



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:03 AM UTC

PDB ID : 3WA0 / pdb_00003wa0
Title : Crystal structure of merlin complexed with DCAF1/VprBP
Authors : Mori, T.; Gotoh, S.; Shirakawa, M.; Hakoshima, T.
Deposited on : 2013-04-20
Resolution : 2.31 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

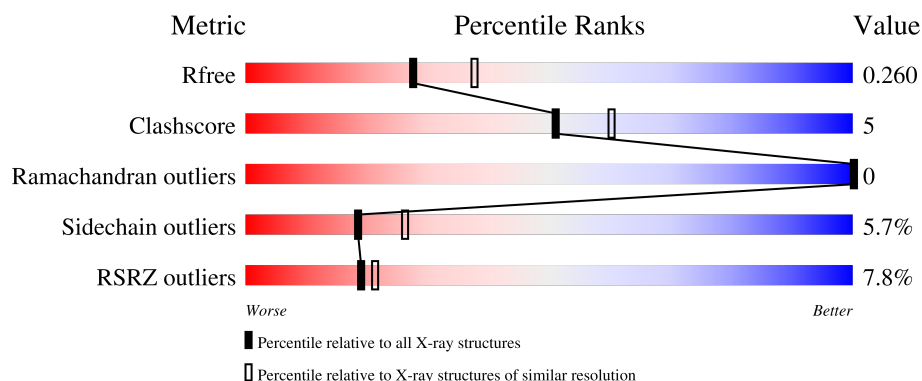
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	301	9% 79% 13% • •
1	B	301	8% 80% 14% • •
1	C	301	5% 81% 15% • •
1	D	301	11% 80% 17% • •
1	E	301	5% 83% 13% • •

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Mol	Chain	Length	Quality of chain
1	F	301	6% 82% 13%
2	G	96	2% 7% 89%
2	H	96	4% 5% 5% 89%
3	I	7	100%
4	J	8	88% 12%
5	K	6	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15373 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 Merlin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2409	1559	402	435	13			
1	B	290	Total	C	N	O	S	0	0	0
			2412	1562	400	437	13			
1	C	293	Total	C	N	O	S	0	0	0
			2435	1575	406	441	13			
1	D	295	Total	C	N	O	S	0	0	0
			2457	1592	409	443	13			
1	E	292	Total	C	N	O	S	0	0	0
			2429	1572	404	440	13			
1	F	291	Total	C	N	O	S	0	0	0
			2427	1572	403	439	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	expression tag	UNP P46662
A	15	PRO	-	expression tag	UNP P46662
A	16	LEU	-	expression tag	UNP P46662
A	17	GLY	-	expression tag	UNP P46662
A	18	SER	-	expression tag	UNP P46662
B	14	GLY	-	expression tag	UNP P46662
B	15	PRO	-	expression tag	UNP P46662
B	16	LEU	-	expression tag	UNP P46662
B	17	GLY	-	expression tag	UNP P46662
B	18	SER	-	expression tag	UNP P46662
C	14	GLY	-	expression tag	UNP P46662
C	15	PRO	-	expression tag	UNP P46662
C	16	LEU	-	expression tag	UNP P46662
C	17	GLY	-	expression tag	UNP P46662
C	18	SER	-	expression tag	UNP P46662
D	14	GLY	-	expression tag	UNP P46662
D	15	PRO	-	expression tag	UNP P46662

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Chain	Residue	Modelled	Actual	Comment	Reference
D	16	LEU	-	expression tag	UNP P46662
D	17	GLY	-	expression tag	UNP P46662
D	18	SER	-	expression tag	UNP P46662
E	14	GLY	-	expression tag	UNP P46662
E	15	PRO	-	expression tag	UNP P46662
E	16	LEU	-	expression tag	UNP P46662
E	17	GLY	-	expression tag	UNP P46662
E	18	SER	-	expression tag	UNP P46662
F	14	GLY	-	expression tag	UNP P46662
F	15	PRO	-	expression tag	UNP P46662
F	16	LEU	-	expression tag	UNP P46662
F	17	GLY	-	expression tag	UNP P46662
F	18	SER	-	expression tag	UNP P46662

- Molecule 2 is a protein called Protein VPRBP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	11	Total	C	N	O	0	0	0
			80	50	11	19			
2	H	11	Total	C	N	O	0	0	0
			76	48	12	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1411	GLY	-	expression tag	UNP Q9Y4B6
G	1412	PRO	-	expression tag	UNP Q9Y4B6
G	1413	LEU	-	expression tag	UNP Q9Y4B6
G	1414	GLY	-	expression tag	UNP Q9Y4B6
G	1415	SER	-	expression tag	UNP Q9Y4B6
G	1416	TYR	-	expression tag	UNP Q9Y4B6
H	1411	GLY	-	expression tag	UNP Q9Y4B6
H	1412	PRO	-	expression tag	UNP Q9Y4B6
H	1413	LEU	-	expression tag	UNP Q9Y4B6
H	1414	GLY	-	expression tag	UNP Q9Y4B6
H	1415	SER	-	expression tag	UNP Q9Y4B6
H	1416	TYR	-	expression tag	UNP Q9Y4B6

