



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:54 AM UTC

PDB ID : 6ABH / pdb_00006abh
Title : Structure of a natural red emitting luciferase from Phrixothrix hirtus (P1 crystal form)
Authors : Carrasco-Lopez, C.; Panjikar, S.; Naumov, P.; Rabeh, W.
Deposited on : 2018-07-21
Resolution : 3.05 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

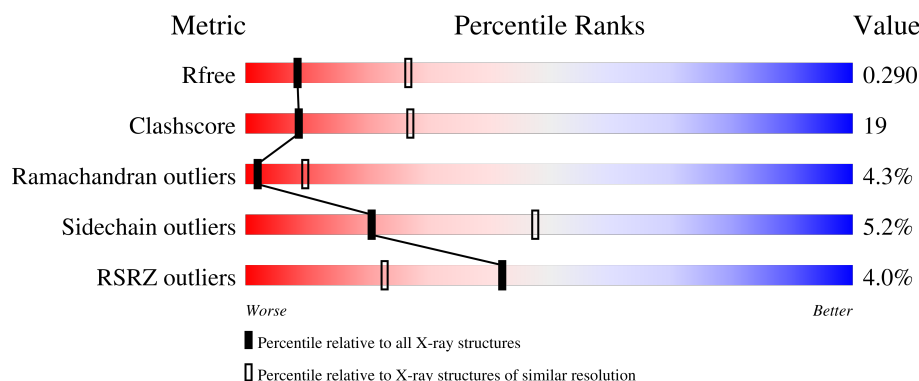
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	546	2% 44% 21% • • 31%
1	B	546	4% 47% 23% • • 26%
1	C	546	3% 45% 26% • 25%
1	D	546	4% 47% 28% 5% • 19%
1	E	546	2% 41% 28% • • 27%

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Mol	Chain	Length	Quality of chain
1	F	546	 3% 49% 24% •• 24%
1	G	546	 3% 46% 23% •• 27%
1	H	546	 3% 41% 27% • 27%

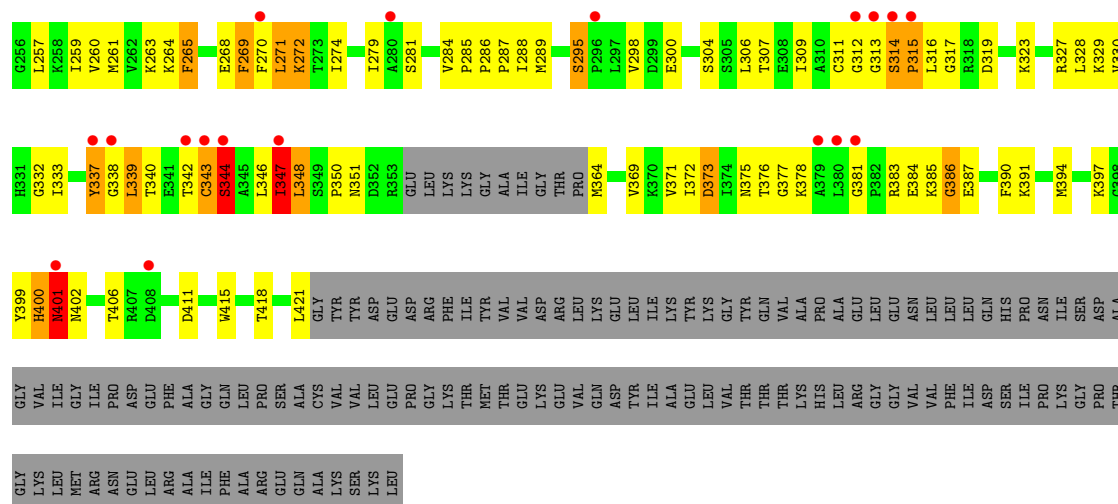
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25451 atoms, of which 0 are hydrogens and 0 are deuteriums.

