



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2024 – 08:35 PM EDT

PDB ID : 6N4X  
Title : Metabotropic Glutamate Receptor 5 Apo Form Ligand Binding Domain  
Authors : Koehl, A.; Hu, H.; Feng, D.; Sun, B.; Weis, W.I.; Skiniotis, G.S.; Mathiesen, J.M.; Kobilka, B.K.  
Deposited on : 2018-11-20  
Resolution : 4.00 Å(reported)

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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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

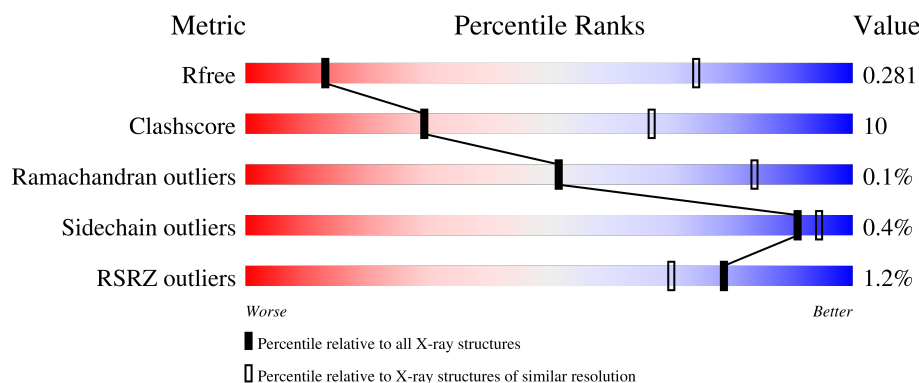
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	877	 45% 13% 42%
1	B	877	 43% 13% 44%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7736 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 Metabotropic glutamate receptor 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3897	2456	666	739	36			
1	B	487	Total	C	N	O	S	0	0	0
			3754	2362	646	712	34			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P41594
A	-4	LYS	-	expression tag	UNP P41594
A	-3	THR	-	expression tag	UNP P41594
A	-2	ILE	-	expression tag	UNP P41594
A	-1	ILE	-	expression tag	UNP P41594
A	0	ALA	-	expression tag	UNP P41594
A	1	LEU	-	expression tag	UNP P41594
A	2	SER	-	expression tag	UNP P41594
A	3	TYR	-	expression tag	UNP P41594
A	4	ILE	-	expression tag	UNP P41594
A	5	PHE	-	expression tag	UNP P41594
A	6	CYS	-	expression tag	UNP P41594
A	7	LEU	-	expression tag	UNP P41594
A	8	VAL	-	expression tag	UNP P41594
A	9	PHE	-	expression tag	UNP P41594
A	10	ALA	-	expression tag	UNP P41594
A	11	ASP	-	expression tag	UNP P41594
A	12	TYR	-	expression tag	UNP P41594
A	13	LYS	-	expression tag	UNP P41594
A	14	ASP	-	expression tag	UNP P41594
A	15	ASP	-	expression tag	UNP P41594
A	16	ASP	-	expression tag	UNP P41594
A	17	ASP	-	expression tag	UNP P41594
A	18	ALA	-	expression tag	UNP P41594
A	19	ALA	-	expression tag	UNP P41594

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Chain	Residue	Modelled	Actual	Comment	Reference
A	866	HIS	-	expression tag	UNP P41594
A	867	HIS	-	expression tag	UNP P41594
A	868	HIS	-	expression tag	UNP P41594
A	869	HIS	-	expression tag	UNP P41594
A	870	HIS	-	expression tag	UNP P41594
A	871	HIS	-	expression tag	UNP P41594
B	-5	MET	-	initiating methionine	UNP P41594
B	-4	LYS	-	expression tag	UNP P41594
B	-3	THR	-	expression tag	UNP P41594
B	-2	ILE	-	expression tag	UNP P41594
B	-1	ILE	-	expression tag	UNP P41594
B	0	ALA	-	expression tag	UNP P41594
B	1	LEU	-	expression tag	UNP P41594
B	2	SER	-	expression tag	UNP P41594
B	3	TYR	-	expression tag	UNP P41594
B	4	ILE	-	expression tag	UNP P41594
B	5	PHE	-	expression tag	UNP P41594
B	6	CYS	-	expression tag	UNP P41594
B	7	LEU	-	expression tag	UNP P41594
B	8	VAL	-	expression tag	UNP P41594
B	9	PHE	-	expression tag	UNP P41594
B	10	ALA	-	expression tag	UNP P41594
B	11	ASP	-	expression tag	UNP P41594
B	12	TYR	-	expression tag	UNP P41594
B	13	LYS	-	expression tag	UNP P41594
B	14	ASP	-	expression tag	UNP P41594
B	15	ASP	-	expression tag	UNP P41594
B	16	ASP	-	expression tag	UNP P41594
B	17	ASP	-	expression tag	UNP P41594
B	18	ALA	-	expression tag	UNP P41594
B	19	ALA	-	expression tag	UNP P41594
B	866	HIS	-	expression tag	UNP P41594
B	867	HIS	-	expression tag	UNP P41594
B	868	HIS	-	expression tag	UNP P41594
B	869	HIS	-	expression tag	UNP P41594
B	870	HIS	-	expression tag	UNP P41594
B	871	HIS	-	expression tag	UNP P41594

