



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 10:00 PM BST

PDB ID : 5OA0  
Title : Crystal structure of mutant AChBP in complex with strychnine (T53F, Q74R, Y110A, I135S, W164F)  
Authors : Dawson, A.; Hunter, W.N.; de Souza, J.O.; Trumper, P.  
Deposited on : 2017-06-20  
Resolution : 2.60 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

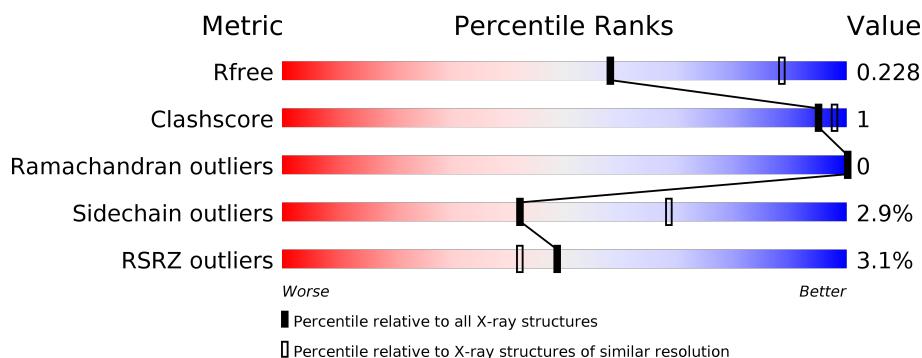
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	249	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	249	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	249	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>• •</div> <div>18%</div> </div> </div>
1	D	249	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>•</div> <div>18%</div> </div> </div>
1	E	249	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>•</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8561 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	2	0
			1640	1038	267	325	10			
1	B	210	Total	C	N	O	S	0	1	0
			1666	1051	276	329	10			
1	C	205	Total	C	N	O	S	0	0	0
			1630	1031	267	323	9			
1	D	205	Total	C	N	O	S	0	1	0
			1634	1034	267	323	10			
1	E	211	Total	C	N	O	S	0	1	0
			1677	1060	277	330	10			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	PHE	THR	engineered mutation	UNP Q8WSF8
A	60	VAL	ALA	conflict	UNP Q8WSF8
A	74	ARG	GLN	engineered mutation	UNP Q8WSF8
A	110	ALA	TYR	engineered mutation	UNP Q8WSF8
A	135	SER	ILE	engineered mutation	UNP Q8WSF8
A	155	VAL	ALA	conflict	UNP Q8WSF8
A	164	PHE	TRP	engineered mutation	UNP Q8WSF8
A	237	GLU	-	expression tag	UNP Q8WSF8
A	238	ASN	-	expression tag	UNP Q8WSF8
A	239	LEU	-	expression tag	UNP Q8WSF8
A	240	TYR	-	expression tag	UNP Q8WSF8
A	241	PHE	-	expression tag	UNP Q8WSF8
A	242	GLN	-	expression tag	UNP Q8WSF8
A	243	GLY	-	expression tag	UNP Q8WSF8
A	244	HIS	-	expression tag	UNP Q8WSF8
A	245	HIS	-	expression tag	UNP Q8WSF8
A	246	HIS	-	expression tag	UNP Q8WSF8
A	247	HIS	-	expression tag	UNP Q8WSF8
A	248	HIS	-	expression tag	UNP Q8WSF8

