



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:47 PM GMT

PDB ID : 1YKP
Title : Protocatechuate 3,4-Dioxygenase Y408H mutant bound to DHB
Authors : Brown, C.K.; Ohlendorf, D.H.
Deposited on : 2005-01-18
Resolution : 2.41 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

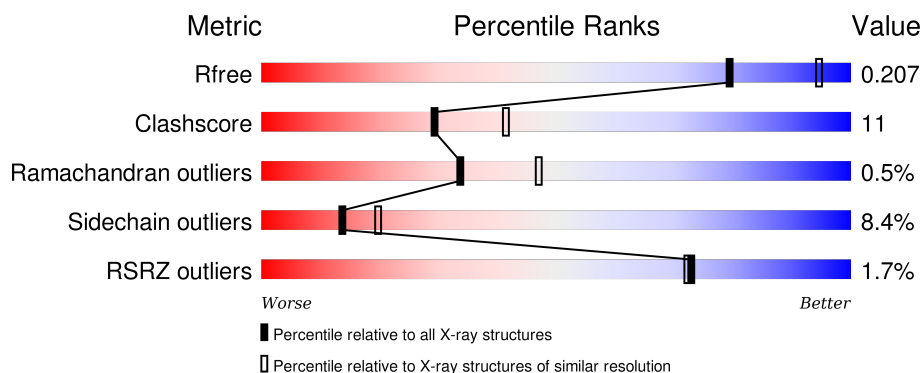
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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	200	<div> <div>2%</div> <div>54% 35% 11% .</div> </div>
1	C	200	<div> <div>2%</div> <div>47% 43% 8% .</div> </div>
1	E	200	<div> <div>2%</div> <div>47% 42% 10% .</div> </div>
1	G	200	<div> <div>2%</div> <div>56% 31% 10% .</div> </div>
1	I	200	<div> <div>2%</div> <div>51% 41% 7% .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	200	
2	B	238	
2	D	238	
2	F	238	
2	H	238	
2	J	238	
2	L	238	

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
4	DHB	A	550	-	-	X	X
4	DHB	D	1550	-	-	-	X
4	DHB	F	2550	-	-	-	X
4	DHB	H	3550	-	-	X	X
4	DHB	J	4550	-	-	-	X
4	DHB	L	5550	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21546 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	C	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	G	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	I	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	K	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	B	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	D	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	F	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	H	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	J	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	L	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	TYR	ENGINEERED	UNP P00437

Continued on next page...

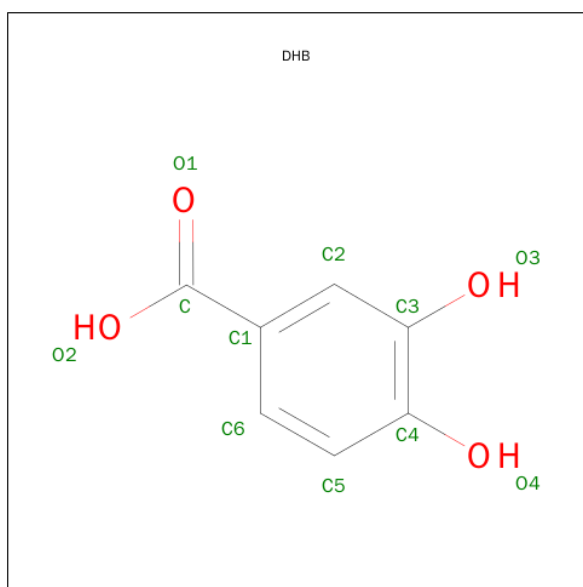
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
D	408	HIS	TYR	ENGINEERED	UNP P00437
D	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
F	408	HIS	TYR	ENGINEERED	UNP P00437
F	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
H	408	HIS	TYR	ENGINEERED	UNP P00437
H	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
J	408	HIS	TYR	ENGINEERED	UNP P00437
J	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
L	408	HIS	TYR	ENGINEERED	UNP P00437
L	429	CME	CYS	MODIFIED RESIDUE	UNP P00437

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0
3	H	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	L	1	Total Fe 1 1	0	0
3	F	1	Total Fe 1 1	0	0

- Molecule 4 is 3,4-DIHYDROXYBENZOIC ACID (three-letter code: DHB) (formula: C₇H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	7	4		
4	D	1	Total	C	O	0	0
			11	7	4		
4	F	1	Total	C	O	0	0
			11	7	4		
4	H	1	Total	C	O	0	0
			11	7	4		
4	J	1	Total	C	O	0	0
			11	7	4		
4	L	1	Total	C	O	0	0
			11	7	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	B	83	Total	O	0	0
			83	83		
5	C	45	Total	O	0	0
			45	45		
5	D	87	Total	O	0	0
			87	87		
5	E	49	Total	O	0	0
			49	49		
5	F	82	Total	O	0	0
			82	82		

Continued on next page...

