



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2016 – 11:01 PM EDT

PDB ID : 5E62  
Title : HEF-mut with Tr323 complex  
Authors : Song, H.; Qi, J.; Shi, Y.; Gao, G.F.  
Deposited on : 2015-10-09  
Resolution : 2.20 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-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

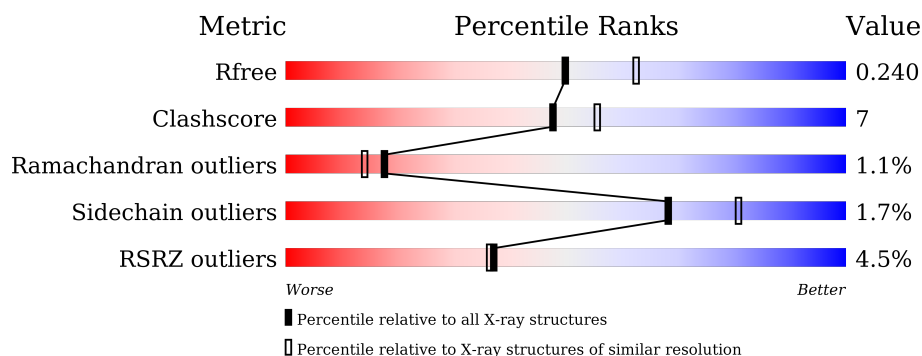
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	427	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	C	427	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	B	149	<div> <div>12%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
2	D	149	<div> <div>9%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9821 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 Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3240	2039	540	639	22			
1	C	424	Total	C	N	O	S	0	0	0
			3240	2039	540	639	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	SER	engineered mutation	UNP K9LG83
A	356	ALA	ASP	engineered mutation	UNP K9LG83
A	359	ALA	HIS	engineered mutation	UNP K9LG83
C	57	ALA	SER	engineered mutation	UNP K9LG83
C	356	ALA	ASP	engineered mutation	UNP K9LG83
C	359	ALA	HIS	engineered mutation	UNP K9LG83

- Molecule 2 is a protein called Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	0	0
			1110	695	194	217	4			
2	D	149	Total	C	N	O	S	0	0	0
			1110	695	194	217	4			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



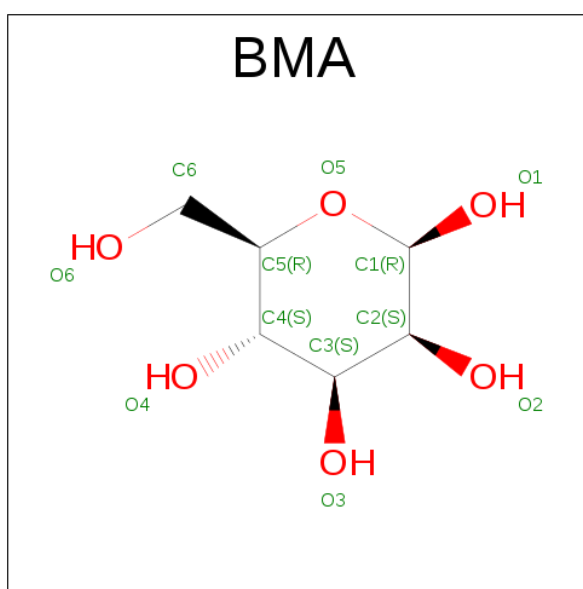
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



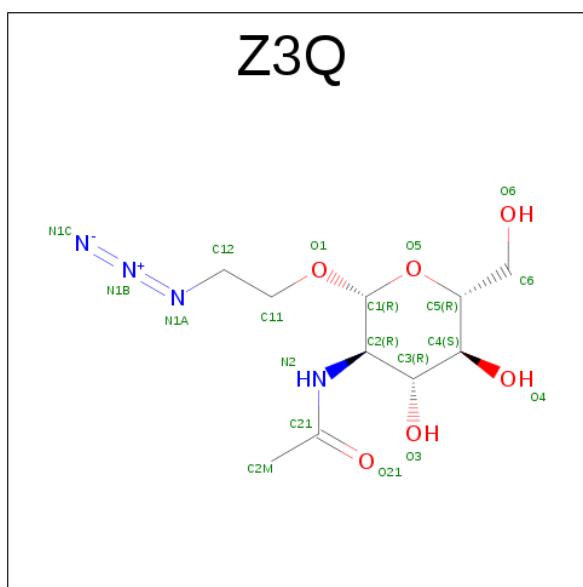
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



