Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 03:03 AM EDT

PDB ID	:	5VNN
Title	:	Crystal structure of Sec23a/Sec24a/Sec22 complexed with 4-phenylbutyric acid (50mM soaking)
Authors	:	Ma, W.; Goldberg, J.
Deposited on	:	2017-05-01
Resolution	:	2.50 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

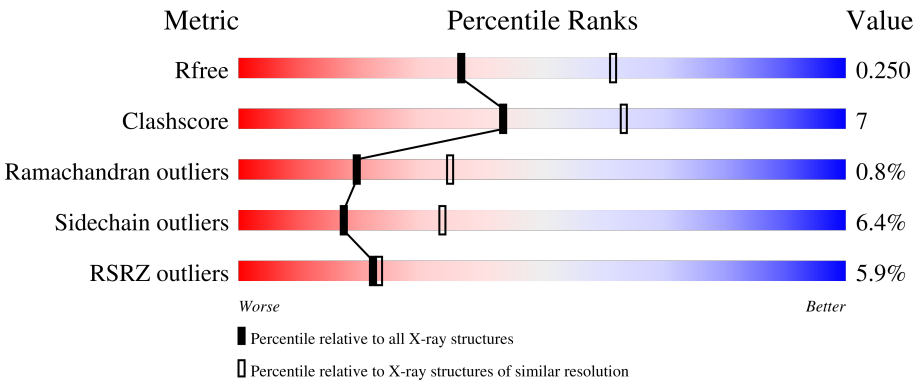
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	4%, 74%, 16%, •, 9%
2	B	748	4%, 78%, 18%, • •
3	C	157	20%, 66%, 18%, •, 13%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	699	5532	3526	953	1014	39	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	731	5780	3690	983	1073	34	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

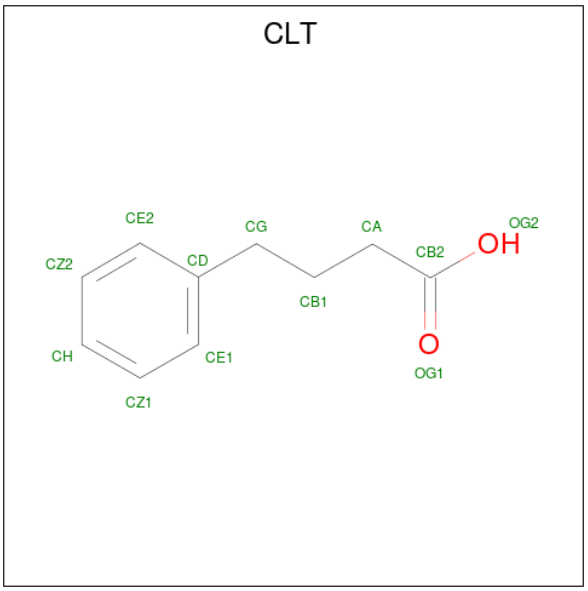
- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	137	1103	708	182	205	8	0	0	0

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

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

- Molecule 5 is 4-PHENYL-BUTANOIC ACID (three-letter code: CLT) (formula: $C_{10}H_{12}O_2$).



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

- Molecule 6 is water.

