



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:27 PM UTC

PDB ID : 1VYH / pdb_00001vyh
Title : PAF-AH Holoenzyme: Lis1/Alfa2
Authors : Tarricone, C.; Perrina, F.; Monzani, S.; Massimiliano, L.; Knapp, S.; Tsai, L.-H.; Derewenda, Z.S.; Musacchio, A.
Deposited on : 2004-04-30
Resolution : 3.40 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

<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

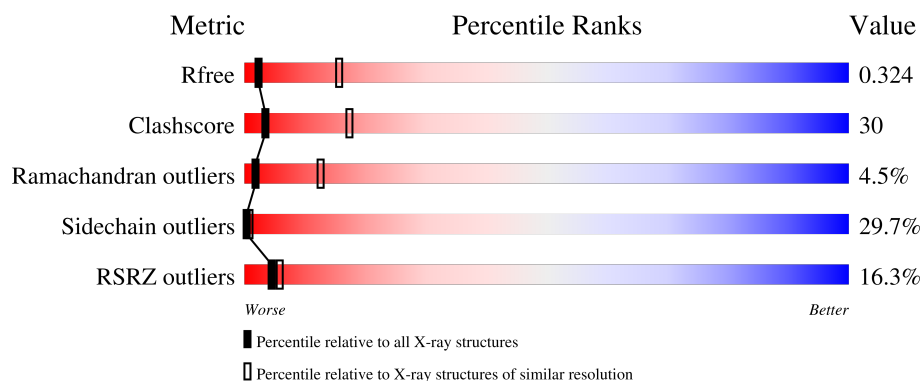
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	229	
1	B	229	
1	E	229	
1	F	229	
1	I	229	

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Mol	Chain	Length	Quality of chain
1	J	229	
1	M	229	
1	N	229	
1	Q	229	
1	R	229	
2	C	410	
2	D	410	
2	G	410	
2	H	410	
2	K	410	
2	L	410	
2	O	410	
2	P	410	
2	S	410	
2	T	410	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41590 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 PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	B	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	E	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	F	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	I	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	J	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	M	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	N	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	Q	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			
1	R	218	Total	C	N	O	S	0	0	0
			1705	1083	302	312	8			

- Molecule 2 is a protein called PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	D	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	G	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	K	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	L	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	O	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	P	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	S	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			
2	T	310	Total	C	N	O	S	0	0	0
			2454	1546	433	456	19			

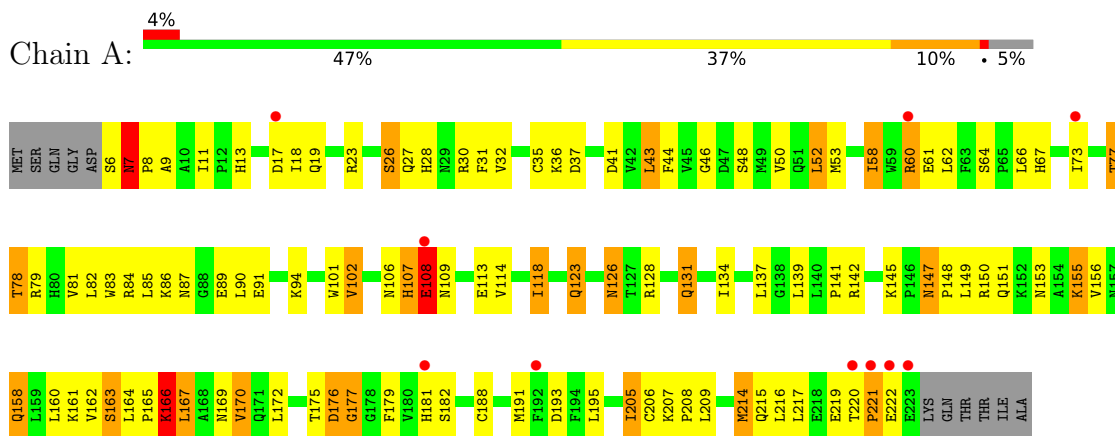
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	199	SER	ALA	conflict	UNP P43034
C	276	ARG	GLU	conflict	UNP P43034
D	199	SER	ALA	conflict	UNP P43034
D	276	ARG	GLU	conflict	UNP P43034
G	199	SER	ALA	conflict	UNP P43034
G	276	ARG	GLU	conflict	UNP P43034
H	199	SER	ALA	conflict	UNP P43034
H	276	ARG	GLU	conflict	UNP P43034
K	199	SER	ALA	conflict	UNP P43034
K	276	ARG	GLU	conflict	UNP P43034
L	199	SER	ALA	conflict	UNP P43034
L	276	ARG	GLU	conflict	UNP P43034
O	199	SER	ALA	conflict	UNP P43034
O	276	ARG	GLU	conflict	UNP P43034
P	199	SER	ALA	conflict	UNP P43034
P	276	ARG	GLU	conflict	UNP P43034
S	199	SER	ALA	conflict	UNP P43034
S	276	ARG	GLU	conflict	UNP P43034
T	199	SER	ALA	conflict	UNP P43034
T	276	ARG	GLU	conflict	UNP P43034

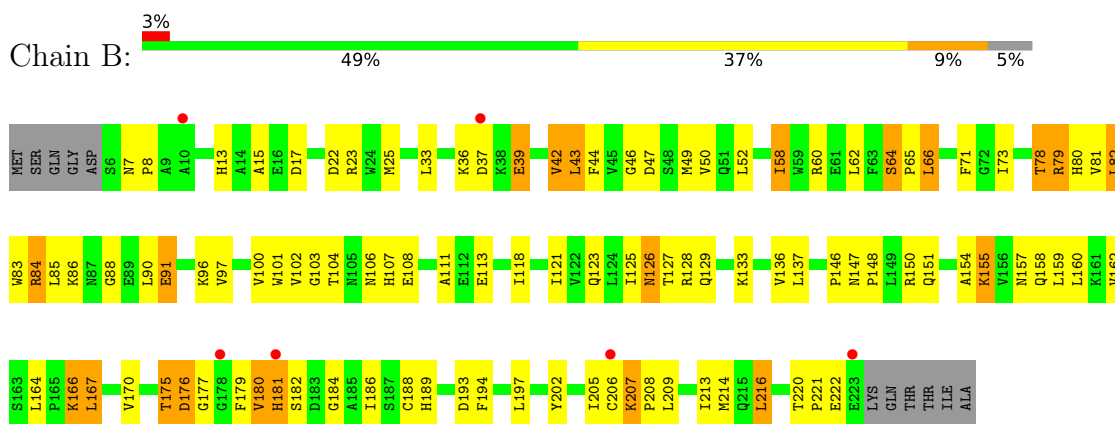
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