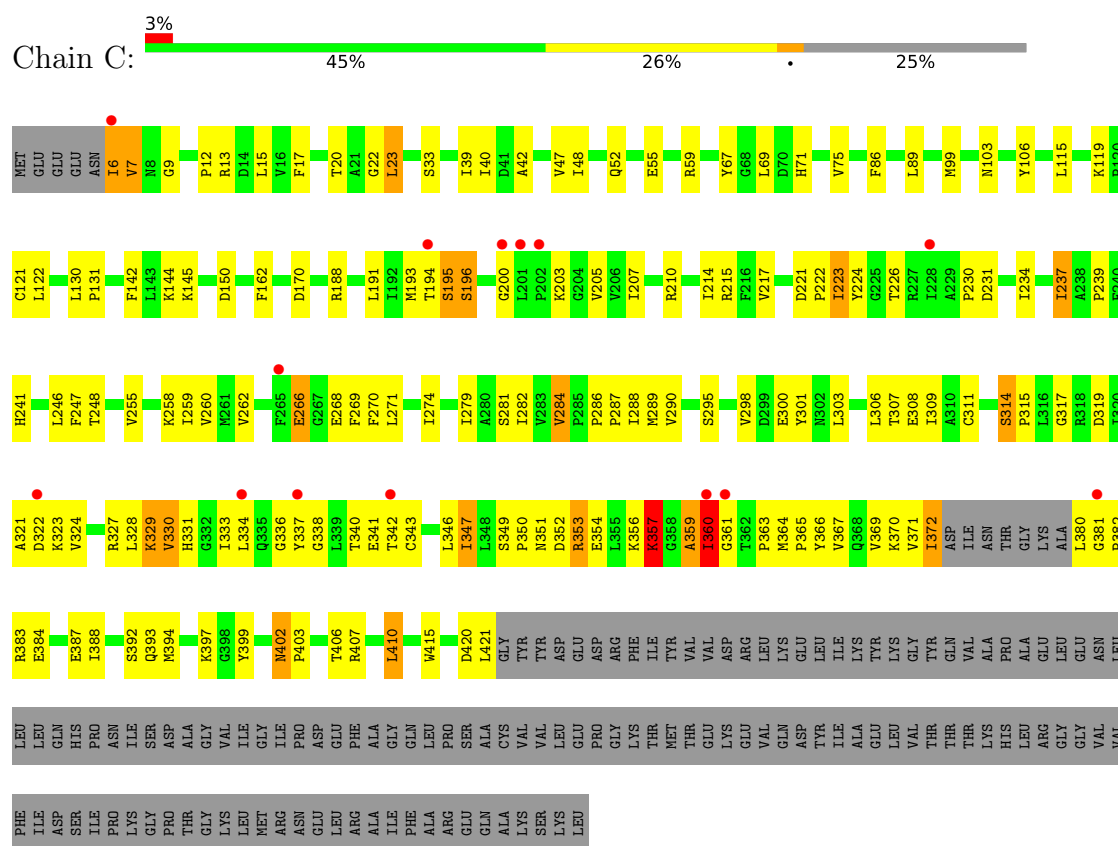
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Red-bioluminescence eliciting luciferase.

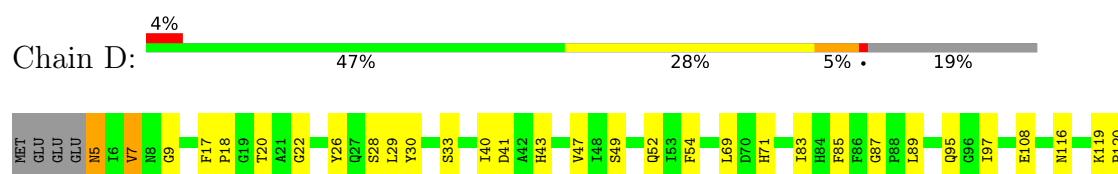
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2955	1915	487	535	18			
1	B	405	Total	C	N	O	S	0	0	0
			3170	2047	527	577	19			
1	C	409	Total	C	N	O	S	0	0	0
			3199	2069	531	580	19			
1	D	442	Total	C	N	O	S	0	0	0
			3480	2251	576	634	19			
1	E	398	Total	C	N	O	S	0	0	0
			3110	2011	515	565	19			
1	F	417	Total	C	N	O	S	0	0	0
			3262	2107	541	595	19			
1	G	401	Total	C	N	O	S	0	0	0
			3137	2030	519	570	18			
1	H	400	Total	C	N	O	S	0	0	0
			3138	2028	517	575	18			