- Molecule 3 is a protein called Protein VPRBP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	7	Total	C	N	O	0	0	0
			35	21	7	7			

- Molecule 4 is a protein called Protein VPRBP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	8	Total	C	N	O	0	0	0
			40	24	8	8			

- Molecule 5 is a protein called Protein VPRBP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	6	Total	C	N	O	0	0	0
			30	18	6	6			

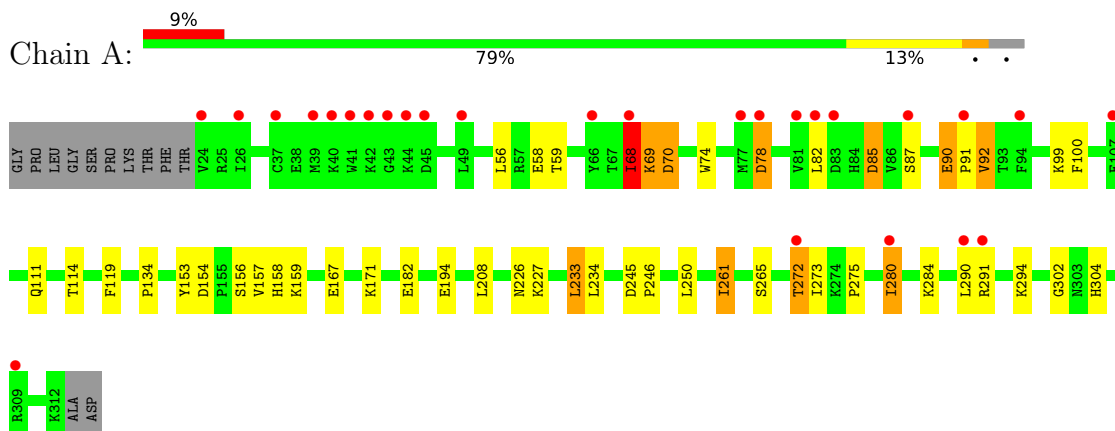
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total	O	0	0
			70	70		
6	B	85	Total	O	0	0
			85	85		
6	C	102	Total	O	0	0
			102	102		
6	D	94	Total	O	0	0
			94	94		
6	E	86	Total	O	0	0
			86	86		
6	F	105	Total	O	0	0
			105	105		
6	H	1	Total	O	0	0
			1	1		

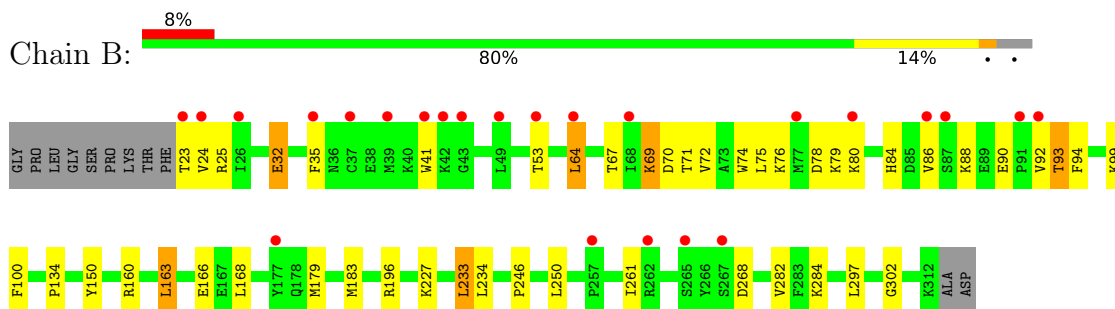
3 Residue-property plots [i](#)

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.

