



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 08:34 PM BST

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)

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

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

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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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

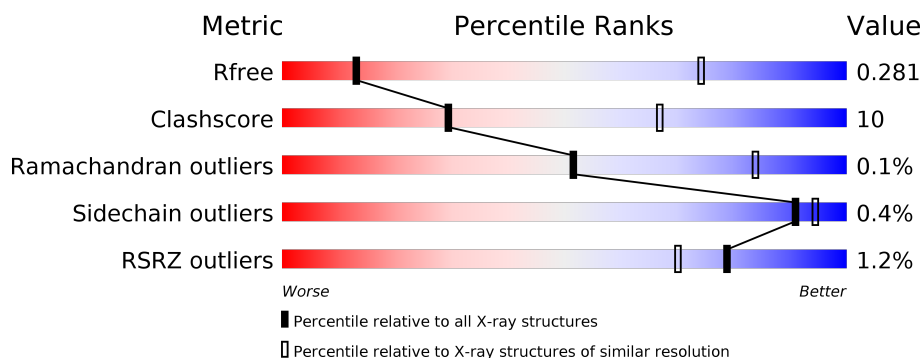
# 1 Overall quality at a glance

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 on 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	<div> <div>%</div> <div> <div></div> <div>45%</div> <div>13%</div> <div>42%</div> </div> </div>
1	B	877	<div> <div>%</div> <div> <div></div> <div>43%</div> <div>13%</div> <div>44%</div> </div> </div>

## 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		

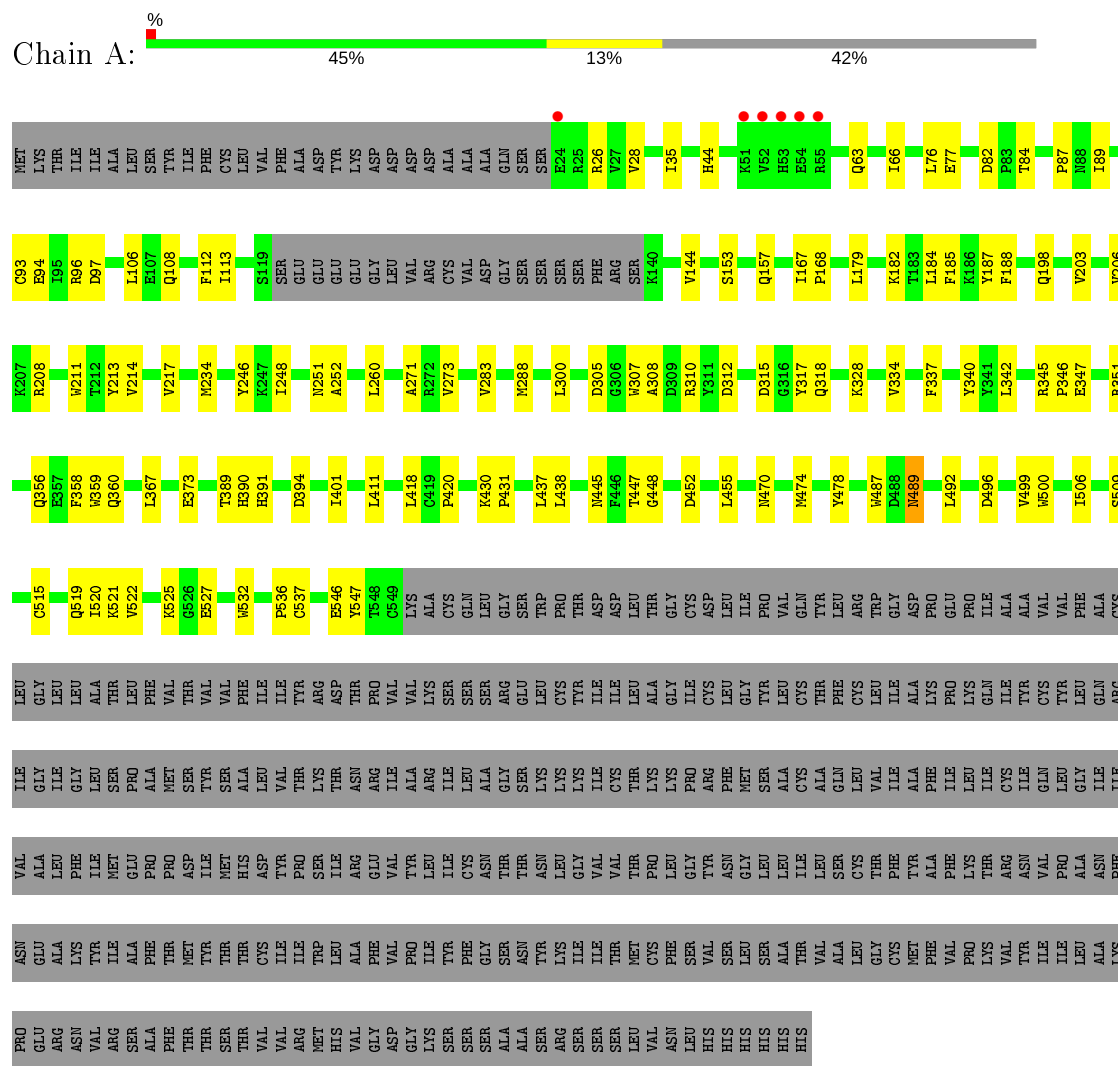
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

