



wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 01:18 PM GMT

PDB ID : 4GK5
Title : Crystal structure of human Rev3-Rev7-Rev1-Polkappa complex
Authors : Tao, J.; Min, X.; Wei, X.
Deposited on : 2012-08-10
Resolution : 3.21 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>

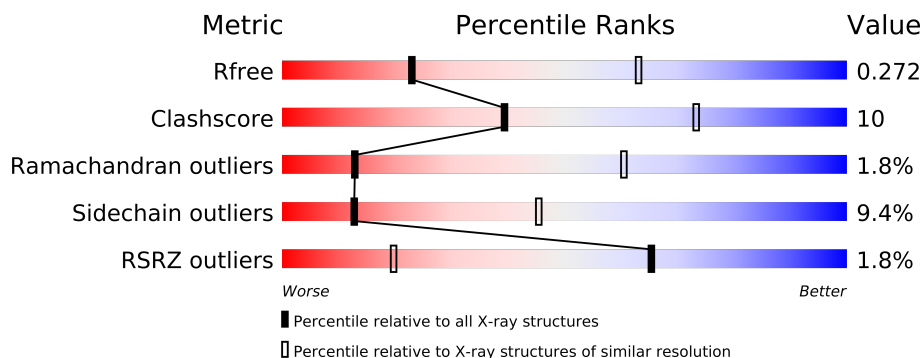
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 3.21 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}	66092	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)

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.

Mol	Chain	Length	Quality of chain
1	A	238	
1	B	238	
2	C	52	
2	D	52	
3	E	136	
3	F	136	
4	G	10	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5058 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 Mitotic spindle assembly checkpoint protein MAD2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1605	1037	270	288	10			
1	B	190	Total	C	N	O	S	0	0	0
			1546	999	261	276	10			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	EXPRESSION TAG	UNP Q9UI95
A	-14	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	-13	SER	-	EXPRESSION TAG	UNP Q9UI95
A	-12	SER	-	EXPRESSION TAG	UNP Q9UI95
A	-11	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-10	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-9	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-8	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-7	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-6	HIS	-	EXPRESSION TAG	UNP Q9UI95
A	-5	SER	-	EXPRESSION TAG	UNP Q9UI95
A	-4	GLN	-	EXPRESSION TAG	UNP Q9UI95
A	-3	ASP	-	EXPRESSION TAG	UNP Q9UI95
A	-2	PRO	-	EXPRESSION TAG	UNP Q9UI95
A	-1	ASN	-	EXPRESSION TAG	UNP Q9UI95
A	0	SER	-	EXPRESSION TAG	UNP Q9UI95
A	124	ALA	ARG	ENGINEERED MUTATION	UNP Q9UI95
A	212	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	213	SER	-	EXPRESSION TAG	UNP Q9UI95
A	214	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	215	SER	-	EXPRESSION TAG	UNP Q9UI95
A	216	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	217	SER	-	EXPRESSION TAG	UNP Q9UI95
A	218	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	219	SER	-	EXPRESSION TAG	UNP Q9UI95

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Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLY	-	EXPRESSION TAG	UNP Q9UI95
A	221	SER	-	EXPRESSION TAG	UNP Q9UI95
A	222	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-15	MET	-	EXPRESSION TAG	UNP Q9UI95
B	-14	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	-13	SER	-	EXPRESSION TAG	UNP Q9UI95
B	-12	SER	-	EXPRESSION TAG	UNP Q9UI95
B	-11	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-10	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-9	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-8	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-7	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-6	HIS	-	EXPRESSION TAG	UNP Q9UI95
B	-5	SER	-	EXPRESSION TAG	UNP Q9UI95
B	-4	GLN	-	EXPRESSION TAG	UNP Q9UI95
B	-3	ASP	-	EXPRESSION TAG	UNP Q9UI95
B	-2	PRO	-	EXPRESSION TAG	UNP Q9UI95
B	-1	ASN	-	EXPRESSION TAG	UNP Q9UI95
B	0	SER	-	EXPRESSION TAG	UNP Q9UI95
B	124	ALA	ARG	ENGINEERED MUTATION	UNP Q9UI95
B	212	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	213	SER	-	EXPRESSION TAG	UNP Q9UI95
B	214	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	215	SER	-	EXPRESSION TAG	UNP Q9UI95
B	216	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	217	SER	-	EXPRESSION TAG	UNP Q9UI95
B	218	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	219	SER	-	EXPRESSION TAG	UNP Q9UI95
B	220	GLY	-	EXPRESSION TAG	UNP Q9UI95
B	221	SER	-	EXPRESSION TAG	UNP Q9UI95
B	222	HIS	-	EXPRESSION TAG	UNP Q9UI95

