



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:46 PM GMT

PDB ID : 5E0I
Title : Crystal structure of the HBV capsid Y132A mutant (VCID 8772) in complex with NVR10-001E2 at 1.95Å resolution
Authors : Lukacs, C.M.; Abendroth, J.; Klumpp, K.
Deposited on : 2015-09-28
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

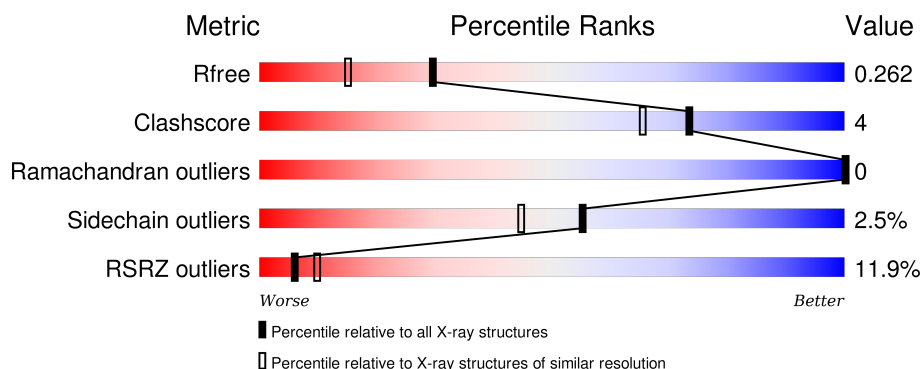
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 ≥ 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	157	<div> <div>8%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	B	157	<div> <div>10%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	C	157	<div> <div>15%</div> <div>82%</div> <div>10%</div> <div>.</div> <div>7%</div> </div>
1	D	157	<div> <div>15%</div> <div>83%</div> <div>8%</div> <div>.</div> <div>8%</div> </div>
1	E	157	<div> <div>13%</div> <div>82%</div> <div>10%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	157	<div><div></div><div>7%</div><div>77%</div><div>9%</div><div>•</div><div>13%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7532 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	1	0
			1212	787	197	223	5			
1	B	154	Total	C	N	O	S	0	1	0
			1208	785	197	221	5			
1	C	146	Total	C	N	O	S	0	1	0
			1147	748	185	209	5			
1	D	145	Total	C	N	O	S	0	0	0
			1132	739	183	205	5			
1	E	144	Total	C	N	O	S	0	1	0
			1123	730	182	206	5			
1	F	137	Total	C	N	O	S	0	2	0
			1090	711	176	198	5			

There are 54 discrepancies between the modelled and reference sequences:

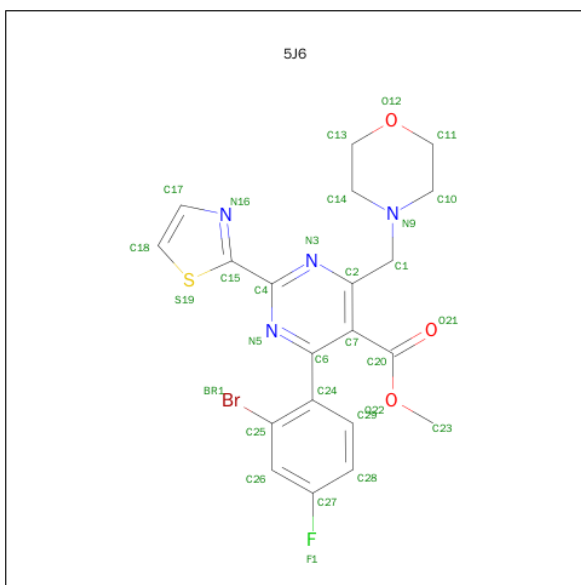
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P03147
A	132	ALA	TYR	engineered mutation	UNP P03147
A	150	LYS	-	expression tag	UNP P03147
A	151	LEU	-	expression tag	UNP P03147
A	152	GLU	-	expression tag	UNP P03147
A	153	ASN	-	expression tag	UNP P03147
A	154	LEU	-	expression tag	UNP P03147
A	155	TYR	-	expression tag	UNP P03147
A	156	PHE	-	expression tag	UNP P03147
B	0	SER	-	expression tag	UNP P03147
B	132	ALA	TYR	engineered mutation	UNP P03147
B	150	LYS	-	expression tag	UNP P03147
B	151	LEU	-	expression tag	UNP P03147
B	152	GLU	-	expression tag	UNP P03147
B	153	ASN	-	expression tag	UNP P03147
B	154	LEU	-	expression tag	UNP P03147
B	155	TYR	-	expression tag	UNP P03147

