



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:26 PM GMT

PDB ID : 4EZC  
Title : Crystal Structure of the UT-B Urea Transporter from Bos Taurus  
Authors : Cao, Y.; Levin, E.J.; Zhou, M.; New York Consortium on Membrane Protein Structure (NYCOMPS)  
Deposited on : 2012-05-02  
Resolution : 2.36 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

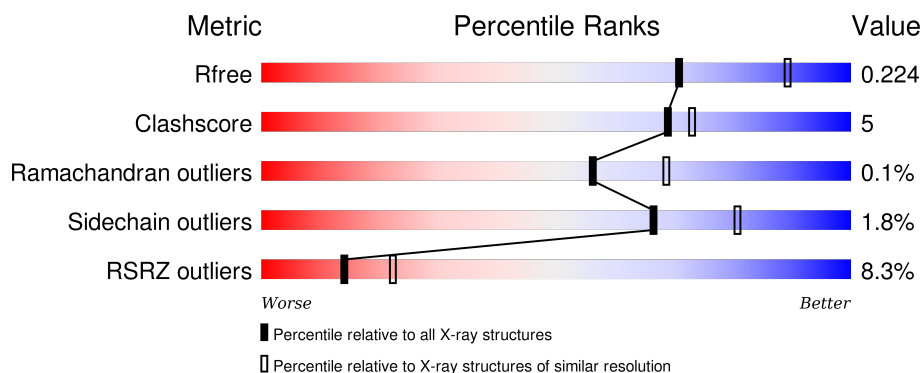
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


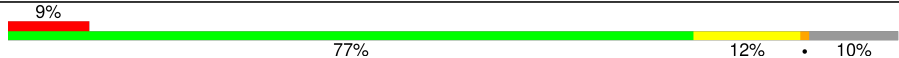

The reported resolution of this entry is 2.36 Å.

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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	384	
1	B	384	
1	C	384	

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
3	BOG	A	403	-	-	-	X
3	BOG	A	404	-	-	-	X
3	BOG	A	405	-	-	-	X
3	BOG	A	406	-	-	-	X
3	BOG	B	404	-	-	-	X
3	BOG	C	404	-	-	-	X
3	BOG	C	405	-	-	-	X
3	BOG	C	406	-	-	-	X
3	BOG	C	407	-	-	-	X
4	SPL	A	407	-	-	-	X
4	SPL	B	406	-	-	-	X
4	SPL	C	408	-	-	-	X

## 2 Entry composition [i](#)

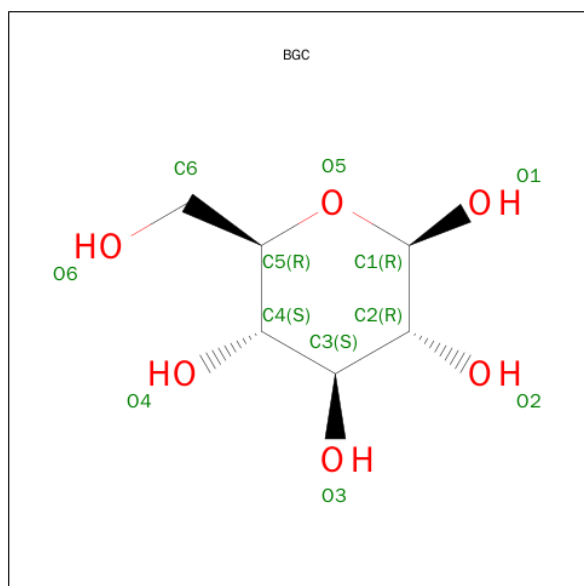
There are 5 unique types of molecules in this entry. The entry contains 8470 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Urea transporter 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2623	1735	407	462	19			
1	B	346	Total	C	N	O	S	0	0	0
			2634	1741	411	463	19			
1	C	346	Total	C	N	O	S	0	0	0
			2634	1741	411	463	19			

