



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:04 am BST

PDB ID : 5VNL  
Title : Crystal structure of Sec23a/Sec24a/Sec22 complexed with 4-phenylbutyric acid (1mM soaking)  
Authors : Ma, W.; Goldberg, J.  
Deposited on : 2017-04-30  
Resolution : 2.39 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

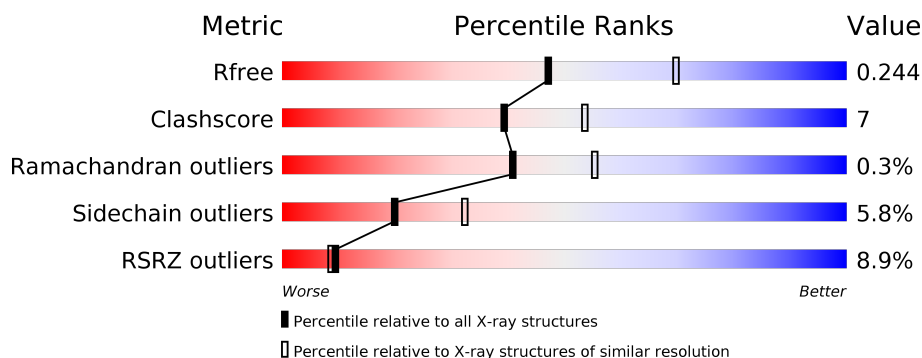
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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>9%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>
2	B	748	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>•</div> <div>•</div> </div> </div>
3	C	157	<div> <div>21%</div> <div> <div></div> <div>66%</div> <div>20%</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 12473 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	699	Total	C	N	O	S	0	0	0
			5536	3527	953	1017	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
			5773	3685	983	1071	34			

There is a discrepancy between the modelled and reference sequences:

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

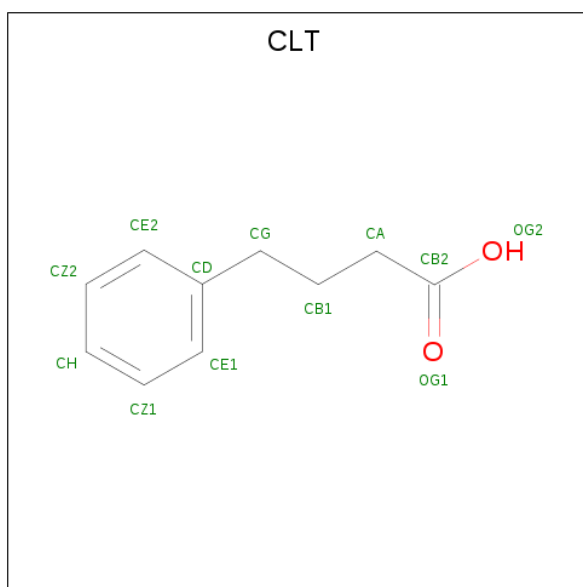
- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	137	Total	C	N	O	S	0	0	0
			1100	705	182	205	8			

