



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2019 – 12:47 PM EDT

PDB ID : 4D5T  
Title : Structure of N-terminally truncated A49 from Vaccinia Virus Western Reserve  
Authors : Neidel, S.; Maluquer de Motes, C.; Mansur, D.S.; Strnadova, P.; Smith, G.L.;  
Graham, S.C.  
Deposited on : 2014-11-07  
Resolution : 1.84 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
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) : rb-20031633

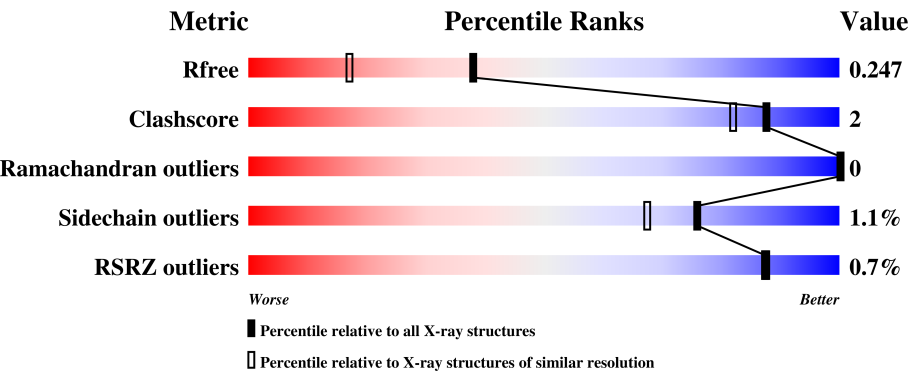
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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 <sub>free</sub>	111664	3313 (1.86-1.82)
Clashscore	122126	3530 (1.86-1.82)
Ramachandran outliers	120053	3495 (1.86-1.82)
Sidechain outliers	120020	3496 (1.86-1.82)
RSRZ outliers	108989	3265 (1.86-1.82)

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	160	<div><div></div><div>88%7%6%</div></div>
1	B	160	<div><div>3%</div><div>91%6%</div></div>
1	C	160	<div><div></div><div>86%8%6%</div></div>
1	D	160	<div><div>%</div><div>88%5%6%</div></div>
1	E	160	<div><div></div><div>88%7%6%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	160	<div><div>%</div><div><div></div><div>85%</div><div>8%</div><div>6%</div></div></div>
1	G	160	<div><div></div><div>86%</div><div>8%</div><div>6%</div></div>
1	H	160	<div><div></div><div>89%</div><div>5%</div><div>6%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11015 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 PROTEIN A49R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	11	0
			1290	812	205	265	8			
1	B	151	Total	C	N	O	S	0	9	0
			1281	805	205	263	8			
1	C	150	Total	C	N	O	S	0	11	0
			1297	816	206	267	8			
1	D	151	Total	C	N	O	S	0	8	0
			1276	804	205	260	7			
1	E	151	Total	C	N	O	S	0	4	0
			1248	791	198	252	7			
1	F	150	Total	C	N	O	S	0	4	0
			1238	784	194	254	6			
1	G	150	Total	C	N	O	S	0	5	0
			1242	787	196	252	7			
1	H	150	Total	C	N	O	S	0	3	0
			1224	777	196	244	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	expression tag	UNP P31037
A	163	GLY	-	expression tag	UNP P31037
A	164	SER	-	expression tag	UNP P31037
A	165	LYS	-	expression tag	UNP P31037
A	166	HIS	-	expression tag	UNP P31037
A	167	HIS	-	expression tag	UNP P31037
A	168	HIS	-	expression tag	UNP P31037
A	169	HIS	-	expression tag	UNP P31037
A	170	HIS	-	expression tag	UNP P31037
A	171	HIS	-	expression tag	UNP P31037
B	12	MET	-	expression tag	UNP P31037
B	163	GLY	-	expression tag	UNP P31037
B	164	SER	-	expression tag	UNP P31037

