



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 01:26 pm GMT

PDB ID : 6GRD
Title : eukaryotic junction-resolving enzyme GEN-1 binding with Cesium
Authors : Lilley, D.M.J.; Liu, Y.; Freeman, D.J.
Deposited on : 2018-06-11
Resolution : 2.66 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

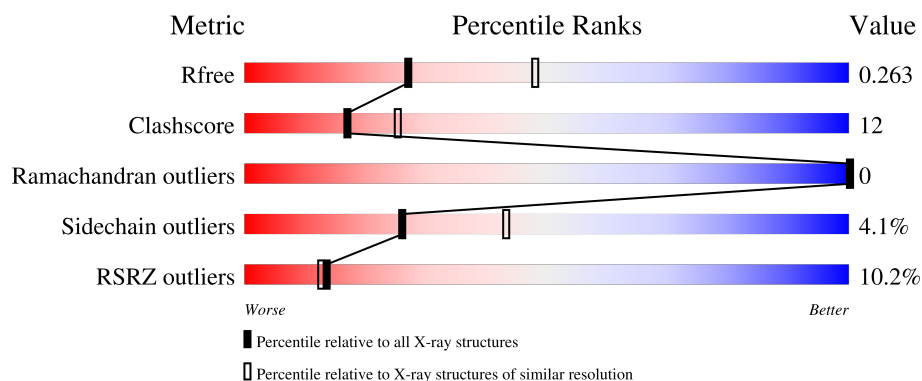
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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}	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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	A	530	<div> <div>8%</div> <div>58%</div> <div>17%</div> <div>23%</div> </div>
2	H	15	<div> <div>7%</div> <div>73%</div> <div>27%</div> </div>
3	R	16	<div> <div>6%</div> <div>62%</div> <div>38%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3688 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 Nuclease-like protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	Se		24	1	0
			3091	1973	531	574	6	7				

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*AP*GP*CP*GP*GP*TP*GP*GP*TP*TP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	15	Total	C	N	O	P		0	0	1
			297	139	56	88	14				

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*AP*CP*CP*CP*AP*CP*CP*AP*CP*CP*GP*CP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	R	16	Total	C	N	O	P		0	0	1
			298	141	54	88	15				

- Molecule 4 is CESIUM ION (three-letter code: CS) (formula: Cs) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cs	1	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	1	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.39Å 97.39Å 119.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.81 – 2.66 68.81 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.81-2.66) 99.9 (68.81-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.244 , 0.262 0.261 , 0.263	Depositor DCC
R_{free} test set	977 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3688	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/3160	0.72	4/4286 (0.1%)
2	H	1.08	1/333 (0.3%)	1.03	0/516
3	R	0.96	0/332	0.91	0/508
All	All	0.71	1/3825 (0.0%)	0.77	4/5310 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	16	DT	O3'-P	6.70	1.69	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	324	LYS	CD-CE-NZ	-6.04	97.81	111.70
1	A	162	LYS	N-CA-C	-5.97	94.88	111.00
1	A	329	LEU	CA-CB-CG	5.85	128.75	115.30

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	A	3091	0	2990	81	0
2	H	297	0	159	4	0
3	R	298	0	167	5	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
All	All	3688	0	3316	86	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 12.

