



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:15 AM GMT

PDB ID : 3DWQ  
Title : Crystal structure of the A-subunit of the AB5 toxin from E. coli with Neu5Gc-2,3Gal-1,3GlcNAc  
Authors : Byres, E.; Paton, A.W.; Paton, J.C.; Lofling, J.C.; Smith, D.F.; Wilce, M.C.J.; Talbot, U.M.; Chong, D.C.; Yu, H.; Huang, S.; Chen, X.; Varki, N.M.; Varki, A.; Rossjohn, J.; Beddoe, T.  
Deposited on : 2008-07-22  
Resolution : 2.10 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

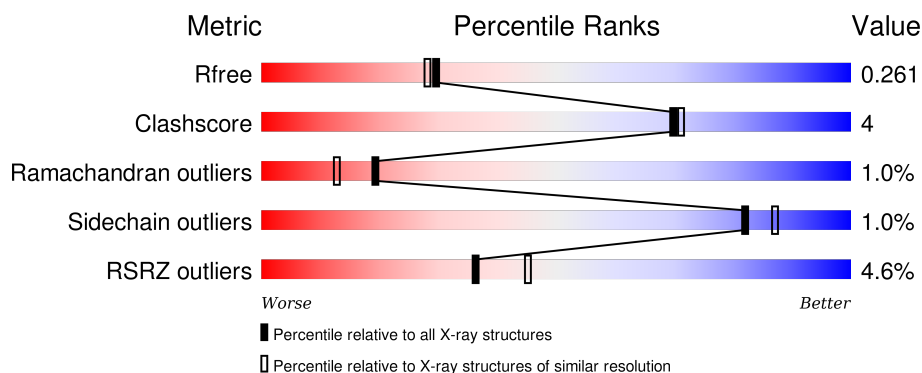
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	126	<div> <div>5%</div> <div>82%</div> <div>10%</div> <div>8%</div> </div>
1	B	126	<div> <div>2%</div> <div>76%</div> <div>16%</div> <div>7%</div> </div>
1	C	126	<div> <div>4%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
1	D	126	<div> <div>4%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
1	E	126	<div> <div>6%</div> <div>89%</div> <div>8%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NGC	A	127	X	-	-	X
2	GAL	A	128	X	-	-	-
2	NGA	A	129	X	-	-	-
2	NGC	C	127	X	-	-	-
2	GAL	C	128	X	-	-	-
2	NGA	C	129	X	-	-	-
2	NGC	D	127	X	-	-	X
2	GAL	D	128	X	-	-	-
2	NGA	D	129	X	-	-	-
2	NGC	E	127	X	-	-	-
2	GAL	E	128	X	-	-	-
2	NGA	E	129	X	-	-	-
4	1PE	A	132	-	-	-	X
4	1PE	B	127	-	-	-	X
4	1PE	D	132	-	-	-	X
4	1PE	D	133	-	-	-	X
4	1PE	E	132	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5380 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 Subtilase cytotoxin, subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			897	573	145	173	6			
1	B	117	Total	C	N	O	S	0	0	0
			905	577	147	175	6			
1	C	120	Total	C	N	O	S	0	0	0
			928	591	150	181	6			
1	D	117	Total	C	N	O	S	0	0	0
			905	577	147	175	6			
1	E	116	Total	C	N	O	S	0	0	0
			897	573	145	173	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	LEU	-	EXPRESSION TAG	UNP Q3ZTX8
A	120	GLU	-	EXPRESSION TAG	UNP Q3ZTX8
A	121	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
A	122	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
A	123	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
A	124	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
A	125	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
A	126	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
B	119	LEU	-	EXPRESSION TAG	UNP Q3ZTX8
B	120	GLU	-	EXPRESSION TAG	UNP Q3ZTX8
B	121	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
B	122	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
B	123	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
B	124	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
B	125	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
B	126	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
C	119	LEU	-	EXPRESSION TAG	UNP Q3ZTX8
C	120	GLU	-	EXPRESSION TAG	UNP Q3ZTX8
C	121	HIS	-	EXPRESSION TAG	UNP Q3ZTX8

