



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:03 AM UTC

PDB ID : 5DFZ / pdb_00005dfz
Title : Structure of Vps34 complex II from *S. cerevisiae*.
Authors : Rostislavleva, K.; Soler, N.; Ohashi, Y.; Zhang, L.; Williams, R.L.
Deposited on : 2015-08-27
Resolution : 4.40 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

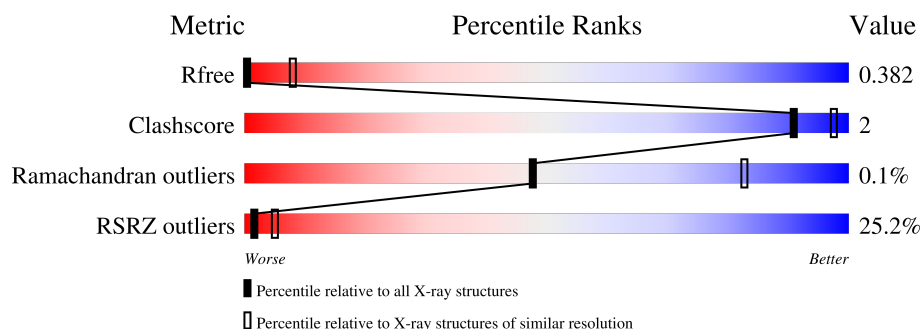
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

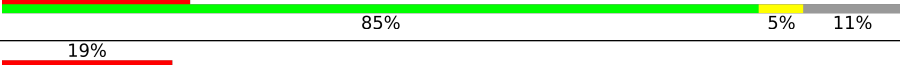
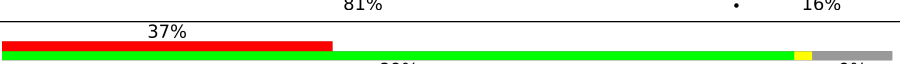
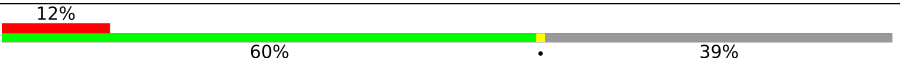
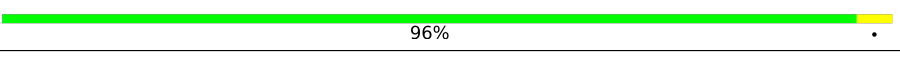
The reported resolution of this entry is 4.40 Å.

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	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	441	
2	C	875	
3	B	1460	
4	E	124	
5	D	559	
6	G	49	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14160 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 Vacuolar protein sorting-associated protein 38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	0	0	0
			1700	1014	343	343			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	GLY	-	expression tag	UNP Q05919
A	441	SER	-	expression tag	UNP Q05919

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase VPS34.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	783	Total	C	N	O	30	0	0
			3888	2322	783	783			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	SER	conflict	UNP P22543
C	241	GLY	ASP	conflict	UNP P22543

- Molecule 3 is a protein called Serine/threonine-protein kinase VPS15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	1224	Total	C	N	O	0	0	0
			6079	3631	1224	1224			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P22219

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	MET	deletion	UNP P22219
B	?	-	ASP	deletion	UNP P22219
B	?	-	ASN	deletion	UNP P22219
B	?	-	ASN	deletion	UNP P22219
B	?	-	THR	deletion	UNP P22219
B	?	-	GLU	deletion	UNP P22219
B	?	-	ILE	deletion	UNP P22219
B	?	-	MET	deletion	UNP P22219
B	?	-	GLU	deletion	UNP P22219
B	1455	GLY	-	expression tag	UNP P22219
B	1456	SER	-	expression tag	UNP P22219
B	1457	SER	-	expression tag	UNP P22219
B	1458	ARG	-	expression tag	UNP P22219
B	1459	PRO	-	expression tag	UNP P22219
B	1460	THR	-	expression tag	UNP P22219
B	1461	THR	-	expression tag	UNP P22219
B	1462	ALA	-	expression tag	UNP P22219
B	1463	SER	-	expression tag	UNP P22219
B	1464	GLU	-	expression tag	UNP P22219
B	1465	ASN	-	expression tag	UNP P22219
B	1466	LEU	-	expression tag	UNP P22219
B	1467	TYR	-	expression tag	UNP P22219
B	1468	PHE	-	expression tag	UNP P22219
B	1469	GLN	-	expression tag	UNP P22219
B	1470	GLY	-	expression tag	UNP P22219

- Molecule 4 is a protein called Nanobody binding *S. cerevisiae* Vps34.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	113	Total	C	N	O	0	0	0
			552	326	113	113			

- Molecule 5 is a protein called Vacuolar protein sorting-associated protein 30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	341	Total	C	N	O	0	0	0
			1696	1014	341	341			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	77	ILE	LYS	conflict	UNP Q02948

