

Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2022 – 07:03 am BST

PDB ID : 7R1O

Title: p62-ZZ domain of the human sequestosome in complex with dusquetide

Authors: Hakansson, M.; Hansson, M.; Logan, D.T.; Rozek, A.; Donini, O.

Deposited on : 2022-02-03

Resolution : 2.20 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 (i) 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 (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \\ & & EDS & : & \textbf{FAILED} \end{array}$

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

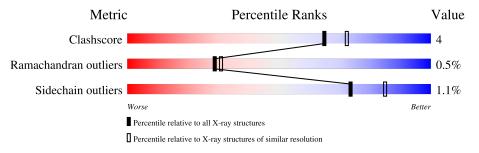
Validation Pipeline (wwPDB-VP) : 2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.20 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(\AA))$
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain	Ĺ
1	AAA	53	89%	11%
1	BBB	53	81%	8% • 9%
1	CCC	53	89%	8% •
1	DDD	53	87%	13%
2	EEE	5	100%	
2	FFF	5	60%	20% 20%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1711 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 Sequestosome-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace			
1	AAA	53	Total	С	N	О	S	0	0	0			
1	AAA	99	397	247	71	72	7	0	0	U			
1	BBB	48	Total	С	N	О	S	0	0	0			
1	מממ	40	351	218	63	64	6	0	0	U			
1	CCC	51	Total	С	N	О	S	0	0	0			
1		91	377	234	68	68	7	0	0	U			
1	מממ	מממ	מממ	DDD	53	Total	С	N	О	S	0	2	0
1	מממ	55	404	252	71	74	7	0	2	U			

• Molecule 2 is a protein called Dusquetide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	EEE	5	Total 39	C 25			0	0	0
2	FFF	4	Total 33	C 22	N 7	O 4	0	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	2	$\begin{array}{cc} \text{Total} & \text{Zn} \\ 2 & 2 \end{array}$	0	0
3	BBB	2	Total Zn 2 2	0	0
3	CCC	2	Total Zn 2 2	0	0
3	DDD	2	$\begin{array}{cc} \text{Total} & \text{Zn} \\ 2 & 2 \end{array}$	0	0

• Molecule 4 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	34	Total O 34 34	0	0
4	BBB	20	Total O 20 20	0	0
4	CCC	11	Total O 11 11	0	0
4	DDD	32	Total O 32 32	0	0
4	EEE	3	Total O 3 3	0	0
4	FFF	2	Total O 2 2	0	0

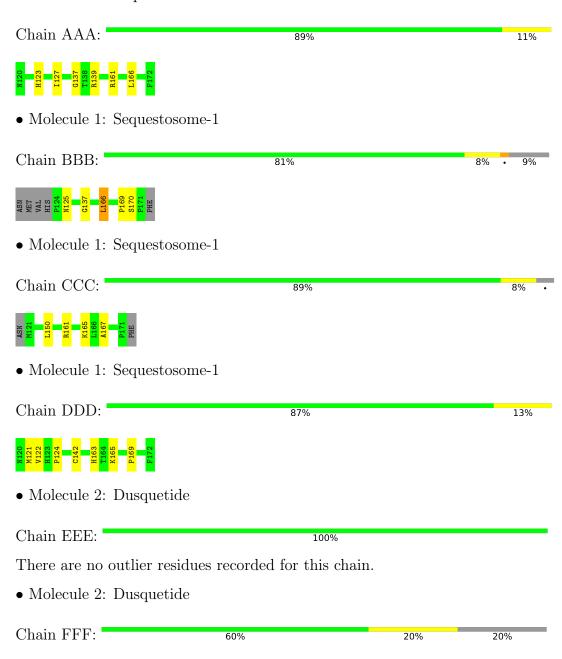


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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 failed to run properly.