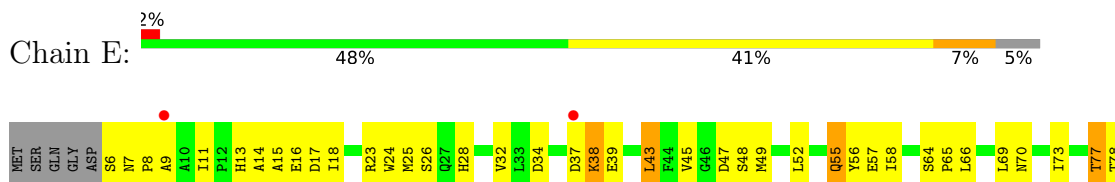
• Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT

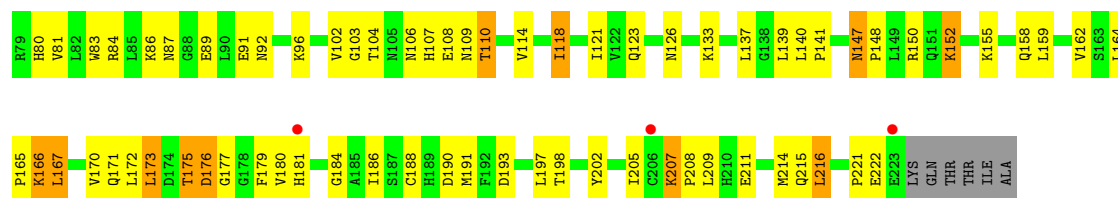


• Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT



• Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT

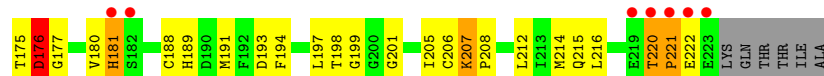
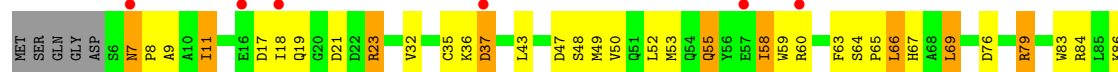




• Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT



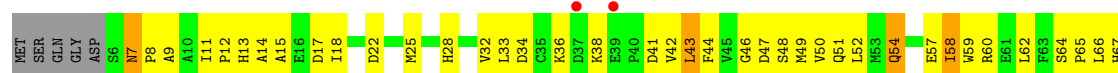
Chain F: 7% 55% 30% 9% 5%



• Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT



Chain I: 3% 44% 44% 7% 5%



• Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT

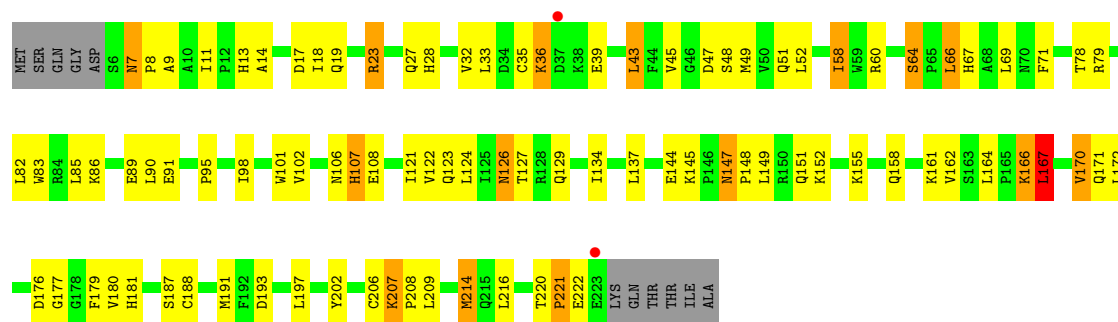


Chain J: 3% 58% 30% 7% 5%

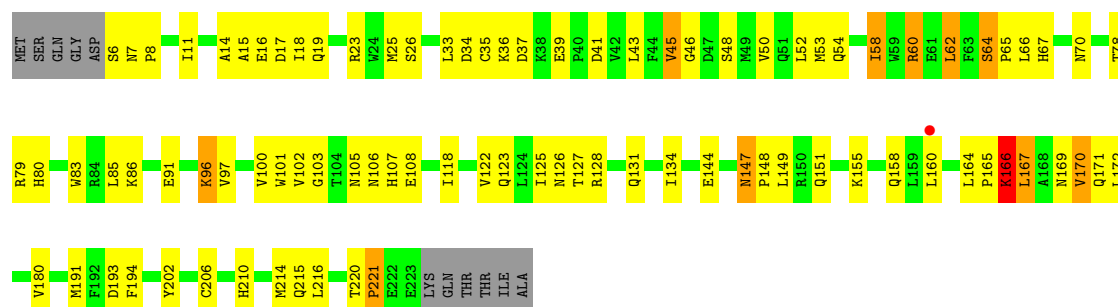




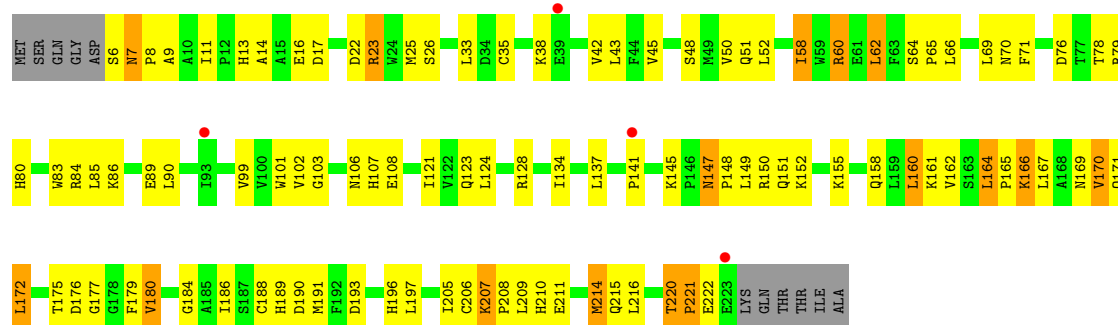
- Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT