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Chain	Residue	Modelled	Actual	Comment	Reference
B	156	PHE	-	expression tag	UNP P03147
C	0	SER	-	expression tag	UNP P03147
C	132	ALA	TYR	engineered mutation	UNP P03147
C	150	LYS	-	expression tag	UNP P03147
C	151	LEU	-	expression tag	UNP P03147
C	152	GLU	-	expression tag	UNP P03147
C	153	ASN	-	expression tag	UNP P03147
C	154	LEU	-	expression tag	UNP P03147
C	155	TYR	-	expression tag	UNP P03147
C	156	PHE	-	expression tag	UNP P03147
D	0	SER	-	expression tag	UNP P03147
D	132	ALA	TYR	engineered mutation	UNP P03147
D	150	LYS	-	expression tag	UNP P03147
D	151	LEU	-	expression tag	UNP P03147
D	152	GLU	-	expression tag	UNP P03147
D	153	ASN	-	expression tag	UNP P03147
D	154	LEU	-	expression tag	UNP P03147
D	155	TYR	-	expression tag	UNP P03147
D	156	PHE	-	expression tag	UNP P03147
E	0	SER	-	expression tag	UNP P03147
E	132	ALA	TYR	engineered mutation	UNP P03147
E	150	LYS	-	expression tag	UNP P03147
E	151	LEU	-	expression tag	UNP P03147
E	152	GLU	-	expression tag	UNP P03147
E	153	ASN	-	expression tag	UNP P03147
E	154	LEU	-	expression tag	UNP P03147
E	155	TYR	-	expression tag	UNP P03147
E	156	PHE	-	expression tag	UNP P03147
F	0	SER	-	expression tag	UNP P03147
F	132	ALA	TYR	engineered mutation	UNP P03147
F	150	LYS	-	expression tag	UNP P03147
F	151	LEU	-	expression tag	UNP P03147
F	152	GLU	-	expression tag	UNP P03147
F	153	ASN	-	expression tag	UNP P03147
F	154	LEU	-	expression tag	UNP P03147
F	155	TYR	-	expression tag	UNP P03147
F	156	PHE	-	expression tag	UNP P03147

- Molecule 2 is methyl 4-(2-bromo-4-fluorophenyl)-6-(morpholin-4-ylmethyl)-2-(1,3-thiazol-2-yl)pyrimidine-5-carboxylate (three-letter code: 5J6) (formula: C₂₀H₁₈BrFN₄O₃S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	Br	C	F	N	O	S	0	0
			30	1	20	1	4	3	1		
2	B	1	Total	Br	C	F	N	O	S	0	0
			30	1	20	1	4	3	1		
2	C	1	Total	Br	C	F	N	O	S	0	0
			30	1	20	1	4	3	1		
2	D	1	Total	Br	C	F	N	O	S	0	0
			30	1	20	1	4	3	1		
2	E	1	Total	Br	C	F	N	O	S	0	0
			30	1	20	1	4	3	1		
2	F	1	Total	Br	C	F	N	O	S	0	0
			30	1	20	1	4	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	83	Total	O	0	0
			83	83		
3	C	72	Total	O	0	0
			72	72		
3	D	65	Total	O	0	0
			65	65		
3	E	69	Total	O	0	0
			69	69		
3	F	69	Total	O	0	0
			69	69		

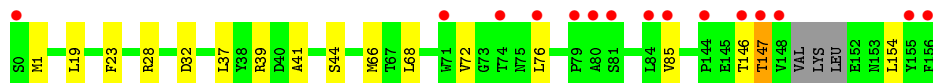
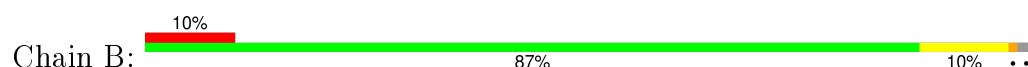
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