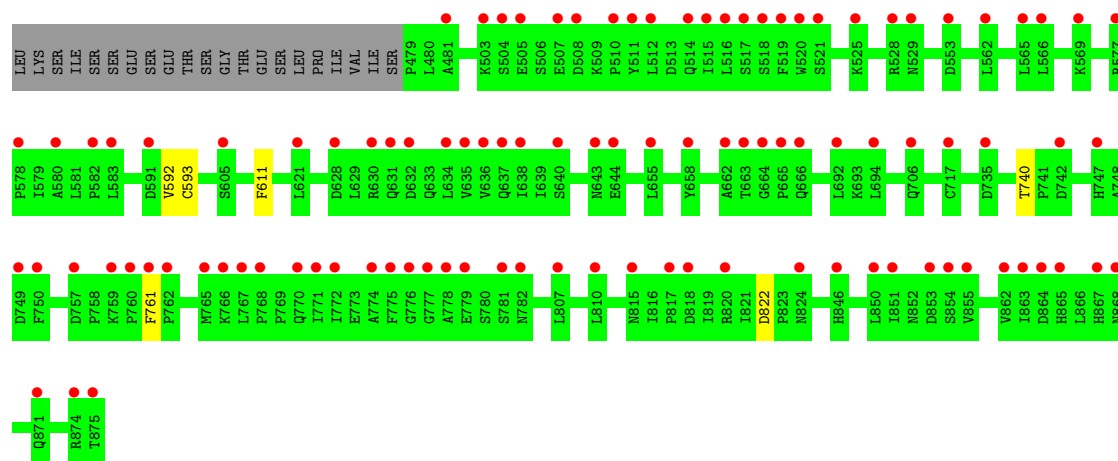
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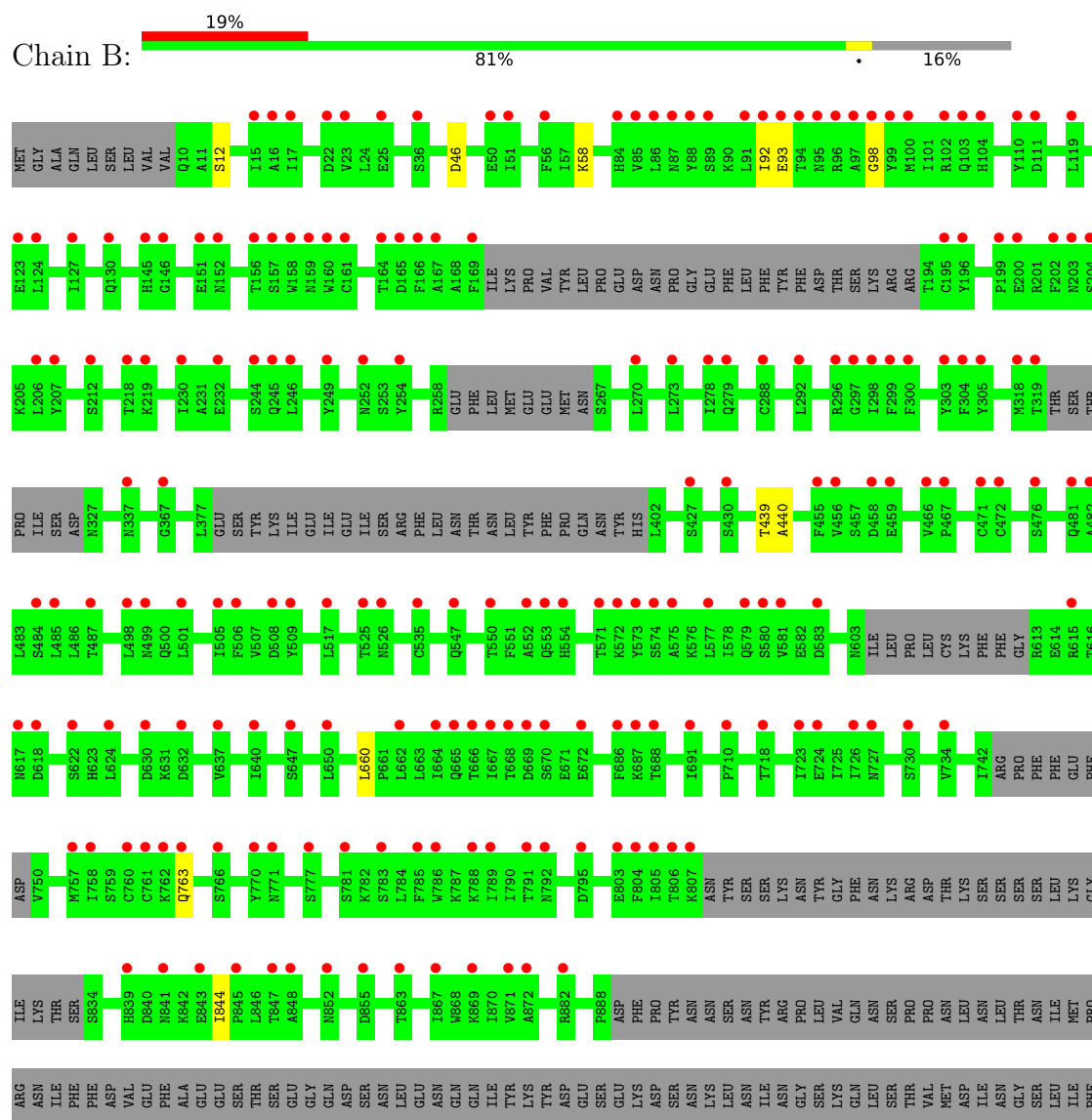
Chain	Residue	Modelled	Actual	Comment	Reference
D	467	ALA	THR	conflict	UNP Q02948
D	549	HIS	TYR	conflict	UNP Q02948
D	558	GLY	-	expression tag	UNP Q02948
D	559	SER	-	expression tag	UNP Q02948

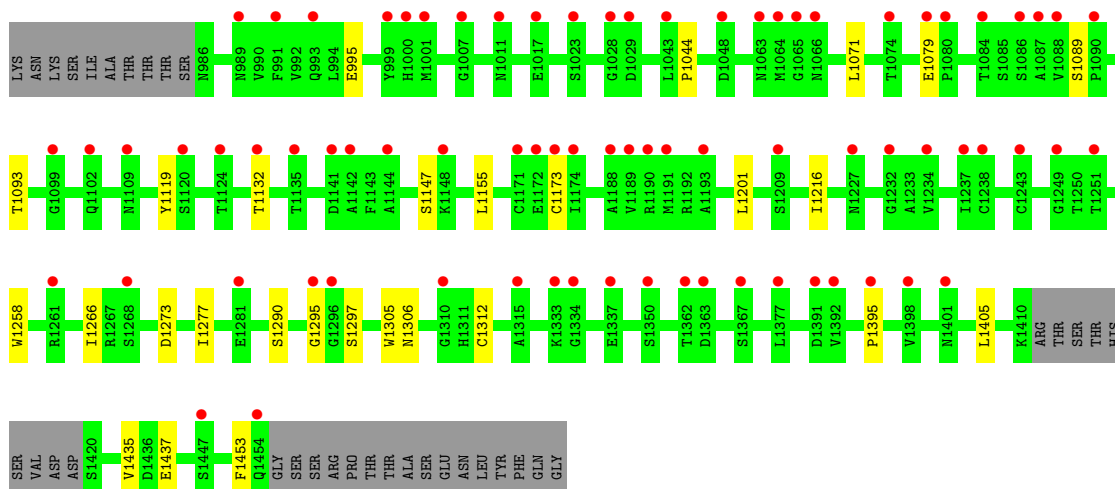
- Molecule 6 is a protein called Putative N-terminal domain of *S. cerevisiae* Vps30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	49	Total	C	N	O	0	0	0
			245	147	49	49			

