



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 11:49 AM EDT

PDB ID : 6CHT / pdb\_00006cht  
Title : HNF4alpha in complex with the corepressor EBP1 fragment  
Authors : Chi, Y.I.; Singh, P.; Lee, I.K.  
Deposited on : 2018-02-22  
Resolution : 3.17 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

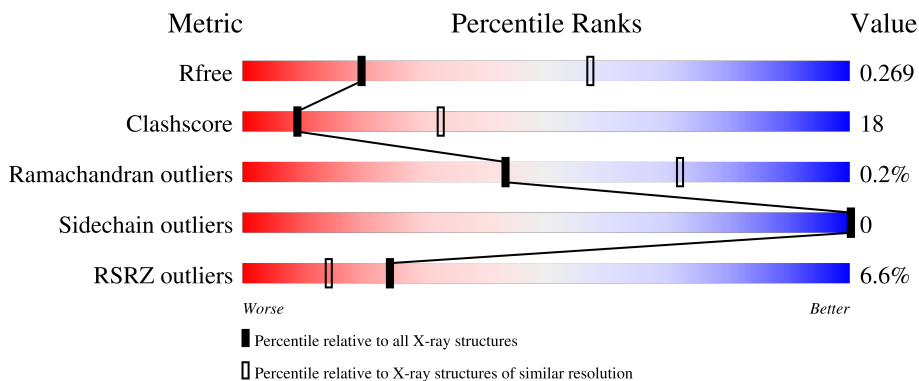
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.17 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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  $\geq 3$ , 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	245	 14% 53% 33% 14%
1	B	245	 56% 28% 16%
1	D	245	 14% 53% 34% 13%
1	E	245	 17% 52% 31% 17%
1	G	245	 4% 53% 33% 15%

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Mol	Chain	Length	Quality of chain
1	H	245	4% 45% 38% 18%
1	J	245	% 49% 36% 15%
1	K	245	50% 32% 18%
1	M	245	9% 48% 34% 18%
1	N	245	7% 42% 37% 21%
1	P	245	7% 44% 38% 18%
1	Q	245	8% 45% 34% 20%
1	S	245	5% 49% 33% 18%
1	T	245	6% 46% 33% 22%
1	V	245	4% 49% 33% 18%
1	W	245	2% 44% 34% 22%
2	C	20	25% 10% 65%
2	F	20	30% 5% 65%
2	I	20	25% 10% 65%
2	L	20	35% 5% 60%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26381 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 Hepatocyte nuclear factor 4-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	210	Total 1681	C 1086	N 278	O 308	S 9	0	0	0
1	B	205	Total 1647	C 1062	N 275	O 301	S 9	0	0	0
1	D	214	Total 1712	C 1104	N 285	O 314	S 9	0	0	0
1	E	204	Total 1639	C 1056	N 274	O 300	S 9	0	0	0
1	G	209	Total 1678	C 1085	N 279	O 305	S 9	0	0	0
1	H	202	Total 1627	C 1050	N 271	O 297	S 9	0	0	0
1	J	209	Total 1678	C 1085	N 279	O 305	S 9	0	0	0
1	K	202	Total 1627	C 1050	N 271	O 297	S 9	0	0	0
1	M	201	Total 1619	C 1046	N 270	O 294	S 9	0	0	0
1	N	193	Total 1557	C 1005	N 257	O 286	S 9	0	0	0
1	P	200	Total 1611	C 1040	N 269	O 293	S 9	0	0	0
1	Q	196	Total 1582	C 1023	N 261	O 289	S 9	0	0	0
1	S	201	Total 1615	C 1042	N 270	O 294	S 9	0	0	0
1	T	192	Total 1554	C 1005	N 256	O 284	S 9	0	0	0
1	V	202	Total 1627	C 1050	N 271	O 297	S 9	0	0	0
1	W	192	Total 1554	C 1005	N 256	O 284	S 9	0	0	0