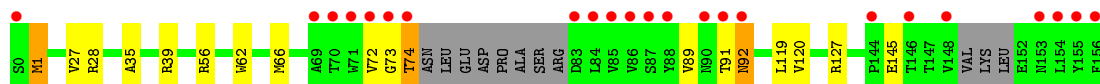
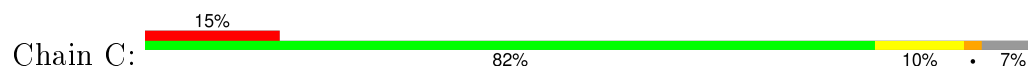
- Molecule 1: Capsid protein



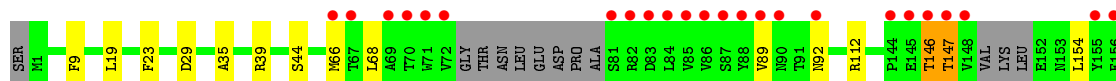
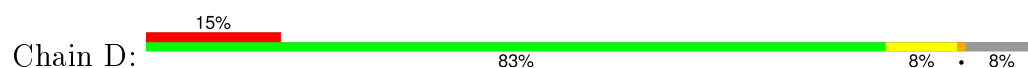
- Molecule 1: Capsid protein



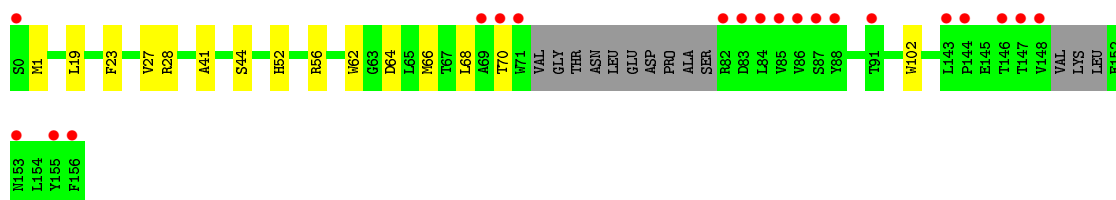
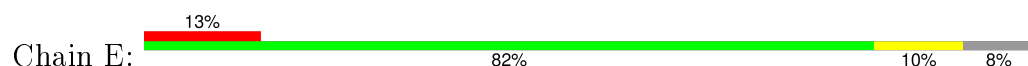
- Molecule 1: Capsid protein



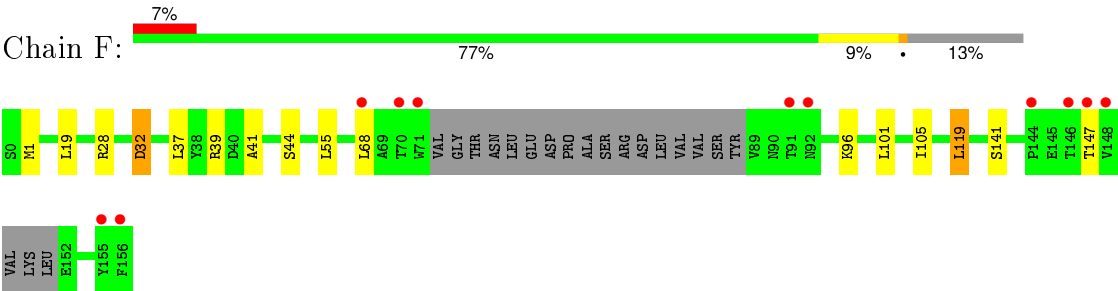
- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



● Molecule 1: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.60Å 88.17Å 102.25Å 90.00° 103.47° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 46.63 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.95) 99.9 (46.63-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.219 , 0.252 0.232 , 0.262	Depositor DCC
R_{free} test set	4810 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	7 of 95947 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7532	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5J6

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	0.74	0/1247	0.74	0/1710
1	B	0.72	0/1244	0.74	0/1708
1	C	0.71	0/1181	0.80	2/1619 (0.1%)
1	D	0.75	0/1166	0.79	1/1599 (0.1%)
1	E	0.75	0/1156	0.76	0/1585
1	F	0.75	0/1123	0.82	1/1538 (0.1%)
All	All	0.74	0/7117	0.78	4/9759 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	29	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	127	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	F	32	ASP	CB-CG-OD2	5.56	123.31	118.30
1	C	56	ARG	NE-CZ-NH1	5.25	122.92	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	92	ASN	Peptide

