Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:27 PM EDT

PDB ID	:	5HLZ
Title	:	Structure of Pro-Activin A Complex at 2.85 A resolution
Authors	:	Wang, X.; Fischer, G.; Hyvonen, M.
Deposited on	:	2016-01-15
Resolution	:	2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

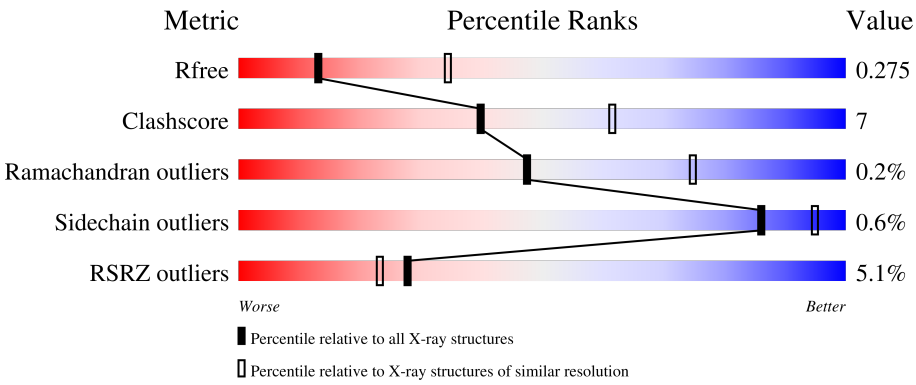
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	270	% 63% 12% 24%
1	C	270	% 61% 14% 24%
1	E	270	2% 63% 13% 24%
1	G	270	2% 62% 13% 24%
2	B	116	8% 53% 21% • 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	116	8% 59% 12% 29%
2	F	116	11% 54% 19% • 26%
2	H	116	9% 53% 17% • 28%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9163 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 Inhibin beta A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	204	1626	1020	295	304	7	0	0	0
1	C	204	1626	1020	295	304	7	0	0	0
1	E	204	1626	1020	295	304	7	0	0	0
1	G	204	1626	1020	295	304	7	0	0	0

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	expression tag	UNP P08476
A	21	SER	-	expression tag	UNP P08476
A	22	HIS	-	expression tag	UNP P08476
A	23	HIS	-	expression tag	UNP P08476
A	24	HIS	-	expression tag	UNP P08476
A	25	HIS	-	expression tag	UNP P08476
A	26	HIS	-	expression tag	UNP P08476
A	27	HIS	-	expression tag	UNP P08476
A	28	SER	-	expression tag	UNP P08476
A	29	MET	-	expression tag	UNP P08476
A	35	SER	CYS	engineered mutation	UNP P08476
A	38	SER	CYS	engineered mutation	UNP P08476
A	?	-	LYS	deletion	UNP P08476
A	?	-	LYS	deletion	UNP P08476
A	?	-	LYS	deletion	UNP P08476
A	?	-	LYS	deletion	UNP P08476
A	?	-	LYS	deletion	UNP P08476
A	?	-	GLU	deletion	UNP P08476
A	?	-	GLU	deletion	UNP P08476
A	?	-	GLU	deletion	UNP P08476
A	?	-	GLY	deletion	UNP P08476

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P08476
A	?	-	GLY	deletion	UNP P08476
A	?	-	LYS	deletion	UNP P08476
A	?	-	LYS	deletion	UNP P08476
A	?	-	LYS	deletion	UNP P08476
A	?	-	GLY	deletion	UNP P08476
A	?	-	GLY	deletion	UNP P08476
A	?	-	GLY	deletion	UNP P08476
A	?	-	GLU	deletion	UNP P08476
A	?	-	GLY	deletion	UNP P08476
A	?	-	GLY	deletion	UNP P08476
A	?	-	ALA	deletion	UNP P08476
A	?	-	GLY	deletion	UNP P08476
A	?	-	ALA	deletion	UNP P08476
A	?	-	ASP	deletion	UNP P08476
A	306	LEU	-	cloning artifact	UNP P08476
A	307	GLU	-	cloning artifact	UNP P08476
A	308	VAL	-	cloning artifact	UNP P08476
A	309	LEU	-	cloning artifact	UNP P08476
A	310	PHE	-	cloning artifact	UNP P08476
A	310A	GLN	-	cloning artifact	UNP P08476
A	310B	GLY	-	cloning artifact	UNP P08476
A	310C	PRO	-	cloning artifact	UNP P08476
C	20	MET	-	expression tag	UNP P08476
C	21	SER	-	expression tag	UNP P08476
C	22	HIS	-	expression tag	UNP P08476
C	23	HIS	-	expression tag	UNP P08476
C	24	HIS	-	expression tag	UNP P08476
C	25	HIS	-	expression tag	UNP P08476
C	26	HIS	-	expression tag	UNP P08476
C	27	HIS	-	expression tag	UNP P08476
C	28	SER	-	expression tag	UNP P08476
C	29	MET	-	expression tag	UNP P08476
C	35	SER	CYS	engineered mutation	UNP P08476
C	38	SER	CYS	engineered mutation	UNP P08476
C	?	-	LYS	deletion	UNP P08476
C	?	-	LYS	deletion	UNP P08476
C	?	-	LYS	deletion	UNP P08476
C	?	-	LYS	deletion	UNP P08476
C	?	-	LYS	deletion	UNP P08476
C	?	-	GLU	deletion	UNP P08476
C	?	-	GLU	deletion	UNP P08476