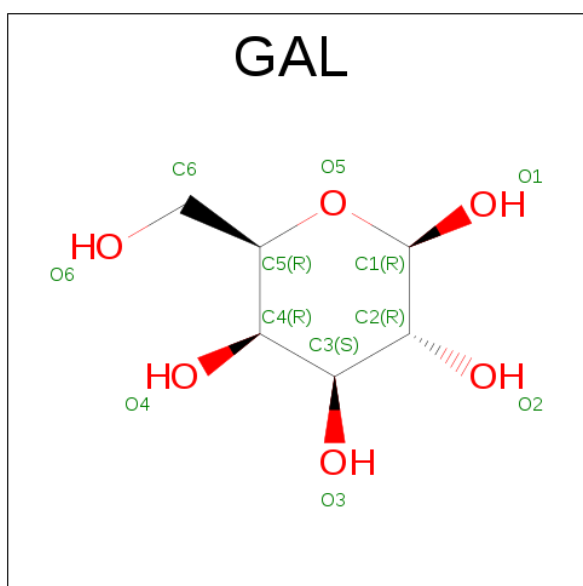
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is 2-azidoethyl 2-(acetylamino)-2-deoxy-beta-D-glucopyranoside (three-letter code: Z3Q) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	10	4	6		
6	C	1	Total	C	N	O	0	0
			20	10	4	6		

- Molecule 7 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



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

- # 5N6
- 
- The chemical structure of 5N6 is a complex molecule featuring a central core with several stereocenters and functional groups. The structure is shown in a 3D representation with wedged and dashed bonds indicating stereochemistry. Key features include:
- A central core with a nitrogen atom (N) and a carbonyl group (C=O).
  - Multiple stereocenters labeled with letters (A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z) and their corresponding configurations (R or S).
  - Functional groups including hydroxyl groups (OH), a carboxylic acid group (COOH), and a carbonyl group (C=O).
  - Various substituents and side chains, including a long chain with a terminal carboxylic acid group (OCB) and a side chain with a terminal hydroxyl group (OH<sub>01</sub>).
- The structure is highly complex and contains many stereocenters, making it difficult to represent accurately in a 2D format. The 3D representation provides a clear view of the molecule's geometry and stereochemistry.

- Molecule 9 is water.

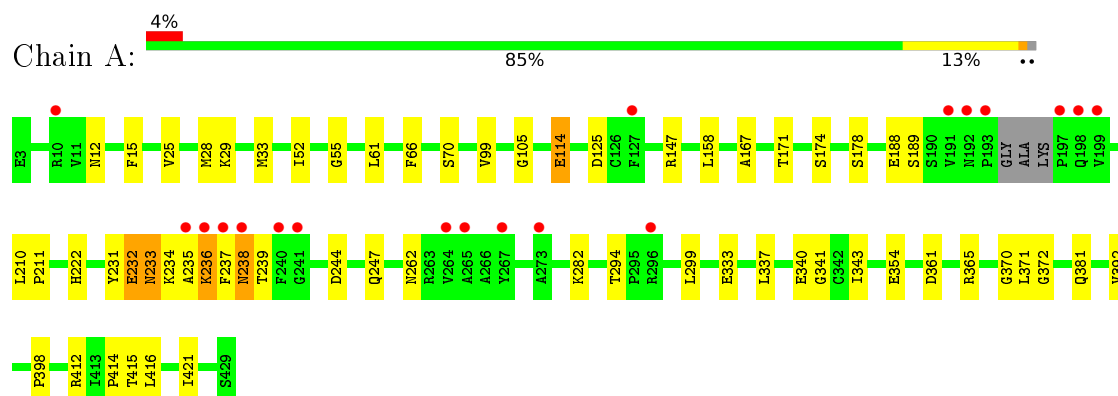
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	239	Total O 239 239	0	0
9	B	66	Total O 66 66	0	0
9	C	280	Total O 280 280	0	0
9	D	44	Total O 44 44	0	0