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



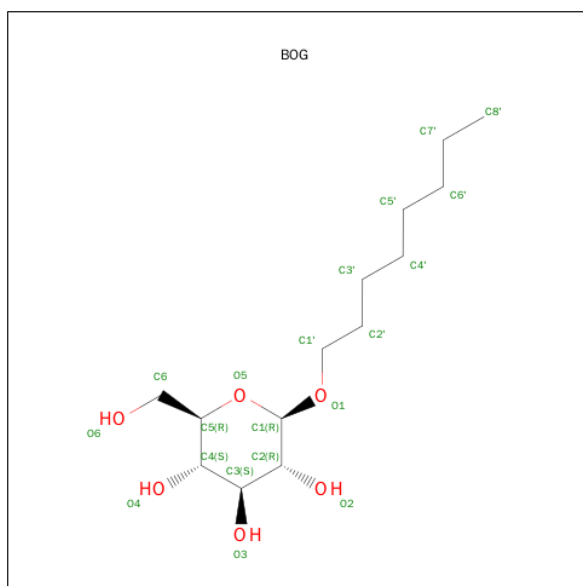
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



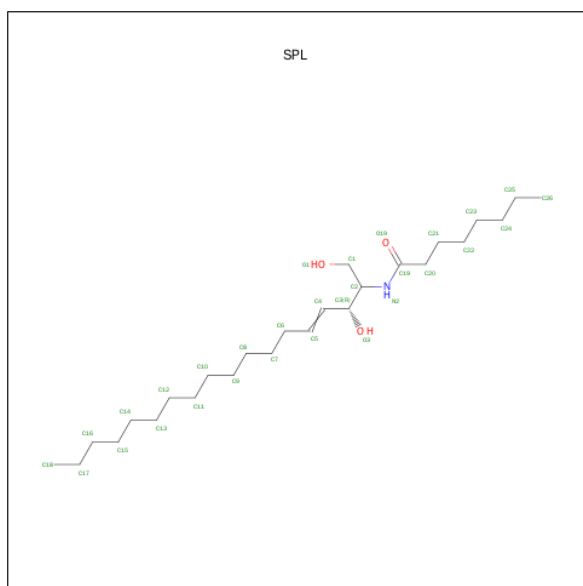
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			20	14	6		
3	C	1	Total	C	O	0	0
			20	14	6		
3	C	1	Total	C	O	0	0
			20	14	6		
3	C	1	Total	C	O	0	0
			20	14	6		

- Molecule 4 is OCTANOIC ACID (2-HYDROXY-1-HYDROXYMETHYL-HEPTADEC-3-ENYL)-AMIDE (three-letter code: SPL) (formula: C<sub>26</sub>H<sub>51</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			30	26	1	3		
4	B	1	Total	C	N	O	0	0
			30	26	1	3		
4	C	1	Total	C	N	O	0	0
			30	26	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	68	Total	O	0	0
			68	68		

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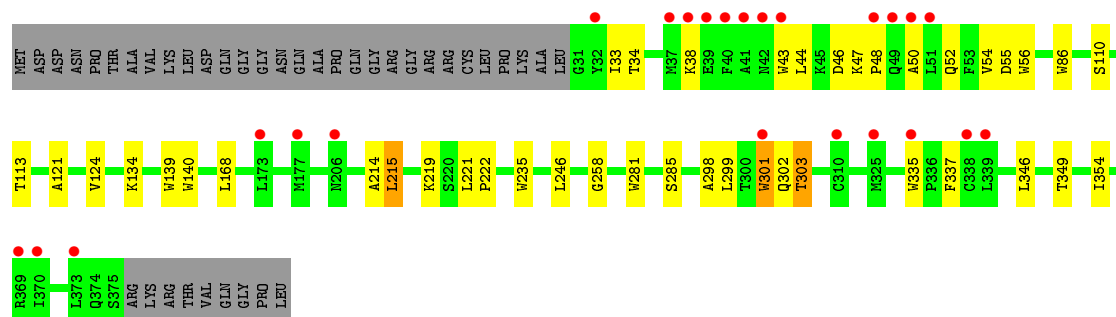
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	66	Total	O	0	0
			66	66		