- 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		

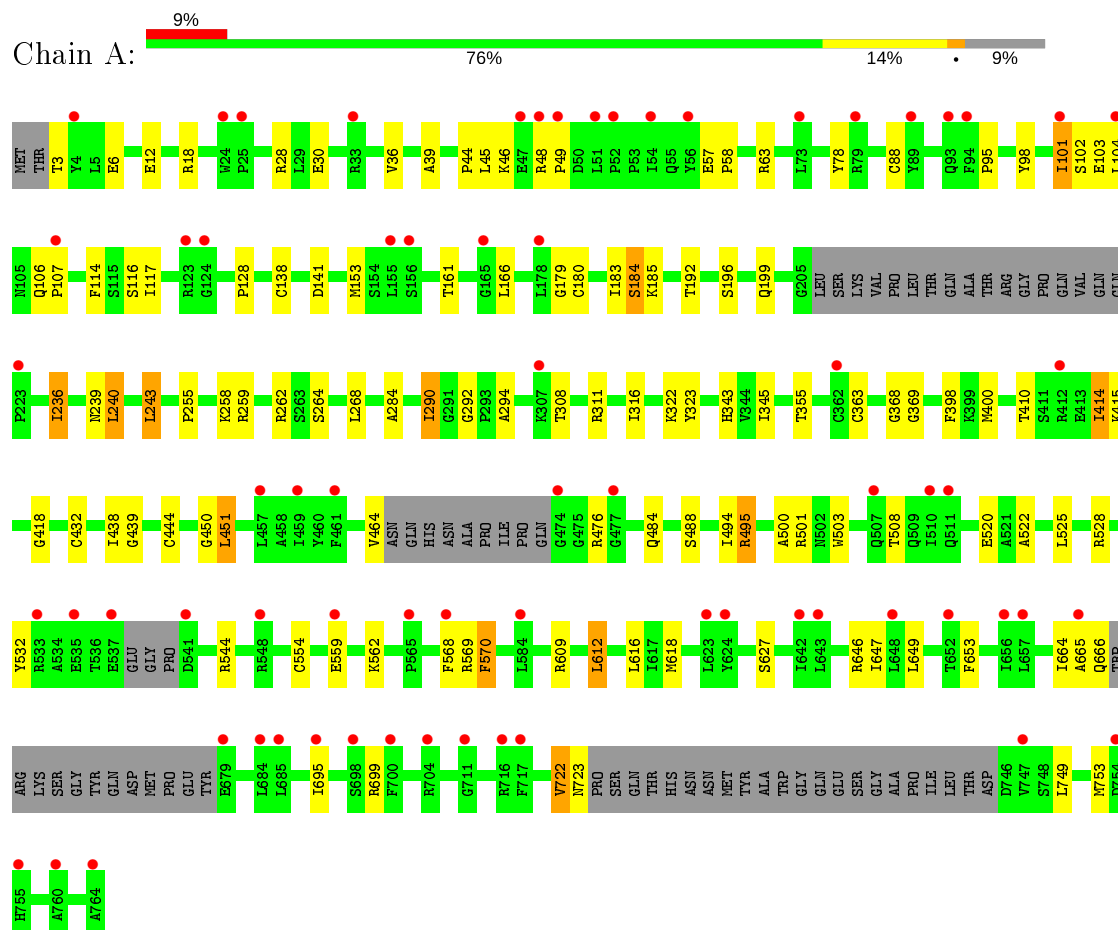
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		
6	B	32	Total	O	0	0
			32	32		
6	C	2	Total	O	0	0
			2	2		

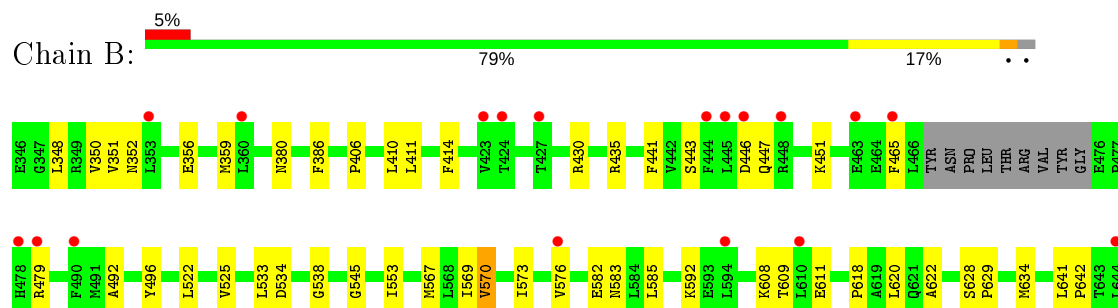
### 3 Residue-property plots [i](#)