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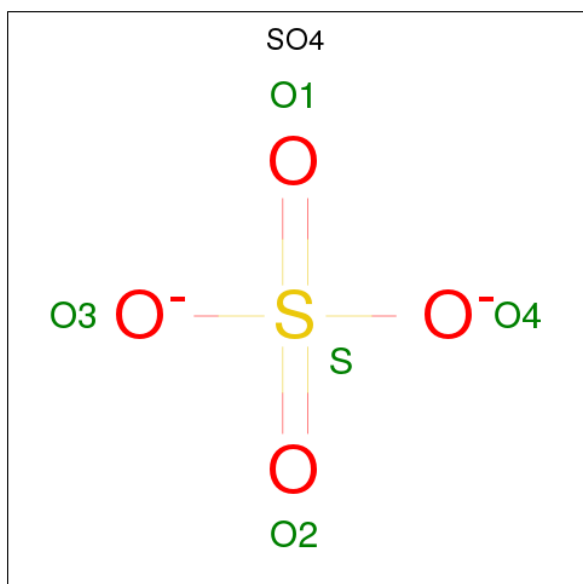
Chain	Residue	Modelled	Actual	Comment	Reference
B	165	LYS	-	expression tag	UNP P31037
B	166	HIS	-	expression tag	UNP P31037
B	167	HIS	-	expression tag	UNP P31037
B	168	HIS	-	expression tag	UNP P31037
B	169	HIS	-	expression tag	UNP P31037
B	170	HIS	-	expression tag	UNP P31037
B	171	HIS	-	expression tag	UNP P31037
C	12	MET	-	expression tag	UNP P31037
C	163	GLY	-	expression tag	UNP P31037
C	164	SER	-	expression tag	UNP P31037
C	165	LYS	-	expression tag	UNP P31037
C	166	HIS	-	expression tag	UNP P31037
C	167	HIS	-	expression tag	UNP P31037
C	168	HIS	-	expression tag	UNP P31037
C	169	HIS	-	expression tag	UNP P31037
C	170	HIS	-	expression tag	UNP P31037
C	171	HIS	-	expression tag	UNP P31037
D	12	MET	-	expression tag	UNP P31037
D	163	GLY	-	expression tag	UNP P31037
D	164	SER	-	expression tag	UNP P31037
D	165	LYS	-	expression tag	UNP P31037
D	166	HIS	-	expression tag	UNP P31037
D	167	HIS	-	expression tag	UNP P31037
D	168	HIS	-	expression tag	UNP P31037
D	169	HIS	-	expression tag	UNP P31037
D	170	HIS	-	expression tag	UNP P31037
D	171	HIS	-	expression tag	UNP P31037
E	12	MET	-	expression tag	UNP P31037
E	163	GLY	-	expression tag	UNP P31037
E	164	SER	-	expression tag	UNP P31037
E	165	LYS	-	expression tag	UNP P31037
E	166	HIS	-	expression tag	UNP P31037
E	167	HIS	-	expression tag	UNP P31037
E	168	HIS	-	expression tag	UNP P31037
E	169	HIS	-	expression tag	UNP P31037
E	170	HIS	-	expression tag	UNP P31037
E	171	HIS	-	expression tag	UNP P31037
F	12	MET	-	expression tag	UNP P31037
F	163	GLY	-	expression tag	UNP P31037
F	164	SER	-	expression tag	UNP P31037
F	165	LYS	-	expression tag	UNP P31037
F	166	HIS	-	expression tag	UNP P31037

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Chain	Residue	Modelled	Actual	Comment	Reference
F	167	HIS	-	expression tag	UNP P31037
F	168	HIS	-	expression tag	UNP P31037
F	169	HIS	-	expression tag	UNP P31037
F	170	HIS	-	expression tag	UNP P31037
F	171	HIS	-	expression tag	UNP P31037
G	12	MET	-	expression tag	UNP P31037
G	163	GLY	-	expression tag	UNP P31037
G	164	SER	-	expression tag	UNP P31037
G	165	LYS	-	expression tag	UNP P31037
G	166	HIS	-	expression tag	UNP P31037
G	167	HIS	-	expression tag	UNP P31037
G	168	HIS	-	expression tag	UNP P31037
G	169	HIS	-	expression tag	UNP P31037
G	170	HIS	-	expression tag	UNP P31037
G	171	HIS	-	expression tag	UNP P31037
H	12	MET	-	expression tag	UNP P31037
H	163	GLY	-	expression tag	UNP P31037
H	164	SER	-	expression tag	UNP P31037
H	165	LYS	-	expression tag	UNP P31037
H	166	HIS	-	expression tag	UNP P31037
H	167	HIS	-	expression tag	UNP P31037
H	168	HIS	-	expression tag	UNP P31037
H	169	HIS	-	expression tag	UNP P31037
H	170	HIS	-	expression tag	UNP P31037
H	171	HIS	-	expression tag	UNP P31037

