



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 13, 2017 – 08:22 AM EDT

PDB ID : 4D5E
Title : Crystal Structure of recombinant wildtype CDH
Authors : Loschonsky, S.; Wacker, T.; Waltzer, S.; Giovannini, P.P.; McLeish, M.J.;
Andrade, S.L.A.; Mueller, M.
Deposited on : unknown
Resolution : 1.43 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

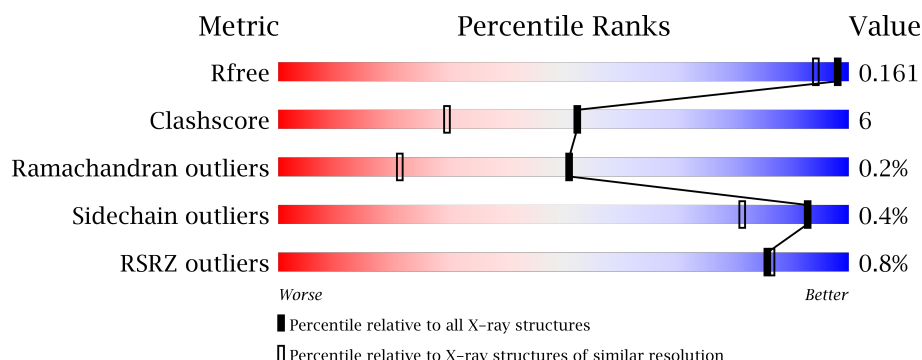
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.43 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}	100719	1367 (1.46-1.42)
Clashscore	112137	1425 (1.46-1.42)
Ramachandran outliers	110173	1405 (1.46-1.42)
Sidechain outliers	110143	1405 (1.46-1.42)
RSRZ outliers	101464	1372 (1.46-1.42)

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. 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	589	 86% 11% ..
1	B	589	 87% 12% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	2PE	A	1598	-	-	-	X
11	2PE	B	1595	-	-	-	X
11	2PE	B	1597	-	-	-	X
4	MES	A	1590[A]	-	-	-	X
4	MES	A	1590[B]	-	-	-	X
4	MES	B	1591	-	-	-	X
7	P6G	A	1593	-	-	-	X
7	P6G	A	1595	-	-	-	X
9	PG4	A	1596	-	-	-	X
9	PG4	A	1599	-	-	-	X
9	PG4	A	1600	-	-	-	X
9	PG4	B	1596	-	-	X	-
9	PG4	B	1602	-	-	-	X

2 Entry composition ⓘ

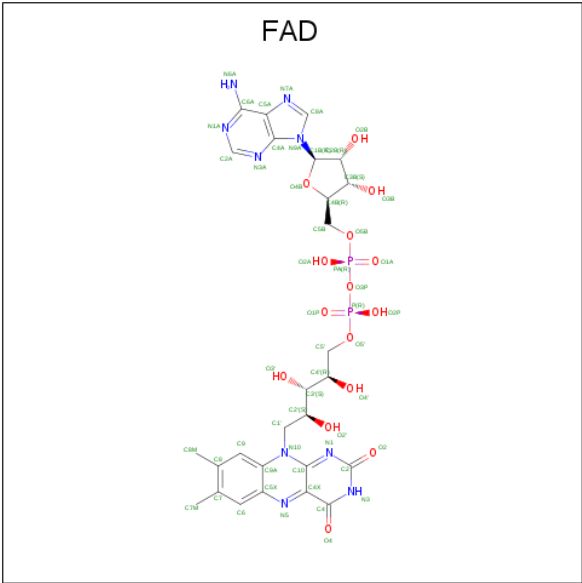
There are 12 unique types of molecules in this entry. The entry contains 10559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYCLOHEXANE-1,2-DIONE HYDROLASE.

