



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 11, 2016 – 04:17 PM EDT

PDB ID : 5AWC  
Title : Crystal structure of human TLR8 in complex with MB-564  
Authors : Tanji, H.; Ohto, U.; Shimizu, T.  
Deposited on : 2015-07-03  
Resolution : 2.50 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-20027790  
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-20027790

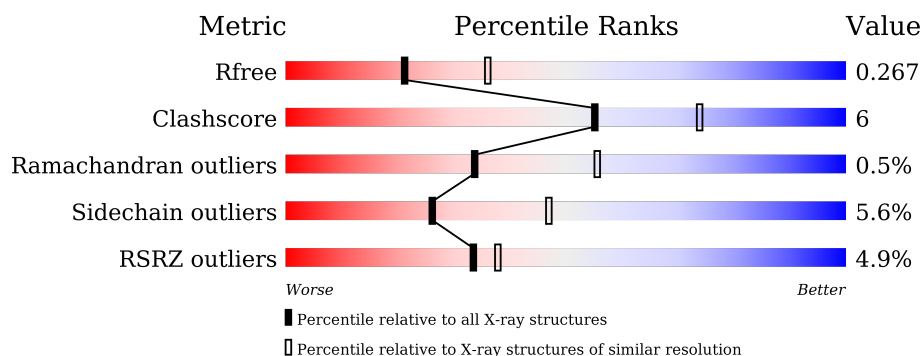
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	811	
1	B	811	
1	C	811	
1	D	811	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	M4D	C	1011	-	-	-	X
4	M4D	D	901	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24478 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	749	Total	C	N	O	S	0	0	0
			6035	3862	1023	1131	19			
1	B	742	Total	C	N	O	S	0	0	0
			5979	3828	1015	1117	19			
1	C	727	Total	C	N	O	S	0	0	0
			5871	3760	998	1094	19			
1	D	724	Total	C	N	O	S	0	0	0
			5836	3735	990	1092	19			

There are 40 discrepancies between the modelled and reference sequences:

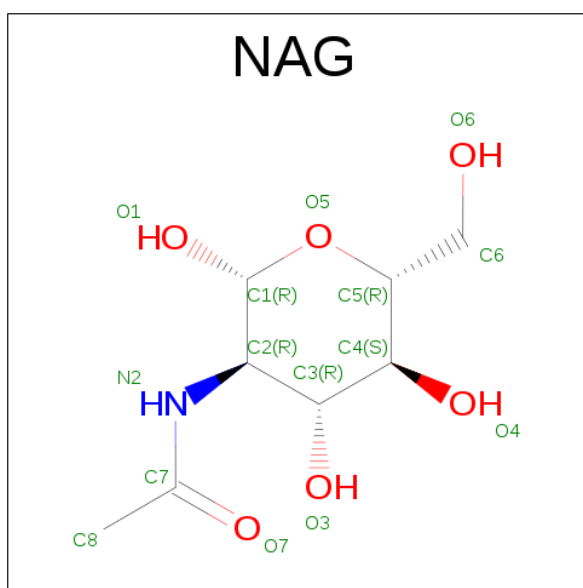
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97
C	23	ARG	-	expression tag	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	SER	-	expression tag	UNP Q9NR97
C	25	PRO	-	expression tag	UNP Q9NR97
C	26	TRP	-	expression tag	UNP Q9NR97
C	828	GLU	-	expression tag	UNP Q9NR97
C	829	PHE	-	expression tag	UNP Q9NR97
C	830	LEU	-	expression tag	UNP Q9NR97
C	831	VAL	-	expression tag	UNP Q9NR97
C	832	PRO	-	expression tag	UNP Q9NR97
C	833	ARG	-	expression tag	UNP Q9NR97
D	23	ARG	-	expression tag	UNP Q9NR97
D	24	SER	-	expression tag	UNP Q9NR97
D	25	PRO	-	expression tag	UNP Q9NR97
D	26	TRP	-	expression tag	UNP Q9NR97
D	828	GLU	-	expression tag	UNP Q9NR97
D	829	PHE	-	expression tag	UNP Q9NR97
D	830	LEU	-	expression tag	UNP Q9NR97
D	831	VAL	-	expression tag	UNP Q9NR97
D	832	PRO	-	expression tag	UNP Q9NR97
D	833	ARG	-	expression tag	UNP Q9NR97

