



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2024 – 02:03 AM EST

PDB ID : 3PCB
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 3-HYDROXYBENZOATE
Authors : Elango, N.; Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-04-25
Resolution : 2.19 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

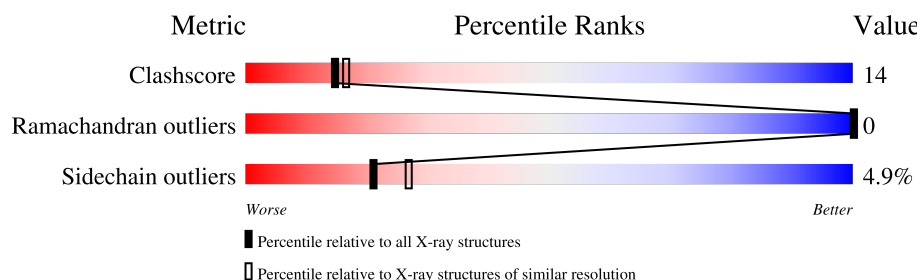
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	71% 24% .
1	B	200	71% 24% .
1	C	200	72% 25% .
1	D	200	71% 25% .
1	E	200	68% 27% . .
1	F	200	66% 29% .
2	M	238	69% 25% . . .
2	N	238	76% 18% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	O	238	<div><div></div><div>68%26%</div><div>...</div></div>
2	P	238	<div><div></div><div>72%20%</div><div>...</div></div>
2	Q	238	<div><div></div><div>68%26%</div><div>..</div></div>
2	R	238	<div><div></div><div>68%24%5%</div><div>.</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22032 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 Protocatechuate 3,4-dioxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	B	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	C	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	D	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	E	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	F	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			

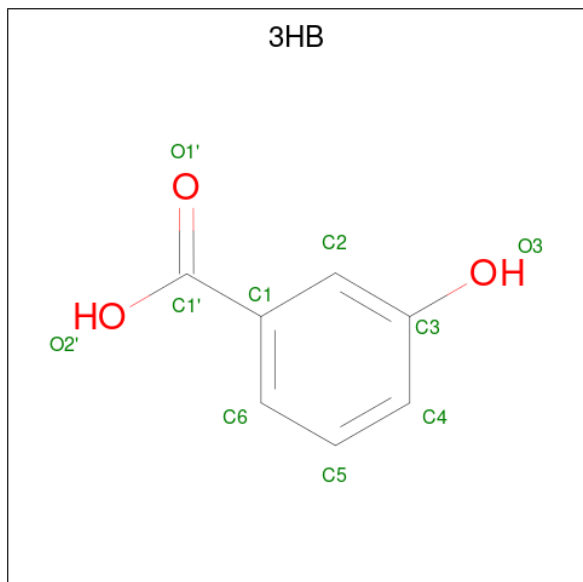
- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			
2	N	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			
2	O	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			
2	P	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			
2	Q	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			
2	R	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0

- Molecule 4 is 3-HYDROXYBENZOIC ACID (three-letter code: 3HB) (formula: C₇H₆O₃).



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

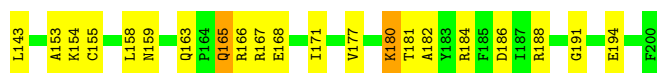
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	C	O	0	0
			10	7	3		
4	P	1	Total	C	O	0	0
			10	7	3		
4	Q	1	Total	C	O	0	0
			10	7	3		
4	Q	1	Total	C	O	0	0
			10	7	3		
4	R	1	Total	C	O	0	0
			10	7	3		
4	R	1	Total	C	O	0	0
			10	7	3		

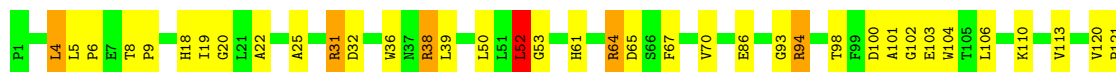
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total	O	0	0
			83	83		
5	M	151	Total	O	0	0
			151	151		
5	B	79	Total	O	0	0
			79	79		
5	N	161	Total	O	0	0
			161	161		
5	C	81	Total	O	0	0
			81	81		
5	O	155	Total	O	0	0
			155	155		
5	D	81	Total	O	0	0
			81	81		
5	P	152	Total	O	0	0
			152	152		
5	E	84	Total	O	0	0
			84	84		
5	Q	153	Total	O	0	0
			153	153		
5	F	80	Total	O	0	0
			80	80		
5	R	156	Total	O	0	0
			156	156		



- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain E: 68% 27% . .



- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain F: 66% 29% .



- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

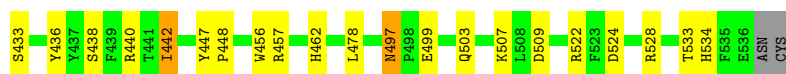
Chain M: 69% 25% . . .