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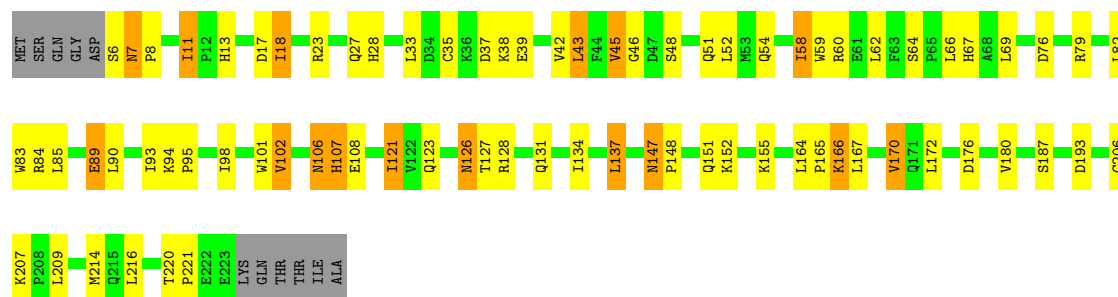


- Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT

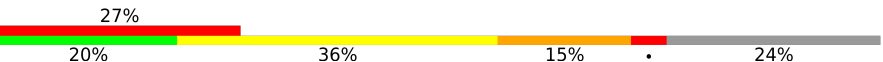


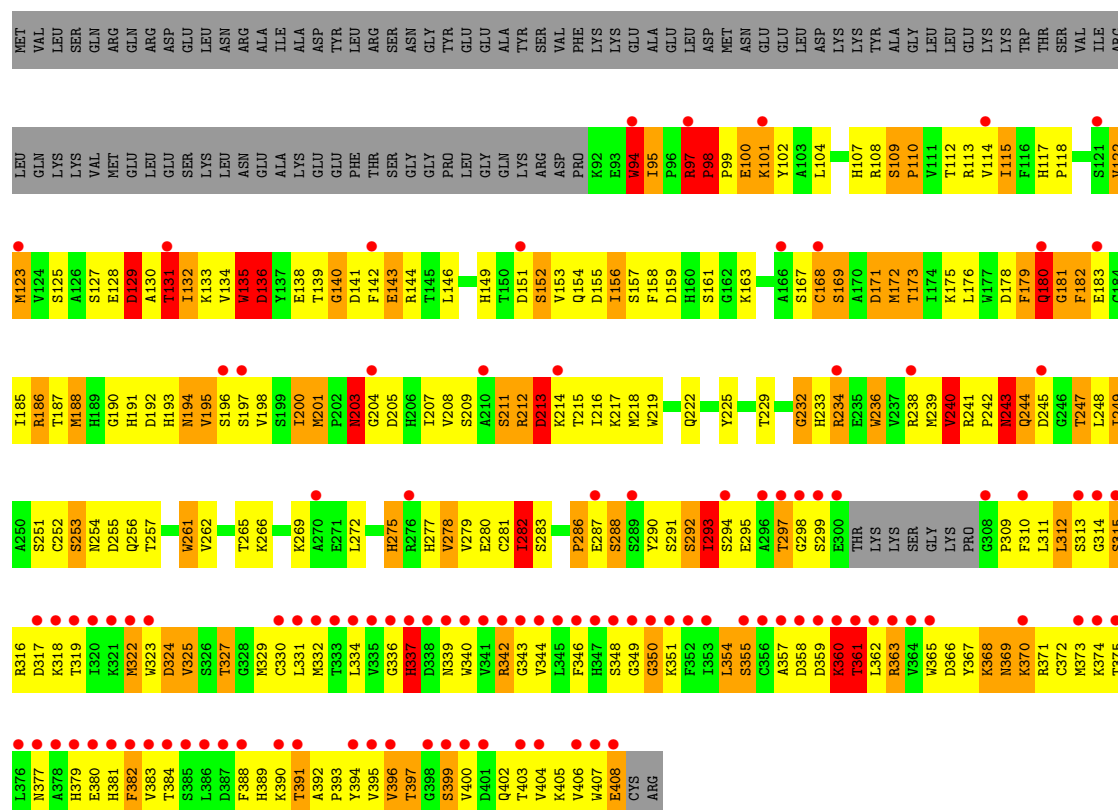
• Molecule 1: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB BETA SUB-UNIT

Chain R: 



• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

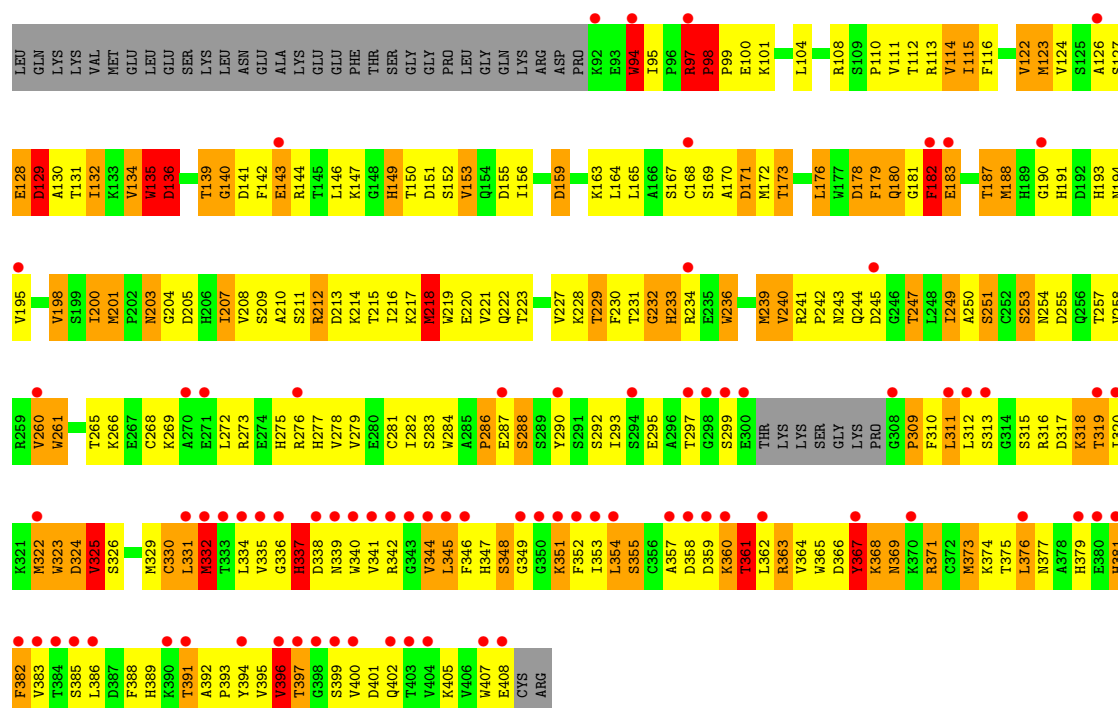
Chain C: 