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP P08476
C	?	-	GLY	deletion	UNP P08476
C	?	-	GLU	deletion	UNP P08476
C	?	-	GLY	deletion	UNP P08476
C	?	-	LYS	deletion	UNP P08476
C	?	-	LYS	deletion	UNP P08476
C	?	-	LYS	deletion	UNP P08476
C	?	-	GLY	deletion	UNP P08476
C	?	-	GLY	deletion	UNP P08476
C	?	-	GLY	deletion	UNP P08476
C	?	-	GLU	deletion	UNP P08476
C	?	-	GLY	deletion	UNP P08476
C	?	-	GLY	deletion	UNP P08476
C	?	-	ALA	deletion	UNP P08476
C	?	-	GLY	deletion	UNP P08476
C	?	-	ALA	deletion	UNP P08476
C	?	-	ASP	deletion	UNP P08476
C	306	LEU	-	cloning artifact	UNP P08476
C	307	GLU	-	cloning artifact	UNP P08476
C	308	VAL	-	cloning artifact	UNP P08476
C	309	LEU	-	cloning artifact	UNP P08476
C	310	PHE	-	cloning artifact	UNP P08476
C	310A	GLN	-	cloning artifact	UNP P08476
C	310B	GLY	-	cloning artifact	UNP P08476
C	310C	PRO	-	cloning artifact	UNP P08476
E	20	MET	-	expression tag	UNP P08476
E	21	SER	-	expression tag	UNP P08476
E	22	HIS	-	expression tag	UNP P08476
E	23	HIS	-	expression tag	UNP P08476
E	24	HIS	-	expression tag	UNP P08476
E	25	HIS	-	expression tag	UNP P08476
E	26	HIS	-	expression tag	UNP P08476
E	27	HIS	-	expression tag	UNP P08476
E	28	SER	-	expression tag	UNP P08476
E	29	MET	-	expression tag	UNP P08476
E	35	SER	CYS	engineered mutation	UNP P08476
E	38	SER	CYS	engineered mutation	UNP P08476
E	?	-	LYS	deletion	UNP P08476
E	?	-	LYS	deletion	UNP P08476
E	?	-	LYS	deletion	UNP P08476
E	?	-	LYS	deletion	UNP P08476
E	?	-	LYS	deletion	UNP P08476

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLU	deletion	UNP P08476
E	?	-	GLU	deletion	UNP P08476
E	?	-	GLU	deletion	UNP P08476
E	?	-	GLY	deletion	UNP P08476
E	?	-	GLU	deletion	UNP P08476
E	?	-	GLY	deletion	UNP P08476
E	?	-	LYS	deletion	UNP P08476
E	?	-	LYS	deletion	UNP P08476
E	?	-	LYS	deletion	UNP P08476
E	?	-	GLY	deletion	UNP P08476
E	?	-	GLY	deletion	UNP P08476
E	?	-	GLY	deletion	UNP P08476
E	?	-	GLU	deletion	UNP P08476
E	?	-	GLY	deletion	UNP P08476
E	?	-	GLY	deletion	UNP P08476
E	?	-	ALA	deletion	UNP P08476
E	?	-	GLY	deletion	UNP P08476
E	?	-	ALA	deletion	UNP P08476
E	?	-	ASP	deletion	UNP P08476
E	306	LEU	-	cloning artifact	UNP P08476
E	307	GLU	-	cloning artifact	UNP P08476
E	308	VAL	-	cloning artifact	UNP P08476
E	309	LEU	-	cloning artifact	UNP P08476
E	310	PHE	-	cloning artifact	UNP P08476
E	310A	GLN	-	cloning artifact	UNP P08476
E	310B	GLY	-	cloning artifact	UNP P08476
E	310C	PRO	-	cloning artifact	UNP P08476
G	20	MET	-	expression tag	UNP P08476
G	21	SER	-	expression tag	UNP P08476
G	22	HIS	-	expression tag	UNP P08476
G	23	HIS	-	expression tag	UNP P08476
G	24	HIS	-	expression tag	UNP P08476
G	25	HIS	-	expression tag	UNP P08476
G	26	HIS	-	expression tag	UNP P08476
G	27	HIS	-	expression tag	UNP P08476
G	28	SER	-	expression tag	UNP P08476
G	29	MET	-	expression tag	UNP P08476
G	35	SER	CYS	engineered mutation	UNP P08476
G	38	SER	CYS	engineered mutation	UNP P08476
G	?	-	LYS	deletion	UNP P08476
G	?	-	LYS	deletion	UNP P08476
G	?	-	LYS	deletion	UNP P08476