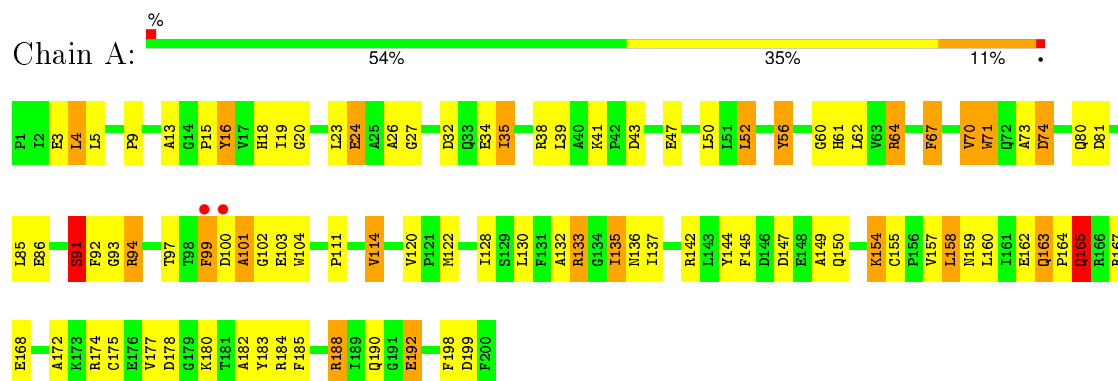
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	49	Total 49	O 49	0	0
5	H	83	Total 83	O 83	0	0
5	I	46	Total 46	O 46	0	0
5	J	85	Total 85	O 85	0	0
5	K	43	Total 43	O 43	0	0
5	L	87	Total 87	O 87	0	0

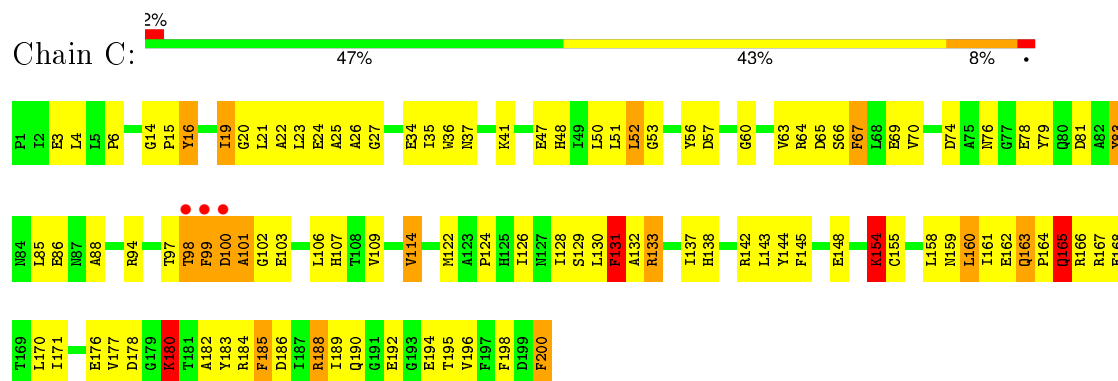
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

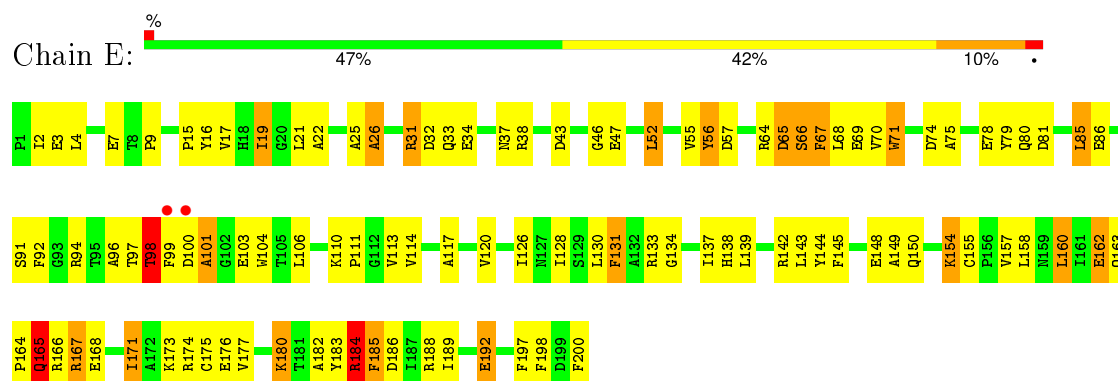
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