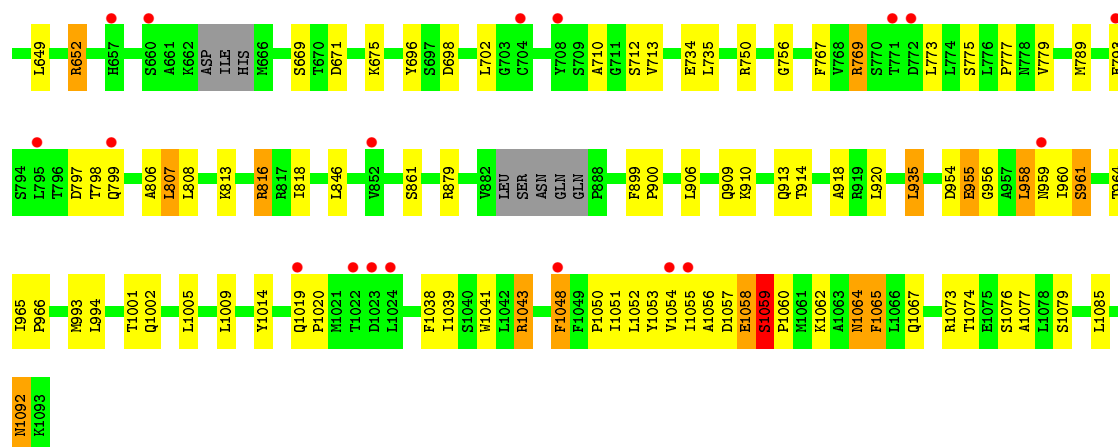
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

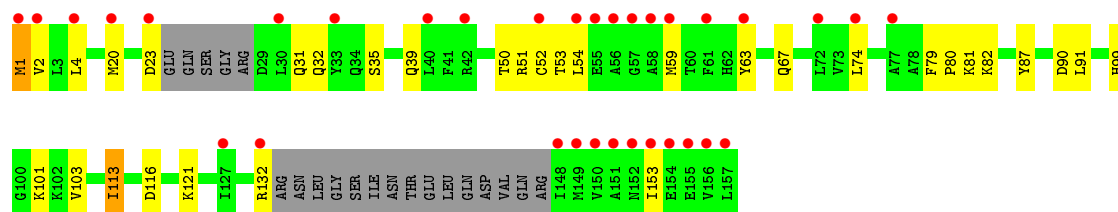


#### • Molecule 2: Protein transport protein Sec24A





• 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, $\alpha$ , $\beta$ , $\gamma$	147.76 Å 96.77 Å 129.59 Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	48.78 – 2.39 48.78 – 2.39	Depositor EDS
% Data completeness (in resolution range)	84.7 (48.78-2.39) 84.7 (48.78-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.39 Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.208 , 0.246 0.208 , 0.244	Depositor DCC
$R_{free}$ test set	2009 reflections (3.29%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12473	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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	0.39	0/5663	0.50	0/7667
2	B	0.45	0/5897	0.54	0/8015
3	C	0.34	0/1119	0.50	0/1506
All	All	0.41	0/12679	0.52	0/17188

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	5536	0	5494	75	0
2	B	5773	0	5822	95	0
3	C	1100	0	1100	18	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	12	0	11	4	0
6	A	16	0	0	2	0
6	B	32	0	0	3	0
6	C	2	0	0	0	0
All	All	12473	0	12427	185	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 7.

