



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 29, 2022 – 03:13 pm GMT

PDB ID : 7QF9
Title : Crystal structure of PDE6D bound to HRas peptide
Authors : Yelland, T.; Ismail, I.
Deposited on : 2021-12-05
Resolution : 1.95 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

<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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.31.3

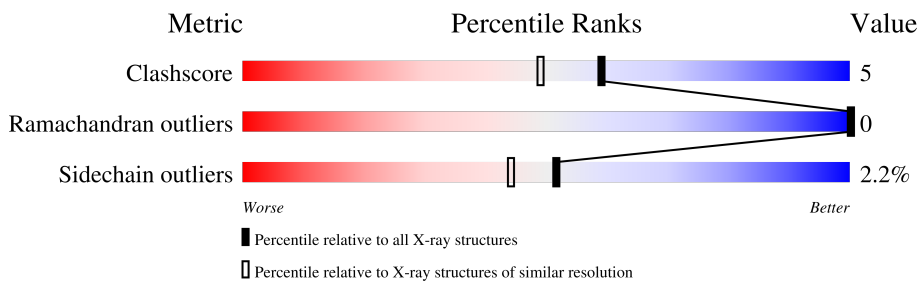
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	149	87% 11% ..
1	BBB	149	88% 11% .
2	EEE	10	50% 10% 10% 30%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2705 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.

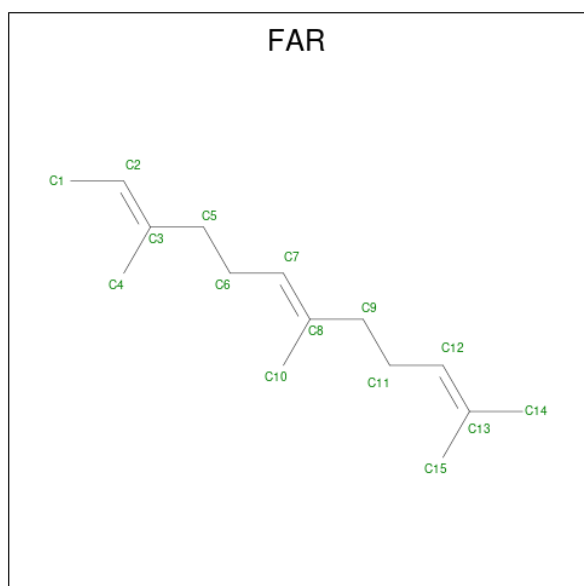
- Molecule 1 is a protein called Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BBB	149	Total	C	N	O	S	0	6	0
			1258	809	212	231	6			
1	AAA	147	Total	C	N	O	S	0	1	0
			1205	774	201	224	6			

- Molecule 2 is a protein called HRas peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	EEE	7	Total	C	N	O	S	0	0	0
			47	26	8	9	4			

- Molecule 3 is FARNESYL (three-letter code: FAR) (formula: C₁₅H₂₆).



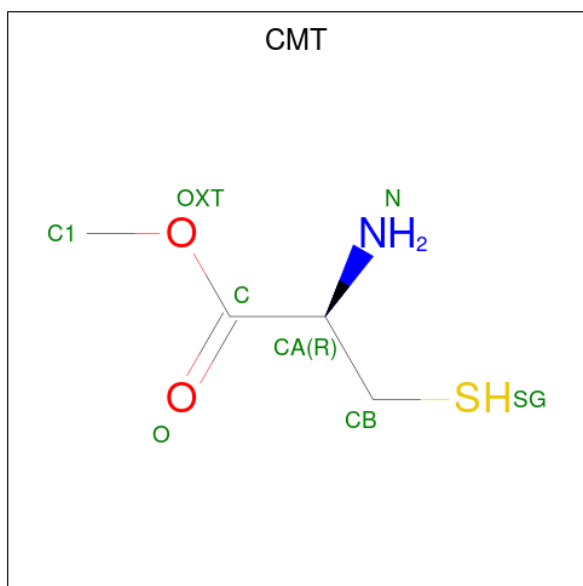
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	BBB	1	Total	C	0	0
			15	15		

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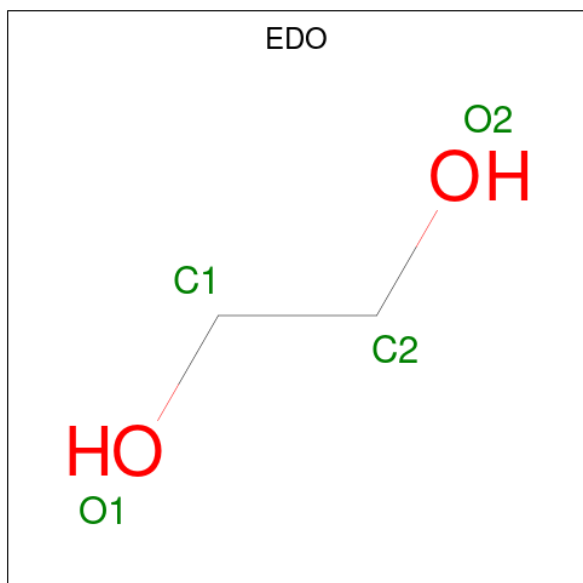
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	EEE	1	Total	C	0	0
			15	15		

- Molecule 4 is O-METHYLCYSTEINE (three-letter code: CMT) (formula: $C_4H_9NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	BBB	1	Total	C	N	O	S	0	0
			8	4	1	2	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	BBB	72	Total O 72 72	0	0
6	AAA	64	Total O 64 64	0	0
6	EEE	1	Total O 1 1	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: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

Chain BBB:  88% 11% .



