



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2023 – 01:49 AM EDT

PDB ID : 3WA0
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

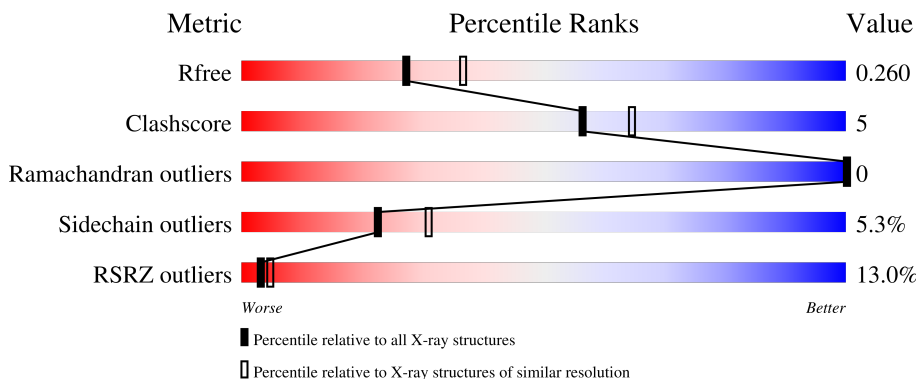
1 Overall quality at a glance

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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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	 15% 81% 12% . .
1	B	301	 13% 81% 13% . .
1	C	301	 8% 83% 14% . .
1	D	301	 13% 83% 15% . .
1	E	301	 12% 85% 11% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	301	
2	G	96	
2	H	96	
3	I	7	
4	J	8	
5	K	6	

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

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

Continued on next page...

Continued from previous page...

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			

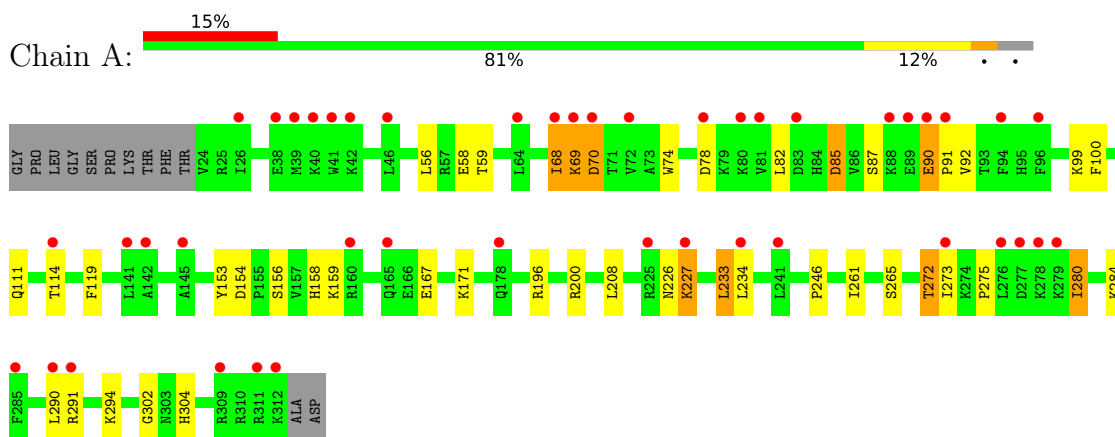
- Molecule 6 is water.

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		

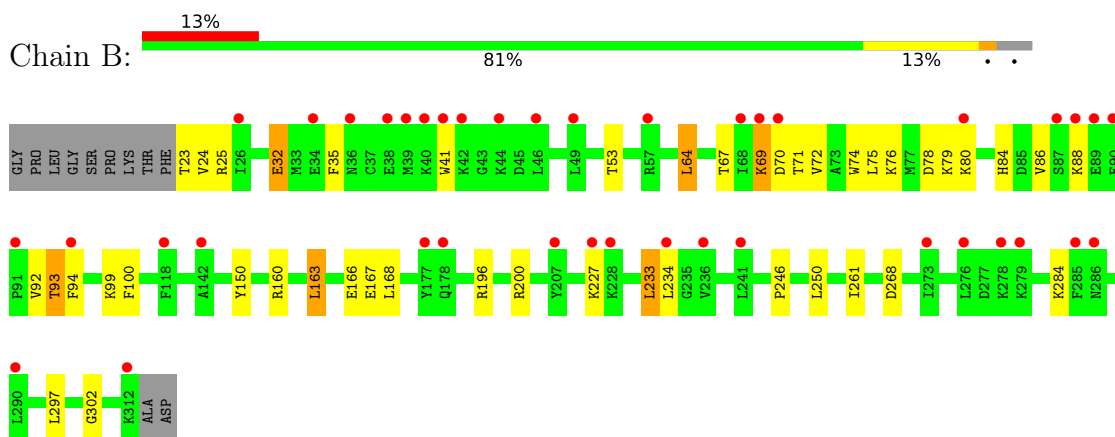
3 Residue-property plots [i](#)