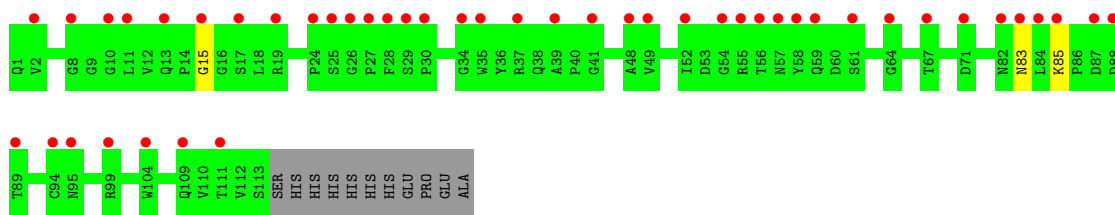


• Molecule 3: Serine/threonine-protein kinase VPS15

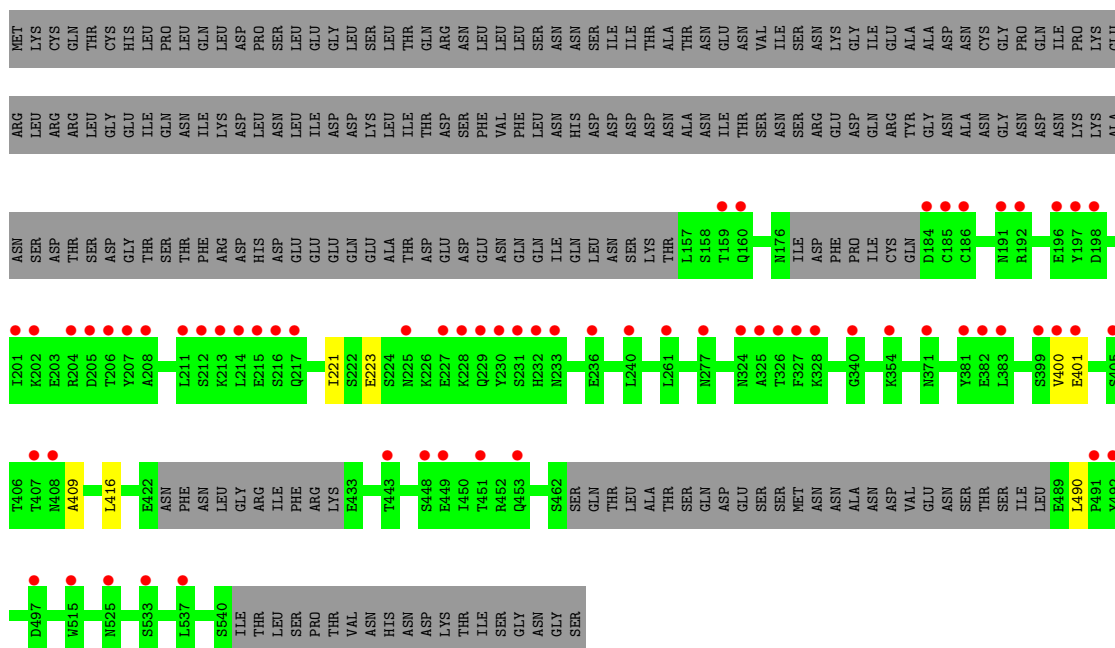




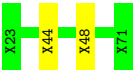
- Molecule 4: Nanobody binding *S. cerevisiae* Vps34



- Molecule 5: Vacuolar protein sorting-associated protein 30



- Molecule 6: Putative N-terminal domain of *S. cerevisiae* Vps30



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	215.18Å 226.84Å 127.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.36 – 4.40 50.36 – 4.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.36-4.40) 99.9 (50.36-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.31	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.368 , 0.376 0.372 , 0.382	Depositor DCC
R_{free} test set	2043 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	254.5	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	14160	wwPDB-VP
Average B, all atoms (Å ²)	258.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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](#)