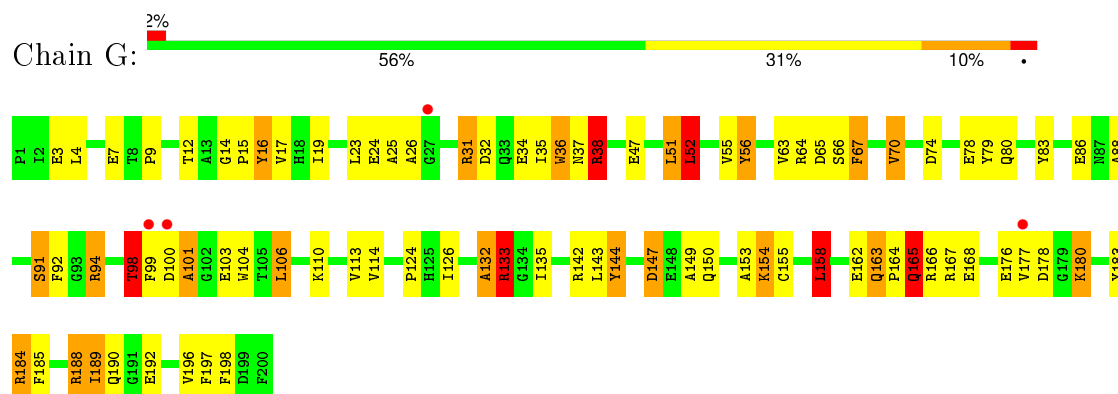
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



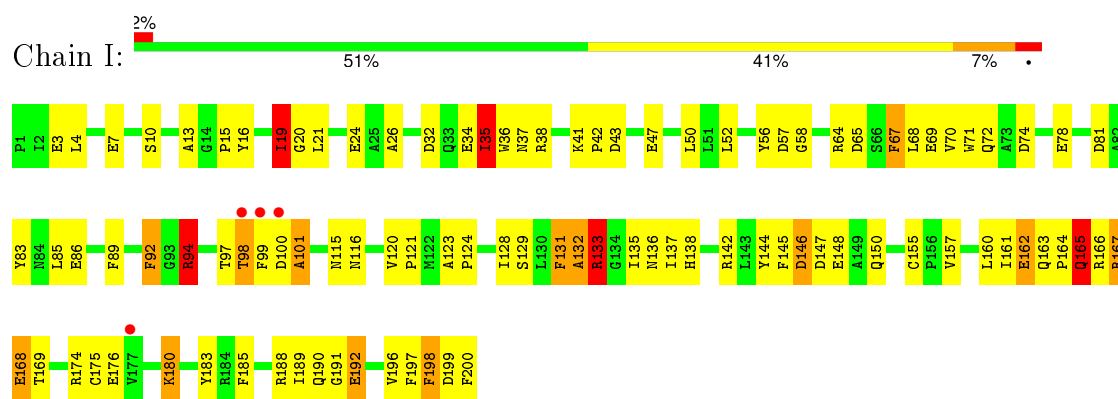
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



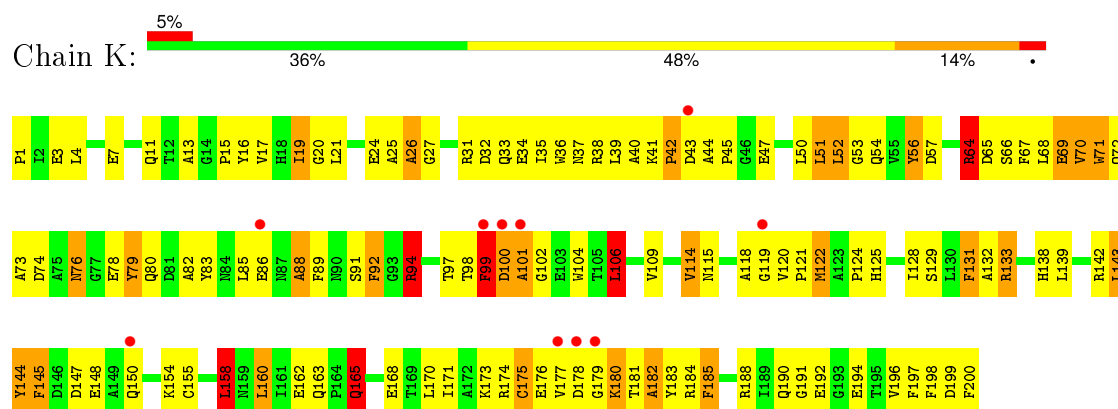
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



