wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:22 PM GMT

PDB ID	:	4HXG
Title	:	Pyrococcus horikoshii acylaminoacyl peptidase (orthorhombic crystal form)
Authors	:	Kiss-Szeman, A.; Menyhard, D.K.; Tichy-Racs, E.; Hornung, B.; Radi, K.; Szeltner, Z.; Domokos, K.; Szamosi, I.; Naray-Szabo, G.; Polgar, L.; Harmat, V.
Deposited on	:	2012-11-09
Resolution	:	2.70 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:

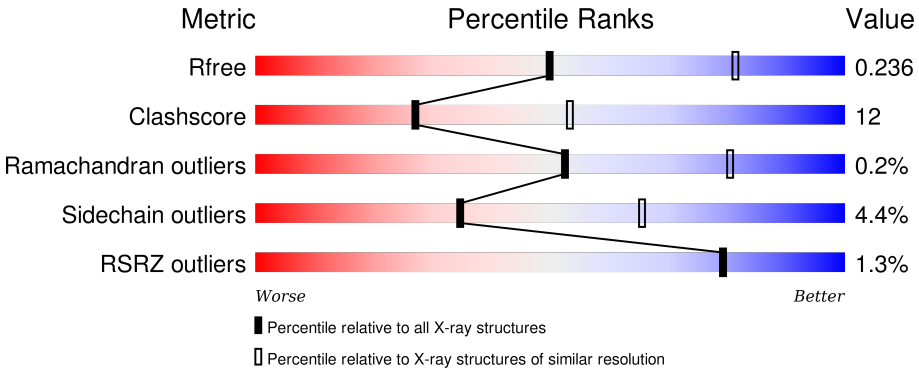
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	622	74% 22%
1	B	622	% 73% 24%
1	C	622	% 71% 26%
1	D	622	75% 22%
1	E	622	77% 20%

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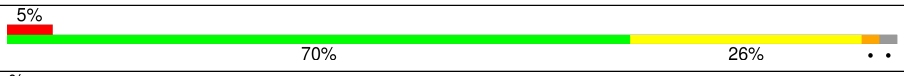
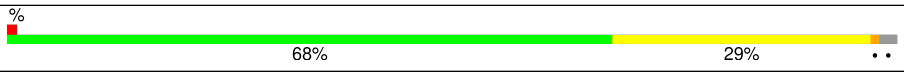
Mol	Chain	Length	Quality of chain
1	F	622	
1	G	622	
1	H	622	
1	I	622	
1	J	622	
1	K	622	
1	L	622	

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	HEZ	A	702	-	-	-	X
2	HEZ	A	703	-	-	-	X
2	HEZ	B	701	-	-	-	X
2	HEZ	B	702	-	-	-	X
2	HEZ	C	701	-	-	-	X
2	HEZ	D	701	-	-	X	-
2	HEZ	D	702	-	-	-	X
2	HEZ	D	703	-	-	-	X
2	HEZ	D	704	-	-	-	X
2	HEZ	D	705	-	-	-	X
2	HEZ	D	706	-	-	-	X
2	HEZ	D	707	-	-	-	X
2	HEZ	E	702	-	-	-	X
2	HEZ	E	703	-	-	-	X
2	HEZ	F	702	-	-	-	X
2	HEZ	F	703	-	-	-	X
2	HEZ	G	701	-	-	-	X
2	HEZ	I	702	-	-	-	X
3	MG	D	710	-	-	-	X
3	MG	E	705	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 59910 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 uncharacterized protein PH0594.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	3	0
			4940	3225	803	900	12			
1	B	612	Total	C	N	O	S	0	2	0
			4926	3211	800	903	12			
1	C	612	Total	C	N	O	S	0	1	0
			4883	3183	791	897	12			
1	D	612	Total	C	N	O	S	0	3	0
			4989	3254	812	911	12			
1	E	613	Total	C	N	O	S	0	2	0
			5005	3259	815	919	12			
1	F	614	Total	C	N	O	S	0	1	0
			4975	3237	814	912	12			
1	G	608	Total	C	N	O	S	0	2	0
			4886	3190	792	892	12			
1	H	609	Total	C	N	O	S	0	0	0
			4866	3168	795	891	12			
1	I	611	Total	C	N	O	S	0	2	0
			4910	3201	794	903	12			
1	J	609	Total	C	N	O	S	0	1	0
			4617	2999	753	853	12			
1	K	610	Total	C	N	O	S	0	1	0
			4659	3017	762	868	12			
1	L	611	Total	C	N	O	S	0	0	0
			4862	3165	784	901	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	466	ALA	SER	ENGINEERED MUTATION	UNP O58323
B	466	ALA	SER	ENGINEERED MUTATION	UNP O58323
C	466	ALA	SER	ENGINEERED MUTATION	UNP O58323
D	466	ALA	SER	ENGINEERED MUTATION	UNP O58323
E	466	ALA	SER	ENGINEERED MUTATION	UNP O58323

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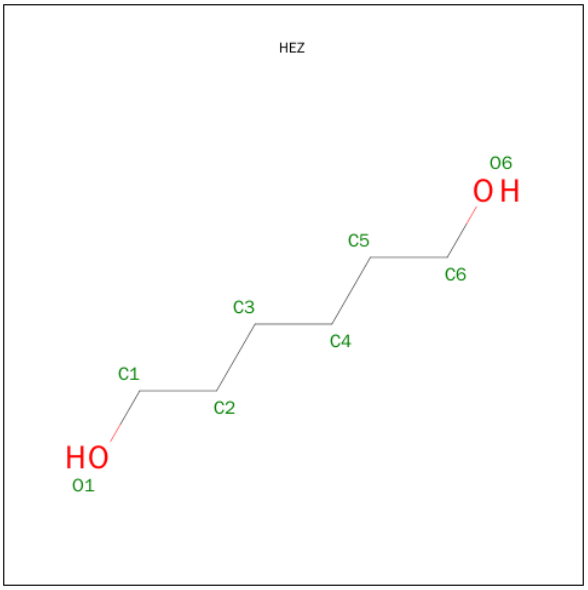
Chain	Residue	Modelled	Actual	Comment	Reference
F	466	ALA	SER	ENGINEERED MUTATION	UNP O58323
G	466	ALA	SER	ENGINEERED MUTATION	UNP O58323
H	466	ALA	SER	ENGINEERED MUTATION	UNP O58323
I	466	ALA	SER	ENGINEERED MUTATION	UNP O58323
J	466	ALA	SER	ENGINEERED MUTATION	UNP O58323
K	466	ALA	SER	ENGINEERED MUTATION	UNP O58323
L	466	ALA	SER	ENGINEERED MUTATION	UNP O58323

