



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 03:02 AM GMT

PDB ID : 3NHQ  
Title : The dark Pfr structure of the photosensory core module of *P. aeruginosa* Bacteriophytochrome  
Authors : Yang, X.; Ren, Z.; Kuk, J.; Moffat, K.  
Deposited on : 2010-06-14  
Resolution : 2.55 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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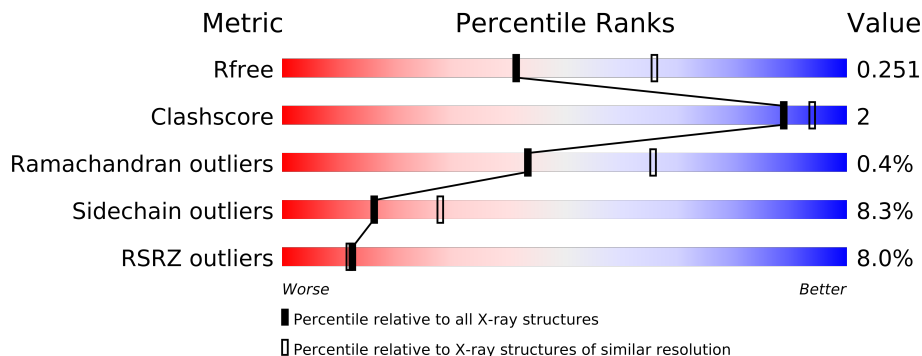
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.55 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))
$R_{free}$	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	505	
1	B	505	
1	C	505	
1	D	505	
1	E	505	
1	F	505	
1	G	505	
1	H	505	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30788 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3790	2386	682	703	19			
1	B	470	Total	C	N	O	S	0	0	0
			3709	2332	665	693	19			
1	C	482	Total	C	N	O	S	0	0	0
			3812	2398	688	707	19			
1	D	480	Total	C	N	O	S	0	0	0
			3801	2391	686	705	19			
1	E	479	Total	C	N	O	S	0	0	0
			3790	2386	683	702	19			
1	F	471	Total	C	N	O	S	0	0	0
			3717	2338	666	694	19			
1	G	482	Total	C	N	O	S	0	1	0
			3816	2401	688	708	19			
1	H	481	Total	C	N	O	S	0	0	0
			3808	2396	687	706	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
A	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
A	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
A	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
B	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
B	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3

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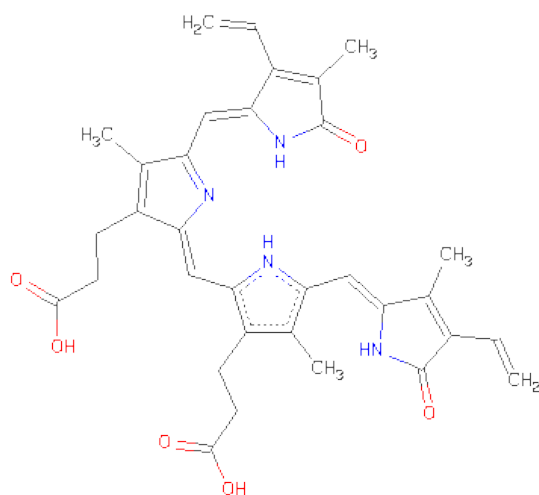
Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
B	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
C	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
C	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
C	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
D	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
D	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
D	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
E	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
E	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
E	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
F	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
F	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
F	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
G	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
G	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
G	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	498	LEU	-	EXPRESSION TAG	UNP Q9HWR3
H	499	GLU	-	EXPRESSION TAG	UNP Q9HWR3
H	500	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	501	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	502	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	503	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	504	HIS	-	EXPRESSION TAG	UNP Q9HWR3
H	505	HIS	-	EXPRESSION TAG	UNP Q9HWR3

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula:  $C_{33}H_{34}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		
2	C	1	Total	C	N	O	0	0
			43	33	4	6		
2	D	1	Total	C	N	O	0	0
			43	33	4	6		
2	E	1	Total	C	N	O	0	0
			43	33	4	6		
2	F	1	Total	C	N	O	0	0
			43	33	4	6		
2	G	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 3 is water.

