



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:34 AM GMT

PDB ID : 2HWE
Title : A COMPARISON OF THE ANTI-RHINOVIRAL DRUG BINDING
POCKET IN HRV14 AND HRV1A
Authors : Kim, K.H.; Rossmann, M.G.
Deposited on : 1994-01-25
Resolution : 3.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

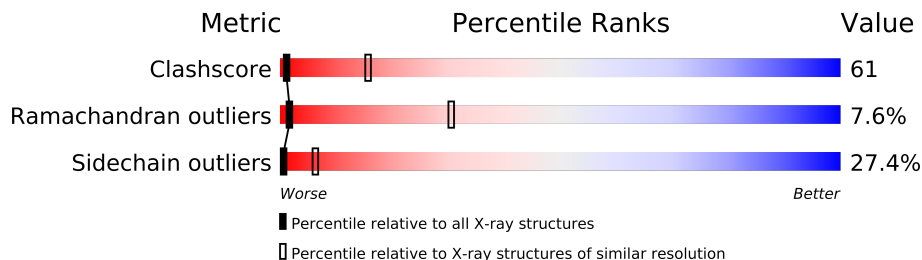
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.80 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	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	287	
2	2	263	
3	3	238	
4	4	44	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6248 atoms, of which 0 are hydrogen and 0 are deuterium.

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 1A COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	283	Total	C	N	O	S	0	0	0
			2262	1431	389	430	12			

- Molecule 2 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	253	Total	C	N	O	S	0	0	0
			1979	1249	349	371	10			

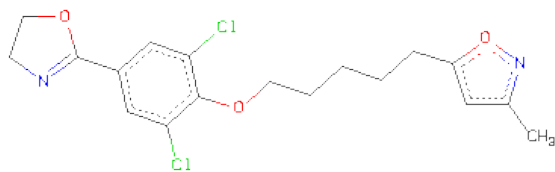
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	238	Total	C	N	O	S	0	0	0
			1831	1169	297	348	17			

- Molecule 4 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	19	Total	C	N	O	0	0	0
			151	96	25	30			

- Molecule 5 is 5-(5-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLY)PHENOXY)PENTYL)-3-METHYLISOXAZOLE (three-letter code: W54) (formula: C₁₈H₂₀Cl₂N₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	1	1	25	18	2	2	3	0	0

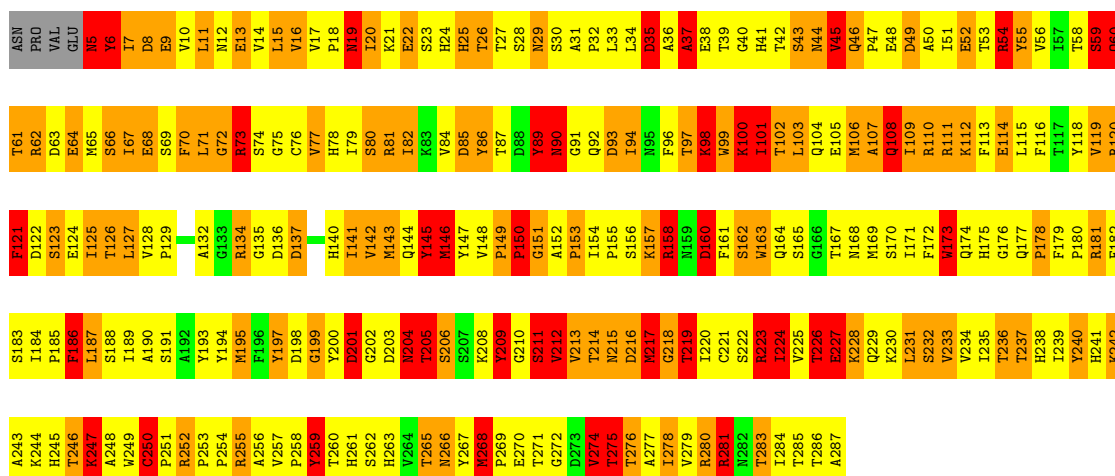
3 Residue-property plots

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.

Note EDS was not executed.