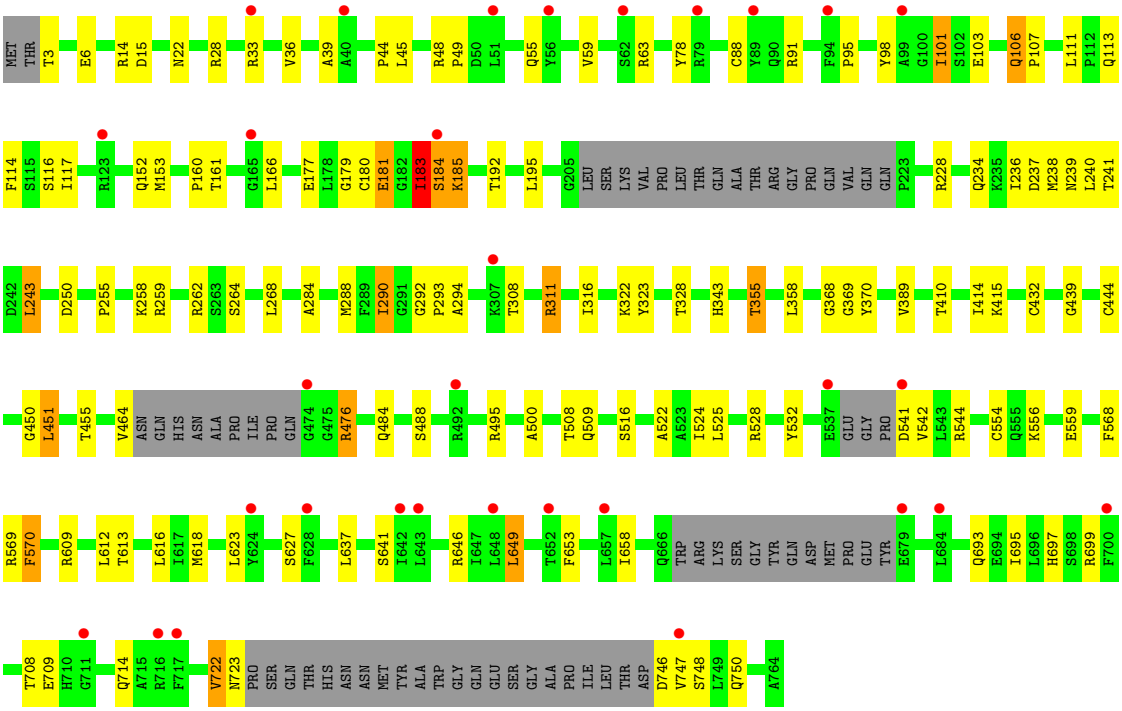
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	22	22	22	0	0
			Total	O		
6	B	18	18	18	0	0
			Total	O		
6	C	4	4	4	0	0

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.

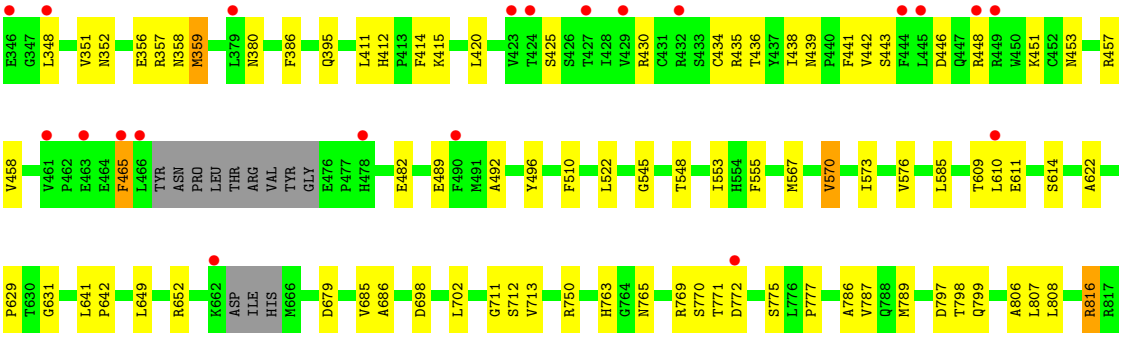
• Molecule 1: Protein transport protein Sec23A

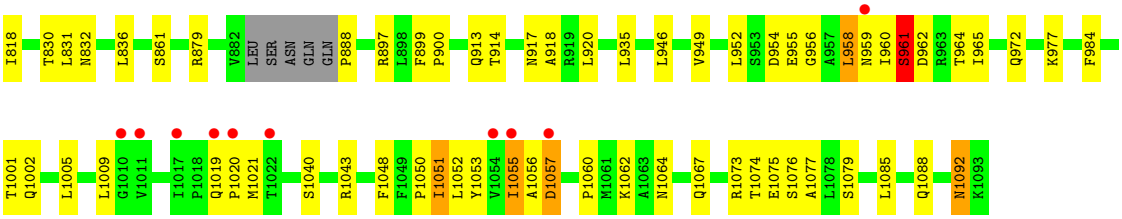
Chain A:



• Molecule 2: Protein transport protein Sec24A

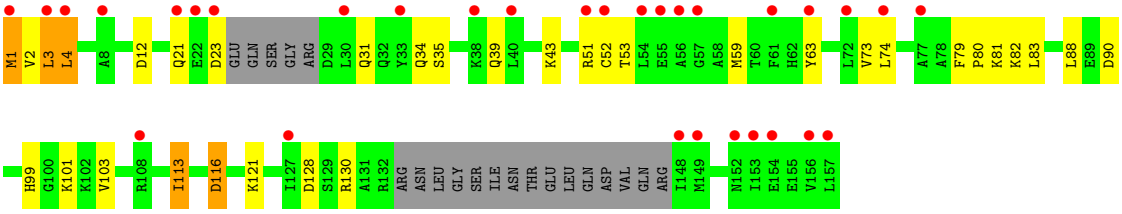
Chain B:





- Molecule 3: Vesicle-trafficking protein SEC22b

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.02Å 97.72Å 128.97Å 90.00° 89.59° 90.00°	Depositor
Resolution (Å)	48.86 – 2.50 48.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	83.5 (48.86-2.50) 83.5 (48.86-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.210 , 0.251 0.211 , 0.250	Depositor DCC
R_{free} test set	2007 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12473	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, CLT

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	0/5659	0.50	0/7662
2	B	0.32	0/5904	0.47	0/8024
3	C	0.24	0/1122	0.42	0/1510
All	All	0.35	0/12685	0.48	0/17196

