



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:09 PM UTC

PDB ID : 2W29 / pdb_00002w29
Title : Gly102Thr mutant of Rv3291c
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Deposited on : 2008-10-25
Resolution : 4.10 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

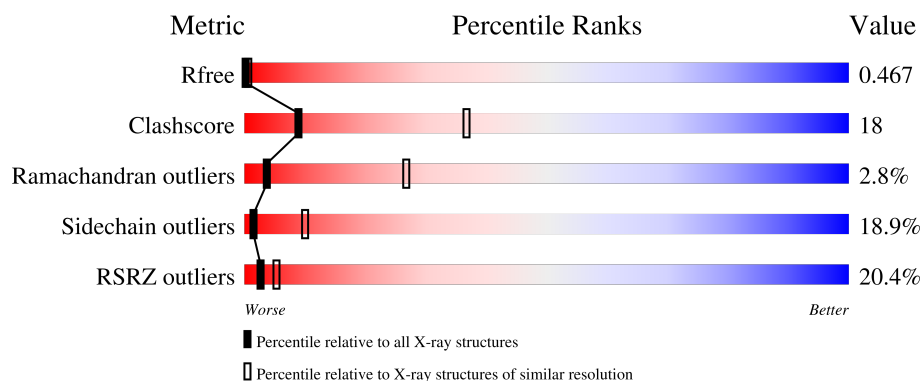
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	150	23% 64% 22% 9% ..
1	B	150	27% 59% 25% 12% ..
1	C	150	11% 61% 27% 7% ..
1	D	150	19% 55% 30% 10% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4488 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 PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1130	699	209	221	1			
1	B	147	Total	C	N	O	S	0	0	0
			1114	691	203	219	1			
1	C	147	Total	C	N	O	S	0	0	0
			1130	699	209	221	1			
1	D	147	Total	C	N	O	S	0	0	0
			1114	691	203	219	1			

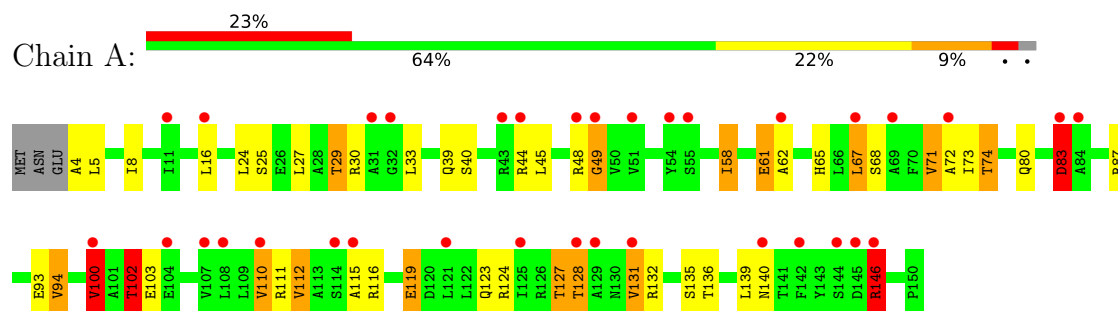
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	THR	GLY	engineered mutation	UNP P96896
B	102	THR	GLY	engineered mutation	UNP P96896
C	102	THR	GLY	engineered mutation	UNP P96896
D	102	THR	GLY	engineered mutation	UNP P96896

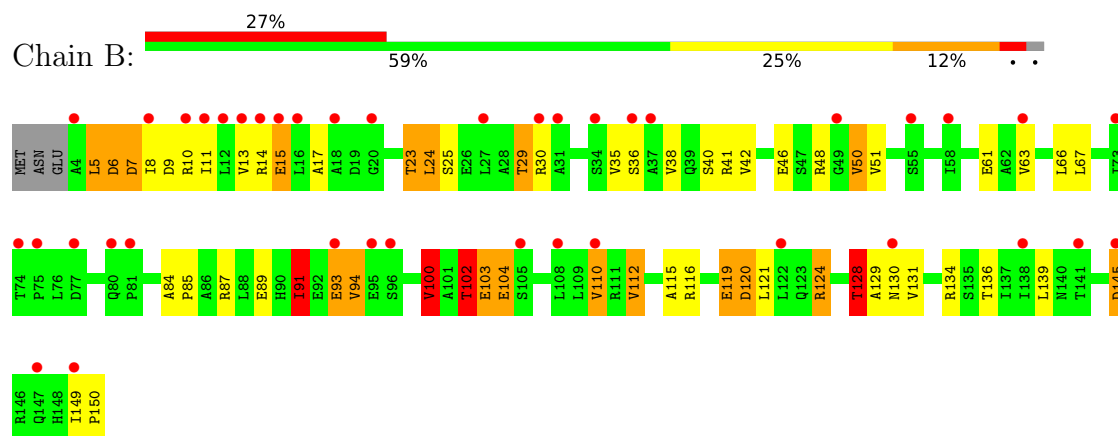
3 Residue-property plots [i](#)

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.