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.

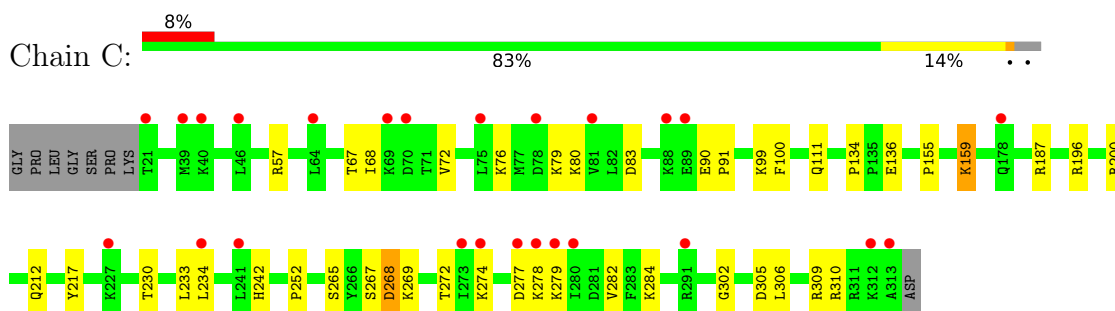
- Molecule 1: Merlin



- Molecule 1: Merlin



- Molecule 1: Merlin



GLY PRO LEU GLY SER TYR ASP ASP THR ASP ASP LEU ASP LEU GLU ASP THR ASP ASP GLN LEU LEU GLU ASP ALA SER GLU LEU GLU ASP ASP ASP ASN ASN ASN ALA GLY GLY ASP GLY ASP ASP ASP PHE SER PRO SER ASP GLU LEU LEU ALA LEU GLU GLY GLY ASP ASP


GLU ASP LEU ASP SER ASP ALA ASP GLU GLU VAL ASP LEU ILE LEU GLY THR ASP SER SER ASP ASN SER ASP L1496 E1497 D1498 L1502 N1505 E1506