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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		

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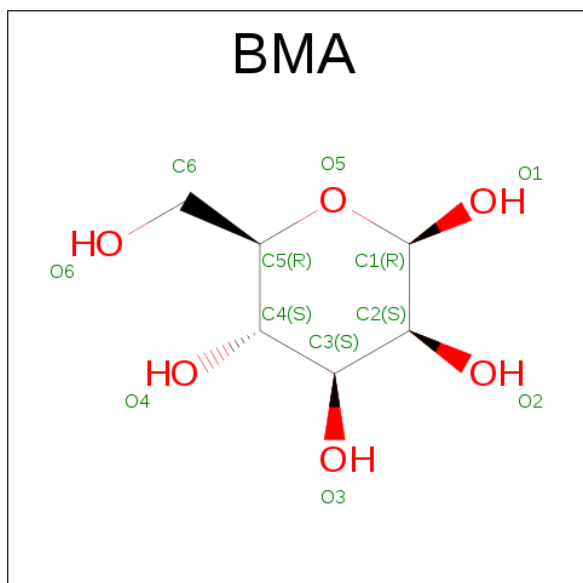
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



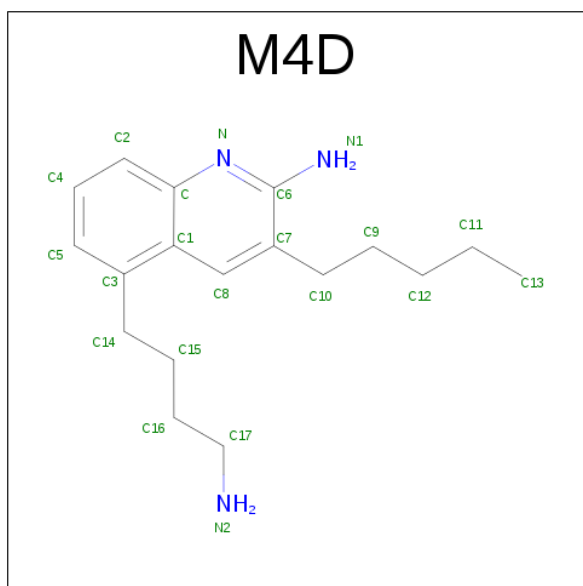
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is 5-(4-azanylbutyl)-3-pentyl-quinolin-2-amine (three-letter code: M4D) (formula: C<sub>18</sub>H<sub>27</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			21	18	3		
4	B	1	Total	C	N	0	0
			21	18	3		
4	C	1	Total	C	N	0	0
			21	18	3		
4	D	1	Total	C	N	0	0
			21	18	3		