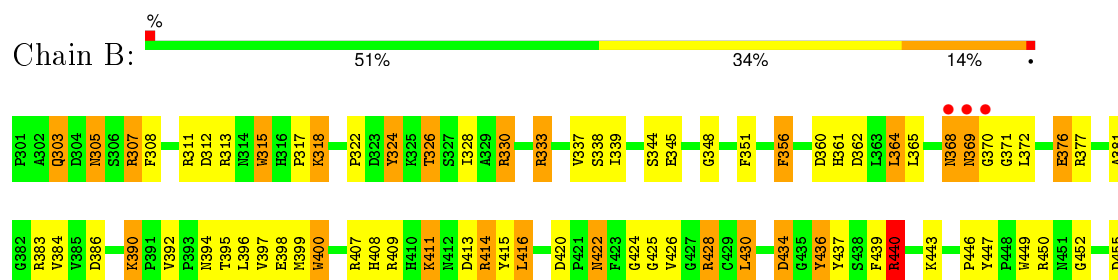
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

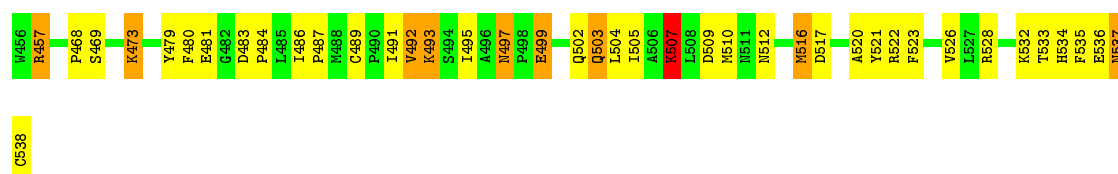


- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

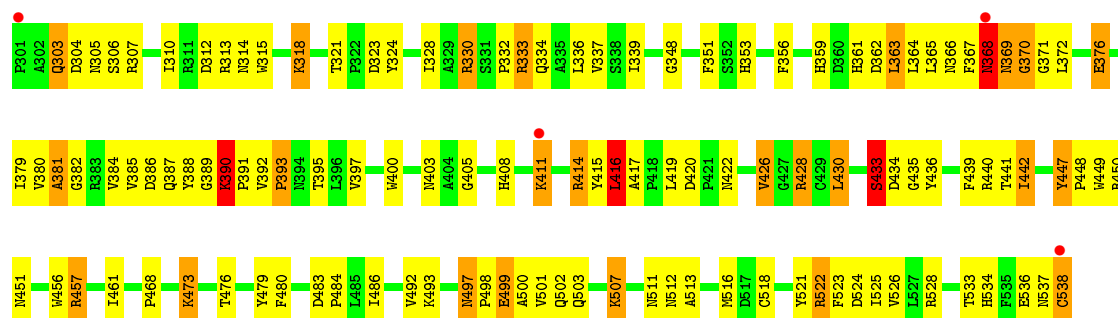


- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

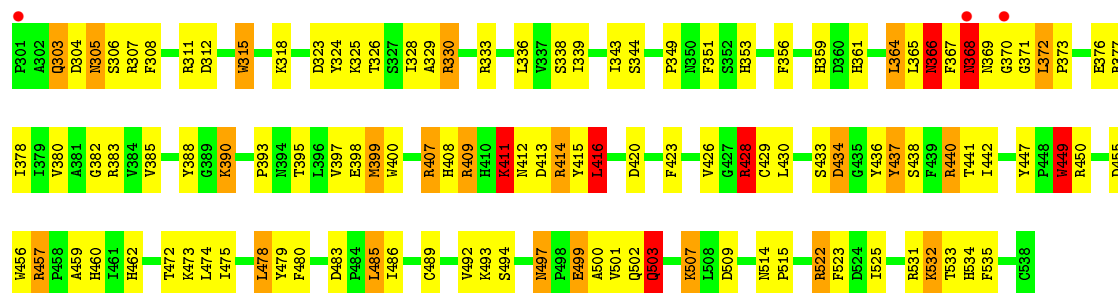




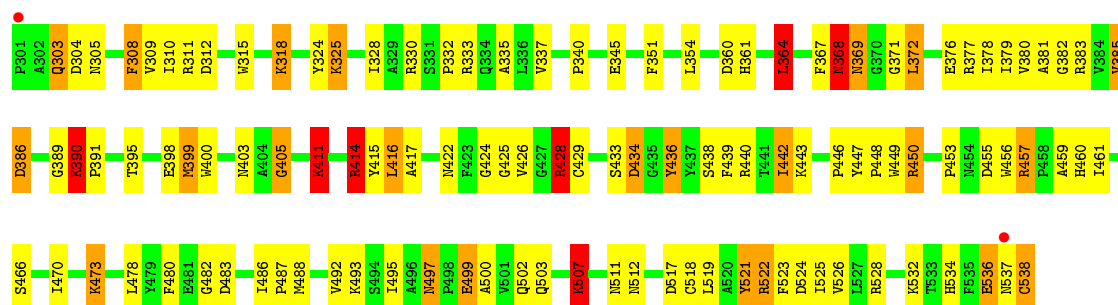
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



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

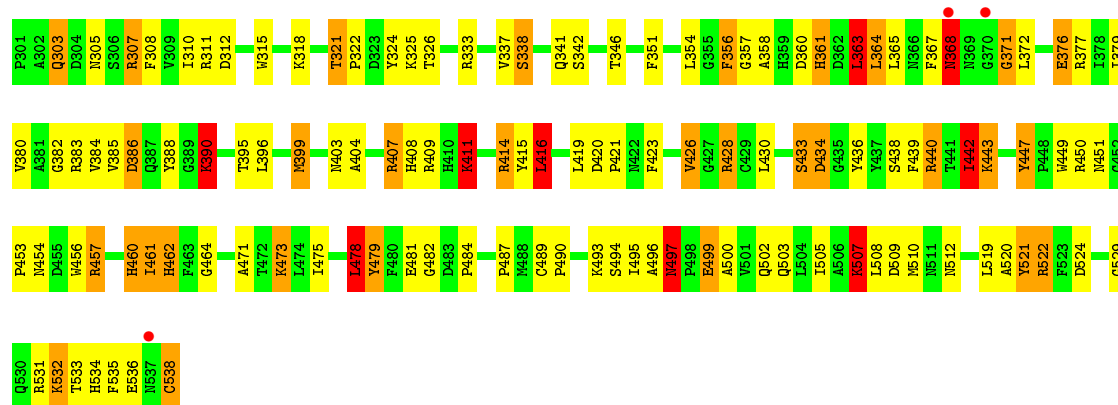


• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

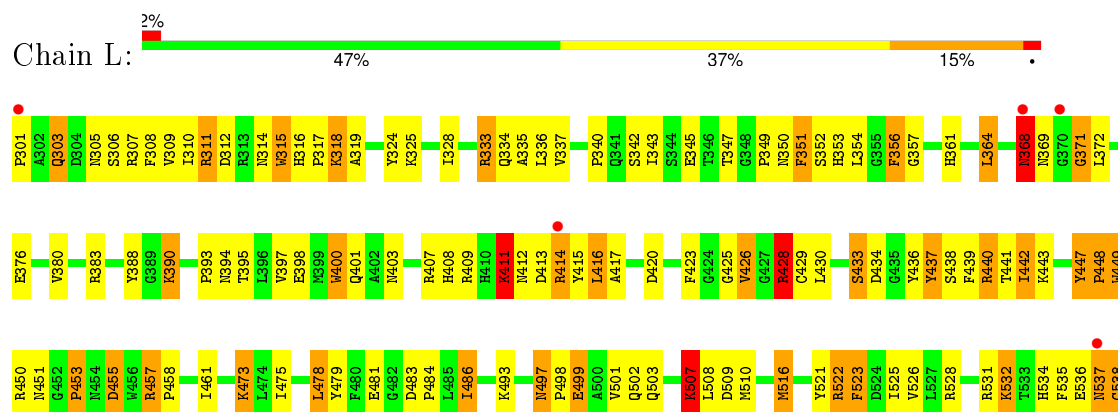


• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain





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



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.19Å 127.97Å 134.18Å 90.00° 97.68° 90.00°	Depositor
Resolution (Å)	30.37 – 2.41 30.37 – 1.95	Depositor EDS
% Data completeness (in resolution range)	72.4 (30.37-2.41) 72.5 (30.37-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.145 , 0.211 0.144 , 0.207	Depositor DCC
R_{free} test set	1209 reflections (1.33%)	DCC
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 190284 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21546	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CME, DHB, FE