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	1212	0	1162	10	0
1	B	1208	0	1157	13	0
1	C	1147	0	1094	10	0
1	D	1132	0	1082	8	0
1	E	1123	0	1063	10	0
1	F	1090	0	1039	12	0
2	A	30	0	18	0	0
2	B	30	0	18	0	0
2	C	30	0	18	2	0
2	D	30	0	18	0	0
2	E	30	0	18	0	0
2	F	30	0	18	0	0
3	A	82	0	0	2	0
3	B	83	0	0	1	0
3	C	72	0	0	0	0
3	D	65	0	0	0	0
3	E	69	0	0	2	0
3	F	69	0	0	1	0
All	All	7532	0	6705	56	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 (56) 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:102:TRP:HZ3	3:E:669:HOH:O	1.46	0.99
1:A:32:ASP:OD2	3:A:601:HOH:O	1.89	0.91
1:E:102:TRP:CZ3	3:E:669:HOH:O	2.23	0.88
1:F:101:LEU:O	1:F:105[B]:ILE:HD13	1.82	0.80
1:B:32:ASP:OD2	3:B:601:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:LEU:HD11	1:F:105[B]:ILE:HD11	1.75	0.69
1:C:73:GLY:O	1:C:74:THR:HG23	1.96	0.65
1:A:1:MET:HG2	1:B:39:ARG:HG3	1.78	0.64
1:A:99:GLN:NE2	3:A:602:HOH:O	2.16	0.59
1:C:66:MET:CE	1:C:89:VAL:HG11	2.34	0.58
1:F:55:LEU:CD1	1:F:105[B]:ILE:HD11	2.34	0.57
1:A:39:ARG:HG3	1:B:1:MET:HG2	1.86	0.57
1:A:81:SER:HA	1:B:76:LEU:HD11	1.86	0.57
1:F:32:ASP:OD2	3:F:601:HOH:O	2.18	0.55
1:D:9:PHE:O	1:D:112:ARG:HD3	2.08	0.54
1:B:68:LEU:HD23	1:B:68:LEU:C	2.28	0.54
1:C:1:MET:HG3	1:D:39:ARG:HG3	1.90	0.53
1:E:41:ALA:O	1:E:44:SER:HB3	2.08	0.53
1:C:27:VAL:HG11	1:C:62:TRP:CE2	2.45	0.52
1:D:68:LEU:C	1:D:68:LEU:HD23	2.32	0.50
1:A:119:LEU:C	1:A:119:LEU:HD23	2.31	0.50
1:C:92:ASN:OD1	1:C:92:ASN:N	2.44	0.50
1:D:35:ALA:O	1:D:39:ARG:HB2	2.13	0.49
1:D:19:LEU:HD13	1:D:23:PHE:CE1	2.47	0.48
1:C:72:VAL:N	1:C:73:GLY:HA3	2.28	0.48
1:E:66:MET:O	1:E:70:THR:HG23	2.13	0.47
1:A:120:VAL:HG11	1:F:37:LEU:HD21	1.97	0.47
1:A:41:ALA:O	1:A:44:SER:HB3	2.15	0.46
1:D:146:THR:HA	1:D:154:LEU:HB2	1.96	0.46
1:F:105[B]:ILE:CD1	1:F:105[B]:ILE:N	2.78	0.46
1:E:68:LEU:HD23	1:F:68:LEU:HD23	1.98	0.45
1:B:72:VAL:HG21	1:B:85:VAL:HG11	1.98	0.45
1:C:66:MET:CE	1:C:89:VAL:CG1	2.94	0.45
1:C:91:THR:HB	1:C:92:ASN:OD1	2.17	0.44
1:A:66:MET:CE	1:A:66:MET:HA	2.47	0.44
1:B:19:LEU:HD13	1:B:23:PHE:CE2	2.53	0.44
1:B:37:LEU:HD21	1:C:120:VAL:HG13	2.00	0.44
1:B:41:ALA:O	1:B:44:SER:HB3	2.18	0.44
1:B:146:THR:HG22	1:B:147:THR:O	2.18	0.44
1:E:1:MET:HG2	1:F:39:ARG:HG3	2.00	0.44
1:F:41:ALA:O	1:F:44:SER:HB3	2.18	0.44
1:B:146:THR:HA	1:B:154:LEU:HB2	2.00	0.43
2:C:500:5J6:C1	2:C:500:5J6:O21	2.66	0.43
1:B:66:MET:CE	1:B:66:MET:HA	2.49	0.43
1:F:55:LEU:CD1	1:F:105[B]:ILE:CD1	2.97	0.42
1:D:66:MET:CE	1:D:89:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ASP:OD2	1:F:96:LYS:NZ	2.47	0.42
1:F:19:LEU:HD11	1:F:119:LEU:HG	2.01	0.42
1:E:27:VAL:HG11	1:E:62:TRP:CE2	2.55	0.41
1:E:52:HIS:O	1:E:56:ARG:HG3	2.21	0.41
1:A:35:ALA:O	1:A:39:ARG:HB2	2.21	0.41
1:D:146:THR:HG23	1:D:147:THR:N	2.36	0.41
1:C:35:ALA:O	1:C:39:ARG:HB2	2.20	0.41
1:E:19:LEU:HD13	1:E:23:PHE:CE1	2.56	0.41
2:C:500:5J6:O21	2:C:500:5J6:H9	2.21	0.40
1:B:147:THR:HG22	1:B:154:LEU:CD1	2.51	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	151/157 (96%)	144 (95%)	7 (5%)	0	100	100
1	B	151/157 (96%)	145 (96%)	6 (4%)	0	100	100
1	C	141/157 (90%)	134 (95%)	7 (5%)	0	100	100
1	D	139/157 (88%)	133 (96%)	6 (4%)	0	100	100
1	E	139/157 (88%)	134 (96%)	5 (4%)	0	100	100
1	F	133/157 (85%)	126 (95%)	7 (5%)	0	100	100
All	All	854/942 (91%)	816 (96%)	38 (4%)	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	130/139 (94%)	129 (99%)	1 (1%)	86	85
1	B	129/139 (93%)	127 (98%)	2 (2%)	70	66
1	C	122/139 (88%)	116 (95%)	6 (5%)	31	15
1	D	121/139 (87%)	118 (98%)	3 (2%)	55	45
1	E	119/139 (86%)	118 (99%)	1 (1%)	86	85
1	F	116/139 (84%)	111 (96%)	5 (4%)	35	20
All	All	737/834 (88%)	719 (98%)	18 (2%)	55	47

