



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 07:33 pm GMT

PDB ID : 5F5O  
Title : Crystal structure of Marburg virus nucleoprotein core domain bound to VP35 regulation peptide  
Authors : Guo, Y.; Liu, B.C.; Liu, X.; Li, G.B.; Wang, W.M.; Dong, S.S.; Wang, W.J.  
Deposited on : 2015-12-04  
Resolution : 2.20 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

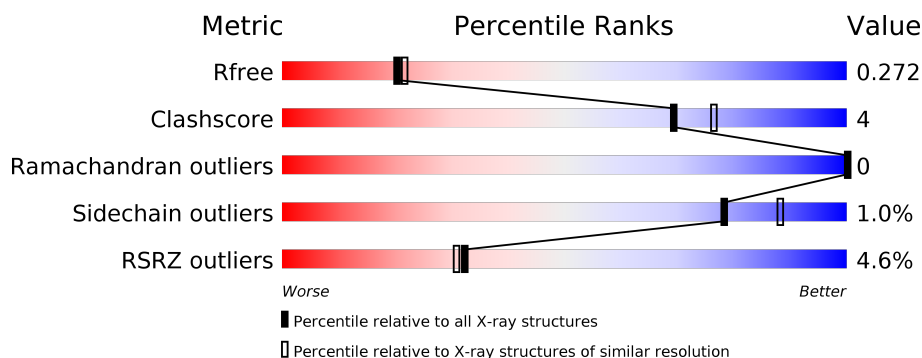
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	373	<div> <div>3%</div> <div>77% 7% • 16%</div> </div>
1	C	373	<div> <div>4%</div> <div>74% 11% 15%</div> </div>
1	E	373	<div> <div>3%</div> <div>73% 11% 16%</div> </div>
2	B	29	<div> <div>3%</div> <div>69% 17% • 10%</div> </div>
2	D	29	<div> <div>7%</div> <div>90% • 7%</div> </div>
2	F	29	<div> <div>17%</div> <div>83% 10% 7%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8248 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2453	1568	425	456	4			
1	C	318	Total	C	N	O	S	0	0	0
			2481	1585	432	460	4			
1	E	315	Total	C	N	O	S	0	0	0
			2451	1568	423	456	4			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q6UY69
A	-1	GLY	-	expression tag	UNP Q6UY69
A	0	SER	-	expression tag	UNP Q6UY69
A	1	SER	-	expression tag	UNP Q6UY69
A	2	HIS	-	expression tag	UNP Q6UY69
A	3	HIS	-	expression tag	UNP Q6UY69
A	4	HIS	-	expression tag	UNP Q6UY69
A	5	HIS	-	expression tag	UNP Q6UY69
A	6	HIS	-	expression tag	UNP Q6UY69
A	7	HIS	-	expression tag	UNP Q6UY69
A	8	SER	-	expression tag	UNP Q6UY69
A	9	SER	-	expression tag	UNP Q6UY69
A	10	GLY	-	expression tag	UNP Q6UY69
A	11	LEU	-	expression tag	UNP Q6UY69
A	12	VAL	-	expression tag	UNP Q6UY69
A	13	PRO	-	expression tag	UNP Q6UY69
A	14	ARG	-	expression tag	UNP Q6UY69
A	15	GLY	-	expression tag	UNP Q6UY69
A	16	SER	-	expression tag	UNP Q6UY69
A	17	HIS	-	expression tag	UNP Q6UY69
A	18	MET	-	expression tag	UNP Q6UY69
C	-2	MET	-	expression tag	UNP Q6UY69
C	-1	GLY	-	expression tag	UNP Q6UY69