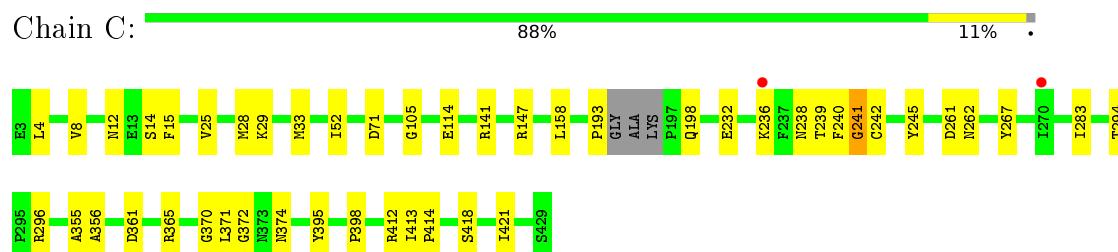
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

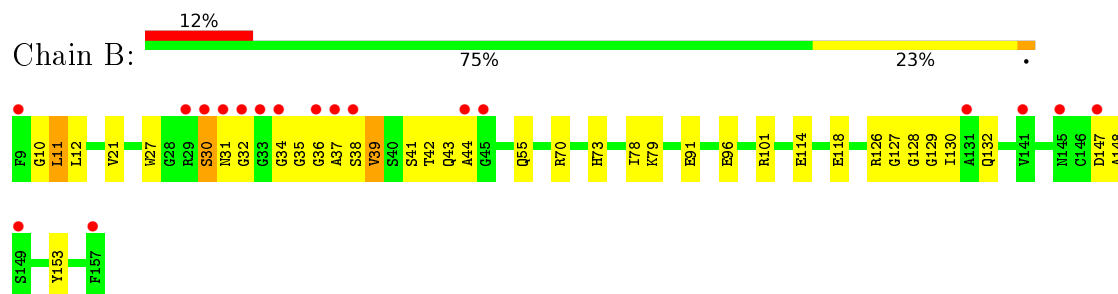
#### • Molecule 1: Hemagglutinin-esterase



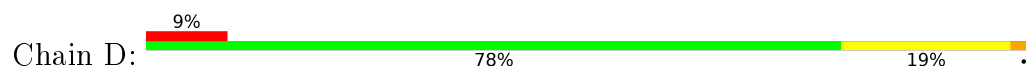
#### • Molecule 1: Hemagglutinin-esterase



#### • Molecule 2: Hemagglutinin-esterase



#### • Molecule 2: Hemagglutinin-esterase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.82Å 164.82Å 164.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.20 49.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.70-2.20) 96.0 (49.70-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.72 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.204 , 0.244 0.201 , 0.240	Depositor DCC
$R_{free}$ test set	3506 reflections (4.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.2	EDS
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 75309 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9821	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, Z3Q, 5N6, GAL, MAN, 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	0.48	0/3315	0.63	1/4494 (0.0%)
1	C	0.46	0/3315	0.61	0/4494
2	B	0.44	0/1127	0.62	0/1515
2	D	0.38	0/1127	0.55	0/1515
All	All	0.46	0/8884	0.61	1/12018 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASN	C-N-CA	-5.47	108.01	121.70

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	3240	0	3114	47	0
1	C	3240	0	3114	38	0
2	B	1110	0	1067	25	0
2	D	1110	0	1067	28	0
3	A	84	0	73	3	0
3	B	42	0	38	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	84	0	74	1	0
3	D	42	0	38	1	0
4	A	22	0	17	2	0
4	C	11	0	9	0	0
5	A	66	0	57	0	0
5	C	33	0	28	0	0
6	A	20	0	0	1	0
6	C	20	0	0	0	0
7	A	11	0	9	3	0
7	C	11	0	9	2	0
8	A	23	0	0	5	0
8	C	23	0	0	2	0
9	A	239	0	0	5	1
9	B	66	0	0	5	1
9	C	280	0	0	7	1
9	D	44	0	0	7	0
All	All	9821	0	8714	132	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 132 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:234:LYS:O	1:A:238:ASN:ND2	1.89	1.06
1:A:244:ASP:OD1	1:A:262:ASN:HB2	1.70	0.92
1:A:29:LYS:NZ	9:A:804:HOH:O	2.05	0.90
8:A:717:5N6:OBW	8:A:717:5N6:OBL	1.90	0.90
2:D:80:ASN:OD1	9:D:801:HOH:O	1.91	0.87