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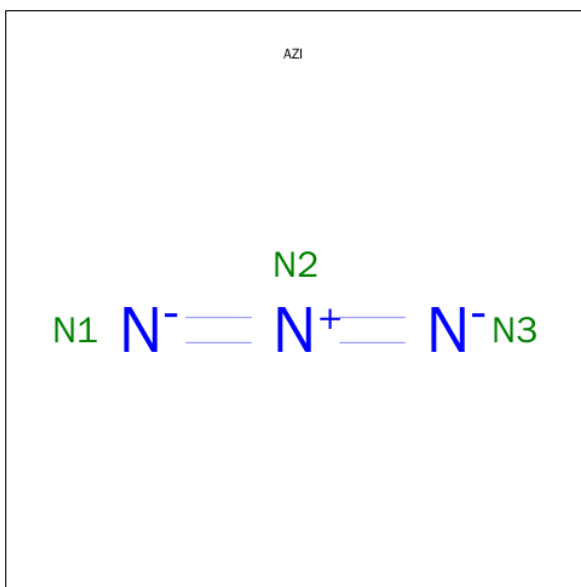
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Chain	Residue	Modelled	Actual	Comment	Reference
C	122	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
C	123	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
C	124	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
C	125	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
C	126	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	119	LEU	-	EXPRESSION TAG	UNP Q3ZTX8
D	120	GLU	-	EXPRESSION TAG	UNP Q3ZTX8
D	121	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	122	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	123	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	124	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	125	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	126	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
E	119	LEU	-	EXPRESSION TAG	UNP Q3ZTX8
E	120	GLU	-	EXPRESSION TAG	UNP Q3ZTX8
E	121	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
E	122	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
E	123	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
E	124	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
E	125	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
E	126	HIS	-	EXPRESSION TAG	UNP Q3ZTX8

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

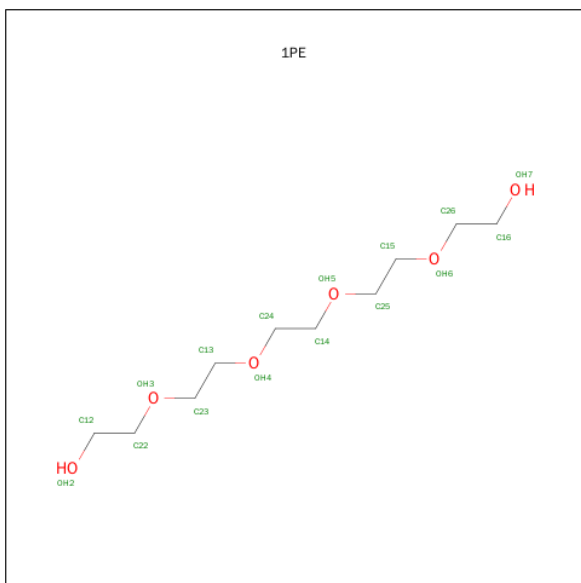
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			46	25	2	19		
2	C	3	Total	C	N	O	0	0
			46	25	2	19		
2	D	3	Total	C	N	O	0	0
			46	25	2	19		
2	E	3	Total	C	N	O	0	0
			46	25	2	19		

- Molecule 3 is N-PROPANOL (three-letter code: AZI, POL) (formula: N<sub>3</sub>, C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			7	3	3	1		
3	C	2	Total	C	N	O	0	0
			7	3	3	1		
3	D	2	Total	C	N	O	0	0
			7	3	3	1		
3	E	2	Total	C	N	O	0	0
			7	3	3	1		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		
4	D	1	Total	C	O	0	0
			16	10	6		
4	D	1	Total	C	O	0	0
			16	10	6		
4	E	1	Total	C	O	0	0
			16	10	6		