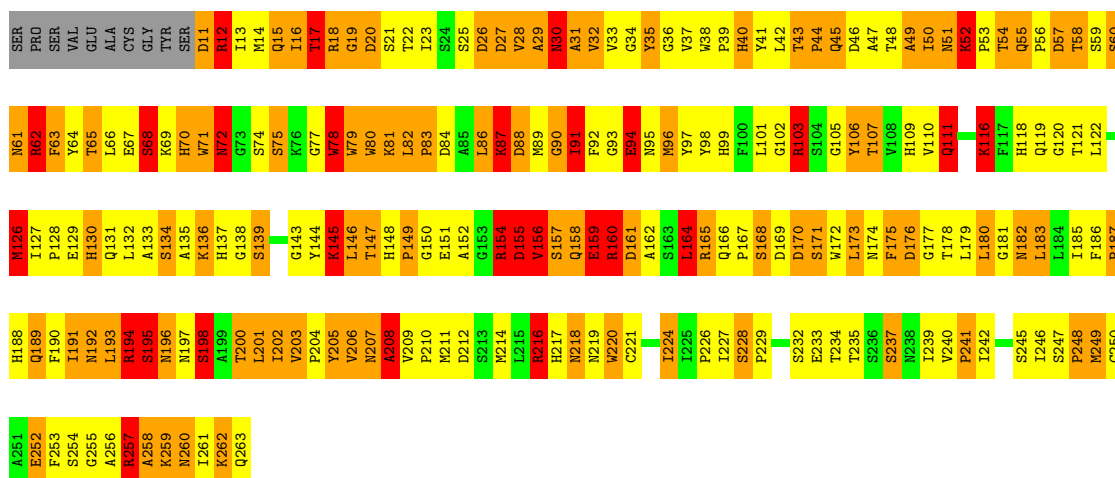
• Molecule 1: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1)

Chain 1:



• Molecule 2: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2)

Chain 2:



• Molecule 3: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3)

Chain 3:

S184	M185	A186	G187	Y188	I189	T190	C191	W192	Y193	Q194	T195	M196	L197	P201	S202	T203	P204	Q205	T206	A207	D208	M209	L210	C211	F212	V213	S214	A215	C216	K217	D218	F219	C220	L221	R222	M223	A224	R225	D226	T227	D228	L229	H230	T231	Q232	S233	G234	P235	L236	E237	Q238								
G121	T122	A123	N124	T125	T126	L127	K128	L129	L130	L131	A132	Y133	T134	P135	P136		D139	E140	P141	T142	T143	R144	K145	L146	A147	M148	G149	G150	T151	H152	V153	V154	W155	D156	V157	G158	L159	Q160	S161	T162	I163	S164	L165	V166	V167	P168	W169		A172	S173	H174	F175	R176	L177	T178	N181	K182	Y183	
G1	L2	P3	V4	Y5	I6	T7	P8	G9	S10	G11	Q12	F13	M14	T15	T16	D17	D18	M19	Q20	S21	P22	C23	A24	L25	P26	W27	K28	E29	I30	T31	S32	E33	I34	S35	I36	P37	G38	E39	V40	K41	N42	L43	I44	E45	M46	C47	Q48	V49	D50	T51	L52	I53	P54	N55	N56	N57	V58	G59	N60

● Molecule 4: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4)

Chain 4:

GLY	ALA	GLY	VAL	SER	ARG	GLN	ASN	VAL	GLY	THR	HIS	SER	THR	GLN	ASN	SER	VAL	SER	ASN	GLY	SER	SER	LEU	ASN	Y26	F27	N28	I29	N30	Y31	F32	K33	D34	A35	A36	S37	S38	G39	A40	S41	R42	L43	D44
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	341.30Å 341.30Å 465.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6248	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W54

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	1.19	8/2322 (0.3%)	2.59	145/3162 (4.6%)
2	2	0.95	0/2033	2.59	151/2770 (5.5%)
3	3	0.93	0/1878	2.46	110/2570 (4.3%)
4	4	1.25	0/154	3.16	21/206 (10.2%)
All	All	1.05	8/6387 (0.1%)	2.57	427/8708 (4.9%)

