



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:54 PM UTC

PDB ID : 5VNK / pdb_00005vnk
Title : Crystal structure of Sec23a/Sec24a/Sec22 complexed with a C-terminal LL sorting motif
Authors : Ma, W.; Goldberg, J.
Deposited on : 2017-04-30
Resolution : 2.55 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

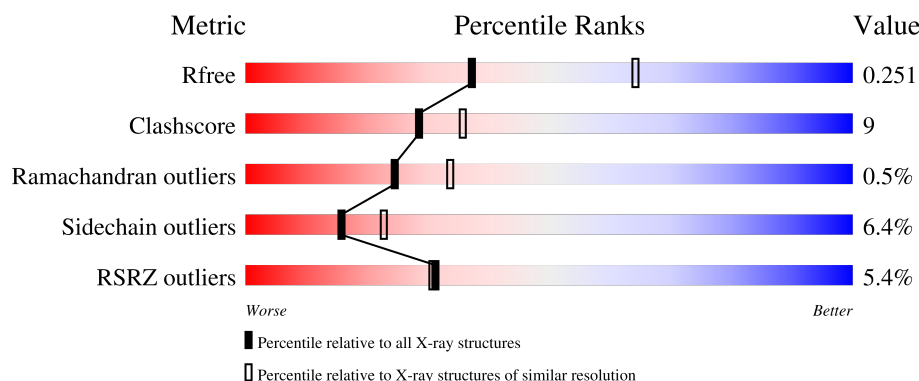
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 $\leq 5\%$. 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	5% 73% 17% • • 7%
2	B	748	5% 76% 19% • •
3	C	157	6% 59% 24% • • 14%
4	D	5	60% 20% 40% 40%

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	ZN	A	801	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12544 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	708	Total	C	N	O	S	0	0	0
			5620	3582	967	1031	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	729	Total	C	N	O	S	0	0	0
			5754	3669	980	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	135	Total	C	N	O	S	0	0	0
			1087	699	177	203	8			

- Molecule 4 is a protein called C-terminal LL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			22	15	3	4			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Zn 1	0	0

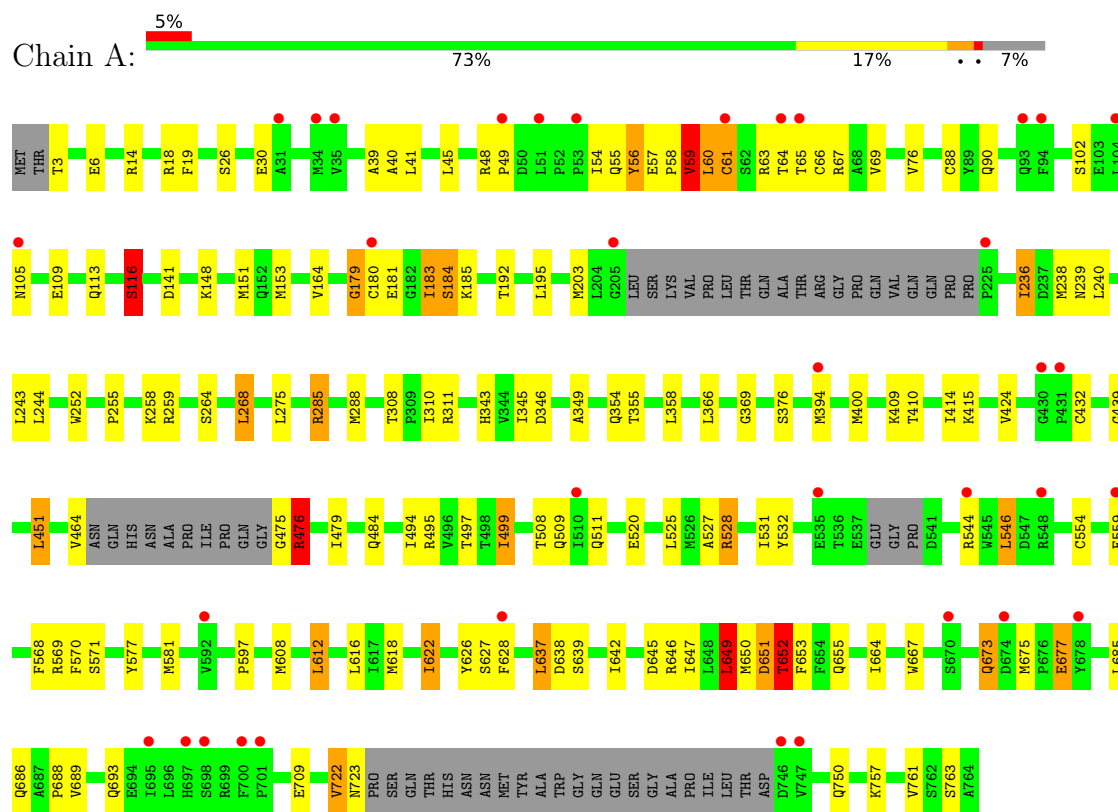
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total 21	O 21	0	0
6	B	35	Total 35	O 35	0	0
6	C	3	Total 3	O 3	0	0