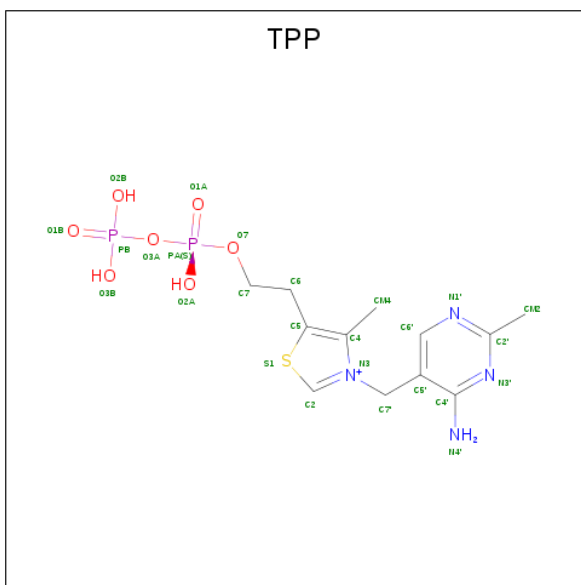
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	22	26	0
			4605	2917	812	851	25			
1	B	587	Total	C	N	O	S	41	21	0
			4598	2913	817	845	23			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



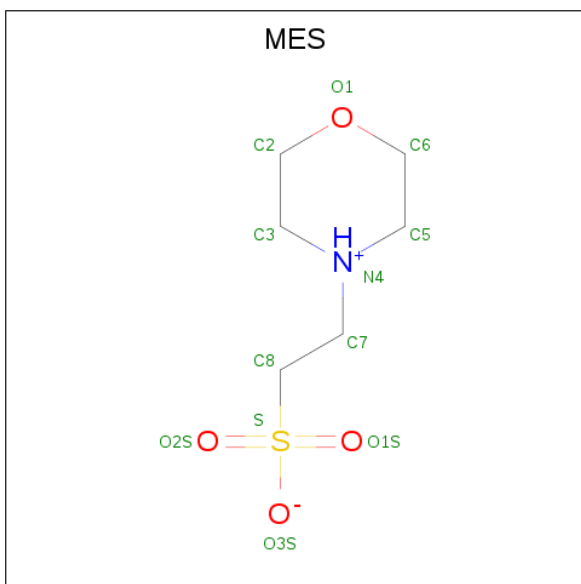
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

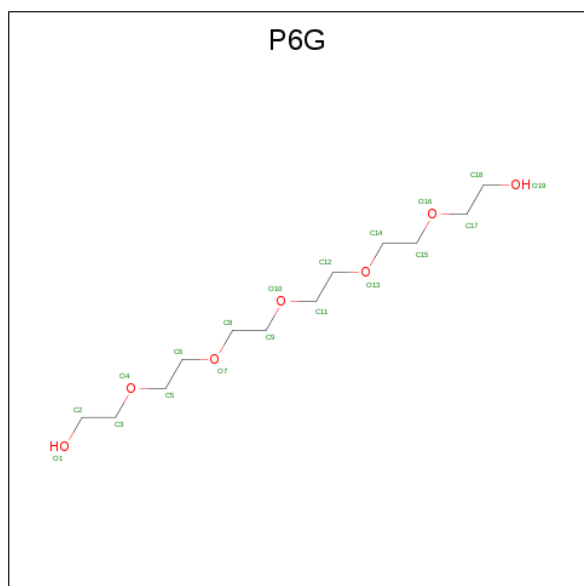
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

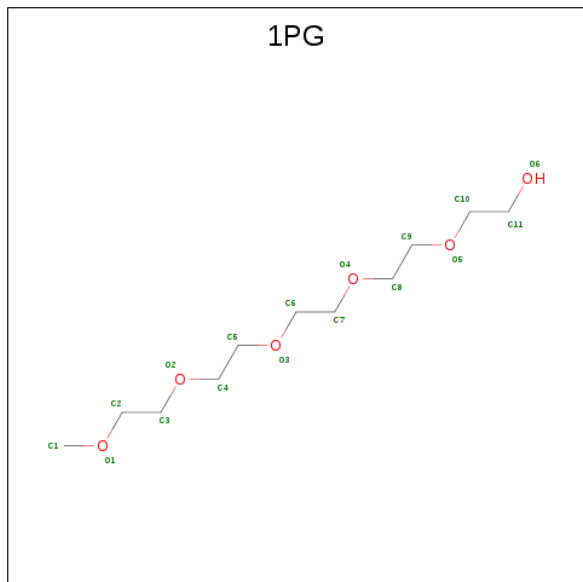
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Mg	0	0
			2	2		
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