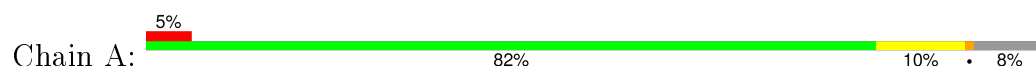
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	112	Total	O	0	0
			112	112		
5	B	103	Total	O	0	0
			103	103		
5	C	108	Total	O	0	0
			108	108		
5	D	107	Total	O	0	0
			107	107		
5	E	126	Total	O	0	0
			126	126		

### 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.

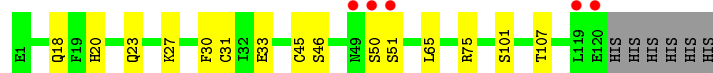
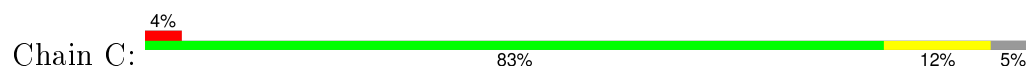
- Molecule 1: Subtilase cytotoxin, subunit B



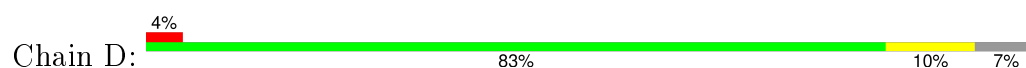
- Molecule 1: Subtilase cytotoxin, subunit B



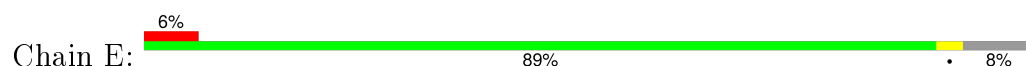
- Molecule 1: Subtilase cytotoxin, subunit B



- Molecule 1: Subtilase cytotoxin, subunit B



- Molecule 1: Subtilase cytotoxin, subunit B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.25Å 97.25Å 163.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.67 – 2.10 29.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	83.8 (29.67-2.10) 83.8 (29.66-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.211 , 0.262 0.211 , 0.261	Depositor DCC
$R_{free}$ test set	2177 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.4	EDS
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 42702 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, NGA, NGC, 1PE, POL, GAL

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	0.38	0/923	0.46	0/1255
1	B	0.39	0/931	0.51	0/1266
1	C	0.38	0/954	0.48	0/1297
1	D	0.37	0/931	0.48	0/1266
1	E	0.39	0/923	0.48	0/1255
All	All	0.38	0/4662	0.48	0/6339

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
2	A	15	0
2	C	15	0
2	D	15	0
2	E	15	0
All	All	60	0

There are no bond length outliers.

There are no bond angle outliers.

All (60) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	127	NGC	C5,C3,C6,C4,C7
2	A	128	GAL	C2,C5,C3,C1,C4
2	A	129	NGA	C2,C5,C3,C1,C4
2	C	127	NGC	C5,C3,C6,C4,C7
2	C	128	GAL	C2,C5,C3,C1,C4
2	C	129	NGA	C2,C5,C3,C1,C4

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Mol	Chain	Res	Type	Atom
2	D	127	NGC	C5,C3,C6,C4,C7
2	D	128	GAL	C2,C5,C3,C1,C4
2	D	129	NGA	C2,C5,C3,C1,C4
2	E	127	NGC	C5,C3,C6,C4,C7
2	E	128	GAL	C2,C5,C3,C1,C4
2	E	129	NGA	C2,C5,C3,C1,C4

There are no planarity outliers.

