



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2016 – 08:06 PM EST

PDB ID : 5K8N  
Title : 5NAA-bound 5-nitroanthranilate aminohydrolase  
Authors : Kalyoncu, S.  
Deposited on : 2016-05-30  
Resolution : 3.23 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028320

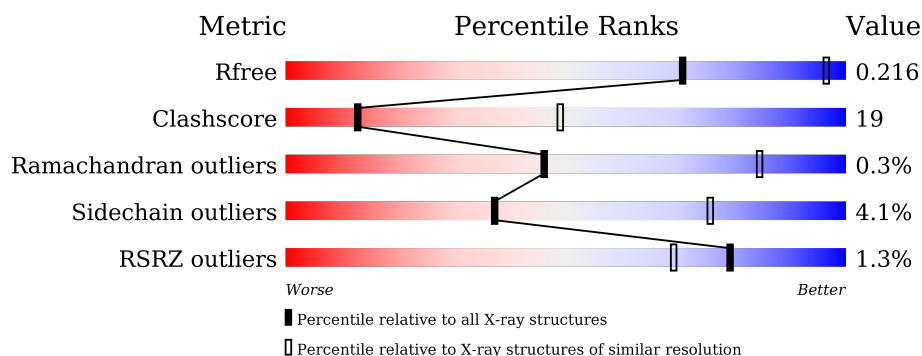
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.23 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))
$R_{free}$	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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. 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	425	<div> <div></div> <div>60%36%..</div> </div>
1	B	425	<div> <div>2%</div> <div>58%40%..</div> </div>
1	C	425	<div> <div>5%</div> <div>62%35%..</div> </div>
1	D	425	<div> <div></div> <div>66%31%..</div> </div>
1	E	425	<div> <div></div> <div>64%33%..</div> </div>
1	F	425	<div> <div>%</div> <div>63%34%..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	425	<div> <div>%</div> <div> </div> <div>60% 36% ..</div> </div>
1	H	425	<div> <div>%</div> <div> </div> <div>63% 34% ..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	6R6	A	501	-	-	-	X
2	6R6	D	501	-	-	-	X
2	6R6	F	501	-	-	-	X
2	6R6	G	501	-	-	-	X

## 2 Entry composition

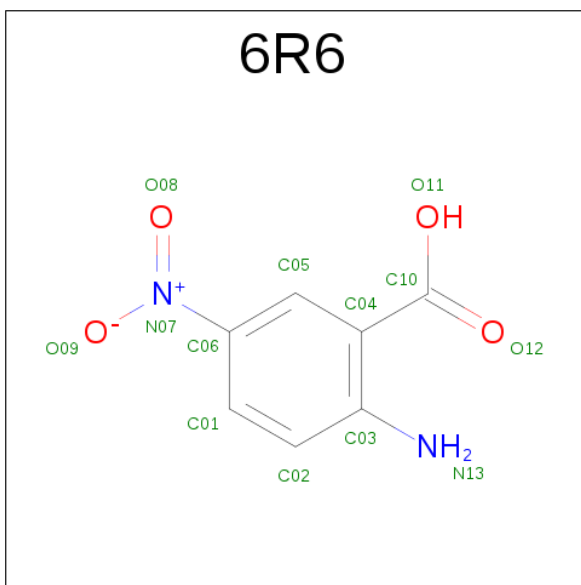
There are 2 unique types of molecules in this entry. The entry contains 25920 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5-nitroanthranilic acid aminohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3227	2042	560	606	19			
1	B	420	Total	C	N	O	S	0	0	0
			3227	2042	560	606	19			
1	C	420	Total	C	N	O	S	0	0	0
			3227	2042	560	606	19			
1	D	420	Total	C	N	O	S	0	0	0
			3227	2042	560	606	19			
1	E	420	Total	C	N	O	S	0	0	0
			3227	2042	560	606	19			
1	F	420	Total	C	N	O	S	0	0	0
			3227	2042	560	606	19			
1	G	420	Total	C	N	O	S	0	0	0
			3227	2042	560	606	19			
1	H	420	Total	C	N	O	S	0	0	0
			3227	2042	560	606	19			

- Molecule 2 is 5-nitroanthranilic acid (three-letter code: 6R6) (formula: C<sub>7</sub>H<sub>6</sub>N<sub>2</sub>O<sub>4</sub>).

