wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:40 AM GMT

PDB ID	:	3FEQ
Title	:	Crystal structure of uncharacterized protein eah89906
Authors	:	Patskovsky, Y.; Bonanno, J.; Romero, R.; Freeman, J.; Lau, C.; Smith, D.; Bain, K.; Wasserman, S.R.; Raushel, F.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-11-30
Resolution	:	2.63 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

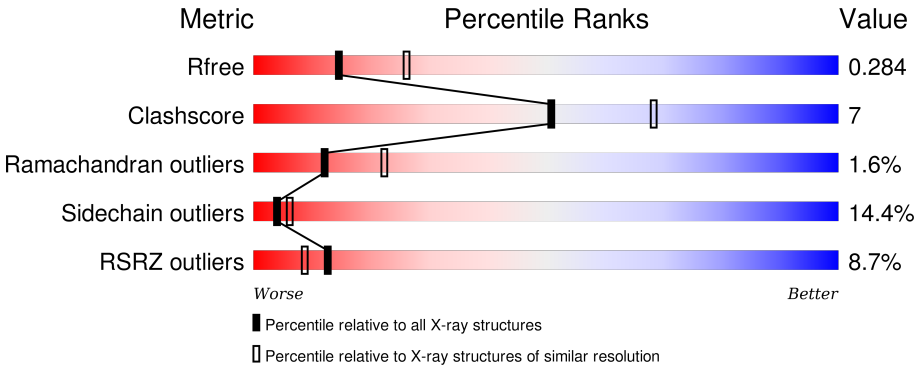
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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}	91344	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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 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 <=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	423	2% 70% 22%
1	B	423	3% 72% 20%
1	C	423	4% 71% 22%
1	D	423	2% 71% 22%
1	E	423	3% 74% 19%

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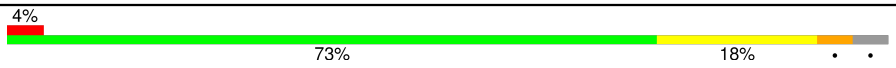
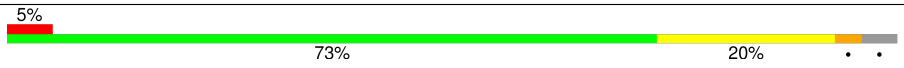
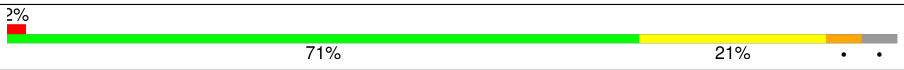
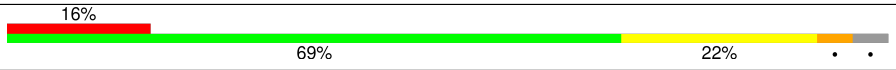
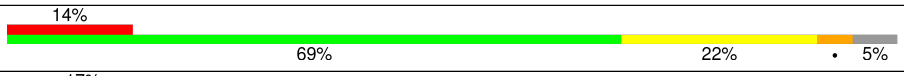
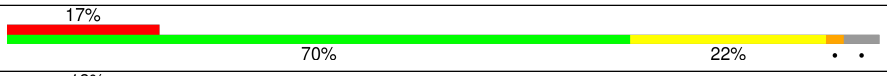
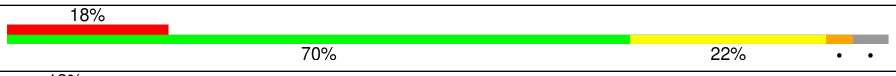
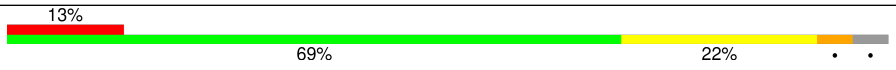
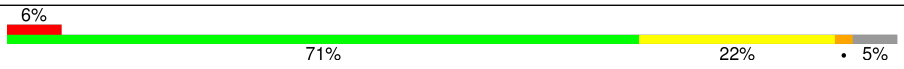
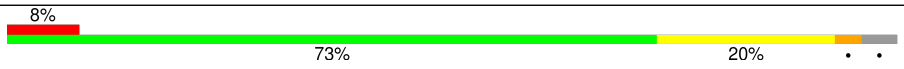
Mol	Chain	Length	Quality of chain
1	F	423	
1	G	423	
1	H	423	
1	I	423	
1	J	423	
1	K	423	
1	L	423	
1	M	423	
1	N	423	
1	O	423	
1	P	423	

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	C	425	-	-	-	X
2	ZN	C	426	-	-	-	X
2	ZN	D	426	-	-	-	X
2	ZN	E	426	-	-	-	X
2	ZN	F	426	-	-	-	X
2	ZN	H	425	-	-	-	X
2	ZN	J	425	-	-	-	X
2	ZN	J	426	-	-	-	X
2	ZN	L	425	-	-	-	X
2	ZN	L	426	-	-	-	X
2	ZN	M	426	-	-	-	X
2	ZN	N	425	-	-	-	X
2	ZN	N	426	-	-	-	X
2	ZN	O	425	-	-	-	X
2	ZN	O	426	-	-	-	X
2	ZN	P	426	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 48417 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 PUTATIVE AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	4	0
			3028	1886	547	580	15			
1	B	405	Total	C	N	O	S	0	6	0
			3040	1894	552	579	15			
1	C	406	Total	C	N	O	S	0	2	0
			3025	1883	550	577	15			
1	D	405	Total	C	N	O	S	0	4	0
			3035	1890	553	577	15			
1	E	405	Total	C	N	O	S	0	4	0
			3026	1883	550	578	15			
1	F	405	Total	C	N	O	S	0	2	0
			3016	1878	546	577	15			
1	G	405	Total	C	N	O	S	0	2	0
			3021	1881	549	576	15			
1	H	405	Total	C	N	O	S	0	2	0
			3016	1878	546	577	15			
1	I	405	Total	C	N	O	S	0	1	0
			3013	1876	546	576	15			
1	J	402	Total	C	N	O	S	0	1	0
			2994	1866	543	571	14			
1	K	403	Total	C	N	O	S	0	1	0
			3000	1869	544	572	15			
1	L	404	Total	C	N	O	S	0	1	0
			3005	1870	545	575	15			
1	M	406	Total	C	N	O	S	0	1	0
			3017	1878	547	577	15			
1	N	404	Total	C	N	O	S	0	1	0
			3003	1869	545	575	14			
1	O	401	Total	C	N	O	S	0	1	0
			2983	1857	542	570	14			
1	P	405	Total	C	N	O	S	0	2	0
			3018	1879	547	577	15			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	N	2	Total Zn 2 2	0	0
2	O	2	Total Zn 2 2	0	0
2	L	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	M	2	Total Zn 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	27	Total O 27 27	0	0
3	C	13	Total O 13 13	0	0