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LYS	deletion	UNP P08476
G	?	-	LYS	deletion	UNP P08476
G	?	-	GLU	deletion	UNP P08476
G	?	-	GLU	deletion	UNP P08476
G	?	-	GLU	deletion	UNP P08476
G	?	-	GLY	deletion	UNP P08476
G	?	-	GLU	deletion	UNP P08476
G	?	-	GLY	deletion	UNP P08476
G	?	-	LYS	deletion	UNP P08476
G	?	-	LYS	deletion	UNP P08476
G	?	-	LYS	deletion	UNP P08476
G	?	-	GLY	deletion	UNP P08476
G	?	-	GLY	deletion	UNP P08476
G	?	-	GLY	deletion	UNP P08476
G	?	-	GLU	deletion	UNP P08476
G	?	-	GLY	deletion	UNP P08476
G	?	-	GLY	deletion	UNP P08476
G	?	-	ALA	deletion	UNP P08476
G	?	-	GLY	deletion	UNP P08476
G	?	-	ALA	deletion	UNP P08476
G	?	-	ASP	deletion	UNP P08476
G	306	LEU	-	cloning artifact	UNP P08476
G	307	GLU	-	cloning artifact	UNP P08476
G	308	VAL	-	cloning artifact	UNP P08476
G	309	LEU	-	cloning artifact	UNP P08476
G	310	PHE	-	cloning artifact	UNP P08476
G	310A	GLN	-	cloning artifact	UNP P08476
G	310B	GLY	-	cloning artifact	UNP P08476
G	310C	PRO	-	cloning artifact	UNP P08476

- Molecule 2 is a protein called Inhibin beta A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	86	674	425	109	128	12	0	0	0
			Total	C	N	O	S			
2	D	82	644	405	104	123	12	0	0	0
			Total	C	N	O	S			
2	F	86	674	425	109	128	12	0	0	0
			Total	C	N	O	S			
2	H	84	657	413	106	126	12	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	2	2	2	0	0
			Total	O		
3	C	2	2	2	0	0
			Total	O		
3	E	2	2	2	0	0
			Total	O		
3	G	4	4	4	0	0

3 Residue-property plots (i)

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: Inhibin beta A chain

Chain A: %
63% 12% 24%

MET SER HIS HIS HIS HIS HIS SER MET SER ALA ALA PRO ASP SER PRO SER SER ALA LEU ALA ALA LEU PRO LYS ASP VAL PRO ASN SER Q51 P52 M65 R71 P72 R88 K89 G99 Y100 V101 E118 S121 E122 I123 I124 S141 L147 A153 K160

V161 P162 K163 R174 Q177 K180 HIS PRO GLN GLY SER LEU ASP THR GLY GLU GLU ALA GLU GLU VAL GLY LEU LYS GLY GLU ARG S202 E203 E208 V211 H219 S224 R229 R241 I242 L256 L257 G258 E283 E286 Q287 S288 Q299 SER GLU ASP HIS

PRO HIS LEU GLU VAL LEU PHE GLN GLY PRO

• Molecule 1: Inhibin beta A chain

Chain C: %
61% 14% 24%

MET SER HIS HIS HIS HIS HIS SER MET SER ALA ALA PRO ASP SER PRO SER SER ALA LEU ALA ALA LEU PRO LYS ASP VAL PRO ASN SER Q51 P52 K59 R71 P72 A81 R88 K89 G93 K94 V95 G96 Y100 E104 S121 I124 T131 S141

L147 A153 E154 K160 A164 R168 T169 K170 R174 K180 HIS PRO GLN GLY SER LEU ASP THR GLY GLU GLU GLU VAL GLY LEU LYS GLY GLU ARG S202 E203 E208 V211 H219 V220 F221 P222 V223 S224 R229 Q233 R241 I242 L256