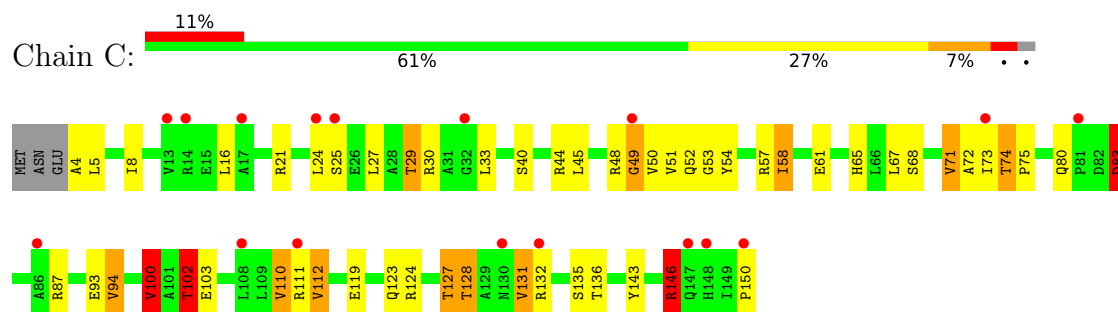
• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN



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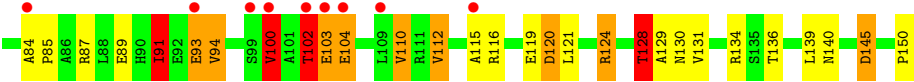
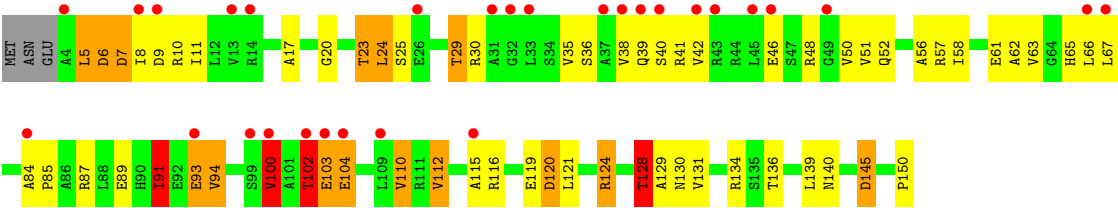


• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN



• Molecule 1: PROBABLE TRANSCRIPTIONAL REGULATORY PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.00Å 185.70Å 119.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.10 20.00 – 4.10	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-4.10) 93.6 (20.00-4.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.99Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.388 , (Not available) 0.466 , 0.467	Depositor DCC
R_{free} test set	337 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	110.1	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	4488	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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

5.1 Standard geometry

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	1.64	7/1144 (0.6%)	1.83	21/1557 (1.3%)
1	B	1.58	5/1128 (0.4%)	1.76	21/1538 (1.4%)
1	C	1.63	6/1144 (0.5%)	1.65	19/1557 (1.2%)
1	D	1.58	5/1128 (0.4%)	1.76	21/1538 (1.4%)
All	All	1.61	23/4544 (0.5%)	1.75	82/6190 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	THR	CA-CB	20.90	1.88	1.53
1	D	102	THR	CA-CB	19.99	1.87	1.53
1	B	102	THR	CA-CB	19.90	1.87	1.53
1	C	102	THR	CA-CB	19.30	1.86	1.53
1	B	91	ILE	CA-CB	6.35	1.60	1.53
1	D	91	ILE	CA-CB	6.18	1.60	1.53
1	A	73	ILE	C-O	6.00	1.30	1.24
1	C	73	ILE	C-O	6.00	1.30	1.24
1	D	130	ASN	N-CA	5.69	1.54	1.46
1	B	124	ARG	N-CA	-5.68	1.39	1.46
1	B	130	ASN	N-CA	5.67	1.54	1.46
1	D	124	ARG	N-CA	-5.64	1.39	1.46
1	A	123	GLN	N-CA	5.46	1.52	1.46
1	C	123	GLN	N-CA	5.44	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	SER	C-O	-5.20	1.17	1.23
1	B	94	VAL	CA-CB	5.19	1.58	1.53
1	C	135	SER	C-O	-5.19	1.17	1.23
1	D	94	VAL	CA-CB	5.18	1.58	1.53
1	C	72	ALA	CA-C	5.15	1.59	1.52
1	A	72	ALA	CA-C	5.14	1.59	1.52
1	A	132	ARG	CG-CD	5.11	1.67	1.52
1	C	132	ARG	CG-CD	5.11	1.67	1.52
1	A	39	GLN	C-O	-5.05	1.17	1.24