• Molecule 1: Sequestosome-1









4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	124.07Å 25.15Å 77.53Å	Depositor
a, b, c, α , β , γ	90.00° 124.92° 90.00°	Depositor
Resolution (Å)	24.63 - 2.20	Depositor
% Data completeness	98.9 (24.63-2.20)	Depositor
(in resolution range)	30.3 (24.00 2.20)	_
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.45 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.178 , 0.243	Depositor
Wilson B-factor (\mathring{A}^2)	26.9	Xtriage
Anisotropy	0.153	Xtriage
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1711	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 17.09% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	Bo	nd angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	AAA	0.80	0/408	1.02	1/552~(0.2%)
1	BBB	0.79	0/360	1.00	0/488
1	CCC	0.73	0/387	0.90	0/525
1	DDD	0.81	0/421	1.00	0/570
2	EEE	0.93	0/39	0.79	0/51
2	FFF	0.72	0/33	0.97	0/44
All	All	0.79	0/1648	0.98	1/2230 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
1	AAA	139	ARG	NE-CZ-NH2	-6.41	117.09	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	AAA	397	0	375	5	0
1	BBB	351	0	336	5	0
1	CCC	377	0	360	3	0
1	DDD	404	0	387	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	EEE	39	0	47	0	0
2	FFF	33	0	42	2	0
3	AAA	2	0	0	0	0
3	BBB	2	0	0	0	0
3	CCC	2	0	0	0	0
3	DDD	2	0	0	0	0
4	AAA	34	0	0	0	0
4	BBB	20	0	0	0	0
4	CCC	11	0	0	0	0
4	DDD	32	0	0	0	0
4	EEE	3	0	0	0	0
4	FFF	2	0	0	0	0
All	All	1711	0	1547	13	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 (13) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:DDD:122:VAL:O	1:DDD:124:PRO:HD3	2.06	0.55
1:CCC:150:LEU:HD12	1:CCC:165:LYS:HE2	1.87	0.55
1:BBB:137:GLY:O	1:BBB:170:SER:HB3	2.07	0.54
1:BBB:166:LEU:HD23	1:BBB:166:LEU:N	2.24	0.52
1:AAA:127:ILE:HD12	2:FFF:3:VAL:HG11	1.96	0.48
1:CCC:167:ALA:HB3	1:DDD:165:LYS:HB2	1.95	0.48
1:AAA:166:LEU:CD2	1:BBB:166:LEU:HD22	2.45	0.46
2:FFF:3:VAL:O	2:FFF:3:VAL:HG23	2.17	0.44
1:AAA:123:HIS:NE2	1:AAA:137:GLY:O	2.48	0.43
1:DDD:142:CYS:SG	1:DDD:163:HIS:HB3	2.59	0.42
1:AAA:166:LEU:HD23	1:BBB:166:LEU:HD22	2.02	0.41
1:AAA:161:ARG:O	1:BBB:169:PRO:HG3	2.21	0.41
1:CCC:161:ARG:O	1:DDD:169:PRO:HB3	2.21	0.41

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	Perce	entiles
1	AAA	51/53~(96%)	50 (98%)	1 (2%)	0	100	100
1	BBB	46/53~(87%)	42 (91%)	3 (6%)	1 (2%)	6	4
1	CCC	$49/53\ (92\%)$	47 (96%)	2 (4%)	0	100	100
1	DDD	53/53~(100%)	47 (89%)	6 (11%)	0	100	100
2	EEE	3/5~(60%)	3 (100%)	0	0	100	100
2	FFF	2/5~(40%)	2 (100%)	0	0	100	100
All	All	$204/222\ (92\%)$	191 (94%)	12 (6%)	1 (0%)	29	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	125	ASN

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	Perce	ntiles
1	AAA	$46/46 \; (100\%)$	46 (100%)	0	100	100
1	BBB	41/46 (89%)	40 (98%)	1 (2%)	49	62
1	CCC	44/46 (96%)	44 (100%)	0	100	100
1	DDD	48/46 (104%)	47 (98%)	1 (2%)	53	67
2	EEE	4/4 (100%)	4 (100%)	0	100	100
2	FFF	4/4~(100%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	187/192 (97%)	185 (99%)	2 (1%)	73 85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	166	LEU
1	DDD	121	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