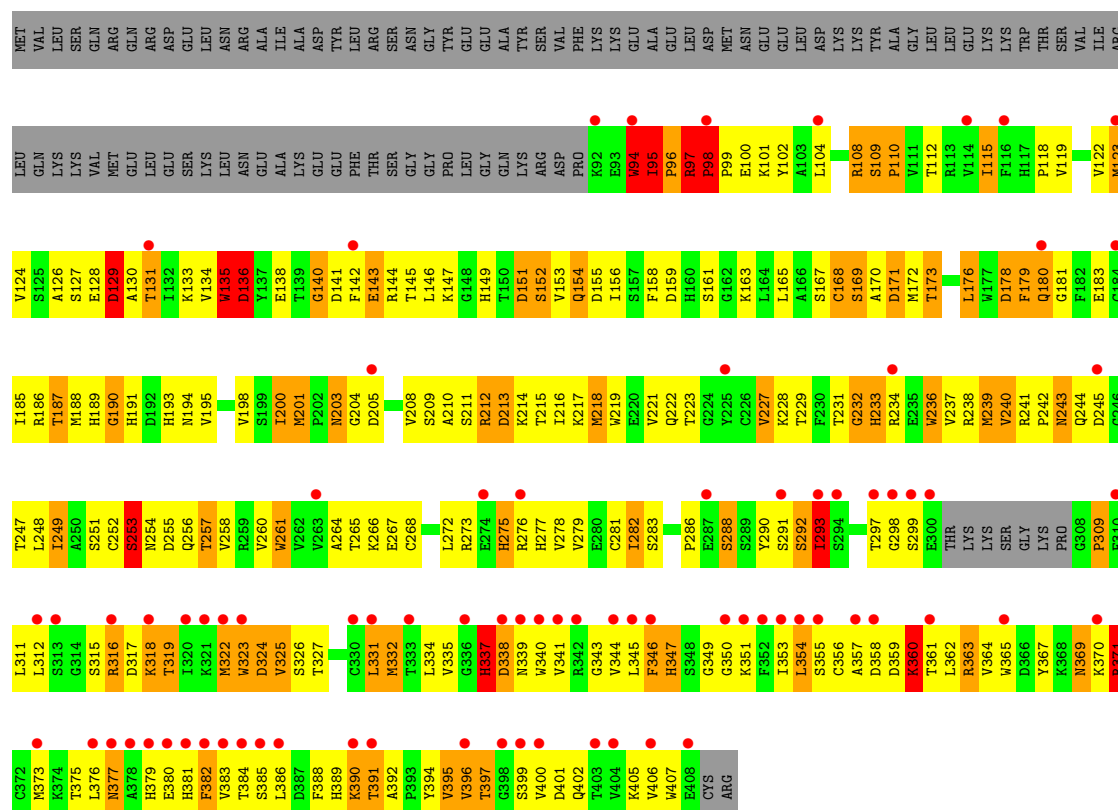
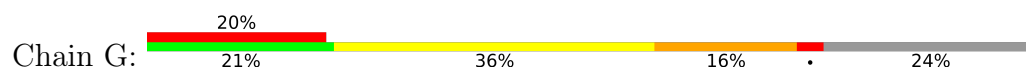
• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

Chain D: 