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:977:HOH:O	9:C:1012:HOH:O[3_554]	1.99	0.21
9:B:807:HOH:O	9:B:829:HOH:O[10_554]	2.19	0.01

## 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	420/427 (98%)	399 (95%)	21 (5%)	0	100	100
1	C	420/427 (98%)	402 (96%)	15 (4%)	3 (1%)	26	25
2	B	147/149 (99%)	124 (84%)	17 (12%)	6 (4%)	3	1
2	D	147/149 (99%)	127 (86%)	16 (11%)	4 (3%)	6	3
All	All	1134/1152 (98%)	1052 (93%)	69 (6%)	13 (1%)	17	14

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	11	LEU
1	C	355	ALA
2	D	128	GLY
2	B	21	VAL
2	B	41	SER

### 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	357/358 (100%)	349 (98%)	8 (2%)	60	72
1	C	357/358 (100%)	355 (99%)	2 (1%)	90	95
2	B	109/109 (100%)	107 (98%)	2 (2%)	66	79
2	D	109/109 (100%)	105 (96%)	4 (4%)	41	50
All	All	932/934 (100%)	916 (98%)	16 (2%)	68	81

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	VAL
2	B	11	LEU
2	D	9	PHE
1	A	238	ASN
2	D	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
2	B	156	ASN
2	D	31	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](#)