ASN
CYS

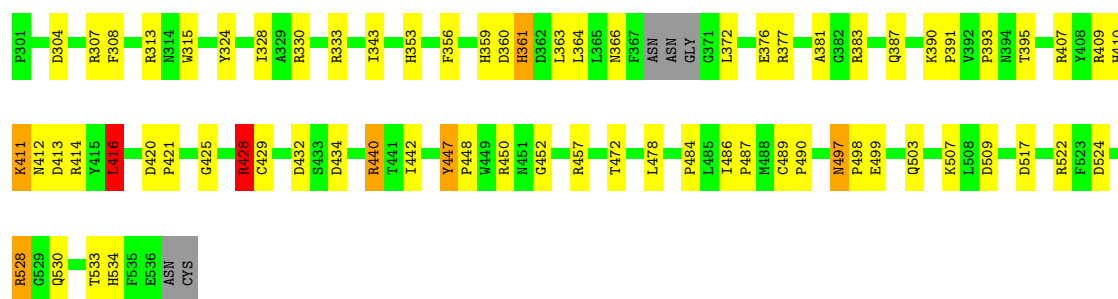
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain N: 76% 18% . .



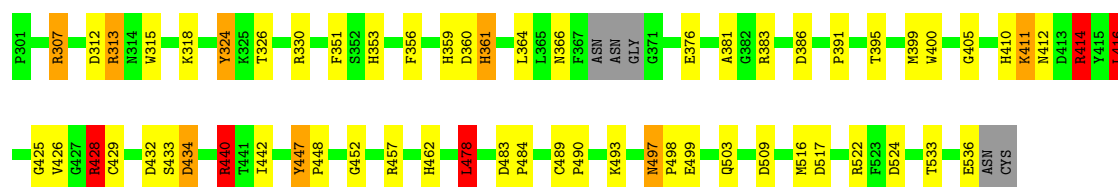
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain O: 68% 26% . . .



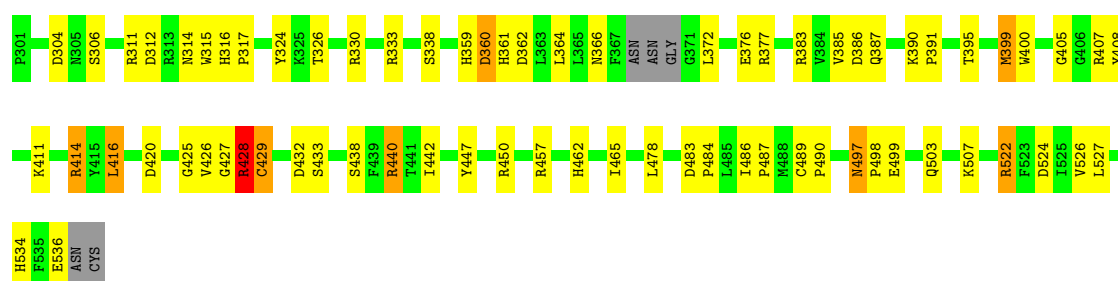
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain P: 72% 20% . . .



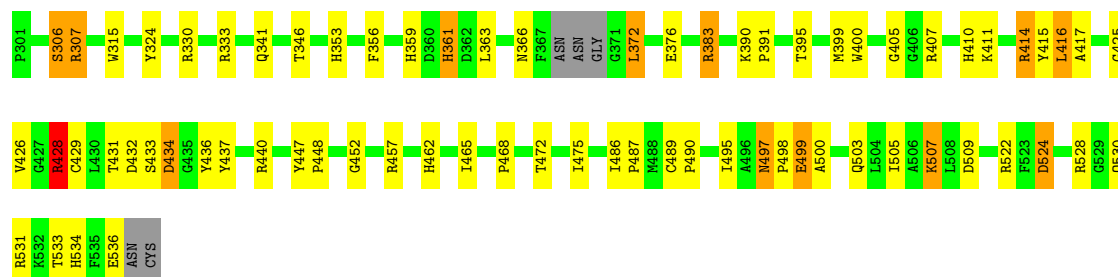
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain Q: 68% 26% . .



• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain R: 68% 24% 5% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.95 Å 127.56 Å 134.31 Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.19	Depositor
% Data completeness (in resolution range)	78.2 (6.00-2.19)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22032	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3HB, FE, CME

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	0.95	1/1611 (0.1%)	1.68	33/2195 (1.5%)
1	B	0.96	2/1611 (0.1%)	1.67	31/2195 (1.4%)
1	C	1.00	0/1611	1.64	22/2195 (1.0%)
1	D	0.99	1/1611 (0.1%)	1.75	28/2195 (1.3%)
1	E	0.99	0/1611	1.54	21/2195 (1.0%)
1	F	1.02	0/1611	1.65	25/2195 (1.1%)
2	M	1.02	0/1888	1.63	28/2569 (1.1%)
2	N	0.99	0/1888	1.61	27/2569 (1.1%)
2	O	0.99	0/1888	1.62	30/2569 (1.2%)
2	P	0.98	1/1888 (0.1%)	1.58	30/2569 (1.2%)
2	Q	1.03	0/1888	1.63	27/2569 (1.1%)
2	R	1.01	0/1888	1.58	26/2569 (1.0%)
All	All	0.99	5/20994 (0.0%)	1.63	328/28584 (1.1%)

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	F	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ARG	CD-NE	-6.59	1.35	1.46
1	D	94	ARG	CD-NE	-6.48	1.35	1.46
1	B	194	GLU	CD-OE2	-5.92	1.19	1.25
2	P	428	ARG	CG-CD	-5.26	1.38	1.51
1	B	94	ARG	CD-NE	-5.07	1.37	1.46

The worst 5 of 328 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	440	ARG	NE-CZ-NH2	-23.68	108.46	120.30
2	N	440	ARG	NE-CZ-NH2	-22.88	108.86	120.30
1	D	94	ARG	NE-CZ-NH2	-21.94	109.33	120.30
1	D	133	ARG	CD-NE-CZ	21.20	153.28	123.60
2	R	440	ARG	NE-CZ-NH2	-19.38	110.61	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	184	ARG	Sidechain

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	1571	0	1499	41	0
1	B	1571	0	1499	42	0
1	C	1571	0	1499	47	0
1	D	1571	0	1499	49	0
1	E	1571	0	1499	50	0
1	F	1571	0	1499	61	0
2	M	1844	0	1796	59	0
2	N	1844	0	1796	29	0
2	O	1844	0	1796	52	0
2	P	1844	0	1796	48	0
2	Q	1844	0	1796	52	0
2	R	1844	0	1796	59	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	M	20	0	10	3	0
4	N	20	0	10	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	20	0	9	2	0
4	P	20	0	9	2	0
4	Q	20	0	10	3	0
4	R	20	0	10	3	0
5	A	83	0	0	0	0
5	B	79	0	0	1	0
5	C	81	0	0	1	0
5	D	81	0	0	2	0
5	E	84	0	0	1	0
5	F	80	0	0	3	0
5	M	151	0	0	5	0
5	N	161	0	0	3	0
5	O	155	0	0	3	0
5	P	152	0	0	3	0
5	Q	153	0	0	6	0
5	R	156	0	0	5	0
All	All	22032	0	19828	554	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 14.

The worst 5 of 554 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:E:165:GLN:H	1:E:165:GLN:NE2	1.26	1.33
1:E:165:GLN:HE21	1:E:165:GLN:N	1.27	1.31
1:F:64:ARG:NH1	1:F:100:ASP:O	1.84	1.10
1:D:64:ARG:NH1	1:D:100:ASP:O	1.85	1.09
2:R:447:TYR:OH	4:R:550:3HB:H4	1.55	1.06

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	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	B	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	C	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	D	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	186 (94%)	12 (6%)	0	100	100
1	F	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
2	M	228/238 (96%)	219 (96%)	9 (4%)	0	100	100
2	N	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
2	O	228/238 (96%)	219 (96%)	9 (4%)	0	100	100
2	P	228/238 (96%)	221 (97%)	7 (3%)	0	100	100
2	Q	228/238 (96%)	222 (97%)	6 (3%)	0	100	100
2	R	228/238 (96%)	216 (95%)	12 (5%)	0	100	100
All	All	2556/2628 (97%)	2457 (96%)	99 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	162/163 (99%)	155 (96%)	7 (4%)	25	32
1	B	162/163 (99%)	154 (95%)	8 (5%)	21	27
1	C	162/163 (99%)	156 (96%)	6 (4%)	29	39
1	D	162/163 (99%)	156 (96%)	6 (4%)	29	39
1	E	162/163 (99%)	153 (94%)	9 (6%)	17	21
1	F	162/163 (99%)	158 (98%)	4 (2%)	42	56
2	M	195/201 (97%)	183 (94%)	12 (6%)	15	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	195/201 (97%)	183 (94%)	12 (6%)	15	18
2	O	195/201 (97%)	185 (95%)	10 (5%)	20	25
2	P	195/201 (97%)	185 (95%)	10 (5%)	20	25
2	Q	195/201 (97%)	185 (95%)	10 (5%)	20	25
2	R	195/201 (97%)	184 (94%)	11 (6%)	17	21
All	All	2142/2184 (98%)	2037 (95%)	105 (5%)	21	27