### 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.

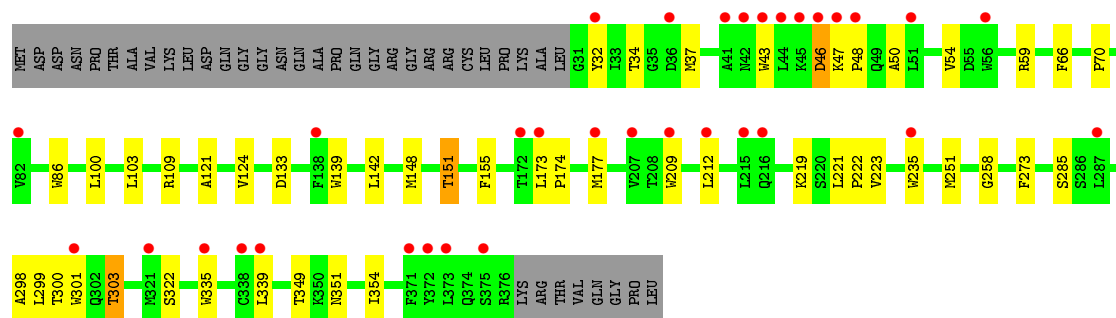
#### • Molecule 1: Urea transporter 1

Chain A: 




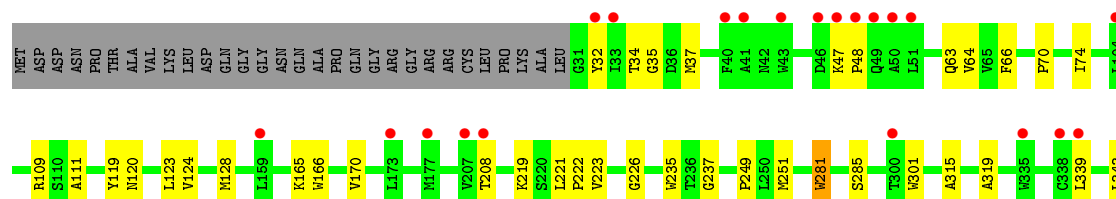
#### • Molecule 1: Urea transporter 1

Chain B: 

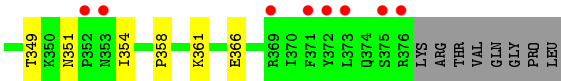


#### • Molecule 1: Urea transporter 1

Chain C: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.70Å 105.64Å 105.87Å 90.00° 99.00° 90.00°	Depositor
Resolution (Å)	42.95 – 2.36 42.95 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.95-2.36) 98.9 (42.95-2.36)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.196 , 0.228 0.193 , 0.224	Depositor DCC
$R_{free}$ test set	3274 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.3	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 66520 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8470	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 4.62% 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: BGC, SPL, BOG

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	0.70	8/2699 (0.3%)	0.65	1/3699 (0.0%)
1	B	0.71	6/2710 (0.2%)	0.64	0/3713
1	C	0.70	4/2710 (0.1%)	0.64	0/3713
All	All	0.70	18/8119 (0.2%)	0.64	1/11125 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	TRP	CD2-CE2	5.96	1.48	1.41
1	B	235	TRP	CD2-CE2	5.84	1.48	1.41
1	A	86	TRP	CD2-CE2	5.84	1.48	1.41
1	B	209	TRP	CD2-CE2	5.72	1.48	1.41
1	C	301	TRP	CD2-CE2	5.53	1.48	1.41
1	B	86	TRP	CD2-CE2	5.46	1.48	1.41
1	A	281	TRP	CD2-CE2	5.43	1.47	1.41
1	B	301	TRP	CD2-CE2	5.40	1.47	1.41
1	B	335	TRP	CD2-CE2	5.37	1.47	1.41
1	C	235	TRP	CD2-CE2	5.37	1.47	1.41
1	A	235	TRP	CD2-CE2	5.37	1.47	1.41
1	B	43	TRP	CD2-CE2	5.28	1.47	1.41
1	A	140	TRP	CD2-CE2	5.27	1.47	1.41
1	A	335	TRP	CD2-CE2	5.26	1.47	1.41
1	A	139	TRP	CD2-CE2	5.25	1.47	1.41
1	C	281	TRP	CD2-CE2	5.18	1.47	1.41
1	C	166	TRP	CD2-CE2	5.18	1.47	1.41
1	A	43	TRP	CD2-CE2	5.03	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	LEU	CA-CB-CG	5.24	127.34	115.30