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	B	28	ARG
1	B	147	THR
1	C	1	MET
1	C	28	ARG
1	C	74	THR
1	C	92	ASN
1	C	119	LEU
1	C	145	GLU
1	D	44	SER
1	D	146	THR
1	D	147	THR
1	E	28	ARG
1	F	1	MET
1	F	28	ARG
1	F	119	LEU
1	F	141	SER
1	F	147	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	92	ASN
1	F	92	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	5J6	A	500	-	33,33,33	2.08	7 (21%)	38,46,46	2.52	11 (28%)
2	5J6	B	500	-	33,33,33	2.33	9 (27%)	38,46,46	2.51	10 (26%)
2	5J6	C	500	-	33,33,33	2.14	6 (18%)	38,46,46	2.55	11 (28%)
2	5J6	D	500	-	33,33,33	2.21	9 (27%)	38,46,46	2.60	12 (31%)
2	5J6	E	500	-	33,33,33	2.13	7 (21%)	38,46,46	2.62	11 (28%)
2	5J6	F	500	-	33,33,33	2.45	9 (27%)	38,46,46	2.57	11 (28%)

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	5J6	A	500	-	-	0/14/26/26	0/4/4/4
2	5J6	B	500	-	-	0/14/26/26	0/4/4/4
2	5J6	C	500	-	-	0/14/26/26	0/4/4/4
2	5J6	D	500	-	-	0/14/26/26	0/4/4/4
2	5J6	E	500	-	-	0/14/26/26	0/4/4/4
2	5J6	F	500	-	-	0/14/26/26	0/4/4/4