- Molecule 3: Protein VPRBP

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Protein VPRBP

Chain J:  88% 12%

X1 X6 X7 X8

- 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) 99.0 (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)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.235 , 0.264 0.230 , 0.260	Depositor DCC
R_{free} test set	6089 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [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	0.35	0/2467	0.52	0/3328
1	B	0.35	0/2470	0.51	0/3334
1	C	0.38	0/2494	0.51	0/3366
1	D	0.36	0/2517	0.53	0/3396
1	E	0.36	0/2488	0.50	0/3359
1	F	0.36	0/2486	0.51	0/3356
2	G	0.46	0/79	0.65	0/106
2	H	0.47	0/75	1.03	1/100 (1.0%)
All	All	0.36	0/15076	0.52	1/20345 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1497	GLU	CB-CA-C	-5.61	99.18	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2409	0	2402	36	0
1	B	2412	0	2405	34	0
1	C	2435	0	2419	24	0
1	D	2457	0	2458	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2429	0	2412	15	0
1	F	2427	0	2419	21	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	147	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 (147) 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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:20:LYS:HG2	1:D:39:MET:HE3	1.81	0.63
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:F:85:ASP:N	1:F:85:ASP:OD1	2.34	0.60
1:B:25:ARG:CD	1:B:93:THR:HG21	2.23	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: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:88:LYS:O	1:F:89:GLU:C	2.42	0.55
1:F:22:PHE:HD2	1:F:39:MET:HE2	1.72	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: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:C:99:LYS:NZ	6:C:439:HOH:O	2.36	0.51
1:B:24:VAL:HG12	1:B:92:VAL:HB	1.93	0.50
1:A:226:ASN:HB2	1:A:227:LYS:HZ1	1.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LYS:O	1:B:88:LYS:HG2	2.12	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: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: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: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: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:C:274:LYS:HZ1	1:C:278:LYS:HD2	1.81	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:C:79:LYS:HZ3	1:C:83:ASP:HB3	1.82	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
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: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:C:134:PRO:HB2	1:E:194:GLU:CD	2.38	0.44
1:D:212:GLN:HA	1:D:217:TYR:CG	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HG	1:B:168:LEU:CD1	2.47	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: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: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:167:GLU:O	1:F:167:GLU:HG3	2.19	0.41
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:A:90:GLU:HA	1:A:91:PRO:C	2.39	0.41
1:F:265:SER:HB2	1:F:272:THR:HB	2.01	0.41
1:D:44:LYS:HA	1:D:77:MET:HE1	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:88:LYS:O	1:E:88:LYS:HG2	2.20	0.40
1:C:212:GLN:HA	1:C:217:TYR:CG	2.56	0.40
1:E:111:GLN:HB3	1:E:113:ILE:HG22	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
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/272 (96%)	247 (95%)	14 (5%)	22	30
1	B	262/272 (96%)	247 (94%)	15 (6%)	20	28
1	C	263/272 (97%)	253 (96%)	10 (4%)	33	46
1	D	267/272 (98%)	254 (95%)	13 (5%)	25	34
1	E	263/272 (97%)	246 (94%)	17 (6%)	17	22
1	F	264/272 (97%)	250 (95%)	14 (5%)	22	31
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%)	1511 (95%)	84 (5%)	22	31