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	0.29	0/1696	0.99	4/2359 (0.2%)
2	C	0.33	0/3885	1.15	32/5418 (0.6%)
3	B	0.30	0/6069	0.95	25/8456 (0.3%)
4	E	0.30	0/551	0.90	2/762 (0.3%)
5	D	0.30	0/1692	0.92	9/2357 (0.4%)
All	All	0.31	0/13893	1.01	72/19352 (0.4%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ALA	CA-C-N	15.92	135.91	120.31
1	A	139	ALA	C-N-CA	15.92	135.91	120.31
2	C	822	ASP	CA-C-N	11.43	134.13	119.84
2	C	822	ASP	C-N-CA	11.43	134.13	119.84
2	C	120	ILE	CA-C-N	-10.55	109.70	120.98
2	C	120	ILE	C-N-CA	-10.55	109.70	120.98
2	C	40	ASN	CA-C-N	10.50	130.11	119.82
2	C	40	ASN	C-N-CA	10.50	130.11	119.82
2	C	16	VAL	CA-C-N	9.90	130.64	120.14
2	C	16	VAL	C-N-CA	9.90	130.64	120.14
3	B	1079	GLU	CA-C-N	9.32	128.93	119.24
3	B	1079	GLU	C-N-CA	9.32	128.93	119.24
2	C	740	THR	CA-C-N	8.95	128.69	119.56
2	C	740	THR	C-N-CA	8.95	128.69	119.56
2	C	275	ASP	CA-C-N	8.80	129.23	120.52
2	C	275	ASP	C-N-CA	8.80	129.23	120.52
2	C	177	LEU	CA-C-N	8.09	127.67	118.85
2	C	177	LEU	C-N-CA	8.09	127.67	118.85
2	C	77	THR	CA-C-N	7.65	129.40	119.84
2	C	77	THR	C-N-CA	7.65	129.40	119.84
5	D	416	LEU	CA-C-N	7.54	127.97	119.83
5	D	416	LEU	C-N-CA	7.54	127.97	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	440	ALA	N-CA-C	-7.33	103.60	112.54
3	B	46	ASP	CA-C-N	7.16	128.79	119.84
3	B	46	ASP	C-N-CA	7.16	128.79	119.84
5	D	223	GLU	N-CA-C	-6.99	104.38	113.12
5	D	401	GLU	N-CA-C	-6.95	104.95	113.50
2	C	51	PHE	CA-C-N	6.95	127.51	120.14
2	C	51	PHE	C-N-CA	6.95	127.51	120.14
3	B	1044	PRO	CA-C-N	6.88	126.49	119.19
3	B	1044	PRO	C-N-CA	6.88	126.49	119.19
2	C	313	TYR	CA-C-N	6.81	124.63	119.66
2	C	313	TYR	C-N-CA	6.81	124.63	119.66
2	C	761	PHE	CA-C-N	6.76	127.35	120.38
2	C	761	PHE	C-N-CA	6.76	127.35	120.38
3	B	844	ILE	CA-C-N	6.43	126.05	119.56
3	B	844	ILE	C-N-CA	6.43	126.05	119.56
2	C	115	ASN	N-CA-C	6.33	120.88	111.96
3	B	12	SER	CA-C-N	6.32	126.51	120.31
3	B	12	SER	C-N-CA	6.32	126.51	120.31
2	C	298	LYS	CA-C-N	6.25	126.44	120.31
2	C	298	LYS	C-N-CA	6.25	126.44	120.31
3	B	58	LYS	CA-C-N	6.11	125.73	119.56
3	B	58	LYS	C-N-CA	6.11	125.73	119.56
5	D	409	ALA	CA-C-N	6.09	126.06	119.78
5	D	409	ALA	C-N-CA	6.09	126.06	119.78
2	C	593	CYS	CA-C-N	6.04	125.75	119.05
2	C	593	CYS	C-N-CA	6.04	125.75	119.05
3	B	1119	TYR	N-CA-C	6.03	119.59	107.41
5	D	490	LEU	CA-C-N	6.03	125.65	119.56
5	D	490	LEU	C-N-CA	6.03	125.65	119.56
4	E	85	LYS	CA-C-N	6.02	125.74	119.05
4	E	85	LYS	C-N-CA	6.02	125.74	119.05
1	A	382	LEU	CA-C-N	6.02	126.18	119.32
1	A	382	LEU	C-N-CA	6.02	126.18	119.32
3	B	995	GLU	CA-C-N	5.92	126.38	119.99
3	B	995	GLU	C-N-CA	5.92	126.38	119.99
2	C	213	LEU	CA-C-N	-5.82	114.62	120.21
2	C	213	LEU	C-N-CA	-5.82	114.62	120.21
3	B	92	ILE	N-CA-C	5.70	115.85	107.75
2	C	822	ASP	N-CA-C	-5.68	105.86	113.25
5	D	400	VAL	CB-CA-C	-5.64	102.03	111.29
3	B	763	GLN	CA-C-N	5.58	124.93	118.85
3	B	763	GLN	C-N-CA	5.58	124.93	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1093	THR	CA-C-N	5.53	125.54	119.90
3	B	1093	THR	C-N-CA	5.53	125.54	119.90
3	B	1089	SER	CA-C-N	5.29	125.27	120.03
3	B	1089	SER	C-N-CA	5.29	125.27	120.03
2	C	314	PRO	CA-C-N	5.26	124.89	119.05
2	C	314	PRO	C-N-CA	5.26	124.89	119.05
3	B	660	LEU	CA-C-N	5.09	124.70	119.56
3	B	660	LEU	C-N-CA	5.09	124.70	119.56

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	1700	0	720	6	0
2	C	3888	0	1633	15	0
3	B	6079	0	2576	13	0
4	E	552	0	253	1	0
5	D	1696	0	715	0	0
6	G	245	0	53	1	0
All	All	14160	0	5950	35	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 2.

All (35) 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:C:130:PHE:HA	2:C:136:THR:HA	1.68	0.74
2:C:6:ILE:HA	2:C:212:GLU:HA	1.68	0.73
2:C:65:LYS:H	2:C:105:SER:HA	1.60	0.66
2:C:23:LYS:HA	2:C:89:ASP:H	1.60	0.64
2:C:140:GLY:HA2	2:C:209:PRO:HA	1.83	0.61
2:C:115:ASN:H	2:C:120:ILE:HA	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:SER:HA	2:C:115:ASN:HA	1.86	0.57
2:C:592:VAL:HA	2:C:611:PHE:HA	1.87	0.56
2:C:25:LEU:HA	2:C:204:LEU:HA	1.88	0.55
3:B:1277:ILE:HA	3:B:1295:GLY:HA3	1.89	0.55
3:B:1290:SER:HA	3:B:1306:ASN:HA	1.88	0.55
3:B:1071:LEU:HA	3:B:1453:PHE:HA	1.89	0.54
3:B:1132:THR:H	3:B:1147:SER:HA	1.73	0.54
3:B:1258:TRP:HA	3:B:1266:ILE:H	1.72	0.53
4:E:15:GLY:HA2	4:E:83:ASN:HA	1.91	0.53
3:B:1305:TRP:HA	3:B:1312:CYS:HA	1.90	0.53
1:A:32:LEU:HA	1:A:66:ARG:HA	1.91	0.52
2:C:45:LEU:O	2:C:49:ASN:N	2.33	0.52
1:A:131:THR:HA	1:A:147:GLY:HA2	1.93	0.51
3:B:1155:LEU:HA	3:B:1173:CYS:HA	1.94	0.49
3:B:1395:PRO:HA	3:B:1405:LEU:HA	1.96	0.47
1:A:28:GLY:HA3	1:A:70:PHE:HA	1.96	0.47
1:A:22:SER:HA	1:A:150:THR:HA	1.98	0.45
2:C:17:PRO:HA	2:C:97:ARG:HA	1.98	0.45
2:C:11:SER:CB	2:C:217:PHE:H	2.30	0.45
2:C:219:GLU:H	3:B:439:THR:CB	2.30	0.44
2:C:141:PHE:HA	2:C:207:GLU:HA	2.00	0.44
1:A:26:ALA:HA	1:A:146:ASP:HA	1.99	0.43
3:B:1201:LEU:HA	3:B:1216:ILE:H	1.84	0.42
2:C:65:LYS:HA	2:C:104:SER:C	2.45	0.41
3:B:1273:ASP:H	3:B:1297:SER:HA	1.86	0.41
3:B:1435:VAL:C	3:B:1437:GLU:H	2.28	0.41
6:G:44:UNK:HA	6:G:48:UNK:HA	2.03	0.41
1:A:395:ILE:C	1:A:397:SER:H	2.28	0.41
3:B:93:GLU:HA	3:B:98:GLY:HA2	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	335/441 (76%)	311 (93%)	24 (7%)	0	100	100
2	C	777/875 (89%)	720 (93%)	56 (7%)	1 (0%)	48	83
3	B	1204/1460 (82%)	1109 (92%)	95 (8%)	0	100	100
4	E	111/124 (90%)	107 (96%)	4 (4%)	0	100	100
5	D	333/559 (60%)	317 (95%)	15 (4%)	1 (0%)	36	71
All	All	2760/3459 (80%)	2564 (93%)	194 (7%)	2 (0%)	48	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	29	LYS
5	D	221	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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, 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	343/441 (77%)	2.02	132 (38%)  	144, 275, 387, 469	0
2	C	777/875 (88%)	1.31	183 (23%)  	19, 256, 386, 550	14 (1%)
3	B	1224/1460 (83%)	1.30	278 (22%)  	135, 227, 330, 441	0
4	E	113/124 (91%)	1.86	46 (40%)  	210, 305, 385, 407	0
5	D	341/559 (61%)	1.14	65 (19%)  	143, 247, 439, 499	0
6	G	0/49	-	-	-	-
All	All	2798/3508 (79%)	1.40	704 (25%)  	19, 246, 380, 550	14 (0%)