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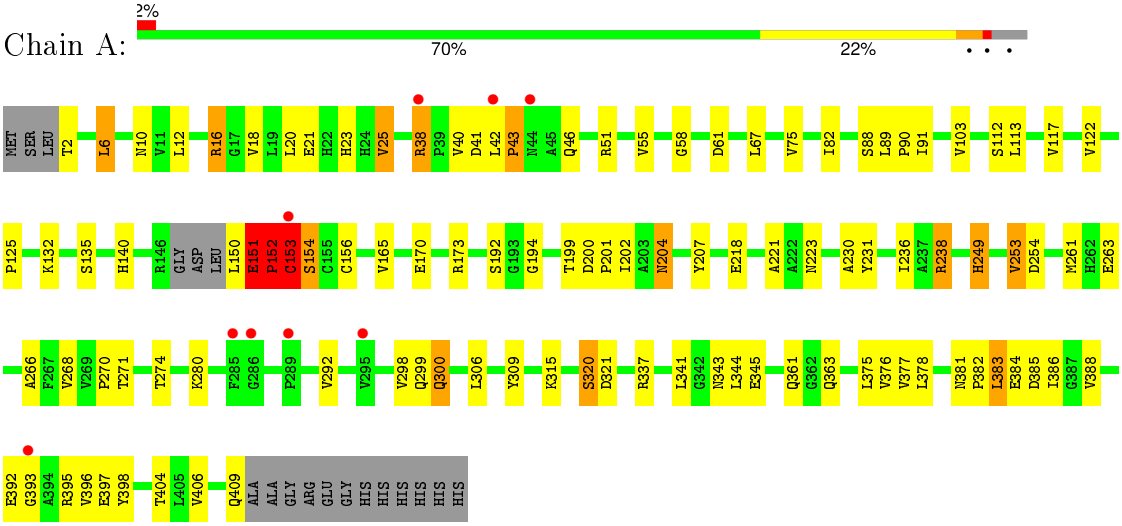
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	20	Total O 20 20	0	0
3	E	18	Total O 18 18	0	0
3	F	17	Total O 17 17	0	0
3	G	16	Total O 16 16	0	0
3	H	6	Total O 6 6	0	0
3	O	2	Total O 2 2	0	0
3	P	2	Total O 2 2	0	0

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 errors 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.

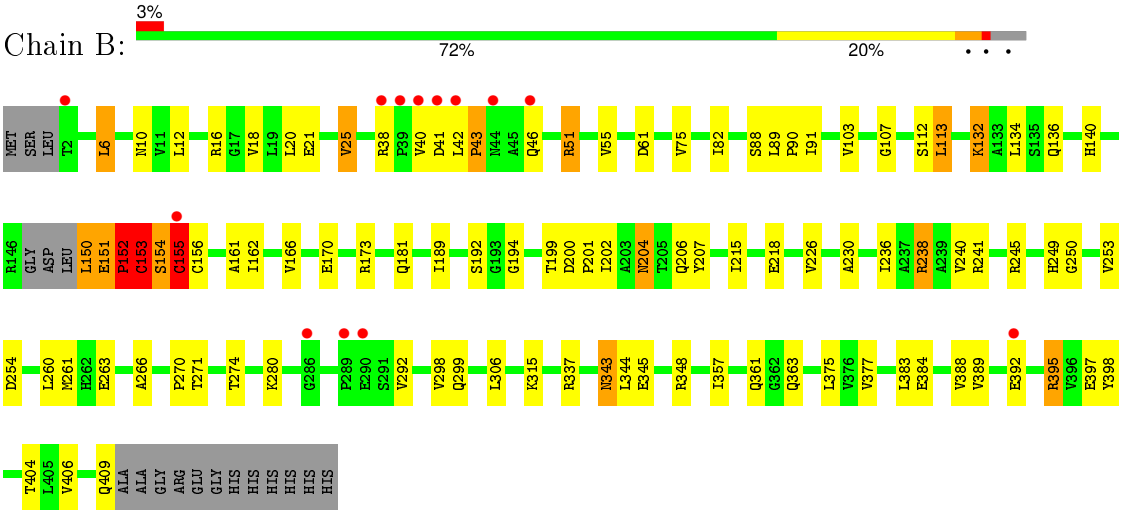
- Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain A:



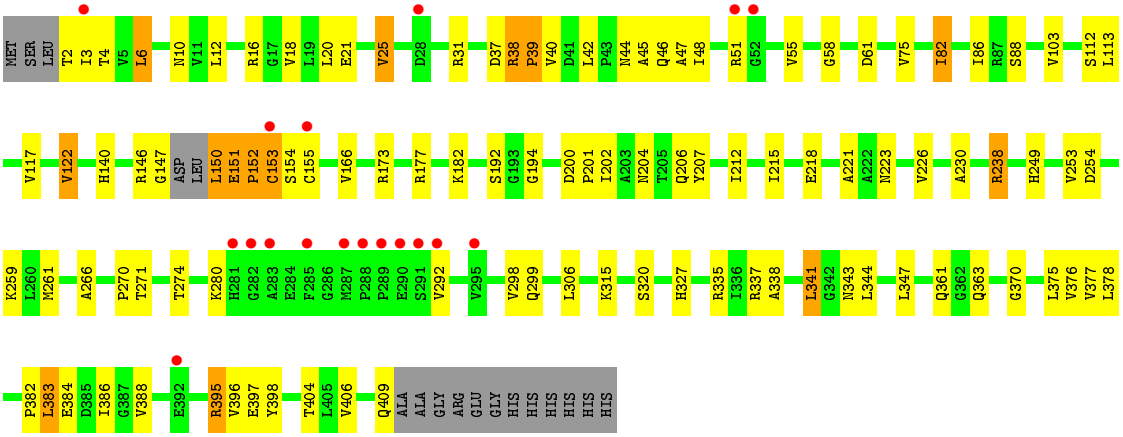
- Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain B:



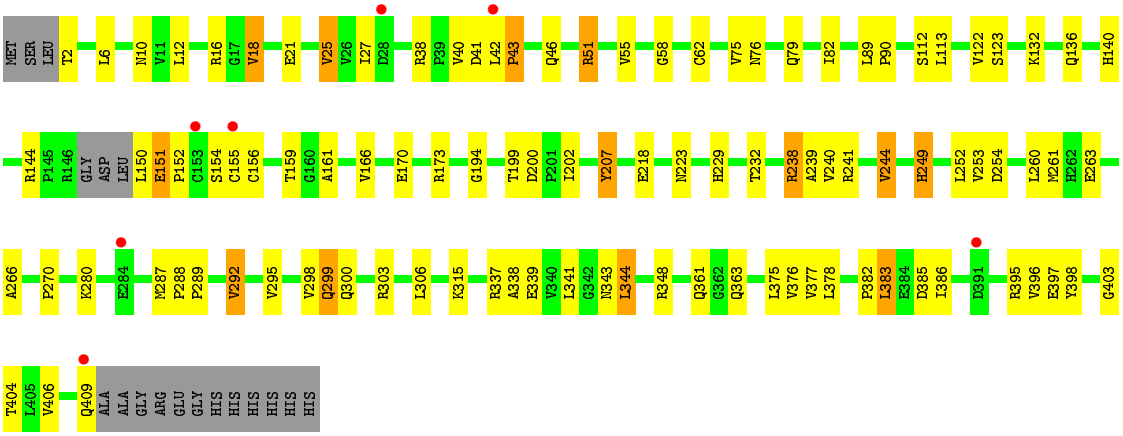
- Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain C:



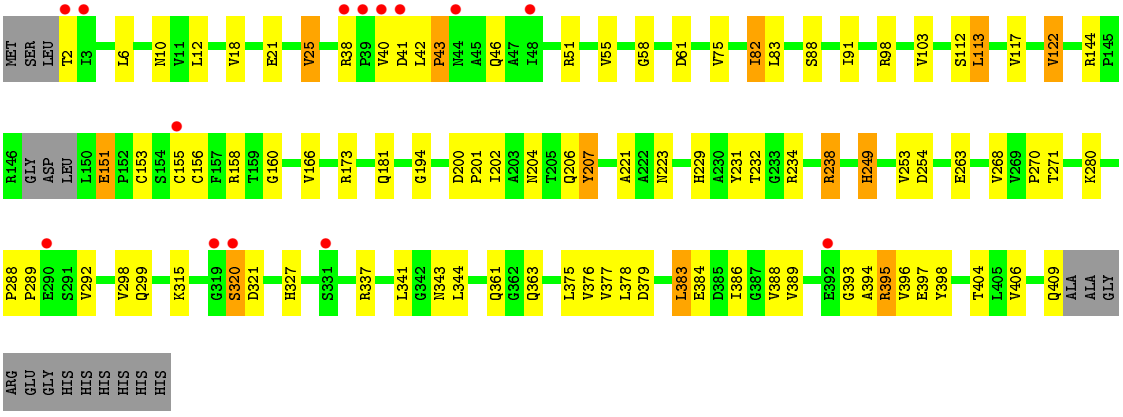
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain D:



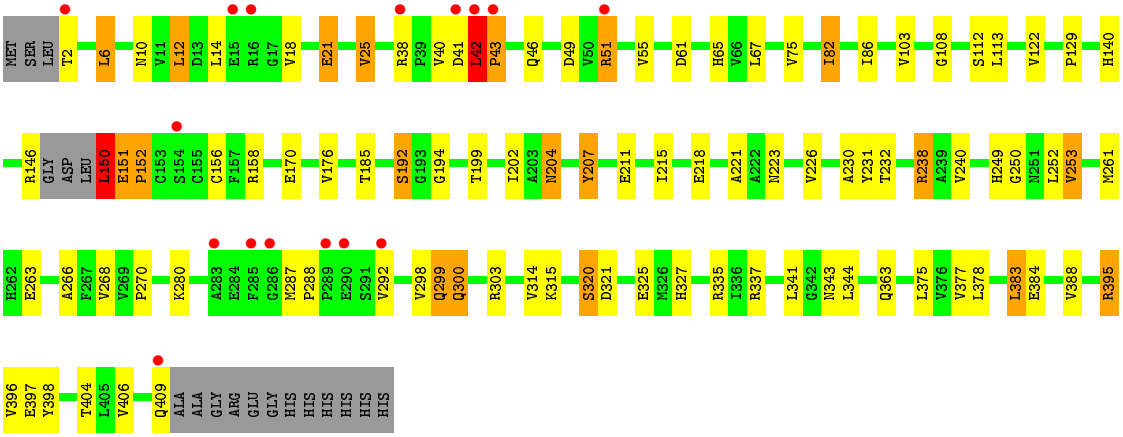
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain E:



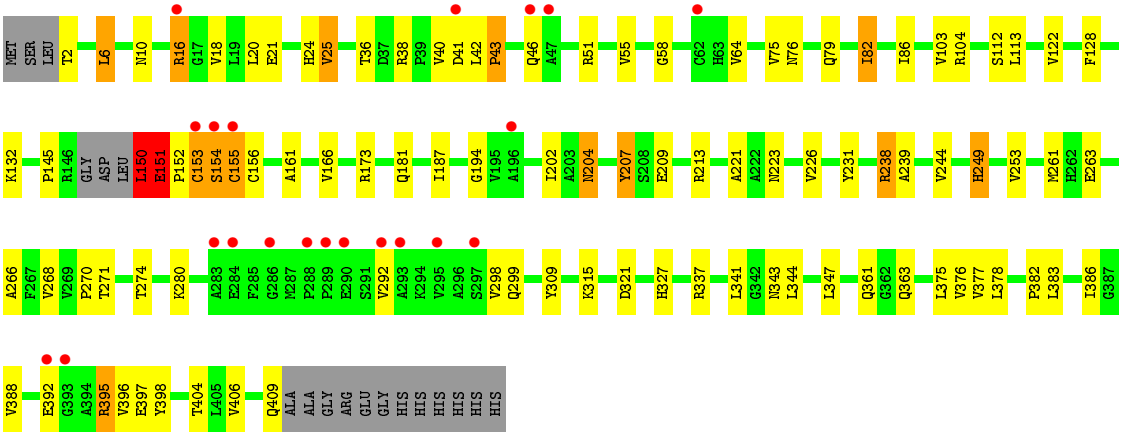
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain F:



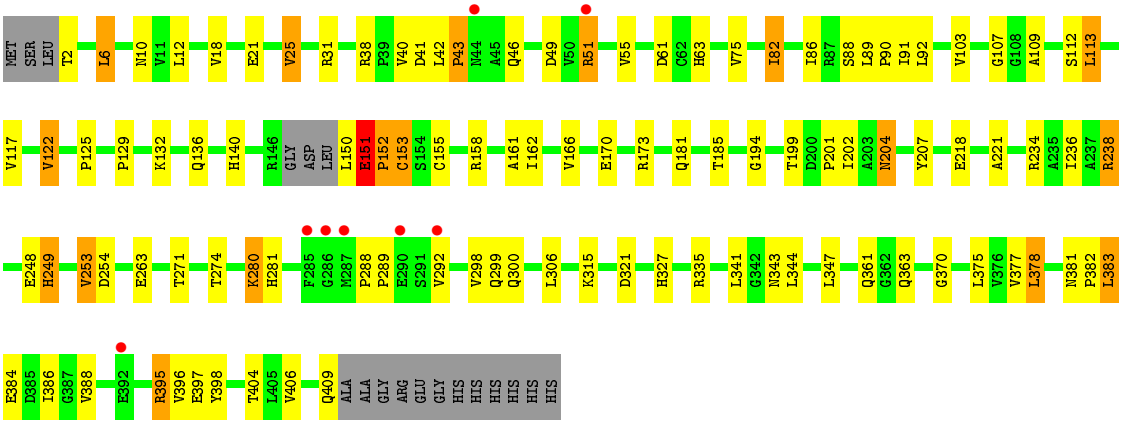
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain G:



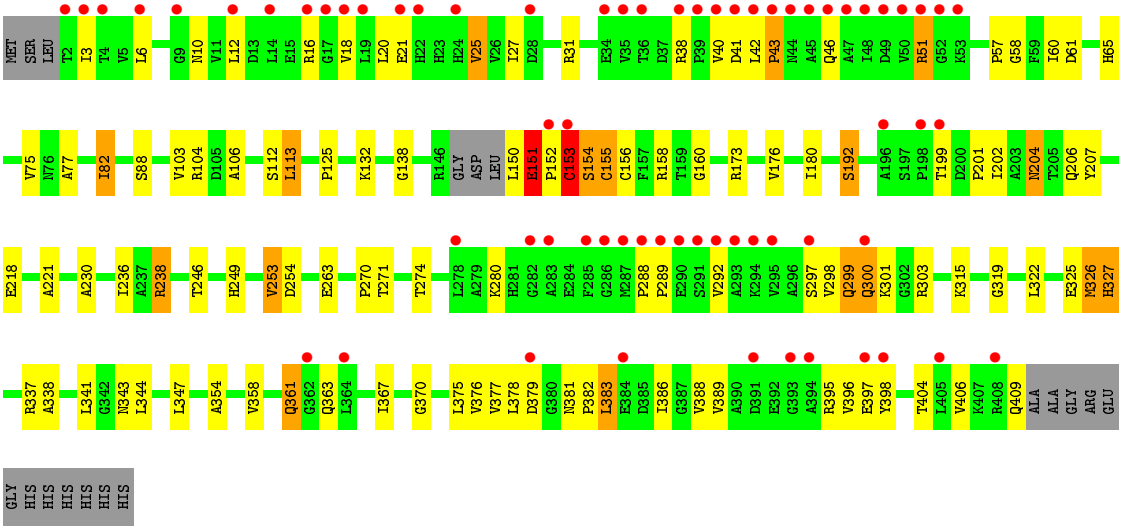
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain H:



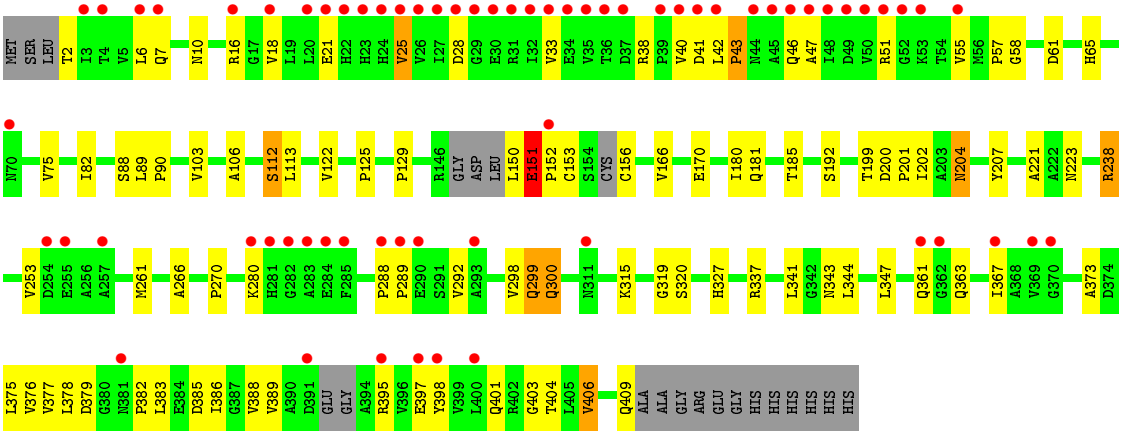
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain I:



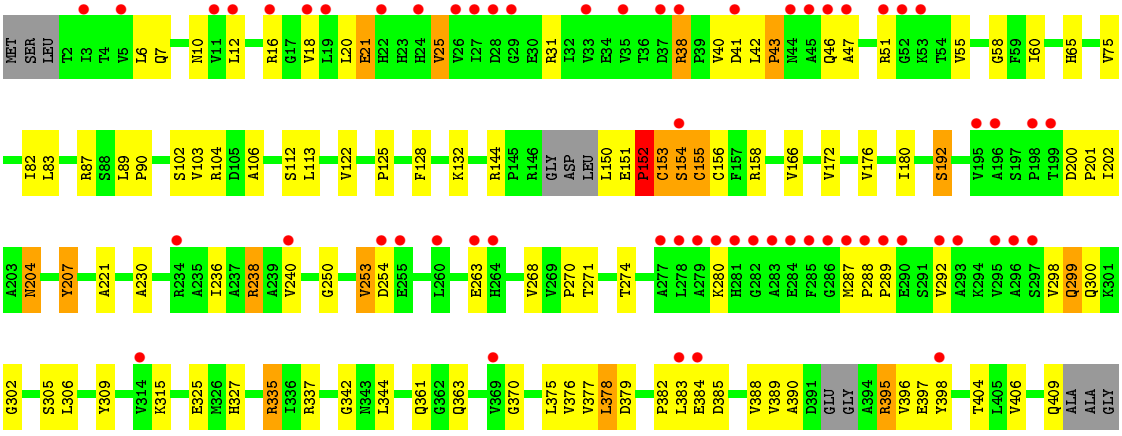
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain J:



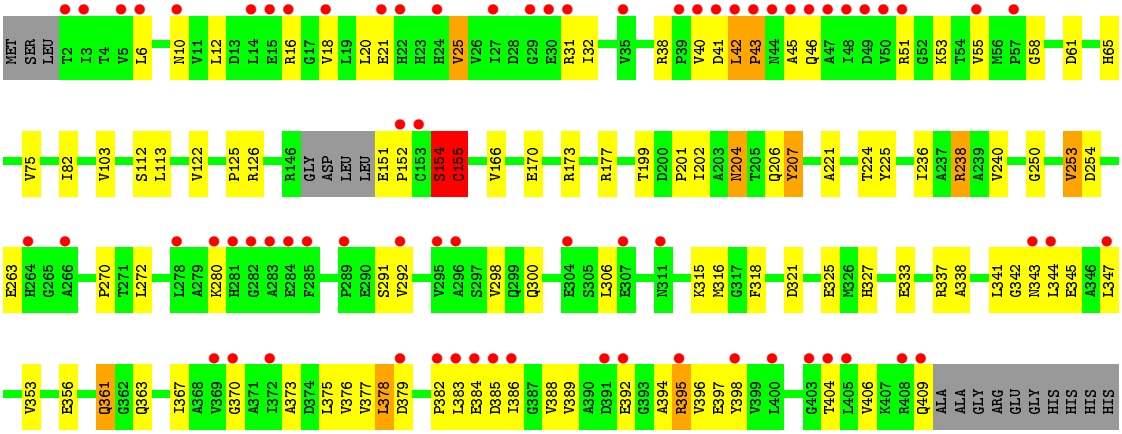
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain K:



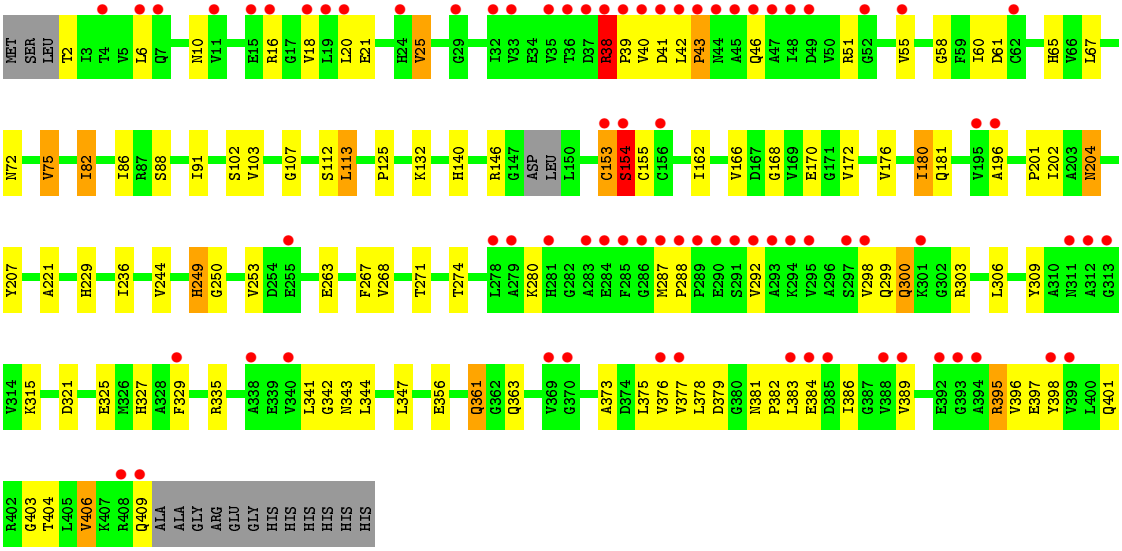
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain L:



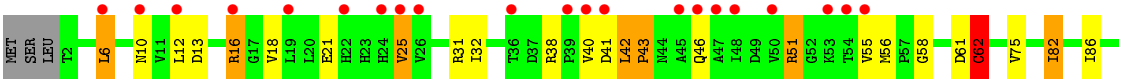
• Molecule 1: PUTATIVE AMIDOHYDROLASE

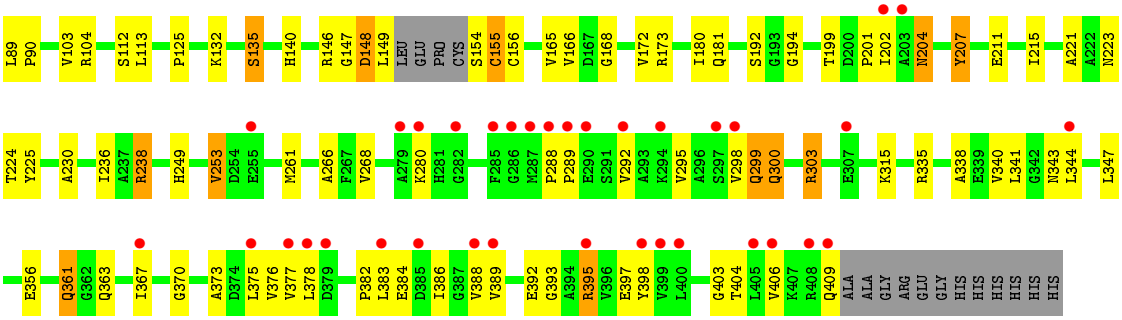
Chain M:



• Molecule 1: PUTATIVE AMIDOHYDROLASE

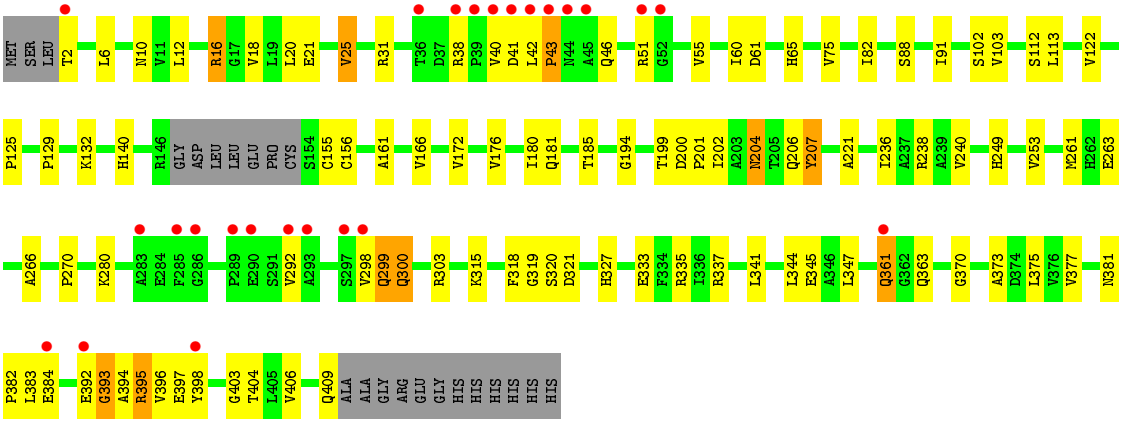
Chain N:





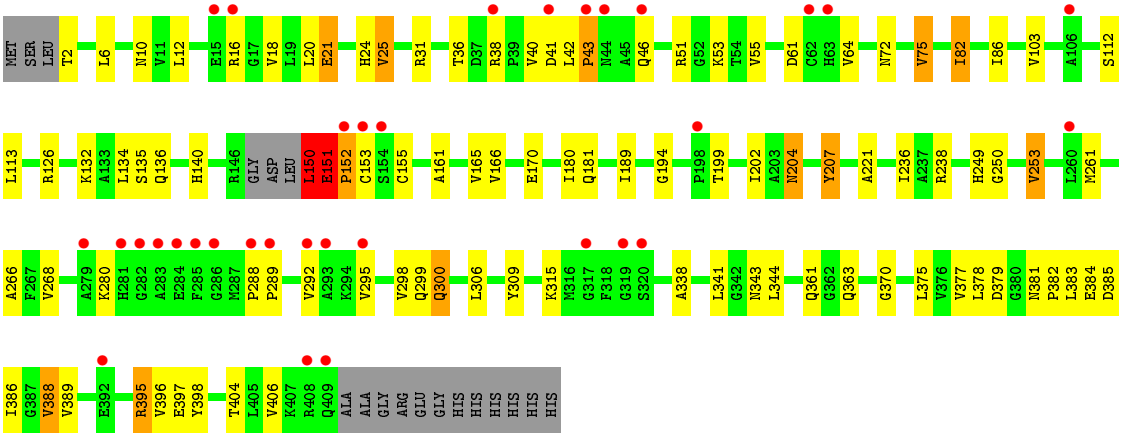
- Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain O:



- Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	113.21Å 108.05Å 171.13Å 81.75° 80.36° 74.40°	Depositor
Resolution (Å)	20.00 – 2.63 35.90 – 2.63	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.63) 93.4 (35.90-2.63)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.281 0.241 , 0.284	Depositor DCC
R_{free} test set	6581 reflections (3.10%)	DCC
Wilson B-factor (Å^2)	41.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.3	EDS
Estimated twinning fraction	0.011 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 219029 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	48417	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	0/3083	0.58	2/4180 (0.0%)
1	B	0.44	0/3102	0.58	1/4205 (0.0%)
1	C	0.43	0/3074	0.55	0/4167
1	D	0.46	1/3090 (0.0%)	0.57	0/4188
1	E	0.43	0/3081	0.58	1/4177 (0.0%)
1	F	0.41	0/3065	0.59	1/4156 (0.0%)
1	G	0.41	0/3070	0.56	0/4162
1	H	0.44	0/3065	0.56	0/4156
1	I	0.46	0/3059	0.56	0/4148
1	J	0.44	0/3038	0.53	0/4117
1	K	0.44	0/3045	0.55	0/4128
1	L	0.43	0/3051	0.54	0/4137
1	M	0.43	0/3063	0.56	0/4153
1	N	0.44	1/3048 (0.0%)	0.54	0/4132
1	O	0.41	0/3028	0.54	0/4105
1	P	0.42	0/3067	0.57	0/4159
All	All	0.43	2/49029 (0.0%)	0.56	5/66470 (0.0%)

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	4
1	B	0	2
1	C	0	3
1	D	0	2
1	E	0	3
1	F	0	2
1	G	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	4
1	I	0	2
1	J	0	3
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	1
1	O	0	3
1	P	0	5
All	All	0	46

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	62	CYS	CB-SG	-6.20	1.71	1.82
1	D	62	CYS	CB-SG	-5.68	1.72	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	238	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	F	42	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	238	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	E	173	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	16	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	GLU	Peptide
1	A	152	PRO	Peptide
1	A	2	THR	Peptide
1	A	38	ARG	Peptide
1	B	38	ARG	Peptide

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	3028	0	3044	47	0
1	B	3040	0	3063	45	0
1	C	3025	0	3041	43	1
1	D	3035	0	3059	43	0
1	E	3026	0	3040	39	0
1	F	3016	0	3030	45	0
1	G	3021	0	3038	38	0
1	H	3016	0	3030	51	0
1	I	3013	0	3025	58	1
1	J	2994	0	3009	39	0
1	K	3000	0	3015	43	0
1	L	3005	0	3014	40	0
1	M	3017	0	3028	51	0
1	N	3003	0	3014	55	0
1	O	2983	0	2996	36	0
1	P	3018	0	3031	40	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
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	24	0	0	0	0
3	B	27	0	0	1	0
3	C	13	0	0	1	0
3	D	20	0	0	1	0
3	E	18	0	0	3	0
3	F	17	0	0	1	0
3	G	16	0	0	1	0
3	H	6	0	0	1	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	48417	0	48477	663	1

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.

The worst 5 of 663 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:H:263:GLU:OE2	1:M:38:ARG:HD2	1.55	1.07
1:I:221:ALA:O	1:K:204:ASN:HB2	1.60	1.01
1:A:16:ARG:HH12	1:A:20:LEU:HD21	1.27	0.97
1:C:221:ALA:O	1:F:204:ASN:HB2	1.72	0.88
1:C:3:ILE:HG23	1:C:45:ALA:HA	1.59	0.85

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ALA:O	1:I:301:LYS:NZ[1_546]	1.98	0.22

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	405/423 (96%)	385 (95%)	13 (3%)	7 (2%)	11	21
1	B	407/423 (96%)	384 (94%)	16 (4%)	7 (2%)	11	21
1	C	404/423 (96%)	380 (94%)	18 (4%)	6 (2%)	13	24
1	D	405/423 (96%)	383 (95%)	17 (4%)	5 (1%)	16	31
1	E	405/423 (96%)	378 (93%)	23 (6%)	4 (1%)	19	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	403/423 (95%)	379 (94%)	19 (5%)	5 (1%)	16	31
1	G	403/423 (95%)	380 (94%)	18 (4%)	5 (1%)	16	31
1	H	403/423 (95%)	374 (93%)	21 (5%)	8 (2%)	9	16
1	I	402/423 (95%)	374 (93%)	20 (5%)	8 (2%)	9	16
1	J	395/423 (93%)	368 (93%)	22 (6%)	5 (1%)	15	28
1	K	398/423 (94%)	369 (93%)	22 (6%)	7 (2%)	11	19
1	L	401/423 (95%)	371 (92%)	21 (5%)	9 (2%)	8	14
1	M	403/423 (95%)	378 (94%)	17 (4%)	8 (2%)	9	16
1	N	401/423 (95%)	367 (92%)	28 (7%)	6 (2%)	13	24
1	O	398/423 (94%)	373 (94%)	18 (4%)	7 (2%)	11	19
1	P	403/423 (95%)	380 (94%)	17 (4%)	6 (2%)	13	24
All	All	6436/6768 (95%)	6023 (94%)	310 (5%)	103 (2%)	12	22