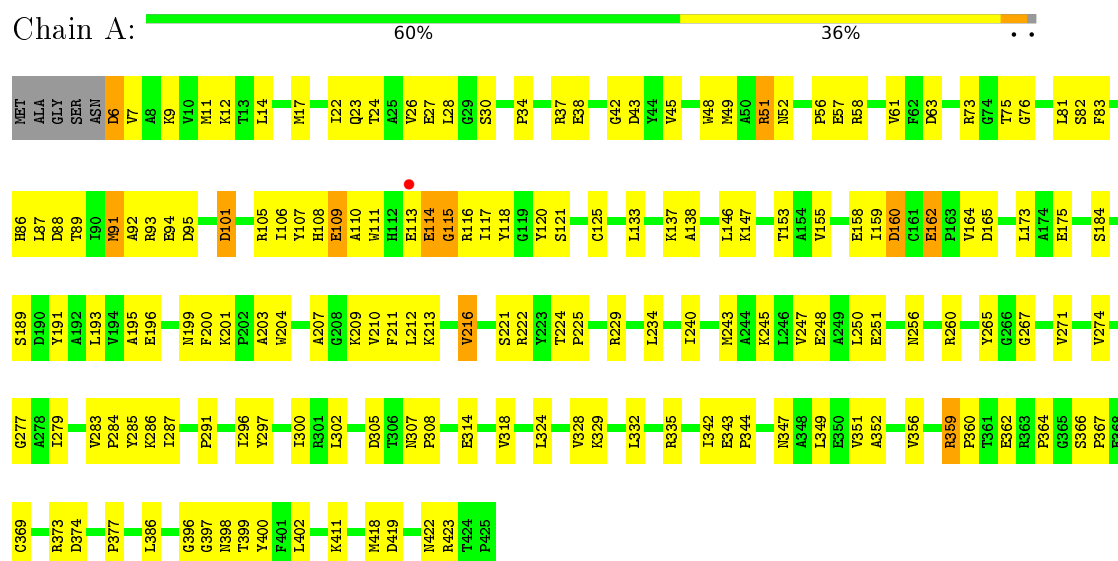


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	2	4		
2	B	1	Total	C	N	O	0	0
			13	7	2	4		
2	C	1	Total	C	N	O	0	0
			13	7	2	4		
2	D	1	Total	C	N	O	0	0
			13	7	2	4		
2	E	1	Total	C	N	O	0	0
			13	7	2	4		
2	F	1	Total	C	N	O	0	0
			13	7	2	4		
2	G	1	Total	C	N	O	0	0
			13	7	2	4		
2	H	1	Total	C	N	O	0	0
			13	7	2	4		

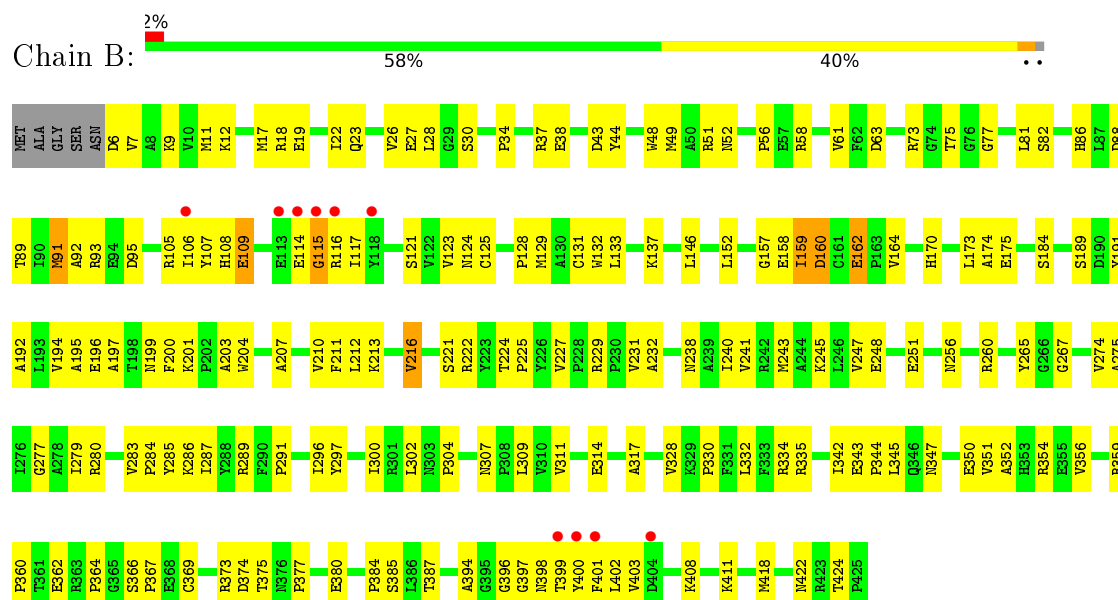
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