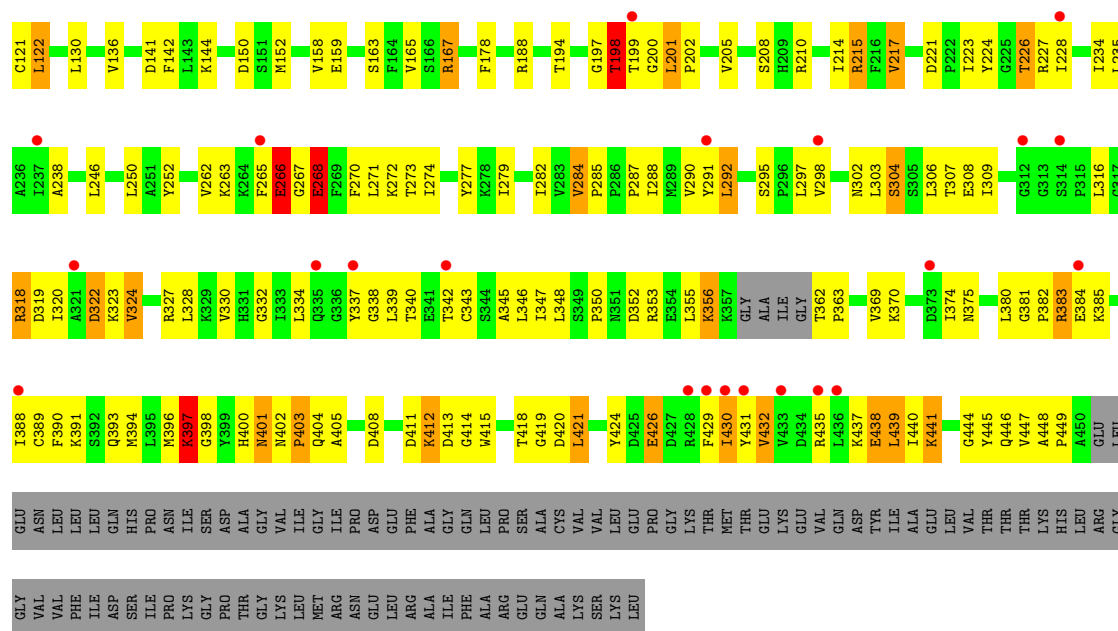


• Molecule 1: Red-bioluminescence eliciting luciferase

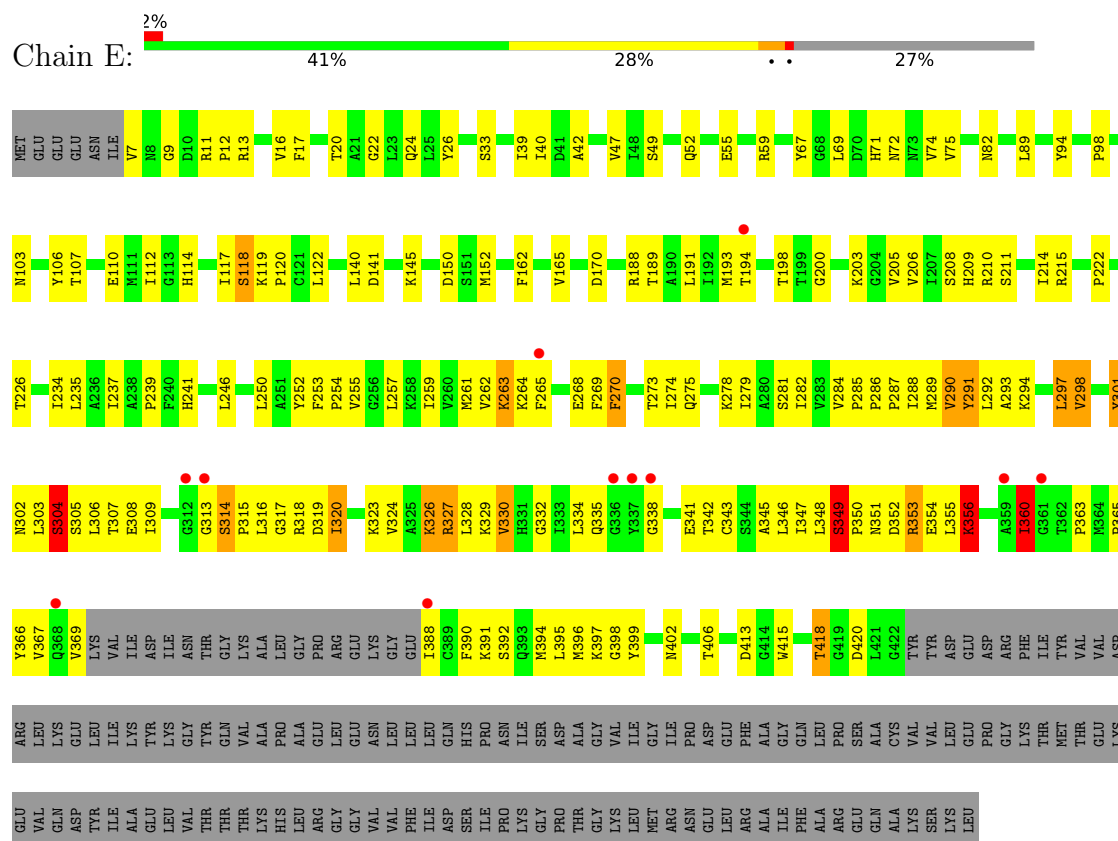


• Molecule 1: Red-bioluminescence eliciting luciferase



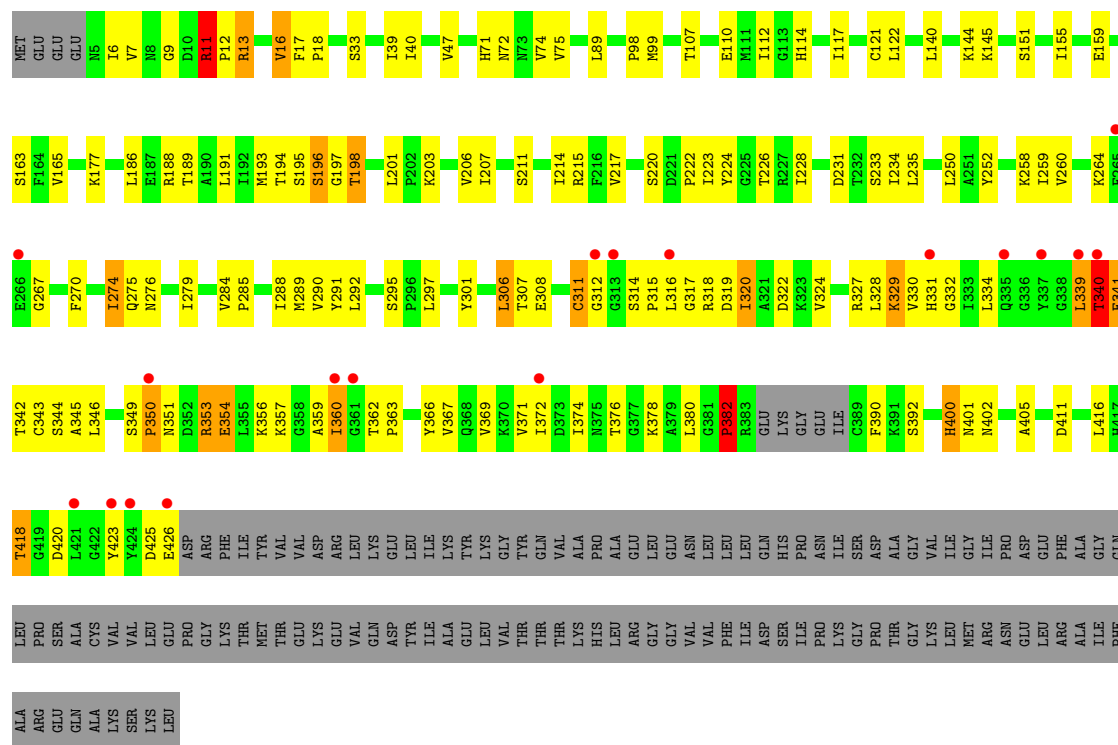


• Molecule 1: Red-bioluminescence eliciting luciferase

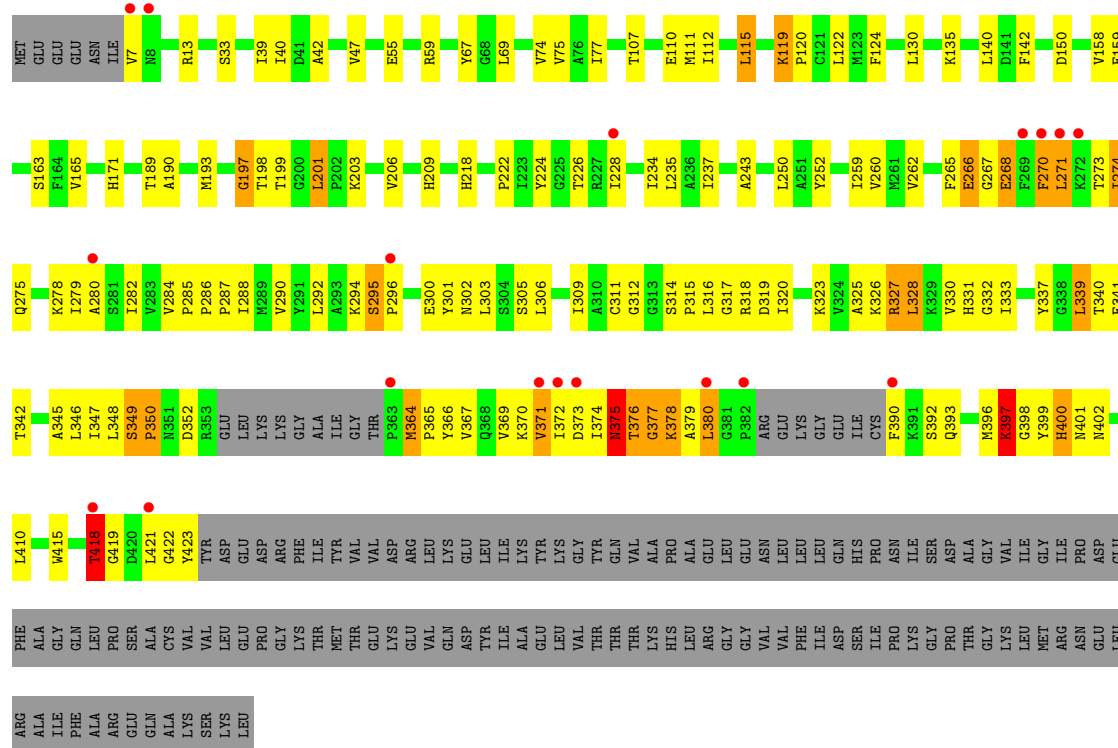


• Molecule 1: Red-bioluminescence eliciting luciferase





• Molecule 1: Red-bioluminescence eliciting luciferase



• Molecule 1: Red-bioluminescence eliciting luciferase



MET	GLU	GLU	GLU	ASN	ILE	V7	H8	G9	P12	R13	D14	L15	V16	F17	T20	A21	G22	L25	S33	Y34	I35	D37	I40	D41	A42	V47	I48	Q52	E55	R59	V74	F85	F86	L89	I90	Q95	G96	I97	N103	Y106	T107	E108	R109																															
E110	H111	I112	L115	K119	P120	K135	L140	D141	F142	L143	K145	V146	I147	V148	I149	D150	I155	V161	F162	V165	D170	H171	A172	F173	D184	P185	L186	E187	L191	I192	M193	S196	G197	T198	I199	G200	L201	P202	K203	G204	R210	S211	I212	T213	I214	R215																												