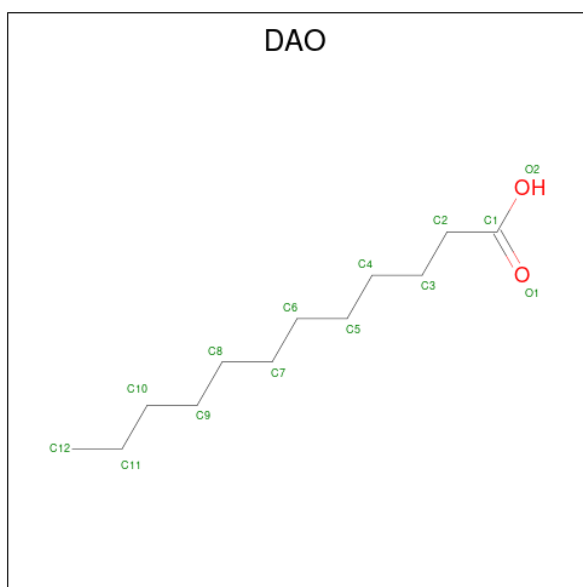
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLY	-	expression tag	UNP P41235
B	138	GLY	-	expression tag	UNP P41235
D	138	GLY	-	expression tag	UNP P41235
E	138	GLY	-	expression tag	UNP P41235
G	138	GLY	-	expression tag	UNP P41235
H	138	GLY	-	expression tag	UNP P41235
J	138	GLY	-	expression tag	UNP P41235
K	138	GLY	-	expression tag	UNP P41235
M	138	GLY	-	expression tag	UNP P41235
N	138	GLY	-	expression tag	UNP P41235
P	138	GLY	-	expression tag	UNP P41235
Q	138	GLY	-	expression tag	UNP P41235
S	138	GLY	-	expression tag	UNP P41235
T	138	GLY	-	expression tag	UNP P41235
V	138	GLY	-	expression tag	UNP P41235
W	138	GLY	-	expression tag	UNP P41235

- Molecule 2 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			52	35	8	9			
2	F	7	Total	C	N	O	0	0	0
			52	35	8	9			
2	I	7	Total	C	N	O	0	0	0
			52	35	8	9			
2	L	8	Total	C	N	O	0	0	0
			61	40	10	11			

- Molecule 3 is LAURIC ACID (CCD ID: DAO) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	12	2		
3	B	1	Total	C	O	0	0
			14	12	2		
3	D	1	Total	C	O	0	0
			14	12	2		
3	E	1	Total	C	O	0	0
			14	12	2		
3	G	1	Total	C	O	0	0
			14	12	2		
3	H	1	Total	C	O	0	0
			14	12	2		
3	J	1	Total	C	O	0	0
			14	12	2		
3	K	1	Total	C	O	0	0
			14	12	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	6	Total	O	0	0
			6	6		
4	D	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

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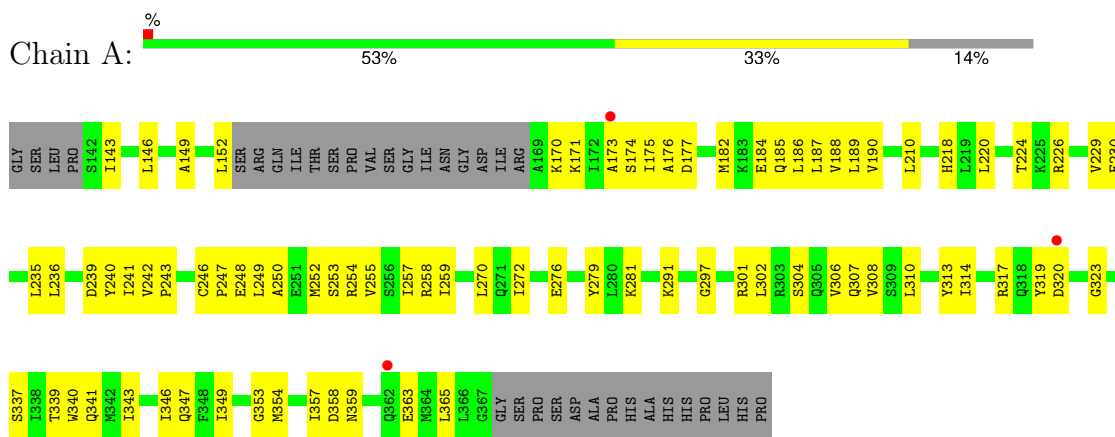
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total O 1 1	0	0
4	G	5	Total O 5 5	0	0
4	H	4	Total O 4 4	0	0
4	J	2	Total O 2 2	0	0
4	K	7	Total O 7 7	0	0
4	L	1	Total O 1 1	0	0
4	M	1	Total O 1 1	0	0
4	N	2	Total O 2 2	0	0
4	Q	1	Total O 1 1	0	0
4	S	2	Total O 2 2	0	0
4	V	2	Total O 2 2	0	0
4	W	2	Total O 2 2	0	0