## 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	897	0	852	8	0
1	B	905	0	858	15	0
1	C	928	0	882	8	0
1	D	905	0	858	12	0
1	E	897	0	852	2	0
2	A	46	0	38	0	0
2	C	46	0	38	2	0
2	D	46	0	38	1	0
2	E	46	0	38	1	0
3	A	7	0	5	0	0
3	C	7	0	5	0	0
3	D	7	0	6	0	0
3	E	7	0	5	0	0
4	A	16	0	22	0	0
4	B	16	0	22	1	0
4	D	32	0	44	1	0
4	E	16	0	22	0	0
5	A	112	0	0	1	0
5	B	103	0	0	2	0
5	C	108	0	0	1	0
5	D	107	0	0	0	0
5	E	126	0	0	1	0
All	All	5380	0	4585	42	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 4.

All (42) 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:C:31:CYS:HB2	5:C:199:HOH:O	1.60	1.02
1:D:10:MET:HE3	1:D:114:ARG:H	1.29	0.97
1:A:47:MET:HB3	1:A:50:SER:HB3	1.57	0.86
1:B:62:ASN:HB3	5:E:189:HOH:O	1.79	0.80
1:D:10:MET:HE3	1:D:114:ARG:N	2.04	0.70
1:D:14:VAL:HG12	1:D:36:GLN:HG3	1.78	0.66
1:D:10:MET:HE2	1:D:75:ARG:HD3	1.80	0.64
1:A:29:TYR:HB3	1:A:47:MET:HG3	1.88	0.56
2:E:127:NGC:O5	2:E:128:GAL:C4	2.54	0.55
1:A:63:GLN:HE22	1:C:65:LEU:HD13	1.72	0.55
2:D:127:NGC:O5	2:D:128:GAL:C4	2.57	0.53
1:B:56:SER:OG	1:E:23:GLN:HB2	2.09	0.52
1:E:30:PHE:CE2	1:E:46:SER:HB3	2.44	0.52
1:B:31:CYS:HB2	5:B:191:HOH:O	2.10	0.51
1:B:92:LEU:HD13	5:B:191:HOH:O	2.11	0.50
2:C:127:NGC:O5	2:C:128:GAL:C4	2.60	0.49
1:D:70:THR:HG22	4:D:132:1PE:H252	1.94	0.49
1:C:18:GLN:HB2	1:C:33:GLU:HB3	1.95	0.48
1:C:30:PHE:CE2	1:C:46:SER:HB3	2.49	0.48
1:D:10:MET:CE	1:D:75:ARG:HD3	2.42	0.47
1:A:56:SER:OG	1:C:23:GLN:HB2	2.14	0.47
1:A:62:ASN:HB3	5:A:140:HOH:O	2.13	0.47
1:B:67:PHE:CG	1:B:74:VAL:HG11	2.50	0.47
1:B:18:GLN:HB2	1:B:33:GLU:HB3	1.97	0.47
1:D:30:PHE:CE2	1:D:46:SER:HB3	2.50	0.46
1:B:30:PHE:CE2	1:B:46:SER:HB3	2.51	0.46
1:B:23:GLN:HB2	1:D:56:SER:OG	2.15	0.46
1:B:70:THR:HG22	4:B:127:1PE:H152	1.98	0.46
1:B:20:HIS:HD2	1:D:101:SER:OG	1.99	0.45
1:B:75:ARG:HB3	1:B:101:SER:HB2	1.99	0.45
1:B:47:MET:HB3	1:B:50:SER:HB3	1.98	0.45
1:B:29:TYR:HB3	1:B:47:MET:HG3	1.99	0.45
1:D:75:ARG:HB3	1:D:101:SER:HB2	1.98	0.45
1:C:31:CYS:SG	1:C:45:CYS:SG	3.15	0.44
1:B:37:SER:HA	1:B:39:GLY:N	2.33	0.44
1:A:30:PHE:CE2	1:A:46:SER:HB3	2.53	0.43
1:A:101:SER:OG	1:C:20:HIS:CD2	2.71	0.43
1:D:29:TYR:HB3	1:D:47:MET:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ARG:HB3	1:C:101:SER:HB2	2.00	0.42
1:A:103:CYS:HA	1:A:109:CYS:HA	2.02	0.41
1:B:20:HIS:CD2	1:D:101:SER:OG	2.74	0.41
2:C:127:NGC:H2A	2:C:128:GAL:H2	2.02	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	114/126 (90%)	110 (96%)	2 (2%)	2 (2%)	11	5
1	B	115/126 (91%)	109 (95%)	5 (4%)	1 (1%)	21	15
1	C	118/126 (94%)	115 (98%)	1 (1%)	2 (2%)	11	5
1	D	115/126 (91%)	112 (97%)	3 (3%)	0	100	100
1	E	114/126 (90%)	112 (98%)	1 (1%)	1 (1%)	21	15
All	All	576/630 (91%)	558 (97%)	12 (2%)	6 (1%)	19	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	SER
1	A	51	SER
1	C	50	SER
1	A	50	SER
1	E	51	SER
1	B	51	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	98/108 (91%)	97 (99%)	1 (1%)	82	87
1	B	99/108 (92%)	98 (99%)	1 (1%)	82	87
1	C	102/108 (94%)	100 (98%)	2 (2%)	63	68
1	D	99/108 (92%)	98 (99%)	1 (1%)	82	87
1	E	98/108 (91%)	98 (100%)	0	100	100
All	All	496/540 (92%)	491 (99%)	5 (1%)	82	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	B	37	SER
1	C	27	LYS
1	C	107	THR
1	D	40	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	72	GLN
1	B	20	HIS
1	B	26	ASN
1	B	63	GLN
1	B	72	GLN
1	C	20	HIS
1	C	63	GLN
1	C	72	GLN
1	C	117	ASN
1	D	49	ASN
1	E	63	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 ⓘ