36 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	701	1,3	14,14,15	0.40	0	15,19,21	0.95	1 (6%)
3	NAG	A	702	3,4	14,14,15	0.29	0	15,19,21	0.68	0
4	BMA	A	703	3,5	11,11,12	0.90	1 (9%)	15,15,17	2.78	6 (40%)
5	MAN	A	704	5,4	11,11,12	0.40	0	15,15,17	1.30	1 (6%)
5	MAN	A	705	5	11,11,12	0.38	0	15,15,17	1.04	0
5	MAN	A	706	5	11,11,12	0.32	0	15,15,17	1.23	2 (13%)
3	NAG	A	707	1,3	14,14,15	0.41	0	15,19,21	0.88	0
3	NAG	A	708	3,4	14,14,15	0.53	0	15,19,21	1.77	4 (26%)
4	BMA	A	709	3,5	11,11,12	0.61	0	15,15,17	3.27	6 (40%)
5	MAN	A	710	5,4	11,11,12	0.46	0	15,15,17	2.02	3 (20%)
5	MAN	A	711	5	11,11,12	0.34	0	15,15,17	0.82	0
5	MAN	A	712	4	11,11,12	0.47	0	15,15,17	1.03	0
3	NAG	A	713	1,3	14,14,15	0.75	1 (7%)	15,19,21	1.44	3 (20%)
3	NAG	A	714	3	14,14,15	0.29	0	15,19,21	1.36	3 (20%)
6	Z3Q	A	715	7	19,20,20	1.66	2 (10%)	22,26,26	3.79	7 (31%)
7	GAL	A	716	8,6	11,11,12	0.97	0	15,15,17	2.13	5 (33%)
8	5N6	A	717	7	20,23,24	1.82	5 (25%)	20,32,35	1.43	4 (20%)
3	NAG	B	701	3,2	14,14,15	0.42	0	15,19,21	0.79	0
3	NAG	B	702	3	14,14,15	0.37	0	15,19,21	1.45	2 (13%)
3	NAG	B	703	2	14,14,15	0.37	0	15,19,21	1.49	4 (26%)
3	NAG	C	701	1,3	14,14,15	0.44	0	15,19,21	0.79	0
3	NAG	C	702	3,4	14,14,15	0.48	0	15,19,21	1.24	1 (6%)
4	BMA	C	703	3,5	11,11,12	0.48	0	15,15,17	1.05	1 (6%)
5	MAN	C	704	5,4	11,11,12	0.49	0	15,15,17	1.72	5 (33%)
5	MAN	C	705	5	11,11,12	0.39	0	15,15,17	0.70	0
5	MAN	C	706	5	11,11,12	0.50	0	15,15,17	1.01	0
3	NAG	C	707	1,3	14,14,15	0.48	0	15,19,21	1.08	2 (13%)
3	NAG	C	708	3	14,14,15	0.48	0	15,19,21	0.81	0
3	NAG	C	709	1,3	14,14,15	0.36	0	15,19,21	1.10	1 (6%)
3	NAG	C	710	3	14,14,15	0.34	0	15,19,21	1.25	2 (13%)
6	Z3Q	C	711	7	19,20,20	1.16	2 (10%)	22,26,26	1.06	2 (9%)
7	GAL	C	712	8,6	11,11,12	1.18	0	15,15,17	1.39	3 (20%)
8	5N6	C	713	7	20,23,24	2.39	9 (45%)	20,32,35	0.90	1 (5%)
3	NAG	D	701	3,2	14,14,15	0.42	0	15,19,21	0.92	1 (6%)
3	NAG	D	702	3	14,14,15	0.47	0	15,19,21	1.48	2 (13%)
3	NAG	D	703	2	14,14,15	0.31	0	15,19,21	1.47	2 (13%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	702	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	703	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	704	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	705	5	-	0/2/19/22	0/1/1/1
5	MAN	A	706	5	-	0/2/19/22	0/1/1/1
3	NAG	A	707	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	708	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	709	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	710	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	711	5	-	0/2/19/22	0/1/1/1
5	MAN	A	712	4	-	0/2/19/22	0/1/1/1
3	NAG	A	713	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	714	3	-	0/6/23/26	0/1/1/1
6	Z3Q	A	715	7	-	1/12/32/32	0/1/1/1
7	GAL	A	716	8,6	-	0/2/19/22	0/1/1/1
8	5N6	A	717	7	-	0/17/37/41	0/1/1/1
3	NAG	B	701	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3	-	0/6/23/26	0/1/1/1
3	NAG	B	703	2	-	0/6/23/26	0/1/1/1
3	NAG	C	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	702	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	703	3,5	-	0/2/19/22	0/1/1/1
5	MAN	C	704	5,4	-	0/2/19/22	0/1/1/1
5	MAN	C	705	5	-	0/2/19/22	0/1/1/1
5	MAN	C	706	5	-	0/2/19/22	0/1/1/1
3	NAG	C	707	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	708	3	-	0/6/23/26	0/1/1/1
3	NAG	C	709	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	710	3	-	0/6/23/26	0/1/1/1
6	Z3Q	C	711	7	-	0/12/32/32	0/1/1/1
7	GAL	C	712	8,6	-	0/2/19/22	0/1/1/1
8	5N6	C	713	7	-	0/17/37/41	0/1/1/1
3	NAG	D	701	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	702	3	-	0/6/23/26	0/1/1/1
3	NAG	D	703	2	-	0/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	715	Z3Q	N1B-N1A	-5.82	1.07	1.23
8	C	713	5N6	CBB-CBA	-4.74	1.48	1.53
8	C	713	5N6	OBY-CBB	-4.55	1.33	1.43
8	A	717	5N6	CBB-CBA	-4.09	1.49	1.53
6	C	711	Z3Q	N1B-N1A	-4.00	1.12	1.23

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	715	Z3Q	O5-C1-O1	-11.41	82.64	109.99
6	A	715	Z3Q	C1-C2-N2	-11.16	90.00	111.01
4	A	709	BMA	C2-C3-C4	-8.34	96.51	111.05
4	A	703	BMA	C1-O5-C5	-6.63	102.39	112.14
4	A	703	BMA	O2-C2-C3	-6.13	97.83	110.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	715	Z3Q	C11-O1-C1-C2

There are no ring outliers.