E283 E286 Q287 L293 A297 R298 Q299 SER GLU ASP HIS PRO HIS LEU GLU VAL LEU PHE GLN GLY PRO

• Molecule 1: Inhibin beta A chain

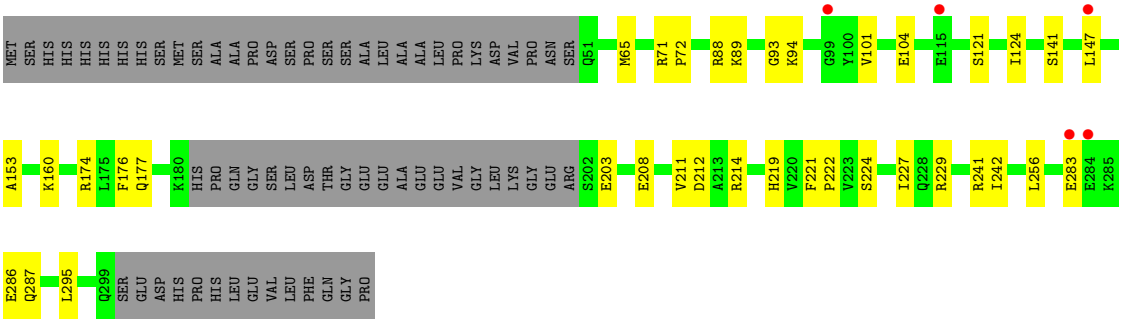
Chain E: 2%
63% 13% 24%

MET SER HIS HIS HIS HIS HIS SER MET SER ALA ALA PRO ASP SER PRO SER SER ALA LEU ALA ALA LEU PRO LYS ASP VAL PRO ASN SER Q51 P52 M65 R71 P72 R88 K89 G93 G96 G99 Y100 V101 E104 R109 I124 S141 K142 A153

K160 N165 R166 T167 R174 Q177 K180 HIS PRO GLN GLY SER LEU ASP THR GLY GLU GLU GLU ALA GLU GLU VAL GLY LEU LYS GLY GLU ARG S202 E203 E208 V211 H219 V220 F221 P222 V223 S224 I227 Q228 R229 R241 I242 L256 E283 E284 K285 E286

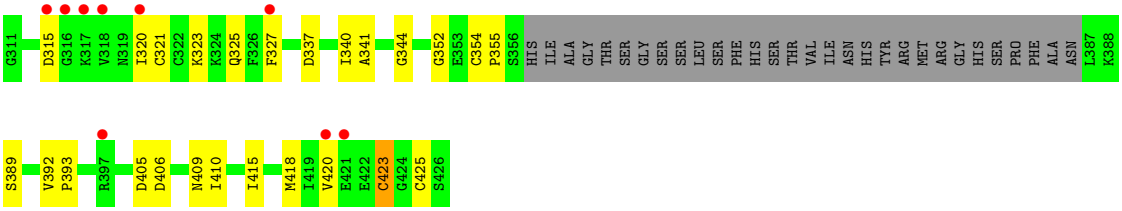
• Molecule 1: Inhibin beta A chain

Chain G:



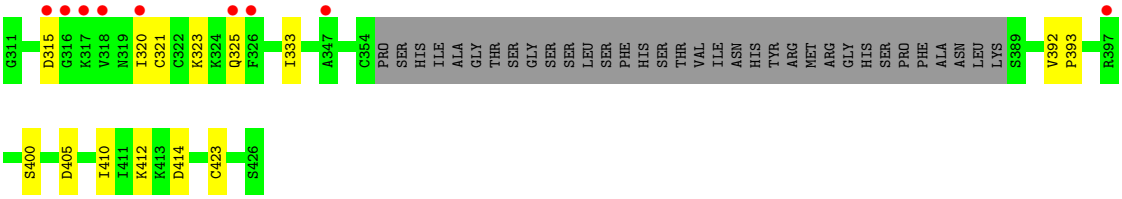
• Molecule 2: Inhibin beta A chain

Chain B:



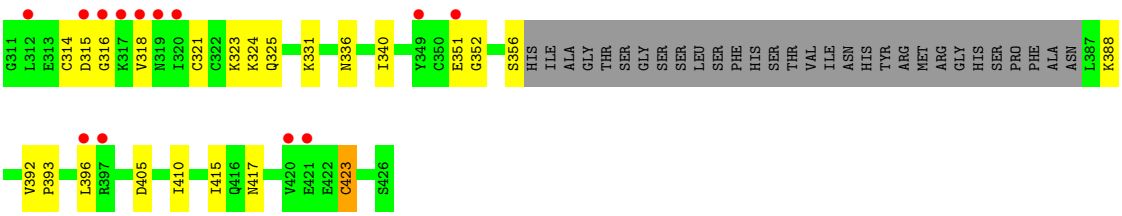
• Molecule 2: Inhibin beta A chain

Chain D:



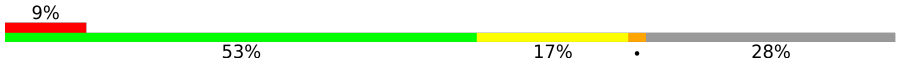
• Molecule 2: Inhibin beta A chain

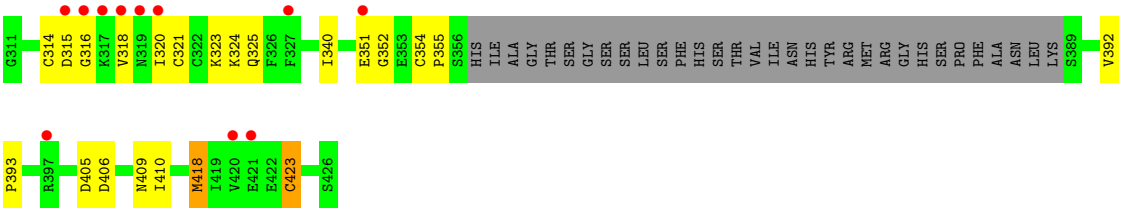
Chain F:



• Molecule 2: Inhibin beta A chain

Chain H:


9%
53%
17%
28%


G311 C314 D315 G316 K317 V318 N319 I320 C321 C322 K323 K324 Q325 F326 F327 I340 E351 G352 E353 C354 P355 S356 HIS ILE ALA GLY THR SER GLY SER SER LEU SER PHE HIS SER THR VAL ILE ASN HIS TYR ARG MET ARG GLY HIS SER PRO PHE ALA ASN LEU LYS S389 V392
P393 R397 D405 D406 N409 I410 M418 I419 V420 E421 E422 C423 S426

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	47.23Å 47.23Å 445.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.90 – 2.85 40.90 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.90-2.85) 92.7 (40.90-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.10pre_2084: ???)	Depositor
R, R_{free}	0.220 , 0.274 0.220 , 0.275	Depositor DCC
R_{free} test set	1338 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	62.1	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l 0.469 for h,-h-k,-l 0.469 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9163	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.26	0/1648	0.43	0/2214
1	C	0.26	0/1648	0.43	0/2214
1	E	0.27	0/1648	0.43	0/2214
1	G	0.27	0/1648	0.45	0/2214
2	B	0.28	0/688	0.44	0/923
2	D	0.27	0/657	0.47	0/881
2	F	0.26	0/688	0.42	0/923
2	H	0.27	0/671	0.45	0/901
All	All	0.27	0/9296	0.44	0/12484

