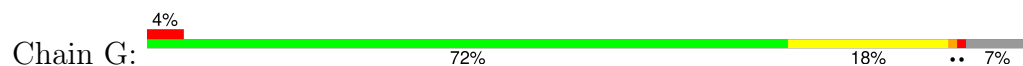
- Molecule 1: STAM-binding protein



- Molecule 1: STAM-binding protein



- Molecule 1: STAM-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.49Å 67.36Å 113.17Å 90.00° 112.44° 90.00°	Depositor
Resolution (Å)	47.15 – 2.50 47.15 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.15-2.50) 99.0 (47.15-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.193 , 0.229 0.189 , 0.224	Depositor DCC
R_{free} test set	2480 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9740	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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	0.52	0/1408	0.94	7/1911 (0.4%)
1	B	0.51	0/1408	0.92	5/1911 (0.3%)
1	C	0.55	0/1416	1.11	6/1923 (0.3%)
1	D	0.52	0/1408	1.22	15/1911 (0.8%)
1	E	0.50	0/1385	0.98	4/1879 (0.2%)
1	F	0.48	0/1385	0.94	6/1879 (0.3%)
1	G	0.55	1/1385 (0.1%)	1.17	15/1879 (0.8%)
All	All	0.52	1/9795 (0.0%)	1.05	58/13293 (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	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	382	HIS	N-CA	-5.71	1.39	1.46

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	401	ASP	CA-C-N	-18.21	101.63	120.38
1	C	401	ASP	C-N-CA	-18.21	101.63	120.38
1	D	401	ASP	CA-C-N	-15.42	104.50	120.38
1	D	401	ASP	C-N-CA	-15.42	104.50	120.38
1	D	250	THR	N-CA-C	14.99	127.34	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	250	THR	CA-C-N	11.60	142.84	121.97
1	D	250	THR	C-N-CA	11.60	142.84	121.97
1	G	381	ASP	CA-C-N	11.42	135.29	120.44
1	G	381	ASP	C-N-CA	11.42	135.29	120.44
1	E	401	ASP	CA-C-N	-10.08	109.99	120.38
1	E	401	ASP	C-N-CA	-10.08	109.99	120.38
1	G	382	HIS	N-CA-CB	-9.32	96.49	110.01
1	E	402	PRO	CA-C-N	8.65	129.19	119.93
1	E	402	PRO	C-N-CA	8.65	129.19	119.93
1	C	253	GLY	N-CA-C	7.89	126.27	115.30
1	G	253	GLY	N-CA-C	7.55	125.80	115.30
1	G	382	HIS	CA-CB-CG	7.02	120.82	113.80
1	A	402	PRO	CA-C-N	6.56	126.95	119.93
1	A	402	PRO	C-N-CA	6.56	126.95	119.93
1	G	381	ASP	CA-C-O	6.52	127.46	120.55
1	G	391	ARG	N-CA-C	6.41	121.07	107.67
1	G	381	ASP	O-C-N	6.39	128.89	122.12
1	D	384	LEU	N-CA-C	6.37	118.22	111.28
1	D	250	THR	CA-C-O	6.21	127.54	121.14
1	G	411	VAL	N-CA-C	6.13	116.70	108.11
1	B	368	SER	CA-C-N	6.04	125.75	119.05
1	B	368	SER	C-N-CA	6.04	125.75	119.05
1	D	396	HIS	CA-C-N	6.02	125.99	120.21
1	D	396	HIS	C-N-CA	6.02	125.99	120.21
1	A	368	SER	CA-C-N	5.83	125.97	119.32
1	A	368	SER	C-N-CA	5.83	125.97	119.32
1	F	253	GLY	N-CA-C	-5.75	107.71	115.36
1	F	368	SER	CA-C-N	5.54	125.20	119.05
1	F	368	SER	C-N-CA	5.54	125.20	119.05