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	THR	CA-CB-OG1	26.67	149.61	109.60
1	A	102	THR	CA-CB-CG2	-22.24	72.69	110.50
1	B	102	THR	CB-CA-C	-14.98	80.62	110.42
1	D	102	THR	CB-CA-C	-14.97	80.63	110.42
1	C	102	THR	CB-CA-C	-14.84	80.88	110.42
1	B	129	ALA	CA-C-N	-14.65	100.85	123.12
1	B	129	ALA	C-N-CA	-14.65	100.85	123.12
1	D	129	ALA	CA-C-N	-14.59	100.95	123.12
1	D	129	ALA	C-N-CA	-14.59	100.95	123.12
1	D	102	THR	N-CA-CB	-13.29	88.03	110.49
1	B	102	THR	N-CA-CB	-13.26	88.08	110.49
1	C	102	THR	N-CA-CB	-12.68	89.07	110.49
1	D	91	ILE	CB-CA-C	12.31	124.53	111.23
1	B	91	ILE	CB-CA-C	12.20	124.41	111.23
1	A	102	THR	N-CA-CB	10.73	128.62	110.49
1	B	129	ALA	N-CA-C	-7.84	99.22	110.59
1	D	129	ALA	N-CA-C	-7.77	99.32	110.59
1	B	128	THR	N-CA-C	7.71	119.46	111.14
1	D	128	THR	N-CA-C	7.69	119.44	111.14
1	A	71	VAL	CB-CA-C	7.44	119.59	110.73
1	C	71	VAL	CB-CA-C	7.42	119.56	110.73
1	B	129	ALA	O-C-N	-7.24	114.21	122.68
1	D	129	ALA	O-C-N	-7.24	114.22	122.68
1	C	83	ASP	N-CA-CB	-7.12	99.28	110.46
1	A	83	ASP	N-CA-CB	-7.06	99.37	110.46
1	C	49	GLY	N-CA-C	7.00	122.37	114.67
1	A	49	GLY	N-CA-C	6.97	122.34	114.67
1	D	130	ASN	CB-CA-C	6.57	121.92	111.73
1	D	145	ASP	N-CA-C	6.57	120.23	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ASN	CB-CA-C	6.51	121.82	111.73
1	B	145	ASP	N-CA-C	6.49	120.13	111.30
1	A	110	VAL	N-CA-CB	-6.06	101.51	111.45
1	C	110	VAL	N-CA-CB	-6.06	101.51	111.45
1	B	50	VAL	N-CA-C	5.88	116.52	110.82
1	D	50	VAL	N-CA-C	5.83	116.48	110.82
1	A	127	THR	N-CA-C	5.70	118.70	111.69
1	C	127	THR	N-CA-C	5.70	118.70	111.69
1	C	131	VAL	N-CA-CB	-5.64	101.36	111.92
1	A	131	VAL	N-CA-CB	-5.64	101.38	111.92
1	A	146	ARG	CB-CA-C	5.62	120.69	111.41
1	B	100	VAL	N-CA-CB	-5.62	101.96	112.36
1	C	146	ARG	CB-CA-C	5.57	120.61	111.41
1	D	110	VAL	N-CA-CB	-5.57	102.31	111.44
1	D	100	VAL	N-CA-CB	-5.56	102.08	112.36
1	B	110	VAL	N-CA-CB	-5.54	102.36	111.44
1	A	112	VAL	CB-CA-C	5.48	120.34	110.48
1	A	58	ILE	N-CA-C	5.47	116.86	108.71
1	D	94	VAL	N-CA-CB	5.46	117.80	111.90
1	C	58	ILE	N-CA-C	5.45	116.83	108.71
1	C	100	VAL	CG1-CB-CG2	5.44	122.77	110.80
1	A	94	VAL	N-CA-C	5.44	116.19	107.98
1	B	94	VAL	N-CA-CB	5.43	117.77	111.90
1	A	100	VAL	CG1-CB-CG2	5.42	122.73	110.80
1	C	112	VAL	CB-CA-C	5.42	120.23	110.48
1	C	83	ASP	N-CA-C	5.41	119.88	113.28
1	C	94	VAL	N-CA-C	5.40	116.13	107.98
1	B	112	VAL	CB-CA-C	5.38	118.98	111.40
1	A	30	ARG	N-CA-C	5.37	118.05	111.82
1	A	80	GLN	CA-C-N	-5.37	114.42	119.90
1	A	80	GLN	C-N-CA	-5.37	114.42	119.90
1	A	83	ASP	N-CA-C	5.36	119.82	113.28
1	D	112	VAL	CB-CA-C	5.35	118.95	111.40
1	C	61	GLU	N-CA-C	5.30	117.47	111.11
1	A	61	GLU	N-CA-C	5.29	117.46	111.11
1	B	48	ARG	N-CA-C	-5.26	102.83	110.24
1	C	30	ARG	N-CA-C	5.26	117.92	111.82
1	D	120	ASP	N-CA-C	5.25	116.68	111.07
1	B	134	ARG	CA-C-N	-5.21	115.12	122.94
1	B	134	ARG	C-N-CA	-5.21	115.12	122.94
1	D	48	ARG	N-CA-C	-5.19	102.92	110.24
1	D	134	ARG	CA-C-N	-5.18	115.17	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	134	ARG	C-N-CA	-5.18	115.17	122.94
1	C	80	GLN	CA-C-N	-5.15	114.45	119.76
1	C	80	GLN	C-N-CA	-5.15	114.45	119.76
1	B	120	ASP	N-CA-C	5.15	116.58	111.07
1	B	131	VAL	N-CA-C	5.11	116.72	108.85
1	D	131	VAL	N-CA-C	5.10	116.71	108.85
1	C	119	GLU	N-CA-CB	5.10	117.61	110.12
1	A	119	GLU	N-CA-CB	5.09	117.61	110.12
1	B	100	VAL	CB-CA-C	5.08	118.89	110.30
1	D	100	VAL	CB-CA-C	5.07	118.88	110.30
1	A	74	THR	CB-CA-C	5.03	117.56	110.02

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	GLY	Peptide
1	A	83	ASP	Peptide
1	C	49	GLY	Peptide
1	C	83	ASP	Peptide

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	1130	0	1134	33	31
1	B	1114	0	1108	71	0
1	C	1130	0	1133	51	0
1	D	1114	0	1108	83	7
All	All	4488	0	4483	166	38

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 18.