F216	V217	H218	P222	I228	T232	S233	I234	L235	A236	L246	F247	T248	A249	L250	A251	Y252	K258	I259	V260	H261	V262	F265	E266	G267	E268	F269	F270	L271	I274	I279	A280	S281	I282	V283	V284	P285	P286	P287	I288	N289	V290	A293	K294	S295	V298	L303	S304	S305																										
L306	I309	A310	C311	S314	F315	G317	R318	D319	I320	K323	V324	A325	K326	R327	L328	K329	V330	H331	G332	I333	L334	G335	G336	Y337	G338	L339	T340	E341	T406	R407	C343	S344	A345	L346	I347	G348	S349	P350	L355	K356	G357	G358	A359	I360	G361	T362	P363	K364	V367	G368	VAL	LYS	VAL	ASP	ARG																			
ASP	ILE	ASN	THR	GLY	LYS	ALA	LEU	GLY	PRO	ARG	GLN	VAL	GLU	LYS	ALA	PRO	GLY	GLU	ALA	ILE	F390	Q393	M394	L395	M396	K397	G398	Y399	H400	N401	N402	P403	Q404	A405	T406	R407	D408	A409	L410	D413	G414	W415	S349	P350	L355	K356	G357	G358	A359	I360	G361	T362	P363	K364	V367	G368	VAL	LYS	VAL	ASP	ARG													
LEU	LYS	GLU	LEU	THR	ILE	LYS	TYR	LEU	LYS	GLY	THR	THR	GLN	VAL	ALA	PRO	GLY	GLU	ALA	ILE	CYS	Q393	M394	L395	M396	K397	G398	Y399	H400	N401	N402	P403	Q404	A405	T406	R407	D408	A409	L410	D413	G414	W415	S349	P350	L355	K356	G357	G358	A359	I360	G361	T362	P363	K364	V367	G368	VAL	LYS	VAL	ASP	ARG													