1	F	254	LEU	N-CA-C	-5.53	100.87	109.72
1	A	401	ASP	CA-C-N	5.53	140.26	127.00
1	A	401	ASP	C-N-CA	5.53	140.26	127.00
1	C	254	LEU	N-CA-C	5.51	118.72	109.95
1	D	393	LYS	CA-C-N	-5.50	114.36	121.96
1	D	393	LYS	C-N-CA	-5.50	114.36	121.96
1	D	251	ILE	CA-C-N	-5.44	111.15	121.54
1	D	251	ILE	C-N-CA	-5.44	111.15	121.54
1	G	315	ASN	N-CA-C	5.34	122.17	110.80
1	G	386	GLU	N-CA-C	5.25	117.09	111.36
1	B	396	HIS	CA-C-N	5.23	125.23	120.21
1	B	396	HIS	C-N-CA	5.23	125.23	120.21
1	G	368	SER	CA-C-N	5.23	124.86	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	368	SER	C-N-CA	5.23	124.86	119.05
1	B	251	ILE	N-CA-C	5.20	114.76	107.37
1	D	251	ILE	CG1-CB-CG2	-5.16	95.22	110.70
1	C	250	THR	CA-C-N	5.13	128.08	120.74
1	C	250	THR	C-N-CA	5.13	128.08	120.74
1	F	402	PRO	CA-C-N	5.13	125.42	119.93
1	F	402	PRO	C-N-CA	5.13	125.42	119.93
1	G	390	CYS	N-CA-C	5.09	117.59	109.96
1	A	401	ASP	C-N-CD	-5.06	109.47	120.60
1	D	250	THR	CB-CA-C	-5.04	101.48	113.02
1	G	316	GLU	N-CA-C	5.02	121.50	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	401	ASP	Peptide

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	1373	0	1351	17	0
1	B	1373	0	1352	17	0
1	C	1381	0	1361	21	0
1	D	1373	0	1352	20	0
1	E	1351	0	1326	21	0
1	F	1351	0	1325	12	0
1	G	1351	0	1326	28	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
3	A	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	3	0
3	C	34	0	0	7	0
3	D	29	0	0	5	0
3	E	17	0	0	5	0
3	F	14	0	0	1	0
3	G	24	0	0	8	0
All	All	9740	0	9393	124	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 7.

All (124) 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:G:382:HIS:CE1	1:G:402:PRO:HB2	1.92	1.04
1:A:357:MET:HE3	1:E:415:ASP:H	1.26	1.00
1:E:362:SER:OG	3:E:169:HOH:O	1.86	0.93
1:G:326:GLN:NE2	3:G:76:HOH:O	2.00	0.93
1:G:382:HIS:HE1	1:G:402:PRO:HB2	1.30	0.92
1:G:362:SER:OG	3:G:122:HOH:O	1.87	0.92
1:B:340:GLN:NE2	3:B:25:HOH:O	2.00	0.91
1:C:265:PRO:O	3:C:39:HOH:O	1.86	0.90
1:A:388:SER:O	1:A:391:ARG:NH2	2.09	0.85
1:G:424:ARG:O	3:G:173:HOH:O	1.95	0.84
1:D:382:HIS:O	3:D:109:HOH:O	1.93	0.84
1:C:318:GLU:OE2	3:C:120:HOH:O	1.96	0.83
1:E:315:ASN:ND2	3:E:80:HOH:O	2.10	0.82
1:C:250:THR:HG22	1:C:251:ILE:H	1.46	0.80
1:C:399:SER:OG	3:C:87:HOH:O	1.99	0.78
1:G:263:LEU:HD11	1:G:299:VAL:HG21	1.66	0.77
1:D:390:CYS:SG	3:D:136:HOH:O	2.43	0.77
1:C:362:SER:OG	3:C:154:HOH:O	2.04	0.76
1:C:287:GLY:HA2	1:C:297:THR:HG22	1.69	0.74
1:G:391:ARG:NH1	3:G:137:HOH:O	2.18	0.74
1:D:269:GLN:NE2	3:D:163:HOH:O	2.21	0.73
1:C:339:THR:OG1	3:C:94:HOH:O	2.07	0.73
1:A:357:MET:HE3	1:E:415:ASP:N	2.05	0.68