All (185) 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:1057:ASP:H	2:B:1060:PRO:HG3	1.35	0.92
2:B:446:ASP:O	2:B:447:GLN:HG2	1.74	0.87
2:B:958:LEU:HB3	2:B:964:THR:HG23	1.55	0.87
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.65	0.78
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.67	0.76
2:B:993:MET:HE3	2:B:1064:ASN:HD21	1.50	0.75
2:B:1057:ASP:O	2:B:1060:PRO:CD	2.35	0.75
1:A:259:ARG:NH2	1:A:308:THR:O	2.19	0.75
3:C:4:LEU:CD1	3:C:20:MET:HG2	2.17	0.75
2:B:1059:SER:N	2:B:1060:PRO:CD	2.50	0.73
2:B:993:MET:CE	2:B:1064:ASN:HD21	2.02	0.73
2:B:1074:THR:HG23	2:B:1076:SER:H	1.54	0.72
2:B:994:LEU:HB3	2:B:1054:VAL:HG22	1.72	0.71
2:B:1057:ASP:N	2:B:1060:PRO:HG3	2.05	0.70
2:B:960:ILE:HD13	2:B:960:ILE:N	2.07	0.69
1:A:114:PHE:HB3	1:A:117:ILE:HD13	1.76	0.68
2:B:879:ARG:NH1	2:B:1092:ASN:OD1	2.27	0.68
1:A:410:THR:HB	1:A:414:ILE:HB	1.76	0.67
2:B:1057:ASP:HB3	2:B:1060:PRO:HD3	1.74	0.67
2:B:1014:TYR:OH	2:B:1057:ASP:OD1	2.06	0.67
1:A:3:THR:HG22	1:A:6:GLU:H	1.59	0.66
3:C:80:PRO:HB3	3:C:82:LYS:HE3	1.77	0.66
2:B:808:LEU:HD22	5:B:1102:CLT:HE1	1.78	0.66
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.76	0.66
1:A:78:TYR:CD2	1:A:102:SER:C	2.69	0.66
2:B:1057:ASP:O	2:B:1060:PRO:HD2	1.95	0.65
2:B:965:ILE:HD13	2:B:1041:TRP:HB2	1.78	0.65
1:A:106:GLN:HB2	1:A:107:PRO:HD2	1.77	0.65
3:C:4:LEU:HD13	3:C:20:MET:HG2	1.79	0.65
1:A:63:ARG:HH11	1:A:88:CYS:HB2	1.62	0.64
2:B:955:GLU:OE1	2:B:955:GLU:N	2.31	0.64
2:B:609:THR:HG22	2:B:611:GLU:H	1.63	0.63
2:B:993:MET:CE	2:B:1064:ASN:ND2	2.62	0.63
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.14	0.63
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.79	0.62
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.80	0.62
2:B:1058:GLU:C	2:B:1060:PRO:HD2	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.82	0.62
2:B:1059:SER:N	2:B:1060:PRO:HD2	2.13	0.62
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.82	0.61
2:B:956:GLY:HA3	2:B:965:ILE:O	1.99	0.61
1:A:128:PRO:O	6:A:902:HOH:O	2.16	0.61
1:A:520:GLU:OE1	6:A:901:HOH:O	2.16	0.61
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.83	0.60
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.64	0.60
2:B:958:LEU:HD23	2:B:958:LEU:O	2.01	0.60
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.82	0.60
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.37	0.59
1:A:749:LEU:O	1:A:753:MET:HG2	2.02	0.59
2:B:534:ASP:OD1	2:B:592:LYS:NZ	2.24	0.58
1:A:45:LEU:HA	1:A:495:ARG:NH1	2.19	0.57
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.87	0.57
2:B:1062:LYS:O	2:B:1062:LYS:HG2	2.05	0.56
1:A:520:GLU:HB3	1:A:616:LEU:HD11	1.88	0.56
2:B:538:GLY:O	6:B:1201:HOH:O	2.18	0.56
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.87	0.56
3:C:113:ILE:O	3:C:116:ASP:HB2	2.04	0.56
1:A:476:ARG:HA	1:A:501:ARG:O	2.05	0.56
2:B:443:SER:HB2	2:B:451:LYS:HB3	1.88	0.56
3:C:54:LEU:HD13	3:C:153:ILE:HG13	1.87	0.56
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.89	0.55
1:A:368:GLY:HA3	1:A:450:GLY:O	2.06	0.55
1:A:101:ILE:HD11	1:A:106:GLN:HA	1.86	0.55