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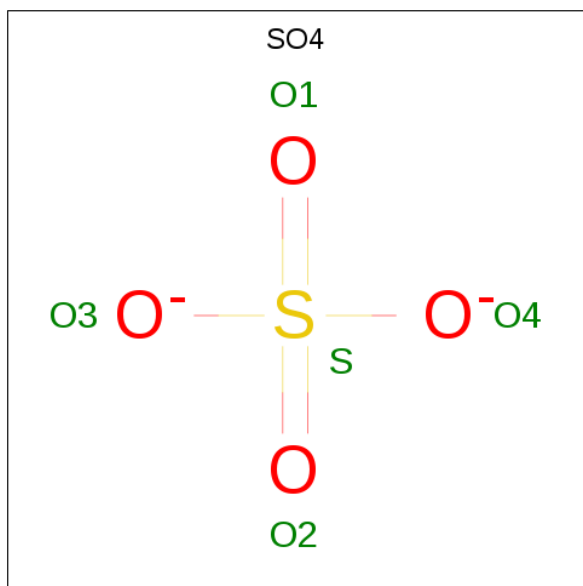
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q6UY69
C	1	SER	-	expression tag	UNP Q6UY69
C	2	HIS	-	expression tag	UNP Q6UY69
C	3	HIS	-	expression tag	UNP Q6UY69
C	4	HIS	-	expression tag	UNP Q6UY69
C	5	HIS	-	expression tag	UNP Q6UY69
C	6	HIS	-	expression tag	UNP Q6UY69
C	7	HIS	-	expression tag	UNP Q6UY69
C	8	SER	-	expression tag	UNP Q6UY69
C	9	SER	-	expression tag	UNP Q6UY69
C	10	GLY	-	expression tag	UNP Q6UY69
C	11	LEU	-	expression tag	UNP Q6UY69
C	12	VAL	-	expression tag	UNP Q6UY69
C	13	PRO	-	expression tag	UNP Q6UY69
C	14	ARG	-	expression tag	UNP Q6UY69
C	15	GLY	-	expression tag	UNP Q6UY69
C	16	SER	-	expression tag	UNP Q6UY69
C	17	HIS	-	expression tag	UNP Q6UY69
C	18	MET	-	expression tag	UNP Q6UY69
E	-2	MET	-	expression tag	UNP Q6UY69
E	-1	GLY	-	expression tag	UNP Q6UY69
E	0	SER	-	expression tag	UNP Q6UY69
E	1	SER	-	expression tag	UNP Q6UY69
E	2	HIS	-	expression tag	UNP Q6UY69
E	3	HIS	-	expression tag	UNP Q6UY69
E	4	HIS	-	expression tag	UNP Q6UY69
E	5	HIS	-	expression tag	UNP Q6UY69
E	6	HIS	-	expression tag	UNP Q6UY69
E	7	HIS	-	expression tag	UNP Q6UY69
E	8	SER	-	expression tag	UNP Q6UY69
E	9	SER	-	expression tag	UNP Q6UY69
E	10	GLY	-	expression tag	UNP Q6UY69
E	11	LEU	-	expression tag	UNP Q6UY69
E	12	VAL	-	expression tag	UNP Q6UY69
E	13	PRO	-	expression tag	UNP Q6UY69
E	14	ARG	-	expression tag	UNP Q6UY69
E	15	GLY	-	expression tag	UNP Q6UY69
E	16	SER	-	expression tag	UNP Q6UY69
E	17	HIS	-	expression tag	UNP Q6UY69
E	18	MET	-	expression tag	UNP Q6UY69

- Molecule 2 is a protein called Peptide from Polymerase cofactor VP35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	26	Total	C	N	O	S	0	0	0
			200	127	31	40	2			
2	D	27	Total	C	N	O	S	0	0	0
			208	131	33	42	2			
2	F	27	Total	C	N	O	S	0	0	0
			208	132	32	41	3			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		
4	B	8	Total	O	0	0
			8	8		
4	C	69	Total	O	0	0
			69	69		
4	D	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	75	Total	O	0	0
			75	75		
4	F	3	Total	O	0	0
			3	3		

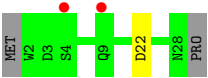
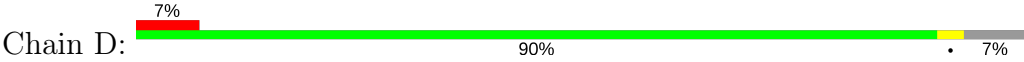