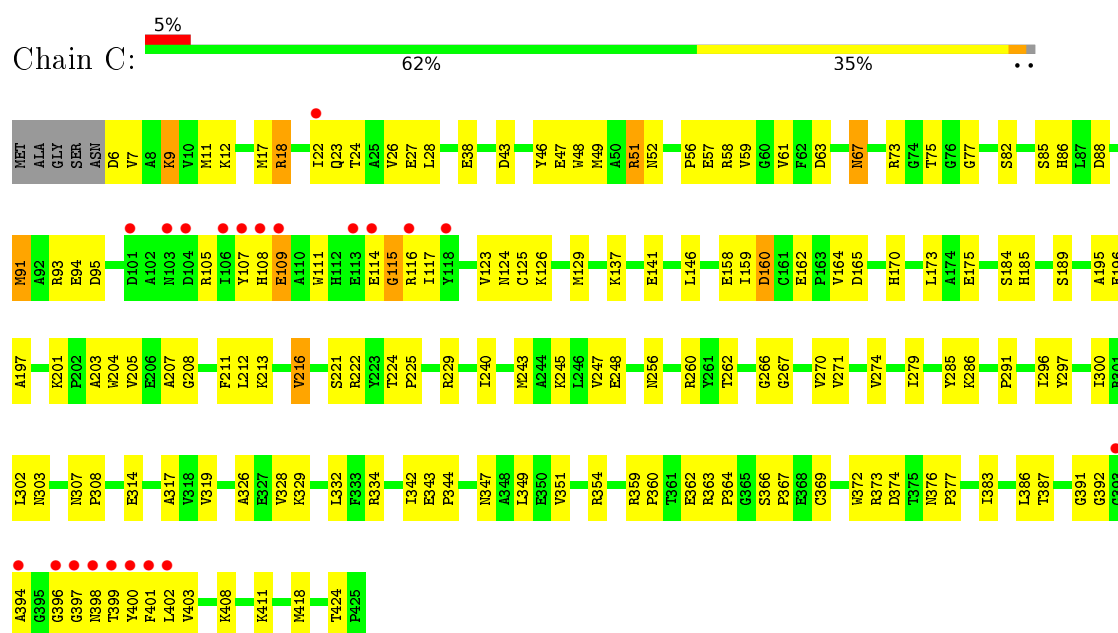
#### • Molecule 1: 5-nitroanthranilic acid aminohydrolase