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 (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	5532	0	5489	75	0
2	B	5780	0	5835	74	0
3	C	1103	0	1109	20	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	12	0	11	5	0
6	A	22	0	0	2	0
6	B	18	0	0	1	0
6	C	4	0	0	1	0
All	All	12473	0	12444	166	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 (166) 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:A:627:SER:HB3	1:A:646:ARG:HG3	1.65	0.79
2:B:770:SER:O	2:B:771:THR:C	2.15	0.77
1:A:183:ILE:O	1:A:184:SER:OG	2.04	0.73
1:A:183:ILE:HG22	1:A:184:SER:N	2.01	0.73
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.70	0.73
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.72	0.71
1:A:101:ILE:HD11	1:A:107:PRO:HD3	1.72	0.70
1:A:259:ARG:NH2	1:A:308:THR:O	2.25	0.69
2:B:1074:THR:HG23	2:B:1076:SER:H	1.59	0.67
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.58	0.67
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.58	0.67
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.77	0.66
2:B:609:THR:HG22	2:B:611:GLU:H	1.61	0.66
2:B:380:ASN:HA	2:B:441:PHE:HZ	1.64	0.63
2:B:750:ARG:NH1	2:B:772:ASP:O	2.29	0.62
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.65	0.62
1:A:111:LEU:HB3	1:A:113:GLN:OE1	1.99	0.62
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.82	0.62
1:A:63:ARG:HH11	1:A:88:CYS:HB2	1.65	0.61
2:B:358:ASN:HA	2:B:972:GLN:OE1	2.00	0.61
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.84	0.59
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.84	0.59
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.85	0.59
1:A:250:ASP:O	3:C:130:ARG:NH1	2.30	0.58
2:B:439:ASN:OD1	2:B:453:ASN:ND2	2.36	0.58
3:C:12:ASP:OD1	3:C:12:ASP:N	2.33	0.58
3:C:34:GLN:NE2	6:C:201:HOH:O	2.36	0.57
2:B:1053:TYR:HB2	2:B:1055:ILE:HG13	1.87	0.57
1:A:3:THR:HG22	1:A:6:GLU:H	1.70	0.57
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.40	0.57
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.86	0.57
2:B:420:LEU:HD21	2:B:489:GLU:HB2	1.87	0.56
2:B:443:SER:HB2	2:B:451:LYS:HB3	1.87	0.56
1:A:113:GLN:OE1	1:A:113:GLN:N	2.27	0.55
1:A:98:TYR:O	1:A:101:ILE:HB	2.07	0.54
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.90	0.54
2:B:965:ILE:O	2:B:965:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:VAL:HG13	2:B:356:GLU:HG3	1.90	0.54
2:B:808:LEU:HD22	5:B:1101:CLT:HE1	1.90	0.53
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.90	0.53
1:A:183:ILE:O	1:A:184:SER:CB	2.55	0.53
1:A:693:GLN:O	1:A:697:HIS:HD2	1.92	0.53
2:B:1043:ARG:NH2	2:B:1050:PRO:O	2.41	0.53
2:B:1055:ILE:O	2:B:1057:ASP:N	2.41	0.53
1:A:747:VAL:HG12	1:A:748:SER:N	2.23	0.53
2:B:642:PRO:HG2	2:B:702:LEU:HD21	1.91	0.53
1:A:63:ARG:NH1	1:A:88:CYS:O	2.42	0.53
2:B:359:MET:SD	2:B:359:MET:N	2.81	0.53
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.91	0.52
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.90	0.52
1:A:750:GLN:OE1	1:A:750:GLN:N	2.42	0.52
2:B:750:ARG:HH21	5:B:1101:CLT:CB2	2.22	0.52
2:B:553:ILE:HB	2:B:570:VAL:HG13	1.91	0.52
2:B:949:VAL:HA	2:B:952:LEU:HD21	1.92	0.52
2:B:711:GLY:O	2:B:765:ASN:ND2	2.32	0.52
1:A:15:ASP:OD1	1:A:116:SER:OG	2.25	0.52
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.92	0.52
3:C:113:ILE:O	3:C:116:ASP:HB2	2.09	0.51
1:A:48:ARG:HB2	1:A:49:PRO:CD	2.41	0.51
1:A:649:LEU:HD22	1:A:658:ILE:HG12	1.92	0.51
3:C:35:SER:O	3:C:39:GLN:HG2	2.10	0.51
2:B:1005:LEU:HD23	2:B:1009:LEU:HD12	1.93	0.51
1:A:288:MET:HG2	1:A:290:ILE:HD13	1.93	0.51
1:A:746:ASP:O	6:A:901:HOH:O	2.18	0.50
1:A:641:SER:O	1:A:646:ARG:NH2	2.40	0.50
2:B:958:LEU:HB3	2:B:964:THR:HG23	1.92	0.50
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.94	0.50
2:B:888:PRO:O	2:B:1088:GLN:NE2	2.45	0.50
2:B:1019:GLN:O	2:B:1055:ILE:HG23	2.11	0.49
3:C:52:CYS:SG	3:C:53:THR:N	2.85	0.49
1:A:22:ASN:HB2	1:A:516:SER:HB2	1.93	0.49
1:A:541:ASP:OD1	1:A:542:VAL:N	2.46	0.49
2:B:358:ASN:CA	2:B:972:GLN:OE1	2.61	0.49
3:C:59:MET:HB3	3:C:74:LEU:HD11	1.95	0.49
1:A:33:ARG:O	1:A:556:LYS:NZ	2.47	0.48
2:B:358:ASN:ND2	2:B:977:LYS:NZ	2.62	0.48
2:B:446:ASP:C	2:B:448:ARG:H	2.15	0.48
2:B:955:GLU:OE1	2:B:955:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:954:ASP:O	2:B:958:LEU:HD11	2.14	0.47
1:A:262:ARG:NH2	6:A:908:HOH:O	2.46	0.47
2:B:510:PHE:HB2	2:B:548:THR:HG22	1.96	0.47