All (86) 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:A:42:TRP:HB3	1:A:46:ILE:CD1	1.59	1.29
1:A:42:TRP:CB	1:A:46:ILE:HD12	1.73	1.18
1:A:39:MSE:HE1	1:A:76:PHE:HB3	1.22	1.11
1:A:42:TRP:CE3	1:A:46:ILE:HD11	2.02	0.95
1:A:42:TRP:CB	1:A:46:ILE:CD1	2.40	0.90
1:A:316:TRP:CE2	1:A:324:LYS:NZ	2.39	0.89
1:A:42:TRP:HB3	1:A:46:ILE:HD12	0.88	0.85
1:A:369:ARG:HE	1:A:371:HIS:HB2	1.41	0.82
1:A:15:ARG:NH2	1:A:157:SER:OG	2.13	0.79
1:A:42:TRP:CD2	1:A:46:ILE:HD11	2.18	0.78
1:A:17:SER:HA	1:A:168:HIS:HA	1.66	0.77
2:H:22:DG:N2	3:R:9:DC:O2	2.19	0.75
1:A:39:MSE:CE	1:A:76:PHE:HB3	2.12	0.75
1:A:369:ARG:NH2	1:A:442:TRP:CD1	2.57	0.73
1:A:316:TRP:CZ2	1:A:324:LYS:NZ	2.58	0.72
1:A:369:ARG:NE	1:A:371:HIS:HB2	2.05	0.70
1:A:387:ALA:HB2	1:A:435:PRO:HB2	1.76	0.68
2:H:21:DG:H1'	2:H:22:DG:H5'	1.76	0.66
1:A:167:THR:OG1	1:A:168:HIS:HD2	1.78	0.66
1:A:225:LEU:HD11	1:A:271:MSE:HE1	1.76	0.65
2:H:22:DG:N1	3:R:9:DC:N3	2.42	0.65
1:A:357:GLU:O	1:A:360:THR:HG22	2.01	0.61
1:A:42:TRP:CG	1:A:46:ILE:HD11	2.36	0.61
1:A:42:TRP:CA	1:A:46:ILE:HD12	2.30	0.60
1:A:225:LEU:O	1:A:225:LEU:HD12	2.02	0.60
1:A:257:THR:OG1	2:H:27:DT:O3'	2.19	0.59
1:A:369:ARG:HE	1:A:371:HIS:CB	2.14	0.59
1:A:333:LEU:HB3	1:A:389:LEU:HD21	1.86	0.58
1:A:215:GLN:HA	1:A:218:LYS:HE3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:HIS:HE1	1:A:124:GLU:OE1	1.87	0.57
1:A:248:ARG:HG3	1:A:260:LYS:HA	1.87	0.56
1:A:42:TRP:CB	1:A:46:ILE:HD11	2.33	0.55
1:A:192:VAL:O	1:A:196:SER:HB3	2.07	0.54
1:A:39:MSE:HE1	1:A:76:PHE:CB	2.16	0.54
1:A:20:LYS:HD2	1:A:375:ASP:HB2	1.90	0.54
1:A:369:ARG:NH2	1:A:442:TRP:NE1	2.56	0.53
1:A:66:ARG:NH2	1:A:166:PRO:HD2	2.24	0.53
1:A:21:LEU:HD11	1:A:171:LEU:HD12	1.89	0.53
1:A:42:TRP:CG	1:A:46:ILE:CD1	2.92	0.53
1:A:303:ILE:HD11	1:A:333:LEU:HD21	1.91	0.52
1:A:9:GLU:O	1:A:182:SER:HB3	2.10	0.51
1:A:106:LEU:HD13	1:A:309:PHE:CE2	2.46	0.51
1:A:167:THR:OG1	1:A:168:HIS:CD2	2.61	0.51
1:A:46:ILE:HG23	1:A:59:THR:OG1	2.11	0.50
1:A:293:GLN:O	1:A:293:GLN:HG3	2.10	0.50
1:A:385:ILE:HG22	1:A:388:GLU:H	1.75	0.50
1:A:358:GLU:HG2	1:A:452:VAL:HA	1.93	0.50
1:A:299:SER:O	1:A:299:SER:OG	2.22	0.50
1:A:44:PHE:O	3:R:15:DA:H2'	2.11	0.49
1:A:49:ALA:O	1:A:50:ARG:HD2	2.12	0.49
1:A:130:GLN:O	1:A:130:GLN:HG3	2.12	0.49
1:A:82:ASN:HB2	1:A:119:GLY:HA2	1.93	0.49
1:A:316:TRP:CD2	1:A:324:LYS:NZ	2.77	0.48
1:A:358:GLU:HG2	1:A:452:VAL:HG12	1.94	0.47
1:A:106:LEU:HD13	1:A:309:PHE:CZ	2.50	0.47
1:A:224:GLU:O	1:A:228:ILE:HG12	2.15	0.47
1:A:57:ILE:HG13	1:A:102:MSE:HG2	1.97	0.46
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.80	0.46
1:A:358:GLU:OE1	1:A:454:VAL:HG22	2.16	0.46
1:A:46:ILE:HG22	1:A:56:ALA:HA	1.97	0.45
1:A:359:SER:HA	1:A:362:VAL:O	2.15	0.45
1:A:35:LEU:HD23	1:A:37:ILE:HD11	1.98	0.45
1:A:225:LEU:CD1	1:A:271:MSE:HE1	2.46	0.44
1:A:118:PRO:HG2	1:A:282:VAL:C	2.39	0.43
1:A:385:ILE:CG2	1:A:388:GLU:HB3	2.48	0.43
1:A:39:MSE:HE2	1:A:39:MSE:HB2	1.59	0.43
1:A:218:LYS:NZ	1:A:254:PHE:O	2.23	0.43
1:A:42:TRP:HE3	1:A:46:ILE:HD11	1.73	0.43
1:A:21:LEU:HA	1:A:21:LEU:HD23	1.86	0.43
1:A:319:ARG:CZ	1:A:399:GLU:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:NH1	1:A:399:GLU:HB2	2.34	0.42
1:A:46:ILE:CG2	1:A:56:ALA:HA	2.49	0.42
1:A:259:HIS:HB3	1:A:262:LEU:HB2	2.01	0.42
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.77	0.42
1:A:283:SER:HB3	1:A:287:THR:HB	2.02	0.42
1:A:24:ASP:O	1:A:28:GLN:HG3	2.20	0.41
1:A:195:MSE:HE2	1:A:208:CYS:SG	2.61	0.41
1:A:49:ALA:HB3	1:A:55:PRO:HB2	2.03	0.41
1:A:65:VAL:HG11	1:A:328:VAL:O	2.20	0.41
1:A:178:ALA:O	1:A:183:GLY:HA2	2.21	0.41
3:R:2:DC:H2'	3:R:3:DC:H6	1.85	0.41
3:R:6:DC:H2''	3:R:7:DC:O4'	2.21	0.41
1:A:144:THR:H	1:A:144:THR:HG23	1.58	0.40
1:A:231:ALA:O	1:A:232:ASP:C	2.58	0.40
1:A:75:ILE:HD11	1:A:115:HIS:HB2	2.03	0.40
1:A:215:GLN:CA	1:A:218:LYS:HE3	2.51	0.40