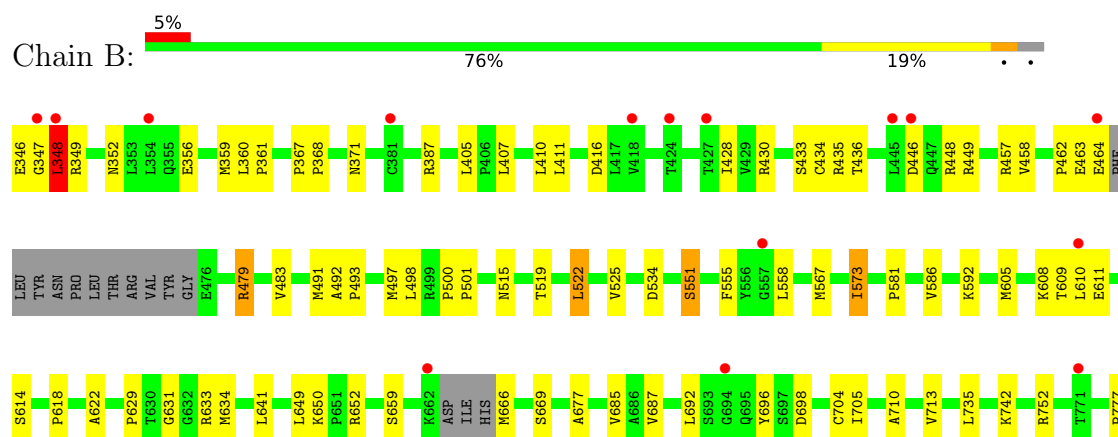
3 Residue-property plots [i](#)

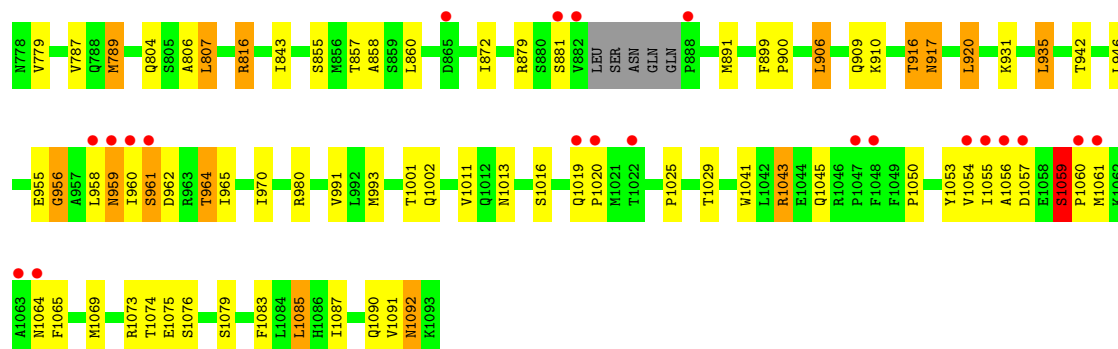
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

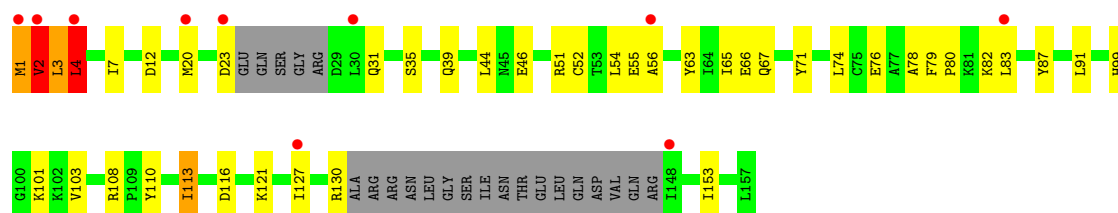


• Molecule 2: Protein transport protein Sec24A

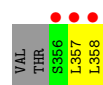
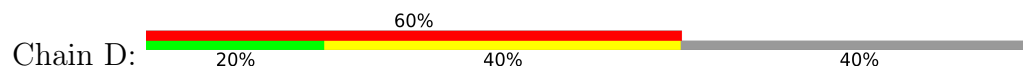




• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: C-terminal LL



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.18Å 97.61Å 130.55Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	130.55 – 2.55 130.55 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.1 (130.55-2.55) 99.1 (130.55-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.196 , 0.251 0.199 , 0.251	Depositor DCC
R_{free} test set	3041 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12544	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.49	6/5751 (0.1%)	0.53	11/7786 (0.1%)
2	B	0.36	4/5877 (0.1%)	0.50	10/7989 (0.1%)
3	C	0.27	1/1106 (0.1%)	0.53	3/1489 (0.2%)
4	D	0.28	0/21	0.53	0/26
All	All	0.42	11/12755 (0.1%)	0.52	24/17290 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1056	ALA	N-CA	-7.22	1.37	1.46
2	B	956	GLY	C-O	-6.43	1.17	1.23
1	A	184	SER	C-O	-6.27	1.16	1.24
2	B	964	THR	C-O	-6.09	1.17	1.24
1	A	59	VAL	C-O	-6.03	1.16	1.24
1	A	651	ASP	C-O	-5.97	1.16	1.24
1	A	649	LEU	C-O	-5.54	1.17	1.24
3	C	4	LEU	C-O	-5.34	1.17	1.24
2	B	965	ILE	C-O	-5.29	1.18	1.24
1	A	54	ILE	C-O	-5.13	1.18	1.24
1	A	57	GLU	C-N	-5.00	1.27	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1064	ASN	N-CA-C	-10.85	100.06	113.18
2	B	965	ILE	CA-C-N	-8.08	112.03	120.03
2	B	965	ILE	C-N-CA	-8.08	112.03	120.03
3	C	3	LEU	N-CA-C	7.41	120.33	109.07
1	A	60	LEU	N-CA-C	6.74	119.96	109.52
1	A	184	SER	CA-C-N	-6.49	111.41	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	SER	C-N-CA	-6.49	111.41	123.03
2	B	959	ASN	N-CA-C	6.27	118.12	111.28
1	A	180	CYS	N-CA-C	6.07	120.29	113.01
1	A	476	ARG	N-CA-C	6.06	123.71	110.80
2	B	1056	ALA	N-CA-C	-6.01	99.01	108.63
2	B	348	LEU	N-CA-C	-6.00	105.27	112.59
3	C	3	LEU	CA-C-N	5.88	132.78	121.54
3	C	3	LEU	C-N-CA	5.88	132.78	121.54
2	B	1059	SER	N-CA-C	5.67	122.33	109.81
1	A	179	GLY	N-CA-C	5.63	122.60	114.10
1	A	116	SER	N-CA-C	-5.61	100.04	109.07
2	B	961	SER	CB-CA-C	-5.61	110.13	116.63
2	B	858	ALA	N-CA-C	5.35	122.19	110.80
1	A	61	CYS	N-CA-C	-5.32	102.52	110.23
1	A	652	THR	CA-C-N	5.29	131.64	121.54
1	A	652	THR	C-N-CA	5.29	131.64	121.54
1	A	55	GLN	N-CA-C	5.25	117.98	110.68
2	B	349	ARG	N-CA-C	5.02	116.58	110.41