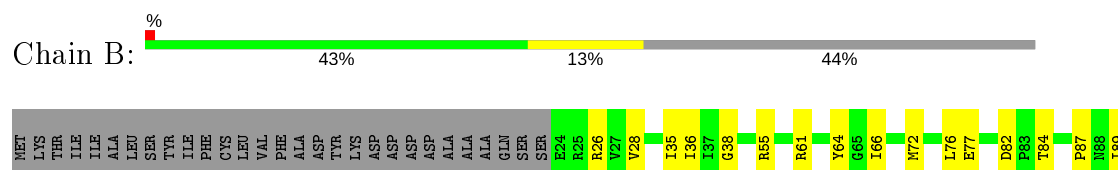
### 3 Residue-property plots

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



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THR	THR	VAL	LEU	TRP	V499	Q360	D195	C93
PHE	PHE	ILE	ILE	GLY	V499	Q360	D195	C93
TYR	TYR	ALA	ALA	ASP	V500	L367	Q198	E94
ALA	ALA	LYS	LYS	PRO	S501			I95
VAL	VAL	PRO	PRO	GLU	K502	F370	V203	R96
PRO	PRO	LYS	LYS	PRO	K503	P371	D204	L106
LYS	LYS	GLN	GLN	ILE	K506	Q372	I205	E107
VAL	VAL	ILE	ILE	ALA	I506	E373	I206	Q108
TYR	ASN	ILE	TYR	ALA	S509	R374	R207	S109
ILE	VAL	GLN	CYS	VAL			R208	I110
ILE	VAL	LEU	TYR	VAL	C515	T389		E111
LEU	ALA	GLY	LEU	PHE		H390		F112
ALA	ASN	ILE	GLN	ALA		H391		I113
LYS	PHE	ILE	ARG	CYS	Q519	T382		R114
PRO	ASN	VAL	ILE	LEU	K520	Q393		D115
GLU	GLU	ALA	GLY	GLY	I521	D394		S116
ARG	ALA	LEU	ILE	LEU	K525	K397		L117
ASN	LYS	PHE	GLY	LEU				I118
VAL	TYR	ILE	LEU	ALA	T533	I401		SER
ARG	ILE	MET	SER	THR				SER
SER	ALA	GLU	PRO	LEU	P536	I404		GLU
ALA	PHE	PRO	ALA	PHE	CYS			GLU
PHE	THR	PRO	MET	VAL				GLU
THR	MET	ASP	SER	THR	LYS	I411		GLU
THR	TYR	ILE	TYR	VAL				GLY
SER	THR	MET	SER	VAL				LEU
THR	THR	HIS	SER	PHE	L418	L418		VAL
VAL	THR	ASP	GLU	ILE	C419	C419		VAL
VAL	VAL	ILE	ILE	ILE	P420	P420		ARG
ARG	ILE	TYR	VAL	ILE	G421	G421		CYS
MET	ILE	PRO	THR	TYR	Y422	Y422		VAL
HIS	THR	SER	LYS	ARG				ASP
VAL	LEU	ILE	THR	ASP	A428	A428		GLY
VAL	ALA	ARG	THR	THR	P429	P429		GLY
GLY	PHE	GLU	ASN	THR	K430	K430		SER
ASP	ASP	VAL	ILE	VAL	P431	P431		SER
GLY	PRO	TYR	ALA	VAL				SER
LYS	ILE	LEU	ARG	LYS	L437	L437		SER
SER	TYR	ILE	ILE	SER	L438	L438		PHE
SER	PHE	CYS	LEU	SER				ARG
SER	GLY	ASN	ALA	SER	G448	G448		SER
ALA	ALA	THR	GLY	ARG				ARG
SER	ASN	THR	LYS	GLU	D452	D452		K140
ARG	LYS	ASN	LYS	LEU				K141
SER	ILE	LEU	LYS	CYS	R465	R465		P142
SER	ILE	GLY	LYS	THR				I143
SER	ILE	VAL	ILE	ILE	N470	N470		V144
LEU	THR	VAL	CYS	LEU				G145
LEU	MET	THR	THR	LEU	P474	P474		Q157
VAL	CYS	PRO	LYS	ALA	GLY	GLY		P168
ASN	PHE	LEU	LYS	GLY	LYS	LYS		
LEU	SER	GLY	PRO	ILE	ASP	ASP		L179
HIS	VAL	TYR	ARG	CYS	THR	THR		K182
HIS	SER	ASN	PHE	LEU	CYS	CYS		T183
HIS	LEU	GLY	MET	GLY	ILE	ILE		I184
HIS	SER	LEU	SER	TYR	PRO	PRO		F185
ALA	ALA	LEU	LEU	LEU	V487	V487		R186
THR	THR	ILE	CYS	CYS	D486	D486		F187
VAL	VAL	LEU	ALA	THR	R489	R489		Y187
ALA	ALA	SER	GLN	PHE				F188
LEU	LEU	CYS	LEU	CYS	D496	D496		

## 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: MG, NAG

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.