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

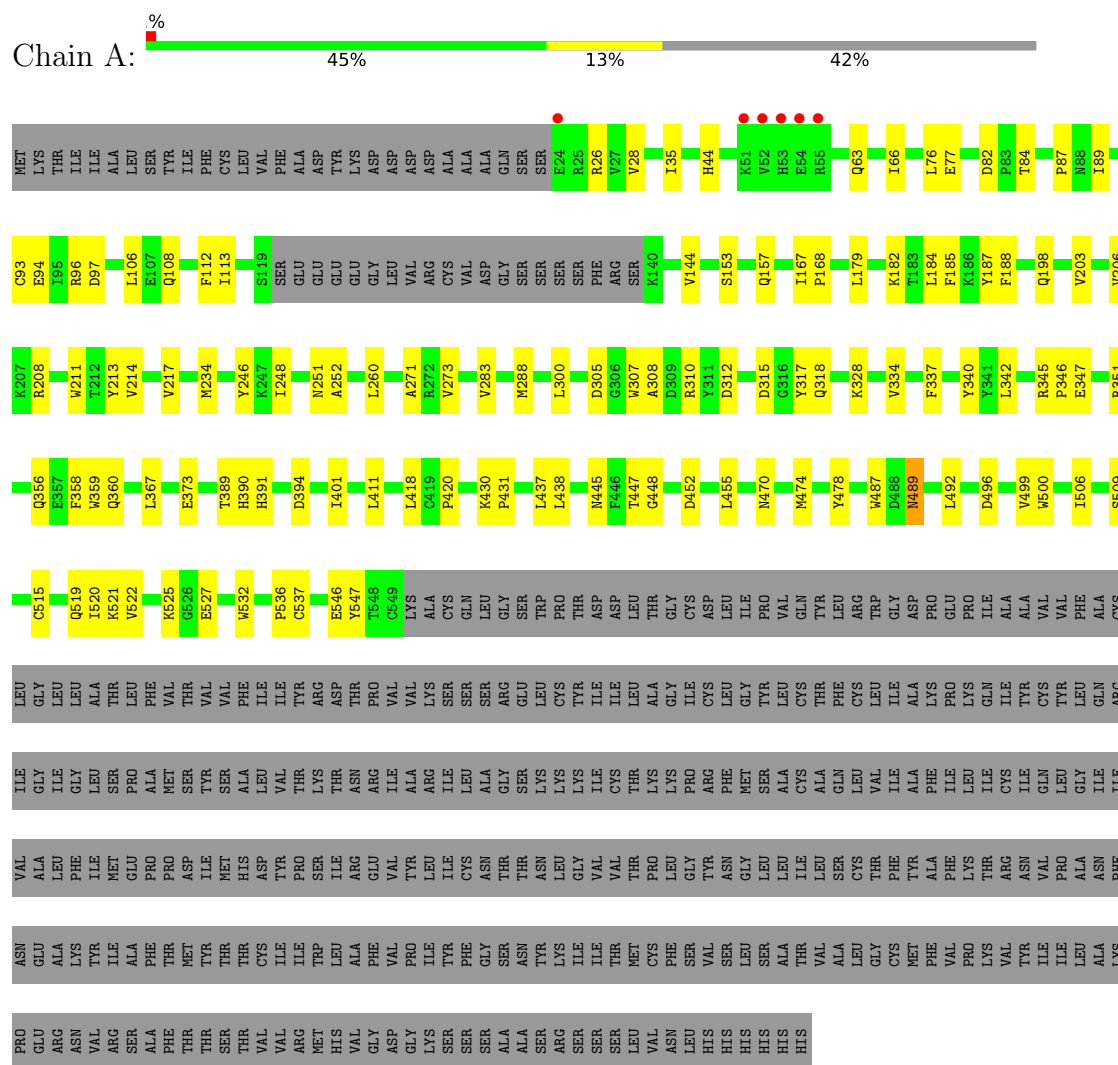
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