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	5620	0	5567	97	0
2	B	5754	0	5795	97	0
3	C	1087	0	1091	31	0
4	D	22	0	23	2	0
5	A	1	0	0	2	0
5	B	1	0	0	0	0
6	A	21	0	0	2	0
6	B	35	0	0	10	0
6	C	3	0	0	0	0
All	All	12544	0	12476	219	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 (219) 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:61:CYS:SG	5:A:801:ZN:ZN	1.52	0.98
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.57	0.86
2:B:551:SER:OG	2:B:611:GLU:OE1	1.94	0.85
3:C:1:MET:H1	3:C:76:GLU:HB2	1.38	0.84
1:A:60:LEU:HD21	1:A:69:VAL:HG22	1.62	0.80
2:B:1057:ASP:HB2	2:B:1060:PRO:HD3	1.64	0.79
3:C:1:MET:N	3:C:1:MET:HE3	1.98	0.79
1:A:60:LEU:HD23	1:A:69:VAL:HA	1.65	0.78
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.48	0.78
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.65	0.77
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.66	0.76
2:B:961:SER:OG	2:B:962:ASP:OD1	2.04	0.75
1:A:259:ARG:NH2	1:A:308:THR:O	2.19	0.75
1:A:61:CYS:HG	5:A:801:ZN:ZN	0.41	0.73
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.72	0.72
1:A:63:ARG:NH1	1:A:90:GLN:HB2	2.07	0.70
1:A:432:CYS:SG	6:A:916:HOH:O	2.50	0.69
3:C:1:MET:N	3:C:76:GLU:HB2	2.07	0.69
2:B:1074:THR:HG23	2:B:1076:SER:H	1.58	0.69
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.75	0.68
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.77	0.67
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.77	0.66
1:A:60:LEU:CD2	1:A:69:VAL:HG22	2.25	0.66
2:B:804:GLN:OE1	6:B:1201:HOH:O	2.14	0.65
1:A:3:THR:HG22	1:A:6:GLU:H	1.62	0.65
2:B:1025:PRO:O	6:B:1202:HOH:O	2.14	0.65
2:B:958:LEU:HD12	2:B:958:LEU:N	2.12	0.64
2:B:931:LYS:NZ	6:B:1207:HOH:O	2.31	0.64
2:B:806:ALA:HB3	4:D:358:LEU:HD11	1.80	0.63
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.81	0.63
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.81	0.63
1:A:56:TYR:OH	1:A:109:GLU:OE2	2.17	0.63
1:A:508:THR:HG22	1:A:511:GLN:OE1	1.99	0.62
2:B:1054:VAL:HG12	2:B:1054:VAL:O	1.99	0.62
1:A:102:SER:O	1:A:105:ASN:O	2.17	0.62
3:C:1:MET:H1	3:C:1:MET:HE3	1.65	0.62
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:MET:HE1	3:C:78:ALA:HB3	1.82	0.62
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.82	0.62
2:B:371:ASN:OD1	6:B:1204:HOH:O	2.16	0.61
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.82	0.61
3:C:1:MET:HE3	3:C:1:MET:H3	1.65	0.60
2:B:891:MET:O	6:B:1203:HOH:O	2.15	0.60
1:A:626:TYR:HB2	1:A:647:ILE:HB	1.82	0.60
1:A:61:CYS:O	1:A:67:ARG:HA	2.01	0.60
2:B:430:ARG:HD3	2:B:435:ARG:HH21	1.66	0.60
1:A:183:ILE:HD13	2:B:605:MET:CE	2.32	0.59
2:B:959:ASN:O	2:B:959:ASN:ND2	2.35	0.59
2:B:962:ASP:OD1	2:B:962:ASP:N	2.27	0.59
2:B:1055:ILE:O	2:B:1057:ASP:N	2.35	0.59
4:D:357:LEU:H	4:D:357:LEU:HD23	1.67	0.59
1:A:475:GLY:O	1:A:476:ARG:HB2	2.03	0.58
2:B:348:LEU:HD12	2:B:348:LEU:O	2.04	0.57
1:A:61:CYS:SG	1:A:88:CYS:SG	3.02	0.57
3:C:113:ILE:O	3:C:116:ASP:HB2	2.04	0.57
1:A:26:SER:H	1:A:509:GLN:NE2	2.04	0.56
1:A:673:GLN:HG2	1:A:685:LEU:HD12	1.85	0.56
3:C:35:SER:O	3:C:39:GLN:HG2	2.06	0.56
2:B:872:ILE:HD12	2:B:1090:GLN:HB2	1.88	0.56
2:B:1043:ARG:HB3	2:B:1050:PRO:HD2	1.88	0.55
1:A:67:ARG:O	1:A:409:LYS:NZ	2.38	0.55
1:A:528:ARG:HA	1:A:608:MET:HE1	1.89	0.55
2:B:405:LEU:HD22	2:B:843:ILE:HD13	1.89	0.55
2:B:1073:ARG:NH2	6:B:1209:HOH:O	2.40	0.55
1:A:410:THR:HB	1:A:414:ILE:HB	1.88	0.54
2:B:955:GLU:OE1	2:B:955:GLU:N	2.40	0.54
1:A:354:GLN:HE22	1:A:597:PRO:HD2	1.72	0.54
2:B:446:ASP:C	2:B:448:ARG:H	2.14	0.54
1:A:116:SER:OG	1:A:497:THR:OG1	1.81	0.54
3:C:54:LEU:HD13	3:C:153:ILE:HD13	1.89	0.54
2:B:906:LEU:HD13	2:B:942:THR:HG21	1.90	0.54
2:B:491:MET:HE2	3:C:108:ARG:HD3	1.88	0.54
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.89	0.53