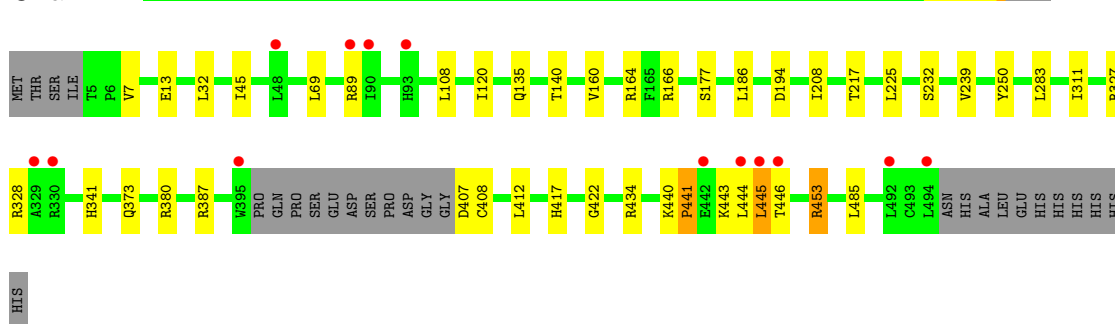
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	16	Total	O	0	0
			16	16		
3	C	44	Total	O	0	0
			44	44		
3	D	14	Total	O	0	0
			14	14		
3	E	15	Total	O	0	0
			15	15		
3	F	7	Total	O	0	0
			7	7		
3	G	37	Total	O	0	0
			37	37		
3	H	7	Total	O	0	0
			7	7		

### 3 Residue-property plots

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.

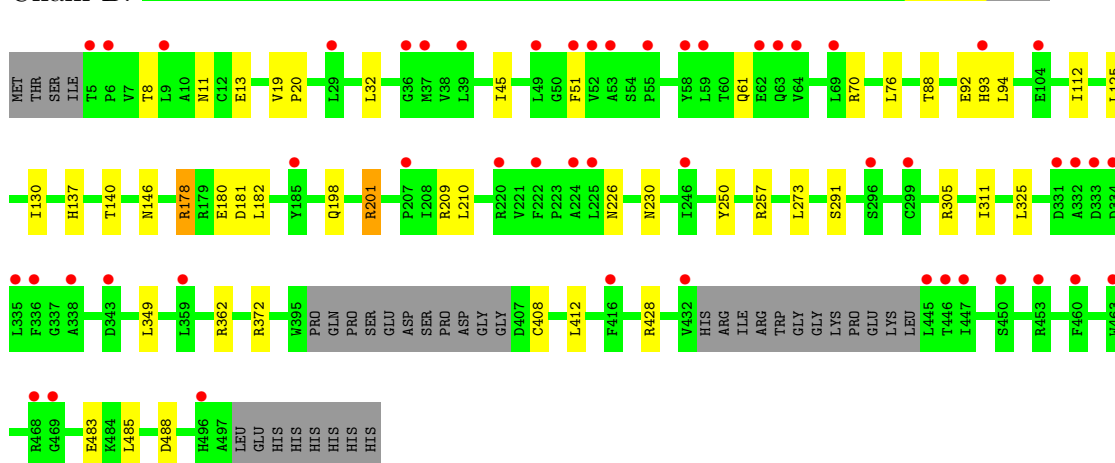
- Molecule 1: Bacteriophytochrome

Chain A:



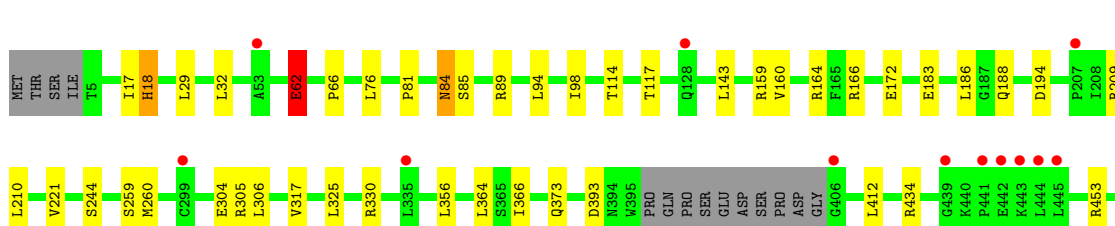
- Molecule 1: Bacteriophytochrome

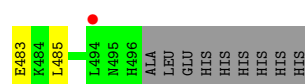
Chain B:



- Molecule 1: Bacteriophytochrome

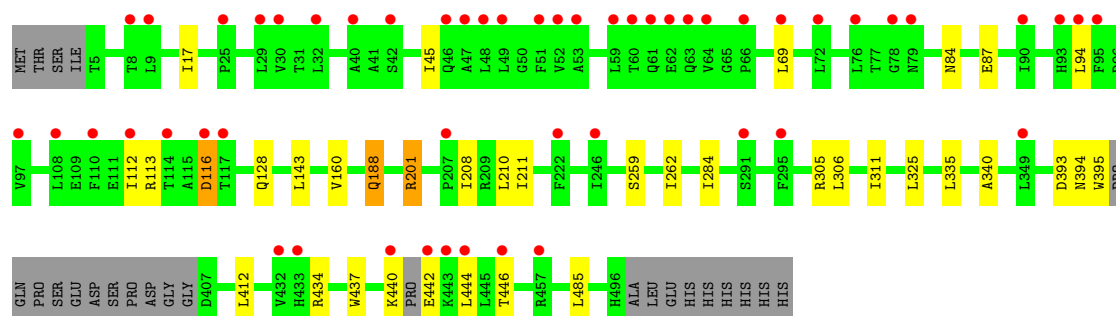
Chain C:





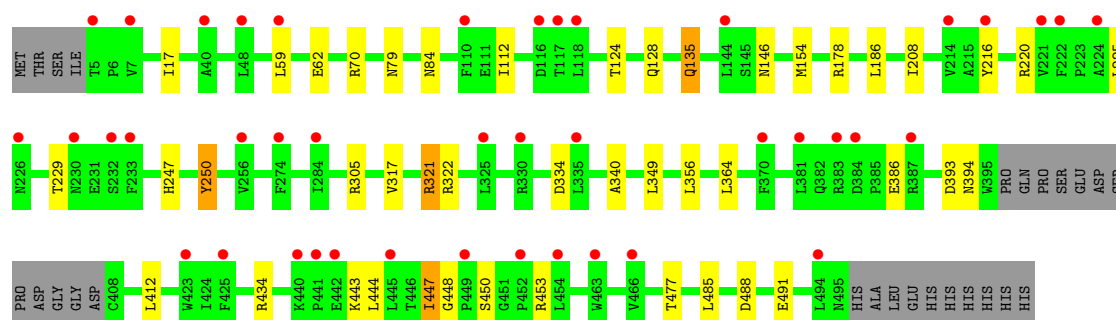
• Molecule 1: Bacteriophytochrome

Chain D:



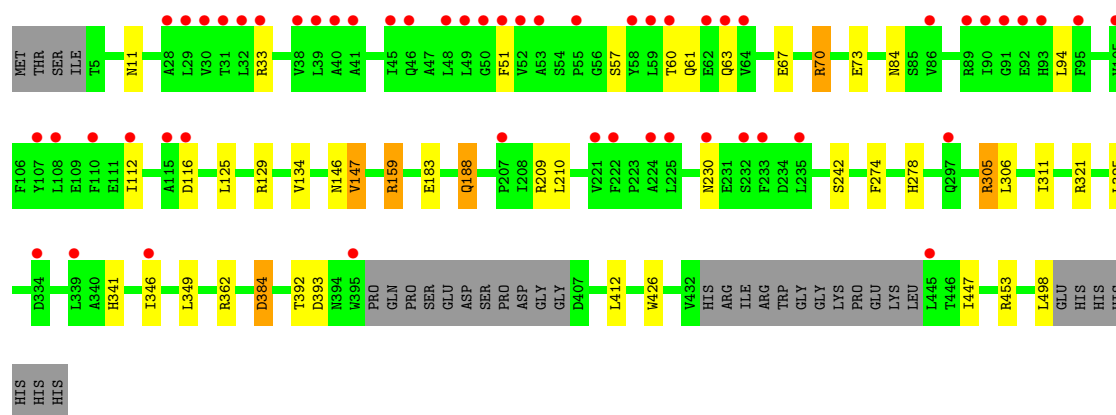
• Molecule 1: Bacteriophytochrome

Chain E:



• Molecule 1: Bacteriophytochrome

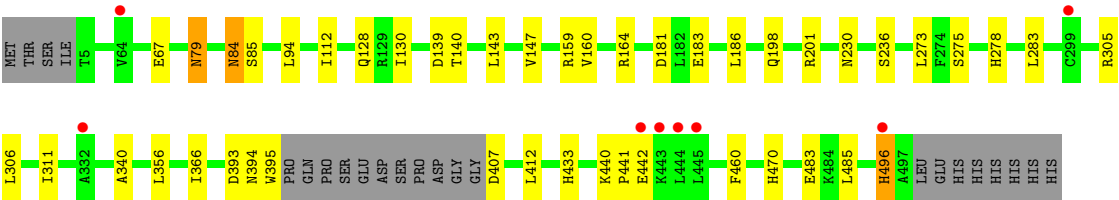
Chain F:



• Molecule 1: Bacteriophytochrome

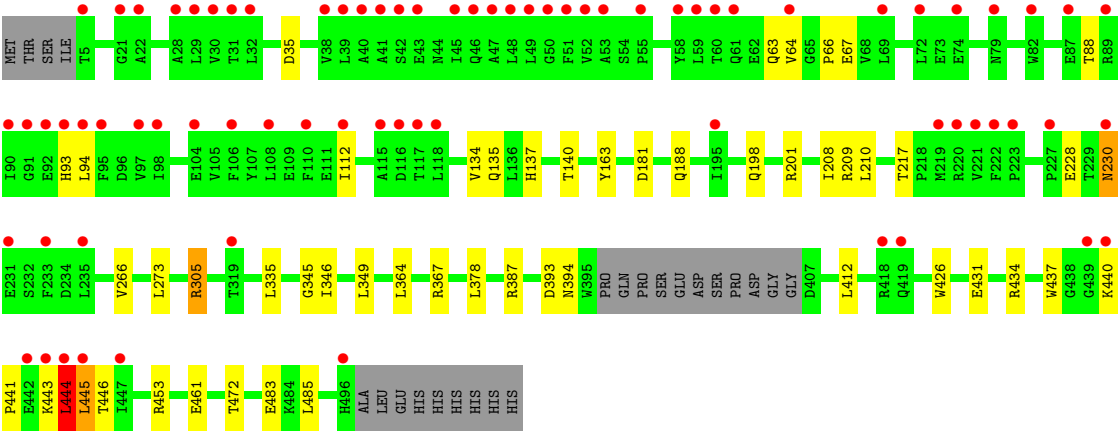
Chain G:





• Molecule 1: Bacteriophytochrome

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.38Å 162.98Å 436.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 2.55 49.49 – 2.53	Depositor EDS
% Data completeness (in resolution range)	82.9 (48.48-2.55) 81.3 (49.49-2.53)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.215 , 0.258 0.209 , 0.251	Depositor DCC
$R_{free}$ test set	7427 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 148657 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	30788	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BLA

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	0/3874	0.48	0/5258
1	B	0.24	0/3789	0.45	0/5144
1	C	0.25	0/3897	0.46	0/5289
1	D	0.24	0/3884	0.45	0/5269
1	E	0.23	0/3874	0.45	0/5258
1	F	0.23	0/3797	0.45	0/5155
1	G	0.25	0/3904	0.47	0/5299
1	H	0.24	0/3893	0.44	0/5284
All	All	0.24	0/30912	0.46	0/41956