- Molecule 2 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0
2	F	1	Total C O 8 6 2	0	0
2	F	1	Total C O 8 6 2	0	0
2	F	1	Total C O 8 6 2	0	0
2	G	1	Total C O 8 6 2	0	0
2	H	1	Total C O 8 6 2	0	0
2	I	1	Total C O 8 6 2	0	0
2	I	1	Total C O 8 6 2	0	0
2	K	1	Total C O 8 6 2	0	0
2	L	1	Total C O 8 6 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Mg 2 2	0	0
3	E	3	Total Mg 3 3	0	0
3	H	2	Total Mg 2 2	0	0
3	B	1	Total Mg 1 1	0	0
3	I	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	L	2	Total Mg 2 2	0	0
3	F	3	Total Mg 3 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	149	Total O 152 152	0	3
5	B	85	Total O 86 86	0	1
5	C	59	Total O 60 60	0	1
5	D	221	Total O 221 221	0	0
5	E	188	Total O 191 191	0	3
5	F	155	Total O 156 156	0	1

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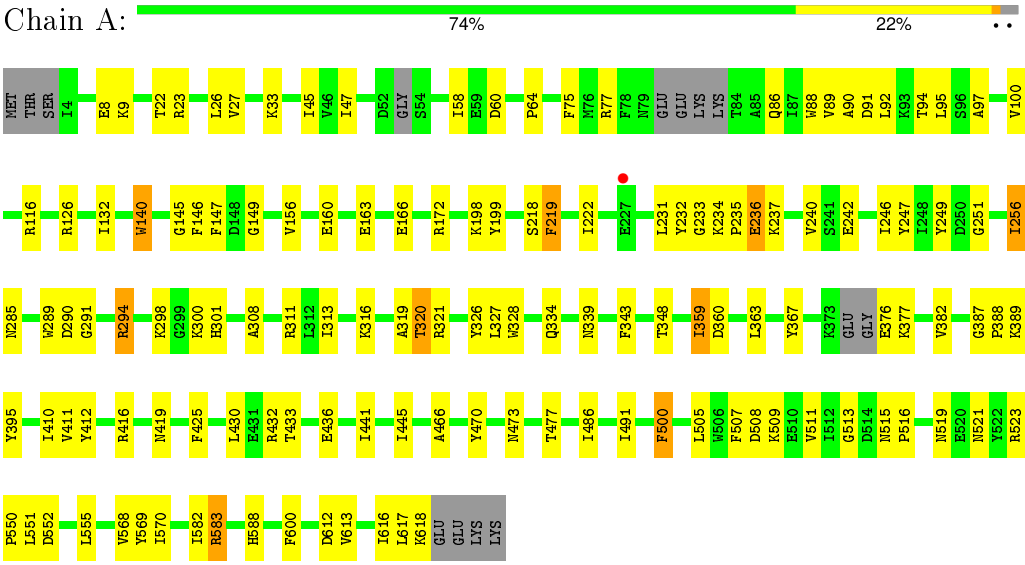
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	76	Total O 79 79	0	3
5	H	58	Total O 58 58	0	0
5	I	77	Total O 78 78	0	1
5	J	17	Total O 17 17	0	0
5	K	11	Total O 12 12	0	1
5	L	51	Total O 51 51	0	0

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.

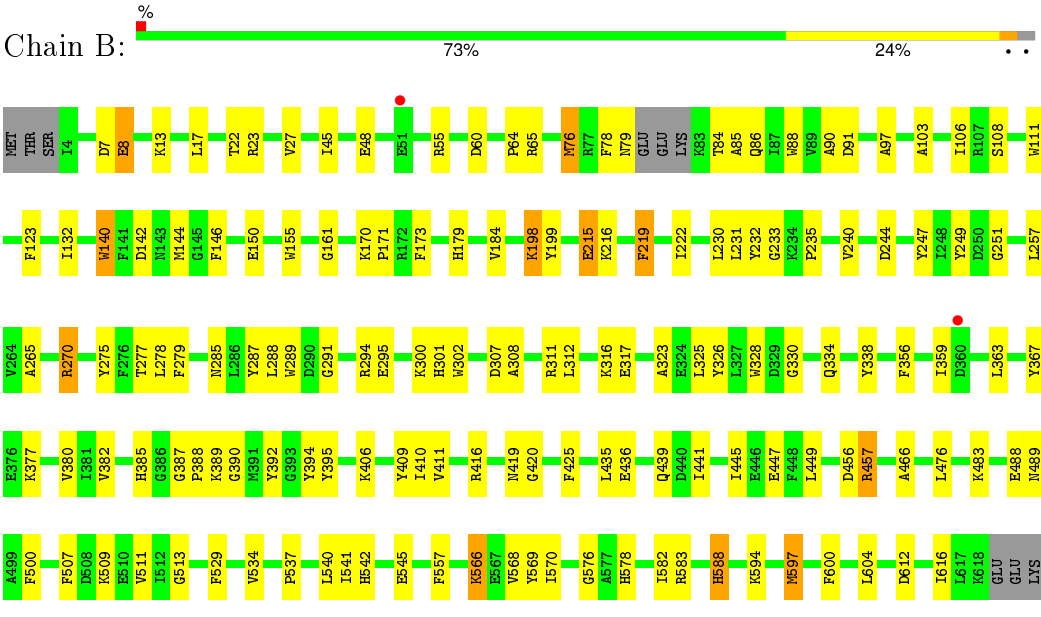
- Molecule 1: Putative uncharacterized protein PH0594

Chain A:



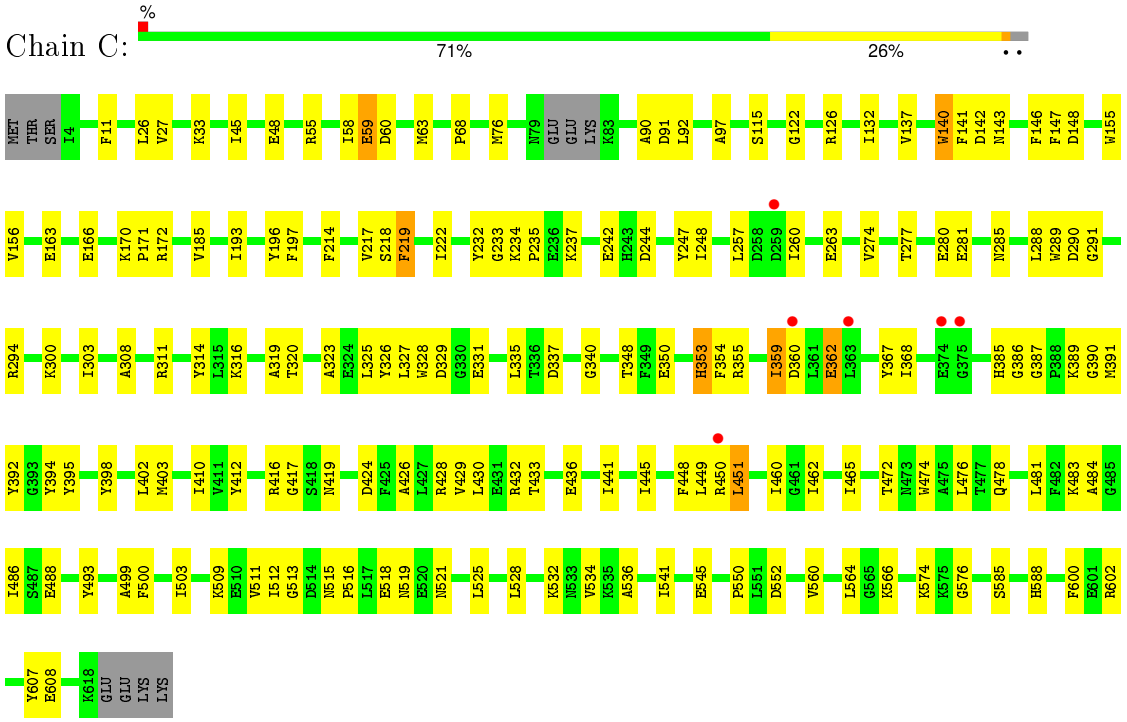
- Molecule 1: Putative uncharacterized protein PH0594

