



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:03 PM GMT

PDB ID : 1RVF
Title : FAB COMPLEXED WITH INTACT HUMAN RHINOVIRUS
Authors : Smith, T.J.
Deposited on : 1996-09-05
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

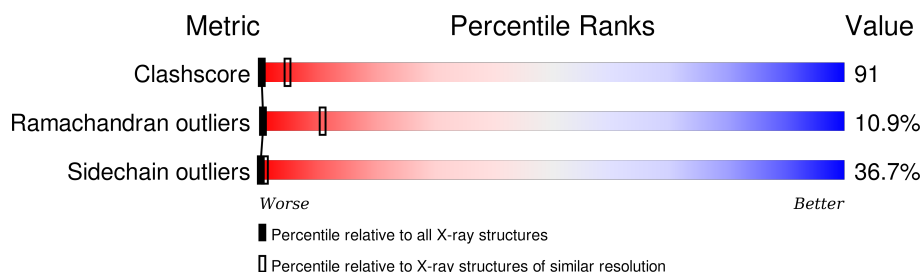
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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))
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	289	
2	2	262	
3	3	236	
4	4	68	
5	L	110	
6	H	119	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8019 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 HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	273	Total	C	N	O	S	0	0	0
			2170	1373	375	414	8			

- Molecule 2 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	255	Total	C	N	O	S	0	0	0
			1952	1238	330	372	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	CONFLICT	UNP P03303

- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	236	Total	C	N	O	S	0	0	0
			1849	1184	305	353	7			

- Molecule 4 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	40	Total	C	N	O	S	0	0	0
			297	186	47	62	2			

- Molecule 5 is a protein called FAB 17-IA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	110	Total	C	N	O	S	0	0	0
			834	524	139	166	5			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	14	PHE	SER	CONFLICT	UNP X79906
L	15	PRO	LEU	CONFLICT	UNP X79906
L	18	LYS	ARG	CONFLICT	UNP X79906
L	21	ILE	MET	CONFLICT	UNP X79906
L	24	SER	THR	CONFLICT	UNP X79906
L	26	THR	SER	CONFLICT	UNP X79906
L	?	-	SER	DELETION	UNP X79906
L	?	-	SER	DELETION	UNP X79906
L	31	ASN	SER	CONFLICT	UNP X79906
L	33	MET	LEU	CONFLICT	UNP X79906
L	36	PHE	TYR	CONFLICT	UNP X79906
L	42	THR	SER	CONFLICT	UNP X79906
L	51	SER	THR	CONFLICT	UNP X79906
L	77	ARG	SER	CONFLICT	UNP X79906
L	89	GLN	HIS	CONFLICT	UNP X79906
L	91	ARG	TYR	CONFLICT	UNP X79906
L	92	SER	HIS	CONFLICT	UNP X79906
L	93	SER	ARG	CONFLICT	UNP X79906
L	94	TYR	PHE	CONFLICT	UNP X79906
L	96	ILE	HIS	CONFLICT	UNP X79906
L	100	SER	GLY	CONFLICT	UNP X79906

- Molecule 6 is a protein called FAB 17-IA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	119	Total	C	N	O	S	0	0	0
			917	579	153	181	4			

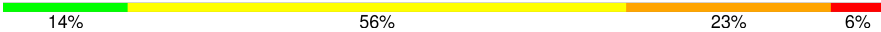
There are 25 discrepancies between the modelled and reference sequences:

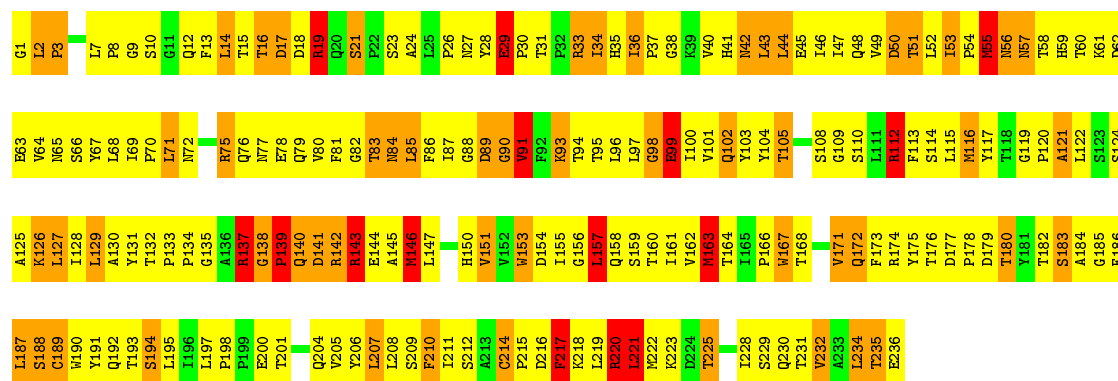
Chain	Residue	Modelled	Actual	Comment	Reference
H	2	GLY	ILE	CONFLICT	UNP S38950
H	9	ALA	PRO	CONFLICT	UNP S38950
H	16	SER	ALA	CONFLICT	UNP S38950
H	28	ALA	THR	CONFLICT	UNP S38950
H	30	SER	THR	CONFLICT	UNP S38950
H	31	SER	ASP	CONFLICT	UNP S38950
H	32	PHE	TYR	CONFLICT	UNP S38950
H	33	TRP	TYR	CONFLICT	UNP S38950
H	34	VAL	ILE	CONFLICT	UNP S38950
H	35	ASN	HIS	CONFLICT	UNP S38950

Continued on next page...

Continued from previous page...

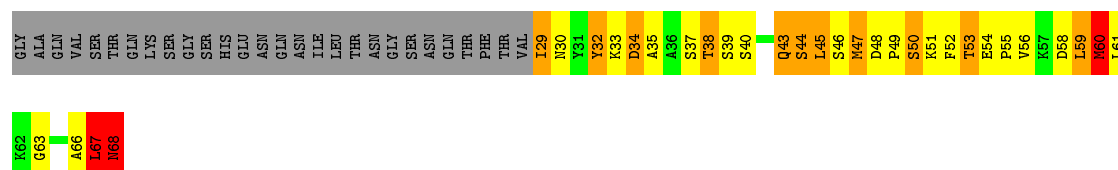
Chain	Residue	Modelled	Actual	Comment	Reference
H	43	GLN	GLU	CONFLICT	UNP S38950
H	50	GLN	TRP	CONFLICT	UNP S38950
H	54	ASP	SER	CONFLICT	UNP S38950
H	56	ASP	ASN	CONFLICT	UNP S38950
H	57	ASN	THR	CONFLICT	UNP S38950
H	61	GLY	GLU	CONFLICT	UNP S38950
H	71	ALA	VAL	CONFLICT	UNP S38950
H	73	LYS	THR	CONFLICT	UNP S38950
H	76	THR	SER	CONFLICT	UNP S38950
H	82A	TYR	SER	CONFLICT	UNP S38950
H	95	SER	GLY	CONFLICT	UNP S38950
H	97	ASN	-	INSERTION	UNP S38950
H	98	TYR	-	INSERTION	UNP S38950
H	99	PRO	LYS	CONFLICT	UNP S38950
H	100I	TYR	PHE	CONFLICT	UNP S38950

Chain 3: 



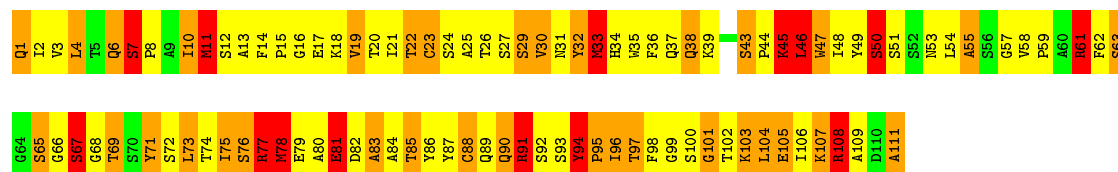
• Molecule 4: HUMAN RHINOVIRUS 14 COAT PROTEIN

Chain 4: 




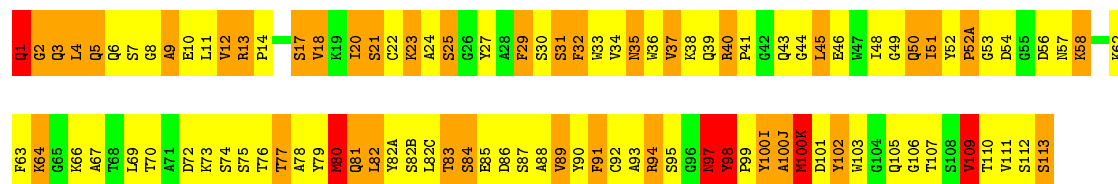
• Molecule 5: FAB 17-IA

Chain L: 