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	2
1	B	0	1
1	C	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	ASP	Peptide
1	A	441	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	92	GLU	Peptide
1	C	62	GLU	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3790	0	0	7	0
1	B	3709	0	0	10	0
1	C	3812	0	0	10	0
1	D	3801	0	0	11	0
1	E	3790	0	0	7	0
1	F	3717	0	0	10	0
1	G	3816	0	0	11	0
1	H	3808	0	0	10	0
2	A	43	0	0	0	0
2	B	43	0	0	1	0
2	C	43	0	0	2	0
2	D	43	0	0	1	0
2	E	43	0	0	2	0
2	F	43	0	0	2	0
2	G	43	0	0	1	0
2	H	43	0	0	1	0
3	A	61	0	0	0	0
3	B	16	0	0	0	0
3	C	44	0	0	2	0
3	D	14	0	0	1	0
3	E	15	0	0	0	0
3	F	7	0	0	0	0
3	G	37	0	0	0	0
3	H	7	0	0	0	0
All	All	30788	0	0	71	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

The worst 5 of 71 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:70:ARG:NH1	1:F:70:ARG:CG	2.60	0.65
1:D:201:ARG:NH1	1:D:201:ARG:CG	2.60	0.64
1:G:159:ARG:NH1	1:G:183:GLU:O	2.29	0.64
1:H:346:ILE:O	1:H:426:TRP:CZ3	2.51	0.64
1:G:198:GLN:NE2	1:G:201:ARG:NH1	2.47	0.62

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	475/505 (94%)	442 (93%)	30 (6%)	3 (1%)	33	54
1	B	464/505 (92%)	436 (94%)	28 (6%)	0	100	100
1	C	478/505 (95%)	455 (95%)	20 (4%)	3 (1%)	33	54
1	D	474/505 (94%)	451 (95%)	23 (5%)	0	100	100
1	E	475/505 (94%)	452 (95%)	22 (5%)	1 (0%)	56	78
1	F	465/505 (92%)	436 (94%)	27 (6%)	2 (0%)	43	66
1	G	479/505 (95%)	460 (96%)	18 (4%)	1 (0%)	56	78
1	H	477/505 (94%)	444 (93%)	28 (6%)	5 (1%)	22	37
All	All	3787/4040 (94%)	3576 (94%)	196 (5%)	15 (0%)	43	66

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	LEU
1	H	444	LEU
1	H	445	LEU
1	E	443	LYS
1	A	441	PRO

### 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	408/431 (95%)	377 (92%)	31 (8%)	19	33
1	B	400/431 (93%)	365 (91%)	35 (9%)	14	25
1	C	410/431 (95%)	376 (92%)	34 (8%)	16	28
1	D	409/431 (95%)	384 (94%)	25 (6%)	26	44
1	E	408/431 (95%)	369 (90%)	39 (10%)	12	21
1	F	401/431 (93%)	366 (91%)	35 (9%)	15	26
1	G	411/431 (95%)	380 (92%)	31 (8%)	19	33
1	H	410/431 (95%)	370 (90%)	40 (10%)	12	20
All	All	3257/3448 (94%)	2987 (92%)	270 (8%)	16	28

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	444	LEU
1	E	364	LEU
1	H	230	ASN
1	E	17	ILE
1	E	178	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 ligands are modelled in this entry.