All (704) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	97	ALA	18.6
3	B	94	THR	14.1
3	B	104	HIS	12.7
3	B	103	GLN	12.5
1	A	20	ASN	12.2
1	A	79	ALA	12.0
3	B	218	THR	12.0
3	B	93	GLU	11.9
3	B	96	ARG	11.4
1	A	66	ARG	11.2
1	A	80	SER	11.0
5	D	229	GLN	10.4
2	C	517	SER	10.2
3	B	95	ASN	10.0
1	A	81	THR	9.9
1	A	214	SER	9.7
3	B	89	SER	9.7
2	C	867	HIS	9.6
2	C	292	ASN	9.4

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Mol	Chain	Res	Type	RSRZ
3	B	1080	PRO	9.2
3	B	993	GLN	9.2
3	B	146	GLY	9.0
3	B	806	THR	8.8
3	B	1189	VAL	8.7
2	C	777	GLY	8.7
1	A	85	LEU	8.5
3	B	575	ALA	8.3
1	A	120	ASP	8.3
1	A	215	LEU	8.3
5	D	400	VAL	8.1
1	A	64	SER	8.0
1	A	77	THR	8.0
3	B	499	ASN	8.0
2	C	423	SER	7.8
1	A	111	TRP	7.7
1	A	62	SER	7.4
2	C	578	PRO	7.3
2	C	516	LEU	7.3
2	C	772	ILE	7.3
2	C	818	ASP	7.1
2	C	5	ASN	7.0
1	A	67	LYS	7.0
1	A	22	SER	7.0
2	C	420	SER	6.8
3	B	786	TRP	6.8
5	D	231	SER	6.8
5	D	230	TYR	6.8
2	C	293	LEU	6.8
2	C	326	SER	6.7
2	C	863	ILE	6.6
1	A	33	ILE	6.6
2	C	875	THR	6.6
3	B	17	ILE	6.5
5	D	212	SER	6.4
3	B	553	GLN	6.4
4	E	94	CYS	6.4
1	A	119	ILE	6.3
1	A	116	THR	6.3
1	A	63	GLY	6.2
3	B	88	TYR	6.2
3	B	1087	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
2	C	504	SER	6.1
1	A	121	LEU	6.1
2	C	35	SER	6.1
5	D	216	SER	6.1
2	C	325	GLY	6.1
2	C	850	LEU	6.1
3	B	805	ILE	6.0
1	A	31	LYS	6.0
3	B	1173	CYS	6.0
2	C	515	ILE	6.0
1	A	389	TYR	5.9
1	A	25	ARG	5.8
2	C	394	ARG	5.8
5	D	228	LYS	5.8
1	A	29	ASP	5.7
1	A	78	GLY	5.7
3	B	199	PRO	5.7
2	C	630	ARG	5.6
2	C	340	ALA	5.6
2	C	776	GLY	5.5
1	A	65	LEU	5.5
1	A	126	PRO	5.4
2	C	632	ASP	5.4
4	E	49	VAL	5.4
3	B	36	SER	5.4
3	B	766	SER	5.3
3	B	305	TYR	5.3
5	D	215	GLU	5.3
2	C	577	ARG	5.3
2	C	6	ILE	5.3
3	B	637	VAL	5.2
1	A	48	GLU	5.2
1	A	260	HIS	5.2
2	C	359	VAL	5.2
4	E	29	SER	5.2
3	B	298	ILE	5.2
2	C	4	ASN	5.2
3	B	624	LEU	5.1
4	E	28	PHE	5.1
3	B	552	ALA	5.1
4	E	2	VAL	5.1
2	C	514	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
4	E	48	ALA	5.0
1	A	30	SER	5.0
2	C	521	SER	5.0
3	B	303	TYR	5.0
3	B	92	ILE	5.0
1	A	146	ASP	4.9
2	C	518	SER	4.9
3	B	687	LYS	4.9
1	A	261	SER	4.9
2	C	424	ASP	4.9
3	B	686	PHE	4.9
5	D	205	ASP	4.9
2	C	55	ASP	4.8
3	B	337	ASN	4.8
1	A	71	GLN	4.8
3	B	727	ASN	4.8
1	A	84	VAL	4.8
2	C	637	GLN	4.8
3	B	127	ILE	4.8
1	A	148	SER	4.8
3	B	872	ALA	4.8
1	A	138	ASN	4.8
3	B	1102	GLN	4.7
1	A	129	GLU	4.7
3	B	839	HIS	4.7
3	B	1132	THR	4.7
2	C	519	PHE	4.7
1	A	118	THR	4.7
3	B	297	GLY	4.6
1	A	61	GLN	4.6
1	A	213	LEU	4.6
1	A	26	ALA	4.6
1	A	82	MET	4.6
3	B	803	GLU	4.6
3	B	1088	VAL	4.6
3	B	618	ASP	4.6
3	B	804	PHE	4.6
2	C	428	SER	4.6
1	A	139	ALA	4.6
3	B	1144	ALA	4.6
1	A	43	CYS	4.5
3	B	579	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
3	B	785	PHE	4.5
2	C	665	PRO	4.5
5	D	324	ASN	4.5
3	B	145	HIS	4.5
5	D	381	TYR	4.5
3	B	99	TYR	4.5
3	B	124	LEU	4.5
5	D	233	ASN	4.5
3	B	1295	GLY	4.5
1	A	290	ASP	4.5
3	B	1188	ALA	4.4
3	B	789	ILE	4.4
2	C	768	PRO	4.4
2	C	761	PHE	4.4
4	E	58	TYR	4.4
2	C	767	LEU	4.4
4	E	87	ASP	4.4
3	B	640	ILE	4.4
2	C	393	ASN	4.4
3	B	102	ARG	4.3
3	B	98	GLY	4.3
1	A	115	CYS	4.3
3	B	1084	THR	4.3
3	B	123	GLU	4.3
4	E	10	GLY	4.3
4	E	26	GLY	4.3
3	B	991	PHE	4.3
5	D	497	ASP	4.3
5	D	232	HIS	4.3
2	C	274	ASN	4.3
2	C	562	LEU	4.2
1	A	75	LYS	4.2
3	B	1011	ASN	4.2
4	E	95	ASN	4.2
4	E	61	SER	4.2
1	A	216	LYS	4.2
1	A	69	SER	4.2
1	A	34	LYS	4.2
5	D	202	LYS	4.2
2	C	566	LEU	4.1
3	B	50	GLU	4.1
3	B	574	SER	4.1

