



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:18 pm BST

PDB ID : 5VNM  
Title : Crystal structure of Sec23a/Sec24a/Sec22 complexed with 4-phenylbutyric acid (15mM soaking)  
Authors : Ma, W.; Goldberg, J.  
Deposited on : 2017-04-30  
Resolution : 2.77 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 : 2.11  
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) : 2.11

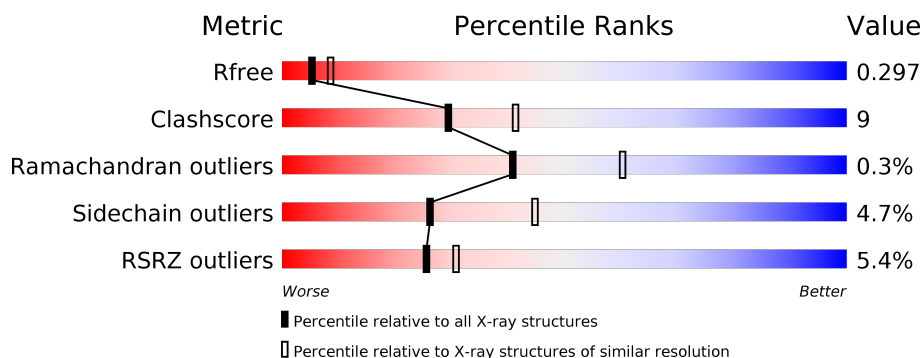
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	764	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>•</div> <div>9%</div> </div> </div>
2	B	748	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>••</div> </div> </div>
3	C	157	<div> <div>10%</div> <div> <div></div> <div>68%</div> <div>17%</div> <div>••</div> <div>13%</div> </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
5	CLT	B	1102	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12446 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	698	Total	C	N	O	S	0	0	0
			5523	3521	949	1014	39			

- Molecule 2 is a protein called Protein transport protein Sec24A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5774	3687	980	1073	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1056	ALA	ARG	conflict	UNP O95486

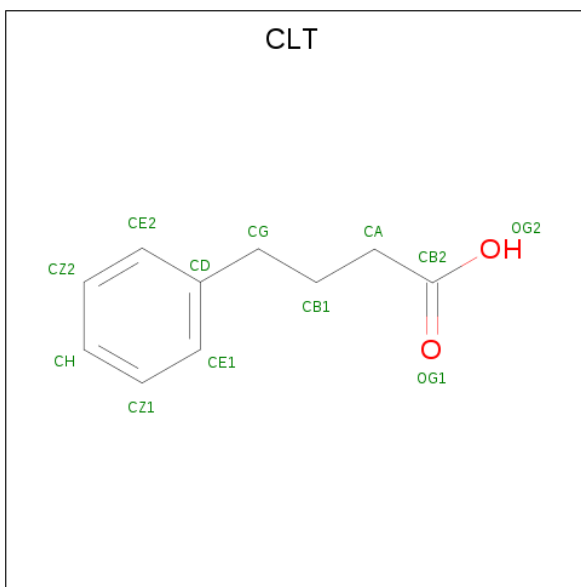
- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	137	Total	C	N	O	S	0	0	0
			1095	701	182	205	7			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 4-PHENYL-BUTANOIC ACID (three-letter code: CLT) (formula: C<sub>10</sub>H<sub>12</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			12	10	2		