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0


- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	152	Total O 152 152	0	0
3	B	113	Total O 113 113	0	0
3	C	126	Total O 126 126	0	0
3	D	87	Total O 87 87	0	0
3	E	129	Total O 129 129	0	0
3	F	95	Total O 95 95	0	0
3	G	110	Total O 110 110	0	0
3	H	82	Total O 82 82	0	0

### 3 Residue-property plots [i](#)

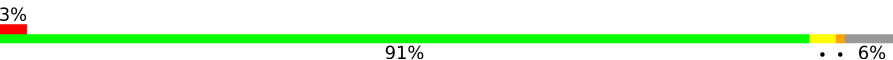
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: PROTEIN A49R

Chain A: 




- Molecule 1: PROTEIN A49R

Chain B: 




- Molecule 1: PROTEIN A49R

Chain C: 




- Molecule 1: PROTEIN A49R

Chain D: 




- Molecule 1: PROTEIN A49R

Chain E: 



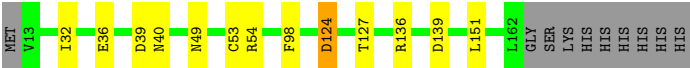
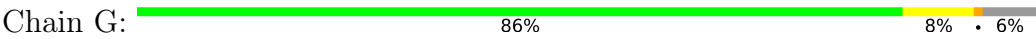
- Molecule 1: PROTEIN A49R

Chain F: 

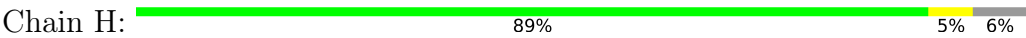




• Molecule 1: PROTEIN A49R



• Molecule 1: PROTEIN A49R



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.29Å 45.63Å 160.26Å 90.00° 98.74° 90.00°	Depositor
Resolution (Å)	45.71 – 1.84 45.71 – 1.84	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.71-1.84) 97.6 (45.71-1.84)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 1.84Å)	Xtrriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.206 , 0.239 0.215 , 0.247	Depositor DCC
$R_{free}$ test set	5665 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtrriage
Anisotropy	0.289	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6125e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.88	0/1308	0.95	4/1775 (0.2%)
1	B	0.86	0/1296	0.87	2/1758 (0.1%)
1	C	0.90	0/1312	0.98	6/1779 (0.3%)
1	D	0.86	0/1291	0.87	4/1750 (0.2%)
1	E	0.91	2/1263 (0.2%)	0.90	0/1714
1	F	0.81	0/1253	0.85	2/1702 (0.1%)
1	G	0.89	0/1263	0.89	2/1715 (0.1%)
1	H	0.82	0/1239	0.84	0/1683
All	All	0.87	2/10225 (0.0%)	0.90	20/13876 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	148	GLU	CD-OE2	-5.75	1.19	1.25
1	E	36	GLU	CD-OE2	5.49	1.31	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	A	141	ASP	CB-CG-OD2	-8.76	110.42	118.30
1	C	141	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	G	124	ASP	CB-CG-OD2	6.58	124.23	118.30
1	A	98	PHE	CB-CG-CD1	-6.44	116.29	120.80
1	A	147	ARG	CB-CA-C	-6.12	98.16	110.40
1	F	136	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	147	ARG	CB-CA-C	-6.08	98.25	110.40
1	A	147	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	G	136	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	98	PHE	CB-CG-CD1	-5.54	116.92	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	D	98	PHE	CB-CG-CD1	-5.45	116.99	120.80
1	F	54	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	D	36	GLU	CG-CD-OE1	5.37	129.04	118.30
1	C	147	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	54	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	54	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	36	GLU	CG-CD-OE2	-5.05	108.20	118.30
1	C	147	ARG	CD-NE-CZ	5.02	130.63	123.60