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	2.51	85/1611 (5.3%)	1.92	41/2195 (1.9%)
1	C	2.54	101/1611 (6.3%)	2.13	53/2195 (2.4%)
1	E	2.62	114/1611 (7.1%)	1.96	51/2195 (2.3%)
1	G	2.63	102/1611 (6.3%)	1.93	40/2195 (1.8%)
1	I	2.62	98/1611 (6.1%)	1.98	39/2195 (1.8%)
1	K	2.85	136/1611 (8.4%)	1.98	44/2195 (2.0%)
2	B	2.40	81/1922 (4.2%)	2.02	55/2615 (2.1%)
2	D	2.46	96/1922 (5.0%)	1.97	53/2615 (2.0%)
2	F	2.41	98/1922 (5.1%)	2.02	45/2615 (1.7%)
2	H	2.38	82/1922 (4.3%)	1.98	60/2615 (2.3%)
2	J	2.52	102/1922 (5.3%)	1.93	59/2615 (2.3%)
2	L	2.64	112/1922 (5.8%)	1.93	52/2615 (2.0%)
All	All	2.55	1207/21198 (5.7%)	1.98	592/28860 (2.1%)

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	A	0	4
1	C	0	7
1	E	0	5
1	G	0	6
1	I	0	4
1	K	0	9
2	B	0	9
2	D	0	6
2	F	0	6
2	H	0	5
2	J	0	8

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	6
All	All	0	75

The worst 5 of 1207 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	532	LYS	CA-CB	16.40	1.90	1.53
2	L	324	TYR	CD1-CE1	16.37	1.64	1.39
1	K	47	GLU	CD-OE2	16.05	1.43	1.25
2	L	426	VAL	CB-CG2	-15.90	1.19	1.52
2	L	436	TYR	CD2-CE2	15.03	1.61	1.39

The worst 5 of 592 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	333	ARG	NE-CZ-NH1	-23.73	108.43	120.30
1	C	133	ARG	NE-CZ-NH1	23.63	132.11	120.30
1	C	94	ARG	NE-CZ-NH1	21.29	130.95	120.30
2	F	440	ARG	NE-CZ-NH2	-20.66	109.97	120.30
2	F	333	ARG	NE-CZ-NH1	-20.45	110.08	120.30

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	TYR	Sidechain
1	A	18	HIS	Mainchain
1	A	35	ILE	Mainchain
1	A	56	TYR	Sidechain
2	B	324	TYR	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	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1571	0	1499	30	0
1	E	1571	0	1499	33	0
1	G	1571	0	1499	32	1
1	I	1571	0	1499	27	0
1	K	1571	0	1499	37	0
2	B	1877	0	1823	43	0
2	D	1877	0	1822	43	0
2	F	1877	0	1822	52	0
2	H	1877	0	1823	52	0
2	J	1877	0	1822	58	0
2	L	1877	0	1822	54	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	A	11	0	4	6	0
4	D	11	0	4	1	0
4	F	11	0	4	1	0
4	H	11	0	4	6	0
4	J	11	0	4	3	0
4	L	11	0	4	3	0
5	A	47	0	0	0	0
5	B	83	0	0	1	0
5	C	45	0	0	0	0
5	D	87	0	0	2	0
5	E	49	0	0	0	1
5	F	82	0	0	2	0
5	G	49	0	0	0	0
5	H	83	0	0	2	0
5	I	46	0	0	0	0
5	J	85	0	0	6	0
5	K	43	0	0	0	0
5	L	87	0	0	2	0
All	All	21546	0	19952	457	1

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 11.