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	1	0	7

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	146	MET	C-N	-15.38	0.98	1.34
1	1	213	VAL	C-N	11.92	1.61	1.34
1	1	98	LYS	C-N	-8.12	1.15	1.34
1	1	218	GLY	CA-C	-6.87	1.40	1.51
1	1	223	ARG	C-N	6.80	1.49	1.34

The worst 5 of 427 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	98	LYS	O-C-N	-28.02	77.86	122.70
2	2	62	ARG	CD-NE-CZ	24.81	158.33	123.60
1	1	134	ARG	NE-CZ-NH1	24.02	132.31	120.30
2	2	216	ARG	NE-CZ-NH2	-22.09	109.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	280	ARG	NE-CZ-NH2	-20.40	110.10	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	110	ARG	Mainchain
1	1	150	PRO	Peptide
1	1	186	PHE	Mainchain
1	1	211	SER	Mainchain
1	1	98	LYS	Mainchain,Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2262	0	2191	387	1486
2	2	1979	0	1920	211	738
3	3	1831	0	1809	234	1610
4	4	151	0	136	16	345
5	1	25	0	20	3	49
All	All	6248	0	6076	756	2841

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 61.

The worst 5 of 756 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:154:ILE:HG23	1:1:221:CYS:SG	1.55	1.47
1:1:101:ILE:H	1:1:101:ILE:CD1	1.07	1.44
1:1:108:GLN:NE2	3:3:226:ASP:OD2	1.69	1.24
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.23
1:1:218:GLY:O	1:1:219:THR:CG2	1.89	1.21

The worst 5 of 2841 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	Distance(Å)	Clash(Å)
1:1:39:THR:N	3:3:30:PRO:CD[12_555]	0.04	2.16
1:1:25:HIS:C	1:1:223:ARG:N[12_555]	0.17	2.03
1:1:243:ALA:N	3:3:215:ALA:N[12_555]	0.21	1.99
2:2:38:TRP:CE3	2:2:210:PRO:CG[12_555]	0.26	1.94
3:3:10:SER:CB	3:3:140:GLU:CA[12_555]	0.32	1.88

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	1	281/287 (98%)	206 (73%)	51 (18%)	24 (8%)	1	27
2	2	251/263 (95%)	201 (80%)	35 (14%)	15 (6%)	2	39
3	3	236/238 (99%)	179 (76%)	37 (16%)	20 (8%)	1	27
4	4	17/44 (39%)	9 (53%)	7 (41%)	1 (6%)	2	39
All	All	785/832 (94%)	595 (76%)	130 (17%)	60 (8%)	2	30

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	59	SER
1	1	72	GLY
1	1	107	ALA
1	1	108	GLN
1	1	114	GLU

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	1	254/258 (98%)	182 (72%)	72 (28%)	0	5
2	2	219/227 (96%)	159 (73%)	60 (27%)	0	6
3	3	209/209 (100%)	156 (75%)	53 (25%)	1	8
4	4	15/35 (43%)	9 (60%)	6 (40%)	0	1
All	All	697/729 (96%)	506 (73%)	191 (27%)	0	6

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	63	PHE
2	2	159	GLU
3	3	211	CYS
2	2	68	SER
2	2	103	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	111	GLN
2	2	197	ASN
3	3	124	ASN
2	2	192	ASN
2	2	207	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

1 ligand is 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	$\# Z > 2$
5	W54	1	500	-	27,27,27	2.81	4 (14%)	36,36,36	2.75	8 (22%)

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
5	W54	1	500	-	-	0/12/20/20	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	500	W54	C2A-N3A	11.69	1.43	1.27
5	1	500	W54	C4A-N3A	-6.52	1.36	1.47
5	1	500	W54	O1A-C2A	-4.03	1.29	1.36
5	1	500	W54	O1A-C5A	-2.79	1.38	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	500	W54	O1A-C2A-N3A	-8.88	109.94	118.38
5	1	500	W54	O1A-C2A-C4B	8.07	124.04	115.61
5	1	500	W54	C4A-N3A-C2A	6.18	112.81	106.68
5	1	500	W54	O1B-C1B-C6B	-5.66	115.18	121.08
5	1	500	W54	O1B-C1B-C2B	3.97	125.22	121.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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.