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	5J6	C24-C25	-2.95	1.37	1.39
2	E	500	5J6	BR1-C25	-2.63	1.83	1.89
2	F	500	5J6	C15-S19	-2.04	1.70	1.73
2	D	500	5J6	C1-N9	2.04	1.51	1.47
2	F	500	5J6	C26-C27	2.04	1.41	1.37
2	B	500	5J6	C28-C27	2.13	1.41	1.37
2	A	500	5J6	C28-C27	2.13	1.41	1.37
2	B	500	5J6	C24-C25	2.18	1.40	1.39
2	D	500	5J6	C15-N16	2.29	1.34	1.31
2	F	500	5J6	C24-C6	2.34	1.51	1.49
2	E	500	5J6	C24-C6	2.41	1.52	1.49
2	C	500	5J6	C4-N5	2.88	1.41	1.34
2	B	500	5J6	C15-N16	3.08	1.35	1.31
2	F	500	5J6	C24-C25	3.17	1.41	1.39
2	E	500	5J6	C4-N5	3.35	1.42	1.34
2	C	500	5J6	C15-N16	3.36	1.36	1.31
2	B	500	5J6	C24-C6	3.42	1.53	1.49
2	D	500	5J6	O22-C20	3.43	1.41	1.33
2	D	500	5J6	C4-N5	3.46	1.42	1.34
2	A	500	5J6	O22-C20	3.46	1.41	1.33
2	A	500	5J6	C15-N16	3.49	1.36	1.31
2	E	500	5J6	O22-C20	3.54	1.41	1.33
2	D	500	5J6	C24-C6	3.56	1.53	1.49
2	A	500	5J6	C4-N5	3.61	1.42	1.34
2	F	500	5J6	C4-N5	3.76	1.43	1.34
2	C	500	5J6	O22-C20	3.88	1.42	1.33
2	B	500	5J6	O22-C20	3.95	1.42	1.33
2	E	500	5J6	C7-C2	3.96	1.47	1.41
2	F	500	5J6	O22-C20	3.99	1.42	1.33
2	B	500	5J6	C4-N5	4.28	1.44	1.34
2	C	500	5J6	C7-C2	4.35	1.48	1.41
2	C	500	5J6	C7-C6	4.46	1.49	1.41
2	D	500	5J6	C7-C2	4.50	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	5J6	C7-C6	4.56	1.49	1.41
2	B	500	5J6	C7-C2	4.64	1.48	1.41
2	A	500	5J6	C7-C2	4.66	1.48	1.41
2	B	500	5J6	C7-C6	4.66	1.49	1.41
2	F	500	5J6	C7-C6	4.83	1.50	1.41
2	E	500	5J6	C7-C6	4.97	1.50	1.41
2	F	500	5J6	C7-C2	5.35	1.49	1.41
2	D	500	5J6	C7-C6	5.42	1.51	1.41
2	A	500	5J6	C6-N5	6.48	1.45	1.34
2	D	500	5J6	C6-N5	6.53	1.45	1.34
2	B	500	5J6	C6-N5	7.33	1.46	1.34
2	E	500	5J6	C6-N5	7.38	1.46	1.34
2	C	500	5J6	C6-N5	7.92	1.47	1.34
2	F	500	5J6	C6-N5	8.58	1.48	1.34

