



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:51 pm GMT

PDB ID : 3RZU
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

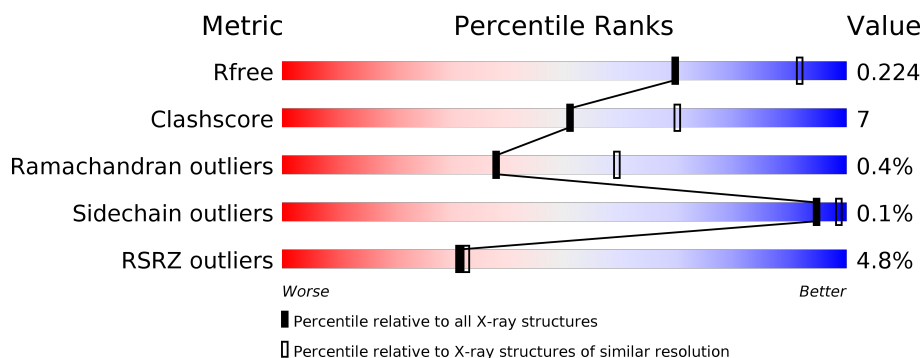
1 Overall quality at a glance

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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>81% 13% 6%</div> <div> <div>6%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	187	<div> <div>83%</div> <div>11%</div> <div>6%</div> </div>
1	C	187	<div> <div>79%</div> <div>14%</div> <div>5%</div> </div>
1	D	187	<div> <div>78%</div> <div>16%</div> <div>6%</div> </div>
1	E	187	<div> <div>75%</div> <div>17%</div> <div>7%</div> </div>
1	F	187	<div> <div>82%</div> <div>10%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	187	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	1	-	-	-	X
2	ZN	B	3	-	-	-	X
2	ZN	C	5	-	-	-	X
2	ZN	E	9	-	-	-	X
2	ZN	G	13	-	-	-	X

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 (three-letter code: ZN) (formula: Zn).

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

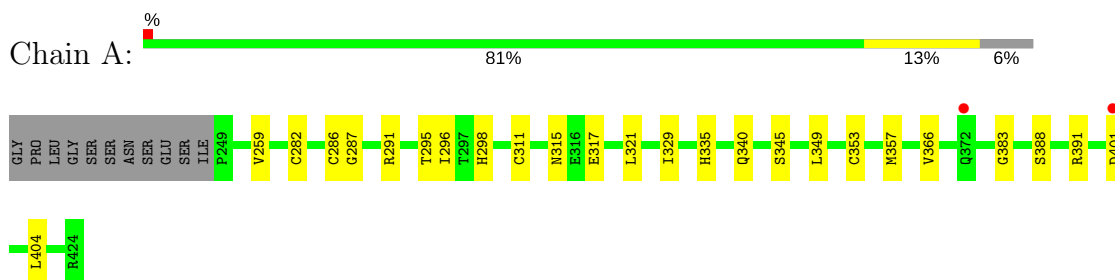
- Molecule 3 is water.

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

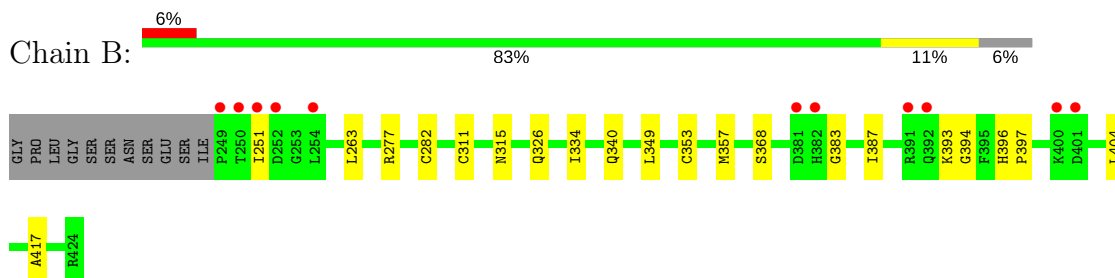
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