1:E:318:GLU:OE2	3:E:100:HOH:O	2.11	0.68
1:B:340:GLN:O	1:B:368:SER:OG	2.11	0.67
1:C:381:ASP:OD1	3:C:41:HOH:O	2.14	0.65
1:F:280:GLU:OE2	3:F:155:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:353:CYS:O	1:G:357:MET:HG2	1.97	0.64
1:G:315:ASN:ND2	1:G:318:GLU:OE1	2.31	0.64
1:G:387:ILE:O	3:G:159:HOH:O	2.15	0.63
1:G:263:LEU:HD13	1:G:418:VAL:HG11	1.80	0.62
1:A:315:ASN:HB2	1:B:417:ALA:HB3	1.80	0.62
1:E:326:GLN:NE2	3:E:132:HOH:O	2.32	0.61
1:A:259:VAL:HG22	1:A:296:ILE:HD12	1.84	0.59
1:G:387:ILE:HD11	1:G:404:LEU:HD13	1.84	0.59
1:C:353:CYS:O	1:C:357:MET:HG2	2.04	0.57
1:A:383:GLY:HA2	1:A:404:LEU:HD22	1.85	0.57
1:F:254:LEU:HB3	1:F:361:GLU:HG3	1.86	0.57
1:C:351:THR:OG1	3:C:139:HOH:O	2.18	0.56
1:E:387:ILE:HD11	1:E:404:LEU:HD13	1.88	0.56
1:F:353:CYS:O	1:F:357:MET:HG2	2.05	0.55
1:C:344:LEU:HD22	1:C:348:ASP:HB3	1.88	0.55
1:G:315:ASN:O	1:G:317:GLU:N	2.34	0.55
1:D:259:VAL:HG22	1:D:296:ILE:HD12	1.88	0.55
1:A:282:CYS:HB3	1:A:311[A]:CYS:SG	2.47	0.54
1:G:383:GLY:HA2	1:G:404:LEU:HD22	1.89	0.54
1:E:282:CYS:HB3	1:E:311[B]:CYS:SG	2.48	0.54
1:B:326:GLN:NE2	3:B:21:HOH:O	2.42	0.53
1:A:353:CYS:O	1:A:357:MET:HG2	2.07	0.53
1:E:302:PRO:HB3	1:E:319:LEU:HD11	1.90	0.53
1:E:372:GLN:HE21	1:G:397:PRO:HG3	1.75	0.52
1:G:259:VAL:HG22	1:G:296:ILE:HD12	1.92	0.52
1:E:259:VAL:HG22	1:E:296:ILE:HD12	1.93	0.51
1:C:250:THR:OG1	1:C:254:LEU:O	2.24	0.51
1:D:416:ARG:HD2	3:D:92:HOH:O	2.11	0.50
1:E:353:CYS:O	1:E:357:MET:HG2	2.11	0.50
1:C:401:ASP:O	1:C:403:PRO:HD3	2.12	0.50
1:F:381:ASP:O	1:F:385:GLU:HG3	2.12	0.50
1:D:353:CYS:O	1:D:357:MET:HG2	2.12	0.49
1:B:282:CYS:HB3	1:B:311[A]:CYS:SG	2.52	0.49
1:B:357:MET:HE2	1:B:388:SER:HB3	1.94	0.49
1:C:322:ILE:HD12	1:G:277:ARG:HG3	1.93	0.49
1:E:290:MET:O	1:E:291:ARG:HG2	2.13	0.49
1:G:282:CYS:HB3	1:G:311[A]:CYS:SG	2.54	0.48
1:C:259:VAL:HG22	1:C:296:ILE:HD12	1.96	0.48
1:F:259:VAL:HG22	1:F:296:ILE:HD12	1.96	0.47
1:F:302:PRO:HB3	1:F:319:LEU:HD11	1.94	0.47
3:E:80:HOH:O	1:F:416:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:ASN:HD21	1:G:318:GLU:CD	2.22	0.47
1:F:255:ARG:O	1:F:361:GLU:HG2	2.14	0.47
1:B:349:LEU:HB3	1:B:387:ILE:HD13	1.97	0.47
1:D:396:HIS:HA	1:D:397:PRO:HD3	1.76	0.46
1:C:256:HIS:CE1	1:C:412:THR:HG1	2.26	0.46
1:E:383:GLY:HA2	1:E:404:LEU:HD22	1.97	0.46
1:A:286:CYS:HB2	1:A:298:HIS:HB2	1.98	0.46
1:E:263:LEU:HD21	1:E:334:ILE:HD12	1.98	0.45
1:E:284:ILE:HG13	1:E:319:LEU:HD23	1.98	0.45
1:C:250:THR:HG22	1:C:251:ILE:N	2.25	0.45
1:D:282:CYS:HB3	1:D:311[B]:CYS:SG	2.56	0.45
1:B:263:LEU:HD21	1:B:334:ILE:HD12	1.98	0.45