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 (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	1626	0	1676	23	0
1	C	1626	0	1676	26	0
1	E	1626	0	1676	22	0
1	G	1626	0	1676	23	0
2	B	674	0	640	19	0
2	D	644	0	604	12	0
2	F	674	0	640	16	0
2	H	657	0	616	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	C	2	0	0	1	0
3	E	2	0	0	0	0
3	G	4	0	0	1	0
All	All	9163	0	9204	133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (133) 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:H:393:PRO:HA	2:H:423:CYS:HB3	1.57	0.86
2:F:393:PRO:HA	2:F:423:CYS:HB3	1.58	0.83
2:D:393:PRO:HA	2:D:423:CYS:HB3	1.59	0.82
2:F:405:ASP:OD2	1:G:141:SER:OG	2.00	0.80
2:B:392:VAL:HG21	2:D:392:VAL:HG21	1.63	0.79
1:A:283:GLU:HB2	1:A:286:GLU:HB3	1.67	0.77
2:B:323:LYS:NZ	2:B:325:GLN:OE1	2.20	0.74
2:H:405:ASP:OD2	1:E:141:SER:OG	2.06	0.74
2:B:405:ASP:OD2	1:C:141:SER:OG	2.02	0.74
2:H:321:CYS:HA	2:H:352:GLY:HA3	1.73	0.71
2:F:392:VAL:HG21	2:H:392:VAL:HG21	1.73	0.71
2:H:340:ILE:HG22	1:G:101:VAL:HG11	1.72	0.70
1:E:203:GLU:OE2	1:E:241:ARG:NH1	2.25	0.69
1:A:177:GLN:OE1	1:A:229:ARG:NH1	2.24	0.69
1:A:101:VAL:HG11	2:B:340:ILE:HG22	1.75	0.69
1:A:141:SER:OG	2:D:405:ASP:OD2	2.09	0.69
2:D:323:LYS:NZ	2:D:325:GLN:OE1	2.25	0.67
1:C:203:GLU:OE2	1:C:241:ARG:NH1	2.29	0.66
1:A:174:ARG:NH2	1:A:208:GLU:OE2	2.30	0.65
1:A:203:GLU:OE2	1:A:241:ARG:NH1	2.30	0.64
1:C:283:GLU:HB2	1:C:286:GLU:HB3	1.80	0.63
1:G:71:ARG:NH1	1:G:72:PRO:O	2.31	0.63
1:A:177:GLN:HE22	1:A:229:ARG:HH22	1.47	0.62
1:G:283:GLU:HB2	1:G:286:GLU:HB3	1.81	0.62
1:A:71:ARG:NH1	1:A:72:PRO:O	2.32	0.61
1:A:160:LYS:HD3	1:A:286:GLU:OE2	2.00	0.61
1:C:168:ARG:NH1	1:C:170:LYS:O	2.33	0.61
1:E:283:GLU:HB2	1:E:286:GLU:HB3	1.82	0.61
1:C:287:GLN:NE2	3:C:401:HOH:O	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:340:ILE:HG22	1:E:101:VAL:HG11	1.84	0.60
1:E:71:ARG:NH1	1:E:72:PRO:O	2.33	0.60
2:H:323:LYS:NZ	2:H:325:GLN:OE1	2.33	0.59
1:C:88:ARG:HH21	1:C:89:LYS:HD3	1.67	0.59
1:A:121:SER:HB2	1:A:147:LEU:HD11	1.86	0.58
1:G:121:SER:HB2	1:G:147:LEU:HD21	1.85	0.57
1:G:203:GLU:OE2	1:G:241:ARG:NH1	2.38	0.56
1:C:153:ALA:HB3	1:C:224:SER:HA	1.87	0.56
1:E:153:ALA:HB3	1:E:224:SER:HA	1.87	0.56
1:G:93:GLY:HA2	1:G:104:GLU:H	1.71	0.56
1:G:88:ARG:HH21	1:G:89:LYS:HD3	1.69	0.56
2:F:324:LYS:HZ2	2:F:351:GLU:HB3	1.71	0.56
2:F:324:LYS:NZ	2:F:351:GLU:HB3	2.21	0.56
1:C:131:THR:O	1:E:142:LYS:NZ	2.34	0.56
1:E:51:GLN:HB2	1:E:52:PRO:HD3	1.87	0.55
2:H:324:LYS:NZ	2:H:351:GLU:HB3	2.21	0.55
2:B:410:ILE:HB	1:C:124:ILE:HB	1.89	0.55
1:C:174:ARG:NH2	1:C:208:GLU:OE2	2.40	0.55
1:G:174:ARG:NH2	1:G:208:GLU:OE2	2.40	0.55
1:A:124:ILE:HB	2:D:410:ILE:HB	1.87	0.55
1:E:174:ARG:NH2	1:E:208:GLU:OE2	2.41	0.54
1:A:88:ARG:HH21	1:A:89:LYS:HD3	1.73	0.54
2:D:400:SER:OG	2:D:414:ASP:OD1	2.26	0.53
1:E:177:GLN:OE1	1:E:229:ARG:NH2	2.40	0.53
1:G:153:ALA:HB3	1:G:224:SER:HA	1.91	0.53
1:E:88:ARG:HH21	1:E:89:LYS:HD3	1.74	0.52
2:H:314:CYS:HA	2:H:318:VAL:HG11	1.92	0.52
2:B:392:VAL:HG11	2:D:392:VAL:HG11	1.90	0.52
2:H:410:ILE:HB	1:E:124:ILE:HB	1.92	0.52
1:G:177:GLN:OE1	1:G:229:ARG:NH2	2.43	0.51
2:F:314:CYS:HA	2:F:318:VAL:HG11	1.93	0.51
1:C:147:LEU:HD13	1:C:297:ALA:HB3	1.93	0.51
1:C:121:SER:HB2	1:C:147:LEU:HD11	1.92	0.51
2:F:410:ILE:HB	1:G:124:ILE:HB	1.93	0.51
1:C:71:ARG:NH1	1:C:72:PRO:O	2.43	0.51
1:C:229:ARG:NH2	1:C:233:GLN:OE1	2.44	0.51
1:E:93:GLY:HA2	1:E:104:GLU:H	1.75	0.50
1:G:287:GLN:NE2	3:G:401:HOH:O	2.44	0.50
2:F:323:LYS:HZ3	2:F:325:GLN:CD	2.13	0.50