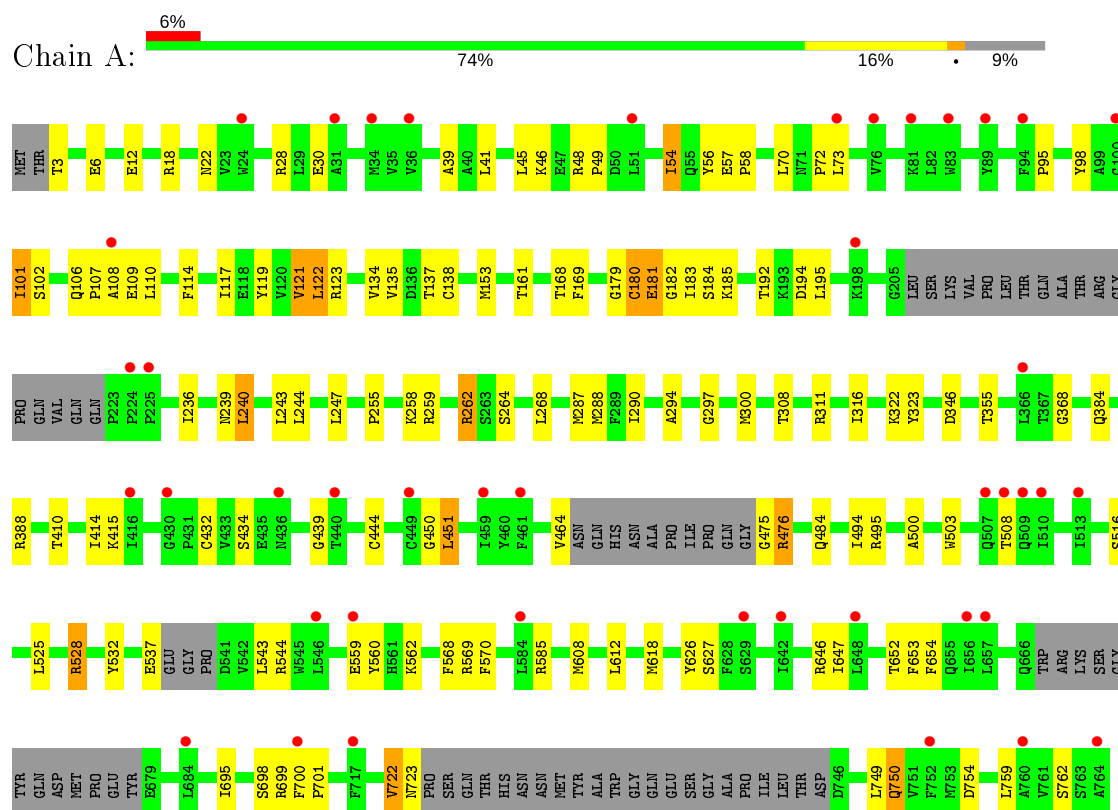
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	B	28	Total	O	0	0
			28	28		
6	C	1	Total	O	0	0
			1	1		

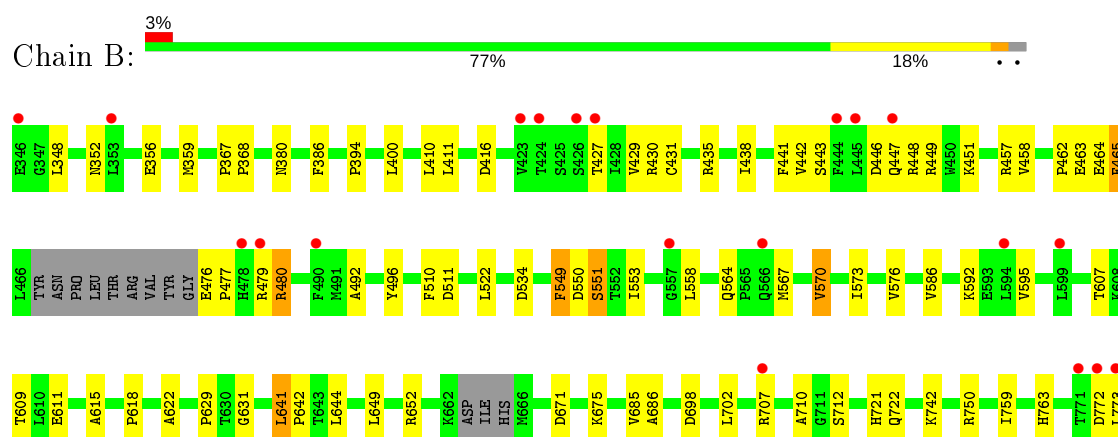
### 3 Residue-property plots [i](#)

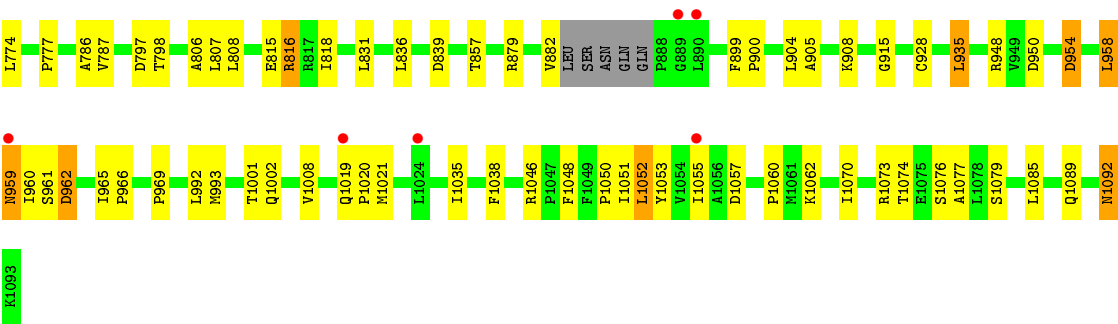
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Protein transport protein Sec23A