All (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
1:A:522:VAL:HG22	1:A:547:TYR:HA	1.72	0.70
1:B:419:CYS:HB3	1:B:422:TYR:HB2	1.74	0.69
1:B:198:GLN:HE22	1:B:305:ASP:H	1.40	0.69
1:A:182:LYS:NZ	1:A:188:PHE:O	2.27	0.67
1:A:198:GLN:HE22	1:A:305:ASP:H	1.42	0.66
1:B:182:LYS:NZ	1:B:188:PHE:O	2.29	0.65
1:A:82:ASP:OD2	1:A:84:THR:OG1	2.11	0.64
1:A:94:GLU:OE2	1:A:96:ARG:NH2	2.32	0.63
1:A:447:THR:HG21	1:B:428:ALA:HB2	1.80	0.63
1:B:213:TYR:O	1:B:509:SER:OG	2.16	0.63
1:B:106:LEU:HD21	1:B:157:GLN:HB3	1.81	0.61
1:A:198:GLN:NE2	1:A:305:ASP:H	1.97	0.61
1:B:525:LYS:HG2	1:B:533:THR:HG23	1.82	0.61
1:A:345:ARG:HD3	1:A:346:PRO:HD2	1.83	0.60
1:A:106:LEU:HD21	1:A:157:GLN:HB3	1.83	0.60
1:B:311:TYR:OH	1:B:480:ASP:OD1	2.16	0.60
1:B:109:SER:HA	1:B:112:PHE:HD2	1.65	0.60
1:A:520:ILE:HD13	1:A:546:GLU:O	2.02	0.60
1:B:345:ARG:HD3	1:B:346:PRO:HD2	1.84	0.59
1:A:35:ILE:HG23	1:A:144:VAL:HG21	1.83	0.59
1:A:310:ARG:HG2	1:A:312:ASP:OD1	2.03	0.59
1:B:208:ARG:NH1	1:B:496:ASP:OD1	2.31	0.58
1:B:342:LEU:HD21	1:B:391:HIS:CG	2.39	0.57
1:B:35:ILE:HG23	1:B:144:VAL:HG21	1.86	0.57
1:A:487:TRP:HD1	1:A:492:LEU:HD13	1.71	0.56
1:A:213:TYR:O	1:A:509:SER:OG	2.22	0.56
1:A:342:LEU:HD21	1:A:391:HIS:CG	2.41	0.55
1:A:525:LYS:HG3	1:A:527:GLU:H	1.71	0.55
1:A:26:ARG:HD2	1:A:108:GLN:NE2	2.21	0.55
1:A:168:PRO:HG2	1:A:437:LEU:HD23	1.88	0.55
1:A:203:VAL:HG21	1:A:234:MET:HB2	1.89	0.54
1:A:208:ARG:NH1	1:A:496:ASP:OD1	2.27	0.54
1:A:340:TYR:OH	1:A:351:ARG:NH2	2.33	0.54
1:A:28:VAL:HG11	1:A:94:GLU:HG3	1.88	0.54
1:A:519:GLN:HB3	1:A:536:PRO:HA	1.89	0.54
1:B:198:GLN:NE2	1:B:305:ASP:H	2.04	0.54
1:B:206:VAL:HG13	1:B:211:TRP:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLU:OE2	1:B:96:ARG:NH2	2.41	0.53
1:A:520:ILE:HG13	1:A:521:LYS:H	1.74	0.53
1:B:203:VAL:HG21	1:B:234:MET:HB2	1.90	0.53
1:B:82:ASP:OD2	1:B:84:THR:OG1	2.13	0.53
1:A:345:ARG:HG3	1:A:347:GLU:H	1.74	0.53
1:B:109:SER:O	1:B:113:ILE:HG12	2.09	0.53
1:A:182:LYS:HZ3	1:A:188:PHE:HB3	1.73	0.52
1:B:288:MET:HG2	1:B:317:TYR:CZ	2.45	0.52
1:B:345:ARG:HG3	1:B:347:GLU:H	1.74	0.52
1:A:44:HIS:ND1	1:A:97:ASP:OD2	2.42	0.51
1:A:500:TRP:CD1	1:A:506:ILE:HG12	2.46	0.51
1:A:273:VAL:HG22	1:A:300:LEU:HD23	1.93	0.51
1:A:519:GLN:HB3	1:A:537:CYS:H	1.76	0.51
1:A:334:VAL:HG21	1:A:401:ILE:HD12	1.94	0.50
1:B:179:LEU:HD13	1:B:188:PHE:CZ	2.47	0.50