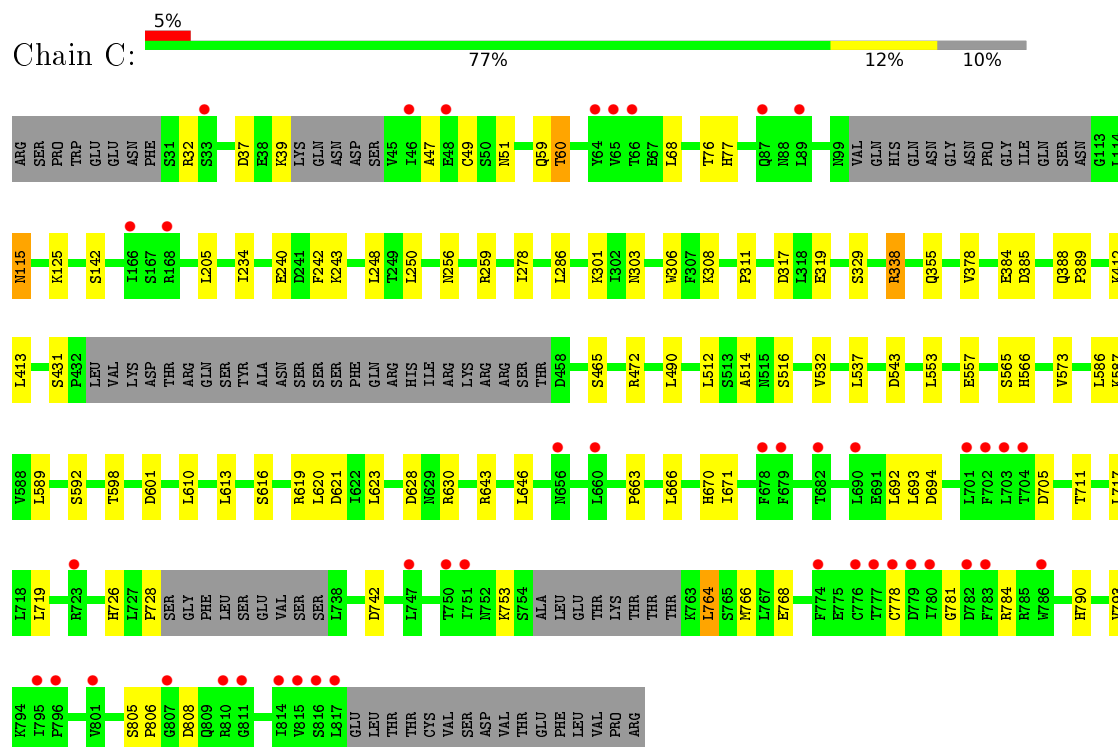


- Molecule 5 is water.

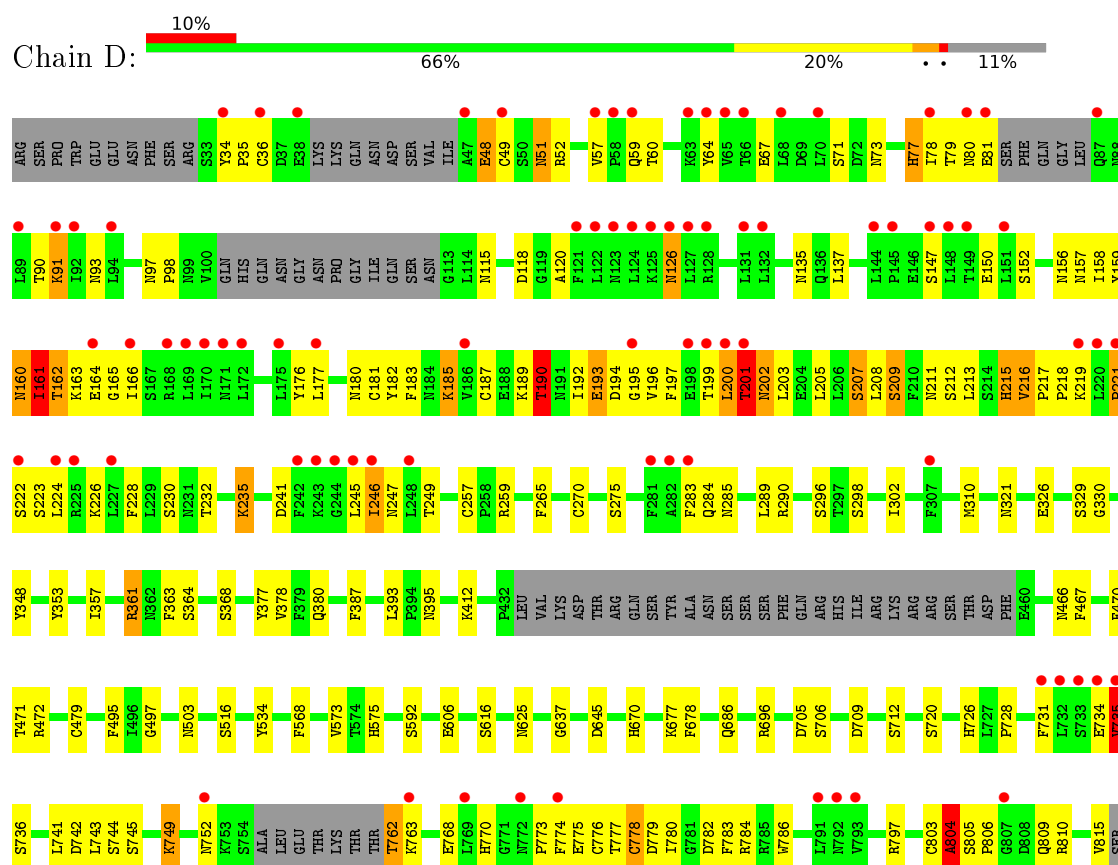
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total 38	O 38	0	0
5	B	42	Total 42	O 42	0	0
5	C	21	Total 21	O 21	0	0
5	D	22	Total 22	O 22	0	0