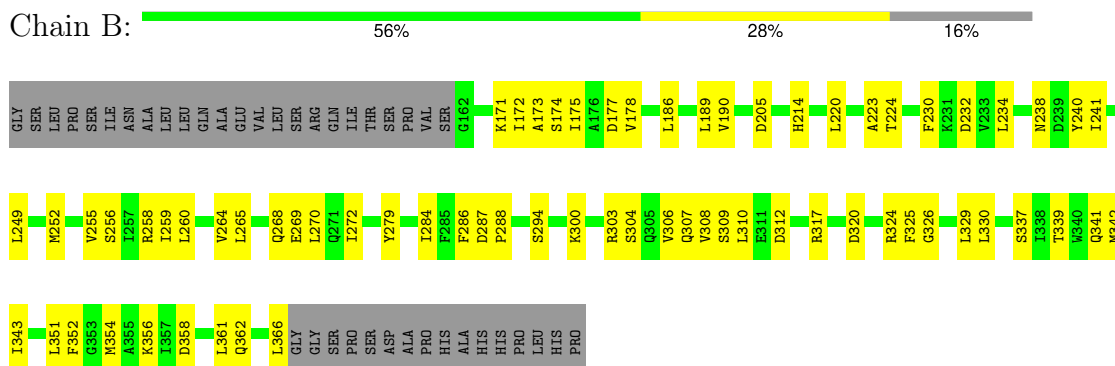
### 3 Residue-property plots [i](#)

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.

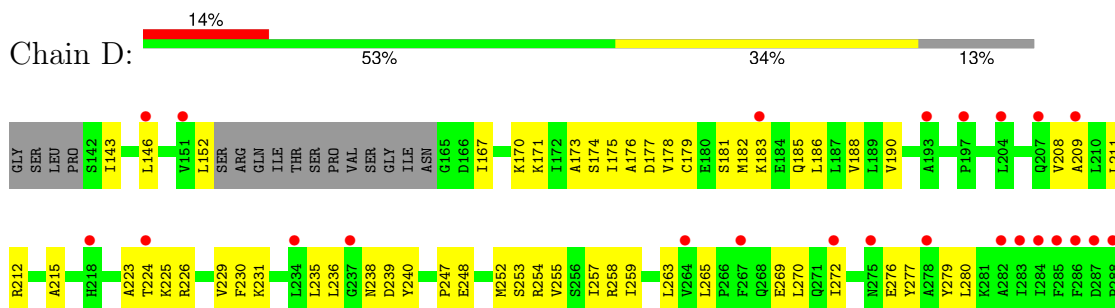
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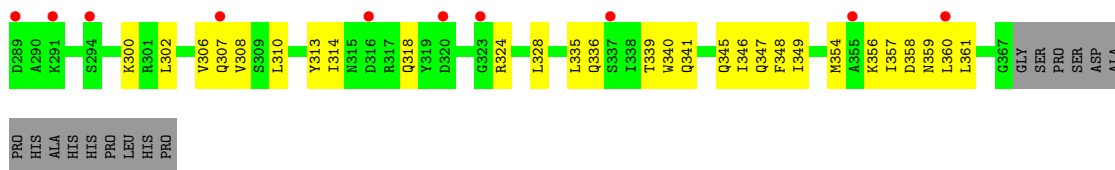