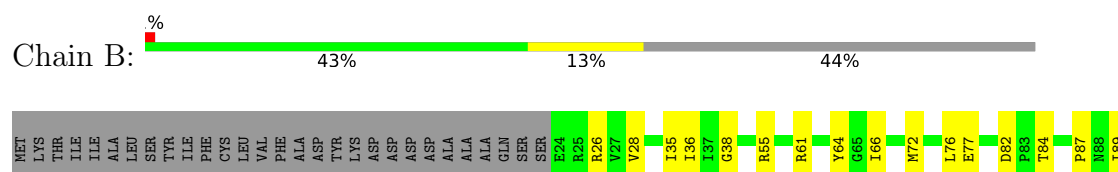
### 3 Residue-property plots

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: Metabotropic glutamate receptor 5



#### • Molecule 1: Metabotropic glutamate receptor 5



THR	THR	VAL	LEU	TRP	V499	K503	K502	W501	L367	Q360	D195	C93
CYS	PHE	ILE	ILE	GLY	LEU	ILE	ALA	ASP	ALA	GLY	GLY	E94
MET	TYR	ALA	ALA	PRO	LYS	PRO	LYS	LYS	PRO	GLU	GLU	I95
VAL	PHE	ILE	ILE	GLY	ILE	ILE	ILE	ILE	ILE	ILE	ILE	R96
PRO	LYS	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	L106
LYS	THR	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	E107
VAL	ARG	CYS	CYS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	Q108
TYR	ASN	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	S109
ILE	VAL	GLN	CYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	I110
ILE	PRO	GLY	ILE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	E111
LEU	ALA	ILE	ILE	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F112
ALA	ASN	ILE	GLN	ALA	ARG	ARG	ARG	ARG	ARG	ARG	ARG	I113
LYS	PHE	ILE	ILE	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	R114
PRO	ASN	VAL	ILE	LEU	ILE	ILE	ILE	ILE	ILE	ILE	ILE	D115
GLU	GLU	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	S116
ARG	ALA	LEU	ILE	LEU	ILE	ILE	ILE	ILE	ILE	ILE	ILE	L117
ASN	LYS	PHE	GLY	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	I118
VAL	TYR	ILE	ILE	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	SER
ARG	ILE	MET	SER	THR	THR	THR	THR	THR	THR	THR	THR	SER
ARG	ALA	GLU	PRO	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	GLU
SER	ALA	PHE	PRO	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	GLU
PHE	THR	THR	PRO	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLU
THR	MET	ILE	ILE	THR	THR	THR	THR	THR	THR	THR	THR	GLY
THR	THR	MET	SER	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY
SER	THR	THR	SER	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	LEU
THR	THR	HIS	THR	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	VAL
VAL	THR	VAL	THR	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	VAL
GLY	ASP	GLY	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ARG
ASP	GLY	GLY	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	CYS
GLY	GLY	GLY	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
LYS	ILE	ILE	ILE	THR	THR	THR	THR	THR	THR	THR	THR	VAL
SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASP
SER	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY
SER	GLY	ASN	ASN	SER	SER	SER	SER	SER	SER	SER	SER	SER
ALA	ALA	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ASN	THR	THR	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ASP
SER	TYR	ASN	LYS	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ASP
ARG	LYS	ILE	LYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	GLY
SER	ILE	GLY	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR
SER	ILE	VAL	VAL	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	THR
SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	P141
SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	P142
SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	T143
LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	V144
ASN	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	G145
LEU	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	Q157
HIS	HIS	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	P168
HIS	HIS	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	L179
HIS	HIS	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	K182
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	T183
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	L184
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F185
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F186
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	R187
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F188
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F189
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F190
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F191
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HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F194
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F195
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HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F197
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F198
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F199
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HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F206
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F207
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F208
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F209
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F210
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F211
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F212
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F213
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HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F215
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HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F219
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F220
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HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F223
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HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F226
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F227
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HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F230
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HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F239
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F240
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F241
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HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F243
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HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F246
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HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F248
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F249
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F250
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F251
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HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F253
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F254
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F255
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F256
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F257
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F258
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F259
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F260
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F261
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F262
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F263
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F264
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F265
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F266
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F267
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F268
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F269
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F270
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F271
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F272
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F273
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F274
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F275
HIS	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	F276
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	F277
HIS	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F278
HIS	HIS	VAL	VAL	VAL								