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:B:102:THR:CA	1:B:102:THR:CB	1.87	1.53
1:D:102:THR:CA	1:D:102:THR:CB	1.87	1.50
1:A:102:THR:CB	1:A:102:THR:CA	1.88	1.48
1:C:102:THR:CA	1:C:102:THR:CB	1.86	1.47
1:A:102:THR:CA	1:A:102:THR:CG2	2.04	1.33
1:A:136:THR:CG2	1:B:102:THR:HG23	1.61	1.28
1:C:136:THR:CG2	1:D:102:THR:HG23	1.68	1.22
1:C:136:THR:HG23	1:D:102:THR:HG23	1.26	1.17
1:D:102:THR:CB	1:D:102:THR:C	2.20	1.14
1:B:102:THR:CB	1:B:102:THR:C	2.20	1.14
1:B:14:ARG:HD3	1:B:149:ILE:HB	1.29	1.13
1:C:102:THR:CB	1:C:102:THR:C	2.20	1.12
1:B:139:LEU:HD13	1:D:119:GLU:HB2	1.32	1.10
1:A:102:THR:CG2	1:A:102:THR:HA	1.82	1.10
1:B:102:THR:HB	1:B:103:GLU:N	1.67	1.09
1:C:102:THR:HB	1:C:103:GLU:N	1.68	1.09
1:D:102:THR:HB	1:D:103:GLU:N	1.67	1.09
1:B:139:LEU:HD22	1:D:115:ALA:O	1.51	1.08
1:A:136:THR:HG23	1:B:102:THR:HG23	1.03	1.00
1:A:102:THR:HA	1:A:102:THR:HG23	1.40	0.99
1:B:139:LEU:CD1	1:D:119:GLU:HB2	1.97	0.94
1:C:102:THR:CB	1:C:103:GLU:N	2.31	0.93
1:A:136:THR:CG2	1:B:102:THR:CG2	2.46	0.93
1:C:136:THR:CG2	1:D:102:THR:CG2	2.50	0.90
1:D:102:THR:CB	1:D:102:THR:N	2.35	0.89
1:B:102:THR:CB	1:B:102:THR:N	2.35	0.89
1:C:136:THR:HG21	1:D:102:THR:HG23	1.53	0.89
1:B:100:VAL:HG13	1:B:102:THR:OG1	1.75	0.87
1:A:102:THR:CA	1:A:102:THR:HG22	2.02	0.86
1:A:136:THR:HG23	1:B:102:THR:CG2	1.98	0.86
1:C:102:THR:C	1:C:102:THR:HB	1.95	0.84
1:B:139:LEU:O	1:D:116:ARG:HB3	1.80	0.82
1:C:136:THR:HG21	1:D:102:THR:CG2	2.08	0.82
1:B:66:LEU:CD1	1:D:66:LEU:CD1	2.56	0.82
1:D:102:THR:C	1:D:102:THR:HB	2.01	0.82
1:D:100:VAL:HG13	1:D:102:THR:OG1	1.79	0.81
1:B:102:THR:CB	1:B:103:GLU:N	2.38	0.81
1:D:124:ARG:O	1:D:128:THR:HG23	1.82	0.80
1:B:66:LEU:HD12	1:D:66:LEU:HD13	1.64	0.80
1:B:14:ARG:CZ	1:B:149:ILE:O	2.29	0.79
1:C:136:THR:HG23	1:D:102:THR:CG2	2.11	0.79
1:B:66:LEU:HD13	1:D:66:LEU:CD1	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:HG21	1:B:102:THR:HG23	1.60	0.78
1:B:124:ARG:O	1:B:128:THR:HG23	1.82	0.78
1:B:102:THR:C	1:B:102:THR:HB	2.00	0.78
1:D:102:THR:CB	1:D:103:GLU:N	2.39	0.78
1:B:66:LEU:HD13	1:D:66:LEU:HD12	1.66	0.76
1:C:102:THR:HB	1:C:103:GLU:H	1.45	0.76
1:B:139:LEU:HD13	1:D:119:GLU:CB	2.13	0.76
1:A:136:THR:HG21	1:B:102:THR:CG2	2.14	0.76
1:C:146:ARG:HH21	1:D:89:GLU:HG2	1.50	0.76
1:C:124:ARG:O	1:C:128:THR:HG23	1.88	0.73
1:D:42:VAL:O	1:D:46:GLU:HG3	1.89	0.73
1:A:124:ARG:O	1:A:128:THR:HG23	1.88	0.73
1:B:42:VAL:O	1:B:46:GLU:HG3	1.89	0.73
1:B:139:LEU:HD23	1:D:115:ALA:HB1	1.71	0.73
1:B:14:ARG:HD3	1:B:149:ILE:CB	2.13	0.72
1:B:124:ARG:O	1:B:128:THR:CG2	2.38	0.71
1:C:146:ARG:NH2	1:D:89:GLU:O	2.21	0.71
1:B:102:THR:HB	1:B:103:GLU:H	1.56	0.71
1:B:116:ARG:HD2	1:D:140:ASN:CG	2.15	0.70
1:C:51:VAL:HG22	1:D:58:ILE:CD1	2.22	0.70
1:D:124:ARG:O	1:D:128:THR:CG2	2.38	0.70
1:D:102:THR:HB	1:D:103:GLU:H	1.54	0.69
1:A:102:THR:CB	1:A:102:THR:C	2.66	0.68
1:B:66:LEU:CD1	1:D:66:LEU:HD13	2.22	0.68
1:B:100:VAL:CG1	1:B:102:THR:OG1	2.45	0.65
1:B:139:LEU:CD2	1:D:115:ALA:O	2.36	0.64
1:C:50:VAL:HG22	1:D:62:ALA:HB1	1.80	0.63
1:B:139:LEU:O	1:D:116:ARG:CB	2.47	0.63
1:C:146:ARG:NH2	1:D:89:GLU:HG2	2.14	0.62
1:A:102:THR:CB	1:A:103:GLU:N	2.62	0.62
1:D:100:VAL:CG1	1:D:102:THR:OG1	2.48	0.62
1:D:91:ILE:HD11	1:D:93:GLU:HG2	1.82	0.62
1:C:102:THR:CB	1:C:103:GLU:H	2.04	0.61
1:B:91:ILE:HD11	1:B:93:GLU:HG2	1.82	0.61
1:A:102:THR:CA	1:A:102:THR:HG23	2.02	0.61
1:B:116:ARG:HA	1:D:139:LEU:O	2.01	0.60
1:A:146:ARG:NH2	1:B:89:GLU:O	2.34	0.60
1:D:7:ASP:HA	1:D:10:ARG:HB2	1.85	0.59
1:A:102:THR:HG22	1:A:102:THR:C	2.28	0.58
1:C:54:TYR:CE2	1:D:56:ALA:HB2	2.38	0.58