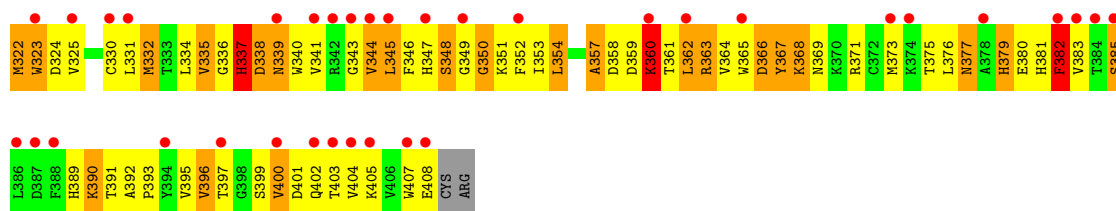


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

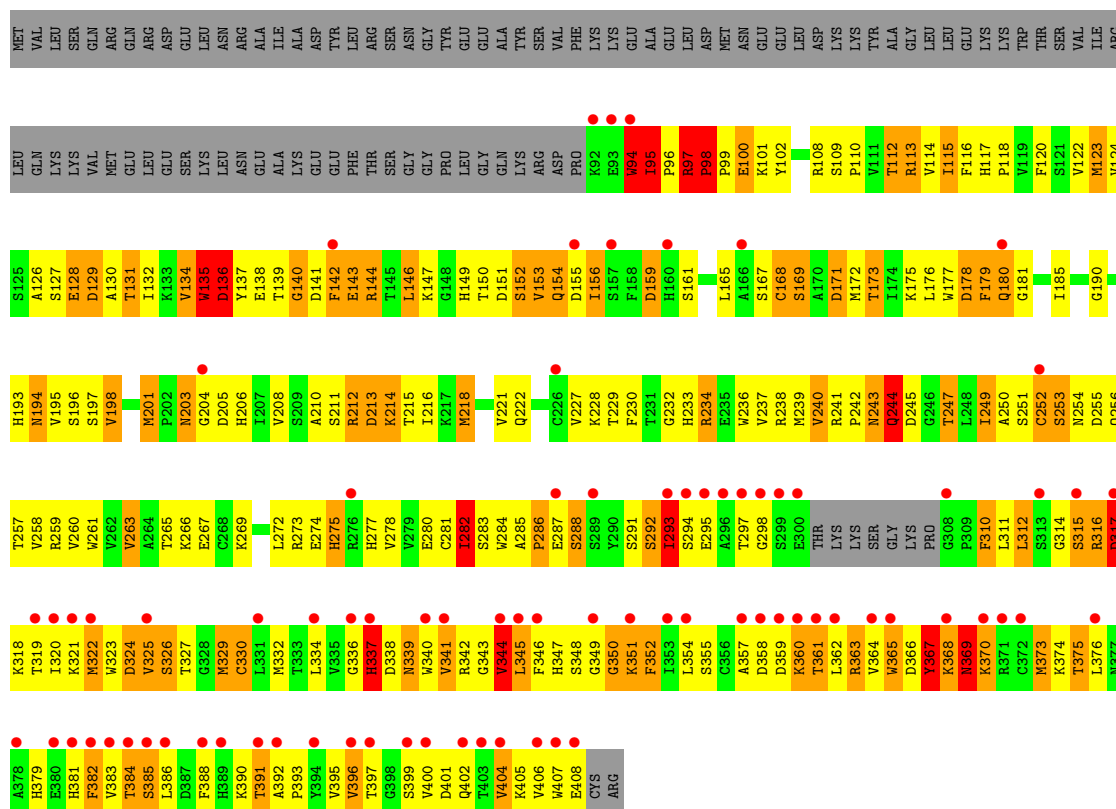
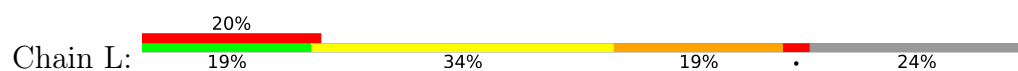


Chain H:

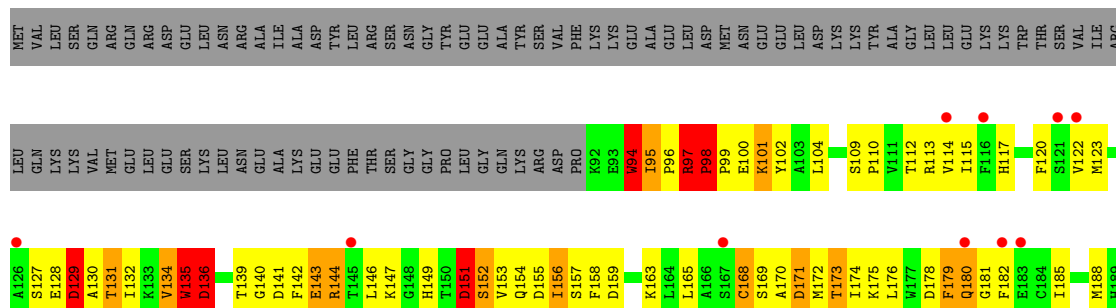
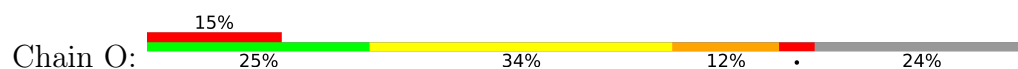