1:F:368:SER:HB2	1:F:373:GLU:HG2	1.99	0.45
1:A:345:SER:O	1:A:349:LEU:HG	2.16	0.45
1:A:340:GLN:NE2	1:D:290:MET:HG2	2.32	0.45
1:B:277:ARG:HD3	1:D:318:GLU:HG2	1.98	0.44
1:A:315:ASN:HB2	1:B:417:ALA:CB	2.45	0.44
1:E:321:LEU:HD23	1:E:321:LEU:HA	1.84	0.44
1:E:277:ARG:HG3	1:F:322:ILE:HD12	1.98	0.44
1:A:287:GLY:HA3	1:A:295:THR:O	2.17	0.44
1:C:334:ILE:HD11	1:C:367:CYS:SG	2.58	0.44
1:D:385:GLU:N	3:D:109:HOH:O	2.18	0.44
1:G:314:GLU:O	1:G:316:GLU:N	2.44	0.44
1:A:340:GLN:HE21	1:D:290:MET:HG2	1.82	0.43
1:D:394:GLY:O	1:D:396:HIS:ND1	2.51	0.43
1:B:251:ILE:HD12	1:B:251:ILE:N	2.34	0.43
1:B:383:GLY:HA2	1:B:404:LEU:HD22	2.00	0.43
1:D:299:VAL:HB	1:D:420:ILE:HG12	2.00	0.43
1:B:315:ASN:HB2	1:D:417:ALA:HB3	2.00	0.43
1:D:263:LEU:HD21	1:D:334:ILE:HD12	2.00	0.43
1:E:287:GLY:HA3	1:E:295:THR:O	2.18	0.43
1:G:299:VAL:HB	1:G:420:ILE:HG12	2.00	0.43
1:B:353:CYS:O	1:B:357:MET:HG2	2.18	0.43
1:C:301:ILE:HB	1:C:422:ASP:HA	2.01	0.43
1:G:316:GLU:HA	1:G:319:LEU:HD13	2.01	0.43
1:G:382:HIS:HE1	1:G:402:PRO:CB	2.17	0.43
1:G:388:SER:O	3:G:124:HOH:O	2.21	0.43
1:A:335:HIS:CE1	1:A:366:VAL:HG22	2.54	0.43
1:E:289:LEU:HD11	1:E:292:ASN:HA	2.01	0.42
1:B:393:LYS:N	3:B:160:HOH:O	2.52	0.42
1:E:370:LYS:HE2	1:G:392:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLU:O	1:A:321:LEU:HD13	2.20	0.42
1:G:340:GLN:OE1	3:G:85:HOH:O	2.22	0.42
1:A:291:ARG:HD2	1:A:291:ARG:HA	1.82	0.42
3:A:133:HOH:O	1:D:291:ARG:HG2	2.19	0.42
1:D:250:THR:HB	1:D:251:ILE:H	1.31	0.42
1:C:250:THR:CG2	1:C:251:ILE:H	2.23	0.41
1:F:387:ILE:HD11	1:F:404:LEU:HD13	2.02	0.41
1:B:393:LYS:HG2	1:B:394:GLY:N	2.34	0.41
1:B:396:HIS:HA	1:B:397:PRO:HD3	1.83	0.41
1:D:383:GLY:HA2	1:D:404:LEU:HD22	2.01	0.41
1:F:301:ILE:HA	1:F:302:PRO:HD3	1.85	0.41
1:C:282:CYS:HB3	1:C:311[B]:CYS:SG	2.60	0.41
1:D:287:GLY:HA3	1:D:295:THR:O	2.21	0.40
1:G:261:GLY:N	1:G:414:VAL:O	2.48	0.40
1:G:277:ARG:NH1	3:G:78:HOH:O	2.49	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	175/187 (94%)	172 (98%)	3 (2%)	0	100	100
1	B	175/187 (94%)	171 (98%)	4 (2%)	0	100	100
1	C	176/187 (94%)	169 (96%)	6 (3%)	1 (1%)	21	38
1	D	175/187 (94%)	167 (95%)	7 (4%)	1 (1%)	21	38
1	E	172/187 (92%)	166 (96%)	5 (3%)	1 (1%)	21	38
1	F	172/187 (92%)	167 (97%)	5 (3%)	0	100	100
1	G	172/187 (92%)	167 (97%)	3 (2%)	2 (1%)	10	20
All	All	1217/1309 (93%)	1179 (97%)	33 (3%)	5 (0%)	30	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	251	ILE
1	G	315	ASN
1	G	316	GLU
1	E	402	PRO
1	C	250	THR

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	159/167 (95%)	158 (99%)	1 (1%)	78	91