VAL	GLN	ASP	TYR	ILE	ILE	ALA	GLU	LEU	VAL	THR	THR	THR	THR	LYS	HIS	LEU	ARG	GLY	GLY	VAL	VAL	PHE	ILE	ASP	SER	ILE	PRO	LYS	GLY	PRO	THR	GLY	VAL	LYS	LEU	MET	ARG	ILE	PRO	ASP	ASN	GLU	LEU	LEU	ARG	ALA	ALA	ILE	GLY	PHE	GLN	ALA	LEU	PRO	ARG	GLU	GLN	ALA	CYS	LYS	VAL	VAL	LEU	GLY	PRO	GLY	LYS	THR	MET	THR	GLU	LYS	ASP	GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	105.70Å 121.17Å 129.44Å 61.86° 68.35° 74.17°	Depositor
Resolution (Å)	48.76 – 3.05 48.76 – 3.05	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.76-3.05) 94.2 (48.76-3.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.240 , 0.285 0.260 , 0.290	Depositor DCC
R_{free} test set	955 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25451	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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	0.77	0/3026	1.13	16/4100 (0.4%)
1	B	0.73	0/3245	1.07	17/4398 (0.4%)
1	C	0.75	0/3275	1.10	7/4438 (0.2%)
1	D	0.81	1/3563 (0.0%)	1.13	17/4829 (0.4%)
1	E	0.69	0/3185	1.08	13/4318 (0.3%)
1	F	0.75	1/3340 (0.0%)	1.17	21/4528 (0.5%)
1	G	0.72	0/3213	1.08	13/4356 (0.3%)
1	H	0.76	0/3215	1.17	17/4359 (0.4%)
All	All	0.75	2/26062 (0.0%)	1.12	121/35326 (0.3%)

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	B	0	1
1	D	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	120	PRO	C-O	-5.83	1.17	1.23
1	F	196	SER	CA-C	5.83	1.55	1.52

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	341	GLU	N-CA-C	-15.38	78.05	110.80
1	H	349	SER	CA-C-N	12.75	132.73	119.85
1	H	349	SER	C-N-CA	12.75	132.73	119.85
1	H	398	GLY	N-CA-C	-12.23	98.88	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	305	SER	N-CA-C	-10.14	100.65	113.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	11	ARG	Sidechain
1	D	167	ARG	Sidechain
1	D	215	ARG	Sidechain
1	D	318	ARG	Sidechain

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	2955	0	2990	111	0
1	B	3170	0	3205	100	0
1	C	3199	0	3246	120	0
1	D	3480	0	3513	144	0
1	E	3110	0	3143	135	0
1	F	3262	0	3293	105	0
1	G	3137	0	3167	108	0
1	H	3138	0	3150	145	0
All	All	25451	0	25707	956	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 19.