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Mol	Chain	Res	Type	RSRZ
5	D	453	GLN	4.1
5	D	159	THR	4.1
4	E	88	ASP	4.1
2	C	275	ASP	4.1
3	B	577	LEU	4.0
1	A	114	LEU	4.0
5	D	533	SER	4.0
3	B	791	THR	4.0
2	C	342	THR	4.0
3	B	164	THR	4.0
2	C	569	LYS	4.0
2	C	421	THR	4.0
1	A	70	PHE	4.0
3	B	1337	GLU	4.0
3	B	1048	ASP	4.0
2	C	643	ASN	4.0
1	A	393	SER	4.0
2	C	846	HIS	4.0
1	A	112	CYS	3.9
3	B	245	GLN	3.9
3	B	22	ASP	3.9
3	B	665	GLN	3.9
3	B	151	GLU	3.9
3	B	498	LEU	3.9
3	B	1190	ARG	3.9
5	D	515	TRP	3.8
3	B	246	LEU	3.8
2	C	396	LYS	3.8
3	B	1395	PRO	3.8
4	E	27	PRO	3.8
2	C	510	PRO	3.8
2	C	628	ASP	3.8
3	B	244	SER	3.8
2	C	391	ALA	3.8
2	C	747	HIS	3.8
3	B	845	PRO	3.8
3	B	688	THR	3.8
3	B	482	ALA	3.8
1	A	27	ASN	3.7
2	C	38	ILE	3.7
1	A	130	ASP	3.7
1	A	76	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
5	D	492	TYR	3.7
5	D	211	LEU	3.7
1	A	217	ASN	3.7
3	B	724	GLU	3.7
4	E	17	SER	3.6
3	B	723	ILE	3.6
1	A	24	PHE	3.6
2	C	528	ARG	3.6
3	B	1066	ASN	3.6
3	B	119	LEU	3.6
3	B	795	ASP	3.6
2	C	640	SER	3.6
3	B	204	SER	3.6
5	D	326	THR	3.6
3	B	278	ILE	3.6
3	B	1296	GLY	3.6
4	E	83	ASN	3.5
3	B	1249	GLY	3.5
1	A	143	ASP	3.5
2	C	762	PRO	3.5
3	B	525	THR	3.5
4	E	56	THR	3.5
5	D	225	ASN	3.5
2	C	407	LEU	3.5
2	C	338	LYS	3.5
3	B	670	SER	3.5
4	E	57	ASN	3.5
2	C	216	VAL	3.5
1	A	144	LEU	3.5
3	B	252	ASN	3.5
1	A	21	ILE	3.5
3	B	726	ILE	3.5
2	C	360	LEU	3.5
2	C	864	ASP	3.5
2	C	422	PHE	3.4
2	C	343	LYS	3.4
2	C	778	ALA	3.4
2	C	782	ASN	3.4
1	A	400	PRO	3.4
5	D	451	THR	3.4
3	B	807	LYS	3.4
2	C	41	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	334	LEU	3.4
3	B	279	GLN	3.4
2	C	79	TYR	3.4
2	C	397	LYS	3.4
1	A	58	SER	3.4
3	B	1447	SER	3.4
2	C	175	THR	3.4
3	B	788	LYS	3.4
3	B	630	ASP	3.4
3	B	1310	GLY	3.4
3	B	1334	GLY	3.4
1	A	83	ILE	3.4
3	B	249	TYR	3.3
1	A	267	LEU	3.3
3	B	1227	ASN	3.3
4	E	11	LEU	3.3
3	B	550	THR	3.3
5	D	443	THR	3.3
2	C	427	ASN	3.3
5	D	371	ASN	3.3
5	D	449	GLU	3.3
1	A	390	GLY	3.3
3	B	777	SER	3.3
3	B	554	HIS	3.3
3	B	783	SER	3.3
3	B	165	ASP	3.2
3	B	763	GLN	3.2
4	E	104	TRP	3.2
3	B	1000	HIS	3.2
2	C	706	GLN	3.2
2	C	508	ASP	3.2
3	B	157	SER	3.2
1	A	87	LEU	3.2
2	C	188	LEU	3.2
3	B	318	MET	3.2
1	A	376	GLN	3.2
3	B	573	TYR	3.2
1	A	89	GLY	3.1
3	B	1174	ILE	3.1
3	B	1238	CYS	3.1
3	B	1029	ASP	3.1
3	B	1172	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	125	GLN	3.1
5	D	214	LEU	3.1
3	B	156	THR	3.1
2	C	37	LYS	3.1
2	C	413	ALA	3.1
2	C	694	LEU	3.1
5	D	186	CYS	3.1
5	D	206	THR	3.1
1	A	68	LEU	3.1
3	B	615	ARG	3.1
2	C	117	SER	3.1
2	C	855	VAL	3.1
3	B	1392	VAL	3.0
2	C	431	THR	3.0
1	A	359	VAL	3.0
2	C	759	LYS	3.0
3	B	1333	LYS	3.0
4	E	99	ARG	3.0
1	A	378	PHE	3.0
5	D	448	SER	3.0
1	A	145	ILE	3.0
5	D	191	ASN	3.0
3	B	130	GLN	3.0
2	C	582	PRO	3.0
2	C	520	TRP	3.0
2	C	211	LEU	3.0
3	B	668	THR	3.0
2	C	760	PRO	3.0
3	B	1099	GLY	3.0
3	B	841	ASN	3.0
3	B	200	GLU	3.0
3	B	160	TRP	2.9
1	A	405	ASP	2.9
5	D	382	GLU	2.9
2	C	717	CYS	2.9
4	E	41	GLY	2.9
1	A	117	TYR	2.9
4	E	24	PRO	2.9
3	B	459	GLU	2.9
3	B	1148	LYS	2.9
2	C	775	PHE	2.9
3	B	110	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	553	ASP	2.9
4	E	84	LEU	2.9