1	B	159/167 (95%)	157 (99%)	2 (1%)	61	82
1	C	160/167 (96%)	160 (100%)	0	100	100
1	D	159/167 (95%)	159 (100%)	0	100	100
1	E	156/167 (93%)	156 (100%)	0	100	100
1	F	156/167 (93%)	156 (100%)	0	100	100
1	G	156/167 (93%)	156 (100%)	0	100	100
All	All	1105/1169 (94%)	1102 (100%)	3 (0%)	86	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	ILE
1	B	251	ILE
1	B	259	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	D	340	GLN
1	D	382	HIS

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Mol	Chain	Res	Type
1	E	382	HIS
1	F	256	HIS
1	F	325	GLN
1	F	382	HIS
1	G	315	ASN
1	G	382	HIS

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 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	176/187 (94%)	-0.08	3 (1%) 69 65	26, 47, 97, 124	1 (0%)
1	B	176/187 (94%)	0.13	5 (2%) 55 50	27, 56, 111, 123	1 (0%)
1	C	177/187 (94%)	0.05	6 (3%) 48 43	27, 49, 94, 112	1 (0%)
1	D	176/187 (94%)	0.07	5 (2%) 55 50	31, 52, 107, 132	1 (0%)
1	E	173/187 (92%)	0.15	5 (2%) 53 49	29, 56, 107, 127	1 (0%)
1	F	173/187 (92%)	0.16	4 (2%) 61 57	33, 59, 105, 126	1 (0%)
1	G	173/187 (92%)	0.28	7 (4%) 42 38	30, 62, 108, 123	1 (0%)
All	All	1224/1309 (93%)	0.11	35 (2%) 53 49	26, 55, 105, 132	7 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	402	PRO	3.7
1	D	249	PRO	3.6
1	C	248	ILE	3.5
1	C	249	PRO	3.4
1	A	249	PRO	3.3
1	D	395	PHE	3.1
1	D	251	ILE	3.0
1	C	250	THR	3.0
1	F	395	PHE	2.9
1	F	402	PRO	2.9
1	E	382	HIS	2.7
1	B	249	PRO	2.7
1	C	315	ASN	2.5
1	E	402	PRO	2.5
1	G	320	PHE	2.4
1	G	382	HIS	2.4
1	B	403	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	395	PHE	2.3
1	B	401	ASP	2.3
1	D	250	THR	2.2
1	C	402	PRO	2.2
1	F	291	ARG	2.2
1	E	384	LEU	2.2
1	A	395	PHE	2.1
1	C	251	ILE	2.1
1	E	388	SER	2.1
1	E	395	PHE	2.1
1	B	399	SER	2.1
1	G	357	MET	2.1
1	G	256	HIS	2.1
1	G	315	ASN	2.0
1	G	379	LEU	2.0
1	A	251	ILE	2.0
1	F	252	ASP	2.0
1	G	403	PRO	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(Å ²)	Q<0.9
2	ZN	E	10	1/1	0.97	0.08	90,90,90,90	0
2	ZN	G	14	1/1	0.98	0.04	64,64,64,64	0
2	ZN	D	7	1/1	0.99	0.07	40,40,40,40	0
2	ZN	D	8	1/1	0.99	0.05	65,65,65,65	0
2	ZN	E	9	1/1	0.99	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	2	1/1	0.99	0.05	53,53,53,53	0
2	ZN	F	12	1/1	0.99	0.07	81,81,81,81	0
2	ZN	B	4	1/1	0.99	0.07	73,73,73,73	0
2	ZN	C	5	1/1	1.00	0.05	35,35,35,35	0
2	ZN	C	6	1/1	1.00	0.05	45,45,45,45	0
2	ZN	F	11	1/1	1.00	0.04	49,49,49,49	0
2	ZN	B	3	1/1	1.00	0.08	45,45,45,45	0
2	ZN	G	13	1/1	1.00	0.05	39,39,39,39	0
2	ZN	A	1	1/1	1.00	0.07	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.