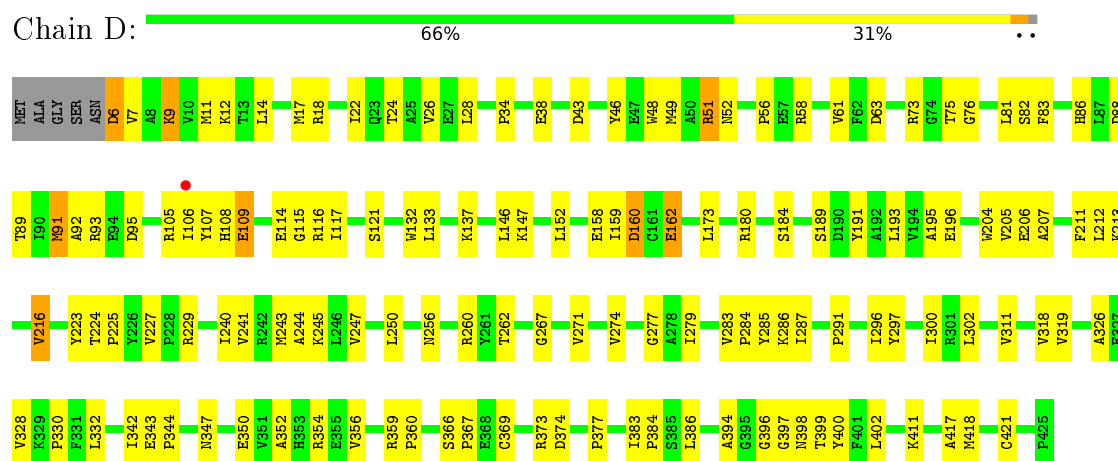
#### • Molecule 1: 5-nitroanthranilic acid aminohydrolase



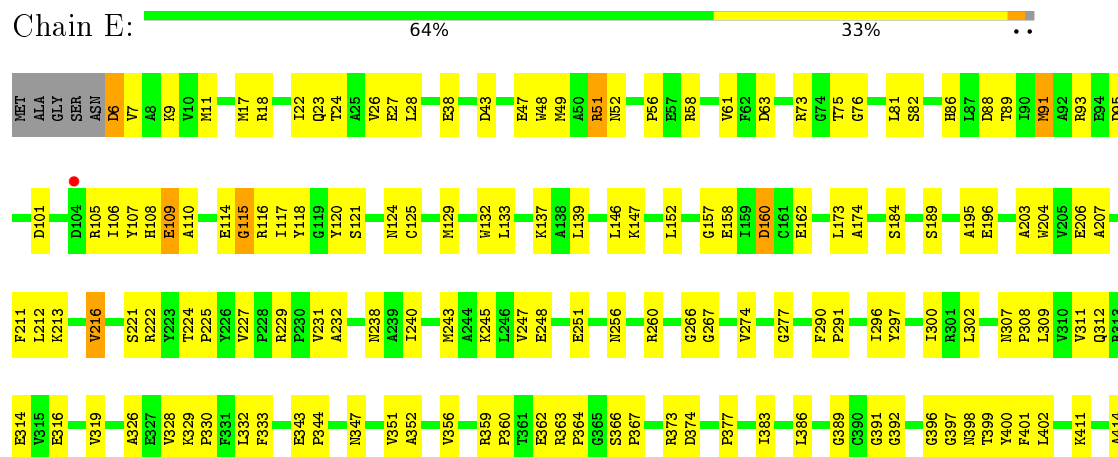
#### • Molecule 1: 5-nitroanthranilic acid aminohydrolase



- Molecule 1: 5-nitroanthranilic acid aminohydrolase



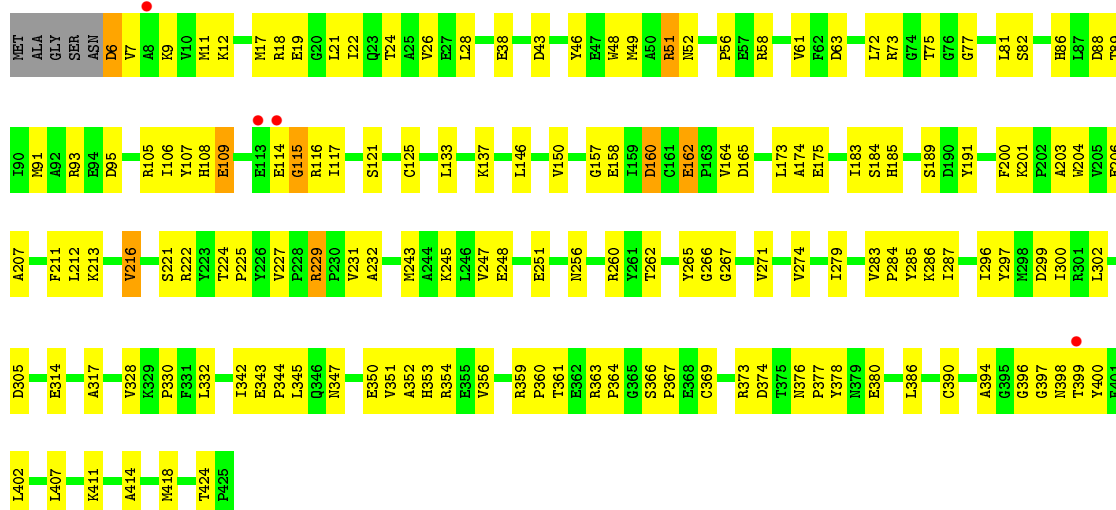
- Molecule 1: 5-nitroanthranilic acid aminohydrolase