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	2623	0	2665	18	0
1	B	2634	0	2678	35	0
1	C	2634	0	2678	24	0
2	A	24	0	24	0	0
2	B	36	0	36	2	0
2	C	36	0	36	0	0
3	A	80	0	112	1	0
3	B	40	0	56	0	0
3	C	80	0	112	0	0
4	A	30	0	51	1	0
4	B	30	0	51	2	0
4	C	30	0	51	0	0
5	A	59	0	0	0	0
5	B	68	0	0	0	0
5	C	66	0	0	3	0
All	All	8470	0	8550	77	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 5.

All (77) 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:349:THR:HG22	1:B:351:ASN:H	1.46	0.80
1:B:298:ALA:O	1:B:303:THR:HG21	1.84	0.78
1:A:33:ILE:HD13	1:A:246:LEU:HD11	1.68	0.75
1:B:349:THR:CG2	1:B:351:ASN:H	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:NH1	1:B:70:PRO:HD3	2.06	0.71
1:A:298:ALA:O	1:A:303:THR:HG21	1.91	0.70
1:B:151:THR:HG23	1:B:155:PHE:CD2	2.31	0.66
1:B:151:THR:HG23	1:B:155:PHE:CE2	2.35	0.62
1:B:148:MET:O	1:B:151:THR:HB	2.00	0.61
1:C:349:THR:HG21	1:C:354:ILE:HB	1.80	0.61
1:B:46:ASP:HB2	1:B:47:LYS:HE3	1.83	0.60
1:B:299:LEU:HA	1:B:303:THR:HG21	1.84	0.59
1:C:124:VAL:HG12	1:C:128:MET:SD	2.43	0.58
1:A:215:LEU:HD11	1:A:219:LYS:HE3	1.86	0.58
1:B:349:THR:CG2	1:B:351:ASN:HB3	2.33	0.57
1:A:299:LEU:HA	1:A:303:THR:HG21	1.85	0.57
1:C:219:LYS:O	1:C:223:VAL:HG23	2.05	0.57
4:B:406:SPL:H101	1:C:343:LEU:HD13	1.87	0.57
1:A:121:ALA:HA	1:A:124:VAL:HB	1.86	0.56
1:A:349:THR:HG21	1:A:354:ILE:HB	1.89	0.55
1:C:120:ASN:O	1:C:124:VAL:HG23	2.06	0.55
4:A:407:SPL:H92	1:B:339:LEU:HB3	1.88	0.54
1:A:52:GLN:O	1:A:55:ASP:HB3	2.07	0.54
1:A:214:ALA:HB2	3:A:404:BOG:H1'2	1.90	0.54
1:C:111:ALA:HB3	5:C:551:HOH:O	2.09	0.52
1:B:299:LEU:HA	1:B:303:THR:CG2	2.40	0.52
1:C:32:TYR:O	1:C:37:MET:HG2	2.11	0.51
4:B:406:SPL:H92	1:C:339:LEU:HB3	1.93	0.51
1:A:258:GLY:O	1:A:285:SER:HB3	2.10	0.51
1:B:349:THR:HG22	1:B:351:ASN:N	2.22	0.51
1:B:47:LYS:HB3	1:B:48:PRO:CD	2.41	0.51
1:C:226:GLY:HA3	5:C:559:HOH:O	2.09	0.51
1:B:151:THR:CG2	1:B:155:PHE:CE2	2.94	0.50
1:C:249:PRO:HD2	1:C:366:GLU:OE1	2.11	0.50
1:A:301:TRP:HB3	1:A:302:GLN:OE1	2.12	0.49
1:A:215:LEU:CD1	1:A:219:LYS:HE3	2.43	0.48
1:B:349:THR:HG21	1:B:351:ASN:HB3	1.94	0.48
1:B:219:LYS:O	1:B:223:VAL:HG23	2.14	0.47
1:B:139:TRP:H	2:B:403:BGC:H6C2	1.80	0.47
1:C:64:VAL:HG13	1:C:123:LEU:HD11	1.97	0.47
1:C:165:LYS:HA	1:C:165:LYS:HD2	1.64	0.47
1:A:44:LEU:HG	1:A:52:GLN:HG2	1.96	0.47
1:B:173:LEU:O	1:B:177:MET:HG3	2.15	0.47
1:B:47:LYS:HB3	1:B:48:PRO:HD2	1.97	0.46
1:C:47:LYS:HB3	1:C:48:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:HB3	1:B:222:PRO:CD	2.46	0.46
1:B:300:THR:OG1	1:B:303:THR:HB	2.16	0.46
1:B:349:THR:HG21	1:B:354:ILE:HD12	1.97	0.45
1:C:221:LEU:HB3	1:C:222:PRO:CD	2.46	0.45
1:B:32:TYR:O	1:B:37:MET:HG2	2.17	0.45
1:C:170:VAL:HG22	5:C:501:HOH:O	2.17	0.44
1:C:63:GLN:HB2	1:C:119:TYR:HB3	2.00	0.44
1:A:56:TRP:CE2	1:A:113:THR:HG22	2.52	0.44
1:B:173:LEU:N	1:B:174:PRO:CD	2.80	0.44
1:A:47:LYS:HB3	1:A:48:PRO:HD2	2.00	0.44
1:A:50:ALA:O	1:A:54:VAL:HG23	2.19	0.43
1:B:109:ARG:HD2	1:B:109:ARG:HA	1.67	0.43
1:C:285:SER:OG	1:C:315:ALA:HB2	2.18	0.43
1:C:70:PRO:O	1:C:74:ILE:HG13	2.19	0.43
1:A:168:LEU:HD11	1:A:346:LEU:HD21	2.01	0.43
1:C:66:PHE:HB2	1:C:251:MET:HE1	2.01	0.43
1:B:212:LEU:HD13	1:B:273:PHE:CE1	2.54	0.43
1:B:151:THR:CG2	1:B:155:PHE:CD2	3.00	0.43
1:C:351:ASN:HB3	1:C:354:ILE:HD12	2.01	0.42
1:C:47:LYS:HB3	1:C:48:PRO:CD	2.49	0.42
1:B:121:ALA:HA	1:B:124:VAL:HB	2.00	0.42
1:B:139:TRP:H	2:B:403:BGC:C6	2.33	0.42
1:C:281:TRP:CH2	1:C:319:ALA:HB2	2.54	0.41
1:C:358:PRO:HG2	1:C:361:LYS:HB2	2.03	0.41
1:B:50:ALA:O	1:B:54:VAL:HG23	2.19	0.41
1:B:258:GLY:O	1:B:285:SER:HB3	2.19	0.41
1:B:299:LEU:HD12	1:B:303:THR:HG22	2.02	0.41
1:A:134:LYS:HA	1:A:134:LYS:HD2	1.82	0.41
1:A:221:LEU:HB3	1:A:222:PRO:HD3	2.03	0.41
1:C:222:PRO:O	1:C:237:GLY:HA3	2.20	0.41
1:B:100:LEU:HA	1:B:103:LEU:HD12	2.02	0.41
1:B:66:PHE:HB2	1:B:251:MET:CE	2.51	0.41

There are no symmetry-related clashes.