13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NAG	1	0
4	A	703	BMA	1	0
3	A	708	NAG	1	0
4	A	709	BMA	1	0
3	A	713	NAG	1	0
6	A	715	Z3Q	1	0
7	A	716	GAL	3	0
8	A	717	5N6	5	0
3	B	702	NAG	2	0
3	C	709	NAG	1	0
7	C	712	GAL	2	0
8	C	713	5N6	2	0
3	D	702	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	424/427 (99%)	-0.18	19 (4%) 37 36	28, 40, 98, 144	0
1	C	424/427 (99%)	-0.48	2 (0%) 91 91	24, 36, 60, 78	0
2	B	149/149 (100%)	0.51	18 (12%) 6 5	26, 55, 120, 198	0
2	D	149/149 (100%)	0.53	13 (8%) 13 12	30, 51, 127, 190	0
All	All	1146/1152 (99%)	-0.11	52 (4%) 37 36	24, 40, 98, 198	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	32	GLY	17.9
2	B	37	ALA	14.5
2	D	33	GLY	14.2
2	B	34	GLY	14.1
2	D	37	ALA	11.0

### 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
3	NAG	B	702	14/15	0.94	0.12	0.32	43,48,56,58	0
3	NAG	D	702	14/15	0.94	0.12	0.17	36,44,50,54	0
8	5N6	C	713	23/24	0.96	0.13	0.02	43,52,60,62	0
3	NAG	B	701	14/15	0.94	0.10	-0.02	30,35,39,41	0
3	NAG	C	709	14/15	0.96	0.11	-0.14	51,52,64,68	0
5	MAN	A	706	11/12	0.92	0.09	-0.50	32,38,42,46	0
8	5N6	A	717	23/24	0.94	0.18	-0.63	71,81,85,87	0
5	MAN	C	706	11/12	0.94	0.09	-0.63	38,40,45,48	0
3	NAG	D	701	14/15	0.96	0.09	-1.03	29,34,36,36	0
3	NAG	A	713	14/15	0.94	0.09	-1.14	60,63,69,72	0
3	NAG	A	714	14/15	0.81	0.13	-	58,65,73,79	0
6	Z3Q	A	715	20/20	0.61	0.61	-	129,139,148,148	0
5	MAN	C	704	11/12	0.96	0.07	-	30,34,39,41	0
4	BMA	C	703	11/12	0.93	0.09	-	33,35,39,41	0
5	MAN	A	711	11/12	0.89	0.16	-	52,58,65,65	0
5	MAN	A	705	11/12	0.93	0.09	-	37,40,43,44	0
7	GAL	C	712	11/12	0.85	0.22	-	68,84,101,102	0
5	MAN	C	705	11/12	0.94	0.09	-	41,46,52,59	0
3	NAG	A	708	14/15	0.95	0.10	-	31,36,38,39	0
3	NAG	C	707	14/15	0.98	0.08	-	25,30,36,39	0
3	NAG	C	710	14/15	0.90	0.10	-	53,57,63,68	0
3	NAG	C	708	14/15	0.91	0.14	-	39,46,51,52	0
3	NAG	A	702	14/15	0.93	0.12	-	36,42,46,50	0
3	NAG	C	702	14/15	0.96	0.09	-	28,33,38,40	0
4	BMA	A	703	11/12	0.95	0.10	-	35,38,42,43	0
3	NAG	C	701	14/15	0.96	0.08	-	34,37,41,42	0
5	MAN	A	710	11/12	0.94	0.11	-	42,47,48,51	0
3	NAG	A	707	14/15	0.96	0.08	-	29,37,40,42	0
3	NAG	B	703	14/15	0.86	0.21	-	70,77,81,82	0
3	NAG	D	703	14/15	0.78	0.25	-	88,99,103,103	0
4	BMA	A	709	11/12	0.88	0.17	-	43,47,54,60	0
6	Z3Q	C	711	20/20	0.45	0.66	-	109,126,133,138	0
7	GAL	A	716	11/12	0.77	0.31	-	96,109,120,121	0
3	NAG	A	701	14/15	0.95	0.09	-	38,40,49,50	0
5	MAN	A	704	11/12	0.97	0.09	-	28,32,37,38	0
5	MAN	A	712	11/12	0.93	0.09	-	39,42,47,47	0

## 6.5 Other polymers

There are no such residues in this entry.