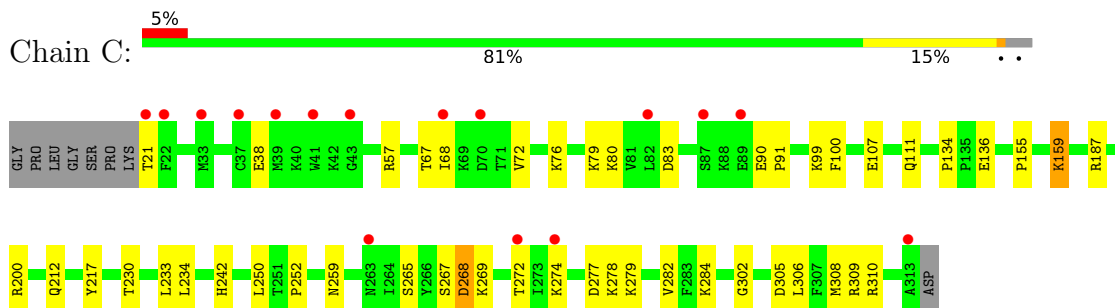
• Molecule 1: Merlin



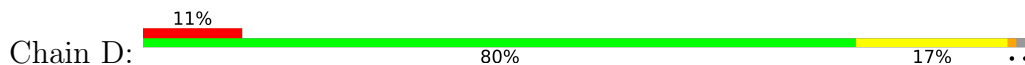
• Molecule 1: Merlin

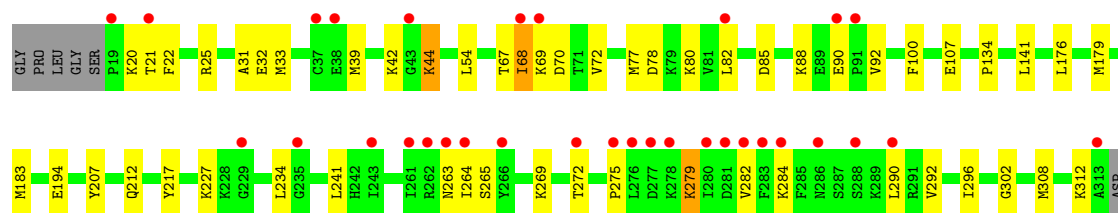


• Molecule 1: Merlin

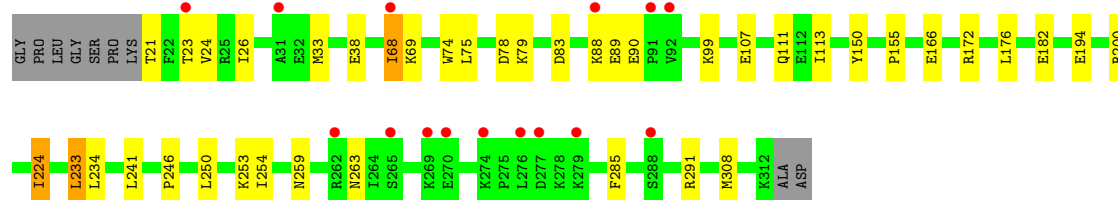
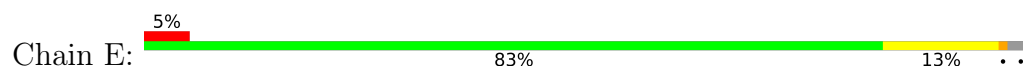


• Molecule 1: Merlin

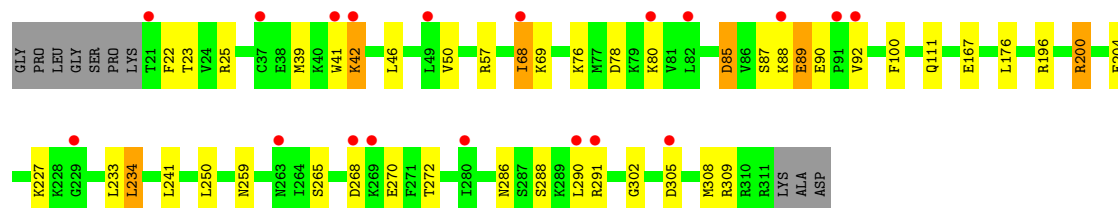
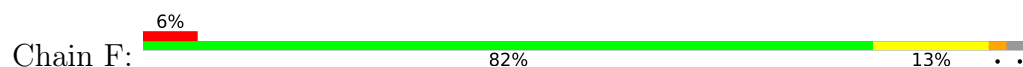