1:A:14:ARG:O	1:A:48:ARG:NH1	2.47	0.47
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.97	0.47
1:A:370:TYR:HE2	1:A:389:VAL:HG13	1.80	0.47
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.54	0.47
2:B:686:ALA:HB2	2:B:777:PRO:HB2	1.97	0.47
2:B:958:LEU:H	2:B:958:LEU:HD22	1.79	0.47
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.96	0.47
3:C:73:VAL:HB	3:C:88:LEU:HD21	1.96	0.47
1:A:78:TYR:CG	1:A:103:GLU:HG3	2.51	0.46
1:A:78:TYR:CD1	1:A:103:GLU:HG3	2.50	0.46
1:A:410:THR:HB	1:A:414:ILE:HB	1.97	0.46
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.51	0.46
2:B:913:GLN:HE21	2:B:918:ALA:HB2	1.80	0.46
3:C:39:GLN:O	3:C:43:LYS:HG2	2.16	0.46
2:B:438:ILE:HD12	2:B:442:VAL:HG11	1.96	0.46
1:A:311:ARG:HH21	1:A:358:LEU:HB3	1.81	0.45
1:A:322:LYS:HE3	1:A:323:TYR:CZ	2.51	0.45
3:C:80:PRO:HB3	3:C:82:LYS:HE3	1.99	0.45
3:C:128:ASP:OD1	3:C:130:ARG:HG2	2.15	0.45
2:B:631:GLY:HA2	2:B:685:VAL:HG22	1.97	0.45
1:A:559:GLU:O	1:A:568:PHE:HA	2.16	0.45
1:A:160:PRO:HB3	1:A:234:GLN:HB3	1.97	0.45
2:B:348:LEU:HD13	2:B:836:LEU:HD11	1.99	0.45
2:B:357:ARG:HG2	2:B:357:ARG:O	2.16	0.45
1:A:14:ARG:HG2	1:A:48:ARG:HH12	1.82	0.45
2:B:492:ALA:HB1	2:B:496:TYR:HB2	1.99	0.44
1:A:44:PRO:HD2	1:A:455:THR:O	2.17	0.44
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.53	0.44
1:A:106:GLN:CB	1:A:107:PRO:CD	2.95	0.44
1:A:368:GLY:HA3	1:A:450:GLY:O	2.18	0.44
1:A:722:VAL:HG13	1:A:723:ASN:N	2.33	0.44
2:B:879:ARG:NH1	2:B:1092:ASN:OD1	2.51	0.44
1:A:181:GLU:O	1:A:181:GLU:HG2	2.18	0.43
1:A:264:SER:HB2	1:A:294:ALA:HB2	2.00	0.43
1:A:237:ASP:OD1	1:A:238:MET:N	2.51	0.43
2:B:457:ARG:HG3	2:B:458:VAL:N	2.33	0.43
2:B:412:HIS:CE1	2:B:415:LYS:HB2	2.54	0.43
2:B:946:LEU:HD11	2:B:984:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:961:SER:HB2	2:B:962:ASP:H	1.73	0.43
1:A:166:LEU:HD23	1:A:243:LEU:HD13	2.00	0.43
1:A:623:LEU:HD22	1:A:637:LEU:HD23	2.00	0.43
2:B:430:ARG:HD3	2:B:435:ARG:HH21	1.83	0.43
2:B:818:ILE:HD13	5:B:1101:CLT:HZ1	1.99	0.43
2:B:959:ASN:O	2:B:961:SER:N	2.52	0.43
3:C:99:HIS:O	3:C:103:VAL:HG23	2.19	0.43
1:A:264:SER:HB3	1:A:288:MET:HE1	2.01	0.43
1:A:708:THR:HB	1:A:714:GLN:HB2	2.01	0.42
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	2.01	0.42
1:A:695:ILE:HD11	1:A:699:ARG:NH2	2.33	0.42
2:B:1051:ILE:H	2:B:1051:ILE:HD13	1.83	0.42
2:B:1064:ASN:HA	2:B:1067:GLN:HG3	2.01	0.42
3:C:3:LEU:HD11	3:C:21:GLN:HB2	2.01	0.42
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.55	0.42
2:B:352:ASN:O	2:B:356:GLU:HG2	2.19	0.42
2:B:357:ARG:O	2:B:359:MET:HE3	2.20	0.42
1:A:36:VAL:HG11	1:A:522:ALA:HB1	2.01	0.41
3:C:1:MET:HA	3:C:79:PHE:CD1	2.55	0.41
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.71	0.41
1:A:618:MET:HG2	1:A:653:PHE:HB3	2.02	0.41
2:B:482:GLU:OE1	2:B:482:GLU:N	2.44	0.41
1:A:152:GLN:NE2	1:A:241:THR:O	2.48	0.41
2:B:899:PHE:HB3	2:B:900:PRO:HD3	2.02	0.41
1:A:290:ILE:HG23	1:A:292:GLY:H	1.86	0.41
3:C:4:LEU:O	3:C:73:VAL:HA	2.20	0.41
2:B:545:GLY:HA3	2:B:585:LEU:HD23	2.02	0.41
2:B:806:ALA:HB3	5:B:1101:CLT:HZ2	2.02	0.41
1:A:177:GLU:HB3	1:A:185:LYS:HG3	2.03	0.41
1:A:181:GLU:O	1:A:181:GLU:CG	2.69	0.41
1:A:369:GLY:O	1:A:609:ARG:NH2	2.53	0.41
1:A:524:ILE:HD11	1:A:616:LEU:HD23	2.02	0.41
1:A:114:PHE:HB3	1:A:117:ILE:HD12	2.02	0.41
2:B:395:GLN:NE2	6:B:1202:HOH:O	2.53	0.41
2:B:830:THR:HG22	2:B:832:ASN:H	1.86	0.41
2:B:954:ASP:C	2:B:956:GLY:H	2.24	0.41
1:A:476:ARG:HD2	1:A:500:ALA:HB1	2.03	0.41
2:B:434:CYS:SG	2:B:436:THR:OG1	2.69	0.41
3:C:4:LEU:HD23	3:C:74:LEU:HB3	2.02	0.41
1:A:28:ARG:HH11	1:A:28:ARG:HB3	1.85	0.40
1:A:101:ILE:HD11	1:A:107:PRO:CD	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:555:PHE:HZ	2:B:622:ALA:HB1	1.85	0.40
1:A:284:ALA:HB3	1:A:343:HIS:CD2	2.56	0.40
1:A:290:ILE:HD12	1:A:290:ILE:HA	1.80	0.40
3:C:80:PRO:HB2	3:C:83:LEU:HG	2.02	0.40
1:A:293:PRO:HA	1:A:355:THR:O	2.21	0.40
2:B:806:ALA:HB1	5:B:1101:CLT:HH	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	687/764 (90%)	649 (94%)	32 (5%)	6 (1%)	17	31
2	B	723/748 (97%)	666 (92%)	52 (7%)	5 (1%)	22	39
3	C	131/157 (83%)	121 (92%)	9 (7%)	1 (1%)	19	35
All	All	1541/1669 (92%)	1436 (93%)	93 (6%)	12 (1%)	19	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	465	PHE
2	B	1056	ALA
3	C	4	LEU
1	A	59	VAL
1	A	181	GLU
1	A	184	SER
1	A	476	ARG
2	B	961	SER
1	A	722	VAL
2	B	960	ILE
2	B	1055	ILE