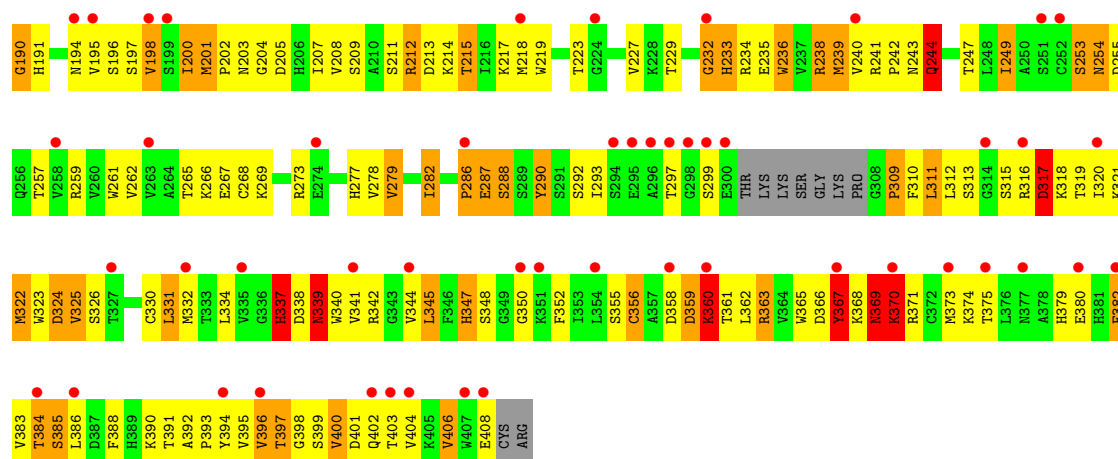


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

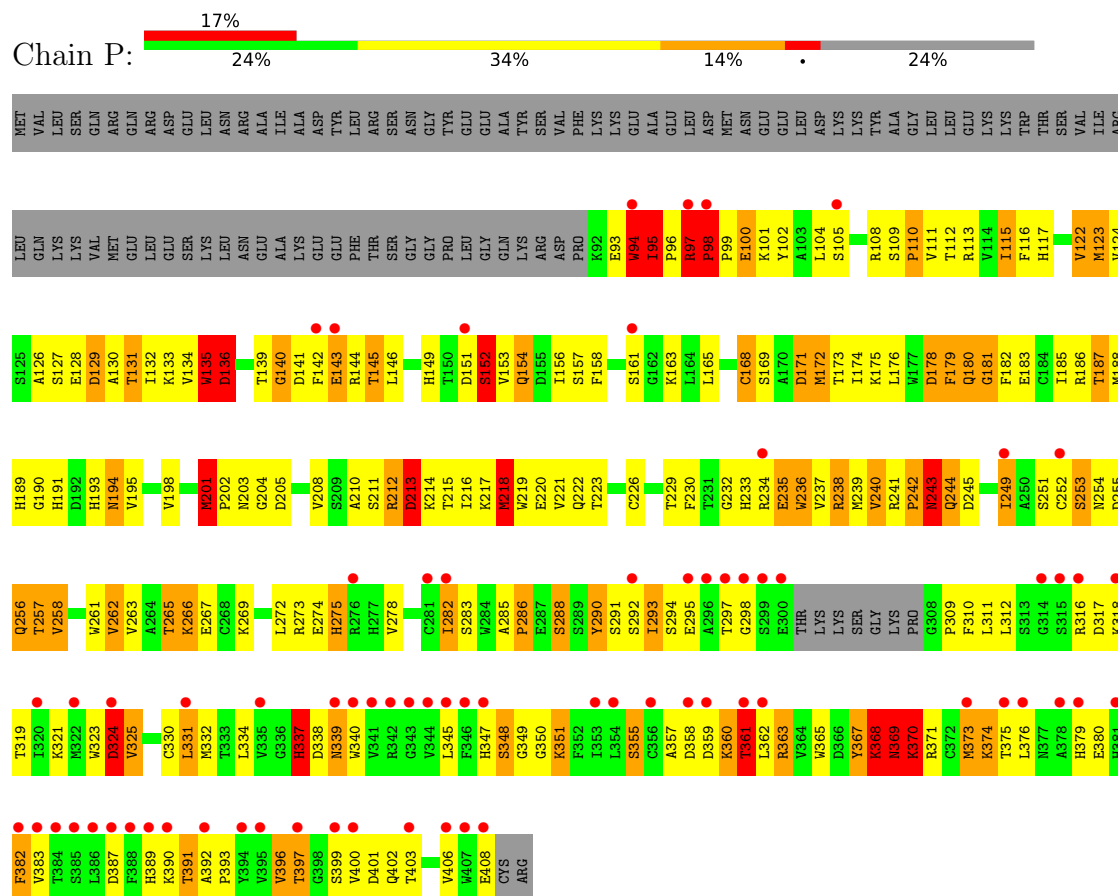


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

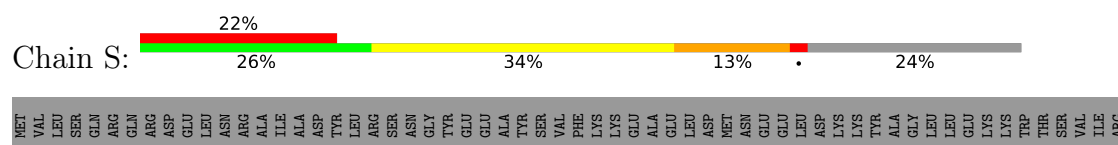


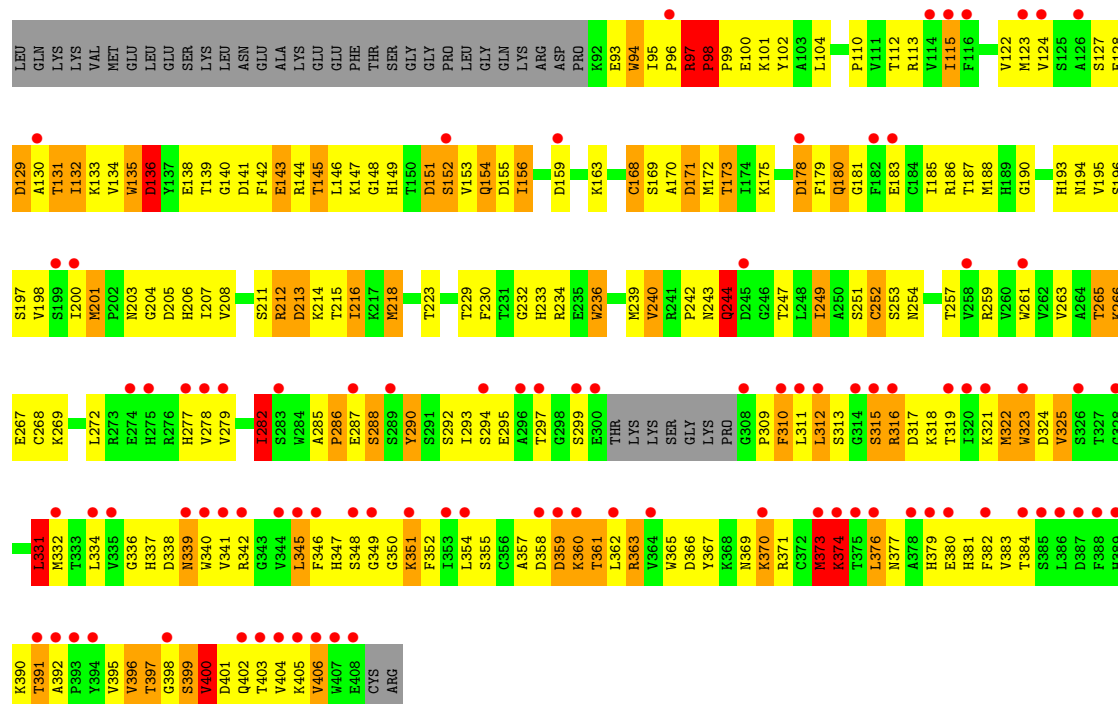


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT

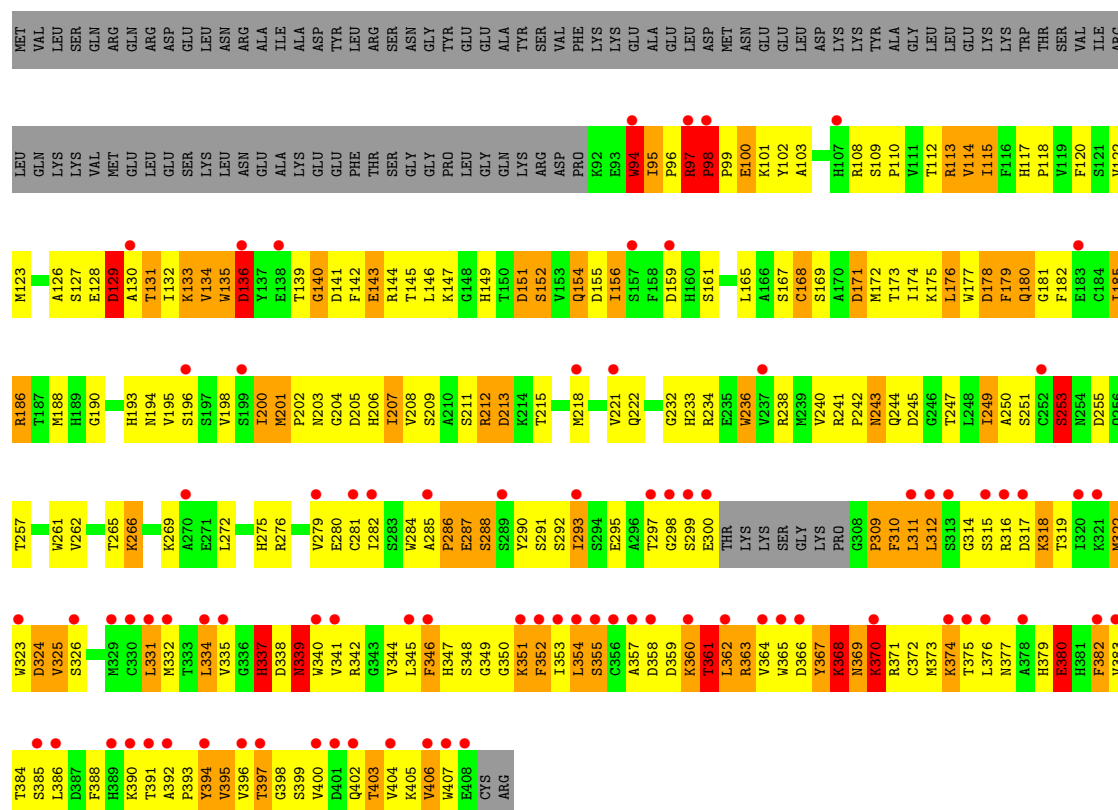
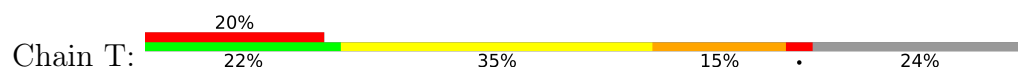


• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT





• Molecule 2: PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE IB ALPHA SUB-UNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	205.77Å 101.22Å 246.13Å 90.00° 98.06° 90.00°	Depositor
Resolution (Å)	200.00 – 3.40 200.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (200.00-3.40) 96.9 (200.00-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.264 , 0.307 0.304 , 0.324	Depositor DCC
R_{free} test set	5399 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	88.3	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	41590	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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

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	1.01	0/1742	1.19	11/2364 (0.5%)
1	B	0.79	0/1742	1.10	4/2364 (0.2%)
1	E	0.92	0/1742	1.11	5/2364 (0.2%)
1	F	1.09	2/1742 (0.1%)	1.21	8/2364 (0.3%)
1	I	0.81	0/1742	1.11	8/2364 (0.3%)
1	J	0.76	3/1742 (0.2%)	1.04	2/2364 (0.1%)
1	M	0.63	0/1742	1.01	4/2364 (0.2%)
1	N	0.58	0/1742	1.00	2/2364 (0.1%)
1	Q	0.55	0/1742	0.96	2/2364 (0.1%)
1	R	0.56	0/1742	0.96	3/2364 (0.1%)
2	C	1.12	6/2518 (0.2%)	1.39	27/3414 (0.8%)
2	D	0.89	5/2518 (0.2%)	1.28	19/3414 (0.6%)
2	G	0.88	2/2518 (0.1%)	1.29	24/3414 (0.7%)
2	H	1.06	4/2518 (0.2%)	1.38	21/3414 (0.6%)