- Molecule 1: Hepatocyte nuclear factor 4-alpha

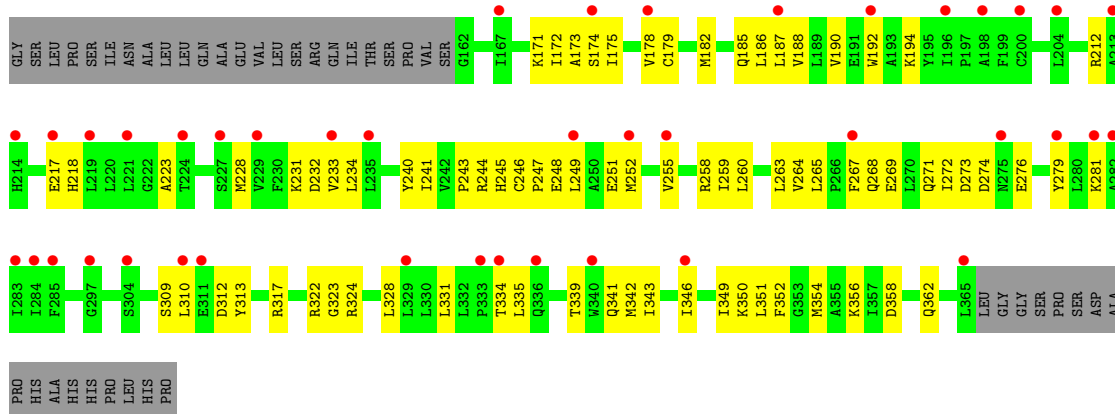


- Molecule 1: Hepatocyte nuclear factor 4-alpha

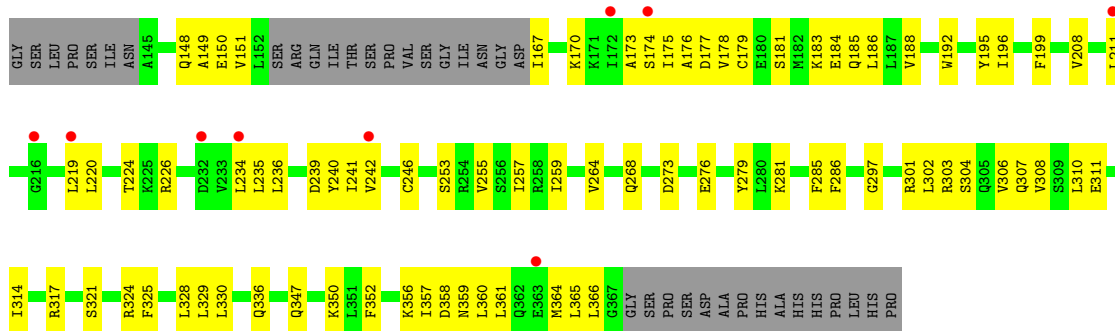




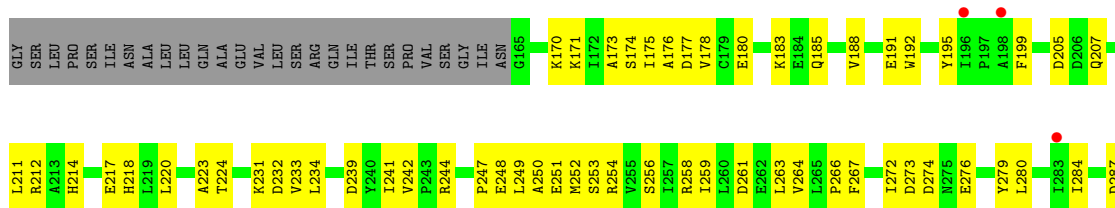
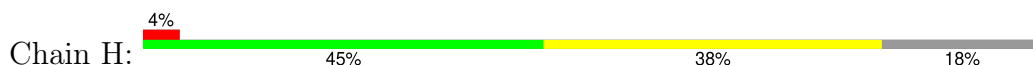
● Molecule 1: Hepatocyte nuclear factor 4-alpha