1:G:212:ASP:OD1	1:G:214:ARG:HG3	2.12	0.50
1:C:51:GLN:HB2	1:C:52:PRO:HD3	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:THR:C	1:E:142:LYS:HZ1	2.15	0.49
1:A:211:VAL:HB	1:A:219:HIS:CE1	2.46	0.49
1:G:160:LYS:HD3	1:G:286:GLU:OE2	2.12	0.48
1:A:177:GLN:HE22	1:A:229:ARG:NH2	2.10	0.48
1:G:176:PHE:HB3	1:G:203:GLU:HG2	1.94	0.48
1:A:118:GLU:HA	2:D:414:ASP:HB2	1.95	0.48
2:H:324:LYS:HZ2	2:H:351:GLU:HB3	1.79	0.48
1:C:242:ILE:HD12	1:C:256:LEU:HD22	1.96	0.48
2:F:315:ASP:N	2:F:315:ASP:OD1	2.46	0.47
2:F:356:SER:HA	2:F:388:LYS:HG3	1.96	0.47
2:B:406:ASP:HB3	2:B:409:ASN:HD22	1.80	0.47
1:G:94:LYS:HG2	1:G:104:GLU:HB2	1.96	0.47
1:A:51:GLN:HB2	1:A:52:PRO:HD3	1.96	0.47
1:A:101:VAL:HG13	2:B:341:ALA:HB2	1.97	0.46
2:F:324:LYS:HZ3	2:F:351:GLU:HG2	1.79	0.46
1:C:160:LYS:HD3	1:C:286:GLU:OE2	2.15	0.46
1:G:227:ILE:HG21	1:G:295:LEU:HD13	1.96	0.46
2:H:315:ASP:N	2:H:315:ASP:OD1	2.48	0.46
1:C:93:GLY:HA2	1:C:104:GLU:H	1.80	0.46
2:F:321:CYS:HA	2:F:352:GLY:HA3	1.97	0.46
1:A:122:GLU:HB2	2:D:412:LYS:HB3	1.98	0.45
1:A:153:ALA:HB3	1:A:224:SER:HA	1.98	0.45
2:B:415:ILE:HB	2:B:418:MET:HG3	1.98	0.44
1:E:160:LYS:HD3	1:E:286:GLU:OE2	2.17	0.44
2:B:321:CYS:HA	2:B:352:GLY:HA3	1.98	0.44
2:B:315:ASP:N	2:B:315:ASP:OD1	2.49	0.44
1:C:94:LYS:HG2	1:C:104:GLU:HB2	2.00	0.43
1:E:211:VAL:HB	1:E:219:HIS:CE1	2.52	0.43
1:G:211:VAL:HB	1:G:219:HIS:CE1	2.53	0.43
2:B:327:PHE:CZ	2:B:344:GLY:HA3	2.54	0.43
2:H:354:CYS:HA	2:H:355:PRO:HD3	1.91	0.43
1:C:211:VAL:HB	1:C:219:HIS:CE1	2.54	0.43
1:E:242:ILE:HD12	1:E:256:LEU:HD22	2.00	0.43
1:A:162:PRO:HB2	1:A:163:LYS:HD2	2.00	0.43
2:F:415:ILE:HG21	1:E:65:MET:HB3	2.01	0.43
2:D:315:ASP:N	2:D:315:ASP:OD1	2.51	0.43
2:H:320:ILE:HG13	2:H:321:CYS:N	2.34	0.43
1:A:288:SER:HB2	1:C:81:ALA:HB1	2.01	0.43
2:B:393:PRO:HA	2:B:423:CYS:HB3	2.01	0.43
2:B:393:PRO:HB3	2:B:420:VAL:HG13	2.01	0.43
1:A:242:ILE:HD12	1:A:256:LEU:HD22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:396:LEU:HB3	2:F:417:ASN:HA	2.01	0.42
2:H:406:ASP:HB3	2:H:409:ASN:HD22	1.85	0.42
1:E:283:GLU:O	1:E:287:GLN:N	2.53	0.42
2:D:320:ILE:HG13	2:D:321:CYS:N	2.34	0.42
1:E:165:ASN:OD1	1:E:167:THR:HG22	2.19	0.42
2:D:333:ILE:HG23	1:C:59:LYS:HE2	2.02	0.42
2:H:418:MET:HE3	1:G:65:MET:HG3	2.01	0.42
1:E:227:ILE:HG21	1:E:295:LEU:HD13	2.01	0.42
1:G:283:GLU:O	1:G:287:GLN:N	2.53	0.42
2:F:331:LYS:HG2	2:F:336:ASN:ND2	2.36	0.41
2:H:324:LYS:HZ3	2:H:351:GLU:HG2	1.86	0.41
1:C:154:GLU:O	1:C:293:LEU:HD12	2.21	0.41
2:B:320:ILE:HG13	2:B:321:CYS:N	2.36	0.41
1:C:283:GLU:O	1:C:287:GLN:N	2.54	0.41
2:B:337:ASP:OD1	2:B:337:ASP:N	2.51	0.41
2:B:389:SER:OG	2:B:425:CYS:HB3	2.20	0.41
1:E:221:PHE:HA	1:E:222:PRO:HD3	1.74	0.41
1:G:242:ILE:HD12	1:G:256:LEU:HD22	2.03	0.41
2:B:354:CYS:HA	2:B:355:PRO:HD3	1.93	0.40
1:C:221:PHE:HA	1:C:222:PRO:HD3	1.80	0.40
1:G:221:PHE:HA	1:G:222:PRO:HD3	1.76	0.40
1:A:65:MET:HB3	2:B:415:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/270 (74%)	194 (97%)	6 (3%)	0	100	100
1	C	200/270 (74%)	196 (98%)	4 (2%)	0	100	100
1	E	200/270 (74%)	194 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	200/270 (74%)	194 (97%)	6 (3%)	0	100	100
2	B	82/116 (71%)	79 (96%)	3 (4%)	0	100	100
2	D	78/116 (67%)	76 (97%)	2 (3%)	0	100	100
2	F	82/116 (71%)	80 (98%)	1 (1%)	1 (1%)	13	35
2	H	80/116 (69%)	76 (95%)	3 (4%)	1 (1%)	12	33
All	All	1122/1544 (73%)	1089 (97%)	31 (3%)	2 (0%)	47	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	316	GLY
2	H	316	GLY