The worst 5 of 956 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:A:201:LEU:HD22	1:A:202:PRO:CD	1.45	1.47
1:A:201:LEU:CD2	1:A:202:PRO:HD3	1.59	1.30
1:F:340:THR:OG1	1:F:344:SER:HA	1.29	1.29
1:G:370:LYS:HD2	1:G:415:TRP:CE3	1.72	1.24
1:D:319:ASP:O	1:D:323:LYS:HG3	1.43	1.17

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	371/546 (68%)	329 (89%)	29 (8%)	13 (4%)	3	13
1	B	401/546 (73%)	352 (88%)	28 (7%)	21 (5%)	1	8
1	C	405/546 (74%)	359 (89%)	27 (7%)	19 (5%)	2	9
1	D	438/546 (80%)	374 (85%)	44 (10%)	20 (5%)	2	9
1	E	394/546 (72%)	349 (89%)	31 (8%)	14 (4%)	2	12
1	F	413/546 (76%)	362 (88%)	36 (9%)	15 (4%)	2	12
1	G	395/546 (72%)	339 (86%)	35 (9%)	21 (5%)	1	7
1	H	396/546 (72%)	345 (87%)	36 (9%)	15 (4%)	2	12
All	All	3213/4368 (74%)	2809 (87%)	266 (8%)	138 (4%)	2	10

5 of 138 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	GLU
1	A	335	GLN
1	A	401	ASN
1	A	403	PRO
1	B	316	LEU

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	328/471 (70%)	312 (95%)	16 (5%)	22	50
1	B	352/471 (75%)	337 (96%)	15 (4%)	26	53
1	C	355/471 (75%)	339 (96%)	16 (4%)	24	52
1	D	384/471 (82%)	362 (94%)	22 (6%)	18	45
1	E	345/471 (73%)	327 (95%)	18 (5%)	21	48
1	F	361/471 (77%)	344 (95%)	17 (5%)	23	51
1	G	348/471 (74%)	328 (94%)	20 (6%)	18	45
1	H	347/471 (74%)	324 (93%)	23 (7%)	15	40
All	All	2820/3768 (75%)	2673 (95%)	147 (5%)	21	48

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	371	VAL
1	H	417	HIS
1	G	380	LEU
1	H	217	VAL
1	D	7	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	242	HIS
1	F	8	ASN
1	H	27	GLN
1	E	351	ASN
1	F	335	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 [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	377/546 (69%)	0.05	9 (2%) 59 37	49, 71, 150, 244	0
1	B	405/546 (74%)	0.25	23 (5%) 29 15	43, 86, 182, 250	0
1	C	409/546 (74%)	0.12	14 (3%) 48 27	50, 76, 169, 239	0
1	D	442/546 (80%)	0.14	22 (4%) 34 17	41, 68, 155, 256	0
1	E	398/546 (72%)	0.17	11 (2%) 55 32	58, 84, 179, 239	0
1	F	417/546 (76%)	0.08	18 (4%) 40 21	45, 72, 160, 221	0
1	G	401/546 (73%)	0.22	18 (4%) 38 20	30, 74, 163, 223	0
1	H	400/546 (73%)	0.13	14 (3%) 47 26	50, 74, 170, 260	0
All	All	3249/4368 (74%)	0.15	129 (3%) 42 23	30, 77, 170, 260	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	TYR	7.1
1	D	429	PHE	5.3
1	F	423	TYR	5.2
1	G	372	ILE	4.8
1	D	384	GLU	4.7

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.