12 carbohydrates 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	NGC	A	127	2	17,21,22	0.64	0	18,29,32	1.87	3 (16%)
2	GAL	A	128	2	11,11,12	0.60	0	14,15,17	1.76	2 (14%)
2	NGA	A	129	3,2	14,14,15	1.01	1 (7%)	15,19,21	0.71	0
2	NGC	C	127	2	17,21,22	0.66	0	18,29,32	2.26	6 (33%)
2	GAL	C	128	2	11,11,12	0.70	0	14,15,17	1.53	2 (14%)
2	NGA	C	129	3,2	14,14,15	0.97	1 (7%)	15,19,21	1.04	1 (6%)
2	NGC	D	127	2	17,21,22	0.71	0	18,29,32	2.19	5 (27%)
2	GAL	D	128	2	11,11,12	0.76	0	14,15,17	1.63	1 (7%)
2	NGA	D	129	3,2	14,14,15	1.03	1 (7%)	15,19,21	0.91	0
2	NGC	E	127	2	17,21,22	0.78	0	18,29,32	2.96	7 (38%)
2	GAL	E	128	2	11,11,12	0.58	0	14,15,17	1.85	3 (21%)
2	NGA	E	129	3,2	14,14,15	1.01	1 (7%)	15,19,21	1.67	4 (26%)