• Molecule 1: Toll-like receptor 8



• Molecule 1: Toll-like receptor 8



LEU
GLU
LEU
THR
THR
CYS
VAL
SER
ASP
VAL
THR
GLU
PHE
LEU
VAL
PRO
ARG

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.40 Å 140.18 Å 169.60 Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	47.48 – 2.50 47.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.7 (47.48-2.50) 94.7 (47.48-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.209 , 0.269 0.212 , 0.267	Depositor DCC
$R_{free}$ test set	6664 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24478	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: BMA, NAG, M4D

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	1/6159 (0.0%)	0.77	5/8351 (0.1%)
1	B	0.57	0/6102	0.74	0/8272
1	C	0.53	0/5992	0.71	2/8122 (0.0%)
1	D	0.56	0/5956	0.73	4/8076 (0.0%)
All	All	0.57	1/24209 (0.0%)	0.74	11/32821 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	PRO	N-CD	5.08	1.54	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	217	PRO	C-N-CD	6.40	141.84	128.40
1	A	270	CYS	CA-CB-SG	6.22	125.20	114.00
1	D	216	VAL	C-N-CD	6.14	141.29	128.40
1	C	338	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	A	225	ARG	NE-CZ-NH1	5.89	123.25	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	779	ASP	Peptide
1	C	242	PHE	Peptide
1	D	161	ILE	Peptide
1	D	201	THR	Peptide
1	D	803	CYS	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	6035	0	6028	62	1
1	B	5979	0	5969	57	1
1	C	5871	0	5857	37	0
1	D	5836	0	5817	148	0
2	A	126	0	112	2	0
2	B	112	0	99	0	0
2	C	112	0	99	0	0
2	D	112	0	99	1	0
3	A	22	0	20	0	0
3	B	22	0	20	0	0
3	C	22	0	20	0	0
3	D	22	0	20	0	0
4	A	21	0	0	1	0
4	B	21	0	0	1	0
4	C	21	0	0	1	0
4	D	21	0	0	0	0
5	A	38	0	0	2	0
5	B	42	0	0	0	0
5	C	21	0	0	0	0
5	D	22	0	0	0	0
All	All	24478	0	24160	302	1

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 6.

The worst 5 of 302 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:D:197:PHE:O	1:D:200:LEU:CD2	1.64	1.43
1:D:197:PHE:O	1:D:200:LEU:HD22	1.15	1.15
1:D:181:CYS:SG	1:D:187:CYS:CB	2.36	1.14
1:D:162:THR:HG1	1:D:164:GLU:HG2	1.01	1.09
1:D:177:LEU:O	1:D:208:LEU:HA	1.52	1.09

All (1) 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:A:709:ASP:OD1	1:B:338:ARG:NH2[2_546]	2.13	0.07

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/811 (91%)	691 (93%)	47 (6%)	3 (0%)	39	61
1	B	732/811 (90%)	675 (92%)	55 (8%)	2 (0%)	46	68
1	C	715/811 (88%)	655 (92%)	58 (8%)	2 (0%)	46	68
1	D	712/811 (88%)	612 (86%)	93 (13%)	7 (1%)	19	34
All	All	2900/3244 (89%)	2633 (91%)	253 (9%)	14 (0%)	34	55

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	ILE
1	D	190	THR
1	D	284	GLN
1	B	735	VAL
1	D	246	ILE



### 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	696/755 (92%)	659 (95%)	37 (5%)	28	50
1	B	689/755 (91%)	658 (96%)	31 (4%)	34	59
1	C	676/755 (90%)	642 (95%)	34 (5%)	30	53
1	D	673/755 (89%)	622 (92%)	51 (8%)	16	30
All	All	2734/3020 (90%)	2581 (94%)	153 (6%)	26	47