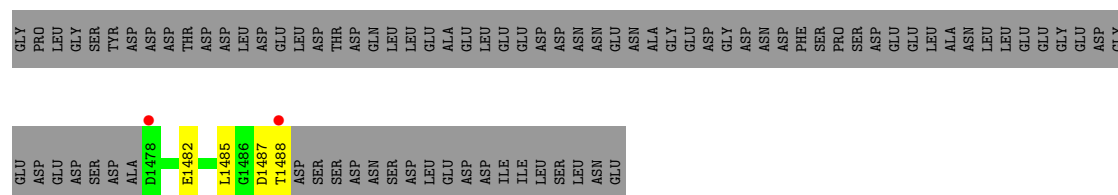
• Molecule 1: Merlin



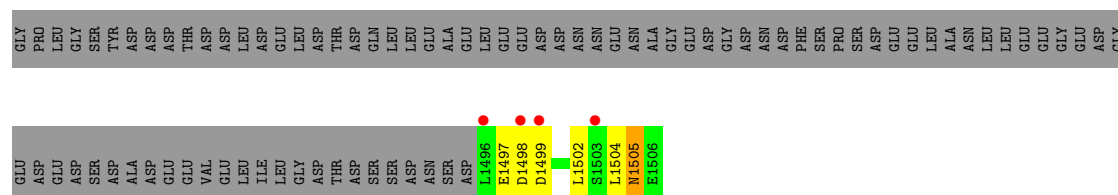
• Molecule 1: Merlin



• Molecule 2: Protein VPRBP



• Molecule 2: Protein VPRBP



• Molecule 3: Protein VPRBP

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Protein VPRBP

Chain J:  88% 12%



- Molecule 5: Protein VPRBP

Chain K:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.36Å 135.76Å 238.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.07 – 2.31 20.07 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.07-2.31) 98.8 (20.07-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.235 , 0.264 0.230 , 0.260	Depositor DCC
R_{free} test set	6149 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15373	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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	0.45	0/2467	0.81	4/3328 (0.1%)
1	B	0.45	0/2470	0.81	2/3334 (0.1%)
1	C	0.47	0/2494	0.78	0/3366
1	D	0.45	0/2517	0.81	3/3396 (0.1%)
1	E	0.45	0/2488	0.77	0/3359
1	F	0.44	0/2486	0.77	1/3356 (0.0%)
2	G	0.61	0/79	0.78	0/106
2	H	0.73	0/75	1.50	5/100 (5.0%)
All	All	0.45	0/15076	0.80	15/20345 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1499	ASP	N-CA-C	6.95	118.96	108.46
1	A	157	VAL	N-CA-C	6.67	116.80	110.53
1	A	68	ILE	CB-CA-C	-6.27	101.81	110.96
1	F	89	GLU	N-CA-C	-5.91	101.56	110.24
1	D	312	LYS	N-CA-C	5.84	120.91	113.55
2	H	1497	GLU	CB-CA-C	-5.65	99.18	110.42
1	B	134	PRO	CA-C-N	5.44	124.89	119.24
1	B	134	PRO	C-N-CA	5.44	124.89	119.24
2	H	1498	ASP	N-CA-C	-5.38	104.38	111.96
1	D	31	ALA	N-CA-C	5.22	116.22	108.60
1	A	245	ASP	CA-C-N	5.20	125.51	119.47
1	A	245	ASP	C-N-CA	5.20	125.51	119.47
1	D	312	LYS	CB-CA-C	-5.15	101.35	109.34
2	H	1504	LEU	N-CA-C	5.02	119.36	112.68
2	H	1505	ASN	N-CA-C	5.00	116.99	109.23

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	2409	0	2402	37	0
1	B	2412	0	2405	35	0
1	C	2435	0	2419	25	0
1	D	2457	0	2458	24	0
1	E	2429	0	2412	17	0
1	F	2427	0	2419	22	0
2	G	80	0	70	5	0
2	H	76	0	68	2	0
3	I	35	0	9	0	0
4	J	40	0	10	1	0
5	K	30	0	9	0	0
6	A	70	0	0	1	0
6	B	85	0	0	0	0
6	C	102	0	0	1	0
6	D	94	0	0	0	0
6	E	86	0	0	2	0
6	F	105	0	0	0	0
6	H	1	0	0	0	0
All	All	15373	0	14681	154	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 5.

