



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:16 AM UTC

PDB ID : 2XV4 / pdb_00002xv4
Title : Structure of Human RPC62 (partial)
Authors : Lefevre, S.; Legrand, P.; Fribourg, S.
Deposited on : 2010-10-22
Resolution : 2.95 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

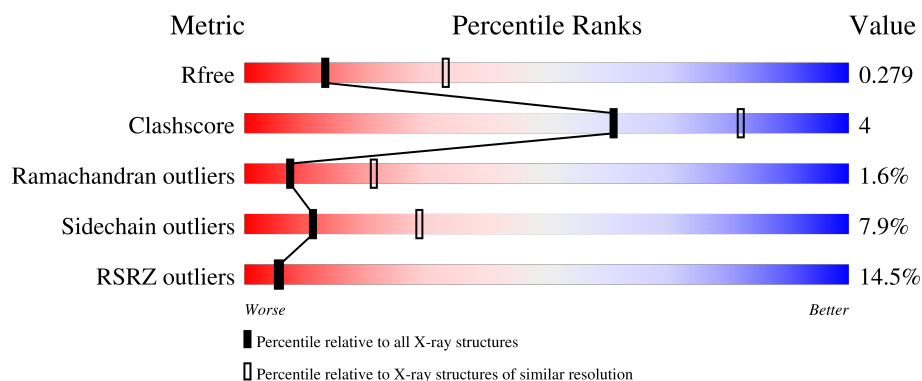
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	S	534	11% 58% 15% • 25%

2 Entry composition [i](#)

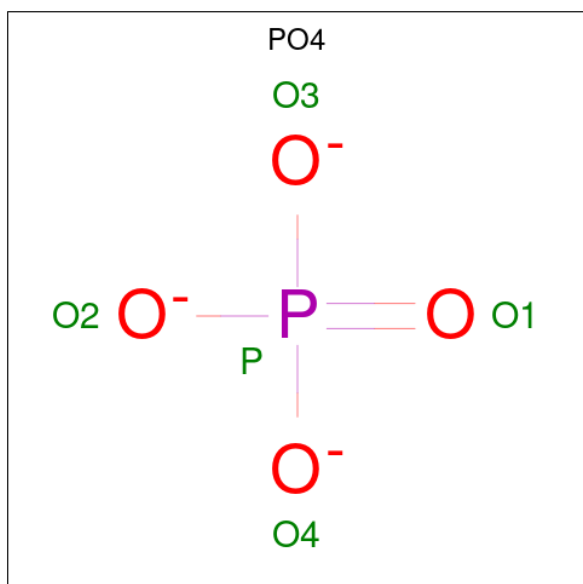
There are 3 unique types of molecules in this entry. The entry contains 3217 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	399	Total	C	N	O	S	0	0	0
			3184	2014	555	596	19			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	S	1	Total	O	P	0	0
			4	3	1		
2	S	1	Total	O	P	0	0
			5	4	1		
2	S	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	19	Total	O	0	0
			19	19		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.54Å 69.92Å 75.97Å 90.00° 112.84° 90.00°	Depositor
Resolution (Å)	70.01 – 2.95 70.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.01-2.95) 99.8 (70.01-2.95)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.228 , 0.256 0.237 , 0.279	Depositor DCC
R_{free} test set	846 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	84.2	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 87.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3217	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: PO4