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Mol	Chain	Res	Type
1	A	183	ILE

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	608/666 (91%)	574 (94%)	34 (6%)	21 40
2	B	662/678 (98%)	618 (93%)	44 (7%)	16 32
3	C	120/138 (87%)	109 (91%)	11 (9%)	9 18
All	All	1390/1482 (94%)	1301 (94%)	89 (6%)	17 33

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	91	ARG
1	A	101	ILE
1	A	106	GLN
1	A	153	MET
1	A	161	THR
1	A	180	CYS
1	A	183	ILE
1	A	185	LYS
1	A	192	THR
1	A	228	ARG
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	328	THR
1	A	355	THR
1	A	451	LEU

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Mol	Chain	Res	Type
1	A	484	GLN
1	A	488	SER
1	A	495	ARG
1	A	508	THR
1	A	509	GLN
1	A	528	ARG
1	A	544	ARG
1	A	569	ARG
1	A	570	PHE
1	A	612	LEU
1	A	613	THR
1	A	649	LEU
1	A	709	GLU
2	B	359	MET
2	B	386	PHE
2	B	411	LEU
2	B	414	PHE
2	B	425	SER
2	B	465	PHE
2	B	522	LEU
2	B	570	VAL
2	B	573	ILE
2	B	610	LEU
2	B	614	SER
2	B	641	LEU
2	B	652	ARG
2	B	679	ASP
2	B	712	SER
2	B	713	VAL
2	B	769	ARG
2	B	775	SER
2	B	787	VAL
2	B	789	MET
2	B	797	ASP
2	B	798	THR
2	B	799	GLN
2	B	807	LEU
2	B	816	ARG
2	B	831	LEU
2	B	861	SER
2	B	897	ARG
2	B	914	THR

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Mol	Chain	Res	Type
2	B	917	ASN
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	1040	SER
2	B	1048	PHE
2	B	1051	ILE
2	B	1052	LEU
2	B	1057	ASP
2	B	1075	GLU
2	B	1085	LEU
2	B	1092	ASN
3	C	1	MET
3	C	2	VAL
3	C	3	LEU
3	C	31	GLN
3	C	51	ARG
3	C	81	LYS
3	C	90	ASP
3	C	101	LYS
3	C	113	ILE
3	C	116	ASP
3	C	121	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	296	GLN
1	A	655	GLN
1	A	697	HIS
2	B	358	ASN
2	B	913	GLN