All (154) 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:25:ARG:HB3	1:B:93:THR:CG2	1.69	1.23
1:A:68:ILE:HD13	1:A:291:ARG:NH1	1.59	1.17
1:B:25:ARG:CB	1:B:93:THR:HG23	1.78	1.12
1:B:25:ARG:HD3	1:B:93:THR:HG21	1.34	1.10
1:A:68:ILE:CD1	1:A:291:ARG:NH1	2.28	0.95
1:A:68:ILE:HD13	1:A:291:ARG:HH12	1.31	0.93
1:A:304:HIS:CD2	2:G:1485:LEU:HD22	2.03	0.92
1:A:68:ILE:CD1	1:A:291:ARG:HH11	1.82	0.90
1:B:25:ARG:HD3	1:B:93:THR:CG2	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:THR:HB	1:F:90:GLU:OE2	1.78	0.82
1:B:25:ARG:HB3	1:B:93:THR:HG23	0.86	0.78
1:A:304:HIS:CG	2:G:1485:LEU:HD22	2.19	0.78
1:A:68:ILE:HD12	1:A:291:ARG:HH11	1.49	0.76
1:C:80:LYS:HG3	1:C:83:ASP:HB2	1.72	0.71
1:B:179:MET:HE2	1:B:183:MET:HB3	1.72	0.71
1:E:79:LYS:HE2	1:E:83:ASP:HB3	1.72	0.71
1:F:68:ILE:HD11	1:F:291:ARG:HE	1.57	0.69
1:D:227:LYS:HB2	1:D:284:LYS:HE3	1.74	0.69
1:A:87:SER:O	1:A:92:VAL:HG22	1.94	0.67
1:B:78:ASP:HB2	2:G:1487:ASP:O	1.93	0.67
1:D:22:PHE:CE2	1:D:92:VAL:HG21	2.30	0.66
1:A:265:SER:HB2	1:A:272:THR:HG23	1.78	0.65
1:B:25:ARG:CB	1:B:93:THR:CG2	2.54	0.64
1:A:261:ILE:HD12	1:A:273:ILE:HG23	1.81	0.63
1:F:25:ARG:N	1:F:92:VAL:O	2.27	0.62
1:B:163:LEU:HG	1:B:168:LEU:HD11	1.82	0.62
1:B:69:LYS:O	1:B:70:ASP:HB2	2.00	0.61
1:B:25:ARG:CD	1:B:93:THR:HG21	2.23	0.60
1:F:88:LYS:O	1:F:89:GLU:C	2.42	0.60
1:B:25:ARG:CD	1:B:93:THR:CG2	2.77	0.60
1:F:42:LYS:HA	1:F:80:LYS:HA	1.84	0.59
1:F:85:ASP:N	1:F:85:ASP:OD1	2.34	0.59
1:A:227:LYS:HD2	1:A:284:LYS:HB2	1.82	0.59
1:D:22:PHE:HE2	1:D:92:VAL:HG21	1.68	0.58
1:B:261:ILE:O	2:H:1505:ASN:ND2	2.38	0.57
1:C:265:SER:OG	1:C:272:THR:OG1	2.22	0.57
1:E:172:ARG:NH1	6:E:473:HOH:O	2.37	0.56
1:B:79:LYS:HG2	1:B:80:LYS:O	2.06	0.56
1:E:68:ILE:HD12	1:E:291:ARG:NH1	2.20	0.56
1:A:85:ASP:N	1:A:85:ASP:OD1	2.39	0.56
1:C:67:THR:HG22	1:C:72:VAL:HG12	1.89	0.55
1:F:76:LYS:NZ	1:F:78:ASP:HB2	2.21	0.55
1:A:154:ASP:H	1:A:158:HIS:CE1	2.25	0.54
1:B:93:THR:O	1:B:94:PHE:CD1	2.60	0.54
1:A:171:LYS:NZ	6:A:466:HOH:O	2.40	0.54
1:B:25:ARG:CG	1:B:93:THR:CG2	2.85	0.54
1:A:56:LEU:HD13	1:A:114:THR:HG22	1.88	0.54
1:A:69:LYS:O	1:A:70:ASP:HB2	2.09	0.53
1:A:304:HIS:CG	2:G:1485:LEU:CD2	2.92	0.53
1:C:274:LYS:HZ1	1:C:278:LYS:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LYS:HG2	1:D:77:MET:HE3	1.93	0.51
1:A:111:GLN:HB2	1:A:114:THR:HG23	1.92	0.51
1:C:90:GLU:HG3	1:C:91:PRO:HA	1.91	0.51
1:B:24:VAL:HG12	1:B:92:VAL:HB	1.93	0.50
1:A:233:LEU:HD22	1:A:246:PRO:HA	1.93	0.50
1:B:76:LYS:HD2	2:G:1488:THR:HA	1.92	0.50
1:F:234:LEU:HD21	1:F:241:LEU:HD22	1.93	0.50
1:F:100:PHE:CZ	1:F:302:GLY:HA3	2.46	0.50
1:A:58:GLU:OE1	1:A:114:THR:HG21	2.12	0.49
1:B:88:LYS:O	1:B:88:LYS:HG2	2.12	0.49
1:D:20:LYS:HG2	1:D:39:MET:HE3	1.93	0.49
1:B:100:PHE:CZ	1:B:302:GLY:HA3	2.48	0.48
1:E:233:LEU:HD22	1:E:246:PRO:HA	1.95	0.48
1:C:134:PRO:HB2	1:E:194:GLU:CD	2.38	0.48
1:D:42:LYS:HE3	1:D:44:LYS:HB2	1.94	0.48
1:A:78:ASP:OD1	1:A:78:ASP:N	2.38	0.48
1:C:79:LYS:HZ3	1:C:83:ASP:HB3	1.79	0.48
1:B:233:LEU:HD22	1:B:246:PRO:HA	1.96	0.48
1:C:155:PRO:HG2	1:F:196:ARG:HG2	1.95	0.48
1:D:179:MET:HB3	1:D:183:MET:HB2	1.96	0.47
1:B:25:ARG:NH2	1:B:32:GLU:OE2	2.44	0.47
1:A:226:ASN:HB2	1:A:227:LYS:NZ	2.30	0.47
1:B:35:PHE:CE1	1:B:53:THR:HG21	2.49	0.47
1:D:25:ARG:NH2	1:D:32:GLU:OE2	2.34	0.47
1:B:74:TRP:CD1	1:B:99:LYS:HE3	2.49	0.47
1:F:68:ILE:HD11	1:F:291:ARG:NE	2.27	0.47
1:E:26:ILE:HB	1:E:33:MET:HB2	1.97	0.47
1:A:167:GLU:O	1:A:167:GLU:HG3	2.16	0.46
1:A:90:GLU:HA	1:A:91:PRO:C	2.39	0.46
1:E:74:TRP:CD1	1:E:99:LYS:HE3	2.50	0.46
1:B:64:LEU:HD12	1:B:64:LEU:HA	1.84	0.46
1:D:33:MET:HE1	1:D:54:LEU:HD21	1.98	0.46
1:A:294:LYS:HD3	1:A:294:LYS:HA	1.62	0.46
1:C:272:THR:HG22	1:C:284:LYS:HG2	1.99	0.45
1:D:269:LYS:NZ	1:D:290:LEU:HD11	2.32	0.45
1:A:272:THR:HB	1:A:284:LYS:HG2	1.98	0.45
1:B:64:LEU:HD23	1:B:75:LEU:HD22	1.98	0.45