All (84) 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	82	LEU
1	A	85	ASP
1	A	90	GLU
1	A	196	ARG
1	A	200	ARG
1	A	227	LYS
1	A	233	LEU
1	A	234	LEU
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	93	THR
1	B	163	LEU
1	B	167	GLU
1	B	196	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	200	ARG
1	B	233	LEU
1	B	234	LEU
1	B	250	LEU
1	B	268	ASP
1	C	68	ILE
1	C	159	LYS
1	C	196	ARG
1	C	200	ARG
1	C	230	THR
1	C	233	LEU
1	C	234	LEU
1	C	267	SER
1	C	268	ASP
1	C	282	VAL
1	D	21	THR
1	D	44	LYS
1	D	69	LYS
1	D	70	ASP
1	D	72	VAL
1	D	78	ASP
1	D	90	GLU
1	D	107	GLU
1	D	196	ARG
1	D	234	LEU
1	D	241	LEU
1	D	279	LYS
1	D	308	MET
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	85	ASP
1	E	90	GLU
1	E	107	GLU
1	E	176	LEU
1	E	200	ARG
1	E	224	ILE
1	E	225	ARG
1	E	233	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	234	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	196	ARG
1	F	200	ARG
1	F	233	LEU
1	F	234	LEU
1	F	250	LEU
1	F	268	ASP
1	F	288	SER
1	F	290	LEU
2	G	1482	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	298	GLN
1	F	65	GLN
1	F	263	ASN
1	F	286	ASN
1	F	298	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	289/301 (96%)	0.72	44 (15%) 2 3	33, 59, 104, 130	0
1	B	290/301 (96%)	0.73	40 (13%) 2 4	29, 57, 109, 125	0
1	C	293/301 (97%)	0.51	25 (8%) 10 15	29, 54, 91, 108	0
1	D	295/301 (98%)	0.65	40 (13%) 3 4	30, 62, 101, 129	0
1	E	292/301 (97%)	0.56	36 (12%) 4 6	29, 57, 92, 110	0
1	F	291/301 (96%)	0.67	42 (14%) 2 3	27, 54, 104, 115	0
2	G	11/96 (11%)	1.04	2 (18%) 1 1	56, 68, 92, 94	0
2	H	11/96 (11%)	1.26	2 (18%) 1 1	65, 68, 100, 102	0
3	I	0/7	-	-	-	-
4	J	0/8	-	-	-	-
5	K	0/6	-	-	-	-
All	All	1772/2019 (87%)	0.65	231 (13%) 3 5	27, 57, 101, 130	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	LYS	10.5
1	C	313	ALA	6.9
1	D	281	ASP	6.3
1	E	279	LYS	6.2
1	D	280	ILE	5.7
1	F	279	LYS	5.5
1	A	278	LYS	5.4
1	D	284	LYS	5.3
1	A	83	ASP	5.2
1	D	277	ASP	5.1
1	B	38	GLU	5.1
1	E	278	LYS	5.1
1	B	40	LYS	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	279	LYS	4.9
1	B	42	LYS	4.7
1	F	280	ILE	4.6
1	A	291	ARG	4.6
1	A	41	TRP	4.6
1	D	40	LYS	4.5
1	A	64	LEU	4.5
1	B	70	ASP	4.5
1	F	40	LYS	4.4
1	B	312	LYS	4.4
1	A	279	LYS	4.3
2	H	1498	ASP	4.3
1	D	313	ALA	4.3
1	A	42	LYS	4.3
1	F	291	ARG	4.3
1	E	276	LEU	4.3
1	F	229	GLY	4.3
1	D	229	GLY	4.2
1	C	88	LYS	4.2
1	D	227	LYS	4.2
1	A	46	LEU	4.1
1	A	312	LYS	4.1
1	F	46	LEU	4.1
1	C	39	MET	4.1
1	F	21	THR	4.1
1	C	241	LEU	4.1
1	D	234	LEU	4.1
1	A	88	LYS	4.0
1	B	227	LYS	4.0
1	F	268	ASP	4.0
1	B	290	LEU	4.0
1	B	178	GLN	4.0
1	B	46	LEU	3.9
1	D	19	PRO	3.9
1	F	290	LEU	3.9
1	B	90	GLU	3.8
1	F	90	GLU	3.8
1	F	64	LEU	3.8
1	E	291	ARG	3.8
1	F	88	LYS	3.8
1	D	288	SER	3.7
1	B	34	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	39	MET	3.7
1	D	241	LEU	3.7
1	E	46	LEU	3.6
1	B	39	MET	3.6
1	F	228	LYS	3.6
1	D	274	LYS	3.6
1	E	277	ASP	3.5
1	D	278	LYS	3.5
1	F	234	LEU	3.5