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)

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	1101	-	12,12,12	0.65	0	14,14,14	0.96	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	1101	-	-	2/6/6/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	CLT	CB1-CA-CB2-OG2
5	B	1101	CLT	CB1-CA-CB2-OG1

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1101	CLT	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	699/764 (91%)	0.33	31 (4%)	34	37	42, 70, 109, 136	0
2	B	731/748 (97%)	0.36	31 (4%)	36	39	42, 64, 110, 173	0
3	C	137/157 (87%)	1.17	31 (22%)	0	0	61, 94, 132, 157	0
All	All	1567/1669 (93%)	0.41	93 (5%)	22	23	42, 69, 113, 173	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1055	ILE	18.1
3	C	57	GLY	9.0
3	C	157	LEU	7.2
3	C	153	ILE	6.7
3	C	1	MET	6.5
2	B	424	THR	6.4
2	B	445	LEU	6.3
2	B	772	ASP	5.6
1	A	684	LEU	5.6
2	B	959	ASN	5.4
1	A	717	PHE	4.9
2	B	1019	GLN	4.7
3	C	23	ASP	4.6
2	B	465	PHE	4.5
3	C	3	LEU	4.4
3	C	54	LEU	4.3
3	C	149	MET	4.3
1	A	700	PHE	4.3
3	C	21	GLN	4.1
2	B	427	THR	4.0
3	C	33	TYR	3.6
3	C	156	VAL	3.6
1	A	657	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	747	VAL	3.6
2	B	423	VAL	3.5
3	C	56	ALA	3.5
1	A	184	SER	3.4
1	A	89	TYR	3.4
1	A	648	LEU	3.3
3	C	148	ILE	3.3
3	C	77	ALA	3.1
2	B	448	ARG	3.1
2	B	432	ARG	3.1
2	B	444	PHE	3.1
3	C	52	CYS	3.0
3	C	108	ARG	3.0
2	B	346	GLU	2.9
1	A	541	ASP	2.9
3	C	127	ILE	2.9
1	A	123	ARG	2.8
2	B	449	ARG	2.8
2	B	478	HIS	2.8
3	C	22	GLU	2.7
1	A	537	GLU	2.7
1	A	474	GLY	2.7
3	C	40	LEU	2.7
3	C	61	PHE	2.7
2	B	1022	THR	2.7
2	B	1054	VAL	2.6
1	A	79	ARG	2.6
2	B	662	LYS	2.6
2	B	461	VAL	2.6
1	A	165	GLY	2.5
1	A	716	ARG	2.5
3	C	51	ARG	2.4
1	A	40	ALA	2.4
3	C	74	LEU	2.4
2	B	463	GLU	2.4
3	C	38	LYS	2.4
1	A	643	LEU	2.3
3	C	4	LEU	2.3
1	A	99	ALA	2.3
3	C	152	ASN	2.3
3	C	55	GLU	2.3
1	A	51	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	94	PHE	2.3
1	A	33	ARG	2.2
3	C	72	LEU	2.2
1	A	642	ILE	2.2
2	B	490	PHE	2.2
2	B	348	LEU	2.2
1	A	679	GLU	2.2
2	B	1017	ILE	2.2
2	B	379	LEU	2.2
1	A	711	GLY	2.2
3	C	154	GLU	2.2
1	A	56	TYR	2.2
1	A	628	PHE	2.2
2	B	466	LEU	2.2
2	B	1011	VAL	2.1
2	B	1057	ASP	2.1
3	C	8	ALA	2.1
1	A	624	TYR	2.1
2	B	1010	GLY	2.1
1	A	62	SER	2.1
3	C	63	TYR	2.1
2	B	610	LEU	2.1
1	A	652	THR	2.1
2	B	429	VAL	2.1
1	A	492	ARG	2.0
2	B	1020	PRO	2.0
1	A	307	LYS	2.0
3	C	30	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 monosaccharides 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, 95th 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^2)	Q<0.9
4	ZN	B	1102	1/1	0.78	0.31	146,146,146,146	0
4	ZN	A	801	1/1	0.82	0.31	236,236,236,236	0
5	CLT	B	1101	12/12	0.82	0.32	102,104,112,112	0

6.5 Other polymers (i)

There are no such residues in this entry.