2:B:1054:VAL:O	2:B:1054:VAL:HG12	2.05	0.55
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.89	0.55
2:B:806:ALA:HB1	5:B:1102:CLT:HH	1.88	0.55
3:C:59:MET:HB3	3:C:74:LEU:HD11	1.88	0.55
1:A:48:ARG:HB2	1:A:49:PRO:CD	2.37	0.55
2:B:1057:ASP:C	2:B:1060:PRO:CD	2.76	0.54
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.48	0.54
1:A:78:TYR:CD2	1:A:103:GLU:N	2.76	0.54
1:A:101:ILE:HD11	1:A:107:PRO:HD3	1.90	0.54
2:B:583:ASN:N	6:B:1207:HOH:O	2.40	0.53
1:A:695:ILE:HD11	1:A:699:ARG:NH2	2.23	0.53
1:A:78:TYR:HD2	1:A:102:SER:C	2.12	0.52
2:B:1057:ASP:O	2:B:1060:PRO:CG	2.57	0.52
2:B:958:LEU:HA	2:B:964:THR:HA	1.91	0.52
2:B:756:GLY:HA2	2:B:793:GLU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1064:ASN:O	2:B:1067:GLN:N	2.37	0.52
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.92	0.52
2:B:671:ASP:OD2	2:B:675:LYS:HE3	2.10	0.52
2:B:913:GLN:HE21	2:B:918:ALA:HB2	1.75	0.52
2:B:993:MET:HE1	2:B:1064:ASN:ND2	2.25	0.51
1:A:500:ALA:O	1:A:501:ARG:NH1	2.39	0.51
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.92	0.51
2:B:1055:ILE:O	2:B:1056:ALA:C	2.49	0.51
2:B:1057:ASP:C	2:B:1060:PRO:HD3	2.31	0.51
3:C:4:LEU:HD11	3:C:20:MET:CE	2.41	0.51
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.92	0.51
2:B:620:LEU:HD22	2:B:634:MET:HE3	1.93	0.51
1:A:63:ARG:HD2	1:A:88:CYS:SG	2.52	0.50
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.93	0.50
1:A:322:LYS:HE3	1:A:323:TYR:CZ	2.46	0.50
3:C:35:SER:O	3:C:39:GLN:HG2	2.11	0.50
1:A:196:SER:OG	1:A:199:GLN:HG3	2.12	0.49
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.47	0.49
1:A:12:GLU:HG2	1:A:46:LYS:NZ	2.28	0.49
1:A:562:LYS:NZ	1:A:562:LYS:HB3	2.27	0.49
2:B:553:ILE:HB	2:B:570:VAL:HG13	1.94	0.48
2:B:1064:ASN:HD22	2:B:1064:ASN:C	2.16	0.48
2:B:806:ALA:HB3	5:B:1102:CLT:HZ2	1.96	0.48
2:B:652:ARG:HH12	2:B:669:SER:HB3	1.79	0.48
2:B:628:SER:HB3	2:B:629:PRO:HD3	1.96	0.47
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.30	0.47
3:C:1:MET:HA	3:C:79:PHE:CD1	2.49	0.47
2:B:582:GLU:N	6:B:1207:HOH:O	2.46	0.47
2:B:966:PRO:HG2	2:B:1038:PHE:HB2	1.97	0.47
1:A:166:LEU:HD23	1:A:243:LEU:HD13	1.97	0.47
2:B:380:ASN:HA	2:B:441:PHE:HZ	1.79	0.47
1:A:559:GLU:O	1:A:568:PHE:HA	2.15	0.47
2:B:994:LEU:HD23	2:B:1054:VAL:HG22	1.97	0.46
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.96	0.46
2:B:959:ASN:HB3	2:B:960:ILE:HD13	1.96	0.46
1:A:101:ILE:HD12	1:A:102:SER:H	1.81	0.46
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.96	0.46
2:B:958:LEU:CD2	2:B:958:LEU:C	2.84	0.46
1:A:104:LEU:HA	1:A:104:LEU:HD23	1.75	0.46
1:A:36:VAL:HG11	1:A:522:ALA:HB1	1.98	0.46
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.50	0.46
2:B:525:VAL:HG22	2:B:735:LEU:HD11	1.98	0.46
2:B:909:GLN:HG2	2:B:910:LYS:N	2.31	0.46
1:A:345:ILE:O	1:A:369:GLY:HA3	2.17	0.45
1:A:28:ARG:NH1	1:A:28:ARG:HB3	2.31	0.45
2:B:573:ILE:HD13	2:B:573:ILE:HA	1.81	0.45
2:B:352:ASN:O	2:B:356:GLU:HG2	2.17	0.45
2:B:750:ARG:CZ	2:B:773:LEU:HD13	2.47	0.45
2:B:1059:SER:N	2:B:1060:PRO:HD3	2.31	0.44
1:A:665:ALA:O	1:A:666:GLN:C	2.55	0.44
2:B:642:PRO:HG2	2:B:702:LEU:HD21	1.99	0.44