1:B:15:GLU:OE2	1:B:15:GLU:HA	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:CA	1:D:139:LEU:O	2.51	0.58
1:C:51:VAL:HG22	1:D:58:ILE:HD13	1.84	0.58
1:C:146:ARG:HH22	1:D:89:GLU:C	2.12	0.57
1:C:16:LEU:HD21	1:C:27:LEU:HD11	1.85	0.57
1:A:16:LEU:HD21	1:A:27:LEU:HD11	1.85	0.57
1:B:6:ASP:O	1:B:9:ASP:HB2	2.06	0.56
1:B:7:ASP:HA	1:B:10:ARG:HB2	1.85	0.56
1:C:54:TYR:CD2	1:D:56:ALA:HB2	2.40	0.56
1:B:91:ILE:C	1:B:91:ILE:HD12	2.31	0.56
1:D:102:THR:N	1:D:102:THR:OG1	2.39	0.56
1:D:91:ILE:C	1:D:91:ILE:HD12	2.31	0.56
1:B:102:THR:N	1:B:102:THR:OG1	2.38	0.55
1:D:6:ASP:O	1:D:9:ASP:HB2	2.05	0.55
1:C:100:VAL:HG22	1:D:136:THR:HG22	1.88	0.55
1:A:146:ARG:HH21	1:B:89:GLU:HG2	1.71	0.55
1:B:116:ARG:HD2	1:D:140:ASN:OD1	2.07	0.55
1:C:124:ARG:O	1:C:128:THR:CG2	2.54	0.54
1:C:150:PRO:HG3	1:D:65:HIS:CE1	2.42	0.54
1:B:67:LEU:HD11	1:D:67:LEU:HD21	1.89	0.54
1:A:124:ARG:O	1:A:128:THR:CG2	2.54	0.54
1:C:68:SER:OG	1:C:111:ARG:HD3	2.08	0.54
1:C:83:ASP:HB3	1:C:87:ARG:HD2	1.91	0.53
1:C:146:ARG:HH21	1:D:89:GLU:CG	2.20	0.53
1:B:115:ALA:HB2	1:D:67:LEU:HD23	1.90	0.53
1:B:139:LEU:HA	1:D:115:ALA:HB1	1.90	0.53
1:C:102:THR:CA	1:C:102:THR:CG2	2.82	0.53
1:A:68:SER:OG	1:A:111:ARG:HD3	2.08	0.53
1:A:83:ASP:HB3	1:A:87:ARG:HD2	1.90	0.53
1:A:102:THR:CB	1:A:103:GLU:H	2.21	0.52
1:B:8:ILE:HB	1:B:41:ARG:NH2	2.24	0.52
1:A:4:ALA:O	1:A:48:ARG:NH2	2.43	0.52
1:C:65:HIS:CE1	1:D:150:PRO:HG3	2.44	0.52
1:A:102:THR:CG2	1:A:102:THR:C	2.81	0.52
1:C:4:ALA:O	1:C:48:ARG:NH2	2.43	0.51
1:D:8:ILE:HB	1:D:41:ARG:NH2	2.24	0.51
1:C:52:GLN:N	1:D:57:ARG:O	2.31	0.51
1:A:100:VAL:HG22	1:B:136:THR:HG22	1.93	0.50
1:A:146:ARG:NH2	1:B:89:GLU:HG2	2.26	0.50
1:A:65:HIS:CE1	1:B:150:PRO:HG3	2.46	0.50
1:C:54:TYR:HA	1:D:56:ALA:HA	1.94	0.50
1:B:115:ALA:HB2	1:D:67:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ARG:NH2	1:D:89:GLU:CG	2.75	0.49
1:B:116:ARG:HB2	1:D:139:LEU:O	2.13	0.49
1:B:139:LEU:HA	1:D:115:ALA:CB	2.43	0.48
1:C:100:VAL:HG13	1:C:102:THR:OG1	2.13	0.48
1:A:62:ALA:HB1	1:B:50:VAL:HG22	1.95	0.48
1:C:8:ILE:HG21	1:C:33:LEU:HD11	1.96	0.48
1:D:23:THR:O	1:D:24:LEU:C	2.57	0.47
1:C:21:ARG:NH1	1:D:20:GLY:O	2.47	0.47
1:C:57:ARG:O	1:D:52:GLN:HG3	2.15	0.47
1:C:58:ILE:HD12	1:D:17:ALA:HB2	1.97	0.47
1:B:119:GLU:HB2	1:D:139:LEU:HD13	1.97	0.47
1:B:23:THR:O	1:B:24:LEU:C	2.57	0.46
1:C:54:TYR:CD2	1:D:56:ALA:CB	2.99	0.46
1:A:8:ILE:HG21	1:A:33:LEU:HD11	1.96	0.45
1:B:102:THR:HB	1:B:104:GLU:H	1.81	0.45
1:A:58:ILE:HD13	1:B:13:VAL:HB	1.98	0.45
1:B:119:GLU:HB2	1:D:139:LEU:CD1	2.47	0.45
1:C:50:VAL:HG22	1:D:62:ALA:CB	2.47	0.45
1:C:53:GLY:O	1:D:57:ARG:N	2.34	0.45
1:B:102:THR:CA	1:B:102:THR:CG2	2.84	0.45
1:D:8:ILE:HB	1:D:41:ARG:HH21	1.83	0.44
1:A:58:ILE:HD12	1:B:17:ALA:HB2	1.98	0.44
1:C:74:THR:HA	1:C:75:PRO:HD3	1.91	0.44
1:D:102:THR:HB	1:D:104:GLU:H	1.83	0.43
1:D:102:THR:CA	1:D:102:THR:CG2	2.84	0.43
1:C:146:ARG:NH2	1:D:89:GLU:HA	2.34	0.43
1:B:91:ILE:HD11	1:B:121:LEU:HD11	2.01	0.42
1:B:149:ILE:HA	1:B:150:PRO:HD3	1.86	0.42
1:B:14:ARG:NE	1:B:149:ILE:O	2.52	0.42
1:D:91:ILE:HD11	1:D:121:LEU:HD11	2.01	0.42
1:C:146:ARG:HH22	1:D:89:GLU:HA	1.84	0.42
1:B:124:ARG:O	1:B:128:THR:HG22	2.18	0.42
1:C:143:TYR:OH	1:D:85:PRO:O	2.26	0.42
1:C:146:ARG:HH22	1:D:89:GLU:CA	2.33	0.42
1:B:8:ILE:HB	1:B:41:ARG:HH21	1.83	0.42
1:C:54:TYR:CE2	1:D:56:ALA:CB	3.02	0.42
1:A:25:SER:O	1:A:29:THR:HG23	2.21	0.41
1:B:67:LEU:HD12	1:B:115:ALA:HA	2.02	0.41
1:B:84:ALA:N	1:B:85:PRO:CD	2.84	0.41
1:D:84:ALA:N	1:D:85:PRO:CD	2.84	0.41
1:C:25:SER:O	1:C:29:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ARG:O	1:D:128:THR:HG22	2.18	0.41