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	5J6	C24-C6-C7	-8.31	108.52	124.11
2	A	500	5J6	C24-C6-N5	-8.17	102.07	114.67
2	F	500	5J6	C24-C6-C7	-8.07	108.95	124.11
2	F	500	5J6	C24-C6-N5	-8.04	102.26	114.67
2	D	500	5J6	C24-C6-N5	-8.00	102.34	114.67
2	C	500	5J6	C24-C6-C7	-7.89	109.30	124.11
2	A	500	5J6	C24-C6-C7	-7.68	109.69	124.11
2	E	500	5J6	C24-C6-C7	-7.52	109.99	124.11
2	D	500	5J6	C24-C6-C7	-7.38	110.25	124.11
2	E	500	5J6	C24-C6-N5	-7.37	103.30	114.67
2	B	500	5J6	C24-C6-N5	-7.13	103.68	114.67
2	C	500	5J6	C24-C6-N5	-6.69	104.34	114.67
2	E	500	5J6	C7-C6-N5	-6.24	112.14	121.97
2	D	500	5J6	C7-C6-N5	-5.87	112.72	121.97
2	C	500	5J6	C7-C6-N5	-5.73	112.95	121.97
2	A	500	5J6	C7-C6-N5	-4.91	114.23	121.97
2	F	500	5J6	C7-C6-N5	-4.89	114.26	121.97
2	C	500	5J6	C2-C1-N9	-4.80	106.42	113.53
2	B	500	5J6	C7-C6-N5	-4.10	115.51	121.97
2	B	500	5J6	C2-C1-N9	-3.95	107.68	113.53
2	A	500	5J6	C7-C2-N3	-3.60	117.58	122.36
2	E	500	5J6	C2-C1-N9	-3.18	108.83	113.53
2	D	500	5J6	C2-C1-N9	-3.17	108.84	113.53
2	D	500	5J6	C7-C2-N3	-3.17	118.16	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	5J6	C28-C27-C26	-3.16	119.30	123.32
2	F	500	5J6	C28-C27-C26	-3.15	119.33	123.32
2	D	500	5J6	C28-C27-C26	-3.13	119.34	123.32
2	B	500	5J6	C7-C2-N3	-2.99	118.39	122.36
2	B	500	5J6	C28-C27-C26	-2.77	119.80	123.32
2	A	500	5J6	C2-C1-N9	-2.72	109.50	113.53
2	A	500	5J6	C28-C27-C26	-2.64	119.96	123.32
2	F	500	5J6	C2-C1-N9	-2.64	109.62	113.53
2	C	500	5J6	C7-C2-N3	-2.49	119.06	122.36
2	A	500	5J6	C6-C7-C20	-2.46	117.35	121.74
2	C	500	5J6	C28-C27-C26	-2.37	120.31	123.32
2	F	500	5J6	O22-C20-O21	-2.34	118.60	123.45
2	B	500	5J6	O22-C20-O21	-2.26	118.77	123.45
2	A	500	5J6	C11-C10-N9	-2.23	106.70	110.11
2	F	500	5J6	C11-C10-N9	-2.22	106.71	110.11
2	E	500	5J6	C6-C7-C20	-2.21	117.80	121.74
2	D	500	5J6	C6-C7-C20	-2.08	118.03	121.74
2	E	500	5J6	C7-C2-N3	-2.07	119.61	122.36
2	D	500	5J6	F1-C27-C28	2.18	122.00	118.53
2	A	500	5J6	C6-N5-C4	2.19	119.19	117.32
2	F	500	5J6	O22-C20-C7	2.24	117.13	112.26
2	C	500	5J6	C10-N9-C14	2.28	113.98	108.87
2	D	500	5J6	C15-C4-N5	2.36	119.53	116.68
2	C	500	5J6	O22-C20-C7	2.40	117.48	112.26
2	B	500	5J6	C27-C26-C25	2.48	121.28	117.69
2	E	500	5J6	C23-O22-C20	2.77	121.28	115.84
2	D	500	5J6	C27-C26-C25	2.86	121.82	117.69
2	B	500	5J6	C15-C4-N5	2.97	120.26	116.68
2	C	500	5J6	C15-C4-N5	3.19	120.53	116.68
2	F	500	5J6	C15-C4-N5	3.23	120.58	116.68
2	F	500	5J6	C23-O22-C20	3.24	122.19	115.84
2	D	500	5J6	C6-N5-C4	3.41	120.24	117.32
2	A	500	5J6	C17-N16-C15	3.46	112.46	103.97
2	A	500	5J6	C15-C4-N5	3.46	120.86	116.68
2	E	500	5J6	C15-C4-N5	3.48	120.87	116.68
2	D	500	5J6	C17-N16-C15	3.75	113.17	103.97
2	F	500	5J6	C17-N16-C15	3.79	113.27	103.97
2	E	500	5J6	C17-N16-C15	3.81	113.32	103.97
2	C	500	5J6	C6-N5-C4	3.87	120.63	117.32
2	C	500	5J6	C17-N16-C15	3.94	113.64	103.97
2	E	500	5J6	C6-N5-C4	4.15	120.87	117.32
2	B	500	5J6	C17-N16-C15	4.37	114.68	103.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	5J6	2	0