- Molecule 2 is a protein called DNA polymerase zeta catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total 151	C 95	N 25	O 29	S 2	0	0	0
2	D	20	Total 151	C 95	N 25	O 29	S 2	0	0	0

- Molecule 3 is a protein called DNA repair protein REV1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	96	Total	C	N	O	S	0	0	0
			778	500	121	152	5			
3	F	93	Total	C	N	O	S	0	0	0
			756	487	118	146	5			

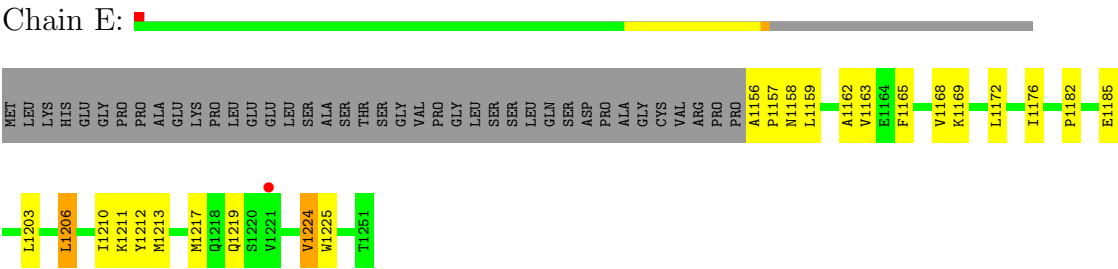
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1116	MET	-	EXPRESSION TAG	UNP Q9UBZ9
F	1116	MET	-	EXPRESSION TAG	UNP Q9UBZ9

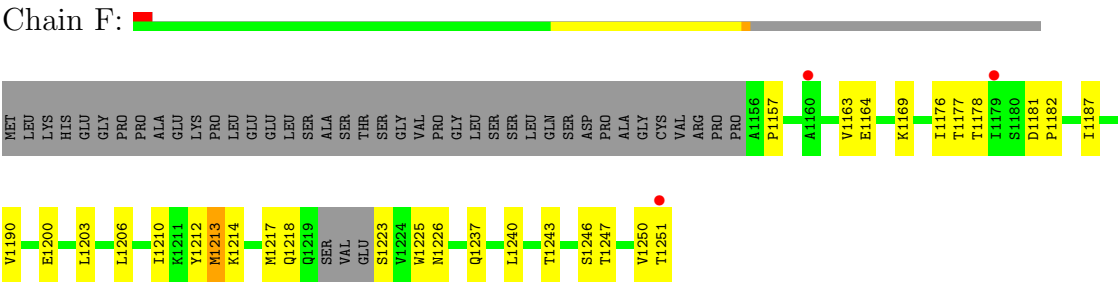
- Molecule 4 is a protein called DNA polymerase kappa.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	8	Total	C	N	O	0	0	0
			71	46	13	12			