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	1290	0	1250	15	0
1	B	1281	0	1242	3	1
1	C	1297	0	1261	7	0
1	D	1276	0	1247	4	1
1	E	1248	0	1231	4	1
1	F	1238	0	1210	12	1
1	G	1242	0	1222	6	0
1	H	1224	0	1206	4	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
3	A	152	0	0	5	0
3	B	113	0	0	2	0
3	C	126	0	0	3	0
3	D	87	0	0	1	0
3	E	129	0	0	1	0
3	F	95	0	0	1	0
3	G	110	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	82	0	0	1	0
All	All	11015	0	9869	45	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (45) 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:A:32[A]:ILE:HG22	1:F:151:LEU:HD11	1.54	0.89
1:A:32[A]:ILE:HG22	1:F:151:LEU:CD1	2.10	0.81
1:C:103:LYS:NZ	1:G:139[B]:ASP:OD2	2.16	0.78
1:C:104[B]:ASP:OD1	3:C:2088:HOH:O	2.04	0.75
1:A:41[B]:ASP:OD1	3:A:2040:HOH:O	2.09	0.70
1:A:32[A]:ILE:CG2	1:F:151:LEU:HD11	2.22	0.69
1:C:41[A]:ASP:OD1	3:C:2036:HOH:O	2.11	0.69
1:B:74[A]:GLN:NE2	3:B:2049:HOH:O	2.28	0.65
1:A:32[B]:ILE:HD11	1:F:32:ILE:HG21	1.79	0.63
1:A:123:PRO:HG3	1:G:124:ASP:OD1	2.01	0.60
1:A:104[B]:ASP:OD1	3:A:2103:HOH:O	2.16	0.60
1:A:32[B]:ILE:HD11	1:F:32:ILE:CG2	2.31	0.60
1:E:136:ARG:NH1	3:E:2109:HOH:O	2.35	0.60
1:G:49:ASN:OD1	1:G:54:ARG:NH1	2.37	0.57
1:H:49:ASN:OD1	1:H:54:ARG:NH1	2.39	0.56
1:D:100[A]:SER:OG	3:D:2047:HOH:O	2.18	0.55
1:B:49:ASN:OD1	1:B:54:ARG:NH1	2.39	0.54
1:A:74[B]:GLN:CD	3:A:2073:HOH:O	2.45	0.54
1:D:49:ASN:OD1	1:D:54:ARG:NH1	2.40	0.53
1:A:49:ASN:OD1	1:A:54:ARG:NH1	2.41	0.52
1:C:49:ASN:OD1	1:C:54:ARG:NH1	2.42	0.52
1:F:49:ASN:OD1	1:F:54:ARG:NH1	2.42	0.51
1:H:28[B]:SER:OG	1:H:154:SER:HB2	2.11	0.51
1:B:74[A]:GLN:CD	3:B:2049:HOH:O	2.49	0.51
3:A:2114:HOH:O	1:D:15:GLY:N	2.42	0.50
1:E:32[A]:ILE:HD12	1:E:147:ARG:HG3	1.93	0.50
1:E:49:ASN:OD1	1:E:54:ARG:NH1	2.44	0.50
1:A:74[B]:GLN:NE2	3:A:2073:HOH:O	2.45	0.49
1:A:123:PRO:HB2	1:G:127:THR:OG1	2.13	0.48
1:A:32[B]:ILE:CD1	1:F:32:ILE:HG21	2.43	0.48
1:A:32[A]:ILE:HG13	1:A:151:LEU:HD21	1.99	0.45
1:C:131:GLU:HB3	3:C:2100:HOH:O	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32[A]:ILE:HG13	1:C:151:LEU:HD21	2.00	0.44
1:H:29:GLN:NE2	3:H:2015:HOH:O	2.50	0.43
1:F:56:ASN:OD1	1:F:58[B]:ASP:HB2	2.18	0.43
1:F:81:LEU:HD23	1:F:81:LEU:C	2.39	0.43
1:F:103:LYS:HE2	3:F:2069:HOH:O	2.19	0.42
1:H:32:ILE:HG13	1:H:151:LEU:HD21	2.02	0.42
1:G:32:ILE:HG13	1:G:151:LEU:HD21	2.03	0.41
1:A:32[A]:ILE:HG22	1:F:151:LEU:HD13	2.00	0.41
1:D:81:LEU:C	1:D:81:LEU:HD23	2.41	0.41
1:G:39[A]:ASP:OD1	1:G:40:ASN:N	2.53	0.41
1:F:31:VAL:HG11	1:F:150:ILE:HD13	2.02	0.41
1:C:81:LEU:HD23	1:C:81:LEU:C	2.41	0.41
1:E:32[B]:ILE:HG13	1:E:151:LEU:HD21	2.03	0.40