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	S	0.87	2/3225 (0.1%)	1.53	22/4350 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	355	GLN	CD-OE1	5.33	1.33	1.23
1	S	244	GLN	CD-OE1	5.17	1.33	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	229	PRO	N-CA-CB	8.50	111.95	102.60
1	S	34	GLN	N-CA-C	7.93	115.35	108.22
1	S	260	ASP	CA-CB-CG	7.87	120.47	112.60
1	S	101	ASP	N-CA-C	-7.45	103.66	112.89
1	S	428	ILE	N-CA-C	7.16	117.24	110.30
1	S	309	ASP	CA-CB-CG	6.34	118.94	112.60
1	S	510	ASP	CA-CB-CG	6.28	118.88	112.60
1	S	422	TYR	N-CA-C	6.24	124.09	110.80
1	S	262	THR	N-CA-C	-6.08	104.21	111.69
1	S	73	VAL	N-CA-CB	5.81	116.86	110.53
1	S	421	PHE	CA-C-N	5.53	132.10	121.54
1	S	421	PHE	C-N-CA	5.53	132.10	121.54
1	S	246	PHE	CA-CB-CG	5.33	119.13	113.80
1	S	55	CYS	CA-C-N	5.30	127.23	120.56
1	S	55	CYS	C-N-CA	5.30	127.23	120.56
1	S	42	ASP	CA-CB-CG	5.21	117.81	112.60
1	S	118	MET	CA-C-N	5.20	127.20	120.44
1	S	118	MET	C-N-CA	5.20	127.20	120.44
1	S	275	GLU	CA-C-N	5.15	129.49	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	275	GLU	C-N-CA	5.15	129.49	122.90
1	S	29	ILE	CA-C-N	5.02	127.45	120.63
1	S	29	ILE	C-N-CA	5.02	127.45	120.63

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	S	3184	0	3222	27	0
2	S	14	0	0	0	0
3	S	19	0	0	1	0
All	All	3217	0	3222	27	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 (27) 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:S:429:LEU:HD21	1:S:433:ARG:HH11	1.68	0.58
1:S:347:THR:HA	1:S:350:LEU:HD12	1.88	0.56
1:S:310:GLN:NE2	3:S:2016:HOH:O	2.39	0.52
1:S:54:LEU:O	1:S:58:VAL:HG23	2.09	0.52
1:S:324:GLY:HA2	1:S:334:TYR:HA	1.93	0.50
1:S:317:ASP:OD2	1:S:319:PRO:HD2	2.13	0.49
1:S:260:ASP:O	1:S:261:GLN:HB2	2.14	0.48
1:S:308:LEU:HA	1:S:311:TYR:CD2	2.49	0.48
1:S:285:THR:HB	1:S:336:ILE:H	1.80	0.47
1:S:273:MET:CG	1:S:288:LEU:HD21	2.46	0.46
1:S:362:CYS:HA	1:S:365:ILE:HD12	1.98	0.45
1:S:315:LEU:HD11	1:S:334:TYR:HE1	1.82	0.45
1:S:273:MET:HG3	1:S:288:LEU:HD21	1.99	0.44
1:S:96:LYS:HB2	1:S:104:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:8:LEU:HD11	1:S:443:ILE:HG22	2.00	0.44
1:S:7:LYS:HE3	1:S:11:LEU:HD11	1.99	0.44
1:S:312:LEU:HA	1:S:315:LEU:HD12	1.99	0.44
1:S:105:LEU:HD22	1:S:128:ARG:NH1	2.34	0.43
1:S:517:ASP:HA	1:S:520:ILE:HB	2.00	0.43
1:S:512:SER:O	1:S:516:VAL:HG23	2.18	0.43
1:S:269:THR:HG21	1:S:297:LEU:HD23	2.00	0.42
1:S:443:ILE:HD12	1:S:520:ILE:HD12	2.02	0.41
1:S:99:TYR:HB2	1:S:103:GLY:HA3	2.02	0.41
1:S:315:LEU:HD21	1:S:334:TYR:HD1	1.85	0.40
1:S:428:ILE:HD13	1:S:428:ILE:H	1.86	0.40
1:S:40:ALA:HA	1:S:50:VAL:HG21	2.02	0.40
1:S:96:LYS:O	1:S:99:TYR:O	2.39	0.40

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	S	385/534 (72%)	362 (94%)	17 (4%)	6 (2%)	7 21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	229	PRO
1	S	231	ASP
1	S	422	TYR
1	S	100	SER
1	S	277	THR
1	S	230	ASP