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	NGC	A	127	2	5/5/8/9	0/15/36/40	0/1/1/1
2	GAL	A	128	2	5/5/4/5	0/2/19/22	0/1/1/1
2	NGA	A	129	3,2	5/5/5/7	0/6/23/26	0/1/1/1
2	NGC	C	127	2	5/5/8/9	0/15/36/40	1/1/1/1
2	GAL	C	128	2	5/5/4/5	0/2/19/22	0/1/1/1
2	NGA	C	129	3,2	5/5/5/7	0/6/23/26	0/1/1/1
2	NGC	D	127	2	5/5/8/9	0/15/36/40	1/1/1/1
2	GAL	D	128	2	5/5/4/5	0/2/19/22	0/1/1/1
2	NGA	D	129	3,2	5/5/5/7	0/6/23/26	0/1/1/1
2	NGC	E	127	2	5/5/8/9	0/15/36/40	1/1/1/1
2	GAL	E	128	2	5/5/4/5	0/2/19/22	0/1/1/1
2	NGA	E	129	3,2	5/5/5/7	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	129	NGA	C7-N2	3.04	1.46	1.34
2	A	129	NGA	C7-N2	3.09	1.46	1.34
2	D	129	NGA	C7-N2	3.12	1.46	1.34
2	E	129	NGA	C7-N2	3.15	1.46	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	127	NGC	C2-C3-C4	-3.99	107.03	111.47
2	D	127	NGC	C2-C3-C4	-3.43	107.66	111.47
2	A	128	GAL	O3-C3-C2	-2.51	105.47	110.00
2	C	127	NGC	C2-C3-C4	-2.33	108.87	111.47
2	E	128	GAL	C2-C3-C4	-2.29	107.15	111.04
2	E	129	NGA	C8-C7-N2	-2.26	111.78	116.11
2	C	129	NGA	C8-C7-N2	-2.22	111.86	116.11
2	E	127	NGC	C11-C10-N4	-2.22	112.30	116.21
2	A	127	NGC	C6-C5-C4	2.03	117.39	114.32
2	C	127	NGC	C7-C6-C5	2.08	117.18	113.01
2	E	129	NGA	C3-C4-C5	2.17	113.97	110.20
2	E	129	NGA	O7-C7-N2	2.18	126.31	121.86
2	D	127	NGC	C5-C4-N4	2.47	115.38	111.07
2	C	128	GAL	C1-O5-C5	2.50	115.42	112.25
2	C	127	NGC	C5-C4-N4	2.58	115.57	111.07
2	E	128	GAL	C1-O5-C5	2.75	115.74	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	127	NGC	C7-C6-C5	2.89	118.81	113.01
2	E	127	NGC	C3-C4-N4	2.95	116.81	110.41
2	E	129	NGA	C2-N2-C7	4.06	128.26	123.04
2	D	127	NGC	C6-C5-C4	4.11	120.55	114.32
2	A	127	NGC	C4-N4-C10	4.19	129.58	123.05
2	D	127	NGC	O5-C1-C2	4.22	117.97	109.86
2	E	127	NGC	O5-C1-C2	4.30	118.12	109.86
2	C	127	NGC	C6-C5-C4	4.44	121.04	114.32
2	C	128	GAL	O3-C3-C4	4.46	120.39	110.34
2	C	127	NGC	O5-C1-C2	4.70	118.90	109.86
2	D	127	NGC	C4-N4-C10	4.81	130.55	123.05
2	D	128	GAL	O3-C3-C4	4.98	121.55	110.34
2	C	127	NGC	C4-N4-C10	5.20	131.15	123.05
2	A	127	NGC	O5-C1-C2	5.48	120.40	109.86
2	E	128	GAL	O3-C3-C4	5.56	122.85	110.34
2	E	127	NGC	C6-C5-C4	5.60	122.79	114.32
2	A	128	GAL	C1-C2-C3	5.63	116.20	109.54
2	E	127	NGC	C4-N4-C10	7.69	135.03	123.05

All (60) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	128	GAL	C2
2	A	128	GAL	C5
2	A	128	GAL	C3
2	A	128	GAL	C1
2	A	128	GAL	C4
2	D	127	NGC	C5
2	D	127	NGC	C3
2	D	127	NGC	C6
2	D	127	NGC	C4
2	D	127	NGC	C7
2	E	128	GAL	C2
2	E	128	GAL	C5
2	E	128	GAL	C3
2	E	128	GAL	C1
2	E	128	GAL	C4
2	D	129	NGA	C2
2	D	129	NGA	C5
2	D	129	NGA	C3
2	D	129	NGA	C1
2	D	129	NGA	C4