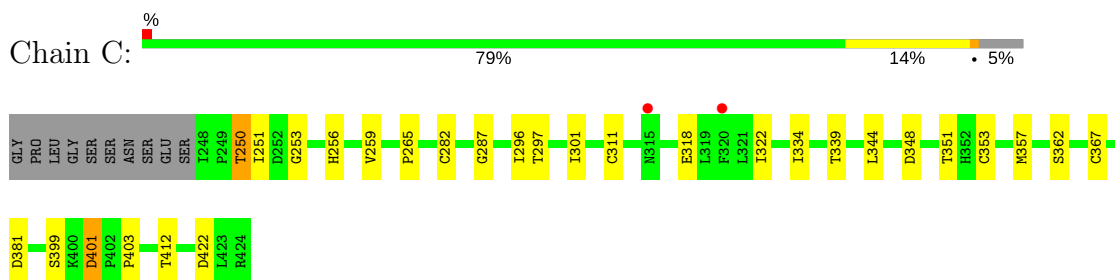
- Molecule 1: STAM-binding protein



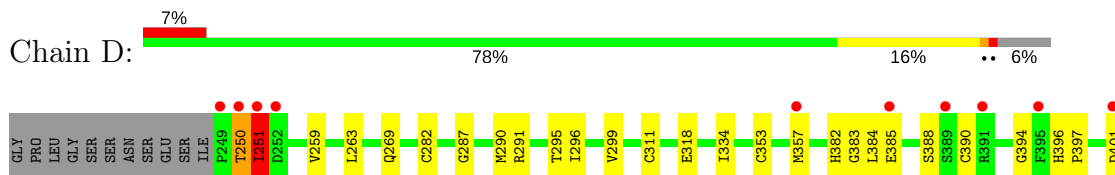
- Molecule 1: STAM-binding protein

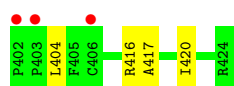


- Molecule 1: STAM-binding protein

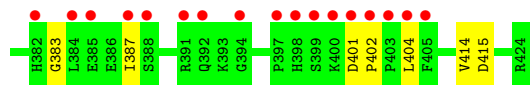
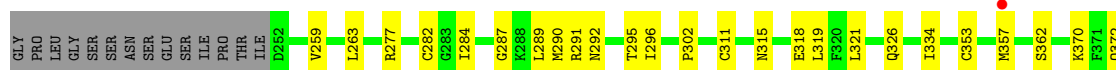
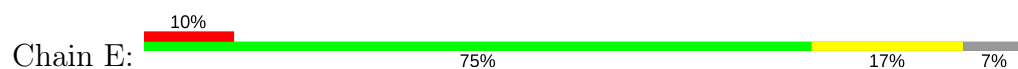


- Molecule 1: STAM-binding protein

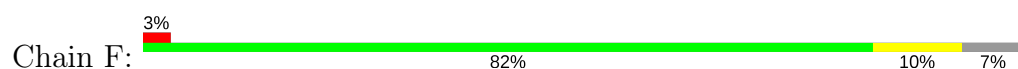




- Molecule 1: STAM-binding protein



- 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: dev_833)	Depositor
R, R_{free}	0.193 , 0.229 0.188 , 0.224	Depositor DCC
R_{free} test set	2478 reflections (5.07%)	DCC
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 , 45.6	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	0.42	0/1408	0.64	1/1911 (0.1%)
1	B	0.40	0/1408	0.58	0/1911
1	C	0.42	0/1416	0.67	2/1923 (0.1%)
1	D	0.41	0/1408	0.75	5/1911 (0.3%)
1	E	0.40	0/1385	0.62	0/1879
1	F	0.37	0/1385	0.64	0/1879
1	G	0.42	0/1385	0.79	4/1879 (0.2%)
All	All	0.41	0/9795	0.67	12/13293 (0.1%)

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	250	THR	C-N-CA	8.46	142.84	121.70
1	G	382	HIS	N-CA-CB	-7.84	96.49	110.60
1	D	251	ILE	CG1-CB-CG2	-7.36	95.22	111.40
1	C	401	ASP	C-N-CD	6.93	142.96	128.40
1	G	381	ASP	CA-C-N	-6.16	103.64	117.20
1	D	250	THR	CA-C-N	-6.14	103.69	117.20
1	D	250	THR	N-CA-C	6.05	127.34	111.00
1	D	401	ASP	C-N-CD	5.84	140.66	128.40
1	G	381	ASP	C-N-CA	5.43	135.29	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	GLY	N-CA-C	5.27	126.27	113.10
1	G	253	GLY	N-CA-C	5.08	125.80	113.10
1	A	401	ASP	C-N-CD	-5.06	109.47	120.60

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	18	0
1	B	1373	0	1352	16	0
1	C	1381	0	1361	20	0
1	D	1373	0	1352	21	0
1	E	1351	0	1326	22	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
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: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: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:A:357:MET:HE3	1:E:415:ASP:H	1.60	0.65
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
1:G:353:CYS:O	1:G:357:MET:HG2	1.97	0.64
1:A:357:MET:HE3	1:E:414:VAL:HA	1.79	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:A:357:MET:CE	1:E:415:ASP:H	2.15	0.59
1:C:353:CYS:O	1:C:357:MET:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:284:ILE:HG13	1:E:319:LEU:HD23	1.98	0.45
1:E:263:LEU:HD21	1:E:334:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:384:LEU:O	1:D:388:SER:OG	2.27	0.42
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:G:315:ASN:HD21	1:G:318:GLU:CD	2.22	0.42
1:E:370:LYS:HE2	1:G:392:GLN:OE1	2.19	0.42
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:HA	1:A:291:ARG:HD2	1.82	0.42
3:A:133:HOH:O	1:D:291:ARG:HG2	2.19	0.42
1:B:393:LYS:HG2	1:B:394:GLY:N	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:277:ARG:NH1	3:G:78:HOH:O	2.49	0.40
1:G:261:GLY:N	1:G:414:VAL:O	2.48	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	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%)	28	48
1	D	175/187 (94%)	167 (95%)	7 (4%)	1 (1%)	28	48
1	E	172/187 (92%)	166 (96%)	5 (3%)	1 (1%)	28	48
1	F	172/187 (92%)	167 (97%)	5 (3%)	0	100	100
1	G	172/187 (92%)	167 (97%)	3 (2%)	2 (1%)	15	27
All	All	1217/1309 (93%)	1179 (97%)	33 (3%)	5 (0%)	38	59