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.08Å 174.10Å 180.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 4.00 49.57 – 4.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.57-4.00) 83.5 (49.57-4.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.14 _3211	Depositor
R, $R_{free}$	0.270 , 0.282 0.268 , 0.281	Depositor DCC
$R_{free}$ test set	1540 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	172.6	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 160.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.064 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	184.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: NAG, MG

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	0.25	0/3985	0.45	0/5407
1	B	0.24	0/3836	0.45	0/5200
All	All	0.25	0/7821	0.45	0/10607

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	3897	0	3649	73	0
1	B	3754	0	3546	71	0
2	A	56	0	52	0	0
2	B	28	0	26	0	0
3	B	1	0	0	0	0
All	All	7736	0	7273	143	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 10.

The worst 5 of 143 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ILE:HD13	1:A:546:GLU:C	1.90	0.90
1:A:77:GLU:OE2	1:A:351:ARG:NH1	2.18	0.76
1:B:77:GLU:OE2	1:B:351:ARG:NH1	2.19	0.74
1:B:360:GLN:HE22	1:B:373:GLU:HA	1.52	0.74
1:A:360:GLN:HE22	1:A:373:GLU:HA	1.53	0.73

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	502/877 (57%)	471 (94%)	31 (6%)	0	100	100
1	B	481/877 (55%)	453 (94%)	27 (6%)	1 (0%)	47	79
All	All	983/1754 (56%)	924 (94%)	58 (6%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	521	LYS

### 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	412/763 (54%)	411 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	399/763 (52%)	397 (100%)	2 (0%)	88	93
All	All	811/1526 (53%)	808 (100%)	3 (0%)	91	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	489	ASN
1	B	465	ARG
1	B	489	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	157	GLN
1	B	166	ASN
1	B	364	GLN
1	B	218	HIS
1	B	244	HIS

### 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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	NAG	A	902	1	14,14,15	0.28	0	17,19,21	0.59	0
2	NAG	A	904	1	14,14,15	0.45	0	17,19,21	0.67	1 (5%)
2	NAG	B	902	1	14,14,15	0.36	0	17,19,21	0.63	1 (5%)
2	NAG	B	903	1	14,14,15	0.44	0	17,19,21	0.56	0
2	NAG	A	901	1	14,14,15	0.35	0	17,19,21	0.46	0
2	NAG	A	903	1	14,14,15	0.35	0	17,19,21	0.48	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
2	NAG	A	902	1	-	0/6/23/26	0/1/1/1
2	NAG	A	904	1	-	2/6/23/26	0/1/1/1
2	NAG	B	902	1	-	0/6/23/26	0/1/1/1
2	NAG	B	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	901	1	-	2/6/23/26	0/1/1/1
2	NAG	A	903	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	NAG	C1-O5-C5	2.22	115.20	112.19
2	A	904	NAG	C1-O5-C5	2.19	115.15	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	NAG	O5-C5-C6-O6
2	A	901	NAG	C4-C5-C6-O6
2	A	904	NAG	O5-C5-C6-O6
2	A	904	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [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	506/877 (57%)	-0.19	6 (1%) 79 70	127, 180, 254, 270	0
1	B	487/877 (55%)	-0.20	6 (1%) 79 70	114, 183, 252, 292	0
All	All	993/1754 (56%)	-0.19	12 (1%) 79 70	114, 181, 254, 292	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	GLU	4.6
1	B	222	ASN	3.8
1	A	51	LYS	3.5
1	B	372	GLN	3.3
1	A	52	VAL	3.2

### 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](#)

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( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	903	14/15	0.59	0.26	214,233,238,244	0
2	NAG	A	901	14/15	0.62	0.28	200,209,217,221	0
2	NAG	B	902	14/15	0.64	0.27	184,210,226,226	0
2	NAG	A	902	14/15	0.72	0.24	200,219,226,230	0
2	NAG	A	904	14/15	0.84	0.16	193,206,212,217	0
2	NAG	B	903	14/15	0.84	0.24	222,240,245,248	0
3	MG	B	901	1/1	0.92	0.10	165,165,165,165	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.