2	C	765	MET	2.9
3	B	843	GLU	2.9
3	B	869	LYS	2.9
3	B	319	THR	2.9
3	B	1350	SER	2.9
5	D	208	ALA	2.9
3	B	304	PHE	2.9
5	D	185	CYS	2.9
2	C	505	GLU	2.9
3	B	1017	GLU	2.9
4	E	109	GLN	2.9
2	C	512	LEU	2.9
2	C	357	VAL	2.9
2	C	817	PRO	2.9
2	C	631	GLN	2.9
1	A	36	TYR	2.8
1	A	137	THR	2.8
2	C	7	THR	2.8
5	D	213	LYS	2.8
2	C	810	LEU	2.8
5	D	401	GLU	2.8
2	C	392	VAL	2.8
1	A	392	THR	2.8
4	E	25	SER	2.8
1	A	264	GLU	2.8
1	A	384	TYR	2.8
2	C	291	ALA	2.8
3	B	852	ASN	2.8
3	B	202	PHE	2.8
3	B	299	PHE	2.8
4	E	111	THR	2.8
3	B	672	GLU	2.8
3	B	867	ILE	2.8
3	B	1086	SER	2.8
5	D	197	TYR	2.8
2	C	339	LYS	2.8
2	C	368	GLU	2.8
3	B	622	SER	2.8
3	B	1023	SER	2.8
2	C	330	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	511	TYR	2.8
2	C	735	ASP	2.8
1	A	122	ASN	2.8
3	B	989	ASN	2.8
2	C	404	GLU	2.8
2	C	871	GLN	2.8
3	B	1074	THR	2.8
5	D	236	GLU	2.8
2	C	433	VAL	2.7
3	B	288	CYS	2.7
1	A	427	LEU	2.7
2	C	658	TYR	2.7
3	B	427	SER	2.7
3	B	487	THR	2.7
5	D	327	PHE	2.7
3	B	669	ASP	2.7
3	B	1363	ASP	2.7
2	C	635	VAL	2.7
3	B	1243	CYS	2.7
1	A	32	LEU	2.7
3	B	16	ALA	2.7
3	B	1193	ALA	2.7
3	B	1209	SER	2.7
1	A	124	LEU	2.7
2	C	341	LEU	2.7
3	B	86	LEU	2.7
3	B	1065	GLY	2.7
1	A	383	PRO	2.7
3	B	476	SER	2.7
3	B	508	ASP	2.7
5	D	277	ASN	2.7
5	D	408	ASN	2.7
2	C	398	ALA	2.7
3	B	232	GLU	2.7
4	E	67	THR	2.7
2	C	662	ALA	2.7
2	C	815	ASN	2.7
3	B	666	THR	2.7
3	B	730	SER	2.7
2	C	771	ILE	2.7
2	C	16	VAL	2.7
4	E	13	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	664	GLY	2.7
5	D	399	SER	2.7
1	A	388	TYR	2.6
3	B	1237	ILE	2.6
3	B	152	ASN	2.6
3	B	1191	MET	2.6
1	A	52	GLY	2.6
5	D	405	SER	2.6
3	B	650	LEU	2.6
2	C	663	THR	2.6
3	B	760	CYS	2.6
3	B	1234	VAL	2.6
3	B	757	MET	2.6
3	B	203	ASN	2.6
1	A	377	ILE	2.6
3	B	571	THR	2.6
3	B	1124	THR	2.6
3	B	547	GLN	2.6
3	B	219	LYS	2.6
2	C	634	LEU	2.6
2	C	666	GLN	2.6
2	C	583	LEU	2.6
2	C	636	VAL	2.6
3	B	292	LEU	2.6
1	A	404	THR	2.6
1	A	266	SER	2.6
2	C	218	ILE	2.6
3	B	467	PRO	2.6
2	C	91	TRP	2.5
3	B	23	VAL	2.5
4	E	37	ARG	2.5
5	D	325	ALA	2.5
2	C	529	ASN	2.5
5	D	328	LYS	2.5
5	D	407	THR	2.5
2	C	565	LEU	2.5
3	B	581	VAL	2.5
2	C	591	ASP	2.5
3	B	161	CYS	2.5
3	B	1171	CYS	2.5
5	D	207	TYR	2.5
3	B	758	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
5	D	217	GLN	2.5
1	A	59	GLU	2.5
3	B	300	PHE	2.5
1	A	381	PRO	2.5
1	A	360	ASN	2.5
4	E	8	GLY	2.5
4	E	19	ARG	2.5
3	B	718	THR	2.5
2	C	854	SER	2.5
4	E	85	LYS	2.5
2	C	395	LEU	2.5
3	B	517	LEU	2.5
3	B	632	ASP	2.5
5	D	340	GLY	2.5
3	B	472	CYS	2.5
3	B	848	ALA	2.5
3	B	484	SER	2.5
2	C	344	LEU	2.5
2	C	779	GLU	2.5
3	B	509	TYR	2.5
1	A	437	ARG	2.5
2	C	383	LYS	2.5
3	B	471	CYS	2.4
1	A	135	THR	2.4
3	B	662	LEU	2.4
2	C	327	ILE	2.4
2	C	749	ASP	2.4
3	B	583	ASP	2.4
3	B	87	ASN	2.4
3	B	617	ASN	2.4
5	D	525	ASN	2.4
1	A	265	LEU	2.4
3	B	1043	LEU	2.4
1	A	285	PHE	2.4
3	B	855	ASP	2.4
5	D	240	LEU	2.4
1	A	150	THR	2.4
2	C	331	ARG	2.4
3	B	1232	GLY	2.4
3	B	167	ALA	2.4
4	E	35	TRP	2.4
3	B	230	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	874	ARG	2.4
3	B	1261	ARG	2.4
3	B	1398	VAL	2.4
1	A	345	LEU	2.4
3	B	169	PHE	2.4
3	B	505	ILE	2.4
3	B	1109	ASN	2.4
1	A	140	PRO	2.4
3	B	273	LEU	2.4