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	39	LYS
1	C	355	GLN
1	D	726	HIS
1	C	51	ASN
1	C	142	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	55	GLN
1	C	284	GLN
1	D	593	HIS
1	C	115	ASN
1	C	191	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](#)

45 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	NAG	A	1001	1,2	14,14,15	0.91	1 (7%)	15,19,21	1.07	1 (6%)
2	NAG	A	1002	3,2	14,14,15	0.88	0	15,19,21	1.28	1 (6%)
3	BMA	A	1003	2	11,11,12	0.84	0	15,15,17	1.69	4 (26%)
2	NAG	A	1004	1,2	14,14,15	1.02	1 (7%)	15,19,21	1.39	2 (13%)
2	NAG	A	1005	2	14,14,15	0.69	0	15,19,21	1.68	2 (13%)
2	NAG	A	1006	1	14,14,15	0.61	0	15,19,21	1.34	2 (13%)
2	NAG	A	1007	1,2	14,14,15	0.66	0	15,19,21	1.79	4 (26%)
2	NAG	A	1008	3,2	14,14,15	0.86	1 (7%)	15,19,21	1.20	1 (6%)
3	BMA	A	1009	2	11,11,12	0.61	0	15,15,17	1.35	1 (6%)
2	NAG	A	1010	1	14,14,15	0.54	0	15,19,21	1.18	2 (13%)
2	NAG	A	1011	1	14,14,15	0.78	1 (7%)	15,19,21	0.92	0
4	M4D	A	1012	-	22,22,22	1.65	3 (13%)	27,28,28	1.23	4 (14%)
4	M4D	B	901	-	22,22,22	1.47	2 (9%)	27,28,28	1.37	4 (14%)
2	NAG	B	902	1,2	14,14,15	0.72	0	15,19,21	1.46	2 (13%)
2	NAG	B	903	3,2	14,14,15	0.64	0	15,19,21	1.01	0
3	BMA	B	904	2	11,11,12	0.84	0	15,15,17	1.59	3 (20%)
2	NAG	B	905	1,2	14,14,15	0.93	1 (7%)	15,19,21	1.52	2 (13%)
2	NAG	B	906	2	14,14,15	0.41	0	15,19,21	1.32	3 (20%)
2	NAG	B	907	1	14,14,15	0.75	0	15,19,21	0.96	0
2	NAG	B	908	1,2	14,14,15	0.63	0	15,19,21	1.40	3 (20%)
2	NAG	B	909	3,2	14,14,15	0.75	0	15,19,21	1.29	1 (6%)
3	BMA	B	910	2	11,11,12	0.61	0	15,15,17	1.45	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	911	1	14,14,15	0.60	0	15,19,21	1.21	2 (13%)
2	NAG	C	1001	1,2	14,14,15	0.96	1 (7%)	15,19,21	1.27	2 (13%)
2	NAG	C	1002	3,2	14,14,15	0.68	0	15,19,21	1.29	2 (13%)
3	BMA	C	1003	2	11,11,12	0.95	1 (9%)	15,15,17	1.64	4 (26%)
2	NAG	C	1004	1,2	14,14,15	0.88	0	15,19,21	1.15	1 (6%)
2	NAG	C	1005	2	14,14,15	0.67	0	15,19,21	1.75	5 (33%)
2	NAG	C	1006	1	14,14,15	0.56	0	15,19,21	1.53	2 (13%)
2	NAG	C	1007	1,2	14,14,15	0.72	1 (7%)	15,19,21	1.49	5 (33%)
2	NAG	C	1008	3,2	14,14,15	1.10	1 (7%)	15,19,21	1.35	3 (20%)
3	BMA	C	1009	2	11,11,12	0.59	0	15,15,17	1.35	2 (13%)
2	NAG	C	1010	1	14,14,15	0.64	0	15,19,21	1.57	3 (20%)
4	M4D	C	1011	-	22,22,22	1.54	3 (13%)	27,28,28	1.19	4 (14%)
4	M4D	D	901	-	22,22,22	1.16	4 (18%)	27,28,28	1.32	2 (7%)
2	NAG	D	902	1,2	14,14,15	0.58	0	15,19,21	1.33	1 (6%)
2	NAG	D	903	3,2	14,14,15	0.88	1 (7%)	15,19,21	1.33	2 (13%)
3	BMA	D	904	2	11,11,12	0.71	0	15,15,17	1.43	2 (13%)
2	NAG	D	905	1,2	14,14,15	0.79	1 (7%)	15,19,21	0.93	0
2	NAG	D	906	2	14,14,15	0.74	0	15,19,21	0.75	0
2	NAG	D	907	1	14,14,15	0.80	0	15,19,21	1.17	1 (6%)
2	NAG	D	908	1,2	14,14,15	0.59	0	15,19,21	1.25	1 (6%)
2	NAG	D	909	3,2	14,14,15	0.93	1 (7%)	15,19,21	1.07	1 (6%)
3	BMA	D	910	2	11,11,12	0.89	0	15,15,17	1.89	3 (20%)
2	NAG	D	911	1	14,14,15	0.51	0	15,19,21	0.95	1 (6%)