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	GLU
1	A	152	PRO
1	A	153	CYS
1	B	151	GLU
1	B	152	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/326 (97%)	268 (84%)	49 (16%)	3	5
1	B	319/326 (98%)	272 (85%)	47 (15%)	4	6
1	C	315/326 (97%)	267 (85%)	48 (15%)	3	5
1	D	317/326 (97%)	270 (85%)	47 (15%)	4	6
1	E	316/326 (97%)	272 (86%)	44 (14%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	315/326 (97%)	266 (84%)	49 (16%)	3 5
1	G	315/326 (97%)	272 (86%)	43 (14%)	4 7
1	H	315/326 (97%)	271 (86%)	44 (14%)	4 7
1	I	314/326 (96%)	270 (86%)	44 (14%)	4 7
1	J	312/326 (96%)	272 (87%)	40 (13%)	5 9
1	K	313/326 (96%)	265 (85%)	48 (15%)	3 5
1	L	313/326 (96%)	268 (86%)	45 (14%)	4 6
1	M	314/326 (96%)	269 (86%)	45 (14%)	4 6
1	N	312/326 (96%)	265 (85%)	47 (15%)	3 5
1	O	310/326 (95%)	266 (86%)	44 (14%)	4 6
1	P	315/326 (97%)	274 (87%)	41 (13%)	5 8
All	All	5032/5216 (96%)	4307 (86%)	725 (14%)	4 6

5 of 725 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	6	LEU
1	I	344	LEU
1	O	341	LEU
1	H	82	ILE
1	H	404	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	300	GLN
1	J	65	HIS
1	O	299	GLN
1	H	361	GLN
1	I	299	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 32 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, 95^{th} 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	405/423 (95%)	-0.08	9 (2%) 65 59	16, 50, 100, 117	0
1	B	405/423 (95%)	0.01	13 (3%) 51 45	11, 48, 102, 119	0
1	C	406/423 (95%)	0.07	18 (4%) 38 31	14, 49, 104, 118	0
1	D	405/423 (95%)	0.02	7 (1%) 73 68	14, 44, 98, 116	0
1	E	405/423 (95%)	0.07	14 (3%) 48 41	14, 47, 102, 119	0
1	F	405/423 (95%)	0.06	16 (3%) 42 35	15, 49, 99, 119	0
1	G	405/423 (95%)	0.13	21 (5%) 31 24	18, 50, 103, 136	0
1	H	405/423 (95%)	0.02	8 (1%) 68 63	12, 46, 100, 119	0
1	I	405/423 (95%)	0.66	66 (16%) 2 1	28, 58, 106, 123	0
1	J	402/423 (95%)	0.63	66 (16%) 2 1	27, 60, 103, 121	0
1	K	403/423 (95%)	0.66	61 (15%) 3 1	25, 59, 103, 119	0
1	L	404/423 (95%)	0.72	72 (17%) 2 1	22, 61, 106, 133	0
1	M	406/423 (95%)	0.85	78 (19%) 2 1	23, 60, 107, 130	0
1	N	404/423 (95%)	0.55	56 (13%) 4 2	21, 58, 106, 121	0
1	O	401/423 (94%)	0.05	25 (6%) 24 18	22, 53, 103, 121	0
1	P	405/423 (95%)	0.23	33 (8%) 15 10	13, 51, 100, 121	0
All	All	6471/6768 (95%)	0.29	563 (8%) 13 9	11, 53, 103, 136	0

The worst 5 of 563 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	290	GLU	8.7
1	M	393	GLY	8.3
1	J	18	VAL	8.0
1	M	398	TYR	7.4
1	J	6	LEU	7.2

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, 95^{th} 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	C	425	1/1	0.97	0.29	7.37	42,42,42,42	1
2	ZN	J	426	1/1	0.95	0.31	5.26	68,68,68,68	1
2	ZN	L	426	1/1	0.94	0.31	4.22	63,63,63,63	1
2	ZN	O	425	1/1	0.96	0.31	4.15	50,50,50,50	1
2	ZN	L	425	1/1	0.93	0.28	4.02	55,55,55,55	1
2	ZN	E	426	1/1	0.94	0.40	4.01	45,45,45,45	1
2	ZN	D	426	1/1	0.93	0.32	3.48	33,33,33,33	1
2	ZN	C	426	1/1	0.96	0.27	3.14	38,38,38,38	1
2	ZN	N	426	1/1	0.89	0.31	3.08	55,55,55,55	1
2	ZN	M	426	1/1	0.93	0.36	3.03	63,63,63,63	1
2	ZN	F	426	1/1	0.84	0.32	3.02	51,51,51,51	1
2	ZN	O	426	1/1	0.85	0.29	2.87	58,58,58,58	1
2	ZN	P	426	1/1	0.95	0.38	2.69	59,59,59,59	1
2	ZN	J	425	1/1	0.93	0.24	2.67	60,60,60,60	1
2	ZN	H	425	1/1	0.98	0.28	2.49	40,40,40,40	1
2	ZN	N	425	1/1	0.88	0.29	2.39	41,41,41,41	1
2	ZN	A	426	1/1	0.96	0.23	1.99	52,52,52,52	1
2	ZN	H	426	1/1	0.95	0.29	1.97	39,39,39,39	1
2	ZN	A	425	1/1	0.98	0.25	1.80	51,51,51,51	1
2	ZN	G	425	1/1	0.97	0.27	1.79	40,40,40,40	1
2	ZN	I	425	1/1	0.97	0.20	1.69	42,42,42,42	1
2	ZN	F	425	1/1	0.95	0.27	1.60	52,52,52,52	1
2	ZN	B	425	1/1	0.95	0.26	1.50	44,44,44,44	1
2	ZN	B	426	1/1	0.97	0.25	1.49	44,44,44,44	1
2	ZN	E	425	1/1	0.97	0.28	1.34	43,43,43,43	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	I	426	1/1	0.84	0.19	1.31	58,58,58,58	1
2	ZN	G	426	1/1	0.98	0.23	0.99	37,37,37,37	1
2	ZN	P	425	1/1	0.88	0.30	0.99	47,47,47,47	1
2	ZN	K	425	1/1	0.92	0.23	0.84	55,55,55,55	1
2	ZN	D	425	1/1	0.95	0.21	0.29	34,34,34,34	1
2	ZN	K	426	1/1	0.95	0.12	-1.58	68,68,68,68	1
2	ZN	M	425	1/1	0.88	0.21	-1.74	50,50,50,50	1

6.5 Other polymers (i)

There are no such residues in this entry.