Chain B:



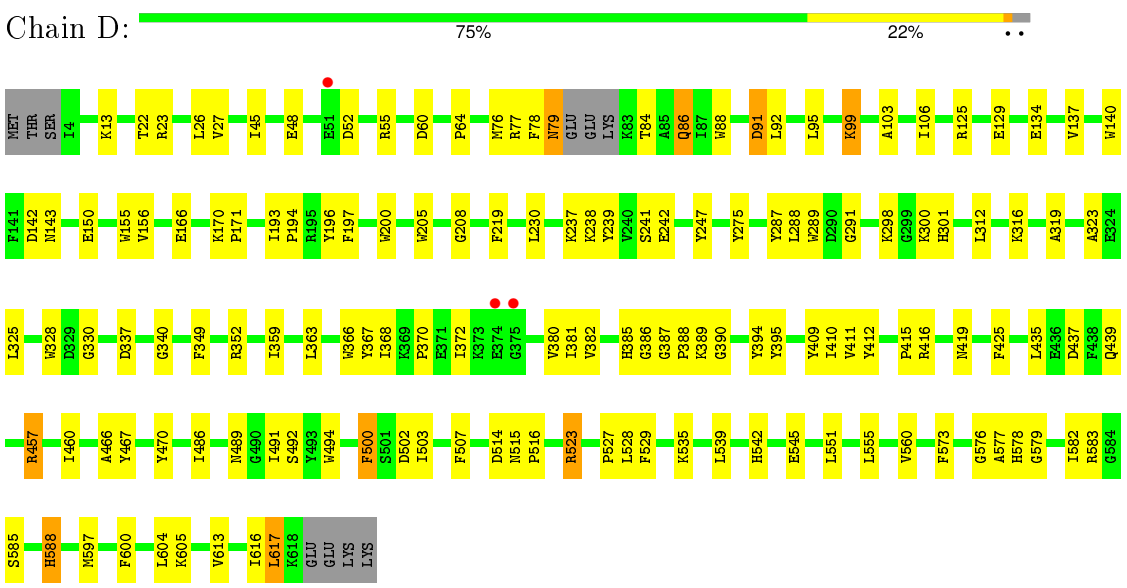
• Molecule 1: Putative uncharacterized protein PH0594

Chain C:



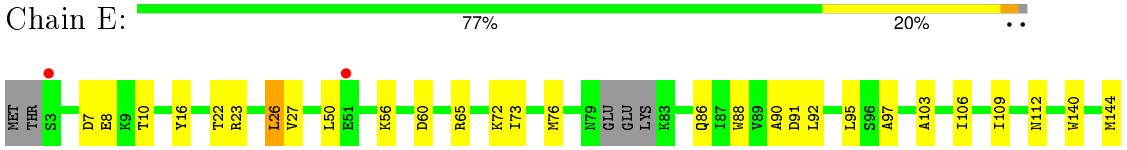
• Molecule 1: Putative uncharacterized protein PH0594

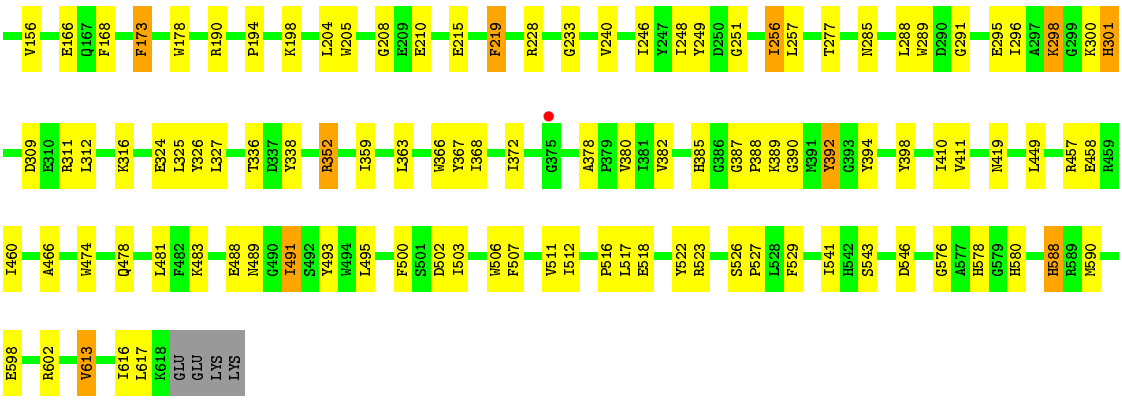
Chain D:



• Molecule 1: Putative uncharacterized protein PH0594

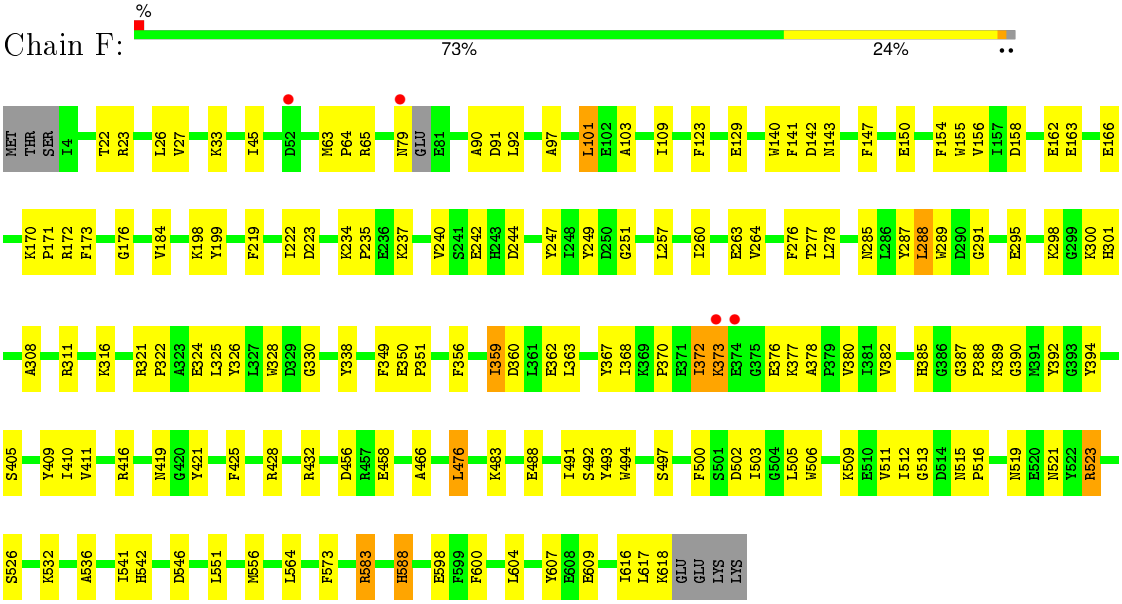
Chain E:





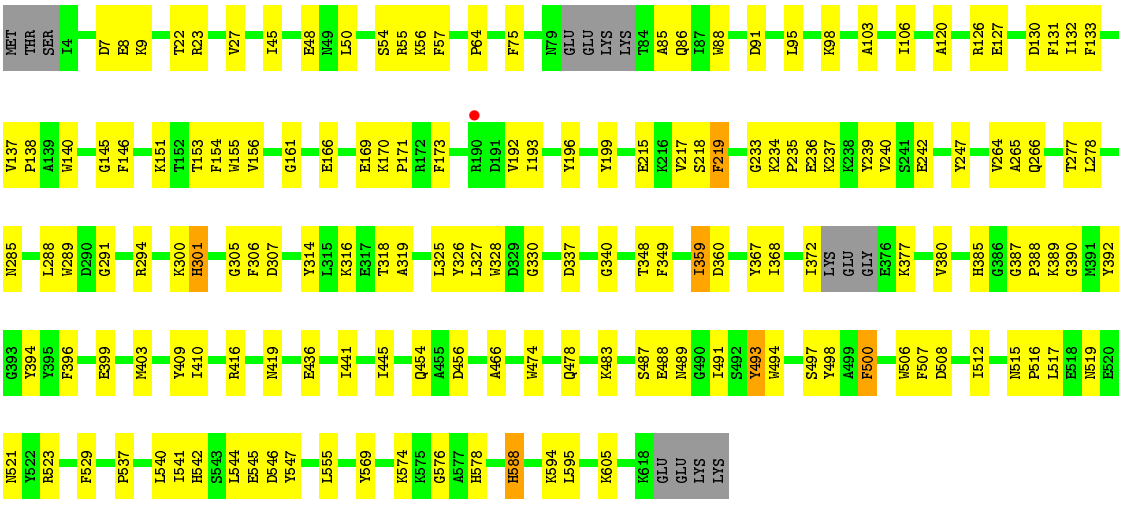
• Molecule 1: Putative uncharacterized protein PH0594

Chain F:



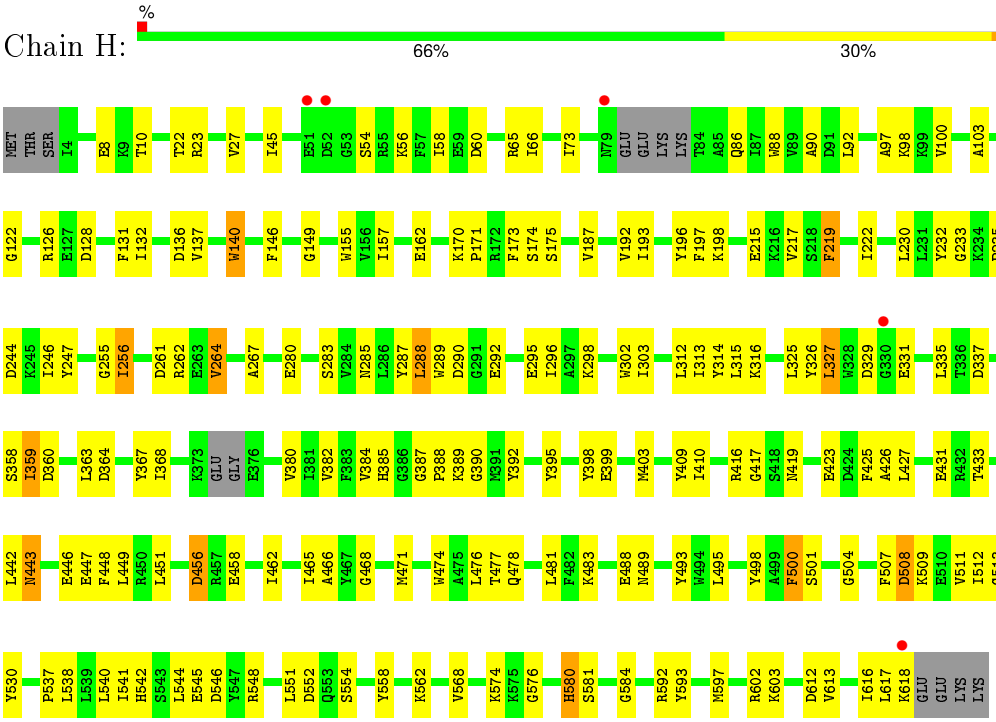
• Molecule 1: Putative uncharacterized protein PH0594

Chain G:



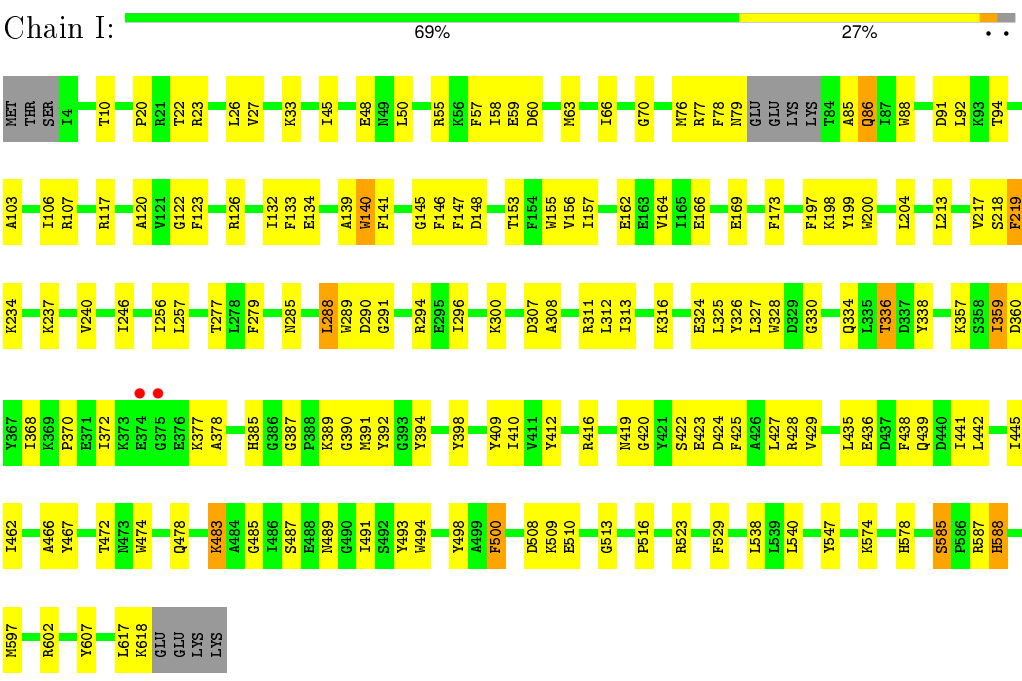
• Molecule 1: Putative uncharacterized protein PH0594

Chain H:



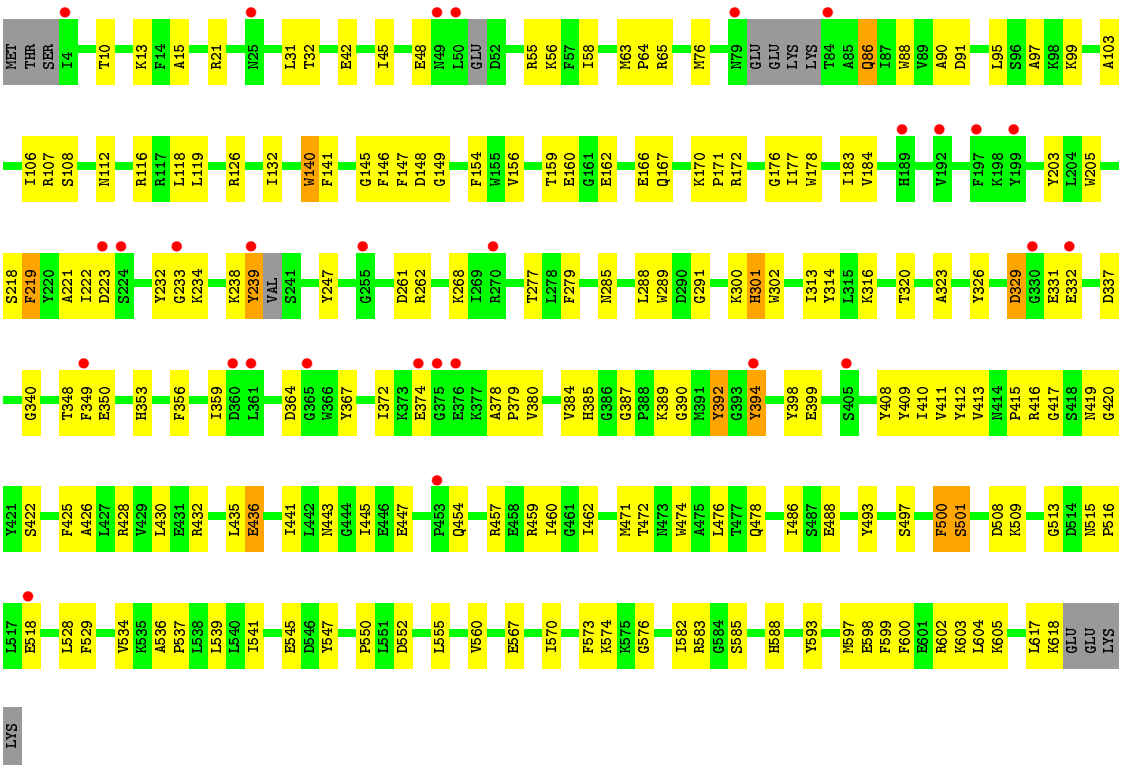
• Molecule 1: Putative uncharacterized protein PH0594

Chain I:



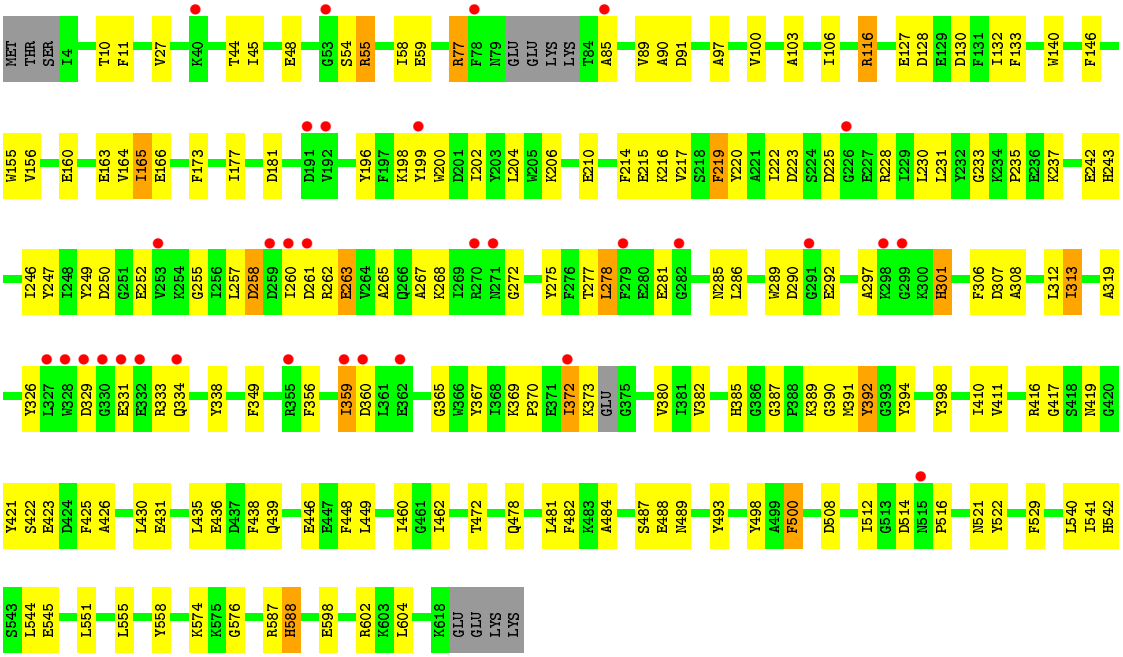
• Molecule 1: Putative uncharacterized protein PH0594

Chain J:



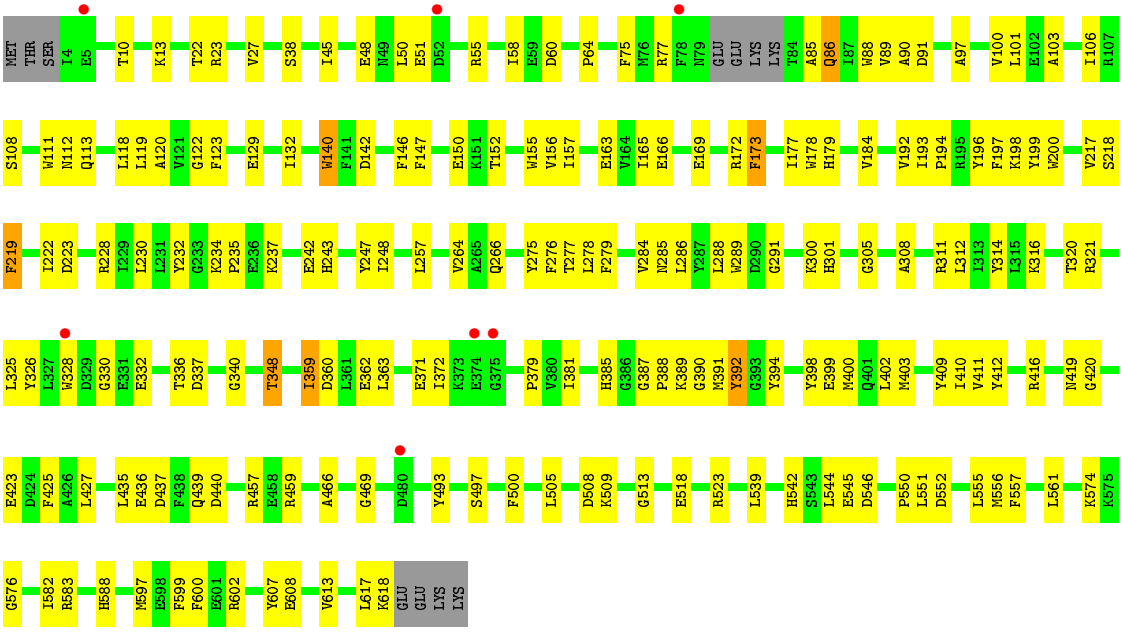
• Molecule 1: Putative uncharacterized protein PH0594

Chain K:



• Molecule 1: Putative uncharacterized protein PH0594

Chain L:


MET THR SER I4 E5 T10 K13 T22 R23 V27 S38 I45 E48 N49 L50 E51 D52 R55 I58 E59 D60 P64 F75 N76 R77 F78 N79 GLU GLU LYS LYS T84 A85 Q86 I87 W88 V89 A90 D91 A97 V100 L101 E102 A103 I106 R107
S108 W111 N112 Q113 L118 L119 A120 V121 G122 F123 E129 I132 W140 F141 D142 F146 F147 E150 K151 T152 W155 V156 I157 E163 V164 I165 E166 E169 R172 F173 I177 W178 H179 V184 V192 I193 P194 R195 Y196 F197 K198 Y199 W200 V217 S218
F219 I222 D223 R228 I229 L230 L231 Y232 G233 K234 P235 E236 K237 E242 H243 Y247 I248 L257 V264 A265 Q266 Y275 F276 T277 L278 F279 V284 N285 L286 Y287 L288 W289 D290 G291 K300 H301 G305 A308 R311 L312 I313 Y314 K315 K316 T320 R321
L325 Y326 L327 W328 D329 G330 E331 E332 T336 D337 G340 T348 I359 D360 L361 E362 L363 E371 I372 K373 E374 G375 P379 Y380 I381 H385 G386 G387 P388 K389 G390 M391 Y392 G393 Y394 Y398 E399 M400 Q401 L402 M403 Y409 I410 V411 Y412 R416 N419 G420
E423 D424 F425 A426 L427 L435 E436 D437 F438 Q439 D440 R457 E458 R459 A466 G469 D480 Y493 S497 F500 L505 D508 K509 G513 E518 R523 L539 H542 S543 L544 E545 D546 P550 L551 D552 L555 M556 F557 L561 K574 K575
G576 I582 R583 H588 M597 E598 F599 F600 E601 R602 Y607 E608 V613 L617 K618 GLU GLU LYS LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.31Å 183.80Å 275.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.70 19.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	87.6 (19.98-2.70) 87.1 (19.98-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.200 , 0.241 0.197 , 0.236	Depositor DCC
R_{free} test set	1906 reflections (0.87%)	DCC
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.6	EDS
Estimated twinning fraction	0.073 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 241056 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	59910	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: MG, HEZ, CL

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	0.33	0/5083	0.54	0/6881
1	B	0.30	0/5068	0.50	0/6869
1	C	0.28	0/5022	0.48	0/6815
1	D	0.35	0/5134	0.55	0/6945
1	E	0.35	0/5147	0.54	0/6964
1	F	0.32	0/5112	0.53	0/6917
1	G	0.29	0/5027	0.48	0/6814
1	H	0.28	0/4999	0.46	0/6779
1	I	0.29	0/5050	0.49	0/6844
1	J	0.25	0/4750	0.44	0/6470
1	K	0.26	0/4790	0.45	0/6513
1	L	0.28	0/4996	0.47	0/6781
All	All	0.30	0/60178	0.50	0/81592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4940	0	4668	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4926	0	4614	104	0
1	C	4883	0	4516	109	0
1	D	4989	0	4741	103	0
1	E	5005	0	4745	91	0
1	F	4975	0	4709	113	0
1	G	4886	0	4563	111	0
1	H	4866	0	4530	149	0
1	I	4910	0	4605	135	0
1	J	4617	0	4007	124	0
1	K	4659	0	4088	137	0
1	L	4862	0	4488	122	0
2	A	24	0	42	3	0
2	B	16	0	28	0	0
2	C	8	0	14	1	0
2	D	64	0	112	12	0
2	E	24	0	42	5	0
2	F	24	0	42	4	0
2	G	8	0	14	4	0
2	H	8	0	14	2	0
2	I	16	0	28	4	0
2	K	8	0	14	0	0
2	L	8	0	14	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	L	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	152	0	0	1	0
5	B	86	0	0	1	0
5	C	60	0	0	0	0
5	D	221	0	0	3	0
5	E	191	0	0	2	0
5	F	156	0	0	2	0
5	G	79	0	0	2	0
5	H	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	78	0	0	0	0
5	J	17	0	0	0	0
5	K	12	0	0	0	0
5	L	51	0	0	0	0
All	All	59910	0	54638	1362	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 12.