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Mol	Chain	Res	Type	Atom
2	C	129	NGA	C2
2	C	129	NGA	C5
2	C	129	NGA	C3
2	C	129	NGA	C1
2	C	129	NGA	C4
2	E	129	NGA	C2
2	E	129	NGA	C5
2	E	129	NGA	C3
2	E	129	NGA	C1
2	E	129	NGA	C4
2	A	129	NGA	C2
2	A	129	NGA	C5
2	A	129	NGA	C3
2	A	129	NGA	C1
2	A	129	NGA	C4
2	C	127	NGC	C5
2	C	127	NGC	C3
2	C	127	NGC	C6
2	C	127	NGC	C4
2	C	127	NGC	C7
2	E	127	NGC	C5
2	E	127	NGC	C3
2	E	127	NGC	C6
2	E	127	NGC	C4
2	E	127	NGC	C7
2	D	128	GAL	C2
2	D	128	GAL	C5
2	D	128	GAL	C3
2	D	128	GAL	C1
2	D	128	GAL	C4
2	A	127	NGC	C5
2	A	127	NGC	C3
2	A	127	NGC	C6
2	A	127	NGC	C4
2	A	127	NGC	C7
2	C	128	GAL	C2
2	C	128	GAL	C5
2	C	128	GAL	C3
2	C	128	GAL	C1
2	C	128	GAL	C4

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	127	NGC	C1-C2-C3-C4-C5-O5
2	D	127	NGC	C1-C2-C3-C4-C5-O5
2	E	127	NGC	C1-C2-C3-C4-C5-O5

6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	127	NGC	2	0
2	C	128	GAL	2	0
2	D	127	NGC	1	0
2	D	128	GAL	1	0
2	E	127	NGC	1	0
2	E	128	GAL	1	0

## 5.6 Ligand geometry [i](#)

13 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	POL	A	130	3,2	3,3,3	0.37	0	2,2,2	0.27	0
3	AZI	A	131	3	0,2,2	0.00	-	0,1,1	0.00	-
4	1PE	A	132	-	15,15,15	0.48	0	14,14,14	0.25	0
4	1PE	B	127	-	15,15,15	0.48	0	14,14,14	0.25	0
3	POL	C	130	3,2	3,3,3	0.40	0	2,2,2	0.22	0
3	AZI	C	131	3	0,2,2	0.00	-	0,1,1	0.00	-
3	POL	D	130	3,2	3,3,3	0.42	0	2,2,2	0.28	0
3	AZI	D	131	3	0,2,2	0.00	-	0,1,1	0.00	-
4	1PE	D	132	-	15,15,15	0.48	0	14,14,14	0.26	0
4	1PE	D	133	-	15,15,15	0.48	0	14,14,14	0.25	0
3	POL	E	130	3,2	3,3,3	0.34	0	2,2,2	0.41	0
3	AZI	E	131	3	0,2,2	0.00	-	0,1,1	0.00	-
4	1PE	E	132	-	15,15,15	0.48	0	14,14,14	0.28	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
3	POL	A	130	3,2	-	0/1/1/1	0/0/0/0
3	AZI	A	131	3	-	0/0/0/0	0/0/0/0
4	1PE	A	132	-	-	0/13/13/13	0/0/0/0
4	1PE	B	127	-	-	0/13/13/13	0/0/0/0
3	POL	C	130	3,2	-	0/1/1/1	0/0/0/0
3	AZI	C	131	3	-	0/0/0/0	0/0/0/0
3	POL	D	130	3,2	-	0/1/1/1	0/0/0/0
3	AZI	D	131	3	-	0/0/0/0	0/0/0/0
4	1PE	D	132	-	-	0/13/13/13	0/0/0/0
4	1PE	D	133	-	-	0/13/13/13	0/0/0/0
3	POL	E	130	3,2	-	0/1/1/1	0/0/0/0
3	AZI	E	131	3	-	0/0/0/0	0/0/0/0
4	1PE	E	132	-	-	0/13/13/13	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	127	1PE	1	0
4	D	132	1PE	1	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	116/126 (92%)	-0.17	6 (5%) 31 39	15, 20, 29, 30	0
1	B	117/126 (92%)	-0.22	3 (2%) 59 66	15, 20, 29, 32	0
1	C	120/126 (95%)	-0.12	5 (4%) 40 49	15, 20, 29, 37	0
1	D	117/126 (92%)	0.02	5 (4%) 39 48	15, 20, 29, 32	0
1	E	116/126 (92%)	0.18	8 (6%) 20 27	15, 20, 28, 30	0
All	All	586/630 (93%)	-0.06	27 (4%) 36 45	15, 20, 29, 37	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	ALA	4.7
1	E	39	GLY	4.3
1	D	37	SER	4.2
1	A	37	SER	4.1
1	E	38	ALA	3.6
1	D	117	ASN	3.5
1	D	38	ALA	3.5
1	C	50	SER	3.3
1	E	32	ILE	3.0
1	C	119	LEU	3.0
1	A	51	SER	2.9
1	B	38	ALA	2.9
1	A	50	SER	2.9
1	A	116	LYS	2.7
1	C	120	GLU	2.7
1	E	37	SER	2.6
1	C	51	SER	2.6
1	E	51	SER	2.6
1	E	60	LEU	2.6
1	D	39	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	44	ALA	2.4
1	E	100	LEU	2.3
1	D	40	SER	2.1
1	B	37	SER	2.1
1	B	31	CYS	2.1
1	A	39	GLY	2.1
1	C	49	ASN	2.0