● Molecule 1: Hepatocyte nuclear factor 4-alpha

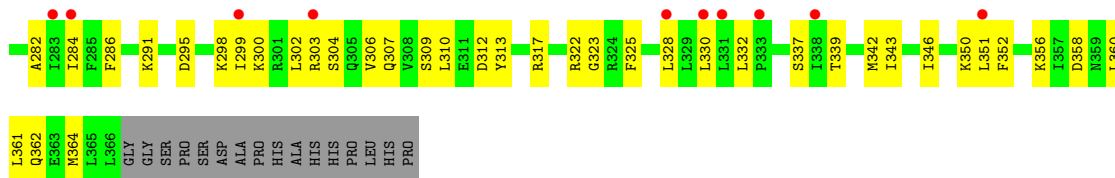


● Molecule 1: Hepatocyte nuclear factor 4-alpha

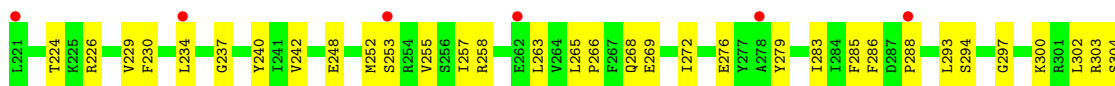




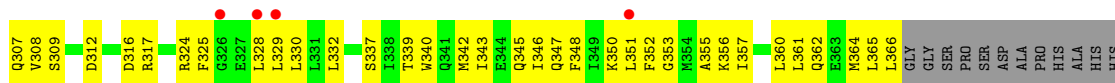
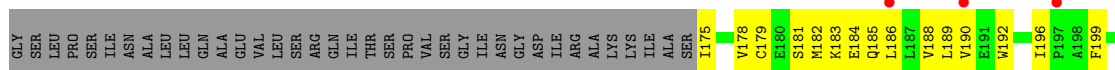




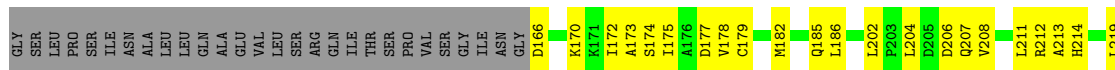
- Molecule 1: Hepatocyte nuclear factor 4-alpha



- Molecule 1: Hepatocyte nuclear factor 4-alpha

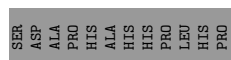
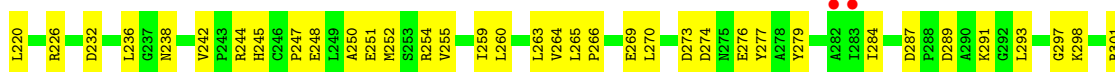
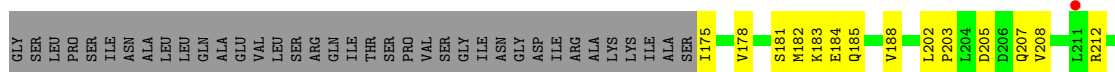
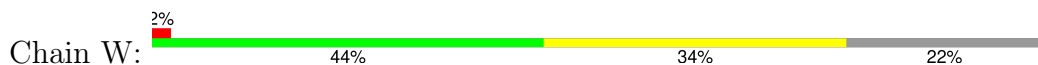


- Molecule 1: Hepatocyte nuclear factor 4-alpha

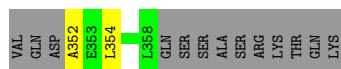




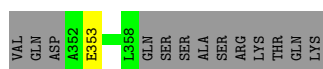
● Molecule 1: Hepatocyte nuclear factor 4-alpha



● Molecule 2: Proliferation-associated protein 2G4



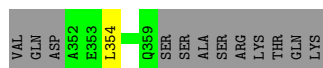
● Molecule 2: Proliferation-associated protein 2G4