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%)	89	97
1	B	159/167 (95%)	159 (100%)	0	100	100
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%)	1104 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	D	382	HIS
1	E	326	GLN
1	E	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [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	176/187 (94%)	-0.04	2 (1%) 80 81	31, 47, 97, 124	0
1	B	176/187 (94%)	0.38	11 (6%) 21 21	31, 56, 111, 123	0
1	C	177/187 (94%)	-0.01	2 (1%) 80 81	33, 49, 94, 112	0
1	D	176/187 (94%)	0.31	13 (7%) 15 15	33, 52, 107, 132	0
1	E	173/187 (92%)	0.42	18 (10%) 7 6	33, 56, 107, 127	0
1	F	173/187 (92%)	0.22	6 (3%) 44 47	38, 59, 105, 126	0
1	G	173/187 (92%)	0.21	7 (4%) 39 41	37, 62, 108, 123	0
All	All	1224/1309 (93%)	0.21	59 (4%) 31 32	31, 55, 105, 132	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	391	ARG	6.4
1	D	401	ASP	5.6
1	B	249	PRO	5.0
1	E	391	ARG	5.0
1	F	391	ARG	4.5
1	F	393	LYS	4.3
1	E	402	PRO	4.2
1	D	251	ILE	4.2
1	G	252	ASP	4.1
1	D	389	SER	4.0
1	G	320	PHE	4.0
1	G	319	LEU	3.8
1	B	401	ASP	3.7
1	E	401	ASP	3.7
1	E	392	GLN	3.6
1	E	400	LYS	3.5
1	E	404	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	252	ASP	3.5
1	F	395	PHE	3.4
1	B	381	ASP	3.4
1	G	391	ARG	3.3
1	F	291	ARG	3.3
1	G	382	HIS	3.2
1	B	400	LYS	3.2
1	E	384	LEU	3.1
1	B	250	THR	3.1
1	E	388	SER	3.0
1	C	315	ASN	3.0
1	G	315	ASN	2.9
1	B	251	ILE	2.8
1	D	249	PRO	2.8
1	A	401	ASP	2.8
1	D	252	ASP	2.8
1	D	395	PHE	2.8
1	D	250	THR	2.7
1	D	357	MET	2.7
1	G	384	LEU	2.7
1	C	320	PHE	2.6
1	B	391	ARG	2.6
1	B	392	GLN	2.6
1	B	254	LEU	2.5
1	E	382	HIS	2.5
1	D	403	PRO	2.5
1	F	389	SER	2.4
1	E	403	PRO	2.4
1	E	405	PHE	2.4
1	E	387	ILE	2.3
1	A	372	GLN	2.3
1	E	385	GLU	2.3
1	E	397	PRO	2.3
1	D	385	GLU	2.2
1	E	399	SER	2.2
1	E	357	MET	2.2
1	E	394	GLY	2.2
1	D	406	CYS	2.1
1	B	382	HIS	2.1
1	E	398	HIS	2.0
1	D	402	PRO	2.0
1	F	357	MET	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	A	1	1/1	1.00	0.20	5.83	36,36,36,36	0
2	ZN	G	13	1/1	1.00	0.18	5.02	39,39,39,39	0
2	ZN	B	3	1/1	1.00	0.19	3.60	45,45,45,45	0
2	ZN	C	5	1/1	0.99	0.17	3.15	35,35,35,35	0
2	ZN	E	9	1/1	0.99	0.17	2.32	46,46,46,46	0
2	ZN	D	7	1/1	0.99	0.18	1.95	40,40,40,40	0
2	ZN	C	6	1/1	1.00	0.19	1.89	45,45,45,45	0
2	ZN	F	11	1/1	1.00	0.17	1.77	49,49,49,49	0
2	ZN	A	2	1/1	0.99	0.17	0.22	53,53,53,53	0
2	ZN	B	4	1/1	0.98	0.12	-0.61	73,73,73,73	0
2	ZN	F	12	1/1	0.99	0.13	-0.66	81,81,81,81	0
2	ZN	G	14	1/1	0.98	0.16	-1.66	64,64,64,64	0
2	ZN	D	8	1/1	0.97	0.11	-2.16	65,65,65,65	0
2	ZN	E	10	1/1	0.95	0.09	-2.17	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.