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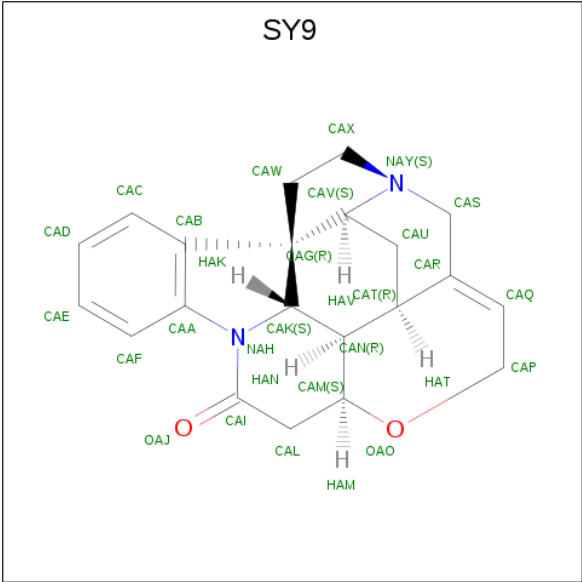
Chain	Residue	Modelled	Actual	Comment	Reference
A	249	HIS	-	expression tag	UNP Q8WSF8
B	53	PHE	THR	engineered mutation	UNP Q8WSF8
B	60	VAL	ALA	conflict	UNP Q8WSF8
B	74	ARG	GLN	engineered mutation	UNP Q8WSF8
B	110	ALA	TYR	engineered mutation	UNP Q8WSF8
B	135	SER	ILE	engineered mutation	UNP Q8WSF8
B	155	VAL	ALA	conflict	UNP Q8WSF8
B	164	PHE	TRP	engineered mutation	UNP Q8WSF8
B	237	GLU	-	expression tag	UNP Q8WSF8
B	238	ASN	-	expression tag	UNP Q8WSF8
B	239	LEU	-	expression tag	UNP Q8WSF8
B	240	TYR	-	expression tag	UNP Q8WSF8
B	241	PHE	-	expression tag	UNP Q8WSF8
B	242	GLN	-	expression tag	UNP Q8WSF8
B	243	GLY	-	expression tag	UNP Q8WSF8
B	244	HIS	-	expression tag	UNP Q8WSF8
B	245	HIS	-	expression tag	UNP Q8WSF8
B	246	HIS	-	expression tag	UNP Q8WSF8
B	247	HIS	-	expression tag	UNP Q8WSF8
B	248	HIS	-	expression tag	UNP Q8WSF8
B	249	HIS	-	expression tag	UNP Q8WSF8
C	53	PHE	THR	engineered mutation	UNP Q8WSF8
C	60	VAL	ALA	conflict	UNP Q8WSF8
C	74	ARG	GLN	engineered mutation	UNP Q8WSF8
C	110	ALA	TYR	engineered mutation	UNP Q8WSF8
C	135	SER	ILE	engineered mutation	UNP Q8WSF8
C	155	VAL	ALA	conflict	UNP Q8WSF8
C	164	PHE	TRP	engineered mutation	UNP Q8WSF8
C	237	GLU	-	expression tag	UNP Q8WSF8
C	238	ASN	-	expression tag	UNP Q8WSF8
C	239	LEU	-	expression tag	UNP Q8WSF8
C	240	TYR	-	expression tag	UNP Q8WSF8
C	241	PHE	-	expression tag	UNP Q8WSF8
C	242	GLN	-	expression tag	UNP Q8WSF8
C	243	GLY	-	expression tag	UNP Q8WSF8
C	244	HIS	-	expression tag	UNP Q8WSF8
C	245	HIS	-	expression tag	UNP Q8WSF8
C	246	HIS	-	expression tag	UNP Q8WSF8
C	247	HIS	-	expression tag	UNP Q8WSF8
C	248	HIS	-	expression tag	UNP Q8WSF8
C	249	HIS	-	expression tag	UNP Q8WSF8
D	53	PHE	THR	engineered mutation	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	60	VAL	ALA	conflict	UNP Q8WSF8
D	74	ARG	GLN	engineered mutation	UNP Q8WSF8
D	110	ALA	TYR	engineered mutation	UNP Q8WSF8
D	135	SER	ILE	engineered mutation	UNP Q8WSF8
D	155	VAL	ALA	conflict	UNP Q8WSF8
D	164	PHE	TRP	engineered mutation	UNP Q8WSF8
D	237	GLU	-	expression tag	UNP Q8WSF8
D	238	ASN	-	expression tag	UNP Q8WSF8
D	239	LEU	-	expression tag	UNP Q8WSF8
D	240	TYR	-	expression tag	UNP Q8WSF8
D	241	PHE	-	expression tag	UNP Q8WSF8
D	242	GLN	-	expression tag	UNP Q8WSF8
D	243	GLY	-	expression tag	UNP Q8WSF8
D	244	HIS	-	expression tag	UNP Q8WSF8
D	245	HIS	-	expression tag	UNP Q8WSF8
D	246	HIS	-	expression tag	UNP Q8WSF8
D	247	HIS	-	expression tag	UNP Q8WSF8
D	248	HIS	-	expression tag	UNP Q8WSF8
D	249	HIS	-	expression tag	UNP Q8WSF8
E	53	PHE	THR	engineered mutation	UNP Q8WSF8
E	60	VAL	ALA	conflict	UNP Q8WSF8
E	74	ARG	GLN	engineered mutation	UNP Q8WSF8
E	110	ALA	TYR	engineered mutation	UNP Q8WSF8
E	135	SER	ILE	engineered mutation	UNP Q8WSF8
E	155	VAL	ALA	conflict	UNP Q8WSF8
E	164	PHE	TRP	engineered mutation	UNP Q8WSF8
E	237	GLU	-	expression tag	UNP Q8WSF8
E	238	ASN	-	expression tag	UNP Q8WSF8
E	239	LEU	-	expression tag	UNP Q8WSF8
E	240	TYR	-	expression tag	UNP Q8WSF8
E	241	PHE	-	expression tag	UNP Q8WSF8
E	242	GLN	-	expression tag	UNP Q8WSF8
E	243	GLY	-	expression tag	UNP Q8WSF8
E	244	HIS	-	expression tag	UNP Q8WSF8
E	245	HIS	-	expression tag	UNP Q8WSF8
E	246	HIS	-	expression tag	UNP Q8WSF8
E	247	HIS	-	expression tag	UNP Q8WSF8
E	248	HIS	-	expression tag	UNP Q8WSF8
E	249	HIS	-	expression tag	UNP Q8WSF8