The worst 5 of 457 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:101:ALA:CB	1:A:101:ALA:CA	1.77	1.62
2:B:507:LYS:CE	2:B:507:LYS:CD	1.78	1.62
1:E:154:LYS:CE	1:E:154:LYS:CD	1.76	1.61
2:F:532:LYS:CB	2:F:532:LYS:CA	1.76	1.61
2:J:390:LYS:CE	2:J:390:LYS:CD	1.77	1.60

All (1) 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)
1:G:150:GLN:CD	5:E:2951:HOH:O[3_445]	2.18	0.02

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	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	34	47
1	C	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	E	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	G	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	I	198/200 (99%)	187 (94%)	10 (5%)	1 (0%)	34	47
1	K	198/200 (99%)	189 (96%)	7 (4%)	2 (1%)	19	27
2	B	235/238 (99%)	223 (95%)	10 (4%)	2 (1%)	21	29
2	D	235/238 (99%)	225 (96%)	9 (4%)	1 (0%)	39	54
2	F	235/238 (99%)	226 (96%)	8 (3%)	1 (0%)	39	54
2	H	235/238 (99%)	223 (95%)	11 (5%)	1 (0%)	39	54
2	J	235/238 (99%)	222 (94%)	12 (5%)	1 (0%)	39	54
2	L	235/238 (99%)	218 (93%)	15 (6%)	2 (1%)	21	29
All	All	2598/2628 (99%)	2467 (95%)	119 (5%)	12 (0%)	34	47

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	368	ASN
2	D	368	ASN
2	F	368	ASN
2	H	368	ASN
2	J	368	ASN

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%)	151 (93%)	11 (7%)	20	30
1	C	162/163 (99%)	149 (92%)	13 (8%)	15	22
1	E	162/163 (99%)	152 (94%)	10 (6%)	23	35
1	G	162/163 (99%)	151 (93%)	11 (7%)	20	30
1	I	162/163 (99%)	151 (93%)	11 (7%)	20	30
1	K	162/163 (99%)	149 (92%)	13 (8%)	15	22
2	B	199/201 (99%)	184 (92%)	15 (8%)	17	26
2	D	199/201 (99%)	179 (90%)	20 (10%)	9	13
2	F	199/201 (99%)	181 (91%)	18 (9%)	12	17
2	H	199/201 (99%)	180 (90%)	19 (10%)	11	15
2	J	199/201 (99%)	177 (89%)	22 (11%)	8	10
2	L	199/201 (99%)	179 (90%)	20 (10%)	9	13
All	All	2166/2184 (99%)	1983 (92%)	183 (8%)	14	20

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	497	ASN
2	H	391	PRO
2	L	395	THR
2	F	522	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	66	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	369	ASN
1	G	165	GLN
2	L	368	ASN
2	F	422	ASN
2	F	503	GLN

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	B	429	2	8,9,10	1.87	3 (37%)	6,9,11	3.64	3 (50%)
2	CME	D	429	2	8,9,10	2.23	3 (37%)	6,9,11	2.17	4 (66%)
2	CME	F	429	2	8,9,10	3.24	3 (37%)	6,9,11	2.20	3 (50%)
2	CME	H	429	2	8,9,10	2.73	5 (62%)	6,9,11	1.92	2 (33%)
2	CME	J	429	2	8,9,10	1.85	3 (37%)	6,9,11	2.10	3 (50%)
2	CME	L	429	2	8,9,10	2.01	2 (25%)	6,9,11	2.97	5 (83%)

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	B	429	2	-	0/5/8/10	0/0/0/0
2	CME	D	429	2	-	0/5/8/10	0/0/0/0
2	CME	F	429	2	-	0/5/8/10	0/0/0/0
2	CME	H	429	2	-	0/5/8/10	0/0/0/0
2	CME	J	429	2	-	0/5/8/10	0/0/0/0
2	CME	L	429	2	-	0/5/8/10	0/0/0/0