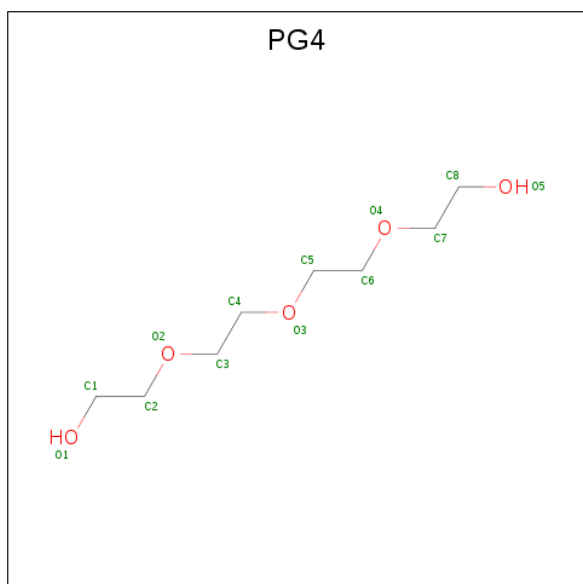
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	8	4		
7	A	1	Total	C	O	0	0
			17	11	6		

- Molecule 8 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula: C₁₁H₂₄O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



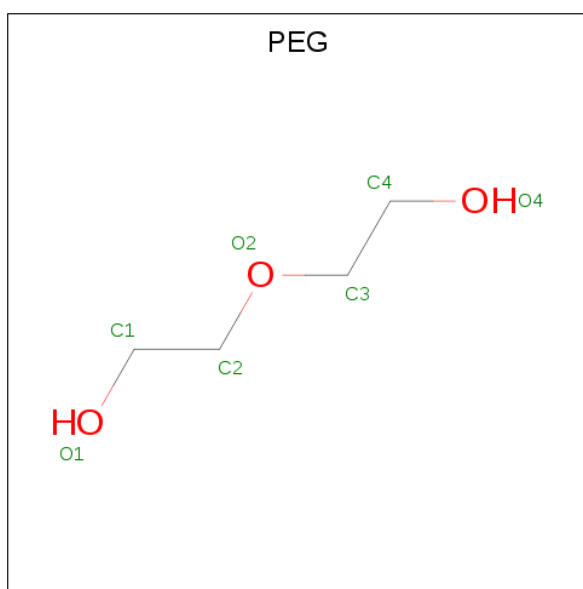
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	7	4		

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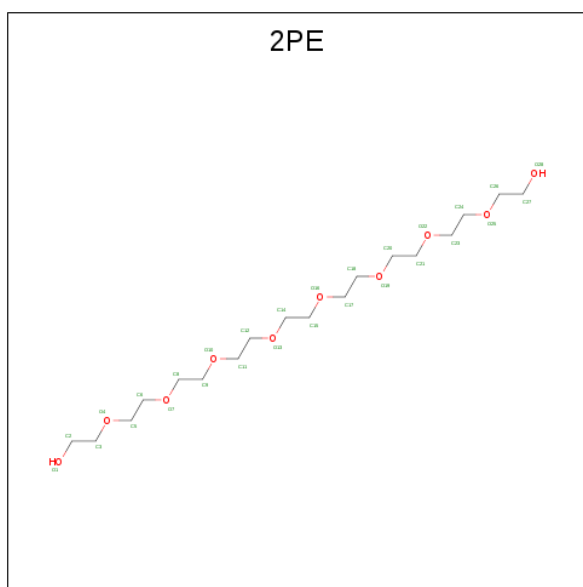
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	4	2		
9	A	1	Total	C	O	0	0
			13	8	5		
9	B	1	Total	C	O	0	0
			11	7	4		
9	B	1	Total	C	O	0	0
			6	4	2		
9	B	1	Total	C	O	0	0
			11	7	4		
9	B	1	Total	C	O	0	0
			8	5	3		
9	B	1	Total	C	O	0	0
			9	6	3		
9	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total 15	C 10	O 5	0	0
11	B	1	Total 19	C 12	O 7	0	0
11	B	1	Total 22	C 14	O 8	0	0