2:B:779:VAL:HG21	2:B:807:LEU:HD21	2.00	0.44
3:C:4:LEU:HB3	3:C:74:LEU:HB3	2.00	0.44
1:A:647:ILE:HG13	1:A:664:ILE:HD12	1.99	0.44
2:B:1053:TYR:CE1	2:B:1062:LYS:HD3	2.53	0.44
3:C:99:HIS:O	3:C:103:VAL:HG23	2.17	0.44
1:A:476:ARG:H	1:A:503:TRP:H	1.65	0.44
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.99	0.43
1:A:63:ARG:NH1	1:A:88:CYS:HB2	2.32	0.43
2:B:767:PHE:CD2	2:B:769:ARG:HD3	2.53	0.43
2:B:993:MET:HE3	2:B:1064:ASN:ND2	2.25	0.43
1:A:666:GLN:H	1:A:666:GLN:HG3	1.66	0.43
2:B:1043:ARG:HB3	2:B:1050:PRO:HD2	1.99	0.43
2:B:807:LEU:O	2:B:818:ILE:HA	2.18	0.43
2:B:954:ASP:C	2:B:956:GLY:H	2.21	0.43
3:C:4:LEU:HD11	3:C:20:MET:HE1	2.00	0.43
2:B:1064:ASN:O	2:B:1065:PHE:C	2.55	0.43
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.54	0.43
2:B:406:PRO:HB2	2:B:846:LEU:HD23	2.00	0.43
3:C:52:CYS:SG	3:C:53:THR:N	2.91	0.43
1:A:722:VAL:HG22	1:A:723:ASN:H	1.84	0.43
1:A:44:PRO:O	1:A:495:ARG:NH1	2.49	0.42
1:A:78:TYR:CE2	1:A:102:SER:O	2.73	0.42
1:A:284:ALA:HB3	1:A:343:HIS:CD2	2.54	0.42
1:A:418:GLY:HA3	1:A:438:ILE:O	2.20	0.42
2:B:545:GLY:HA3	2:B:585:LEU:HD23	2.01	0.42
1:A:185:LYS:HD2	2:B:569:ILE:HD11	2.01	0.42
1:A:618:MET:HG2	1:A:653:PHE:HB3	2.01	0.42
1:A:345:ILE:HG21	1:A:363:CYS:HB3	2.01	0.42
2:B:1005:LEU:HD23	2:B:1009:LEU:HD12	2.02	0.42
2:B:1039:ILE:O	2:B:1043:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:VAL:HG12	2:B:351:VAL:N	2.33	0.42
3:C:54:LEU:HB3	3:C:153:ILE:HB	2.02	0.42
1:A:236:ILE:HD13	1:A:236:ILE:HA	1.80	0.42
2:B:879:ARG:CZ	2:B:1092:ASN:HB3	2.50	0.42
1:A:184:SER:OG	1:A:184:SER:O	2.21	0.42
2:B:1064:ASN:C	2:B:1064:ASN:ND2	2.72	0.42
2:B:492:ALA:HB1	2:B:496:TYR:HB2	2.02	0.42
2:B:710:ALA:HB3	2:B:777:PRO:HD2	2.01	0.41
1:A:415:LYS:HD2	1:A:464:VAL:HG21	2.01	0.41
3:C:87:TYR:CZ	3:C:91:LEU:HD11	2.54	0.41
2:B:965:ILE:HA	2:B:966:PRO:HD2	1.92	0.41
3:C:32:GLN:O	3:C:35:SER:OG	2.31	0.41
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.89	0.41
1:A:106:GLN:HB2	1:A:107:PRO:CD	2.48	0.41
2:B:430:ARG:HD3	2:B:435:ARG:HH21	1.85	0.41
2:B:734:GLU:HA	2:B:1048:PHE:HE1	1.86	0.41
1:A:78:TYR:CE2	1:A:103:GLU:HA	2.55	0.41
1:A:290:ILE:HG23	1:A:292:GLY:H	1.86	0.41
2:B:750:ARG:HH21	5:B:1102:CLT:CB2	2.33	0.41
1:A:183:ILE:HG13	1:A:183:ILE:O	2.20	0.40
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.86	0.40
1:A:368:GLY:C	1:A:609:ARG:HH22	2.25	0.40
1:A:183:ILE:O	1:A:183:ILE:CG1	2.69	0.40
1:A:369:GLY:O	1:A:609:ARG:NH2	2.54	0.40
2:B:533:LEU:HD12	2:B:533:LEU:HA	1.95	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	687/764 (90%)	651 (95%)	35 (5%)	1 (0%)	51 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	723/748 (97%)	678 (94%)	41 (6%)	4 (1%)	25	36
3	C	131/157 (83%)	121 (92%)	10 (8%)	0	100	100
All	All	1541/1669 (92%)	1450 (94%)	86 (6%)	5 (0%)	41	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	961	SER
2	B	1065	PHE
2	B	955	GLU
1	A	722	VAL
2	B	1059	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	610/666 (92%)	582 (95%)	28 (5%)	27	43
2	B	660/678 (97%)	619 (94%)	41 (6%)	18	29
3	C	119/138 (86%)	107 (90%)	12 (10%)	7	11
All	All	1389/1482 (94%)	1308 (94%)	81 (6%)	20	32