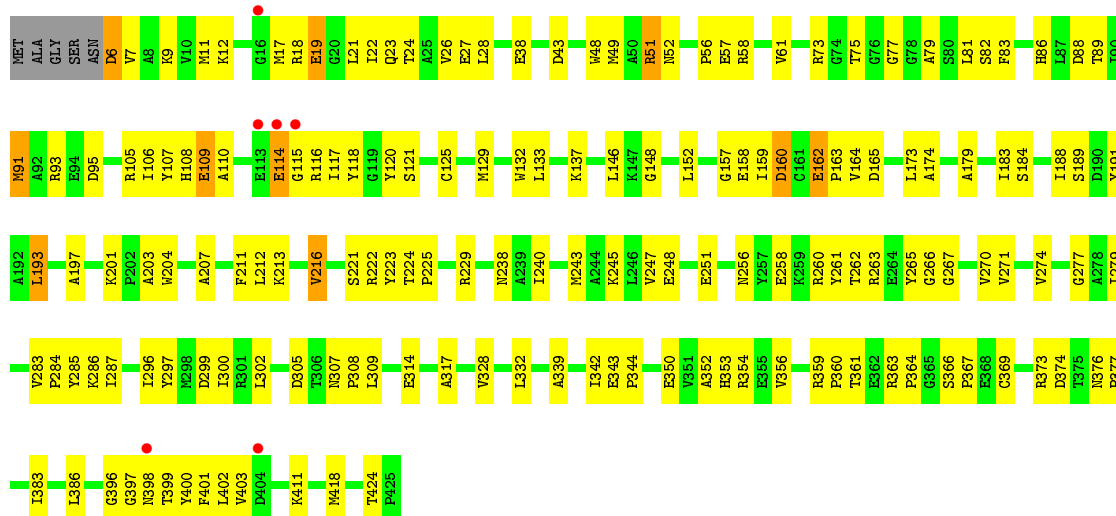
• Molecule 1: 5-nitroanthranilic acid aminohydrolase

Chain F: 63% 34%



• Molecule 1: 5-nitroanthranilic acid aminohydrolase

Chain G: 60% 36%



• Molecule 1: 5-nitroanthranilic acid aminohydrolase

Chain H: 63% 34%





R93	D190	I296	K411
E94	Y191	I297	
D95		I300	A417
	A195	I301	M418
D101	E196	L302	D419
			I420
R105	F200	D305	C421
I106		T306	M422
Y107	A207	N307	R423
H108		P308	T424
E109	F211	L309	P425
A110	L212		
	K213	E314	
E114			
G115	V216	V328	
R116			
I117	S221	L332	
Y118	R222		
G119	Y223	I342	
Y120	T224	E343	
S121	P225	P344	
	Y226		
N124	V227	L349	
C125	P228		
	R229	R359	
L133		P360	
I134	I240		
A135		P364	
A136	M243	G365	
K137	A244	S366	
A138	K245	P367	
L139	L246	E368	
	V247	C369	
L146	E248	S370	
K147		N371	
	E252	G372	
V155	W253	R373	
G156		D374	
G157	N256		
E158		P377	
I159	R260		
D160		I383	
C161	R263	P384	
E162	E264	S385	
P163	Y265	L386	
V164		T387	
D165	V271	Y388	
		G389	
L173	V274	C390	
A174		G391	
E175	I279		
		G396	
A179	Y285	G397	
R180	K286	N398	
	I287	T399	
I183	Y288	Y400	
S184	E289	F401	
H185	F290	L402	
	P291		
S189			