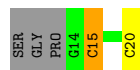
- Molecule 1: Retinal rod rhodopsin-sensitive cGMP 3',5'-cyclic phosphodiesterase subunit delta

Chain AAA:  87% 11% ..



- Molecule 2: HRas peptide

Chain EEE:  50% 10% 10% 30%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	34.63Å 82.79Å 112.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.23 – 1.95	Depositor
% Data completeness (in resolution range)	99.8 (56.23-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.230 , 0.299	Depositor
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.043	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2705	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.03% 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: EDO, CMT, FAR

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	AAA	0.61	0/1231	0.66	0/1660
1	BBB	0.62	0/1289	0.67	0/1743
2	EEE	0.75	0/38	0.73	0/47
All	All	0.62	0/2558	0.66	0/3450

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	1205	0	1190	12	0
1	BBB	1258	0	1238	11	0
2	EEE	47	0	46	1	0
3	BBB	15	0	24	0	0
3	EEE	15	0	24	2	0
4	BBB	8	0	8	2	0
5	AAA	8	0	12	0	0
5	BBB	12	0	18	0	0
6	AAA	64	0	0	1	0
6	BBB	72	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	EEE	1	0	0	0	0
All	All	2705	0	2560	24	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 5.

The worst 5 of 24 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:AAA:50:PRO:HB2	1:AAA:52:LYS:HG2	1.67	0.74
1:AAA:17:LEU:HG	1:AAA:63:LEU:HD11	1.80	0.62
1:AAA:147:LEU:HD21	3:EEE:201:FAR:H52	1.84	0.60
1:BBB:6[B]:GLU:OE2	1:BBB:13:ARG:NH1	2.39	0.56
1:BBB:76[A]:LEU:HD11	1:BBB:92:PHE:HD2	1.72	0.54

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	AAA	146/149 (98%)	144 (99%)	2 (1%)	0	100	100
1	BBB	153/149 (103%)	149 (97%)	4 (3%)	0	100	100
2	EEE	5/10 (50%)	5 (100%)	0	0	100	100
All	All	304/308 (99%)	298 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	132/134 (98%)	130 (98%)	2 (2%)	65	60
1	BBB	137/134 (102%)	134 (98%)	3 (2%)	52	44
2	EEE	5/7 (71%)	4 (80%)	1 (20%)	1	0
All	All	274/275 (100%)	268 (98%)	6 (2%)	52	44

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	5	ASP
1	AAA	52	LYS
2	EEE	15	CYS
1	BBB	20	MET
1	BBB	5	ASP

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](#)

1 non-standard protein/DNA/RNA residue 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
2	CMT	EEE	20	2,3	7,7,7	1.99	1 (14%)	6,8,8	1.37	0

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
2	CMT	EEE	20	2,3	-	2/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EEE	20	CMT	OXT-C	5.05	1.45	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	EEE	20	CMT	N-CA-CB-SG
2	EEE	20	CMT	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
5	EDO	AAA	201	-	3,3,3	0.05	0	2,2,2	0.09	0
5	EDO	BBB	203	-	3,3,3	0.05	0	2,2,2	0.04	0
5	EDO	BBB	204	-	3,3,3	0.06	0	2,2,2	0.06	0
4	CMT	BBB	202	3	7,7,7	2.00	1 (14%)	6,8,8	0.80	0
3	FAR	BBB	201	4	14,14,14	0.24	0	16,16,16	0.17	0
5	EDO	AAA	202	-	3,3,3	0.07	0	2,2,2	0.08	0
3	FAR	EEE	201	2	14,14,14	0.23	0	16,16,16	0.46	0
5	EDO	BBB	205	-	3,3,3	0.06	0	2,2,2	0.06	0

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	EDO	AAA	201	-	-	0/1/1/1	-
5	EDO	BBB	203	-	-	0/1/1/1	-
5	EDO	BBB	204	-	-	1/1/1/1	-
4	CMT	BBB	202	3	-	5/8/8/8	-
3	FAR	BBB	201	4	-	6/14/14/14	-
5	EDO	AAA	202	-	-	0/1/1/1	-
3	FAR	EEE	201	2	-	5/14/14/14	-
5	EDO	BBB	205	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	202	CMT	OXT-C	5.10	1.45	1.33

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	EEE	201	FAR	C7-C8-C9-C11
3	EEE	201	FAR	C10-C8-C9-C11
4	BBB	202	CMT	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
4	BBB	202	CMT	OXT-C-CA-N
4	BBB	202	CMT	CA-C-OXT-C1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	202	CMT	2	0
3	EEE	201	FAR	2	0

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.