- Molecule 2 is STRYCHNINE (three-letter code: SY9) (formula: C<sub>21</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>).



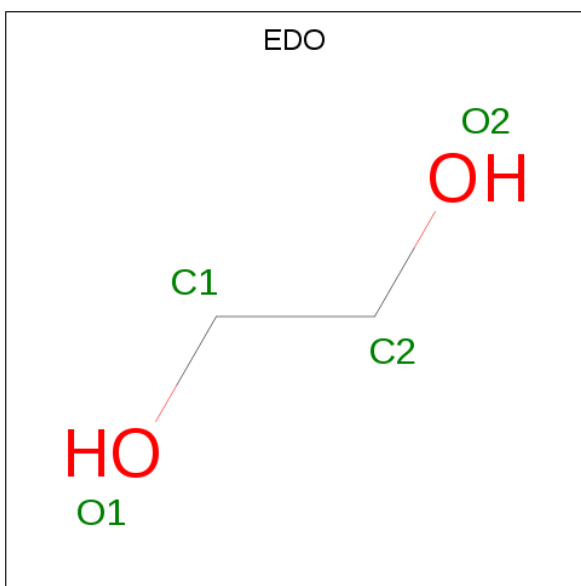
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	21	2	2		
2	C	1	Total	C	N	O	0	0
			25	21	2	2		
2	C	1	Total	C	N	O	0	0
			25	21	2	2		
2	D	1	Total	C	N	O	0	0
			25	21	2	2		
2	E	1	Total	C	N	O	0	0
			25	21	2	2		

- Molecule 3 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
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		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

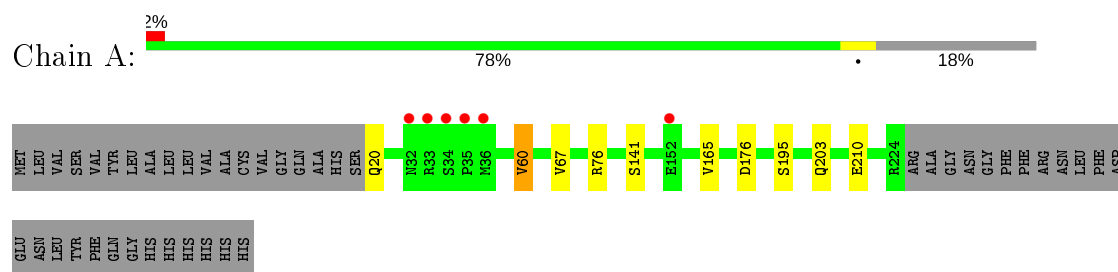
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	28	Total O 28 28	0	0
5	B	21	Total O 21 21	0	0
5	C	15	Total O 15 15	0	0
5	D	22	Total O 22 22	0	0
5	E	27	Total O 27 27	0	0