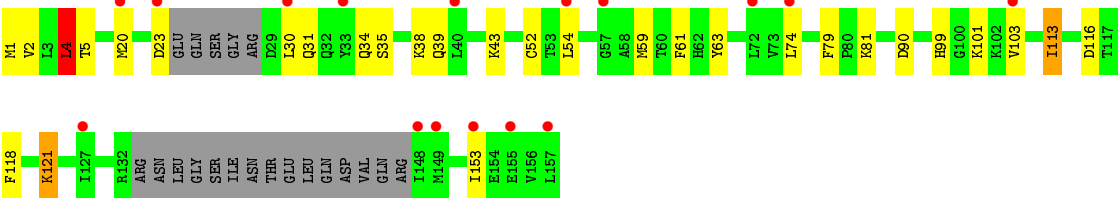


#### • Molecule 2: Protein transport protein Sec24A





• Molecule 3: Vesicle-trafficking protein SEC22b



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.18Å 96.80Å 130.61Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	130.61 – 2.77 130.61 – 2.76	Depositor EDS
% Data completeness (in resolution range)	90.2 (130.61-2.77) 90.2 (130.61-2.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	32.82 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.268 , 0.297 0.268 , 0.297	Depositor DCC
$R_{free}$ test set	1966 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.973	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	12446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLT, ZN

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	0/5650	0.50	0/7651
2	B	0.40	0/5898	0.50	0/8017
3	C	0.33	0/1114	0.48	0/1500
All	All	0.39	0/12662	0.50	0/17168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	5523	0	5478	99	0
2	B	5774	0	5823	120	0
3	C	1095	0	1086	19	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	12	0	11	3	0
6	A	11	0	0	1	0
6	B	28	0	0	8	0
6	C	1	0	0	1	0
All	All	12446	0	12398	235	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 9.