All (2) 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:B:103:LYS:NZ	1:F:139[B]:ASP:OD2[1_545]	2.00	0.20
1:D:103:LYS:NZ	1:E:139[A]:ASP:OD2[1_445]	2.14	0.06

## 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	160/160 (100%)	158 (99%)	2 (1%)	0	100	100
1	B	158/160 (99%)	156 (99%)	2 (1%)	0	100	100
1	C	159/160 (99%)	157 (99%)	2 (1%)	0	100	100
1	D	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
1	E	153/160 (96%)	151 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	152/160 (95%)	149 (98%)	3 (2%)	0	100	100
1	G	153/160 (96%)	150 (98%)	3 (2%)	0	100	100
1	H	151/160 (94%)	149 (99%)	2 (1%)	0	100	100
All	All	1243/1280 (97%)	1225 (99%)	18 (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	151/152 (99%)	151 (100%)	0	100	100
1	B	150/152 (99%)	149 (99%)	1 (1%)	85	80
1	C	153/152 (101%)	153 (100%)	0	100	100
1	D	149/152 (98%)	146 (98%)	3 (2%)	58	43
1	E	146/152 (96%)	143 (98%)	3 (2%)	56	41
1	F	145/152 (95%)	143 (99%)	2 (1%)	69	58
1	G	146/152 (96%)	142 (97%)	4 (3%)	48	30
1	H	142/152 (93%)	141 (99%)	1 (1%)	85	80
All	All	1182/1216 (97%)	1168 (99%)	14 (1%)	76	64

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	GLU
1	D	36	GLU
1	D	53	CYS
1	D	88	ASN
1	E	53[A]	CYS
1	E	53[B]	CYS
1	E	98	PHE
1	F	53	CYS

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Mol	Chain	Res	Type
1	F	98	PHE
1	G	36	GLU
1	G	53[A]	CYS
1	G	53[B]	CYS
1	G	98	PHE
1	H	36	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	29	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
2	SO4	A	1000	-	4,4,4	0.45	0	6,6,6	0.37	0
2	SO4	C	1000	-	4,4,4	0.60	0	6,6,6	0.52	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	D	1000	-	4,4,4	0.48	0	6,6,6	0.88	0
2	SO4	F	1000	-	4,4,4	0.56	0	6,6,6	0.78	0
2	SO4	G	1000	-	4,4,4	0.22	0	6,6,6	0.35	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
2	SO4	A	1000	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1000	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1000	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1000	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1000	-	-	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	151/160 (94%)	-0.29	0 <b>100</b> <b>100</b>	20, 31, 52, 66	0
1	B	151/160 (94%)	-0.18	4 (2%) 56 53	21, 37, 58, 81	0
1	C	150/160 (93%)	-0.25	0 <b>100</b> <b>100</b>	21, 32, 54, 61	0
1	D	151/160 (94%)	-0.18	2 (1%) 77 77	20, 37, 59, 70	0
1	E	151/160 (94%)	-0.22	0 <b>100</b> <b>100</b>	19, 34, 54, 66	0
1	F	150/160 (93%)	-0.05	2 (1%) 77 77	25, 38, 63, 85	0
1	G	150/160 (93%)	-0.23	0 <b>100</b> <b>100</b>	22, 36, 58, 72	0
1	H	150/160 (93%)	-0.15	0 <b>100</b> <b>100</b>	24, 39, 58, 66	0
All	All	1204/1280 (94%)	-0.20	8 (0%) 87 87	19, 35, 58, 85	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	VAL	5.0
1	D	13	VAL	3.7
1	F	14	LEU	3.2
1	D	14	LEU	3.0
1	B	14	LEU	3.0
1	B	33	ALA	2.7
1	B	15	GLY	2.4
1	F	16	TYR	2.2

### 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	F	1000	5/5	0.89	0.17	39,40,49,50	5
2	SO4	D	1000	5/5	0.91	0.17	35,37,41,42	5
2	SO4	G	1000	5/5	0.93	0.23	48,48,50,56	5
2	SO4	C	1000	5/5	0.97	0.07	36,41,45,46	5
2	SO4	A	1000	5/5	0.99	0.05	34,36,40,42	5

### 6.5 Other polymers [i](#)

There are no such residues in this entry.