All (38) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:GLN:CG	1:D:39:GLN:OE1[4_565]	0.43	1.77
1:A:119:GLU:CD	1:A:139:LEU:CB[3_454]	0.70	1.50
1:A:119:GLU:CG	1:A:139:LEU:CB[3_454]	0.92	1.28
1:A:61:GLU:OE1	1:A:116:ARG:NH2[3_454]	0.95	1.25
1:A:119:GLU:CB	1:A:139:LEU:CG[3_454]	0.97	1.23
1:D:39:GLN:NE2	1:D:39:GLN:NE2[4_565]	1.04	1.16
1:A:61:GLU:OE2	1:A:116:ARG:NE[3_454]	1.07	1.13
1:A:119:GLU:OE2	1:A:139:LEU:CA[3_454]	1.18	1.02
1:A:119:GLU:CB	1:A:139:LEU:CD2[3_454]	1.20	1.00
1:A:119:GLU:OE2	1:A:139:LEU:C[3_454]	1.22	0.98
1:D:39:GLN:CD	1:D:39:GLN:OE1[4_565]	1.23	0.97
1:A:61:GLU:CD	1:A:116:ARG:NH2[3_454]	1.26	0.94
1:A:61:GLU:OE2	1:A:116:ARG:CZ[3_454]	1.27	0.93
1:A:119:GLU:CD	1:A:139:LEU:CA[3_454]	1.35	0.85
1:D:39:GLN:CD	1:D:39:GLN:NE2[4_565]	1.44	0.76
1:A:61:GLU:CD	1:A:116:ARG:CZ[3_454]	1.48	0.72
1:D:39:GLN:CG	1:D:39:GLN:CD[4_565]	1.50	0.70
1:A:119:GLU:OE2	1:A:140:ASN:N[3_454]	1.52	0.68
1:A:119:GLU:CG	1:A:139:LEU:CG[3_454]	1.53	0.67
1:A:119:GLU:CB	1:A:139:LEU:CD1[3_454]	1.59	0.61
1:A:119:GLU:OE1	1:A:139:LEU:CB[3_454]	1.62	0.58
1:A:61:GLU:OE1	1:A:116:ARG:CZ[3_454]	1.65	0.55
1:A:119:GLU:CG	1:A:139:LEU:CA[3_454]	1.70	0.50
1:A:119:GLU:OE2	1:A:139:LEU:CB[3_454]	1.75	0.45
1:D:39:GLN:CB	1:D:39:GLN:OE1[4_565]	1.75	0.45
1:A:119:GLU:CA	1:A:139:LEU:CD2[3_454]	1.79	0.41
1:A:119:GLU:OE2	1:A:139:LEU:N[3_454]	1.81	0.39
1:A:119:GLU:CD	1:A:139:LEU:CG[3_454]	1.90	0.30
1:A:119:GLU:CB	1:A:139:LEU:CB[3_454]	1.91	0.29
1:A:119:GLU:OE1	1:A:139:LEU:CG[3_454]	1.96	0.24
1:D:39:GLN:OE1	1:D:39:GLN:OE1[4_565]	2.00	0.20
1:A:119:GLU:CD	1:A:139:LEU:N[3_454]	2.01	0.19
1:A:119:GLU:CG	1:A:139:LEU:CD2[3_454]	2.02	0.18
1:A:61:GLU:OE2	1:A:116:ARG:NH2[3_454]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLU:CD	1:A:116:ARG:NE[3_454]	2.05	0.15
1:A:61:GLU:OE2	1:A:116:ARG:CD[3_454]	2.11	0.09
1:A:61:GLU:OE1	1:A:116:ARG:NH1[3_454]	2.18	0.02
1:A:67:LEU:CG	1:A:115:ALA:CB[3_454]	2.19	0.01