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	429	CME	CB-SG	-7.28	1.56	1.81
2	D	429	CME	CB-SG	-4.92	1.64	1.81
2	H	429	CME	CB-SG	-4.45	1.65	1.81
2	B	429	CME	CB-SG	-3.52	1.69	1.81
2	F	429	CME	CB-CA	-3.43	1.44	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	429	CME	CZ-CE-SD	-4.63	101.84	113.16
2	L	429	CME	CB-SG-SD	-3.40	97.33	103.95
2	B	429	CME	O-C-CA	-3.11	117.38	125.49
2	H	429	CME	CZ-CE-SD	-2.83	106.25	113.16
2	J	429	CME	CZ-CE-SD	-2.72	106.51	113.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	429	CME	1	0
2	H	429	CME	2	0
2	L	429	CME	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	DHB	A	550	3,2	8,11,11	0.88	0	11,15,15	0.87	0
4	DHB	D	1550	3	8,11,11	0.93	0	11,15,15	0.57	0
4	DHB	F	2550	3	8,11,11	1.15	0	11,15,15	0.65	0
4	DHB	H	3550	3	8,11,11	0.92	0	11,15,15	0.60	0
4	DHB	J	4550	3	8,11,11	0.75	0	11,15,15	0.69	0
4	DHB	L	5550	3,2	8,11,11	0.77	0	11,15,15	0.69	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
4	DHB	A	550	3,2	-	0/0/4/4	0/1/1/1
4	DHB	D	1550	3	-	0/0/4/4	0/1/1/1
4	DHB	F	2550	3	-	0/0/4/4	0/1/1/1
4	DHB	H	3550	3	-	0/0/4/4	0/1/1/1
4	DHB	J	4550	3	-	0/0/4/4	0/1/1/1
4	DHB	L	5550	3,2	-	0/0/4/4	0/1/1/1

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.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	550	DHB	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1550	DHB	1	0
4	F	2550	DHB	1	0
4	H	3550	DHB	6	0
4	J	4550	DHB	3	0
4	L	5550	DHB	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 ⓘ

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	200/200 (100%)	-0.71	2 (1%) 84 83	9, 24, 57, 73	0
1	C	200/200 (100%)	-0.67	3 (1%) 76 75	8, 25, 57, 72	0
1	E	200/200 (100%)	-0.60	2 (1%) 84 83	7, 27, 57, 73	0
1	G	200/200 (100%)	-0.61	4 (2%) 68 67	8, 26, 58, 73	0
1	I	200/200 (100%)	-0.51	4 (2%) 68 67	9, 28, 59, 73	0
1	K	200/200 (100%)	-0.27	10 (5%) 32 32	12, 30, 59, 73	0
2	B	237/238 (99%)	-0.84	3 (1%) 79 79	9, 19, 48, 68	0
2	D	237/238 (99%)	-0.83	4 (1%) 73 72	8, 19, 48, 68	0
2	F	237/238 (99%)	-0.88	3 (1%) 79 79	8, 19, 48, 67	0
2	H	237/238 (99%)	-0.92	2 (0%) 87 87	9, 19, 48, 65	0
2	J	237/238 (99%)	-0.87	3 (1%) 79 79	11, 22, 49, 68	0
2	L	237/238 (99%)	-0.77	5 (2%) 67 66	12, 21, 50, 68	0
All	All	2622/2628 (99%)	-0.72	45 (1%) 73 72	7, 23, 56, 73	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	99	PHE	4.6
2	L	301	PRO	4.2
1	G	100	ASP	4.0
1	I	98	THR	3.8
2	F	368	ASN	3.8

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

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(Å ²)	Q<0.9
2	CME	H	429	10/11	0.97	0.09	-	23,31,52,52	0
2	CME	B	429	10/11	0.97	0.10	-	22,30,52,55	0
2	CME	D	429	10/11	0.97	0.11	-	23,32,55,57	0
2	CME	J	429	10/11	0.96	0.09	-	26,33,55,57	0
2	CME	L	429	10/11	0.96	0.13	-	25,34,55,57	0
2	CME	F	429	10/11	0.96	0.10	-	23,31,53,56	0

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(Å ²)	Q<0.9
4	DHB	J	4550	11/11	0.88	0.31	15.06	103,105,106,106	0
4	DHB	H	3550	11/11	0.83	0.28	14.66	100,101,101,102	0
4	DHB	F	2550	11/11	0.83	0.34	13.07	102,102,103,103	0
4	DHB	L	5550	11/11	0.85	0.26	10.91	86,87,88,88	0
4	DHB	A	550	11/11	0.85	0.28	10.06	86,88,88,89	0
4	DHB	D	1550	11/11	0.87	0.23	7.17	77,78,79,79	0
3	FE	F	2600	1/1	0.99	0.09	0.14	57,57,57,57	0
3	FE	J	4600	1/1	0.90	0.07	-0.74	67,67,67,67	0
3	FE	B	600	1/1	0.94	0.08	-1.00	62,62,62,62	0
3	FE	L	5600	1/1	0.92	0.06	-1.52	63,63,63,63	0
3	FE	D	1600	1/1	0.98	0.06	-1.62	54,54,54,54	0
3	FE	H	3600	1/1	0.92	0.04	-3.07	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.