1:B:71:THR:HG22	1:B:72:VAL:O	2.17	0.45
1:A:119:PHE:HA	1:A:208:LEU:HD21	1.99	0.45
1:F:46:LEU:O	1:F:50:VAL:HG23	2.16	0.45
1:D:68:ILE:HD12	1:D:85:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LYS:O	1:D:88:LYS:HG3	2.16	0.45
1:C:76:LYS:HB2	1:C:79:LYS:HB3	1.99	0.45
1:C:159:LYS:HB3	1:C:159:LYS:HE2	1.59	0.45
1:A:194:GLU:CD	1:D:134:PRO:HB2	2.42	0.45
1:B:297:LEU:HD23	2:H:1502:LEU:HD11	1.98	0.45
1:F:87:SER:OG	1:F:89:GLU:HG2	2.17	0.45
1:E:224:ILE:HG12	1:E:285:PHE:CD1	2.51	0.44
1:D:263:ASN:OD1	1:D:264:ILE:N	2.38	0.44
1:D:275:PRO:HD2	1:D:282:VAL:HG12	1.99	0.44
1:B:84:HIS:HB2	1:B:86:VAL:HG12	1.98	0.44
1:D:100:PHE:CZ	1:D:302:GLY:HA3	2.53	0.44
1:D:212:GLN:HA	1:D:217:TYR:CG	2.53	0.44
1:E:150:TYR:OH	1:E:166:GLU:OE2	2.31	0.44
1:F:259:ASN:HA	1:F:308:MET:HE1	1.99	0.44
1:B:163:LEU:HG	1:B:168:LEU:CD1	2.47	0.44
1:C:99:LYS:NZ	6:C:439:HOH:O	2.36	0.44
1:C:268:ASP:HB3	1:C:269:LYS:H	1.56	0.44
1:F:227:LYS:HD3	1:F:227:LYS:HA	1.70	0.44
1:A:100:PHE:CZ	1:A:302:GLY:HA3	2.52	0.44
1:C:277:ASP:OD1	1:C:279:LYS:HG2	2.18	0.44
1:B:79:LYS:HG2	1:B:80:LYS:N	2.33	0.43
1:C:136:GLU:OE1	1:C:187:ARG:NH2	2.52	0.43
1:D:22:PHE:CE1	1:D:82:LEU:HD11	2.53	0.43
1:C:259:ASN:HA	1:C:308:MET:HE1	2.00	0.43
1:C:305:ASP:O	1:C:309:ARG:HG3	2.18	0.43
1:E:253:LYS:HB3	1:E:253:LYS:HE2	1.82	0.43
1:A:74:TRP:CD1	1:A:99:LYS:HE3	2.54	0.43
1:E:263:ASN:HB2	4:J:6:UNK:O	2.19	0.43
1:A:56:LEU:CD1	1:A:114:THR:HG22	2.49	0.43
1:A:290:LEU:HD12	1:A:290:LEU:H	1.84	0.43
1:C:90:GLU:HA	1:C:91:PRO:HA	1.80	0.43
1:A:134:PRO:HB2	1:D:194:GLU:CD	2.44	0.42
1:A:275:PRO:HG2	1:A:280:ILE:HG12	2.00	0.42
1:B:76:LYS:HB2	1:B:79:LYS:HB3	2.01	0.42
1:B:160:ARG:HE	1:B:160:ARG:HB2	1.58	0.42
1:C:57:ARG:N	1:C:111:GLN:OE1	2.42	0.42
1:A:153:TYR:HE2	1:E:155:PRO:HG2	1.84	0.42
1:A:156:SER:O	1:A:159:LYS:HE2	2.20	0.42
1:C:100:PHE:CZ	1:C:302:GLY:HA3	2.54	0.42
1:F:22:PHE:HD2	1:F:39:MET:HE1	1.85	0.42
1:F:167:GLU:O	1:F:167:GLU:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:TYR:OH	1:B:166:GLU:OE2	2.31	0.41
1:D:67:THR:O	1:D:67:THR:HG23	2.19	0.41
1:D:265:SER:HB2	1:D:272:THR:OG1	2.19	0.41
1:F:265:SER:HB2	1:F:272:THR:HB	2.01	0.41
1:F:200:ARG:HD3	1:F:204:GLU:OE2	2.20	0.41
1:D:141:LEU:HB3	1:D:207:TYR:CE2	2.55	0.41
1:B:227:LYS:HD3	1:B:284:LYS:HB2	2.01	0.41
1:C:306:LEU:O	1:C:310:ARG:HG3	2.21	0.41
1:E:182:GLU:OE1	1:E:182:GLU:N	2.51	0.41
1:F:270:GLU:HB2	1:F:286:ASN:ND2	2.35	0.41
1:D:292:VAL:O	1:D:296:ILE:HG13	2.20	0.41
1:A:74:TRP:CG	1:A:99:LYS:HE3	2.56	0.41
1:C:242:HIS:HB3	1:C:252:PRO:HB3	2.02	0.41
1:C:277:ASP:HB2	1:D:279:LYS:HD3	2.02	0.40
1:C:187:ARG:NH1	6:E:443:HOH:O	2.54	0.40
1:E:75:LEU:HD12	1:E:75:LEU:HA	1.95	0.40
1:F:57:ARG:N	1:F:111:GLN:OE1	2.39	0.40
1:F:305:ASP:O	1:F:309:ARG:HG3	2.21	0.40
1:C:212:GLN:HA	1:C:217:TYR:CG	2.56	0.40
1:E:88:LYS:O	1:E:88:LYS:HG2	2.20	0.40
1:E:111:GLN:HB3	1:E:113:ILE:HG22	2.04	0.40
1:E:259:ASN:HA	1:E:308:MET:HE1	2.04	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	287/301 (95%)	283 (99%)	4 (1%)	0	100	100
1	B	288/301 (96%)	287 (100%)	1 (0%)	0	100	100
1	C	291/301 (97%)	289 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	293/301 (97%)	290 (99%)	3 (1%)	0	100	100
1	E	290/301 (96%)	288 (99%)	2 (1%)	0	100	100
1	F	289/301 (96%)	285 (99%)	4 (1%)	0	100	100
2	G	9/96 (9%)	9 (100%)	0	0	100	100
2	H	9/96 (9%)	9 (100%)	0	0	100	100
All	All	1756/1998 (88%)	1740 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	261/272 (96%)	245 (94%)	16 (6%)	17	23
1	B	262/272 (96%)	247 (94%)	15 (6%)	18	26
1	C	263/272 (97%)	250 (95%)	13 (5%)	22	33
1	D	267/272 (98%)	252 (94%)	15 (6%)	19	27
1	E	263/272 (97%)	245 (93%)	18 (7%)	14	19
1	F	264/272 (97%)	251 (95%)	13 (5%)	22	33
2	G	8/85 (9%)	7 (88%)	1 (12%)	4	4
2	H	7/85 (8%)	7 (100%)	0	100	100
All	All	1595/1802 (88%)	1504 (94%)	91 (6%)	18	26