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	101	ILE
1	A	116	SER
1	A	141	ASP
1	A	153	MET
1	A	161	THR
1	A	180	CYS
1	A	184	SER
1	A	192	THR

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Mol	Chain	Res	Type
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	290	ILE
1	A	311	ARG
1	A	316	ILE
1	A	355	THR
1	A	414	ILE
1	A	451	LEU
1	A	488	SER
1	A	495	ARG
1	A	508	THR
1	A	528	ARG
1	A	544	ARG
1	A	569	ARG
1	A	570	PHE
1	A	612	LEU
1	A	649	LEU
2	B	348	LEU
2	B	359	MET
2	B	386	PHE
2	B	411	LEU
2	B	414	PHE
2	B	465	PHE
2	B	479	ARG
2	B	522	LEU
2	B	570	VAL
2	B	608	LYS
2	B	641	LEU
2	B	652	ARG
2	B	712	SER
2	B	713	VAL
2	B	769	ARG
2	B	775	SER
2	B	789	MET
2	B	797	ASP
2	B	798	THR
2	B	799	GLN
2	B	807	LEU
2	B	813	LYS
2	B	816	ARG

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Mol	Chain	Res	Type
2	B	861	SER
2	B	906	LEU
2	B	914	THR
2	B	920	LEU
2	B	935	LEU
2	B	958	LEU
2	B	961	SER
2	B	1001	THR
2	B	1002	GLN
2	B	1043	ARG
2	B	1048	PHE
2	B	1051	ILE
2	B	1052	LEU
2	B	1058	GLU
2	B	1059	SER
2	B	1064	ASN
2	B	1085	LEU
2	B	1092	ASN
3	C	1	MET
3	C	2	VAL
3	C	31	GLN
3	C	50	THR
3	C	51	ARG
3	C	67	GLN
3	C	81	LYS
3	C	90	ASP
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS
3	C	132	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	913	GLN
2	B	1064	ASN

### 5.3.3 RNA ⓘ

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](#)