All (235) 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)
2:B:551:SER:OG	2:B:611:GLU:OE1	1.86	0.93
2:B:773:LEU:O	2:B:774:LEU:HD23	1.68	0.93
1:A:750:GLN:H	1:A:750:GLN:HE21	1.18	0.90
2:B:430:ARG:HH21	2:B:435:ARG:HB3	1.33	0.90
2:B:958:LEU:HD23	2:B:959:ASN:N	1.87	0.88
2:B:430:ARG:NH2	2:B:435:ARG:HB3	1.89	0.87
1:A:109:GLU:N	1:A:109:GLU:OE2	2.08	0.86
1:A:122:LEU:O	1:A:122:LEU:HD23	1.77	0.84
1:A:107:PRO:HB2	1:A:109:GLU:OE1	1.78	0.83
2:B:429:VAL:HG21	2:B:465:PHE:CE1	2.16	0.81
1:A:122:LEU:H	1:A:122:LEU:HD22	1.46	0.81
1:A:183:ILE:HG13	1:A:183:ILE:O	1.78	0.81
2:B:958:LEU:CD2	2:B:959:ASN:N	2.44	0.80
2:B:959:ASN:O	2:B:959:ASN:ND2	2.14	0.80
2:B:958:LEU:N	2:B:958:LEU:HD22	1.96	0.79
1:A:54:ILE:HG21	1:A:119:TYR:CD2	2.18	0.78
2:B:1089:GLN:OE1	6:B:1201:HOH:O	2.02	0.77
2:B:958:LEU:CD2	2:B:959:ASN:H	1.99	0.75
2:B:815:GLU:OE2	6:B:1202:HOH:O	2.04	0.75
1:A:750:GLN:H	1:A:750:GLN:NE2	1.84	0.74
2:B:712:SER:OG	6:B:1203:HOH:O	2.06	0.73
1:A:54:ILE:HG21	1:A:119:TYR:HD2	1.51	0.73
1:A:750:GLN:HE21	1:A:750:GLN:N	1.85	0.73
2:B:1074:THR:HG23	2:B:1076:SER:H	1.53	0.73
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.70	0.72
2:B:609:THR:HG22	2:B:611:GLU:H	1.55	0.71
2:B:510:PHE:C	2:B:549:PHE:HE2	1.95	0.70
2:B:430:ARG:HH21	2:B:435:ARG:CB	2.05	0.69
2:B:773:LEU:C	2:B:774:LEU:HD23	2.12	0.69
2:B:750:ARG:HD3	2:B:772:ASP:O	1.93	0.68
3:C:4:LEU:HD12	3:C:5:THR:N	2.08	0.68
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.74	0.67
1:A:3:THR:HG22	1:A:6:GLU:H	1.58	0.67
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.77	0.67
2:B:839:ASP:OD2	6:B:1205:HOH:O	2.11	0.67
2:B:969:PRO:O	6:B:1206:HOH:O	2.13	0.66
1:A:45:LEU:HA	1:A:495:ARG:NH1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.79	0.65
2:B:1089:GLN:HB2	6:B:1201:HOH:O	1.96	0.65
2:B:958:LEU:H	2:B:958:LEU:HD22	1.59	0.65
2:B:958:LEU:HD22	2:B:959:ASN:H	1.60	0.65
2:B:510:PHE:O	2:B:549:PHE:CD2	2.50	0.65
1:A:101:ILE:HD11	1:A:107:PRO:HD3	1.77	0.64
2:B:510:PHE:C	2:B:549:PHE:CE2	2.70	0.64
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.79	0.63
2:B:808:LEU:HD22	5:B:1102:CLT:HE1	1.80	0.63
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.79	0.63
2:B:446:ASP:O	2:B:447:GLN:HB3	1.99	0.63
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.81	0.62
1:A:70:LEU:HD11	1:A:110:LEU:HD21	1.79	0.62
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.64	0.62
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.82	0.61
2:B:480:ARG:HH11	2:B:480:ARG:CG	2.13	0.61
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.82	0.61
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.16	0.60
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.82	0.60
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.84	0.60
2:B:510:PHE:O	2:B:549:PHE:CE2	2.55	0.59
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.85	0.59
1:A:259:ARG:NH2	1:A:308:THR:O	2.36	0.59
2:B:642:PRO:HG2	2:B:702:LEU:HD21	1.85	0.59
2:B:550:ASP:OD1	2:B:551:SER:N	2.36	0.58
3:C:38:LYS:NZ	6:C:201:HOH:O	2.32	0.58
1:A:476:ARG:N	1:A:503:TRP:HD1	2.01	0.58
2:B:960:ILE:HD12	2:B:965:ILE:HD12	1.85	0.58
2:B:806:ALA:HB1	5:B:1102:CLT:HH	1.85	0.58
1:A:410:THR:HB	1:A:414:ILE:HB	1.86	0.58
1:A:183:ILE:CG1	1:A:183:ILE:O	2.50	0.58
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.39	0.58
2:B:429:VAL:CG2	2:B:465:PHE:CE1	2.87	0.58
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.86	0.57
2:B:965:ILE:HG22	2:B:965:ILE:O	2.02	0.57
1:A:54:ILE:CG2	1:A:119:TYR:HD2	2.16	0.57
1:A:107:PRO:CB	1:A:109:GLU:OE1	2.53	0.57
2:B:950:ASP:OD2	6:B:1207:HOH:O	2.18	0.57
1:A:57:GLU:HG3	1:A:58:PRO:CD	2.35	0.57