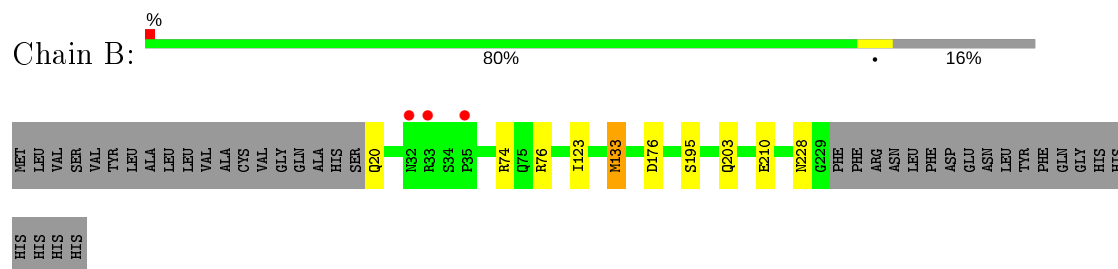
### 3 Residue-property plots [i](#)

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.

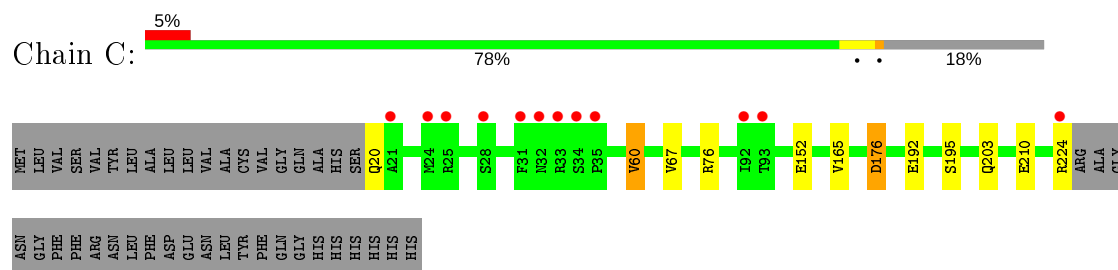
- Molecule 1: Soluble acetylcholine receptor



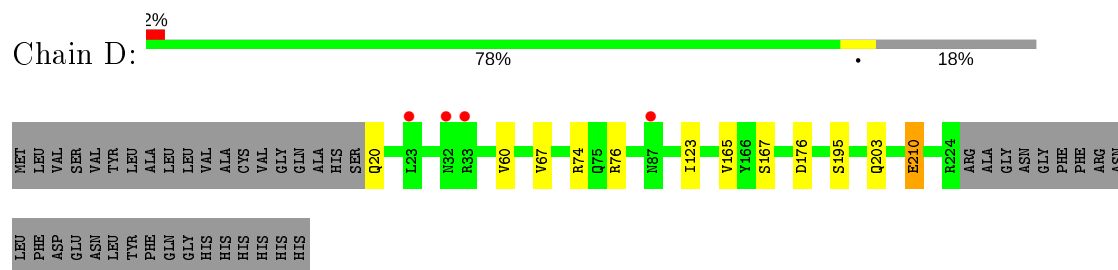
- Molecule 1: Soluble acetylcholine receptor



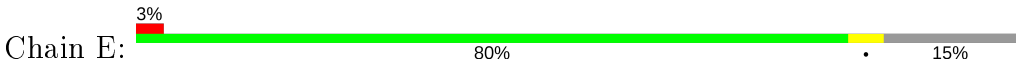
- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor



● Molecule 1: Soluble acetylcholine receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.87Å 74.87Å 185.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.43 – 2.60 37.44 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.43-2.60) 99.1 (37.44-2.60)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.188 , 0.227 0.194 , 0.228	Depositor DCC
$R_{free}$ test set	1676 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l 0.054 for h,-h-k,-l 0.030 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: SY9, NAG, EDO

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	0.51	0/1686	0.72	0/2297
1	B	0.53	0/1709	0.76	2/2326 (0.1%)
1	C	0.50	0/1669	0.74	1/2274 (0.0%)
1	D	0.52	1/1677 (0.1%)	0.74	1/2284 (0.0%)
1	E	0.54	0/1721	0.78	2/2342 (0.1%)
All	All	0.52	1/8462 (0.0%)	0.75	6/11523 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	210	GLU	CG-CD	5.97	1.60	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	225	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	B	133[A]	MET	CA-CB-CG	6.25	123.92	113.30
1	B	133[B]	MET	CA-CB-CG	6.25	123.92	113.30
1	D	210	GLU	OE1-CD-OE2	-5.48	116.73	123.30
1	E	33	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	176	ASP	CB-CG-OD1	5.11	122.90	118.30

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	1640	0	1575	4	0
1	B	1666	0	1599	4	0
1	C	1630	0	1565	4	0
1	D	1634	0	1570	6	0
1	E	1677	0	1609	5	0
2	A	25	0	22	0	0
2	C	50	0	44	0	0
2	D	25	0	22	0	0
2	E	25	0	22	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	8	0	12	1	0
4	B	12	0	18	2	0
4	C	8	0	12	0	0
4	D	8	0	12	0	0
4	E	12	0	18	0	0
5	A	28	0	0	0	0
5	B	21	0	0	0	0
5	C	15	0	0	0	0
5	D	22	0	0	1	0
5	E	27	0	0	0	0
All	All	8561	0	8126	20	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 1.

All (20) 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:B:228:ASN:HD21	4:B:304:EDO:H11	1.62	0.65
1:D:76:ARG:NH2	1:D:176:ASP:OD2	2.33	0.62
1:A:76:ARG:NH2	1:A:176:ASP:OD2	2.34	0.61
1:E:76:ARG:NH2	1:E:176:ASP:OD2	2.34	0.61
1:C:76:ARG:NH2	1:C:176:ASP:OD2	2.34	0.60
1:B:76:ARG:NH2	1:B:176:ASP:OD2	2.34	0.59
1:D:210:GLU:HG2	5:D:718:HOH:O	2.04	0.57
1:C:60:VAL:HG22	1:C:67:VAL:HG22	1.86	0.57
1:E:60:VAL:HG22	1:E:67:VAL:HG22	1.87	0.57
1:A:141:SER:OG	4:A:604:EDO:H21	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG22	1:A:67:VAL:HG22	1.88	0.56
1:D:60:VAL:HG22	1:D:67:VAL:HG22	1.89	0.54
1:D:165:VAL:HG21	1:E:123:ILE:HG21	1.89	0.53
1:B:228:ASN:ND2	4:B:304:EDO:H11	2.24	0.51
1:C:165:VAL:HG21	1:D:123:ILE:HG21	1.95	0.49
1:C:192:GLU:HB3	1:C:224:ARG:HD3	1.95	0.48
1:E:225:ARG:HH11	1:E:225:ARG:CG	2.27	0.47
1:A:165:VAL:HG21	1:B:123:ILE:HG21	1.98	0.45
1:E:91:ASN:HD22	1:E:91:ASN:HA	1.62	0.42
1:D:167:SER:CB	1:D:210:GLU:HG3	2.50	0.41

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	205/249 (82%)	200 (98%)	5 (2%)	0	100	100
1	B	209/249 (84%)	203 (97%)	6 (3%)	0	100	100
1	C	203/249 (82%)	199 (98%)	4 (2%)	0	100	100
1	D	204/249 (82%)	200 (98%)	4 (2%)	0	100	100
1	E	210/249 (84%)	205 (98%)	5 (2%)	0	100	100
All	All	1031/1245 (83%)	1007 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	189/223 (85%)	183 (97%)	6 (3%)	39	65
1	B	190/223 (85%)	183 (96%)	7 (4%)	34	60
1	C	187/223 (84%)	181 (97%)	6 (3%)	39	65
1	D	188/223 (84%)	184 (98%)	4 (2%)	53	77
1	E	191/223 (86%)	185 (97%)	6 (3%)	40	66
All	All	945/1115 (85%)	916 (97%)	29 (3%)	42	66