2:B:1083:PHE:O	2:B:1087:ILE:HG12	2.08	0.53
3:C:7:ILE:HD12	3:C:71:TYR:CD2	2.43	0.53
2:B:909:GLN:HG2	2:B:910:LYS:N	2.24	0.53
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.43	0.53
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:O	1:A:64:THR:C	2.50	0.52
1:A:637:LEU:HD22	1:A:722:VAL:HA	1.92	0.52
2:B:387:ARG:HD2	2:B:935:LEU:HD12	1.92	0.52
2:B:416:ASP:OD1	2:B:742:LYS:NZ	2.40	0.52
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.90	0.52
2:B:872:ILE:HD13	2:B:1087:ILE:HG23	1.92	0.52
1:A:183:ILE:HD13	2:B:605:MET:HE1	1.92	0.51
3:C:80:PRO:HB3	3:C:82:LYS:HE2	1.93	0.51
3:C:44:LEU:HD13	3:C:65:ILE:HD11	1.93	0.51
1:A:479:ILE:HB	1:A:499:ILE:HD11	1.92	0.50
2:B:958:LEU:N	2:B:958:LEU:CD1	2.74	0.50
1:A:366:LEU:HD22	1:A:424:VAL:HG22	1.93	0.50
2:B:980:ARG:NH2	6:B:1211:HOH:O	2.43	0.50
2:B:961:SER:OG	2:B:962:ASP:N	2.45	0.50
1:A:58:PRO:O	1:A:59:VAL:HG23	2.11	0.49
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.94	0.49
3:C:2:VAL:O	3:C:127:ILE:HD11	2.12	0.49
3:C:1:MET:N	3:C:1:MET:CE	2.72	0.49
2:B:956:GLY:C	2:B:958:LEU:HD12	2.38	0.49
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.48	0.48
1:A:311:ARG:H	1:A:311:ARG:HD3	1.79	0.48
1:A:577:TYR:CZ	1:A:581:MET:HE3	2.48	0.48
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.95	0.48
1:A:394:MET:HE3	1:A:394:MET:H	1.78	0.48
1:A:58:PRO:O	1:A:59:VAL:CB	2.62	0.48
2:B:752:ARG:NH1	6:B:1201:HOH:O	2.28	0.48
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.49	0.47
1:A:652:THR:HG22	1:A:655:GLN:H	1.80	0.47
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.95	0.47
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.97	0.47
1:A:622:ILE:HG13	1:A:651:ASP:HB3	1.97	0.47
1:A:14:ARG:O	1:A:48:ARG:NH1	2.48	0.47
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.49	0.47
2:B:433:SER:OG	2:B:457:ARG:HD3	2.15	0.47
2:B:631:GLY:HA2	2:B:685:VAL:HG22	1.97	0.47
3:C:56:ALA:HB2	3:C:153:ILE:HG21	1.95	0.47
1:A:56:TYR:HH	1:A:109:GLU:CD	2.23	0.47
1:A:757:LYS:O	1:A:761:VAL:HG22	2.15	0.47
1:A:628:PHE:HE2	1:A:667:TRP:HZ3	1.63	0.46
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.50	0.46
2:B:462:PRO:O	2:B:464:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:666:MET:HE2	2:B:860:LEU:HB2	1.97	0.46
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.96	0.46
1:A:184:SER:O	1:A:184:SER:OG	2.31	0.46
2:B:677:ALA:HB2	2:B:705:ILE:HA	1.98	0.46
1:A:56:TYR:OH	1:A:109:GLU:CD	2.59	0.46
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.98	0.46
1:A:476:ARG:HH11	1:A:476:ARG:HG2	1.81	0.46
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.97	0.46
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.51	0.46
1:A:63:ARG:HH12	1:A:90:GLN:HB2	1.80	0.46
2:B:879:ARG:CZ	2:B:1092:ASN:HB3	2.46	0.46
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.46	0.46
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.98	0.45
3:C:7:ILE:HD12	3:C:71:TYR:HD2	1.80	0.45
1:A:638:ASP:OD1	1:A:639:SER:N	2.50	0.45
1:A:559:GLU:O	1:A:568:PHE:HA	2.16	0.45
2:B:534:ASP:OD1	2:B:592:LYS:NZ	2.32	0.45
1:A:236:ILE:HD13	1:A:236:ILE:HA	1.73	0.45
2:B:609:THR:HG22	2:B:611:GLU:H	1.80	0.45
2:B:479:ARG:HD2	2:B:479:ARG:HA	1.74	0.45
1:A:527:ALA:O	1:A:531:ILE:HG12	2.17	0.44
2:B:916:THR:HG22	2:B:917:ASN:H	1.82	0.44
2:B:960:ILE:O	2:B:960:ILE:HG22	2.17	0.44
1:A:345:ILE:O	1:A:369:GLY:HA3	2.17	0.44
3:C:55:GLU:O	3:C:153:ILE:HG22	2.18	0.44
1:A:19:PHE:CE1	1:A:40:ALA:HB2	2.52	0.44
3:C:1:MET:HA	3:C:79:PHE:HB2	2.00	0.44
1:A:48:ARG:NH2	6:A:906:HOH:O	2.50	0.43
1:A:63:ARG:O	1:A:66:CYS:N	2.45	0.43
2:B:633:ARG:NH2	6:B:1215:HOH:O	2.50	0.43
2:B:959:ASN:ND2	2:B:959:ASN:C	2.73	0.43
2:B:457:ARG:HG3	2:B:458:VAL:N	2.32	0.43