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	145/150 (97%)	141 (97%)	3 (2%)	1 (1%)	18	55
1	B	145/150 (97%)	132 (91%)	6 (4%)	7 (5%)	2	18
1	C	145/150 (97%)	141 (97%)	3 (2%)	1 (1%)	18	55
1	D	145/150 (97%)	133 (92%)	5 (3%)	7 (5%)	2	18
All	All	580/600 (97%)	547 (94%)	17 (3%)	16 (3%)	4	27

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	THR
1	B	25	SER
1	C	102	THR
1	D	25	SER
1	B	29	THR
1	B	102	THR
1	D	29	THR
1	D	102	THR
1	B	35	VAL
1	D	35	VAL
1	B	5	LEU
1	B	7	ASP
1	B	30	ARG

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Mol	Chain	Res	Type
1	D	5	LEU
1	D	7	ASP
1	D	30	ARG

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	122/127 (96%)	103 (84%)	19 (16%)	2	14
1	B	119/127 (94%)	92 (77%)	27 (23%)	1	6
1	C	122/127 (96%)	102 (84%)	20 (16%)	2	13
1	D	119/127 (94%)	94 (79%)	25 (21%)	1	7
All	All	482/508 (95%)	391 (81%)	91 (19%)	1	10

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	24	LEU
1	A	29	THR
1	A	40	SER
1	A	44	ARG
1	A	45	LEU
1	A	67	LEU
1	A	71	VAL
1	A	74	THR
1	A	83	ASP
1	A	93	GLU
1	A	94	VAL
1	A	100	VAL
1	A	110	VAL
1	A	112	VAL
1	A	127	THR
1	A	128	THR
1	A	131	VAL

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Mol	Chain	Res	Type
1	A	146	ARG
1	B	5	LEU
1	B	6	ASP
1	B	11	ILE
1	B	15	GLU
1	B	23	THR
1	B	24	LEU
1	B	29	THR
1	B	36	SER
1	B	38	VAL
1	B	40	SER
1	B	51	VAL
1	B	61	GLU
1	B	63	VAL
1	B	87	ARG
1	B	91	ILE
1	B	93	GLU
1	B	94	VAL
1	B	100	VAL
1	B	102	THR
1	B	103	GLU
1	B	104	GLU
1	B	110	VAL
1	B	112	VAL
1	B	119	GLU
1	B	120	ASP
1	B	128	THR
1	B	145	ASP
1	C	5	LEU
1	C	24	LEU
1	C	29	THR
1	C	40	SER
1	C	44	ARG
1	C	45	LEU
1	C	67	LEU
1	C	71	VAL
1	C	74	THR
1	C	83	ASP
1	C	93	GLU
1	C	94	VAL
1	C	100	VAL
1	C	102	THR