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	60	VAL
1	A	195	SER
1	A	203	GLN
1	A	210[A]	GLU
1	A	210[B]	GLU
1	B	20	GLN
1	B	74	ARG
1	B	133[A]	MET
1	B	133[B]	MET
1	B	195	SER
1	B	203	GLN
1	B	210	GLU
1	C	20	GLN
1	C	60	VAL
1	C	152	GLU
1	C	195	SER
1	C	203	GLN
1	C	210	GLU
1	D	20	GLN
1	D	74	ARG
1	D	195	SER
1	D	203	GLN
1	E	20	GLN
1	E	91	ASN
1	E	195	SER
1	E	203	GLN
1	E	210	GLU
1	E	225	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	216	ASN
1	B	20	GLN
1	B	216	ASN
1	C	20	GLN
1	C	216	ASN
1	D	20	GLN
1	D	216	ASN
1	E	20	GLN
1	E	91	ASN
1	E	216	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

19 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	SY9	C	602	-	31,31,31	0.28	0	51,51,51	0.46	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	301	1	14,14,15	1.31	2 (14%)	17,19,21	2.66	6 (35%)
2	SY9	A	601	-	31,31,31	0.26	0	51,51,51	0.48	0
2	SY9	D	601	-	31,31,31	0.31	0	51,51,51	0.52	0
2	SY9	C	601	-	31,31,31	0.37	0	51,51,51	0.54	0
4	EDO	A	603	-	3,3,3	0.77	0	2,2,2	0.33	0
4	EDO	C	603	-	3,3,3	0.53	0	2,2,2	0.13	0
3	NAG	A	602	1	14,14,15	0.80	0	17,19,21	1.37	1 (5%)
4	EDO	E	603	-	3,3,3	0.63	0	2,2,2	0.15	0
4	EDO	C	604	-	3,3,3	0.42	0	2,2,2	0.53	0
4	EDO	E	604	-	3,3,3	0.28	0	2,2,2	0.71	0
4	EDO	B	304	-	3,3,3	0.36	0	2,2,2	0.25	0
4	EDO	D	602	-	3,3,3	0.60	0	2,2,2	0.17	0
4	EDO	E	602	-	3,3,3	0.66	0	2,2,2	0.28	0
2	SY9	E	601	-	31,31,31	0.31	0	51,51,51	0.47	0
4	EDO	A	604	-	3,3,3	0.39	0	2,2,2	0.80	0
4	EDO	B	303	-	3,3,3	0.48	0	2,2,2	0.75	0
4	EDO	D	603	-	3,3,3	0.58	0	2,2,2	0.40	0
4	EDO	B	302	-	3,3,3	0.55	0	2,2,2	0.45	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	NAG	B	301	1	-	1/6/23/26	0/1/1/1
4	EDO	C	604	-	-	1/1/1/1	-
4	EDO	A	603	-	-	1/1/1/1	-
4	EDO	C	603	-	-	1/1/1/1	-
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	EDO	E	603	-	-	0/1/1/1	-
4	EDO	B	302	-	-	0/1/1/1	-
4	EDO	B	304	-	-	0/1/1/1	-
4	EDO	D	602	-	-	1/1/1/1	-
4	EDO	E	602	-	-	1/1/1/1	-
4	EDO	E	604	-	-	0/1/1/1	-
4	EDO	B	303	-	-	1/1/1/1	-
4	EDO	D	603	-	-	0/1/1/1	-
4	EDO	A	604	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NAG	C1-C2	3.59	1.57	1.52
3	B	301	NAG	O5-C1	2.27	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	NAG	C1-O5-C5	7.78	122.74	112.19
3	B	301	NAG	O5-C1-C2	4.61	118.57	111.29
3	A	602	NAG	C4-C3-C2	3.89	116.72	111.02
3	B	301	NAG	C2-N2-C7	3.86	128.39	122.90
3	B	301	NAG	C1-C2-N2	2.74	115.16	110.49
3	B	301	NAG	O5-C5-C6	2.47	111.07	107.20
3	B	301	NAG	C4-C3-C2	-2.18	107.82	111.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	EDO	O1-C1-C2-O2
4	C	603	EDO	O1-C1-C2-O2
3	B	301	NAG	C3-C2-N2-C7
4	E	602	EDO	O1-C1-C2-O2
4	D	602	EDO	O1-C1-C2-O2
4	A	604	EDO	O1-C1-C2-O2
4	C	604	EDO	O1-C1-C2-O2
4	B	303	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	304	EDO	2	0
4	A	604	EDO	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