● Molecule 2: Proliferation-associated protein 2G4



● Molecule 2: Proliferation-associated protein 2G4



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.72Å 104.95Å 139.56Å 90.00° 90.61° 90.00°	Depositor
Resolution (Å)	49.63 – 3.17 49.63 – 3.17	Depositor EDS
% Data completeness (in resolution range)	71.6 (49.63-3.17) 71.6 (49.63-3.17)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	644.16 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.262 , 0.274 0.259 , 0.269	Depositor DCC
$R_{free}$ test set	2505 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.1	Xtrriage
Anisotropy	0.153	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 700.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtrriage
Estimated twinning fraction	0.046 for -l,k,h 0.056 for -h,-k,l 0.390 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	26381	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5463e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.22	0/1708	0.51	0/2307
1	B	0.23	0/1675	0.51	0/2262
1	D	0.19	0/1739	0.48	0/2348
1	E	0.20	0/1667	0.50	0/2251
1	G	0.19	0/1705	0.49	0/2302
1	H	0.21	0/1655	0.49	0/2235
1	J	0.21	0/1705	0.52	0/2302
1	K	0.22	0/1655	0.52	0/2235
1	M	0.18	0/1647	0.51	0/2224
1	N	0.17	0/1585	0.45	0/2143
1	P	0.17	0/1639	0.47	0/2213
1	Q	0.20	0/1610	0.45	1/2176 (0.0%)
1	S	0.18	0/1643	0.49	0/2218
1	T	0.18	0/1582	0.45	0/2139
1	V	0.19	0/1655	0.49	0/2235
1	W	0.20	0/1582	0.49	1/2139 (0.0%)
2	C	0.14	0/51	0.37	0/67
2	F	0.12	0/51	0.32	0/67
2	I	0.14	0/51	0.53	0/67
2	L	0.13	0/60	0.47	0/79
All	All	0.20	0/26665	0.49	2/36009 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	242	VAL	CA-C-O	-5.22	117.23	119.94
1	Q	242	VAL	CA-C-O	-5.03	117.33	119.94

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	1681	0	1733	71	1
1	B	1647	0	1694	61	0
1	D	1712	0	1765	62	1
1	E	1639	0	1683	65	0
1	G	1678	0	1735	67	0
1	H	1627	0	1673	68	0
1	J	1678	0	1736	65	0
1	K	1627	0	1673	67	0
1	M	1619	0	1671	66	0
1	N	1557	0	1591	72	0
1	P	1611	0	1660	75	0
1	Q	1582	0	1626	74	0
1	S	1615	0	1663	65	0
1	T	1554	0	1592	68	1
1	V	1627	0	1675	71	0
1	W	1554	0	1592	72	1
2	C	52	0	61	3	0
2	F	52	0	61	1	0
2	I	52	0	61	4	0
2	L	61	0	69	2	0
3	A	14	0	23	1	0
3	B	14	0	23	2	0
3	D	14	0	23	3	0
3	E	14	0	23	2	0
3	G	14	0	23	3	0
3	H	14	0	23	2	0
3	J	14	0	23	2	0
3	K	14	0	23	1	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	4	0	0	0	0
4	J	2	0	0	0	0
4	K	7	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	2	0	0	0	0
4	Q	1	0	0	1	0
4	S	2	0	0	0	0
4	V	2	0	0	1	0
4	W	2	0	0	0	0
All	All	26381	0	27198	983	2

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 18.

The worst 5 of 983 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:M:348:PHE:HE1	1:M:352:PHE:CE2	1.32	1.46
1:M:348:PHE:CE1	1:M:352:PHE:CE2	2.19	1.31
1:A:317:ARG:NE	1:A:319:TYR:CD2	2.25	1.04
1:A:317:ARG:CZ	1:A:319:TYR:CE2	2.51	0.93
1:A:317:ARG:CZ	1:A:319:TYR:CD2	2.53	0.91

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:TYR:OH	1:T:316:ASP:O[2_544]	2.15	0.05
1:A:171:LYS:NZ	1:W:316:ASP:O[2_445]	2.16	0.04