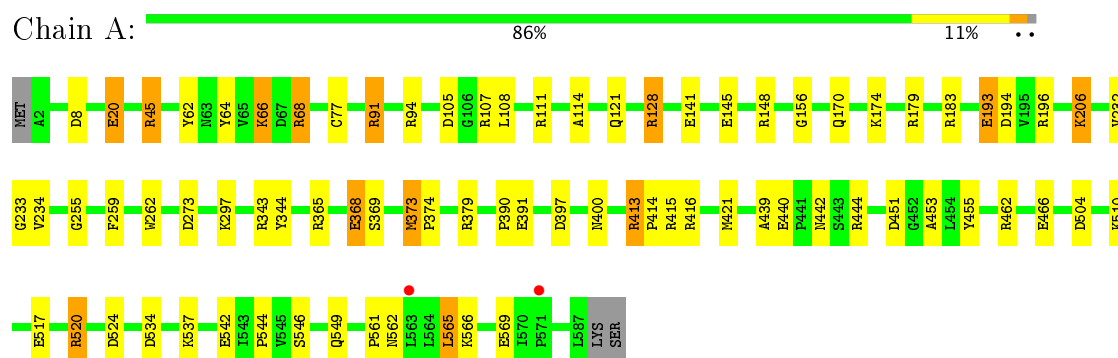
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	539	Total O 539 539	0	0
12	B	431	Total O 431 431	0	0

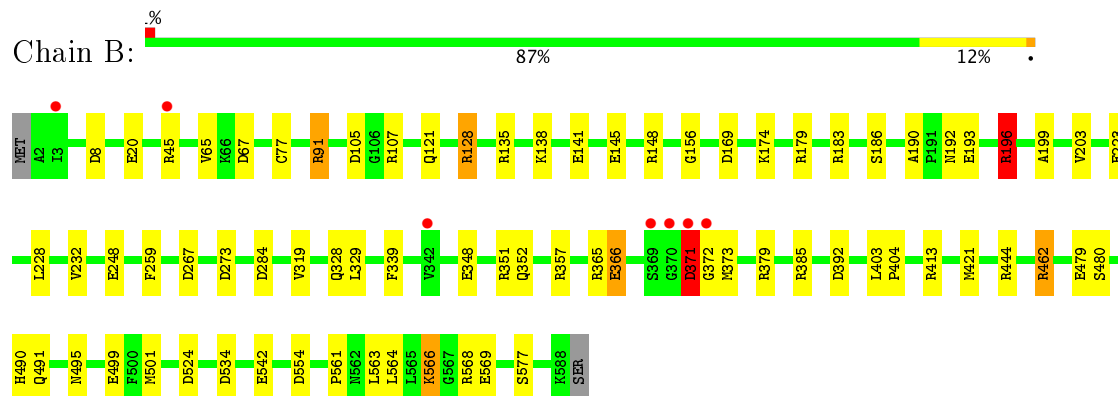
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

• Molecule 1: CYCLOHEXANE-1,2-DIONE HYDROLASE



• Molecule 1: CYCLOHEXANE-1,2-DIONE HYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	123.19Å 123.19Å 143.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.68 – 1.43 46.68 – 1.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.68-1.43) 100.0 (46.68-1.43)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.122 , 0.147 0.138 , 0.161	Depositor DCC
R_{free} test set	10152 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.7	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	0.98	EDS
Total number of atoms	10559	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: MG, P6G, CL, 1PG, PG4, 2PE, MES, TPP, PEG, FAD