## 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	343/384 (89%)	332 (97%)	11 (3%)	0	100	100
1	B	344/384 (90%)	334 (97%)	10 (3%)	0	100	100
1	C	344/384 (90%)	335 (97%)	8 (2%)	1 (0%)	46	55
All	All	1031/1152 (90%)	1001 (97%)	29 (3%)	1 (0%)	56	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	35	GLY

### 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	288/319 (90%)	282 (98%)	6 (2%)	61	76
1	B	289/319 (91%)	282 (98%)	7 (2%)	57	71
1	C	289/319 (91%)	286 (99%)	3 (1%)	82	91
All	All	866/957 (90%)	850 (98%)	16 (2%)	66	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	38	LYS
1	A	46	ASP
1	A	110	SER
1	A	303	THR
1	A	337	PHE
1	B	34	THR
1	B	46	ASP

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Mol	Chain	Res	Type
1	B	133	ASP
1	B	142	LEU
1	B	151	THR
1	B	303	THR
1	B	322	SER
1	C	34	THR
1	C	109	ARG
1	C	208	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

21 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	BGC	A	401	-	12,12,12	0.60	0	17,17,17	0.94	0
2	BGC	A	402	-	12,12,12	0.59	0	17,17,17	1.62	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BOG	A	403	-	20,20,20	0.58	0	25,25,25	0.85	1 (4%)
3	BOG	A	404	-	20,20,20	0.69	0	25,25,25	0.78	0
3	BOG	A	405	-	20,20,20	0.50	0	25,25,25	0.71	1 (4%)
3	BOG	A	406	-	20,20,20	0.59	0	25,25,25	1.04	2 (8%)
4	SPL	A	407	-	28,29,29	0.55	0	27,31,31	1.27	4 (14%)
2	BGC	B	401	-	12,12,12	0.73	0	17,17,17	1.71	5 (29%)
2	BGC	B	402	-	12,12,12	0.63	0	17,17,17	0.84	0
2	BGC	B	403	-	12,12,12	0.59	0	17,17,17	1.32	1 (5%)
3	BOG	B	404	-	20,20,20	0.59	0	25,25,25	0.78	0
3	BOG	B	405	-	20,20,20	0.54	0	25,25,25	0.98	2 (8%)
4	SPL	B	406	-	28,29,29	0.52	0	27,31,31	1.13	3 (11%)
2	BGC	C	401	-	12,12,12	0.43	0	17,17,17	0.65	0
2	BGC	C	402	-	12,12,12	0.52	0	17,17,17	1.56	5 (29%)
2	BGC	C	403	-	12,12,12	0.54	0	17,17,17	0.81	1 (5%)
3	BOG	C	404	-	20,20,20	0.68	1 (5%)	25,25,25	1.01	1 (4%)
3	BOG	C	405	-	20,20,20	0.55	0	25,25,25	0.68	0
3	BOG	C	406	-	20,20,20	0.55	0	25,25,25	0.81	0
3	BOG	C	407	-	20,20,20	0.59	0	25,25,25	0.63	0
4	SPL	C	408	-	28,29,29	0.55	0	27,31,31	1.14	4 (14%)