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.46Å 248.88Å 249.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.28 – 3.23 47.83 – 3.22	Depositor EDS
% Data completeness (in resolution range)	93.8 (46.28-3.23) 93.9 (47.83-3.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.39 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.177 , 0.217 0.173 , 0.216	Depositor DCC
$R_{free}$ test set	2001 reflections (2.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25920	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: 6R6

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	0.62	0/3301	0.64	0/4480
1	B	0.62	0/3301	0.66	0/4480
1	C	0.64	0/3301	0.68	0/4480
1	D	0.63	0/3301	0.65	0/4480
1	E	0.63	0/3301	0.64	0/4480
1	F	0.58	0/3301	0.64	0/4480
1	G	0.59	0/3301	0.64	0/4480
1	H	0.63	0/3301	0.66	0/4480
All	All	0.62	0/26408	0.65	0/35840

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	3227	0	3159	143	0
1	B	3227	0	3159	136	0
1	C	3227	0	3159	126	0
1	D	3227	0	3159	122	0
1	E	3227	0	3159	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3227	0	3159	127	0
1	G	3227	0	3159	134	0
1	H	3227	0	3159	133	0
2	A	13	0	0	2	0
2	B	13	0	0	1	0
2	C	13	0	0	1	0
2	D	13	0	0	1	0
2	E	13	0	0	2	0
2	F	13	0	0	1	0
2	G	13	0	0	1	0
2	H	13	0	0	1	0
All	All	25920	0	25272	984	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 984 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:B:61:VAL:HG13	1:H:173:LEU:HD11	1.36	1.08
1:D:173:LEU:HD11	1:F:61:VAL:HG13	1.37	1.02
1:A:49:MET:HB3	1:A:56:PRO:HG3	1.42	1.00
1:B:22:ILE:HG23	1:B:117:ILE:HD11	1.39	0.99
1:B:173:LEU:HD11	1:H:61:VAL:HG13	1.47	0.96

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	418/425 (98%)	399 (96%)	17 (4%)	2 (0%)	34 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	418/425 (98%)	400 (96%)	17 (4%)	1 (0%)	52	88
1	C	418/425 (98%)	401 (96%)	16 (4%)	1 (0%)	52	88
1	D	418/425 (98%)	401 (96%)	16 (4%)	1 (0%)	52	88
1	E	418/425 (98%)	399 (96%)	18 (4%)	1 (0%)	52	88
1	F	418/425 (98%)	402 (96%)	15 (4%)	1 (0%)	52	88
1	G	418/425 (98%)	402 (96%)	14 (3%)	2 (0%)	34	77
1	H	418/425 (98%)	399 (96%)	17 (4%)	2 (0%)	34	77
All	All	3344/3400 (98%)	3203 (96%)	130 (4%)	11 (0%)	46	84

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLY
1	D	115	GLY
1	E	115	GLY
1	F	115	GLY
1	H	115	GLY

### 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	328/331 (99%)	313 (95%)	15 (5%)	33	73
1	B	328/331 (99%)	315 (96%)	13 (4%)	38	76
1	C	328/331 (99%)	313 (95%)	15 (5%)	33	73
1	D	328/331 (99%)	315 (96%)	13 (4%)	38	76
1	E	328/331 (99%)	316 (96%)	12 (4%)	41	78
1	F	328/331 (99%)	315 (96%)	13 (4%)	38	76
1	G	328/331 (99%)	315 (96%)	13 (4%)	38	76
1	H	328/331 (99%)	314 (96%)	14 (4%)	35	74
All	All	2624/2648 (99%)	2516 (96%)	108 (4%)	37	76