2:B:992:LEU:HB2	2:B:1052:LEU:HB2	1.86	0.57
1:A:45:LEU:HA	1:A:495:ARG:HH12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1053:TYR:HB2	2:B:1055:ILE:HG13	1.87	0.57
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.86	0.56
2:B:549:PHE:N	2:B:549:PHE:CD2	2.71	0.56
1:A:54:ILE:O	1:A:54:ILE:HG22	2.06	0.56
3:C:4:LEU:C	3:C:4:LEU:HD12	2.26	0.56
1:A:122:LEU:N	1:A:122:LEU:HD22	2.16	0.55
1:A:122:LEU:H	1:A:122:LEU:CD2	2.17	0.55
1:A:528:ARG:HA	1:A:608:MET:HE1	1.87	0.55
2:B:427:THR:HG21	2:B:464:GLU:OE1	2.07	0.55
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.89	0.55
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.88	0.54
2:B:948:ARG:NH2	6:B:1207:HOH:O	2.40	0.54
2:B:511:ASP:HA	2:B:549:PHE:CE2	2.42	0.54
2:B:954:ASP:OD1	2:B:954:ASP:N	2.35	0.54
2:B:534:ASP:OD1	2:B:592:LYS:NZ	2.31	0.54
3:C:30:LEU:O	3:C:34:GLN:HB2	2.08	0.54
1:A:476:ARG:N	1:A:503:TRP:CD1	2.75	0.54
1:A:28:ARG:HB3	1:A:28:ARG:NH1	2.23	0.54
1:A:759:LEU:HA	1:A:762:SER:OG	2.07	0.54
2:B:553:ILE:HB	2:B:570:VAL:HG13	1.90	0.54
3:C:59:MET:HB3	3:C:74:LEU:HD11	1.89	0.54
2:B:558:LEU:HD13	2:B:595:VAL:HG12	1.90	0.53
3:C:35:SER:O	3:C:39:GLN:HG2	2.08	0.53
1:A:114:PHE:HB3	1:A:117:ILE:HD12	1.91	0.53
1:A:108:ALA:O	1:A:114:PHE:HB2	2.09	0.52
3:C:54:LEU:HD13	3:C:153:ILE:HG13	1.90	0.52
1:A:722:VAL:HG22	1:A:723:ASN:H	1.75	0.52
2:B:480:ARG:CG	2:B:480:ARG:NH1	2.72	0.52
2:B:1055:ILE:O	2:B:1057:ASP:N	2.42	0.52
3:C:113:ILE:O	3:C:116:ASP:HB2	2.10	0.51
2:B:438:ILE:HD12	2:B:442:VAL:HG11	1.92	0.51
2:B:1019:GLN:O	2:B:1055:ILE:HG23	2.11	0.51
1:A:122:LEU:N	1:A:122:LEU:CD2	2.72	0.51
1:A:475:GLY:CA	1:A:503:TRP:HD1	2.24	0.51
2:B:476:GLU:N	2:B:477:PRO:HD3	2.26	0.50
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.51	0.50
1:A:495:ARG:CZ	6:A:902:HOH:O	2.59	0.50
1:A:72:PRO:HB3	1:A:110:LEU:O	2.11	0.50
1:A:562:LYS:NZ	1:A:562:LYS:HB3	2.26	0.50
2:B:446:ASP:C	2:B:448:ARG:H	2.13	0.50
2:B:446:ASP:HB2	2:B:449:ARG:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLU:H	1:A:109:GLU:CD	2.06	0.49
1:A:322:LYS:HE3	1:A:323:TYR:CZ	2.47	0.49
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.93	0.49
1:A:101:ILE:HD13	1:A:102:SER:H	1.78	0.49
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.77	0.49
1:A:184:SER:OG	1:A:184:SER:O	2.23	0.49
1:A:652:THR:HG22	1:A:654:PHE:H	1.77	0.49
1:A:54:ILE:HG13	1:A:56:TYR:CE2	2.48	0.49
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.95	0.48
2:B:879:ARG:HA	2:B:882:VAL:HG22	1.93	0.48
2:B:430:ARG:HD3	2:B:435:ARG:HH21	1.78	0.48
2:B:686:ALA:HB2	2:B:777:PRO:HB2	1.95	0.48
1:A:134:VAL:HB	1:A:288:MET:HG3	1.95	0.48
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.95	0.48
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.95	0.48
1:A:73:LEU:HD11	1:A:500:ALA:HB2	1.94	0.48
1:A:54:ILE:HG23	1:A:56:TYR:CD2	2.49	0.48
2:B:905:ALA:HB2	2:B:1070:ILE:HD13	1.96	0.48
1:A:28:ARG:HB3	1:A:28:ARG:HH11	1.77	0.48
1:A:384:GLN:O	1:A:388:ARG:HG2	2.14	0.48
2:B:430:ARG:O	2:B:431:CYS:C	2.50	0.48
1:A:22:ASN:HB2	1:A:516:SER:HB2	1.95	0.47
1:A:240:LEU:HD22	1:A:244:LEU:HG	1.96	0.47
1:A:759:LEU:O	1:A:762:SER:OG	2.32	0.47
1:A:107:PRO:HB2	1:A:109:GLU:CD	2.34	0.47
1:A:106:GLN:HB2	1:A:107:PRO:HD2	1.95	0.47
2:B:496:TYR:HD1	2:B:818:ILE:HD11	1.78	0.47
1:A:182:GLY:HA2	2:B:564:GLN:HE22	1.79	0.47
2:B:480:ARG:HH11	2:B:480:ARG:HG3	1.79	0.47
1:A:121:VAL:HG21	1:A:123:ARG:NE	2.30	0.47
2:B:511:ASP:N	2:B:549:PHE:CE2	2.82	0.47
3:C:118:PHE:HA	3:C:121:LYS:HG2	1.95	0.47
1:A:290:ILE:HG21	1:A:355:THR:HG23	1.97	0.47
2:B:380:ASN:HA	2:B:441:PHE:HZ	1.79	0.47
1:A:287:MET:HA	1:A:346:ASP:HB2	1.97	0.47
1:A:559:GLU:O	1:A:568:PHE:HA	2.15	0.47
2:B:549:PHE:N	2:B:549:PHE:HD2	2.11	0.47