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	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1003	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1004	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1005	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1007	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1008	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1009	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1011	1	-	0/6/23/26	0/1/1/1
4	M4D	A	1012	-	-	0/10/10/10	0/2/2/2
4	M4D	B	901	-	-	0/10/10/10	0/2/2/2
2	NAG	B	902	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	903	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	904	2	-	0/2/19/22	0/1/1/1
2	NAG	B	905	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	906	2	-	0/6/23/26	0/1/1/1
2	NAG	B	907	1	-	0/6/23/26	0/1/1/1
2	NAG	B	908	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	909	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	910	2	-	0/2/19/22	0/1/1/1
2	NAG	B	911	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1002	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1003	2	-	0/2/19/22	0/1/1/1
2	NAG	C	1004	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1005	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1006	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1007	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1008	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1009	2	-	0/2/19/22	0/1/1/1
2	NAG	C	1010	1	-	0/6/23/26	0/1/1/1
4	M4D	C	1011	-	-	0/10/10/10	0/2/2/2
4	M4D	D	901	-	-	0/10/10/10	0/2/2/2
2	NAG	D	902	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	903	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	904	2	-	0/2/19/22	0/1/1/1
2	NAG	D	905	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	906	2	-	0/6/23/26	0/1/1/1
2	NAG	D	907	1	-	0/6/23/26	0/1/1/1
2	NAG	D	908	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	909	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	910	2	-	0/2/19/22	0/1/1/1
2	NAG	D	911	1	-	0/6/23/26	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	NAG	O5-C1	-3.25	1.38	1.43
2	C	1008	NAG	O5-C1	-2.99	1.38	1.43
2	A	1004	NAG	C1-C2	-2.39	1.49	1.52
2	A	1001	NAG	O5-C1	-2.34	1.39	1.43
2	D	905	NAG	O5-C1	-2.31	1.40	1.43

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	M4D	C1-C-N	-3.77	119.42	122.89
4	D	901	M4D	C1-C-N	-3.70	119.50	122.89
2	B	905	NAG	C3-C4-C5	-3.27	104.40	110.23
2	C	1005	NAG	C3-C4-C5	-3.18	104.56	110.23
3	C	1003	BMA	C2-C3-C4	-3.13	105.58	111.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	1	0
2	A	1002	NAG	1	0
4	A	1012	M4D	1	0
4	B	901	M4D	1	0
4	C	1011	M4D	1	0
2	D	902	NAG	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	749/811 (92%)	-0.15	7 (0%) 85 88	31, 46, 82, 114	0
1	B	742/811 (91%)	-0.11	9 (1%) 81 83	30, 50, 88, 118	0
1	C	727/811 (89%)	0.17	43 (5%) 26 29	34, 58, 106, 133	0
1	D	724/811 (89%)	0.51	84 (11%) 6 6	34, 72, 121, 150	0
All	All	2942/3244 (90%)	0.10	143 (4%) 33 38	30, 53, 108, 150	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	123	ASN	8.7
1	D	122	LEU	8.1
1	C	64	TYR	7.2
1	D	732	LEU	7.0
1	D	81	GLU	6.6