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Mol	Chain	Res	Type
1	C	110	VAL
1	C	112	VAL
1	C	127	THR
1	C	128	THR
1	C	131	VAL
1	C	146	ARG
1	D	5	LEU
1	D	6	ASP
1	D	11	ILE
1	D	23	THR
1	D	24	LEU
1	D	29	THR
1	D	36	SER
1	D	38	VAL
1	D	40	SER
1	D	51	VAL
1	D	61	GLU
1	D	63	VAL
1	D	87	ARG
1	D	91	ILE
1	D	93	GLU
1	D	94	VAL
1	D	100	VAL
1	D	102	THR
1	D	103	GLU
1	D	104	GLU
1	D	110	VAL
1	D	112	VAL
1	D	120	ASP
1	D	128	THR
1	D	145	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	80	GLN
1	A	130	ASN
1	A	148	HIS
1	B	130	ASN
1	C	65	HIS
1	C	80	GLN

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Mol	Chain	Res	Type
1	C	130	ASN
1	C	147	GLN
1	D	123	GLN
1	D	130	ASN

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 [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	147/150 (98%)	1.39	34 (23%) 2 4	15, 33, 56, 69	0
1	B	147/150 (98%)	1.71	40 (27%) 1 4	14, 36, 95, 99	0
1	C	147/150 (98%)	1.11	17 (11%) 9 12	15, 33, 56, 69	0
1	D	147/150 (98%)	1.23	29 (19%) 3 6	14, 36, 95, 99	0
All	All	588/600 (98%)	1.36	120 (20%) 3 5	14, 34, 88, 99	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	VAL	10.8
1	B	58	ILE	9.4
1	D	39	GLN	8.7
1	A	115	ALA	7.5
1	B	75	PRO	7.3
1	A	129	ALA	5.9
1	B	96	SER	5.6
1	B	31	ALA	5.5
1	A	125	ILE	5.4
1	B	73	ILE	5.3
1	B	63	VAL	4.8
1	B	74	THR	4.7
1	B	49	GLY	4.7
1	A	121	LEU	4.6
1	B	145	ASP	4.4
1	A	144	SER	4.4
1	A	11	ILE	4.3
1	A	55	SER	4.2
1	D	42	VAL	4.2
1	A	62	ALA	4.1
1	B	20	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	138	ILE	3.9
1	C	150	PRO	3.8
1	D	4	ALA	3.8
1	C	32	GLY	3.7
1	B	11	ILE	3.7
1	D	103	GLU	3.6
1	B	8	ILE	3.6
1	D	38	VAL	3.5
1	D	93	GLU	3.5
1	B	4	ALA	3.5
1	C	73	ILE	3.5
1	B	80	GLN	3.5
1	D	14	ARG	3.4
1	B	16	LEU	3.4
1	D	104	GLU	3.3
1	A	140	ASN	3.3
1	B	12	LEU	3.3
1	A	108	LEU	3.3
1	D	49	GLY	3.2
1	A	131	VAL	3.2
1	B	149	ILE	3.2
1	D	115	ALA	3.2
1	D	33	LEU	3.1
1	A	142	PHE	3.1
1	A	49	GLY	3.1
1	A	32	GLY	3.1
1	A	107	VAL	3.1
1	D	40	SER	3.1
1	B	105	SER	3.0
1	A	128	THR	3.0
1	B	130	ASN	2.9
1	A	51	VAL	2.9
1	B	27	LEU	2.9
1	A	100	VAL	2.9
1	C	108	LEU	2.9
1	A	84	ALA	2.9
1	C	132	ARG	2.8
1	A	31	ALA	2.8
1	D	67	LEU	2.8
1	A	104	GLU	2.8
1	C	130	ASN	2.7
1	C	13	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	25	SER	2.7
1	B	81	PRO	2.6
1	C	147	GLN	2.6
1	B	15	GLU	2.5
1	C	49	GLY	2.5
1	A	83	ASP	2.5
1	A	67	LEU	2.5
1	A	54	TYR	2.5
1	D	99	SER	2.5
1	A	145	ASP	2.5
1	A	16	LEU	2.5
1	B	37	ALA	2.5
1	D	102	THR	2.4
1	A	110	VAL	2.4
1	B	55	SER	2.4
1	D	45	LEU	2.4
1	B	95	GLU	2.4
1	D	100	VAL	2.4
1	B	141	THR	2.4
1	D	31	ALA	2.4
1	C	81	PRO	2.4
1	D	26	GLU	2.4
1	B	14	ARG	2.3
1	D	32	GLY	2.3
1	A	48	ARG	2.3
1	D	66	LEU	2.3
1	C	17	ALA	2.3
1	C	148	HIS	2.3
1	D	109	LEU	2.3
1	B	147	GLN	2.2
1	A	43	ARG	2.2
1	C	111	ARG	2.2
1	D	43	ARG	2.2
1	D	46	GLU	2.2
1	A	146	ARG	2.2
1	B	10	ARG	2.2
1	D	84	ALA	2.2
1	A	114	SER	2.2
1	B	77	ASP	2.2
1	A	72	ALA	2.2
1	B	30	ARG	2.2
1	D	13	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	9	ASP	2.1
1	B	108	LEU	2.1
1	B	18	ALA	2.1
1	D	37	ALA	2.1
1	C	14	ARG	2.0
1	B	122	LEU	2.0
1	A	69	ALA	2.0
1	C	86	ALA	2.0
1	D	8	ILE	2.0
1	A	44	ARG	2.0
1	C	24	LEU	2.0
1	B	93	GLU	2.0
1	B	110	VAL	2.0
1	B	34	SER	2.0
1	B	36	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 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.