### 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	205/249 (82%)	-0.23	6 (2%) 51 45	27, 41, 71, 105	0
1	B	210/249 (84%)	-0.08	3 (1%) 75 71	31, 49, 94, 121	0
1	C	205/249 (82%)	0.04	12 (5%) 22 17	33, 53, 91, 116	0
1	D	205/249 (82%)	-0.05	4 (1%) 65 60	28, 46, 77, 117	0
1	E	211/249 (84%)	-0.21	7 (3%) 46 39	25, 41, 79, 108	0
All	All	1036/1245 (83%)	-0.10	32 (3%) 49 42	25, 46, 87, 121	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	ASN	4.1
1	C	33	ARG	4.0
1	C	34	SER	3.9
1	C	31	PHE	3.7
1	C	32	ASN	3.4
1	A	33	ARG	3.2
1	A	34	SER	3.2
1	C	28	SER	3.2
1	B	33	ARG	3.1
1	E	33	ARG	3.1
1	D	33	ARG	3.0
1	E	230	PHE	2.9
1	E	31	PHE	2.9
1	C	21	ALA	2.9
1	C	24	MET	2.8
1	D	87	ASN	2.8
1	E	87	ASN	2.8
1	C	35	PRO	2.6
1	D	32	ASN	2.6
1	C	224	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLU	2.5
1	E	32	ASN	2.4
1	A	36	MET	2.3
1	E	226	ALA	2.3
1	C	92	ILE	2.3
1	A	35	PRO	2.2
1	C	25	ARG	2.2
1	B	35	PRO	2.2
1	C	93	THR	2.2
1	D	23	LEU	2.2
1	E	227	GLY	2.1
1	A	32	ASN	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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
3	NAG	B	301	14/15	0.53	0.38	95,117,129,131	0
3	NAG	A	602	14/15	0.59	0.32	78,94,100,101	0
4	EDO	D	603	4/4	0.84	0.23	51,52,53,56	0
4	EDO	E	604	4/4	0.87	0.20	49,51,53,57	0
4	EDO	B	303	4/4	0.88	0.19	42,43,44,47	0
4	EDO	C	604	4/4	0.90	0.20	55,58,59,65	0
4	EDO	E	603	4/4	0.90	0.16	46,46,47,47	0
2	SY9	C	601	25/25	0.92	0.19	79,88,92,95	0
4	EDO	A	604	4/4	0.92	0.18	40,42,43,44	0
4	EDO	E	602	4/4	0.93	0.21	39,42,44,46	0
4	EDO	B	304	4/4	0.93	0.17	59,63,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SY9	C	602	25/25	0.94	0.16	52,59,64,66	0
4	EDO	B	302	4/4	0.94	0.21	44,51,55,58	0
4	EDO	C	603	4/4	0.94	0.17	46,50,55,58	0
4	EDO	A	603	4/4	0.95	0.32	45,45,46,47	0
2	SY9	E	601	25/25	0.95	0.12	37,45,49,49	0
2	SY9	A	601	25/25	0.96	0.21	31,37,41,42	0
2	SY9	D	601	25/25	0.96	0.19	36,41,44,47	0
4	EDO	D	602	4/4	0.97	0.27	41,43,46,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.