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	BLA	A	900	1	46,46,46	2.60	16 (34%)	65,67,67	1.57	8 (12%)
2	BLA	B	900	1	46,46,46	2.66	15 (32%)	65,67,67	1.62	9 (13%)
2	BLA	C	900	1	46,46,46	2.61	17 (36%)	65,67,67	1.56	8 (12%)
2	BLA	D	900	1	46,46,46	2.65	14 (30%)	65,67,67	1.70	6 (9%)
2	BLA	E	900	1	46,46,46	2.70	16 (34%)	65,67,67	1.59	8 (12%)
2	BLA	F	900	1	46,46,46	2.58	15 (32%)	65,67,67	1.55	9 (13%)
2	BLA	G	900	1	46,46,46	2.65	15 (32%)	65,67,67	1.51	8 (12%)
2	BLA	H	900	1	46,46,46	2.62	14 (30%)	65,67,67	1.52	6 (9%)

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	BLA	A	900	1	-	2/26/74/74	0/4/4/4
2	BLA	B	900	1	-	2/26/74/74	0/4/4/4
2	BLA	C	900	1	-	2/26/74/74	0/4/4/4
2	BLA	D	900	1	-	2/26/74/74	0/4/4/4
2	BLA	E	900	1	-	2/26/74/74	0/4/4/4
2	BLA	F	900	1	-	2/26/74/74	0/4/4/4
2	BLA	G	900	1	-	2/26/74/74	0/4/4/4
2	BLA	H	900	1	-	2/26/74/74	0/4/4/4

The worst 5 of 122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	BLA	CHB-C1B	7.93	1.52	1.34
2	G	900	BLA	CHB-C1B	7.89	1.52	1.34
2	H	900	BLA	CHB-C1B	7.89	1.52	1.34
2	B	900	BLA	CHB-C1B	7.89	1.52	1.34
2	A	900	BLA	CHB-C1B	7.75	1.52	1.34

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	BLA	C1A-CHA-C4D	-7.50	115.29	129.92
2	A	900	BLA	C1A-CHA-C4D	-6.65	116.95	129.92
2	C	900	BLA	C1A-CHA-C4D	-6.06	118.09	129.92
2	B	900	BLA	C4C-CHD-C1D	-5.72	113.88	128.13
2	E	900	BLA	C4C-CHD-C1D	-5.56	114.28	128.13

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	BLA	C1B-CHB-C4A-NA
2	F	900	BLA	C1B-CHB-C4A-NA
2	H	900	BLA	C1B-CHB-C4A-NA
2	G	900	BLA	C4A-CHB-C1B-NB
2	C	900	BLA	C4A-CHB-C1B-NB

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	479/505 (94%)	0.15	13 (2%) 52 55	37, 58, 109, 160	0
1	B	470/505 (93%)	0.70	50 (10%) 7 6	48, 88, 136, 183	0
1	C	482/505 (95%)	0.24	13 (2%) 52 55	39, 61, 102, 147	0
1	D	480/505 (95%)	0.70	52 (10%) 6 6	55, 92, 144, 191	0
1	E	479/505 (94%)	0.57	42 (8%) 10 9	49, 92, 134, 191	0
1	F	471/505 (93%)	0.65	54 (11%) 5 5	41, 81, 144, 171	0
1	G	482/505 (95%)	0.09	8 (1%) 67 70	37, 63, 105, 165	1 (0%)
1	H	481/505 (95%)	0.94	75 (15%) 3 2	55, 95, 158, 207	0
All	All	3824/4040 (94%)	0.51	307 (8%) 12 12	37, 79, 138, 207	1 (0%)

The worst 5 of 307 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	59	LEU	10.9
1	H	51	PHE	9.6
1	B	453	ARG	9.1
1	H	110	PHE	9.1
1	H	53	ALA	8.8

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BLA	E	900	43/43	0.28	1.74	72,92,104,113	0
2	BLA	A	900	43/43	0.17	0.94	34,49,64,77	0
2	BLA	C	900	43/43	0.17	0.52	34,54,68,85	0
2	BLA	B	900	43/43	0.23	0.43	60,76,95,107	0
2	BLA	H	900	43/43	0.20	0.35	64,83,93,105	0
2	BLA	G	900	43/43	0.17	0.34	37,58,68,89	0
2	BLA	F	900	43/43	0.16	-0.07	39,60,70,84	0
2	BLA	D	900	43/43	0.15	-0.44	62,81,95,101	0

## 6.5 Other polymers

There are no such residues in this entry.