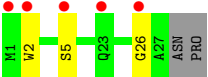
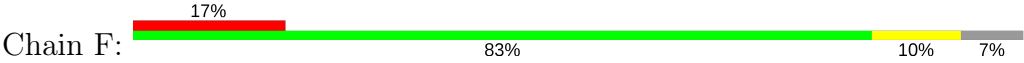
• Molecule 2: Peptide from Polymerase cofactor VP35



• Molecule 2: Peptide from Polymerase cofactor VP35



• Molecule 2: Peptide from Polymerase cofactor VP35





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.40Å 98.40Å 95.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.91 – 2.20 49.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (31.91-2.20) 95.5 (49.20-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.20 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.214 , 0.277 0.211 , 0.272	Depositor DCC
$R_{free}$ test set	2483 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 15.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l 0.358 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
Reported twinning fraction	0.631 for H, K, L 0.369 for K, H, -L	Depositor
Outliers	0 of 50366 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.80	0/2500	0.97	7/3391 (0.2%)
1	C	0.80	0/2528	0.98	7/3428 (0.2%)
1	E	0.73	1/2496 (0.0%)	0.86	3/3384 (0.1%)
2	B	0.84	0/204	0.91	0/275
2	D	0.74	0/212	0.81	0/286
2	F	0.76	0/212	0.92	1/285 (0.4%)
All	All	0.78	1/8152 (0.0%)	0.93	18/11049 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	224	SER	CB-OG	-5.05	1.35	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	GLY	N-CA-C	7.70	132.36	113.10
1	E	187	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	C	309	HIS	N-CA-C	-6.59	93.21	111.00
2	F	5	SER	N-CA-C	6.54	128.66	111.00
1	C	222	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	E	187	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	C	128	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	64	TYR	N-CA-C	6.00	127.21	111.00
1	C	156	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	64	TYR	N-CA-CB	-5.88	100.01	110.60
1	A	309	HIS	CA-C-N	5.50	127.21	116.20
1	A	271	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	E	119	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	309	HIS	N-CA-C	5.22	125.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	208	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	203	LEU	CB-CG-CD2	5.12	119.70	111.00
1	C	40	ASP	CB-CG-OD1	5.03	122.83	118.30

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	2453	0	2485	16	0
1	C	2481	0	2517	19	0
1	E	2451	0	2488	26	0
2	B	200	0	188	6	0
2	D	208	0	194	0	0
2	F	208	0	200	2	0
3	A	5	0	0	0	0
3	C	10	0	0	0	0
4	A	69	0	0	0	0
4	B	8	0	0	0	0
4	C	69	0	0	0	0
4	D	8	0	0	0	0
4	E	75	0	0	1	0
4	F	3	0	0	0	0
All	All	8248	0	8072	65	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 4.