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	BGC	A	401	-	-	0/2/22/22	0/1/1/1
2	BGC	A	402	-	-	0/2/22/22	0/1/1/1
3	BOG	A	403	-	-	0/11/31/31	0/1/1/1
3	BOG	A	404	-	-	0/11/31/31	0/1/1/1
3	BOG	A	405	-	-	0/11/31/31	0/1/1/1
3	BOG	A	406	-	-	0/11/31/31	0/1/1/1
4	SPL	A	407	-	-	0/32/32/32	0/0/0/0
2	BGC	B	401	-	-	0/2/22/22	0/1/1/1
2	BGC	B	402	-	-	0/2/22/22	0/1/1/1
2	BGC	B	403	-	-	0/2/22/22	0/1/1/1
3	BOG	B	404	-	-	0/11/31/31	0/1/1/1
3	BOG	B	405	-	-	0/11/31/31	0/1/1/1
4	SPL	B	406	-	-	0/32/32/32	0/0/0/0
2	BGC	C	401	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	402	-	-	0/2/22/22	0/1/1/1
2	BGC	C	403	-	-	0/2/22/22	0/1/1/1
3	BOG	C	404	-	-	0/11/31/31	0/1/1/1
3	BOG	C	405	-	-	0/11/31/31	0/1/1/1
3	BOG	C	406	-	-	0/11/31/31	0/1/1/1
3	BOG	C	407	-	-	0/11/31/31	0/1/1/1
4	SPL	C	408	-	-	0/32/32/32	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	404	BOG	O1-C1	2.16	1.44	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	BGC	C1-C2-C3	-4.33	103.99	110.43
2	A	402	BGC	C4-C3-C2	-3.27	104.68	110.79
4	A	407	SPL	O3-C3-C4	-3.05	102.21	110.78
4	A	407	SPL	O19-C19-C20	-2.88	117.02	121.98
4	C	408	SPL	O19-C19-C20	-2.67	117.38	121.98
2	B	401	BGC	O5-C1-C2	-2.55	105.72	109.80
4	C	408	SPL	O3-C3-C4	-2.50	103.75	110.78
2	C	402	BGC	C1-C2-C3	-2.48	106.75	110.43
2	B	401	BGC	C4-C3-C2	-2.29	106.51	110.79
2	C	402	BGC	C4-C3-C2	-2.28	106.54	110.79
4	B	406	SPL	O19-C19-C20	-2.17	118.24	121.98
2	C	402	BGC	C6-C5-C4	-2.10	107.83	113.02
3	A	405	BOG	O1-C1-C2	2.04	110.62	108.04
2	C	403	BGC	O5-C5-C6	2.15	111.78	106.36
2	B	401	BGC	O1-C1-C2	2.16	115.01	109.21
4	B	406	SPL	C1-C2-N2	2.24	113.37	109.29
4	C	408	SPL	C1-C2-N2	2.26	113.40	109.29
3	B	405	BOG	C1-C2-C3	2.33	114.56	109.97
2	B	401	BGC	O2-C2-C1	2.35	115.00	109.82
3	B	405	BOG	C4-C3-C2	2.47	115.40	110.79
4	C	408	SPL	C2-N2-C19	2.48	128.20	123.61
3	A	403	BOG	O1-C1-C2	2.48	111.17	108.04
3	A	406	BOG	O5-C5-C4	2.57	114.50	109.68
4	A	407	SPL	C2-N2-C19	2.58	128.39	123.61
3	A	406	BOG	C3-C4-C5	2.62	114.77	110.20
4	A	407	SPL	C1-C2-N2	2.72	114.25	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	BGC	C1-O5-C5	3.02	119.06	113.47