2:B:525:VAL:HG22	2:B:735:LEU:HD11	1.99	0.43
2:B:1041:TRP:O	2:B:1045:GLN:HG2	2.18	0.43
3:C:1:MET:N	3:C:76:GLU:OE1	2.51	0.43
1:A:113:GLN:H	1:A:113:GLN:HG3	1.50	0.43
2:B:407:LEU:HG	2:B:789:MET:HG3	2.00	0.43
2:B:879:ARG:C	2:B:881:SER:H	2.25	0.43
2:B:704:CYS:SG	6:B:1234:HOH:O	2.62	0.43
3:C:80:PRO:HB2	3:C:83:LEU:HG	2.00	0.43
2:B:346:GLU:HB3	2:B:347:GLY:H	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TYR:HD1	1:A:56:TYR:C	2.27	0.43
1:A:618:MET:HE2	1:A:653:PHE:CD1	2.53	0.43
1:A:722:VAL:HG13	1:A:723:ASN:N	2.34	0.43
2:B:1085:LEU:HD12	2:B:1085:LEU:HA	1.86	0.43
1:A:56:TYR:C	1:A:56:TYR:CD1	2.97	0.43
1:A:675:MET:HB3	1:A:677:GLU:HG3	2.00	0.43
2:B:959:ASN:C	2:B:959:ASN:HD22	2.26	0.43
1:A:310:ILE:HG22	1:A:311:ARG:HD3	2.00	0.42
2:B:1060:PRO:O	2:B:1061:MET:HB2	2.19	0.42
1:A:546:LEU:HD12	1:A:546:LEU:HA	1.87	0.42
1:A:484:GLN:HG2	1:A:494:ILE:HG13	2.00	0.42
1:A:689:VAL:O	1:A:693:GLN:HG2	2.20	0.42
3:C:12:ASP:OD1	3:C:12:ASP:N	2.44	0.42
3:C:99:HIS:O	3:C:103:VAL:HG23	2.19	0.42
2:B:666:MET:HE3	2:B:855:SER:HB3	2.00	0.42
1:A:58:PRO:O	1:A:59:VAL:HB	2.19	0.42
2:B:1011:VAL:HG12	2:B:1013:ASN:H	1.84	0.42
2:B:434:CYS:SG	2:B:436:THR:OG1	2.67	0.42
2:B:920:LEU:HD12	2:B:920:LEU:HA	1.90	0.42
3:C:87:TYR:CZ	3:C:91:LEU:HD11	2.54	0.42
1:A:252:TRP:CE2	2:B:581:PRO:HD3	2.55	0.42
1:A:60:LEU:CD2	1:A:69:VAL:HA	2.43	0.42
1:A:268:LEU:HG	1:A:288:MET:SD	2.59	0.42
3:C:51:ARG:NH2	3:C:66:GLU:OE2	2.53	0.42
1:A:285:ARG:NE	1:A:346:ASP:OD2	2.45	0.41
2:B:710:ALA:HB3	2:B:777:PRO:HD2	2.01	0.41
1:A:358:LEU:HD22	1:A:597:PRO:HB3	2.02	0.41
2:B:634:MET:HE2	2:B:687:VAL:HG22	2.03	0.41
1:A:63:ARG:O	1:A:65:THR:N	2.53	0.41
1:A:577:TYR:CE2	1:A:581:MET:HE3	2.54	0.41
1:A:238:MET:HE2	1:A:238:MET:HB3	1.94	0.41
2:B:522:LEU:HD23	2:B:522:LEU:HA	1.90	0.41
2:B:428:ILE:HD13	2:B:493:PRO:HD3	2.03	0.41
2:B:360:LEU:HD12	2:B:361:PRO:HD2	2.03	0.41
2:B:555:PHE:HZ	2:B:622:ALA:HB1	1.85	0.41
1:A:185:LYS:CB	2:B:567:MET:HB3	2.51	0.41
1:A:151:MET:HE3	1:A:244:LEU:HD22	2.03	0.41
1:A:649:LEU:HD12	1:A:650:MET:N	2.36	0.41
2:B:515:ASN:O	2:B:519:THR:HG23	2.21	0.41
2:B:991:VAL:HG21	2:B:1053:TYR:HE1	1.85	0.41
3:C:1:MET:H3	3:C:1:MET:CE	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLU:HB3	1:A:616:LEU:HD11	2.03	0.41
1:A:645:ASP:HA	1:A:664:ILE:HG12	2.03	0.41
2:B:367:PRO:HA	2:B:368:PRO:HD3	1.96	0.41
2:B:910:LYS:HE2	2:B:910:LYS:HB2	1.89	0.41
2:B:956:GLY:O	2:B:958:LEU:CD1	2.69	0.41
1:A:354:GLN:NE2	1:A:597:PRO:HD2	2.35	0.40
2:B:1059:SER:N	2:B:1060:PRO:CD	2.83	0.40
2:B:1087:ILE:O	2:B:1091:VAL:HG23	2.21	0.40
2:B:348:LEU:O	2:B:348:LEU:CG	2.70	0.40
2:B:446:ASP:HB2	2:B:449:ARG:HB2	2.03	0.40
2:B:946:LEU:HD22	2:B:1069:MET:HE1	2.03	0.40
1:A:148:LYS:HE3	1:A:244:LEU:O	2.21	0.40
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.36	0.40
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.88	0.40
1:A:750:GLN:OE1	1:A:750:GLN:N	2.52	0.40
2:B:352:ASN:O	2:B:356:GLU:HG2	2.20	0.40
2:B:500:PRO:HA	2:B:501:PRO:HD3	2.00	0.40
3:C:4:LEU:HD11	3:C:20:MET:HE2	2.03	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	698/764 (91%)	667 (96%)	28 (4%)	3 (0%)	30	39
2	B	721/748 (96%)	680 (94%)	38 (5%)	3 (0%)	30	39
3	C	129/157 (82%)	118 (92%)	9 (7%)	2 (2%)	7	9
4	D	1/5 (20%)	0	1 (100%)	0	100	100
All	All	1549/1674 (92%)	1465 (95%)	76 (5%)	8 (0%)	24	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	4	LEU
1	A	59	VAL
2	B	463	GLU
1	A	476	ARG
2	B	1065	PHE
3	C	2	VAL
1	A	181	GLU
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	617/666 (93%)	579 (94%)	38 (6%)	16	24
2	B	658/678 (97%)	617 (94%)	41 (6%)	16	24
3	C	119/138 (86%)	109 (92%)	10 (8%)	10	14
4	D	2/5 (40%)	2 (100%)	0	100	100
All	All	1396/1487 (94%)	1307 (94%)	89 (6%)	16	23