• Molecule 6: FAB 17-IA

Chain H: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	R 3	Depositor
Cell constants a, b, c, α , β , γ	372.00 Å 372.00 Å 372.00 Å 108.40° 108.40° 108.40°	Depositor
Resolution (Å)	10.00 – 4.00	Depositor
% Data completeness (in resolution range)	64.5 (10.00-4.00)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.212 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8019	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	1.03	1/2228 (0.0%)	1.51	32/3031 (1.1%)
2	2	1.04	2/2001 (0.1%)	1.42	20/2735 (0.7%)
3	3	1.09	4/1898 (0.2%)	1.46	22/2597 (0.8%)
4	4	1.12	2/302 (0.7%)	1.70	6/406 (1.5%)
5	L	1.09	3/854 (0.4%)	1.61	16/1157 (1.4%)
6	H	1.15	3/941 (0.3%)	1.58	16/1272 (1.3%)
All	All	1.07	15/8224 (0.2%)	1.50	112/11198 (1.0%)

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
6	H	0	1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	111	ALA	CA-C	9.21	1.76	1.52
6	H	113	SER	C-OXT	7.97	1.38	1.23
2	2	8	GLY	N-CA	7.97	1.58	1.46
4	4	29	ILE	N-CA	7.16	1.60	1.46
5	L	111	ALA	C-OXT	6.86	1.36	1.23

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	261	PRO	O-C-N	9.93	138.59	122.70
1	1	128	TYR	CB-CG-CD1	9.88	126.92	121.00
4	4	67	LEU	O-C-N	9.24	137.49	122.70
5	L	108	ARG	NE-CZ-NH2	8.57	124.59	120.30
6	H	97	ASN	O-C-N	8.50	136.29	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	H	102	TYR	Sidechain

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	1	2170	0	2107	367	0
2	2	1952	0	1927	317	0
3	3	1849	0	1833	337	0
4	4	297	0	294	40	0
5	L	834	0	814	311	0
6	H	917	0	870	241	0
All	All	8019	0	7845	1439	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 91.

The worst 5 of 1439 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)
5:L:111:ALA:C	5:L:111:ALA:CA	1.76	1.53
5:L:7:SER:CB	5:L:22:THR:HG23	1.50	1.40
6:H:99:PRO:HG2	6:H:100(I):TYR:CE1	1.59	1.38
5:L:6:GLN:HG3	5:L:101:GLY:N	1.40	1.34
5:L:94:TYR:O	5:L:96:ILE:N	1.62	1.31

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	1	271/289 (94%)	205 (76%)	44 (16%)	22 (8%)	1	19
2	2	253/262 (97%)	162 (64%)	56 (22%)	35 (14%)	0	6
3	3	234/236 (99%)	172 (74%)	38 (16%)	24 (10%)	1	12
4	4	38/68 (56%)	23 (60%)	11 (29%)	4 (10%)	1	11
5	L	108/110 (98%)	73 (68%)	19 (18%)	16 (15%)	0	5
6	H	117/119 (98%)	84 (72%)	23 (20%)	10 (8%)	1	17
All	All	1021/1084 (94%)	719 (70%)	191 (19%)	111 (11%)	0	11

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	27	HIS
1	1	45	VAL
1	1	88	THR
1	1	142	TYR
1	1	195	SER

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	1	239/253 (94%)	149 (62%)	90 (38%)	0	1
2	2	223/229 (97%)	141 (63%)	82 (37%)	0	1
3	3	209/209 (100%)	142 (68%)	67 (32%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	33/57 (58%)	19 (58%)	14 (42%)	0	0
5	L	92/92 (100%)	52 (56%)	40 (44%)	0	0
6	H	96/96 (100%)	62 (65%)	34 (35%)	0	1
All	All	892/936 (95%)	565 (63%)	327 (37%)	0	1

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	183	ILE
3	3	48	GLN
6	H	21	SER
2	2	200	VAL
2	2	247	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	190	ASN
3	3	42	ASN
6	H	6	GLN
2	2	262	GLN
3	3	56	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 [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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.