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	2.55	30/4750 (0.6%)	2.17	54/6447 (0.8%)
1	B	2.30	22/4725 (0.5%)	1.79	49/6409 (0.8%)
All	All	2.43	52/9475 (0.5%)	1.99	103/12856 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	4
All	All	1	5

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20[A]	GLU	CD-OE2	-103.26	0.12	1.25
1	A	20[B]	GLU	CD-OE2	-103.26	0.12	1.25
1	B	348	GLU	CD-OE2	-68.21	0.50	1.25
1	B	196[A]	ARG	CZ-NH2	-55.03	0.61	1.33
1	B	196[B]	ARG	CZ-NH2	-55.03	0.61	1.33

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20[A]	GLU	OE1-CD-OE2	-100.02	3.27	123.30
1	A	20[B]	GLU	OE1-CD-OE2	-100.02	3.27	123.30
1	B	196[A]	ARG	NE-CZ-NH1	-63.72	88.44	120.30
1	B	196[B]	ARG	NE-CZ-NH1	-63.72	88.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	GLU	OE1-CD-OE2	28.48	157.48	123.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	371	ASP	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	GLY	Mainchain
1	B	196[A]	ARG	Sidechain
1	B	371	ASP	Mainchain
1	B	372	GLY	Peptide
1	B	480[B]	SER	Peptide

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	A	4605	0	4551	49	0
1	B	4598	0	4549	50	1
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	26	0	16	1	0
3	B	26	0	16	1	0
4	A	24	0	26	4	0
4	B	12	0	13	0	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	29	0	33	9	0
8	A	12	0	14	1	0
9	A	30	0	36	3	0
9	B	53	0	60	12	0
10	A	7	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	15	0	19	1	0
11	B	41	0	54	5	0
12	A	539	0	0	27	1
12	B	431	0	0	15	0
All	All	10559	0	9459	119	2

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 6.

The worst 5 of 119 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:B:379[B]:ARG:HD3	12:B:2286:HOH:O	1.42	1.19
1:B:121[B]:GLN:NE2	12:B:2084:HOH:O	1.70	1.19
1:A:121[B]:GLN:OE1	12:A:2129:HOH:O	1.57	1.18
1:B:259[A]:PHE:CD2	1:B:561:PRO:HD3	1.89	1.06
7:A:1595:P6G:H91	12:A:2530:HOH:O	1.59	1.00

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:2528:HOH:O	12:A:2534:HOH:O[3_445]	2.06	0.14
1:B:366:GLU:OE2	1:B:366:GLU:OE2[8_444]	2.15	0.05

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	610/589 (104%)	599 (98%)	10 (2%)	1 (0%)	51 21
1	B	606/589 (103%)	595 (98%)	10 (2%)	1 (0%)	51 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1216/1178 (103%)	1194 (98%)	20 (2%)	2 (0%)	51	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	CYS
1	B	77	CYS

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	475/453 (105%)	473 (100%)	2 (0%)	93	81
1	B	472/453 (104%)	469 (99%)	3 (1%)	89	69
All	All	947/906 (104%)	942 (100%)	5 (0%)	93	75

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	LEU
1	A	566	LYS
1	B	371	ASP
1	B	542[A]	GLU
1	B	542[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	116	GLN
1	B	495	ASN
1	B	328	GLN
1	A	412	GLN
1	B	153	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 5 are monoatomic - leaving 23 for Mogul analysis.