The worst 5 of 1362 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:K:77:ARG:HH11	1:K:77:ARG:HG2	1.08	1.09
1:I:103:ALA:HB1	1:I:106:ILE:HG13	1.41	1.02
1:I:86:GLN:HG3	1:I:88:TRP:HE1	1.25	1.00
1:B:8:GLU:HG2	1:B:594:LYS:HB2	1.45	0.97
1:J:156:VAL:HB	1:J:166:GLU:HB2	1.50	0.92

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	603/622 (97%)	579 (96%)	23 (4%)	1 (0%)	52 80
1	B	610/622 (98%)	591 (97%)	18 (3%)	1 (0%)	52 80
1	C	609/622 (98%)	580 (95%)	28 (5%)	1 (0%)	52 80
1	D	611/622 (98%)	589 (96%)	21 (3%)	1 (0%)	52 80
1	E	611/622 (98%)	591 (97%)	19 (3%)	1 (0%)	52 80
1	F	611/622 (98%)	588 (96%)	22 (4%)	1 (0%)	52 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	604/622 (97%)	580 (96%)	23 (4%)	1 (0%)	52 80
1	H	603/622 (97%)	566 (94%)	36 (6%)	1 (0%)	52 80
1	I	609/622 (98%)	586 (96%)	22 (4%)	1 (0%)	52 80
1	J	602/622 (97%)	566 (94%)	35 (6%)	1 (0%)	52 80
1	K	605/622 (97%)	568 (94%)	35 (6%)	2 (0%)	46 75
1	L	607/622 (98%)	579 (95%)	27 (4%)	1 (0%)	52 80
All	All	7285/7464 (98%)	6963 (96%)	309 (4%)	13 (0%)	52 80

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	372	ILE
1	A	359	ILE
1	B	359	ILE
1	C	359	ILE
1	D	359	ILE

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	490/548 (89%)	476 (97%)	14 (3%)	50 80
1	B	485/548 (88%)	460 (95%)	25 (5%)	29 58
1	C	473/548 (86%)	461 (98%)	12 (2%)	55 84
1	D	499/548 (91%)	476 (95%)	23 (5%)	33 64
1	E	502/548 (92%)	477 (95%)	25 (5%)	30 60
1	F	496/548 (90%)	479 (97%)	17 (3%)	44 75
1	G	477/548 (87%)	451 (94%)	26 (6%)	27 55
1	H	476/548 (87%)	456 (96%)	20 (4%)	36 68
1	I	485/548 (88%)	466 (96%)	19 (4%)	39 70
1	J	407/548 (74%)	384 (94%)	23 (6%)	25 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	418/548 (76%)	392 (94%)	26 (6%)	23 49
1	L	473/548 (86%)	452 (96%)	21 (4%)	35 65
All	All	5681/6576 (86%)	5430 (96%)	251 (4%)	35 65

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	583	ARG
1	G	588	HIS
1	L	86	GLN
1	G	54	SER
1	G	288	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	478	GLN
1	H	454	GLN
1	K	301	HIS
1	H	86	GLN
1	H	580	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 49 ligands modelled in this entry, 23 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEZ	A	701	-	7,7,7	0.30	0	6,6,6	0.48	0
2	HEZ	A	702	-	7,7,7	0.34	0	6,6,6	0.43	0
2	HEZ	A	703	-	7,7,7	0.31	0	6,6,6	0.44	0
2	HEZ	B	701	-	7,7,7	0.24	0	6,6,6	0.68	0
2	HEZ	B	702	-	7,7,7	0.39	0	6,6,6	0.43	0
2	HEZ	C	701	-	7,7,7	0.25	0	6,6,6	0.67	0
2	HEZ	D	701	-	7,7,7	0.29	0	6,6,6	0.54	0
2	HEZ	D	702	-	7,7,7	0.44	0	6,6,6	0.40	0
2	HEZ	D	703	-	7,7,7	0.31	0	6,6,6	0.52	0
2	HEZ	D	704	-	7,7,7	0.35	0	6,6,6	0.47	0
2	HEZ	D	705	-	7,7,7	0.34	0	6,6,6	0.45	0
2	HEZ	D	706	-	7,7,7	0.39	0	6,6,6	0.31	0
2	HEZ	D	707	-	7,7,7	0.27	0	6,6,6	0.56	0
2	HEZ	D	708	-	7,7,7	0.37	0	6,6,6	0.29	0
2	HEZ	E	701	-	7,7,7	0.28	0	6,6,6	0.60	0
2	HEZ	E	702	-	7,7,7	0.23	0	6,6,6	0.71	0
2	HEZ	E	703	-	7,7,7	0.42	0	6,6,6	0.30	0
2	HEZ	F	701	-	7,7,7	0.33	0	6,6,6	0.56	0
2	HEZ	F	702	-	7,7,7	0.31	0	6,6,6	0.48	0
2	HEZ	F	703	-	7,7,7	0.30	0	6,6,6	0.52	0
2	HEZ	G	701	-	7,7,7	0.28	0	6,6,6	0.56	0
2	HEZ	H	701	-	7,7,7	0.23	0	6,6,6	0.69	0
2	HEZ	I	701	-	7,7,7	0.31	0	6,6,6	0.45	0
2	HEZ	I	702	-	7,7,7	0.28	0	6,6,6	0.62	0
2	HEZ	K	701	-	7,7,7	0.32	0	6,6,6	0.53	0
2	HEZ	L	701	-	7,7,7	0.31	0	6,6,6	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEZ	A	701	-	-	0/5/5/5	0/0/0/0
2	HEZ	A	702	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEZ	A	703	-	-	0/5/5/5	0/0/0/0
2	HEZ	B	701	-	-	0/5/5/5	0/0/0/0
2	HEZ	B	702	-	-	0/5/5/5	0/0/0/0
2	HEZ	C	701	-	-	0/5/5/5	0/0/0/0
2	HEZ	D	701	-	-	0/5/5/5	0/0/0/0
2	HEZ	D	702	-	-	0/5/5/5	0/0/0/0
2	HEZ	D	703	-	-	0/5/5/5	0/0/0/0
2	HEZ	D	704	-	-	0/5/5/5	0/0/0/0
2	HEZ	D	705	-	-	0/5/5/5	0/0/0/0
2	HEZ	D	706	-	-	0/5/5/5	0/0/0/0
2	HEZ	D	707	-	-	0/5/5/5	0/0/0/0
2	HEZ	D	708	-	-	0/5/5/5	0/0/0/0
2	HEZ	E	701	-	-	0/5/5/5	0/0/0/0
2	HEZ	E	702	-	-	0/5/5/5	0/0/0/0
2	HEZ	E	703	-	-	0/5/5/5	0/0/0/0
2	HEZ	F	701	-	-	0/5/5/5	0/0/0/0
2	HEZ	F	702	-	-	0/5/5/5	0/0/0/0
2	HEZ	F	703	-	-	0/5/5/5	0/0/0/0
2	HEZ	G	701	-	-	0/5/5/5	0/0/0/0
2	HEZ	H	701	-	-	0/5/5/5	0/0/0/0
2	HEZ	I	701	-	-	0/5/5/5	0/0/0/0
2	HEZ	I	702	-	-	0/5/5/5	0/0/0/0
2	HEZ	K	701	-	-	0/5/5/5	0/0/0/0
2	HEZ	L	701	-	-	0/5/5/5	0/0/0/0

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.