• Molecule 3: DNA repair protein REV1



• Molecule 3: DNA repair protein REV1



• Molecule 4: DNA polymerase kappa



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.00Å 72.76Å 104.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.21 30.16 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-3.21) 99.2 (30.16-3.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.10 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.232 , 0.281 0.231 , 0.272	Depositor DCC
R_{free} test set	770 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	90.0	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 15469 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5058	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	A	0.63	0/1640	0.87	2/2228 (0.1%)
1	B	0.51	0/1579	0.76	0/2144
2	C	0.68	0/153	0.86	0/207
2	D	0.52	0/153	0.87	0/207
3	E	0.62	0/789	0.82	0/1070
3	F	0.53	0/766	0.74	0/1037
4	G	0.77	0/72	1.02	0/92
All	All	0.58	0/5152	0.81	2/6985 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	153	ARG	NE-CZ-NH2	-5.43	117.59	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	1605	0	1640	38	0
1	B	1546	0	1577	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	151	0	160	5	0
2	D	151	0	160	7	0
3	E	778	0	789	19	0
3	F	756	0	768	13	0
4	G	71	0	70	1	0
All	All	5058	0	5164	98	0

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 10.

The worst 5 of 98 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:TYR:CE2	1:A:53:GLN:HG3	2.21	0.75
2:D:1874:THR:OG1	2:D:1875:ALA:N	2.24	0.71
1:A:32:TYR:CD2	1:A:53:GLN:HG3	2.31	0.66
1:A:138:ASP:HB2	1:A:209:LYS:HE2	1.77	0.66
3:E:1156:ALA:N	3:E:1157:PRO:CD	2.58	0.66

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	194/238 (82%)	186 (96%)	6 (3%)	2 (1%)	22	74
1	B	186/238 (78%)	164 (88%)	18 (10%)	4 (2%)	10	53
2	C	18/52 (35%)	12 (67%)	4 (22%)	2 (11%)	1	5
2	D	18/52 (35%)	13 (72%)	4 (22%)	1 (6%)	3	23
3	E	94/136 (69%)	89 (95%)	5 (5%)	0	100	100
3	F	89/136 (65%)	76 (85%)	11 (12%)	2 (2%)	10	53
4	G	6/10 (60%)	4 (67%)	2 (33%)	0	100	100
All	All	605/862 (70%)	544 (90%)	50 (8%)	11 (2%)	13	60

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1891	MET
2	D	1891	MET
1	A	119	VAL
1	B	118	HIS
1	B	131	SER

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	186/219 (85%)	166 (89%)	20 (11%)	9	37
1	B	178/219 (81%)	162 (91%)	16 (9%)	14	48
2	C	18/49 (37%)	14 (78%)	4 (22%)	1	6
2	D	18/49 (37%)	15 (83%)	3 (17%)	3	14
3	E	90/123 (73%)	86 (96%)	4 (4%)	39	81
3	F	87/123 (71%)	80 (92%)	7 (8%)	17	57
4	G	8/10 (80%)	7 (88%)	1 (12%)	7	30
All	All	585/792 (74%)	530 (91%)	55 (9%)	13	45

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	62	GLN
1	B	165	VAL
3	F	1226	ASN
1	B	115	LEU
1	B	136	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	GLN
1	B	104	GLN
1	B	121	GLN

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Mol	Chain	Res	Type
1	B	10	ASN
1	B	118	HIS

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 ⓘ

There are no ligands in this entry.

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 ⓘ

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	198/238 (83%)	0.14	2 (1%) 79 31	26, 41, 63, 76	0
1	B	190/238 (79%)	0.12	2 (1%) 77 29	38, 59, 76, 80	0
2	C	20/52 (38%)	0.44	1 (5%) 28 6	32, 50, 81, 82	0
2	D	20/52 (38%)	0.51	2 (10%) 8 2	45, 63, 78, 79	0
3	E	96/136 (70%)	0.09	1 (1%) 79 31	26, 44, 65, 71	0
3	F	93/136 (68%)	0.09	3 (3%) 45 10	47, 68, 80, 81	0
4	G	8/10 (80%)	0.86	0 100 100	50, 55, 59, 62	0
All	All	625/862 (72%)	0.15	11 (1%) 65 20	26, 53, 76, 82	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1891	MET	3.7
1	A	90	LYS	3.1
1	B	142	PRO	2.4
3	E	1221	VAL	2.4
3	F	1179	ILE	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.