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	FAD	A	1588	-	51,58,58	1.19	5 (9%)	54,89,89	2.01	9 (16%)
3	TPP	A	1589	6	21,27,27	1.44	2 (9%)	25,40,40	1.58	3 (12%)
4	MES	A	1590[A]	-	12,12,12	3.17	2 (16%)	14,16,16	5.31	6 (42%)
4	MES	A	1590[B]	-	12,12,12	2.07	2 (16%)	14,16,16	3.84	7 (50%)
7	P6G	A	1593	-	11,11,18	0.94	0	10,10,17	1.71	3 (30%)
8	1PG	A	1594	-	11,11,16	0.63	0	10,10,15	0.98	0
7	P6G	A	1595	-	16,16,18	1.31	2 (12%)	15,15,17	2.07	2 (13%)
9	PG4	A	1596	-	10,10,12	1.27	1 (10%)	9,9,11	1.25	0
10	PEG	A	1597	-	6,6,6	0.29	0	5,5,5	1.00	0
11	2PE	A	1598	-	14,14,27	0.75	0	13,13,26	1.32	1 (7%)
9	PG4	A	1599	-	5,5,12	0.59	0	4,4,11	0.66	0
9	PG4	A	1600	-	12,12,12	0.73	0	11,11,11	0.89	0
2	FAD	B	1589	-	51,58,58	1.22	7 (13%)	54,89,89	2.51	11 (20%)
3	TPP	B	1590	6	21,27,27	2.23	3 (14%)	25,40,40	1.59	5 (20%)
4	MES	B	1591	-	12,12,12	1.68	2 (16%)	14,16,16	1.99	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	2PE	B	1595	-	18,18,27	1.19	2 (11%)	17,17,26	1.10	2 (11%)
9	PG4	B	1596	-	10,10,12	2.00	4 (40%)	9,9,11	2.53	3 (33%)
11	2PE	B	1597	-	21,21,27	0.73	0	20,20,26	1.20	1 (5%)
9	PG4	B	1598	-	5,5,12	0.66	0	4,4,11	0.58	0
9	PG4	B	1599	-	10,10,12	0.51	0	9,9,11	0.56	0
9	PG4	B	1600	-	7,7,12	1.04	0	6,6,11	0.40	0
9	PG4	B	1601	-	8,8,12	0.51	0	7,7,11	0.91	0
9	PG4	B	1602	-	7,7,12	1.18	0	6,6,11	0.64	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	FAD	A	1588	-	-	0/28/50/50	0/6/6/6
3	TPP	A	1589	6	-	0/16/17/17	0/2/2/2
4	MES	A	1590[A]	-	-	0/6/14/14	0/1/1/1
4	MES	A	1590[B]	-	-	0/6/14/14	0/1/1/1
7	P6G	A	1593	-	-	0/9/9/16	0/0/0/0
8	1PG	A	1594	-	-	0/9/9/14	0/0/0/0
7	P6G	A	1595	-	-	0/14/14/16	0/0/0/0
9	PG4	A	1596	-	-	0/8/8/10	0/0/0/0
10	PEG	A	1597	-	-	0/4/4/4	0/0/0/0
11	2PE	A	1598	-	-	0/12/12/25	0/0/0/0
9	PG4	A	1599	-	-	0/3/3/10	0/0/0/0
9	PG4	A	1600	-	-	0/10/10/10	0/0/0/0
2	FAD	B	1589	-	-	0/28/50/50	0/6/6/6
3	TPP	B	1590	6	-	0/16/17/17	0/2/2/2
4	MES	B	1591	-	-	0/6/14/14	0/1/1/1
11	2PE	B	1595	-	-	0/16/16/25	0/0/0/0
9	PG4	B	1596	-	-	0/8/8/10	0/0/0/0
11	2PE	B	1597	-	-	0/19/19/25	0/0/0/0
9	PG4	B	1598	-	-	0/3/3/10	0/0/0/0
9	PG4	B	1599	-	-	0/8/8/10	0/0/0/0
9	PG4	B	1600	-	-	0/5/5/10	0/0/0/0
9	PG4	B	1601	-	-	0/6/6/10	0/0/0/0
9	PG4	B	1602	-	-	0/5/5/10	0/0/0/0