2:B:511:ASP:CA	2:B:549:PHE:CE2	2.97	0.47
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.96	0.47
2:B:806:ALA:HB3	5:B:1102:CLT:HZ2	1.97	0.47
2:B:962:ASP:N	2:B:962:ASP:OD1	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.49	0.47
1:A:54:ILE:CG2	1:A:119:TYR:CD2	2.92	0.46
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.97	0.46
2:B:465:PHE:O	2:B:480:ARG:HD2	2.14	0.46
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.97	0.46
3:C:113:ILE:H	3:C:113:ILE:HD13	1.79	0.46
2:B:463:GLU:HG3	2:B:463:GLU:O	2.14	0.46
2:B:721:HIS:CD2	2:B:722:GLN:HG3	2.51	0.46
2:B:959:ASN:O	2:B:961:SER:N	2.47	0.46
1:A:48:ARG:HB2	1:A:49:PRO:CD	2.43	0.46
1:A:56:TYR:CE1	1:A:98:TYR:OH	2.67	0.46
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.98	0.46
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.98	0.46
1:A:194:ASP:OD1	1:A:195:LEU:N	2.49	0.46
1:A:475:GLY:C	1:A:503:TRP:HD1	2.20	0.46
2:B:394:PRO:HG2	2:B:400:LEU:HD13	1.98	0.45
2:B:476:GLU:N	2:B:477:PRO:CD	2.76	0.45
1:A:698:SER:OG	1:A:699:ARG:N	2.49	0.45
1:A:749:LEU:HD12	1:A:749:LEU:HA	1.74	0.45
2:B:352:ASN:O	2:B:356:GLU:HG2	2.16	0.45
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.99	0.44
2:B:966:PRO:HG2	2:B:1038:PHE:HB2	1.99	0.44
1:A:101:ILE:HD11	1:A:107:PRO:CD	2.46	0.44
2:B:915:GLY:HA3	2:B:1076:SER:HB2	1.99	0.44
2:B:476:GLU:HA	2:B:477:PRO:HD2	1.70	0.44
2:B:430:ARG:HD3	2:B:435:ARG:NH2	2.32	0.44
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.33	0.44
1:A:137:THR:OG1	1:A:169:PHE:O	2.35	0.44
2:B:416:ASP:OD1	2:B:742:LYS:NZ	2.47	0.43
1:A:98:TYR:O	1:A:101:ILE:HB	2.18	0.43
1:A:368:GLY:HA3	1:A:450:GLY:O	2.18	0.43
2:B:496:TYR:CD1	2:B:818:ILE:HD11	2.53	0.43
2:B:904:LEU:HD11	2:B:908:LYS:HE3	1.99	0.43
2:B:707:ARG:NH2	2:B:928:CYS:SG	2.87	0.43
2:B:348:LEU:HD13	2:B:836:LEU:HD11	2.00	0.43
2:B:879:ARG:NH1	2:B:1092:ASN:OD1	2.52	0.43
2:B:642:PRO:HD2	2:B:649:LEU:HD12	2.01	0.43
1:A:168:THR:HG21	1:A:247:LEU:HD21	2.01	0.43
1:A:72:PRO:CB	1:A:110:LEU:O	2.67	0.42
1:A:180:CYS:C	1:A:181:GLU:HG2	2.38	0.42
2:B:479:ARG:HD2	2:B:479:ARG:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:MET:HG2	1:A:653:PHE:HB3	1.99	0.42
1:A:543:LEU:HD22	1:A:585:ARG:HB2	2.01	0.42
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.83	0.42
1:A:297:GLY:H	1:A:300:MET:HE2	1.84	0.42
3:C:54:LEU:HB3	3:C:153:ILE:HB	2.01	0.42
2:B:631:GLY:HA2	2:B:685:VAL:HG22	2.02	0.42
2:B:367:PRO:HA	2:B:368:PRO:HD3	1.94	0.42
2:B:759:ILE:HG23	2:B:787:VAL:HG13	2.01	0.42
1:A:415:LYS:HB3	1:A:434:SER:HB2	2.02	0.41
2:B:511:ASP:N	2:B:549:PHE:HE2	2.18	0.41
1:A:626:TYR:HB2	1:A:647:ILE:HB	2.02	0.41
3:C:99:HIS:O	3:C:103:VAL:HG23	2.20	0.41
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.48	0.41
2:B:443:SER:HB2	2:B:451:LYS:HB3	2.03	0.41
2:B:457:ARG:HG3	2:B:458:VAL:N	2.36	0.41
2:B:641:LEU:HD21	2:B:649:LEU:HB2	2.01	0.41
1:A:12:GLU:HG2	1:A:46:LYS:NZ	2.35	0.41
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.55	0.41
1:A:135:VAL:HB	1:A:168:THR:HG22	2.02	0.41
2:B:462:PRO:C	2:B:464:GLU:H	2.24	0.41
3:C:39:GLN:O	3:C:43:LYS:HG2	2.21	0.41
2:B:671:ASP:OD2	2:B:675:LYS:HE3	2.21	0.41
2:B:1046:ARG:HD2	2:B:1050:PRO:HG3	2.02	0.41
1:A:54:ILE:HA	1:A:54:ILE:HD12	1.67	0.41
1:A:700:PHE:HB3	1:A:701:PRO:HD3	2.02	0.41
2:B:641:LEU:HD23	2:B:642:PRO:HD2	2.02	0.41
2:B:1008:VAL:HG13	2:B:1035:ILE:HG21	2.03	0.40
2:B:573:ILE:HD13	2:B:573:ILE:HA	1.90	0.40
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.92	0.40
2:B:615:ALA:HB2	2:B:644:LEU:HD23	2.03	0.40
1:A:695:ILE:HD11	1:A:699:ARG:NH2	2.37	0.40
3:C:4:LEU:HD13	3:C:20:MET:HG2	2.03	0.40
3:C:54:LEU:HB2	3:C:61:PHE:HB2	2.03	0.40
3:C:1:MET:HA	3:C:79:PHE:HB2	2.02	0.40