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

Mol	Chain	Res	Type
1	A	59	THR
1	A	68	ILE
1	A	69	LYS
1	A	70	ASP
1	A	78	ASP

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Mol	Chain	Res	Type
1	A	82	LEU
1	A	85	ASP
1	A	90	GLU
1	A	92	VAL
1	A	182	GLU
1	A	233	LEU
1	A	234	LEU
1	A	250	LEU
1	A	261	ILE
1	A	272	THR
1	A	280	ILE
1	B	23	THR
1	B	32	GLU
1	B	41	TRP
1	B	64	LEU
1	B	67	THR
1	B	69	LYS
1	B	90	GLU
1	B	93	THR
1	B	163	LEU
1	B	196	ARG
1	B	233	LEU
1	B	234	LEU
1	B	250	LEU
1	B	268	ASP
1	B	282	VAL
1	C	21	THR
1	C	38	GLU
1	C	68	ILE
1	C	107	GLU
1	C	159	LYS
1	C	200	ARG
1	C	230	THR
1	C	233	LEU
1	C	234	LEU
1	C	250	LEU
1	C	267	SER
1	C	268	ASP
1	C	282	VAL
1	D	21	THR
1	D	44	LYS
1	D	68	ILE

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Mol	Chain	Res	Type
1	D	69	LYS
1	D	70	ASP
1	D	72	VAL
1	D	78	ASP
1	D	80	LYS
1	D	90	GLU
1	D	107	GLU
1	D	176	LEU
1	D	234	LEU
1	D	241	LEU
1	D	279	LYS
1	D	308	MET
1	E	21	THR
1	E	23	THR
1	E	24	VAL
1	E	38	GLU
1	E	68	ILE
1	E	69	LYS
1	E	78	ASP
1	E	89	GLU
1	E	90	GLU
1	E	107	GLU
1	E	176	LEU
1	E	200	ARG
1	E	224	ILE
1	E	233	LEU
1	E	234	LEU
1	E	241	LEU
1	E	250	LEU
1	E	254	ILE
1	F	41	TRP
1	F	42	LYS
1	F	68	ILE
1	F	69	LYS
1	F	85	ASP
1	F	176	LEU
1	F	200	ARG
1	F	233	LEU
1	F	234	LEU
1	F	250	LEU
1	F	268	ASP
1	F	288	SER

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Mol	Chain	Res	Type
1	F	290	LEU
2	G	1482	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	104	ASN
1	B	298	GLN
1	B	303	ASN
1	C	95	HIS
1	C	298	GLN
1	C	303	ASN
1	D	65	GLN
1	D	147	GLN
1	E	65	GLN
1	E	104	ASN
1	E	263	ASN
1	F	65	GLN
1	F	263	ASN
1	F	286	ASN
1	F	298	GLN