All (65) 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:E:271:ARG:HD3	4:E:452:HOH:O	1.87	0.73
1:E:197:ILE:HD12	1:E:282:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:LEU:HD23	1:E:119:LEU:CD2	2.29	0.62
1:E:318:VAL:HG23	1:E:322:TYR:HB2	1.84	0.59
1:E:116:LEU:HD23	1:E:119:LEU:HD23	1.85	0.59
1:C:269:LEU:HD22	1:C:290:LEU:CD1	2.33	0.58
1:E:246:LEU:HD22	1:E:250:VAL:HG11	1.86	0.58
1:E:309:HIS:CD2	2:F:2:TRP:HB3	2.38	0.57
1:E:28:THR:HG21	1:E:34:ILE:CD1	2.35	0.56
1:E:305:VAL:HG13	1:E:333:GLU:HG3	1.86	0.56
1:A:63:HIS:O	1:A:207:HIS:CD2	2.59	0.55
1:C:274:GLU:O	1:C:277:PRO:HD2	2.08	0.54
1:A:31:GLN:HB3	1:A:62:GLU:OE2	2.07	0.54
1:A:199:GLN:HA	1:A:199:GLN:OE1	2.07	0.54
1:E:199:GLN:NE2	1:E:203:LEU:HD22	2.23	0.54
1:E:144:VAL:HG13	1:E:281:VAL:HG22	1.91	0.53
1:A:303:LEU:HD23	1:A:326:ARG:HD3	1.92	0.52
1:C:197:ILE:O	1:C:201:VAL:HG12	2.11	0.51
1:E:161:HIS:HB3	1:E:167:VAL:HG12	1.92	0.51
1:A:28:THR:HA	1:A:93:ASN:O	2.11	0.51
1:C:154:ALA:O	1:C:158:VAL:HG23	2.11	0.50
1:A:66:ASN:HD21	1:C:66:ASN:HB3	1.77	0.50
1:C:304:GLY:HA3	1:C:329:ALA:HB3	1.94	0.50
1:E:301:ILE:O	1:E:305:VAL:HG23	2.12	0.49
1:A:61:VAL:HG12	1:A:67:SER:HA	1.94	0.49
1:A:229:VAL:HG11	1:A:290:LEU:O	2.12	0.49
1:C:139:PHE:HB2	1:C:186:LEU:HD13	1.95	0.49
1:E:292:HIS:CD2	1:E:316:VAL:HG22	2.48	0.48
1:E:263:LYS:NZ	2:F:26:GLY:O	2.38	0.47
1:A:64:TYR:CZ	1:A:199:GLN:HG3	2.50	0.46
1:E:245:THR:HG22	1:E:246:LEU:O	2.16	0.46
1:E:116:LEU:HD23	1:E:119:LEU:HD21	1.97	0.46
1:C:142:LYS:HB2	1:C:150:SER:HA	1.99	0.45
1:E:139:PHE:HB2	1:E:186:LEU:CD1	2.47	0.44
1:C:197:ILE:HD13	1:C:278:PHE:HB3	2.00	0.44
1:A:197:ILE:HD13	1:A:278:PHE:HB3	2.00	0.44
1:E:99:PHE:O	1:E:102:VAL:HG22	2.18	0.44
1:A:269:LEU:HD21	2:B:15:MET:CE	2.47	0.44
1:E:28:THR:HG21	1:E:34:ILE:HD12	1.99	0.43
1:C:34:ILE:HD12	1:C:98:ARG:C	2.38	0.43
1:C:249:LEU:O	1:C:252:THR:HG23	2.18	0.43
1:A:231:THR:HA	1:A:234:GLU:OE2	2.18	0.43
1:C:214:ILE:O	1:C:218:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:HD22	1:C:290:LEU:HD13	2.01	0.43
1:C:137:SER:HB2	1:C:196:LEU:HD22	2.01	0.42
1:E:276:ALA:N	1:E:277:PRO:CD	2.82	0.42
2:B:2:TRP:NE1	2:B:7:MET:HG3	2.35	0.42
2:B:4:SER:O	2:B:6:TYR:N	2.52	0.42
1:C:336:LEU:C	1:C:337:GLN:OE1	2.58	0.42
1:C:27:ASP:HB3	1:C:92:LYS:HA	2.01	0.42
1:E:62:GLU:OE2	1:E:67:SER:HB2	2.19	0.42
1:A:203:LEU:HD13	1:A:215:SER:HB2	2.01	0.42
1:A:303:LEU:HD23	1:A:326:ARG:CD	2.50	0.42
1:C:247:HIS:O	1:C:250:VAL:HB	2.20	0.42
2:B:3:ASP:O	2:B:4:SER:OG	2.32	0.41
1:E:279:ALA:HB1	1:E:287:ILE:HD13	2.02	0.41
2:B:4:SER:C	2:B:6:TYR:H	2.24	0.41
2:B:4:SER:C	2:B:6:TYR:N	2.73	0.41
1:A:303:LEU:O	1:A:304:GLY:C	2.59	0.41
1:C:203:LEU:O	1:C:207:HIS:NE2	2.53	0.41
1:A:164:GLN:OE1	1:A:166:ILE:HD12	2.21	0.41
1:C:50:ASP:OD1	1:C:50:ASP:C	2.58	0.41
1:E:155:LEU:HA	1:E:155:LEU:HD23	1.94	0.40