### 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 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( $\text{\AA}^2$ )	Q<0.9
4	M4D	C	1011	21/21	0.94	0.21	4.25	48,52,61,63	0
4	M4D	D	901	21/21	0.95	0.19	2.31	35,37,41,43	0
4	M4D	B	901	21/21	0.96	0.20	1.52	39,42,46,47	0
2	NAG	D	911	14/15	0.94	0.17	1.47	58,67,74,74	0
2	NAG	C	1004	14/15	0.98	0.15	0.75	38,41,45,48	0
2	NAG	A	1010	14/15	0.94	0.20	0.74	60,70,81,85	0
4	M4D	A	1012	21/21	0.96	0.17	0.52	32,37,47,49	0
2	NAG	A	1001	14/15	0.98	0.17	0.52	30,33,39,50	0
2	NAG	C	1001	14/15	0.97	0.16	0.51	38,41,44,45	0
2	NAG	A	1011	14/15	0.94	0.19	0.32	59,64,69,69	0
2	NAG	D	908	14/15	0.98	0.15	0.21	37,44,50,55	0
2	NAG	B	902	14/15	0.98	0.17	0.02	35,40,44,46	0
2	NAG	C	1007	14/15	0.97	0.13	-0.22	45,46,50,50	0
2	NAG	A	1004	14/15	0.97	0.14	-0.32	32,34,42,42	0
2	NAG	B	911	14/15	0.95	0.12	-0.35	56,59,67,70	0
2	NAG	C	1008	14/15	0.97	0.13	-0.38	44,49,53,54	0
2	NAG	D	902	14/15	0.95	0.15	-0.39	55,61,69,69	0
2	NAG	B	905	14/15	0.98	0.14	-0.49	34,37,41,47	0
2	NAG	D	903	14/15	0.94	0.15	-0.90	58,66,75,82	0
2	NAG	D	905	14/15	0.96	0.14	-1.02	38,42,44,51	0
2	NAG	A	1007	14/15	0.98	0.12	-1.11	34,37,38,41	0
2	NAG	B	908	14/15	0.96	0.12	-1.16	32,38,40,41	0
2	NAG	A	1002	14/15	0.98	0.12	-1.31	30,34,42,44	0
2	NAG	C	1002	14/15	0.98	0.11	-1.79	39,45,49,52	0
2	NAG	B	903	14/15	0.98	0.14	-1.86	36,45,54,58	0
2	NAG	C	1006	14/15	0.88	0.27	-	74,83,107,117	0
3	BMA	A	1009	11/12	0.86	0.15	-	52,56,63,70	0
3	BMA	D	910	11/12	0.86	0.15	-	53,60,77,78	0
2	NAG	B	907	14/15	0.90	0.16	-	55,62,70,72	0
3	BMA	D	904	11/12	0.88	0.14	-	72,79,85,90	0
2	NAG	A	1008	14/15	0.98	0.17	-	39,44,51,53	0
2	NAG	A	1005	14/15	0.94	0.15	-	43,51,57,60	0
3	BMA	C	1009	11/12	0.92	0.13	-	59,66,77,81	0
2	NAG	C	1005	14/15	0.95	0.11	-	47,55,62,65	0
2	NAG	B	909	14/15	0.98	0.14	-	37,39,47,51	0
2	NAG	B	906	14/15	0.95	0.14	-	53,60,65,66	0
2	NAG	D	909	14/15	0.96	0.13	-	37,47,51,55	0
2	NAG	D	907	14/15	0.91	0.15	-	56,69,82,87	0
2	NAG	C	1010	14/15	0.94	0.15	-	78,82,87,88	0
3	BMA	B	904	11/12	0.90	0.20	-	44,55,60,61	0
3	BMA	C	1003	11/12	0.92	0.11	-	44,54,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	B	910	11/12	0.97	0.09	-	50,55,60,60	0
2	NAG	D	906	14/15	0.95	0.12	-	58,62,67,70	0
3	BMA	A	1003	11/12	0.90	0.12	-	44,48,54,54	0
2	NAG	A	1006	14/15	0.96	0.12	-	56,64,71,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.