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	0.30	0	10,14,14	0.77	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 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1102	CLT	4	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	699/764 (91%)	0.68	70 (10%) 7 6	46, 73, 118, 147	0
2	B	731/748 (97%)	0.58	36 (4%) 29 28	41, 65, 114, 169	0
3	C	137/157 (87%)	1.34	33 (24%) 0 0	56, 94, 141, 162	0
All	All	1567/1669 (93%)	0.69	139 (8%) 9 9	41, 70, 120, 169	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	ARG	9.7
2	B	1055	ILE	8.0
3	C	153	ILE	7.4
3	C	57	GLY	7.0
3	C	1	MET	6.8
2	B	424	THR	6.2
2	B	772	ASP	6.2
2	B	771	THR	6.1
3	C	77	ALA	6.1
3	C	157	LEU	5.9
3	C	20	MET	5.9
3	C	23	ASP	5.7
3	C	148	ILE	5.4
3	C	127	ILE	5.2
1	A	700	PHE	5.1
3	C	149	MET	4.9
2	B	448	ARG	4.8
2	B	1019	GLN	4.7
3	C	56	ALA	4.7
2	B	427	THR	4.7
1	A	79	ARG	4.6
2	B	478	HIS	4.6
1	A	49	PRO	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	959	ASN	4.4
3	C	33	TYR	4.3
1	A	474	GLY	4.3
1	A	679	GLU	4.0
1	A	657	LEU	4.0
1	A	89	TYR	4.0
1	A	94	PHE	4.0
2	B	445	LEU	3.9
3	C	54	LEU	3.8
3	C	152	ASN	3.7
3	C	150	VAL	3.7
2	B	1022	THR	3.6
1	A	684	LEU	3.6
3	C	40	LEU	3.5
3	C	74	LEU	3.5
1	A	104	LEU	3.4
1	A	717	PHE	3.4
3	C	61	PHE	3.4
1	A	642	ILE	3.4
1	A	107	PRO	3.3
2	B	479	ARG	3.3
2	B	1054	VAL	3.3
3	C	132	ARG	3.3
2	B	465	PHE	3.2
3	C	59	MET	3.2
2	B	1048	PHE	3.2
1	A	510	ILE	3.2
3	C	155	GLU	3.1
3	C	4	LEU	3.1
1	A	764	ALA	3.0
3	C	55	GLU	3.0
1	A	704	ARG	3.0
1	A	568	PHE	3.0
1	A	4	TYR	2.9
1	A	507	GLN	2.9
3	C	151	ALA	2.9
2	B	423	VAL	2.9
1	A	73	LEU	2.9
2	B	490	PHE	2.9
1	A	93	GLN	2.9
2	B	660	SER	2.8
1	A	711	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	51	LEU	2.8
1	A	461	PHE	2.7
1	A	537	GLU	2.8
1	A	47	GLU	2.7
1	A	755	HIS	2.7
1	A	52	PRO	2.6
1	A	565	PRO	2.6
1	A	307	LYS	2.6
1	A	559	GLU	2.6
2	B	657	HIS	2.6
1	A	584	LEU	2.6
2	B	793	GLU	2.6
3	C	72	LEU	2.6
1	A	623	LEU	2.6
1	A	56	TYR	2.6
1	A	511	GLN	2.6
1	A	412	ARG	2.5
1	A	223	PRO	2.5
3	C	156	VAL	2.5
2	B	444	PHE	2.4
2	B	708	TYR	2.4
2	B	353	LEU	2.4
3	C	30	LEU	2.4
1	A	541	ASP	2.4
3	C	58	ALA	2.4
2	B	463	GLU	2.4
3	C	42	ARG	2.4
1	A	643	LEU	2.4
1	A	648	LEU	2.4
1	A	695	ILE	2.4
2	B	594	LEU	2.4
3	C	2	VAL	2.4
1	A	165	GLY	2.3
1	A	101	ILE	2.3
1	A	747	VAL	2.3
2	B	799	GLN	2.3
1	A	754	ASP	2.3
1	A	665	ALA	2.3
2	B	446	ASP	2.3
1	A	33	ARG	2.2
1	A	457	LEU	2.2
1	A	624	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	760	ALA	2.2
1	A	25	PRO	2.2
1	A	652	THR	2.2
1	A	178	LEU	2.2
1	A	459	ILE	2.2
2	B	610	LEU	2.2
3	C	154	GLU	2.2
1	A	156	SER	2.2
1	A	124	GLY	2.1
1	A	685	LEU	2.1
1	A	533	ARG	2.1
1	A	656	ILE	2.1
2	B	360	LEU	2.1
2	B	1024	LEU	2.1
1	A	48	ARG	2.1
2	B	1023	ASP	2.1
2	B	704	CYS	2.1
2	B	576	VAL	2.1
1	A	477	GLY	2.1
1	A	54	ILE	2.1
3	C	63	TYR	2.1
1	A	155	LEU	2.0
1	A	716	ARG	2.0
1	A	362	CYS	2.0
3	C	52	CYS	2.0
2	B	852	VAL	2.0
1	A	24	TRP	2.0
1	A	535	GLU	2.0
2	B	644	LEU	2.0
2	B	795	LEU	2.0
1	A	548	ARG	2.0
1	A	698	SER	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	0.68	0.53	119,126,133,133	0
4	ZN	A	801	1/1	0.94	0.16	100,100,100,100	0
4	ZN	B	1101	1/1	0.96	0.15	67,67,67,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.