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	A	400/530 (76%)	377 (94%)	23 (6%)	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	A	318/438 (73%)	305 (96%)	13 (4%)	26	43

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	31	ARG
1	A	130	GLN
1	A	200	TYR
1	A	201	LEU
1	A	208	CYS
1	A	218	LYS
1	A	225	LEU
1	A	229	LYS
1	A	248	ARG
1	A	276	TYR
1	A	311	ARG
1	A	367	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	168	HIS
1	A	215	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

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	400/530 (75%)	0.72	42 (10%) 13 12	36, 71, 98, 111	1 (0%)
2	H	15/15 (100%)	0.06	1 (6%) 25 23	79, 91, 107, 113	0
3	R	16/16 (100%)	0.56	1 (6%) 27 25	85, 96, 114, 117	0
All	All	431/561 (76%)	0.69	44 (10%) 13 13	36, 74, 100, 117	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLN	5.0
1	A	203	ASP	4.9
1	A	97	GLY	4.3
1	A	196	SER	4.2
1	A	299	SER	4.2
1	A	161	SER	4.2
1	A	40	ALA	4.2
1	A	256	ARG	4.0
1	A	200	TYR	3.9
1	A	45	GLN	3.8
1	A	44	PHE	3.5
1	A	228	ILE	3.3
1	A	46	ILE	3.3
1	A	42	TRP	3.2
1	A	355	LYS	3.1
1	A	431	LYS	2.9
1	A	190	VAL	2.8
1	A	356	LYS	2.8
1	A	432	PRO	2.8
1	A	43	GLN	2.7
1	A	400	VAL	2.7
1	A	82	ASN	2.7
1	A	98	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	205	ILE	2.7
1	A	234	GLU	2.6
1	A	199	ASP	2.6
1	A	188	GLY	2.6
2	H	30	DT	2.5
1	A	276	TYR	2.5
1	A	255	PHE	2.5
1	A	103	ALA	2.5
1	A	338	CYS	2.5
1	A	162	LYS	2.4
1	A	163	GLY	2.3
1	A	390	VAL	2.3
1	A	216	ALA	2.3
1	A	231	ALA	2.2
1	A	101	ALA	2.2
1	A	50	ARG	2.1
1	A	201	LEU	2.1
1	A	389	LEU	2.1
1	A	465	SER	2.0
1	A	341	ARG	2.0
3	R	1	DA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.