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NGC	A	127	21/22	0.73	0.23	3.23	66,67,68,68	0
2	NGC	D	127	21/22	0.72	0.22	2.25	45,47,47,48	0
2	NGC	C	127	21/22	0.84	0.17	1.57	32,34,35,36	0
2	NGC	E	127	21/22	0.89	0.13	0.67	22,26,30,31	0
2	NGA	E	129	14/15	0.87	0.12	0.53	27,28,29,30	0
2	GAL	A	128	11/12	0.83	0.25	-	68,69,70,70	0
2	NGA	A	129	14/15	0.72	0.48	-	71,72,72,72	0
2	GAL	E	128	11/12	0.89	0.14	-	25,25,26,28	0
2	NGA	D	129	14/15	0.77	0.38	-	54,56,57,57	0
2	GAL	D	128	11/12	0.85	0.29	-	49,52,52,53	0
2	NGA	C	129	14/15	0.79	0.27	-	47,50,50,50	0
2	GAL	C	128	11/12	0.87	0.24	-	39,44,45,45	0

## 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	1PE	B	127	16/16	0.35	0.38	10.10	82,83,85,85	0
4	1PE	E	132	16/16	0.22	0.39	9.51	76,78,80,80	0
4	1PE	D	132	16/16	0.66	0.23	5.24	57,59,59,59	0
4	1PE	D	133	16/16	0.73	0.27	4.38	70,70,70,70	0
4	1PE	A	132	16/16	0.77	0.19	3.48	51,52,53,53	0
3	POL	C	130	4/4	0.73	0.48	-	51,52,52,53	0
3	AZI	C	131	3/3	0.78	0.44	-	53,53,53,53	0
3	POL	E	130	4/4	0.93	0.12	-	30,31,33,35	0
3	AZI	A	131	3/3	0.62	0.32	-	72,72,72,72	0
3	AZI	E	131	3/3	0.67	0.25	-	36,36,37,37	0
3	POL	D	130	4/4	0.83	0.51	-	57,58,58,59	0
3	POL	A	130	4/4	0.83	0.45	-	72,72,72,72	0
3	AZI	D	131	3/3	0.66	0.54	-	59,59,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.