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	S	353/476 (74%)	325 (92%)	28 (8%)	11	29

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	2	THR
1	S	3	GLN
1	S	36	LEU
1	S	47	LEU
1	S	65	TYR
1	S	67	VAL
1	S	78	GLN
1	S	95	THR
1	S	97	THR
1	S	102	THR
1	S	119	SER
1	S	130	THR
1	S	157	VAL
1	S	233	ILE
1	S	257	ASN
1	S	278	THR
1	S	288	LEU
1	S	303	ILE
1	S	307	VAL
1	S	321	GLU
1	S	368	LEU
1	S	370	LEU
1	S	426	VAL
1	S	428	ILE
1	S	429	LEU
1	S	461	LEU
1	S	497	GLN
1	S	505	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	S	49	GLN
1	S	66	GLN
1	S	155	HIS
1	S	249	GLN
1	S	286	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	PO4	S	1534	-	4,4,4	2.20	1 (25%)	6,6,6	0.81	0
2	PO4	S	1533	-	0,3,4	-	-	0,3,6	-	-
2	PO4	S	1535	-	4,4,4	2.75	2 (50%)	6,6,6	1.22	1 (16%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1535	PO4	P-O1	4.49	1.61	1.50
2	S	1534	PO4	P-O1	3.53	1.58	1.50
2	S	1535	PO4	P-O2	2.34	1.61	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	1535	PO4	O3-P-O1	-2.04	103.75	110.95

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 ⓘ

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	S	399/534 (74%)	0.65	58 (14%) 6 5	62, 98, 153, 176	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	280	SER	6.2
1	S	423	LEU	5.5
1	S	484	LEU	4.6
1	S	420	THR	4.4
1	S	311	TYR	4.4
1	S	318	ASP	4.3
1	S	334	TYR	3.8
1	S	322	PHE	3.8
1	S	323	VAL	3.7
1	S	426	VAL	3.7
1	S	500	GLU	3.6
1	S	324	GLY	3.6
1	S	230	ASP	3.5
1	S	532	LYS	3.5
1	S	474	MET	3.5
1	S	313	THR	3.3
1	S	283	PRO	3.3
1	S	1	MET	3.3
1	S	229	PRO	3.3
1	S	73	VAL	3.3
1	S	302	ASN	3.2
1	S	422	TYR	3.0
1	S	461	LEU	3.0
1	S	259	MET	2.8
1	S	332	GLY	2.8
1	S	306	GLN	2.7
1	S	320	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	S	365	ILE	2.6
1	S	350	LEU	2.6
1	S	431	ALA	2.6
1	S	371	GLN	2.5
1	S	231	ASP	2.5
1	S	366	PHE	2.5
1	S	343	ALA	2.5
1	S	369	VAL	2.4
1	S	419	ARG	2.4
1	S	288	LEU	2.4
1	S	428	ILE	2.4
1	S	333	MET	2.4
1	S	429	LEU	2.4
1	S	285	THR	2.4
1	S	315	LEU	2.4
1	S	325	LYS	2.3
1	S	308	LEU	2.3
1	S	451	GLN	2.3
1	S	471	ILE	2.3
1	S	483	GLN	2.2
1	S	487	ILE	2.2
1	S	370	LEU	2.2
1	S	100	SER	2.2
1	S	132	THR	2.2
1	S	232	GLY	2.2
1	S	304	SER	2.2
1	S	316	ALA	2.1
1	S	528	GLU	2.1
1	S	321	GLU	2.1
1	S	421	PHE	2.1
1	S	162	SER	2.0

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	S	1535	5/5	0.82	0.43	103,106,109,112	0
2	PO4	S	1533	4/5	0.88	0.15	119,123,125,126	0
2	PO4	S	1534	5/5	0.95	0.10	143,148,149,149	0

6.5 Other polymers [i](#)

There are no such residues in this entry.