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	73	ARG
1	E	91	MET
1	H	73	ARG
1	D	95	ASP
1	D	216	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	108	HIS
1	E	108	HIS
1	G	108	HIS
1	C	340	GLN
1	G	307	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 carbohydrates 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
2	6R6	A	501	-	8,13,13	1.46	2 (25%)	11,18,18	1.17	1 (9%)
2	6R6	B	501	-	8,13,13	1.54	2 (25%)	11,18,18	1.67	2 (18%)
2	6R6	C	501	-	8,13,13	1.45	2 (25%)	11,18,18	1.45	3 (27%)
2	6R6	D	501	-	8,13,13	1.42	2 (25%)	11,18,18	2.19	4 (36%)
2	6R6	E	501	-	8,13,13	1.45	2 (25%)	11,18,18	1.29	2 (18%)
2	6R6	F	501	-	8,13,13	1.53	2 (25%)	11,18,18	2.14	3 (27%)
2	6R6	G	501	-	8,13,13	1.54	2 (25%)	11,18,18	1.41	1 (9%)
2	6R6	H	501	-	8,13,13	1.55	3 (37%)	11,18,18	1.09	1 (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	6R6	A	501	-	-	0/4/8/8	0/1/1/1
2	6R6	B	501	-	-	0/4/8/8	0/1/1/1
2	6R6	C	501	-	-	0/4/8/8	0/1/1/1
2	6R6	D	501	-	-	0/4/8/8	0/1/1/1
2	6R6	E	501	-	-	0/4/8/8	0/1/1/1
2	6R6	F	501	-	-	0/4/8/8	0/1/1/1
2	6R6	G	501	-	-	0/4/8/8	0/1/1/1
2	6R6	H	501	-	-	0/4/8/8	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6R6	O08-N07	-2.90	1.17	1.22
2	B	501	6R6	O08-N07	-2.77	1.17	1.22
2	G	501	6R6	O08-N07	-2.76	1.17	1.22
2	E	501	6R6	O08-N07	-2.69	1.17	1.22
2	F	501	6R6	O08-N07	-2.65	1.17	1.22

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	6R6	C05-C06-N07	-2.27	116.75	118.74
2	C	501	6R6	C05-C04-C10	-2.12	116.92	120.16
2	D	501	6R6	C05-C04-C03	2.15	120.68	119.08
2	A	501	6R6	C05-C06-N07	2.19	120.67	118.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	6R6	C01-C06-N07	2.39	121.23	119.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	6R6	2	0
2	B	501	6R6	1	0
2	C	501	6R6	1	0
2	D	501	6R6	1	0
2	E	501	6R6	2	0
2	F	501	6R6	1	0
2	G	501	6R6	1	0
2	H	501	6R6	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 ⓘ

### 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	420/425 (98%)	-0.65	1 (0%) 95 94	9, 25, 59, 79	0
1	B	420/425 (98%)	-0.29	10 (2%) 62 50	12, 29, 81, 110	0
1	C	420/425 (98%)	-0.25	21 (5%) 32 21	9, 28, 86, 114	0
1	D	420/425 (98%)	-0.60	1 (0%) 95 94	11, 26, 66, 89	0
1	E	420/425 (98%)	-0.62	1 (0%) 95 94	10, 25, 59, 85	0
1	F	420/425 (98%)	-0.39	4 (0%) 84 77	11, 30, 67, 85	0
1	G	420/425 (98%)	-0.39	6 (1%) 78 67	10, 28, 70, 93	0
1	H	420/425 (98%)	-0.61	0 100 100	10, 26, 60, 82	0
All	All	3360/3400 (98%)	-0.48	44 (1%) 79 69	9, 27, 71, 114	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	GLU	4.5
1	B	116	ARG	4.1
1	C	114	GLU	4.1
1	B	114	GLU	4.1
1	C	116	ARG	3.7

### 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 [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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	6R6	F	501	13/13	0.96	0.26	3.19	37,44,47,49	0
2	6R6	D	501	13/13	0.93	0.25	2.50	35,48,57,60	0
2	6R6	G	501	13/13	0.95	0.25	2.32	34,44,52,53	0
2	6R6	A	501	13/13	0.95	0.22	2.14	28,34,42,43	0
2	6R6	E	501	13/13	0.93	0.23	1.96	30,38,44,45	0
2	6R6	C	501	13/13	0.86	0.38	1.47	49,61,74,75	0
2	6R6	H	501	13/13	0.96	0.22	1.43	35,43,55,59	0
2	6R6	B	501	13/13	0.90	0.25	0.80	43,47,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.