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1590[A]	MES	C8-S	-10.13	1.62	1.77
3	B	1590	TPP	C4-N3	-8.39	1.32	1.39
4	A	1590[B]	MES	C8-S	-6.06	1.68	1.77
4	B	1591	MES	C8-S	-3.22	1.72	1.77
2	B	1589	FAD	C5'-C4'	-2.92	1.47	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1589	FAD	C4-C4X-C10	-7.53	113.87	119.96
2	B	1589	FAD	C4X-C10-N10	-6.19	116.22	120.52
4	A	1590[A]	MES	O3S-S-C8	-5.73	99.01	106.06
2	A	1588	FAD	N3A-C2A-N1A	-5.37	124.18	128.86
9	B	1596	PG4	C3-O2-C2	-5.23	90.63	113.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1588	FAD	1	0
3	A	1589	TPP	1	0
4	A	1590[A]	MES	1	0
4	A	1590[B]	MES	3	0
7	A	1593	P6G	5	0
8	A	1594	1PG	1	0
7	A	1595	P6G	4	0
9	A	1596	PG4	1	0
10	A	1597	PEG	1	0
11	A	1598	2PE	1	0
9	A	1599	PG4	2	0
2	B	1589	FAD	1	0
3	B	1590	TPP	1	0
11	B	1595	2PE	4	0
9	B	1596	PG4	9	0
11	B	1597	2PE	1	0
9	B	1602	PG4	3	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](#)

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	586/589 (99%)	-0.52	2 (0%)	93 95	7, 11, 22, 47	13 (2%)
1	B	587/589 (99%)	-0.51	7 (1%)	79 79	7, 12, 26, 57	19 (3%)
All	All	1173/1178 (99%)	-0.52	9 (0%)	86 86	7, 11, 24, 57	32 (2%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ILE	4.9
1	A	563[A]	LEU	3.5
1	B	371	ASP	3.1
1	B	45	ARG	3.0
1	B	369	SER	3.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
11	2PE	B	1597	22/28	0.76	0.23	10.02	38,51,71,77	0
7	P6G	A	1593	12/19	0.75	0.16	7.79	36,46,53,57	0
4	MES	A	1590[B]	12/12	0.75	0.30	7.15	24,29,38,40	12
4	MES	A	1590[A]	12/12	0.75	0.30	6.65	23,27,35,38	12
9	PG4	A	1599	6/13	0.68	0.17	6.37	36,40,41,45	0
11	2PE	A	1598	15/28	0.91	0.12	4.11	21,29,42,43	0
7	P6G	A	1595	17/19	0.89	0.10	3.49	19,29,41,46	0
4	MES	B	1591	12/12	0.96	0.18	3.00	18,23,28,31	0
9	PG4	A	1596	11/13	0.90	0.12	2.90	19,26,39,44	0
9	PG4	A	1600	13/13	0.90	0.11	2.88	22,26,34,41	0
11	2PE	B	1595	19/28	0.88	0.14	2.75	21,35,44,45	19
9	PG4	B	1602	8/13	0.87	0.13	2.03	24,33,44,44	0
9	PG4	B	1596	11/13	0.83	0.16	1.85	20,24,41,53	0
8	1PG	A	1594	12/17	0.90	0.17	1.28	30,32,37,37	0
9	PG4	B	1600	8/13	0.90	0.08	1.20	21,23,26,26	0
6	MG	B	1594	1/1	1.00	0.07	1.00	7,7,7,7	0
6	MG	A	1592	1/1	1.00	0.08	0.98	5,5,5,5	0
9	PG4	B	1599	11/13	0.86	0.14	0.65	49,52,61,65	0
9	PG4	B	1601	9/13	0.91	0.10	0.47	34,38,47,49	0
6	MG	B	1593	1/1	0.95	0.08	0.25	38,38,38,38	0
3	TPP	B	1590	26/26	0.99	0.05	-0.43	7,8,9,12	0
3	TPP	A	1589	26/26	0.99	0.06	-0.54	6,7,9,11	0
2	FAD	A	1588	53/53	0.99	0.05	-0.54	6,8,9,10	0
10	PEG	A	1597	7/7	0.94	0.08	-0.56	34,39,42,51	0
2	FAD	B	1589	53/53	0.99	0.05	-0.57	6,8,10,10	0
5	CL	B	1592	1/1	1.00	0.04	-2.35	12,12,12,12	0
5	CL	A	1591	1/1	1.00	0.02	-3.28	14,14,14,14	0
9	PG4	B	1598	6/13	0.79	0.18	-	35,41,48,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.