14 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	HEZ	3	0
2	C	701	HEZ	1	0
2	D	701	HEZ	6	0
2	D	703	HEZ	1	0
2	D	706	HEZ	1	0
2	D	708	HEZ	4	0
2	E	701	HEZ	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	702	HEZ	2	0
2	F	701	HEZ	3	0
2	F	702	HEZ	1	0
2	G	701	HEZ	4	0
2	H	701	HEZ	2	0
2	I	701	HEZ	4	0
2	L	701	HEZ	1	0

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	608/622 (97%)	-0.64	1 (0%)	95	96	30, 50, 75, 93	0
1	B	612/622 (98%)	-0.40	5 (0%)	87	88	38, 62, 89, 126	0
1	C	612/622 (98%)	-0.29	6 (0%)	84	85	47, 70, 98, 126	0
1	D	612/622 (98%)	-0.75	3 (0%)	91	93	23, 39, 62, 109	0
1	E	613/622 (98%)	-0.68	3 (0%)	91	93	27, 44, 67, 108	0
1	F	614/622 (98%)	-0.61	4 (0%)	89	90	26, 49, 73, 103	1 (0%)
1	G	608/622 (97%)	-0.36	1 (0%)	95	96	44, 70, 93, 139	0
1	H	609/622 (97%)	-0.26	5 (0%)	87	88	44, 75, 99, 126	0
1	I	611/622 (98%)	-0.43	2 (0%)	94	95	44, 64, 87, 124	0
1	J	609/622 (97%)	0.28	29 (4%)	34	33	65, 103, 130, 143	4 (0%)
1	K	610/622 (98%)	0.39	32 (5%)	31	30	71, 101, 133, 161	3 (0%)
1	L	611/622 (98%)	-0.15	7 (1%)	82	83	49, 77, 106, 139	0
All	All	7329/7464 (98%)	-0.33	98 (1%)	79	79	23, 65, 113, 161	8 (0%)

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	291	GLY	7.4
1	K	372	ILE	6.2
1	K	330	GLY	4.9
1	K	279	PHE	4.5
1	K	271	ASN	4.1

6.2 Non-standard residues in protein, DNA, RNA chains

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	HEZ	F	702	8/8	0.96	0.31	17.11	17,21,25,27	8
2	HEZ	D	702	8/8	0.93	0.35	14.44	10,14,16,16	8
2	HEZ	B	702	8/8	0.92	0.36	12.73	11,13,17,18	8
2	HEZ	E	702	8/8	0.69	0.41	11.34	67,69,76,77	0
2	HEZ	A	703	8/8	0.84	0.31	10.03	69,71,75,76	0
2	HEZ	D	706	8/8	0.85	0.27	8.73	63,64,65,65	0
2	HEZ	D	705	8/8	0.88	0.23	7.93	60,64,75,77	0
2	HEZ	F	703	8/8	0.93	0.25	6.85	69,70,74,75	0
2	HEZ	D	707	8/8	0.90	0.26	6.66	61,63,64,68	0
2	HEZ	D	703	8/8	0.92	0.17	6.23	63,65,67,68	0
2	HEZ	B	701	8/8	0.87	0.23	4.56	50,56,57,59	0
2	HEZ	G	701	8/8	0.84	0.27	4.12	74,77,79,79	0
2	HEZ	A	702	8/8	0.91	0.21	3.86	47,50,65,67	0
3	MG	D	710	1/1	0.94	0.23	3.36	42,42,42,42	0
2	HEZ	E	703	8/8	0.90	0.21	3.06	54,54,55,56	0
2	HEZ	D	704	8/8	0.92	0.22	2.64	67,71,72,73	0
3	MG	E	705	1/1	0.94	0.19	2.50	29,29,29,29	0
2	HEZ	I	702	8/8	0.89	0.26	2.37	73,74,75,76	0
2	HEZ	C	701	8/8	0.83	0.22	2.14	64,71,73,74	0
2	HEZ	K	701	8/8	0.76	0.28	1.87	74,76,78,78	0
2	HEZ	I	701	8/8	0.90	0.20	1.76	66,70,72,72	0
2	HEZ	A	701	8/8	0.96	0.15	1.69	47,48,49,49	0
2	HEZ	E	701	8/8	0.96	0.14	1.26	36,40,47,47	0
3	MG	D	709	1/1	0.82	0.16	1.18	63,63,63,63	0
2	HEZ	D	708	8/8	0.94	0.17	1.10	50,58,68,69	0
2	HEZ	F	701	8/8	0.95	0.15	1.08	43,45,50,50	0
3	MG	A	705	1/1	0.89	0.13	1.05	60,60,60,60	0
3	MG	B	703	1/1	0.97	0.14	0.97	37,37,37,37	0
2	HEZ	L	701	8/8	0.93	0.17	0.96	57,60,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	I	703	1/1	0.96	0.17	0.91	45,45,45,45	0
2	HEZ	H	701	8/8	0.93	0.17	0.87	58,61,65,67	0
2	HEZ	D	701	8/8	0.95	0.15	0.79	43,43,47,52	0
3	MG	F	705	1/1	0.97	0.14	0.70	32,32,32,32	0
3	MG	H	703	1/1	0.91	0.14	0.62	41,41,41,41	0
3	MG	A	704	1/1	0.99	0.14	0.60	36,36,36,36	0
3	MG	C	702	1/1	0.96	0.15	0.47	60,60,60,60	0
3	MG	L	703	1/1	0.93	0.16	-0.15	66,66,66,66	0
3	MG	F	706	1/1	0.98	0.11	-0.50	67,67,67,67	0
4	CL	D	711	1/1	0.98	0.09	-1.49	47,47,47,47	0
3	MG	H	702	1/1	0.89	0.06	-2.04	81,81,81,81	0
3	MG	C	703	1/1	0.57	0.08	-2.23	93,93,93,93	0
3	MG	F	704	1/1	0.89	0.09	-2.37	80,80,80,80	0
3	MG	G	702	1/1	0.98	0.08	-2.47	34,34,34,34	0
4	CL	F	707	1/1	0.98	0.06	-4.57	44,44,44,44	0
3	MG	G	703	1/1	0.84	0.11	-	82,82,82,82	0
3	MG	L	702	1/1	0.94	0.14	-	80,80,80,80	0
3	MG	I	704	1/1	0.81	0.10	-	75,75,75,75	0
3	MG	E	706	1/1	0.92	0.08	-	44,44,44,44	0
3	MG	E	704	1/1	0.95	0.09	-	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.