1	F	78	ASP	3.5
1	F	87	SER	3.4
1	C	89	GLU	3.4
1	C	40	LYS	3.4
1	B	68	ILE	3.4
1	D	46	LEU	3.4
2	G	1487	ASP	3.4
1	D	21	THR	3.4
1	E	89	GLU	3.4
1	C	78	ASP	3.4
1	C	234	LEU	3.4
1	D	291	ARG	3.4
1	D	75	LEU	3.4
1	A	69	LYS	3.4
1	A	277	ASP	3.3
1	A	90	GLU	3.3
1	E	78	ASP	3.3
1	E	269	LYS	3.3
1	A	68	ILE	3.3
1	D	64	LEU	3.2
1	E	288	SER	3.2
1	C	69	LYS	3.2
1	B	26	ILE	3.2
1	B	41	TRP	3.2
1	E	40	LYS	3.2
1	D	78	ASP	3.2
1	B	80	LYS	3.2
1	D	236	VAL	3.1
1	A	80	LYS	3.1
1	E	228	LYS	3.1
1	A	234	LEU	3.1
1	E	64	LEU	3.1
1	F	75	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	296	ILE	3.1
1	E	274	LYS	3.1
1	E	227	LYS	3.1
1	D	20	LYS	3.0
1	B	228	LYS	3.0
1	F	69	LYS	3.0
1	C	64	LEU	3.0
1	F	41	TRP	3.0
1	D	285	PHE	3.0
1	A	89	GLU	3.0
1	E	90	GLU	2.9
1	B	69	LYS	2.9
1	E	236	VAL	2.9
1	D	289	LYS	2.9
1	A	309	ARG	2.9
1	B	44	LYS	2.8
1	B	279	LYS	2.8
1	A	78	ASP	2.8
1	B	94	PHE	2.8
1	F	227	LYS	2.8
1	F	80	LYS	2.8
1	B	234	LEU	2.8
1	A	38	GLU	2.8
1	E	39	MET	2.7
1	D	68	ILE	2.7
1	D	312	LYS	2.7
1	A	70	ASP	2.7
1	F	22	PHE	2.7
1	D	178	GLN	2.7
1	E	69	LYS	2.7
1	D	225	ARG	2.7
1	F	94	PHE	2.7
1	F	70	ASP	2.7
1	E	24	VAL	2.7
1	A	227	LYS	2.7
1	B	88	LYS	2.7
1	F	269	LYS	2.7
1	C	46	LEU	2.7
1	B	49	LEU	2.6
1	E	88	LYS	2.6
1	B	236	VAL	2.6
1	B	241	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	89	GLU	2.6
1	A	276	LEU	2.6
1	D	94	PHE	2.6
1	F	91	PRO	2.6
1	F	276	LEU	2.6
1	F	26	ILE	2.6
1	A	165	GLN	2.6
2	G	1486	GLY	2.6
1	D	273	ILE	2.5
1	C	21	THR	2.5
1	C	277	ASP	2.5
1	D	253	LYS	2.5
1	F	83	ASP	2.5
1	A	273	ILE	2.5
1	F	241	LEU	2.5
1	A	311	ARG	2.5
1	F	34	GLU	2.4
1	A	72	VAL	2.4
1	F	207	TYR	2.4
1	A	178	GLN	2.4
1	D	268	ASP	2.4
1	E	265	SER	2.4
1	B	57	ARG	2.4
1	B	91	PRO	2.4
1	F	285	PHE	2.4
2	H	1497	GLU	2.4
1	A	225	ARG	2.4
1	F	235	GLY	2.4
1	E	234	LEU	2.4
1	B	273	ILE	2.3
1	C	279	LYS	2.3
1	D	286	ASN	2.3
1	C	291	ARG	2.3
1	E	70	ASP	2.3
1	C	273	ILE	2.3
1	C	178	GLN	2.3
1	E	289	LYS	2.3
1	A	141	LEU	2.3
1	A	285	PHE	2.3
1	B	278	LYS	2.3
1	E	280	ILE	2.3
1	B	177	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	81	VAL	2.3
1	D	290	LEU	2.2
1	A	96	PHE	2.2
1	E	26	ILE	2.2
1	A	290	LEU	2.2
1	B	118	PHE	2.2
1	A	142	ALA	2.2
1	B	36	ASN	2.2
1	E	83	ASP	2.2
1	E	241	LEU	2.2
1	F	281	ASP	2.2
1	A	160	ARG	2.2
1	C	312	LYS	2.2
1	D	269	LYS	2.2
1	E	235	GLY	2.2
1	A	26	ILE	2.2
1	F	224	ILE	2.2
1	C	278	LYS	2.2
1	F	57	ARG	2.2
1	B	87	SER	2.2
1	E	285	PHE	2.2
1	A	114	THR	2.2
1	C	75	LEU	2.2
1	E	75	LEU	2.2
1	E	230	THR	2.1
1	C	280	ILE	2.1
1	A	241	LEU	2.1
1	A	94	PHE	2.1
1	B	285	PHE	2.1
1	D	228	LYS	2.1
1	A	91	PRO	2.1
1	B	207	TYR	2.1
1	F	89	GLU	2.1
1	D	230	THR	2.1
1	F	38	GLU	2.1
1	B	286	ASN	2.1
1	C	227	LYS	2.1
1	F	23	THR	2.1
1	F	79	LYS	2.1
1	A	81	VAL	2.1
1	E	160	ARG	2.0
1	D	38	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	94	PHE	2.0
1	C	274	LYS	2.0
1	B	276	LEU	2.0
1	C	81	VAL	2.0
1	D	80	LYS	2.0
1	C	70	ASP	2.0
1	A	145	ALA	2.0
1	B	142	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.