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	154/157 (98%)	0.39	12 (7%)	16 25	16, 25, 57, 73	0
1	B	154/157 (98%)	0.44	15 (9%)	10 16	16, 26, 59, 73	0
1	C	146/157 (92%)	0.66	23 (15%)	3 4	17, 26, 66, 82	0
1	D	145/157 (92%)	0.70	24 (16%)	2 3	17, 26, 67, 83	0
1	E	144/157 (91%)	0.46	20 (13%)	4 6	16, 25, 60, 71	0
1	F	137/157 (87%)	0.33	11 (8%)	15 24	17, 24, 60, 68	0
All	All	880/942 (93%)	0.50	105 (11%)	6 10	16, 26, 63, 83	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	84	LEU	10.4
1	C	85	VAL	9.2
1	D	85	VAL	7.9
1	C	72	VAL	6.4
1	D	147	THR	5.6
1	D	88	TYR	5.5
1	D	84	LEU	5.3
1	D	86	VAL	5.2
1	D	70	THR	4.9
1	E	156	PHE	4.9
1	B	147	THR	4.9
1	C	86	VAL	4.8
1	C	74	THR	4.6
1	E	84	LEU	4.6
1	D	144	PRO	4.5
1	F	147	THR	4.5
1	C	88	TYR	4.4
1	B	74	THR	4.4
1	B	146	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	71	TRP	4.3
1	D	71	TRP	4.3
1	D	148	VAL	4.2
1	C	156	PHE	4.2
1	F	71	TRP	4.1
1	D	82	ARG	4.1
1	A	147	THR	4.1
1	D	146	THR	4.0
1	C	91	THR	4.0
1	D	83	ASP	4.0
1	E	86	VAL	4.0
1	A	144	PRO	3.9
1	E	88	TYR	3.9
1	A	84	LEU	3.8
1	D	81	SER	3.8
1	B	76	LEU	3.8
1	F	68	LEU	3.8
1	F	144	PRO	3.7
1	E	153	ASN	3.7
1	A	146	THR	3.7
1	D	72	VAL	3.6
1	A	80	ALA	3.6
1	E	147	THR	3.5
1	B	79	PRO	3.5
1	E	144	PRO	3.4
1	D	89	VAL	3.4
1	E	85	VAL	3.4
1	E	87	SER	3.4
1	D	66	MET	3.4
1	E	83	ASP	3.3
1	B	84	LEU	3.3
1	D	155	TYR	3.3
1	B	144	PRO	3.3
1	B	85	VAL	3.2
1	E	69	ALA	3.2
1	A	153	ASN	3.2
1	C	146	THR	3.2
1	C	70	THR	3.2
1	A	74	THR	3.1
1	D	90	ASN	3.1
1	B	148	VAL	3.1
1	E	146	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	80	ALA	3.1
1	D	92	ASN	3.1
1	D	87	SER	3.0
1	B	81	SER	3.0
1	C	144	PRO	2.9
1	D	69	ALA	2.9
1	E	91	THR	2.9
1	B	155	TYR	2.8
1	F	148	VAL	2.8
1	A	155	TYR	2.8
1	E	155	TYR	2.8
1	A	85	VAL	2.8
1	E	0	SER	2.7
1	C	92	ASN	2.7
1	F	156	PHE	2.7
1	F	91	THR	2.7
1	B	0	SER	2.7
1	F	92	ASN	2.7
1	D	67	THR	2.7
1	F	146	THR	2.7
1	D	156	PHE	2.7
1	F	155	TYR	2.6
1	C	153	ASN	2.6
1	A	73	GLY	2.6
1	C	154	LEU	2.5
1	C	71	TRP	2.5
1	C	87	SER	2.5
1	C	83	ASP	2.5
1	B	156	PHE	2.4
1	C	69	ALA	2.4
1	E	70	THR	2.4
1	C	90	ASN	2.4
1	E	148	VAL	2.4
1	A	76	LEU	2.3
1	D	145	GLU	2.3
1	C	0	SER	2.3
1	C	155	TYR	2.3
1	F	70	THR	2.3
1	C	73	GLY	2.3
1	E	82	ARG	2.3
1	B	71	TRP	2.2
1	C	148	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	143	LEU	2.1
1	A	79	PRO	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
2	5J6	E	500	30/30	0.98	0.10	-0.28	18,20,21,22	0
2	5J6	A	500	30/30	0.98	0.10	-0.45	16,19,20,22	0
2	5J6	F	500	30/30	0.99	0.10	-0.51	16,19,21,22	0
2	5J6	C	500	30/30	0.99	0.10	-0.68	18,19,24,25	0
2	5J6	D	500	30/30	0.99	0.10	-1.10	19,20,22,23	0
2	5J6	B	500	30/30	0.99	0.09	-1.21	16,20,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.