1:B:418:LEU:O	1:B:420:PRO:HD3	2.11	0.50
1:B:26:ARG:HD2	1:B:108:GLN:NE2	2.27	0.49
1:B:499:VAL:HG13	1:B:500:TRP:CD1	2.47	0.49
1:B:61:ARG:HG2	1:B:64:TYR:HB2	1.93	0.49
1:A:520:ILE:CD1	1:A:546:GLU:C	2.75	0.49
1:A:499:VAL:HG13	1:A:500:TRP:CD1	2.47	0.49
1:B:36:ILE:HD12	1:B:141:LYS:HB3	1.94	0.49
1:A:448:GLY:N	1:A:452:ASP:O	2.31	0.49
1:B:28:VAL:HG11	1:B:94:GLU:HG3	1.93	0.49
1:B:76:LEU:CD1	1:B:93:CYS:HB3	2.43	0.48
1:B:334:VAL:HG21	1:B:401:ILE:HD12	1.94	0.48
1:A:515:CYS:SG	1:A:532:TRP:NE1	2.85	0.48
1:A:248:ILE:HB	1:A:260:LEU:HD13	1.94	0.48
1:A:474:MET:O	1:A:478:TYR:HB3	2.12	0.48
1:A:418:LEU:O	1:A:420:PRO:HD3	2.13	0.48
1:A:179:LEU:HD13	1:A:188:PHE:CZ	2.49	0.47
1:A:288:MET:HG2	1:A:317:TYR:CZ	2.49	0.47
1:A:445:ASN:HB2	1:A:455:LEU:HD12	1.95	0.47
1:A:206:VAL:HG13	1:A:211:TRP:HB2	1.96	0.47
1:A:144:VAL:HG11	1:A:411:LEU:HD21	1.96	0.47
1:B:168:PRO:HG2	1:B:437:LEU:HD23	1.97	0.47
1:B:76:LEU:HD11	1:B:93:CYS:HB3	1.96	0.47
1:A:76:LEU:CD1	1:A:93:CYS:HB3	2.45	0.47
1:B:28:VAL:HG22	1:B:96:ARG:HG2	1.97	0.47
1:B:489:ASN:C	1:B:489:ASN:HD22	2.18	0.47
1:B:470:ASN:ND2	1:B:499:VAL:HG23	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:TYR:CD1	1:B:438:LEU:HD22	2.50	0.46
1:A:489:ASN:C	1:A:489:ASN:HD22	2.19	0.46
1:B:117:LEU:HD13	1:B:117:LEU:O	2.15	0.45
1:B:87:PRO:O	1:B:89:ILE:HD12	2.16	0.45
1:A:521:LYS:HD3	1:A:537:CYS:HA	1.99	0.45
1:A:187:TYR:CD1	1:A:438:LEU:HD22	2.51	0.45
1:B:502:LYS:HG2	1:B:503:LYS:N	2.32	0.45
1:A:96:ARG:HD3	1:A:108:GLN:HB3	1.98	0.45
1:A:28:VAL:HG22	1:A:96:ARG:HG2	1.97	0.45
1:A:470:ASN:ND2	1:A:499:VAL:HG23	2.31	0.45
1:B:283:VAL:HG11	1:B:307:TRP:CE3	2.52	0.45
1:B:367:LEU:HB3	1:B:370:PHE:CD2	2.51	0.44
1:B:244:HIS:CE1	1:B:246:TYR:CZ	3.05	0.44
1:B:448:GLY:N	1:B:452:ASP:O	2.37	0.44
1:A:389:THR:HG22	1:A:390:HIS:ND1	2.33	0.44
1:B:114:ARG:O	1:B:117:LEU:HB2	2.18	0.44
1:B:184:LEU:HD22	1:B:185:PHE:CZ	2.53	0.44
1:B:356:GLN:O	1:B:360:GLN:HG3	2.18	0.44
1:A:251:ASN:OD1	1:A:252:ALA:N	2.51	0.44
1:B:389:THR:HG22	1:B:390:HIS:ND1	2.32	0.44
1:A:87:PRO:O	1:A:89:ILE:HD12	2.16	0.44
1:B:394:ASP:HB3	1:B:397:MET:HB2	2.00	0.44
1:B:500:TRP:CD1	1:B:506:ILE:HG12	2.52	0.44
1:A:315:ASP:HA	1:A:318:GLN:HE21	1.82	0.44
1:B:144:VAL:HG11	1:B:411:LEU:HD21	2.00	0.44
1:A:94:GLU:HG2	1:A:112:PHE:HE1	1.83	0.44
1:A:356:GLN:O	1:A:360:GLN:HG3	2.18	0.43
1:B:204:ASP:OD2	1:B:487:TRP:HH2	2.01	0.43