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

Mol	Chain	Res	Type
1	A	30	GLU
1	A	41	LEU
1	A	56	TYR
1	A	76	VAL
1	A	116	SER
1	A	141	ASP
1	A	153	MET
1	A	164	VAL
1	A	183	ILE
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	264	SER

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Mol	Chain	Res	Type
1	A	268	LEU
1	A	285	ARG
1	A	376	SER
1	A	400	MET
1	A	451	LEU
1	A	495	ARG
1	A	499	ILE
1	A	528	ARG
1	A	544	ARG
1	A	546	LEU
1	A	569	ARG
1	A	571	SER
1	A	612	LEU
1	A	622	ILE
1	A	637	LEU
1	A	642	ILE
1	A	649	LEU
1	A	652	THR
1	A	673	GLN
1	A	677	GLU
1	A	686	GLN
1	A	709	GLU
1	A	722	VAL
1	A	763	SER
2	B	348	LEU
2	B	359	MET
2	B	411	LEU
2	B	479	ARG
2	B	483	VAL
2	B	497	MET
2	B	498	LEU
2	B	522	LEU
2	B	551	SER
2	B	573	ILE
2	B	608	LYS
2	B	610	LEU
2	B	614	SER
2	B	641	LEU
2	B	650	LYS
2	B	659	SER
2	B	669	SER
2	B	692	LEU