1:E:136:CYS:O	1:E:186:LEU:HD11	2.21	0.40
1:E:196:LEU:HA	1:E:196:LEU:HD23	1.92	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	313/373 (84%)	291 (93%)	22 (7%)	0	100	100
1	C	316/373 (85%)	296 (94%)	20 (6%)	0	100	100
1	E	311/373 (83%)	305 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	24/29 (83%)	21 (88%)	3 (12%)	0	100	100
2	D	25/29 (86%)	24 (96%)	1 (4%)	0	100	100
2	F	25/29 (86%)	23 (92%)	2 (8%)	0	100	100
All	All	1014/1206 (84%)	960 (95%)	54 (5%)	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	270/323 (84%)	269 (100%)	1 (0%)	92	96
1	C	273/323 (84%)	270 (99%)	3 (1%)	76	87
1	E	270/323 (84%)	267 (99%)	3 (1%)	76	87
2	B	22/25 (88%)	21 (96%)	1 (4%)	30	37
2	D	23/25 (92%)	22 (96%)	1 (4%)	32	39
2	F	23/25 (92%)	23 (100%)	0	100	100
All	All	881/1044 (84%)	872 (99%)	9 (1%)	78	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ARG
2	B	6	TYR
1	C	162	GLN
1	C	171	ASN
1	C	338	ARG
2	D	22	ASP
1	E	251	ARG
1	E	291	GLU
1	E	313	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	A	401	-	4,4,4	0.41	0	6,6,6	0.66	0
3	SO4	C	401	-	4,4,4	0.51	0	6,6,6	0.67	0
3	SO4	C	402	-	4,4,4	0.60	0	6,6,6	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	401	-	-	0/0/0/0	0/0/0/0
3	SO4	C	401	-	-	0/0/0/0	0/0/0/0
3	SO4	C	402	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	315/373 (84%)	0.30	12 (3%) 40 38	10, 28, 56, 68	0
1	C	318/373 (85%)	0.48	15 (4%) 31 30	16, 30, 60, 75	0
1	E	315/373 (84%)	0.20	12 (3%) 40 38	15, 30, 55, 74	0
2	B	26/29 (89%)	0.59	1 (3%) 40 38	25, 37, 63, 78	0
2	D	27/29 (93%)	0.60	2 (7%) 14 13	21, 39, 57, 64	0
2	F	27/29 (93%)	0.79	5 (18%) 1 1	15, 32, 52, 53	0
All	All	1028/1206 (85%)	0.35	47 (4%) 32 31	10, 30, 58, 78	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	5	SER	5.0
1	C	243	GLY	5.0
2	D	4	SER	5.0
1	C	97	THR	4.1
1	A	241	ASP	3.6
1	C	315	GLY	3.5
1	C	313	LEU	3.5
2	F	1	MET	3.4
1	E	251	ARG	3.3
1	E	320	GLU	3.3
1	E	319	GLY	3.2
1	E	318	VAL	3.2
1	A	97	THR	3.1
1	C	303	LEU	3.1
1	A	148	ARG	3.1
1	C	321	GLN	3.0
1	A	324	GLN	2.8
1	A	329	ALA	2.8
1	E	313	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	205	THR	2.7
1	C	324	GLN	2.7
1	A	243	GLY	2.7
1	C	325	LEU	2.7
1	E	239	LYS	2.6
1	E	324	GLN	2.5
1	C	328	ALA	2.5
1	C	77	ILE	2.5
1	A	306	ALA	2.5
1	A	250	VAL	2.4
1	A	334	VAL	2.4
2	B	2	TRP	2.4
1	A	96	ALA	2.4
1	C	74	THR	2.4
1	E	67	SER	2.3
1	C	307	THR	2.3
1	C	204	VAL	2.2
2	F	2	TRP	2.2
1	A	317	ASN	2.2
1	C	312	THR	2.2
2	F	26	GLY	2.2
2	F	23	GLN	2.2
1	E	124	SER	2.2
1	E	122	THR	2.2
1	C	203	LEU	2.1
1	E	257	ASN	2.1
2	D	9	GLN	2.0
1	A	203	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	C	402	5/5	0.89	0.23	39,42,46,48	0
3	SO4	C	401	5/5	0.95	0.12	46,47,49,53	0
3	SO4	A	401	5/5	0.96	0.09	36,37,41,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.