1:B:346:PRO:HD3	1:B:359:TRP:CE3	2.53	0.43
1:A:213:TYR:CD2	1:A:271:ALA:HB2	2.54	0.43
1:A:63:GLN:HG2	1:A:394:ASP:HA	2.00	0.43
1:B:430:LYS:HA	1:B:431:PRO:HA	1.86	0.43
1:B:26:ARG:NH2	1:B:55:ARG:O	2.52	0.43
1:B:337:PHE:HD2	1:B:393:GLN:HE21	1.66	0.42
1:B:38:GLY:N	1:B:145:GLY:O	2.52	0.42
1:B:213:TYR:CD2	1:B:271:ALA:HB2	2.55	0.42
1:A:334:VAL:HG12	1:A:337:PHE:H	1.84	0.42
1:A:346:PRO:HD3	1:A:359:TRP:CE3	2.54	0.42
1:B:66:ILE:HG13	1:B:358:PHE:CG	2.54	0.42
1:B:334:VAL:HG12	1:B:337:PHE:H	1.85	0.42
1:A:184:LEU:HD22	1:A:185:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HG13	1:A:358:PHE:CG	2.55	0.42
1:A:283:VAL:HG11	1:A:307:TRP:CE3	2.55	0.41
1:A:308:ALA:HB1	1:A:328:LYS:HA	2.01	0.41
1:B:182:LYS:HZ3	1:B:188:PHE:HB3	1.85	0.41
1:B:280:GLY:HA3	1:B:310:ARG:NH1	2.34	0.41
1:B:515:CYS:HB3	1:B:519:GLN:O	2.20	0.41
1:B:346:PRO:HG3	1:B:359:TRP:CG	2.55	0.41
1:A:214:VAL:HG12	1:A:273:VAL:HB	2.02	0.41
1:B:359:TRP:CD1	1:B:367:LEU:HD21	2.56	0.41
1:B:168:PRO:HA	1:B:187:TYR:HB3	2.03	0.41
1:B:118:ILE:HD12	1:B:142:PRO:HD3	2.03	0.41
1:A:113:ILE:HG22	1:A:167:ILE:HD12	2.03	0.41
1:B:340:TYR:OH	1:B:351:ARG:NH2	2.36	0.41
1:B:72:MET:HA	1:B:404:ILE:HD13	2.03	0.41
1:A:217:VAL:HG22	1:A:246:TYR:HB2	2.02	0.41
1:A:153:SER:O	1:A:157:GLN:NE2	2.54	0.41
1:A:359:TRP:CD1	1:A:367:LEU:HD21	2.55	0.41
1:A:430:LYS:HA	1:A:431:PRO:HA	1.84	0.40
1:B:111:GLU:O	1:B:115:ASP:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	157	GLN
1	A	166	ASN
1	A	198	GLN
1	A	364	GLN
1	B	45	HIS
1	B	74	HIS
1	B	157	GLN
1	B	166	ASN
1	B	198	GLN
1	B	218	HIS
1	B	244	HIS
1	B	364	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	904	1	-	2/6/23/26	0/1/1/1
2	NAG	B	903	1	-	0/6/23/26	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 [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	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

All (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
1	B	371	PRO	2.9
1	B	221	GLY	2.7
1	A	55	ARG	2.7
1	A	24	GLU	2.5
1	A	53	HIS	2.5
1	B	374	ASN	2.4
1	B	195	ASP	2.3

### 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(Å <sup>2</sup> )	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	B	903	14/15	0.84	0.24	222,240,245,248	0
2	NAG	A	904	14/15	0.84	0.16	193,206,212,217	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.