2	C	402	BGC	O5-C5-C4	3.25	115.78	109.68
2	B	403	BGC	C1-O5-C5	3.43	119.82	113.47
4	B	406	SPL	C20-C19-N2	3.48	121.50	115.83
3	C	404	BOG	O1-C1-C2	3.49	112.44	108.04
2	A	402	BGC	O3-C3-C2	3.49	118.19	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	BOG	1	0
4	A	407	SPL	1	0
2	B	403	BGC	2	0
4	B	406	SPL	2	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	345/384 (89%)	0.33	24 (6%)	19 29	38, 54, 97, 132	0
1	B	346/384 (90%)	0.37	33 (9%)	10 17	39, 55, 88, 125	0
1	C	346/384 (90%)	0.34	29 (8%)	14 22	40, 55, 87, 130	0
All	All	1037/1152 (90%)	0.35	86 (8%)	14 22	38, 55, 91, 132	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	ASP	6.6
1	C	51	LEU	6.1
1	B	32	TYR	5.4
1	A	43	TRP	5.2
1	C	33	ILE	5.1
1	B	43	TRP	5.1
1	C	43	TRP	5.0
1	A	301	TRP	4.9
1	C	32	TYR	4.8
1	C	373	LEU	4.7
1	A	32	TYR	4.6
1	A	373	LEU	4.2
1	C	40	PHE	4.2
1	C	47	LYS	4.1
1	A	339	LEU	4.1
1	B	138	PHE	4.1
1	B	51	LEU	4.0
1	C	339	LEU	3.9
1	A	49	GLN	3.9
1	C	372	TYR	3.8
1	C	41	ALA	3.7
1	A	39	GLU	3.6
1	C	48	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	177	MET	3.4
1	C	50	ALA	3.3
1	A	40	PHE	3.3
1	B	235	TRP	3.3
1	A	335	TRP	3.1
1	B	207	VAL	3.1
1	C	46	ASP	3.1
1	A	338	CYS	3.1
1	B	321	MET	3.0
1	A	50	ALA	2.9
1	A	37	MET	2.9
1	B	375	SER	2.9
1	B	173	LEU	2.9
1	A	51	LEU	2.9
1	B	373	LEU	2.8
1	C	173	LEU	2.8
1	B	335	TRP	2.8
1	B	47	LYS	2.8
1	C	353	ASN	2.7
1	B	372	TYR	2.7
1	A	41	ALA	2.7
1	B	56	TRP	2.7
1	C	177	MET	2.7
1	B	212	LEU	2.7
1	B	371	PHE	2.6
1	B	41	ALA	2.6
1	C	159	LEU	2.6
1	C	375	SER	2.5
1	A	369	ARG	2.5
1	B	301	TRP	2.5
1	C	369	ARG	2.5
1	C	335	TRP	2.5
1	C	376	ARG	2.4
1	B	338	CYS	2.4
1	C	207	VAL	2.4
1	B	42	ASN	2.4
1	A	370	ILE	2.4
1	C	104	LEU	2.4
1	B	82	VAL	2.4
1	A	42	ASN	2.3
1	A	38	LYS	2.3
1	C	208	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	339	LEU	2.3
1	C	371	PHE	2.3
1	B	172	THR	2.2
1	C	49	GLN	2.2
1	B	45	LYS	2.2
1	A	173	LEU	2.2
1	B	215	LEU	2.2
1	B	36	ASP	2.2
1	C	352	PRO	2.2
1	C	300	THR	2.2
1	B	209	TRP	2.1
1	B	216	GLN	2.1
1	A	206	ASN	2.1
1	B	44	LEU	2.1
1	A	48	PRO	2.1
1	A	177	MET	2.1
1	B	287	LEU	2.0
1	A	310	CYS	2.0
1	B	48	PRO	2.0
1	A	325	MET	2.0
1	C	338	CYS	2.0