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	686/764 (90%)	652 (95%)	33 (5%)	1 (0%)	51	75
2	B	723/748 (97%)	672 (93%)	50 (7%)	1 (0%)	51	75
3	C	131/157 (83%)	119 (91%)	10 (8%)	2 (2%)	10	18
All	All	1540/1669 (92%)	1443 (94%)	93 (6%)	4 (0%)	41	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	959	ASN
3	C	4	LEU
3	C	2	VAL
1	A	722	VAL

### 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	608/666 (91%)	580 (95%)	28 (5%)	27	46
2	B	661/678 (98%)	631 (96%)	30 (4%)	27	46
3	C	117/138 (85%)	110 (94%)	7 (6%)	19	33
All	All	1386/1482 (94%)	1321 (95%)	65 (5%)	26	45

All (65) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	30	GLU
1	A	54	ILE
1	A	101	ILE
1	A	121	VAL
1	A	122	LEU
1	A	153	MET
1	A	161	THR
1	A	180	CYS
1	A	181	GLU
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	262	ARG
1	A	268	LEU
1	A	311	ARG
1	A	316	ILE
1	A	451	LEU
1	A	476	ARG
1	A	508	THR
1	A	528	ARG
1	A	537	GLU
1	A	544	ARG
1	A	560	TYR
1	A	569	ARG
1	A	570	PHE
1	A	750	GLN
1	A	754	ASP
2	B	359	MET
2	B	386	PHE
2	B	411	LEU
2	B	465	PHE
2	B	480	ARG
2	B	522	LEU
2	B	549	PHE
2	B	551	SER
2	B	570	VAL
2	B	607	THR
2	B	641	LEU
2	B	652	ARG
2	B	797	ASP
2	B	798	THR
2	B	807	LEU