5	D	184	ASP	2.4
2	C	655	LEU	2.4
3	B	501	LEU	2.4
2	C	208	PHE	2.4
3	B	455	PHE	2.4
3	B	158	TRP	2.4
3	B	999	TYR	2.4
3	B	84	HIS	2.4
1	A	147	GLY	2.3
3	B	1454	GLN	2.3
2	C	87	THR	2.3
2	C	367	ALA	2.3
3	B	506	PHE	2.3
2	C	851	ILE	2.3
3	B	647	SER	2.3
4	E	55	ARG	2.3
4	E	30	PRO	2.3
2	C	507	GLU	2.3
3	B	367	GLY	2.3
1	A	269	SER	2.3
2	C	365	SER	2.3
2	C	862	VAL	2.3
2	C	692	LEU	2.3
3	B	458	ASP	2.3
2	C	126	GLU	2.3
3	B	771	ASN	2.3
2	C	820	ARG	2.3
1	A	283	SER	2.3
3	B	206	LEU	2.3
3	B	430	SER	2.3
2	C	853	ASP	2.3
1	A	188	ASN	2.3
2	C	56	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	B	296	ARG	2.3
5	D	354	LYS	2.3
3	B	863	THR	2.3
3	B	91	LEU	2.3
3	B	535	CYS	2.3
3	B	762	LYS	2.3
3	B	882	ARG	2.3
2	C	750	PHE	2.3
3	B	572	LYS	2.3
3	B	1142	ALA	2.3
1	A	113	VAL	2.3
3	B	466	VAL	2.3
1	A	302	GLN	2.3
3	B	195	CYS	2.3
3	B	761	CYS	2.3
1	A	391	SER	2.3
4	E	54	GLY	2.3
1	A	47	LEU	2.3
2	C	580	ALA	2.3
2	C	766	LYS	2.3
3	B	485	LEU	2.3
3	B	871	VAL	2.3
2	C	742	ASP	2.3
1	A	45	PHE	2.2
1	A	403	PHE	2.2
1	A	263	THR	2.2
2	C	781	SER	2.2
1	A	382	LEU	2.2
2	C	39	LEU	2.2
3	B	1141	ASP	2.2
1	A	127	ILE	2.2
3	B	664	ILE	2.2
3	B	770	TYR	2.2
3	B	792	ASN	2.2
3	B	1401	ASN	2.2
3	B	1001	MET	2.2
2	C	865	HIS	2.2
1	A	256	ASP	2.2
5	D	198	ASP	2.2
3	B	691	ILE	2.2
2	C	525	LYS	2.2
1	A	54	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	774	ALA	2.2
5	D	192	ARG	2.2
5	D	491	PRO	2.2
1	A	420	HIS	2.2
1	A	46	ILE	2.2
1	A	151	LEU	2.2
3	B	207	TYR	2.2
3	B	1391	ASP	2.2
1	A	401	LEU	2.2
2	C	621	LEU	2.2
3	B	25	GLU	2.2
3	B	254	TYR	2.2
2	C	824	ASN	2.2
3	B	526	ASN	2.2
3	B	580	SER	2.2
3	B	781	SER	2.2
3	B	1268	SER	2.2
3	B	270	LEU	2.2
5	D	537	LEU	2.2
3	B	1079	GLU	2.2
2	C	387	VAL	2.2
4	E	39	ALA	2.2
1	A	131	THR	2.2
4	E	89	THR	2.2
3	B	1367	SER	2.2
1	A	38	ASP	2.1
2	C	294	ASP	2.1
1	A	422	PHE	2.1
2	C	378	LEU	2.1
2	C	503	LYS	2.1
3	B	1377	LEU	2.1
3	B	1251	THR	2.1
3	B	196	TYR	2.1
1	A	374	ALA	2.1
3	B	1007	GLY	2.1
3	B	1315	ALA	2.1
3	B	1090	PRO	2.1
2	C	807	LEU	2.1
3	B	51	ILE	2.1
3	B	667	ILE	2.1
3	B	1120	SER	2.1
5	D	204	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	E	59	GLN	2.1
1	A	199	GLU	2.1
3	B	1028	GLY	2.1
4	E	15	GLY	2.1
2	C	8	PHE	2.1
3	B	85	VAL	2.1
4	E	82	ASN	2.1
3	B	100	MET	2.1
3	B	1064	MET	2.1
2	C	409	GLN	2.1
2	C	644	GLU	2.1
3	B	1281	GLU	2.1
5	D	261	LEU	2.1
1	A	220	HIS	2.1
2	C	868	ASN	2.1
3	B	1135	THR	2.1
1	A	55	LEU	2.1
5	D	160	GLN	2.1
1	A	253	GLU	2.1
2	C	89	ASP	2.1
3	B	111	ASP	2.1
1	A	193	TYR	2.1
2	C	295	LYS	2.1
3	B	1362	THR	2.1
3	B	56	PHE	2.1
3	B	481	GLN	2.1
3	B	212	SER	2.1
2	C	17	PRO	2.1
2	C	605	SER	2.1
1	A	149	TYR	2.0
4	E	71	ASP	2.0
2	C	369	ILE	2.0
2	C	379	GLY	2.0
4	E	52	ILE	2.0
5	D	201	ILE	2.0
2	C	770	GLN	2.0
3	B	710	PRO	2.0
3	B	847	THR	2.0
5	D	227	GLU	2.0
1	A	307	PHE	2.0
2	C	638	ILE	2.0
3	B	15	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	B	166	PHE	2.0
4	E	34	GLY	2.0
4	E	64	GLY	2.0
2	C	77	THR	2.0
3	B	159	ASN	2.0
3	B	456	VAL	2.0
2	C	481	ALA	2.0
2	C	757	ASP	2.0
2	C	209	PRO	2.0
3	B	734	VAL	2.0
3	B	1063	ASN	2.0
5	D	196	GLU	2.0
5	D	383	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.