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Mol	Chain	Res	Type
2	B	713	VAL
2	B	787	VAL
2	B	789	MET
2	B	807	LEU
2	B	816	ARG
2	B	857	THR
2	B	906	LEU
2	B	916	THR
2	B	917	ASN
2	B	920	LEU
2	B	935	LEU
2	B	964	THR
2	B	970	ILE
2	B	993	MET
2	B	1001	THR
2	B	1002	GLN
2	B	1016	SER
2	B	1029	THR
2	B	1043	ARG
2	B	1059	SER
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	46	GLU
3	C	67	GLN
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS
3	C	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	239	ASN
1	A	256	GLN
1	A	591	GLN
1	A	606	HIS

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Mol	Chain	Res	Type
1	A	610	GLN
1	A	614	GLN
2	B	395	GLN
2	B	478	HIS
2	B	515	ASN
2	B	683	GLN
2	B	727	GLN
2	B	780	ASN
2	B	917	ASN
2	B	959	ASN
2	B	967	GLN
2	B	1002	GLN
2	B	1007	GLN
3	C	36	GLN
3	C	99	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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, 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	708/764 (92%)	0.58	36 (5%) 33 33	38, 69, 112, 158	0
2	B	729/748 (97%)	0.36	36 (4%) 35 34	32, 58, 102, 140	0
3	C	135/157 (85%)	0.75	10 (7%) 20 19	53, 88, 136, 155	0
4	D	3/5 (60%)	3.90	3 (100%) 0 0	140, 140, 141, 143	0
All	All	1575/1674 (94%)	0.50	85 (5%) 31 31	32, 65, 114, 158	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	959	ASN	6.1
2	B	1055	ILE	5.1
3	C	1	MET	4.7
1	A	747	VAL	4.7
1	A	746	ASP	4.7
4	D	356	SER	4.5
4	D	357	LEU	4.4
3	C	127	ILE	4.4
1	A	49	PRO	4.0
2	B	1048	PHE	4.0
1	A	431	PRO	3.9
2	B	888	PRO	3.9
2	B	961	SER	3.6
1	A	430	GLY	3.6
1	A	65	THR	3.5
2	B	1019	GLN	3.4
2	B	958	LEU	3.3
1	A	701	PRO	3.2
3	C	2	VAL	3.2
3	C	148	ILE	3.1
2	B	1047	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	960	ILE	3.1
2	B	445	LEU	3.1
1	A	51	LEU	3.0
1	A	700	PHE	3.0
1	A	180	CYS	3.0
2	B	1056	ALA	3.0
2	B	1061	MET	2.9
1	A	53	PRO	2.9
1	A	592	VAL	2.9
4	D	358	LEU	2.8
2	B	446	ASP	2.8
1	A	205	GLY	2.7
1	A	105	ASN	2.7
1	A	34	MET	2.7
1	A	31	ALA	2.7
2	B	1022	THR	2.6
1	A	94	PHE	2.6
3	C	30	LEU	2.5
1	A	35	VAL	2.5
1	A	225	PRO	2.5
2	B	882	VAL	2.5
1	A	61	CYS	2.5
2	B	347	GLY	2.4
2	B	694	GLY	2.4
1	A	674	ASP	2.4
2	B	1054	VAL	2.4
1	A	698	SER	2.4
1	A	104	LEU	2.4
3	C	4	LEU	2.4
1	A	64	THR	2.3
2	B	418	VAL	2.3
1	A	559	GLU	2.3
2	B	1063	ALA	2.3
3	C	56	ALA	2.3
2	B	427	THR	2.3
2	B	354	LEU	2.3
2	B	1020	PRO	2.3
2	B	881	SER	2.3
2	B	464	GLU	2.3
2	B	865	ASP	2.2
2	B	381	CYS	2.2
1	A	93	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	544	ARG	2.2
1	A	548	ARG	2.2
1	A	670	SER	2.2
2	B	1064	ASN	2.1
2	B	771	THR	2.1
1	A	695	ILE	2.1
2	B	610	LEU	2.1
2	B	1057	ASP	2.1
1	A	628	PHE	2.1
3	C	83	LEU	2.1
3	C	23	ASP	2.1
2	B	1060	PRO	2.1
3	C	20	MET	2.1
2	B	557	GLY	2.1
1	A	535	GLU	2.1
1	A	510	ILE	2.1
2	B	662	LYS	2.1
2	B	348	LEU	2.0
1	A	394	MET	2.0
2	B	424	THR	2.0
1	A	678	TYR	2.0
1	A	697	HIS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	ZN	B	1101	1/1	0.90	0.14	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	A	801	1/1	0.98	0.05	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.