2	K	0.72	2/2518 (0.1%)	1.21	19/3414 (0.6%)
2	L	1.00	4/2518 (0.2%)	1.36	31/3414 (0.9%)
2	O	0.69	1/2518 (0.0%)	1.14	19/3414 (0.6%)
2	P	0.96	5/2518 (0.2%)	1.35	25/3414 (0.7%)
2	S	0.72	1/2518 (0.0%)	1.15	21/3414 (0.6%)
2	T	0.78	2/2518 (0.1%)	1.19	22/3414 (0.6%)
All	All	0.85	37/42600 (0.1%)	1.20	277/57780 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	2
1	F	0	1
2	C	0	3
2	D	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	5
2	H	0	5
2	K	0	4
2	L	0	4
2	O	0	4
2	P	0	4
2	S	0	2
2	T	0	2
All	All	0	44

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	95	ILE	CA-CB	8.83	1.63	1.53
2	C	182	PHE	CA-C	-7.38	1.46	1.52
2	L	329	MET	SD-CE	7.23	1.97	1.79
2	H	95	ILE	CA-CB	7.11	1.61	1.53
1	F	176	ASP	CA-C	-6.95	1.45	1.53

The worst 5 of 277 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	98	PRO	N-CA-C	12.50	125.95	110.70
2	C	98	PRO	N-CA-C	12.49	125.94	110.70
2	L	98	PRO	N-CA-C	12.41	125.84	110.70
2	D	98	PRO	N-CA-C	12.19	125.58	110.70
2	G	98	PRO	N-CA-C	12.16	125.53	110.70

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	THR	Peptide
2	C	135	TRP	Peptide
2	C	337	HIS	Peptide
2	C	97	ARG	Peptide
2	D	97	ARG	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	1705	0	1701	71	0
1	B	1705	0	1701	65	0
1	E	1705	0	1701	60	0
1	F	1705	0	1701	68	0
1	I	1705	0	1701	66	1
1	J	1705	0	1701	57	0
1	M	1705	0	1701	52	0
1	N	1705	0	1701	41	0
1	Q	1705	0	1701	53	0
1	R	1705	0	1701	33	0
2	C	2454	0	2371	229	0
2	D	2454	0	2371	201	0
2	G	2454	0	2371	211	0
2	H	2454	0	2371	209	0
2	K	2454	0	2371	186	0
2	L	2454	0	2371	233	0
2	O	2454	0	2371	156	0
2	P	2454	0	2371	215	0
2	S	2454	0	2371	145	0
2	T	2454	0	2371	169	1
All	All	41590	0	40720	2461	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 30.