## 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	206/245 (84%)	189 (92%)	17 (8%)	0	100	100
1	B	203/245 (83%)	189 (93%)	13 (6%)	1 (0%)	24	57
1	D	210/245 (86%)	190 (90%)	18 (9%)	2 (1%)	12	43
1	E	202/245 (82%)	190 (94%)	12 (6%)	0	100	100
1	G	205/245 (84%)	182 (89%)	23 (11%)	0	100	100
1	H	200/245 (82%)	192 (96%)	7 (4%)	1 (0%)	24	57
1	J	205/245 (84%)	187 (91%)	17 (8%)	1 (0%)	24	57
1	K	200/245 (82%)	185 (92%)	15 (8%)	0	100	100
1	M	199/245 (81%)	178 (89%)	20 (10%)	1 (0%)	24	57
1	N	191/245 (78%)	186 (97%)	5 (3%)	0	100	100
1	P	198/245 (81%)	178 (90%)	20 (10%)	0	100	100
1	Q	194/245 (79%)	183 (94%)	11 (6%)	0	100	100
1	S	199/245 (81%)	173 (87%)	24 (12%)	2 (1%)	12	43
1	T	190/245 (78%)	181 (95%)	9 (5%)	0	100	100
1	V	200/245 (82%)	181 (90%)	19 (10%)	0	100	100
1	W	190/245 (78%)	179 (94%)	11 (6%)	0	100	100
2	C	5/20 (25%)	5 (100%)	0	0	100	100
2	F	5/20 (25%)	5 (100%)	0	0	100	100
2	I	5/20 (25%)	5 (100%)	0	0	100	100
2	L	6/20 (30%)	6 (100%)	0	0	100	100
All	All	3213/4000 (80%)	2964 (92%)	241 (8%)	8 (0%)	43	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	321	SER
1	M	318	GLN
1	S	248	GLU
1	H	232	ASP
1	B	232	ASP

### 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	185/214 (86%)	185 (100%)	0	100	100
1	B	181/214 (85%)	181 (100%)	0	100	100
1	D	188/214 (88%)	188 (100%)	0	100	100
1	E	180/214 (84%)	180 (100%)	0	100	100
1	G	184/214 (86%)	184 (100%)	0	100	100
1	H	179/214 (84%)	179 (100%)	0	100	100
1	J	184/214 (86%)	184 (100%)	0	100	100
1	K	179/214 (84%)	179 (100%)	0	100	100
1	M	178/214 (83%)	178 (100%)	0	100	100
1	N	172/214 (80%)	172 (100%)	0	100	100
1	P	177/214 (83%)	177 (100%)	0	100	100
1	Q	175/214 (82%)	175 (100%)	0	100	100
1	S	177/214 (83%)	177 (100%)	0	100	100
1	T	172/214 (80%)	172 (100%)	0	100	100
1	V	179/214 (84%)	179 (100%)	0	100	100
1	W	172/214 (80%)	172 (100%)	0	100	100
2	C	5/17 (29%)	5 (100%)	0	100	100
2	F	5/17 (29%)	5 (100%)	0	100	100
2	I	5/17 (29%)	5 (100%)	0	100	100
2	L	6/17 (35%)	6 (100%)	0	100	100
All	All	2883/3492 (83%)	2883 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	268	GLN

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Mol	Chain	Res	Type
1	Q	307	GLN
1	V	207	GLN
1	S	245	HIS
1	Q	185	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	DAO	E	500	1	13,13,13	0.68	0	13,13,13	1.26	1 (7%)
3	DAO	D	500	-	13,13,13	0.66	0	13,13,13	1.13	0
3	DAO	H	500	1	13,13,13	0.70	0	13,13,13	1.22	1 (7%)
3	DAO	G	500	1	13,13,13	0.68	0	13,13,13	1.18	1 (7%)
3	DAO	J	500	-	13,13,13	0.68	0	13,13,13	1.20	1 (7%)
3	DAO	B	500	1	13,13,13	0.70	0	13,13,13	1.28	1 (7%)
3	DAO	K	500	1	13,13,13	0.64	0	13,13,13	1.09	0
3	DAO	A	500	1	13,13,13	0.67	0	13,13,13	1.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAO	E	500	1	-	3/11/11/11	-
3	DAO	D	500	-	-	6/11/11/11	-
3	DAO	H	500	1	-	4/11/11/11	-
3	DAO	G	500	1	-	2/11/11/11	-
3	DAO	J	500	-	-	7/11/11/11	-
3	DAO	B	500	1	-	3/11/11/11	-
3	DAO	K	500	1	-	6/11/11/11	-
3	DAO	A	500	1	-	3/11/11/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	DAO	C3-C2-C1	-2.68	107.51	114.51
3	E	500	DAO	C3-C2-C1	-2.66	107.56	114.51
3	J	500	DAO	C3-C2-C1	-2.40	108.24	114.51
3	H	500	DAO	C3-C2-C1	-2.28	108.57	114.51
3	G	500	DAO	O2-C1-C2	2.20	120.94	114.00