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	38	ARG
1	E	4	LEU
2	R	433	SER
1	D	165	GLN
2	P	428	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	497	ASN
2	R	361	HIS
2	P	361	HIS
2	R	503	GLN
2	Q	497	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	CME	P	429	2	8,9,10	0.79	0	6,9,11	1.59	1 (16%)
2	CME	R	429	2	8,9,10	0.74	0	6,9,11	0.74	0
2	CME	Q	429	2	8,9,10	0.75	0	6,9,11	1.36	1 (16%)
2	CME	O	429	2	8,9,10	0.82	0	6,9,11	0.98	0
2	CME	N	429	2	8,9,10	0.52	0	6,9,11	0.58	0
2	CME	M	429	2	8,9,10	0.81	0	6,9,11	0.73	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	CME	P	429	2	-	1/5/8/10	-
2	CME	R	429	2	-	1/5/8/10	-
2	CME	Q	429	2	-	1/5/8/10	-
2	CME	O	429	2	-	1/5/8/10	-
2	CME	N	429	2	-	0/5/8/10	-
2	CME	M	429	2	-	1/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	429	CME	CZ-CE-SD	-2.74	104.21	113.39
2	P	429	CME	CB-SG-SD	2.56	110.49	103.86

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	429	CME	CZ-CE-SD-SG
2	M	429	CME	CZ-CE-SD-SG
2	O	429	CME	CZ-CE-SD-SG
2	P	429	CME	CZ-CE-SD-SG
2	R	429	CME	CZ-CE-SD-SG

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	429	CME	2	0
2	Q	429	CME	3	0
2	O	429	CME	1	0
2	N	429	CME	1	0
2	M	429	CME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\# Z > 2$
4	3HB	R	551	-	10,10,10	1.13	1 (10%)	13,13,13	1.03	2 (15%)
4	3HB	N	550	-	10,10,10	1.34	2 (20%)	13,13,13	1.24	2 (15%)
4	3HB	P	550	-	10,10,10	1.25	1 (10%)	13,13,13	1.19	2 (15%)
4	3HB	Q	551	-	10,10,10	1.24	1 (10%)	13,13,13	1.06	1 (7%)
4	3HB	R	550	-	10,10,10	1.38	2 (20%)	13,13,13	1.70	3 (23%)
4	3HB	M	551	-	10,10,10	1.23	1 (10%)	13,13,13	1.21	2 (15%)
4	3HB	P	551	-	10,10,10	1.29	1 (10%)	13,13,13	1.12	2 (15%)
4	3HB	M	550	-	10,10,10	1.37	2 (20%)	13,13,13	1.19	1 (7%)
4	3HB	O	551	-	10,10,10	1.21	1 (10%)	13,13,13	1.05	1 (7%)
4	3HB	O	550	-	10,10,10	1.36	2 (20%)	13,13,13	1.48	2 (15%)
4	3HB	N	551	-	10,10,10	1.24	1 (10%)	13,13,13	1.27	2 (15%)
4	3HB	Q	550	-	10,10,10	1.50	2 (20%)	13,13,13	1.65	2 (15%)

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
4	3HB	R	551	-	-	0/4/4/4	0/1/1/1
4	3HB	N	550	-	-	0/4/4/4	0/1/1/1
4	3HB	P	550	-	-	0/4/4/4	0/1/1/1
4	3HB	Q	551	-	-	0/4/4/4	0/1/1/1
4	3HB	R	550	-	-	0/4/4/4	0/1/1/1
4	3HB	M	551	-	-	0/4/4/4	0/1/1/1
4	3HB	P	551	-	-	0/4/4/4	0/1/1/1
4	3HB	M	550	-	-	0/4/4/4	0/1/1/1
4	3HB	O	551	-	-	0/4/4/4	0/1/1/1
4	3HB	O	550	-	-	0/4/4/4	0/1/1/1
4	3HB	N	551	-	-	0/4/4/4	0/1/1/1
4	3HB	Q	550	-	-	0/4/4/4	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	551	3HB	C1-C1'	2.82	1.55	1.49
4	Q	550	3HB	C2-C1	2.82	1.43	1.39
4	Q	551	3HB	C1-C1'	2.68	1.55	1.49
4	P	551	3HB	C1-C1'	2.67	1.55	1.49
4	R	551	3HB	C1-C1'	2.55	1.54	1.49

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	550	3HB	O2'-C1'-C1	3.64	124.19	114.84
4	O	550	3HB	O2'-C1'-C1	3.48	123.77	114.84
4	N	551	3HB	O2'-C1'-O1'	-3.39	116.06	123.35
4	M	551	3HB	O2'-C1'-O1'	-3.06	116.78	123.35
4	P	550	3HB	O2'-C1'-C1	2.94	122.38	114.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	550	3HB	1	0
4	P	550	3HB	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	550	3HB	3	0
4	M	550	3HB	3	0
4	O	550	3HB	2	0
4	Q	550	3HB	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.