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	182/237 (77%)	181 (100%)	1 (0%)	88	96
1	C	182/237 (77%)	181 (100%)	1 (0%)	88	96
1	E	182/237 (77%)	182 (100%)	0	100	100
1	G	182/237 (77%)	182 (100%)	0	100	100
2	B	77/102 (76%)	76 (99%)	1 (1%)	69	88
2	D	73/102 (72%)	73 (100%)	0	100	100
2	F	77/102 (76%)	76 (99%)	1 (1%)	69	88
2	H	75/102 (74%)	73 (97%)	2 (3%)	44	74
All	All	1030/1356 (76%)	1024 (99%)	6 (1%)	86	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	423	CYS
2	F	423	CYS
2	H	418	MET
2	H	423	CYS
1	C	229	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	204/270 (75%)	0.04	3 (1%)	73	72	35, 62, 95, 130	0
1	C	204/270 (75%)	0.05	4 (1%)	65	62	37, 62, 94, 126	0
1	E	204/270 (75%)	0.07	5 (2%)	57	54	38, 62, 99, 119	0
1	G	204/270 (75%)	-0.01	5 (2%)	57	54	36, 61, 97, 127	0
2	B	86/116 (74%)	0.45	9 (10%)	6	4	48, 80, 120, 133	0
2	D	82/116 (70%)	0.58	9 (10%)	5	4	47, 78, 120, 132	0
2	F	86/116 (74%)	0.59	13 (15%)	2	1	46, 82, 124, 137	0
2	H	84/116 (72%)	0.54	11 (13%)	3	2	46, 82, 124, 133	0
All	All	1154/1544 (74%)	0.18	59 (5%)	28	23	35, 65, 113, 137	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	318	VAL	7.9
1	G	99	GLY	7.1
1	E	99	GLY	6.2
2	B	316	GLY	6.0
2	H	316	GLY	6.0
2	H	318	VAL	5.9
1	A	99	GLY	5.7
2	D	397	ARG	5.5
2	D	316	GLY	5.5
2	B	318	VAL	5.1
2	F	317	LYS	5.1
2	B	315	ASP	4.9
2	B	317	LYS	4.8
2	H	315	ASP	4.5
2	H	319	ASN	4.4
2	F	316	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	320	ILE	4.0
1	C	164	ALA	3.9
2	B	397	ARG	3.8
2	F	320	ILE	3.8
2	D	315	ASP	3.8
2	F	315	ASP	3.7
2	D	318	VAL	3.7
2	H	320	ILE	3.6
1	G	283	GLU	3.5
2	F	420	VAL	3.4
2	H	317	LYS	3.3
2	D	317	LYS	3.3
2	B	421	GLU	3.2
2	F	397	ARG	3.2
2	B	327	PHE	3.2
2	F	312	LEU	3.1
2	B	320	ILE	3.0
2	F	351	GLU	2.9
1	E	96	GLY	2.9
2	H	397	ARG	2.8
1	C	283	GLU	2.8
1	E	284	GLU	2.6
2	F	319	ASN	2.6
1	C	100	TYR	2.6
2	H	421	GLU	2.5
2	D	347	ALA	2.5
1	G	115	GLU	2.4
2	H	351	GLU	2.4
2	H	420	VAL	2.4
2	D	325	GLN	2.3
2	D	326	PHE	2.3
1	A	283	GLU	2.3
1	E	283	GLU	2.2
2	F	421	GLU	2.2
2	B	420	VAL	2.2
1	G	284	GLU	2.1
2	F	349	TYR	2.1
1	E	109	ARG	2.1
2	H	327	PHE	2.1
1	A	177	GLN	2.1
1	G	147	LEU	2.0
1	C	96	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	396	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.