The worst 5 of 2461 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)
2:L:312:LEU:HD21	2:L:346:PHE:CE1	1.64	1.32
2:K:315:SER:OG	2:K:317:ASP:HB2	1.21	1.27
2:L:312:LEU:CD2	2:L:346:PHE:HE1	1.51	1.24
2:L:239:MET:HE3	2:L:241:ARG:HH21	1.03	1.19
2:D:168:CYS:SG	2:D:198:VAL:HB	1.85	1.16

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:LYS:CB	2:T:300:GLU:O[2_556]	1.91	0.29

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	216/229 (94%)	200 (93%)	14 (6%)	2 (1%)	14	42
1	B	216/229 (94%)	196 (91%)	17 (8%)	3 (1%)	9	31
1	E	216/229 (94%)	192 (89%)	22 (10%)	2 (1%)	14	42
1	F	216/229 (94%)	199 (92%)	15 (7%)	2 (1%)	14	42
1	I	216/229 (94%)	200 (93%)	14 (6%)	2 (1%)	14	42
1	J	216/229 (94%)	197 (91%)	17 (8%)	2 (1%)	14	42
1	M	216/229 (94%)	197 (91%)	16 (7%)	3 (1%)	9	31
1	N	216/229 (94%)	198 (92%)	16 (7%)	2 (1%)	14	42
1	Q	216/229 (94%)	200 (93%)	14 (6%)	2 (1%)	14	42
1	R	216/229 (94%)	199 (92%)	15 (7%)	2 (1%)	14	42
2	C	306/410 (75%)	247 (81%)	35 (11%)	24 (8%)	1	4
2	D	306/410 (75%)	242 (79%)	46 (15%)	18 (6%)	1	8
2	G	306/410 (75%)	238 (78%)	45 (15%)	23 (8%)	1	5
2	H	306/410 (75%)	243 (79%)	38 (12%)	25 (8%)	0	4
2	K	306/410 (75%)	237 (78%)	44 (14%)	25 (8%)	0	4
2	L	306/410 (75%)	243 (79%)	42 (14%)	21 (7%)	1	6
2	O	306/410 (75%)	245 (80%)	43 (14%)	18 (6%)	1	8
2	P	306/410 (75%)	251 (82%)	34 (11%)	21 (7%)	1	6
2	S	306/410 (75%)	242 (79%)	47 (15%)	17 (6%)	1	9
2	T	306/410 (75%)	244 (80%)	43 (14%)	19 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5220/6390 (82%)	4410 (84%)	577 (11%)	233 (4%)	2	12

5 of 233 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	97	ARG
2	C	98	PRO
2	C	143	GLU
2	C	293	ILE
2	C	360	LYS

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	185/197 (94%)	137 (74%)	48 (26%)	0	1
1	B	185/197 (94%)	141 (76%)	44 (24%)	1	2
1	E	185/197 (94%)	140 (76%)	45 (24%)	1	2
1	F	185/197 (94%)	149 (80%)	36 (20%)	1	5
1	I	185/197 (94%)	137 (74%)	48 (26%)	0	1
1	J	185/197 (94%)	151 (82%)	34 (18%)	1	7
1	M	185/197 (94%)	148 (80%)	37 (20%)	1	4
1	N	185/197 (94%)	142 (77%)	43 (23%)	1	2
1	Q	185/197 (94%)	133 (72%)	52 (28%)	0	1
1	R	185/197 (94%)	138 (75%)	47 (25%)	0	1
2	C	274/365 (75%)	184 (67%)	90 (33%)	0	0
2	D	274/365 (75%)	172 (63%)	102 (37%)	0	0
2	G	274/365 (75%)	184 (67%)	90 (33%)	0	0
2	H	274/365 (75%)	182 (66%)	92 (34%)	0	0
2	K	274/365 (75%)	175 (64%)	99 (36%)	0	0
2	L	274/365 (75%)	184 (67%)	90 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	274/365 (75%)	174 (64%)	100 (36%)	0	0
2	P	274/365 (75%)	197 (72%)	77 (28%)	0	1
2	S	274/365 (75%)	183 (67%)	91 (33%)	0	0
2	T	274/365 (75%)	177 (65%)	97 (35%)	0	0
All	All	4590/5620 (82%)	3228 (70%)	1362 (30%)	0	1

5 of 1362 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	182	PHE
1	R	62	LEU
2	O	269	LYS
2	O	179	PHE
2	P	263	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	158	GLN
2	P	254	ASN
1	M	215	GLN
1	N	151	GLN
1	Q	106	ASN

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 [i](#)

There are no ligands in this entry.

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	218/229 (95%)	0.57	10 (4%) 37 27	3, 4, 8, 10	0
1	B	218/229 (95%)	0.29	6 (2%) 55 41	3, 4, 7, 10	0
1	E	218/229 (95%)	0.41	5 (2%) 61 46	3, 4, 8, 10	0
1	F	218/229 (95%)	0.83	15 (6%) 23 18	3, 4, 8, 11	0
1	I	218/229 (95%)	0.20	6 (2%) 55 41	3, 5, 8, 10	0
1	J	218/229 (95%)	0.02	6 (2%) 55 41	3, 5, 7, 10	0
1	M	218/229 (95%)	0.01	2 (0%) 81 68	3, 5, 7, 10	0
1	N	218/229 (95%)	0.11	1 (0%) 87 78	3, 5, 7, 9	0
1	Q	218/229 (95%)	0.23	4 (1%) 67 53	3, 5, 7, 9	0
1	R	218/229 (95%)	0.33	0 100 100	3, 5, 7, 9	0
2	C	310/410 (75%)	1.66	109 (35%) 1 1	3, 5, 63, 78	0
2	D	310/410 (75%)	1.28	80 (25%) 1 3	3, 5, 74, 85	0
2	G	310/410 (75%)	1.28	80 (25%) 1 3	3, 5, 73, 80	0
2	H	310/410 (75%)	1.43	97 (31%) 1 2	3, 5, 65, 82	0
2	K	310/410 (75%)	1.03	54 (17%) 4 5	3, 5, 84, 89	0
2	L	310/410 (75%)	1.34	81 (26%) 1 3	3, 5, 67, 76	0
2	O	310/410 (75%)	1.24	60 (19%) 3 4	3, 5, 90, 94	0
2	P	310/410 (75%)	1.24	71 (22%) 2 4	3, 5, 73, 82	0
2	S	310/410 (75%)	1.43	91 (29%) 1 2	3, 5, 91, 94	0
2	T	310/410 (75%)	1.36	83 (26%) 1 2	3, 5, 91, 95	0
All	All	5280/6390 (82%)	0.90	861 (16%) 4 6	3, 5, 83, 95	0

The worst 5 of 861 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	297	THR	10.3
2	G	299	SER	10.1
2	G	298	GLY	8.8
1	A	223	GLU	8.8
2	L	299	SER	8.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.