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	500	DAO	C1-C2-C3-C4
3	J	500	DAO	C1-C2-C3-C4
3	J	500	DAO	C3-C4-C5-C6
3	D	500	DAO	C6-C7-C8-C9
3	B	500	DAO	C5-C6-C7-C8

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	500	DAO	2	0
3	D	500	DAO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	500	DAO	2	0
3	G	500	DAO	3	0
3	J	500	DAO	2	0
3	B	500	DAO	2	0
3	K	500	DAO	1	0
3	A	500	DAO	1	0

## 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, 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	210/245 (85%)	-0.05	3 (1%) 73 53	18, 46, 87, 107	0
1	B	205/245 (83%)	-0.36	0 100 100	12, 28, 86, 118	0
1	D	214/245 (87%)	1.25	34 (15%) 5 3	73, 127, 199, 208	0
1	E	204/245 (83%)	1.32	41 (20%) 3 2	85, 120, 145, 157	0
1	G	209/245 (85%)	0.75	9 (4%) 40 23	63, 95, 117, 128	0
1	H	202/245 (82%)	0.43	9 (4%) 38 22	25, 62, 101, 124	0
1	J	209/245 (85%)	0.24	2 (0%) 79 62	41, 70, 103, 141	0
1	K	202/245 (82%)	-0.10	0 100 100	18, 40, 81, 99	0
1	M	201/245 (82%)	0.97	21 (10%) 11 7	84, 193, 319, 333	0
1	N	193/245 (78%)	0.91	18 (9%) 14 8	58, 207, 454, 485	0
1	P	200/245 (81%)	0.90	17 (8%) 16 10	118, 152, 235, 277	0
1	Q	196/245 (80%)	0.94	20 (10%) 12 7	69, 209, 377, 395	0
1	S	201/245 (82%)	0.80	13 (6%) 25 14	69, 139, 198, 244	0
1	T	192/245 (78%)	0.77	15 (7%) 19 11	101, 153, 174, 180	0
1	V	202/245 (82%)	0.74	9 (4%) 38 22	89, 129, 164, 192	0
1	W	192/245 (78%)	0.61	5 (2%) 57 36	54, 142, 162, 167	0
2	C	7/20 (35%)	-0.14	0 100 100	76, 79, 90, 95	0
2	F	7/20 (35%)	0.26	0 100 100	127, 137, 150, 152	0
2	I	7/20 (35%)	0.71	0 100 100	188, 189, 191, 191	0
2	L	8/20 (40%)	-0.10	0 100 100	84, 87, 89, 92	0
All	All	3261/4000 (81%)	0.63	216 (6%) 24 14	12, 120, 260, 485	0

The worst 5 of 216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	253	SER	6.2
1	M	329	LEU	5.6
1	Q	253	SER	5.0
1	P	328	LEU	4.7
1	W	282	ALA	4.6

## 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](#)

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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DAO	D	500	14/14	0.95	0.18	78,95,114,119	0
3	DAO	G	500	14/14	0.96	0.14	75,96,103,105	0
3	DAO	J	500	14/14	0.96	0.15	62,80,95,96	0
3	DAO	H	500	14/14	0.97	0.14	41,45,54,56	0
3	DAO	A	500	14/14	0.97	0.12	42,52,70,74	0
3	DAO	E	500	14/14	0.98	0.19	94,108,118,119	0
3	DAO	B	500	14/14	0.98	0.10	21,26,46,47	0
3	DAO	K	500	14/14	0.98	0.10	15,34,44,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.