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers

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	289/301 (96%)	0.64	27 (9%) 14 16	33, 59, 104, 130	0
1	B	290/301 (96%)	0.52	24 (8%) 17 19	29, 57, 109, 125	0
1	C	293/301 (97%)	0.29	16 (5%) 30 33	29, 54, 91, 108	0
1	D	295/301 (98%)	0.48	32 (10%) 11 12	30, 62, 101, 129	0
1	E	292/301 (97%)	0.42	15 (5%) 33 36	29, 57, 92, 110	0
1	F	291/301 (96%)	0.33	19 (6%) 25 27	27, 54, 104, 115	0
2	G	11/96 (11%)	1.09	2 (18%) 3 4	56, 68, 92, 94	0
2	H	11/96 (11%)	2.03	4 (36%) 1 1	65, 68, 100, 102	0
3	I	0/7	-	-	-	-
4	J	0/8	-	-	-	-
5	K	0/6	-	-	-	-
All	All	1772/2019 (87%)	0.46	139 (7%) 19 21	27, 57, 101, 130	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	TRP	4.9
2	H	1496	LEU	4.8
1	B	49	LEU	4.2
1	E	269	LYS	3.9
1	D	313	ALA	3.9
1	C	313	ALA	3.9
1	F	41	TRP	3.8
1	C	37	CYS	3.7
2	H	1498	ASP	3.7
1	D	284	LYS	3.6
1	A	45	ASP	3.5
1	A	43	GLY	3.5
1	B	23	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	274	LYS	3.4
1	C	41	TRP	3.4
1	B	177	TYR	3.3
1	B	43	GLY	3.3
1	F	82	LEU	3.3
1	D	282	VAL	3.3
1	C	21	THR	3.3
1	A	87	SER	3.3
1	A	272	THR	3.2
1	A	94	PHE	3.2
1	C	272	THR	3.2
1	A	291	ARG	3.1
1	B	42	LYS	3.1
1	D	277	ASP	3.1
1	F	280	ILE	3.1
1	D	229	GLY	3.0
1	D	280	ILE	3.0
1	F	268	ASP	3.0
1	B	24	VAL	3.0
1	E	262	ARG	3.0
2	G	1478	ASP	2.9
1	B	262	ARG	2.9
2	G	1488	THR	2.9
1	F	291	ARG	2.9
1	B	53	THR	2.9
1	B	80	LYS	2.9
1	B	86	VAL	2.8
1	E	270	GLU	2.8
1	F	80	LYS	2.8
1	E	91	PRO	2.8
1	D	276	LEU	2.8
1	F	305	ASP	2.7
1	E	276	LEU	2.7
1	B	87	SER	2.7
1	A	42	LYS	2.7
1	F	269	LYS	2.7
1	D	263	ASN	2.7
1	F	92	VAL	2.7
1	D	243	ILE	2.6
1	E	31	ALA	2.6
1	C	89	GLU	2.6
1	D	272	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	280	ILE	2.6
1	B	39	MET	2.6
1	B	91	PRO	2.6
1	B	37	CYS	2.6
1	D	43	GLY	2.6
2	H	1499	ASP	2.6
1	F	21	THR	2.6
1	A	66	TYR	2.6
1	A	68	ILE	2.6
1	B	64	LEU	2.5
1	F	91	PRO	2.5
1	A	40	LYS	2.5
1	B	92	VAL	2.5
1	D	69	LYS	2.5
1	D	264	ILE	2.5
1	A	82	LEU	2.5
1	A	39	MET	2.5
1	F	229	GLY	2.5
1	A	81	VAL	2.5
1	E	265	SER	2.5
1	A	37	CYS	2.5
1	F	42	LYS	2.5
1	D	235	GLY	2.5
1	A	26	ILE	2.4
1	B	41	TRP	2.4
1	C	33	MET	2.4
1	C	87	SER	2.4
1	A	24	VAL	2.4
1	C	68	ILE	2.4
1	E	279	LYS	2.4
1	D	286	ASN	2.4
1	A	91	PRO	2.4
1	C	43	GLY	2.4
1	C	274	LYS	2.4
1	A	49	LEU	2.4
1	D	262	ARG	2.4
1	D	90	GLU	2.4
1	F	37	CYS	2.4
1	D	290	LEU	2.4
1	C	263	ASN	2.3
1	E	277	ASP	2.3
1	D	266	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	82	LEU	2.3
1	E	23	THR	2.3
1	E	92	VAL	2.3
1	A	290	LEU	2.3
1	C	39	MET	2.3
1	B	35	PHE	2.2
1	C	22	PHE	2.2
1	F	290	LEU	2.2
1	B	267	SER	2.2
1	F	68	ILE	2.2
1	A	309	ARG	2.2
1	F	263	ASN	2.2
1	D	38	GLU	2.2
1	D	261	ILE	2.2
1	B	77	MET	2.2
1	D	91	PRO	2.2
1	D	68	ILE	2.1
1	D	82	LEU	2.1
1	A	78	ASP	2.1
1	C	70	ASP	2.1
1	D	281	ASP	2.1
1	A	44	LYS	2.1
1	E	88	LYS	2.1
1	D	19	PRO	2.1
1	B	68	ILE	2.1
1	A	83	ASP	2.1
1	D	37	CYS	2.1
1	B	265	SER	2.1
1	F	49	LEU	2.1
1	D	275	PRO	2.1
1	E	288	SER	2.1
2	H	1503	SER	2.1
1	F	88	LYS	2.1
1	A	77	MET	2.1
1	D	283	PHE	2.1
1	D	21	THR	2.0
1	B	257	PRO	2.0
1	D	278	LYS	2.0
1	A	107	GLU	2.0
1	D	288	SER	2.0
1	B	26	ILE	2.0
1	E	68	ILE	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.