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Mol	Chain	Res	Type
2	B	816	ARG
2	B	831	LEU
2	B	857	THR
2	B	935	LEU
2	B	954	ASP
2	B	958	LEU
2	B	962	ASP
2	B	993	MET
2	B	1001	THR
2	B	1002	GLN
2	B	1048	PHE
2	B	1051	ILE
2	B	1052	LEU
2	B	1085	LEU
2	B	1092	ASN
3	C	4	LEU
3	C	31	GLN
3	C	81	LYS
3	C	90	ASP
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	750	GLN
2	B	564	GLN
2	B	913	GLN
2	B	959	ASN

### 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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
5	CLT	B	1102	-	9,12,12	0.25	0	10,14,14	0.71	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
5	CLT	B	1102	-	-	0/4/6/6	0/1/1/1

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1102	CLT	3	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	698/764 (91%)	0.51	43 (6%)	20 25	46, 81, 125, 161	0
2	B	731/748 (97%)	0.41	26 (3%)	42 51	41, 68, 114, 148	0
3	C	137/157 (87%)	0.70	16 (11%)	4 5	62, 99, 138, 159	0
All	All	1566/1669 (93%)	0.48	85 (5%)	25 31	41, 76, 124, 161	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1055	ILE	8.4
2	B	772	ASP	6.9
3	C	23	ASP	5.6
2	B	424	THR	5.5
3	C	149	MET	5.3
3	C	153	ILE	4.7
3	C	33	TYR	4.6
1	A	510	ILE	4.4
3	C	148	ILE	4.3
1	A	507	GLN	4.0
2	B	445	LEU	4.0
1	A	764	ALA	3.9
1	A	94	PHE	3.8
1	A	648	LEU	3.7
1	A	760	ALA	3.6
1	A	34	MET	3.6
1	A	225	PRO	3.5
3	C	54	LEU	3.5
1	A	76	VAL	3.5
1	A	684	LEU	3.5
1	A	81	LYS	3.4
2	B	771	THR	3.3
1	A	629	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	447	GLN	3.3
2	B	479	ARG	3.2
1	A	700	PHE	3.2
1	A	657	LEU	3.2
1	A	559	GLU	3.1
1	A	89	TYR	3.1
2	B	890	LEU	3.1
2	B	353	LEU	2.9
1	A	642	ILE	2.9
1	A	752	PHE	2.9
3	C	157	LEU	2.9
3	C	40	LEU	2.8
1	A	461	PHE	2.8
2	B	444	PHE	2.8
1	A	73	LEU	2.8
2	B	490	PHE	2.8
3	C	103	VAL	2.7
2	B	959	ASN	2.7
2	B	346	GLU	2.7
2	B	599	LEU	2.7
3	C	30	LEU	2.7
1	A	31	ALA	2.7
1	A	656	ILE	2.7
3	C	127	ILE	2.6
2	B	427	THR	2.6
1	A	546	LEU	2.6
1	A	449	CYS	2.6
2	B	423	VAL	2.6
2	B	1019	GLN	2.6
3	C	155	GLU	2.5
3	C	72	LEU	2.5
1	A	440	THR	2.5
2	B	478	HIS	2.5
2	B	889	GLY	2.4
1	A	100	GLY	2.4
1	A	51	LEU	2.4
1	A	83	TRP	2.4
1	A	508	THR	2.4
2	B	707	ARG	2.4
1	A	224	PRO	2.4
1	A	584	LEU	2.4
1	A	24	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	557	GLY	2.3
1	A	108	ALA	2.3
1	A	509	GLN	2.3
1	A	416	ILE	2.3
1	A	717	PHE	2.2
3	C	57	GLY	2.2
2	B	566	GLN	2.2
2	B	1024	LEU	2.1
2	B	426	SER	2.1
1	A	36	VAL	2.1
2	B	773	LEU	2.1
3	C	20	MET	2.1
3	C	74	LEU	2.1
1	A	513	ILE	2.1
1	A	430	GLY	2.1
2	B	594	LEU	2.1
1	A	459	ILE	2.0
1	A	436	ASN	2.0
1	A	198	LYS	2.0
1	A	366	LEU	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](#)

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. 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( $\text{\AA}^2$ )	Q<0.9
5	CLT	B	1102	12/12	0.67	0.71	99,120,132,134	0
4	ZN	B	1101	1/1	0.88	0.21	99,99,99,99	0
4	ZN	A	801	1/1	0.94	0.12	119,119,119,119	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.