## 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 carbohydrates 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. 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
3	BOG	C	407	20/20	0.74	0.53	11.32	69,134,152,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SPL	B	406	30/30	0.77	0.61	6.09	61,81,92,103	0
3	BOG	A	405	20/20	0.85	0.35	5.40	55,99,115,117	0
3	BOG	A	404	20/20	0.86	0.37	5.26	59,81,85,89	0
3	BOG	C	404	20/20	0.80	0.36	4.82	71,80,91,96	0
4	SPL	C	408	30/30	0.78	0.49	4.48	59,72,88,96	0
4	SPL	A	407	30/30	0.82	0.43	3.98	55,72,82,86	0
3	BOG	A	403	20/20	0.86	0.25	2.84	65,97,125,136	0
3	BOG	C	405	20/20	0.93	0.23	2.51	63,74,81,82	0
3	BOG	C	406	20/20	0.85	0.29	2.39	70,101,109,110	0
3	BOG	A	406	20/20	0.78	0.29	2.34	67,110,129,134	0
3	BOG	B	404	20/20	0.83	0.29	2.25	71,110,122,126	0
3	BOG	B	405	20/20	0.82	0.36	1.93	66,103,129,130	0
2	BGC	B	401	12/12	0.81	0.21	-0.41	74,79,81,83	0
2	BGC	C	402	12/12	0.88	0.16	-	86,96,103,109	0
2	BGC	C	401	12/12	0.88	0.24	-	91,95,101,102	0
2	BGC	A	402	12/12	0.67	0.34	-	74,93,103,112	0
2	BGC	B	402	12/12	0.74	0.25	-	92,102,107,107	0
2	BGC	C	403	12/12	0.85	0.27	-	87,93,104,109	0
2	BGC	B	403	12/12	0.79	0.24	-	68,85,93,95	0
2	BGC	A	401	12/12	0.86	0.16	-	73,80,96,107	0

## 6.5 Other polymers

There are no such residues in this entry.