wwPDB X-ray Structure Validation Summary Report (i)

Sep 18, 2023 – 02:08 PM EDT

PDB ID	:	3PCA
Title	:	STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COMPLEXED WITH 3,4-DIHYDROXYBENZOATE
Authors	:	Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on	:	1997-07-18
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

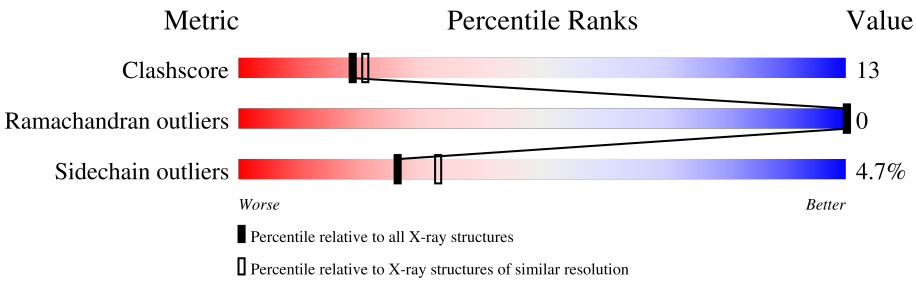
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	72% 24% •
1	B	200	73% 21% 5% •
1	C	200	70% 24% • •
1	D	200	70% 25% • •
1	E	200	65% 30% •
1	F	200	68% 26% 6%
2	M	238	69% 25% • •
2	N	238	73% 21% • •

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Mol	Chain	Length	Quality of chain
2	O	238	70% 24%
2	P	238	71% 22%
2	Q	238	71% 23%
2	R	238	70% 21% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22020 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.

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

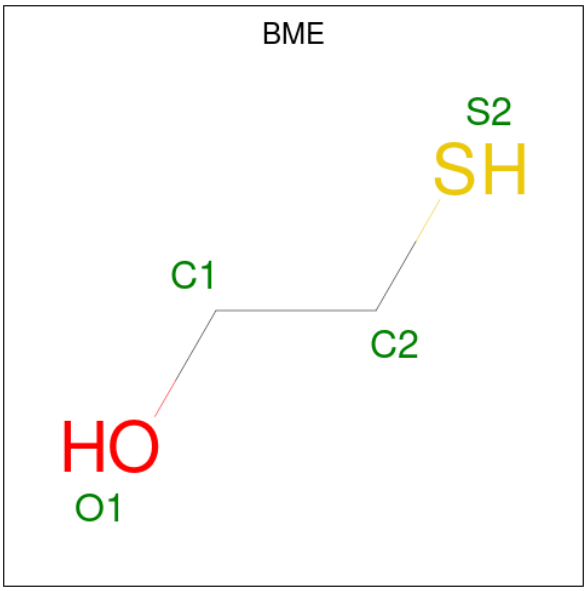
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	233	1840	1171	334	328	7	0	0	0
2	N	233	1840	1171	334	328	7	0	0	0
2	O	233	1840	1171	334	328	7	0	0	0
2	P	233	1840	1171	334	328	7	0	0	0
2	Q	233	1840	1171	334	328	7	0	0	0
2	R	233	1840	1171	334	328	7	0	0	0

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

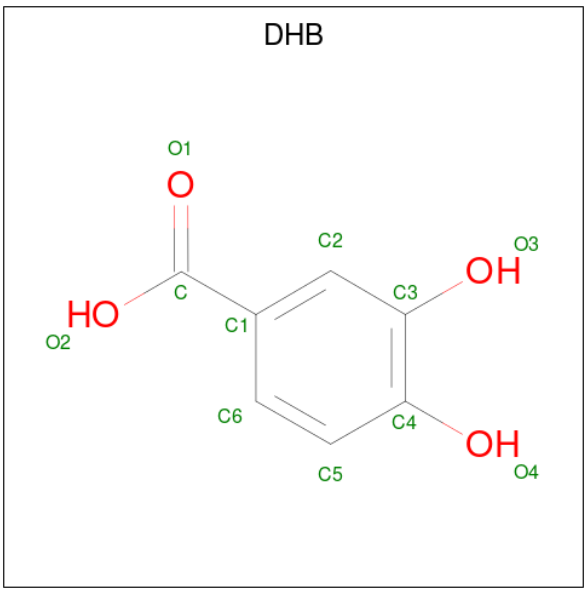
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
3	M	1	1	1	0	0
3	N	1	1	1	0	0
3	O	1	1	1	0	0
3	P	1	1	1	0	0
3	Q	1	1	1	0	0
3	R	1	1	1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	M	1	4	2	1	1	0	0
4	N	1	4	2	1	1	0	0
4	O	1	4	2	1	1	0	0
4	P	1	4	2	1	1	0	0
4	Q	1	4	2	1	1	0	0
4	R	1	4	2	1	1	0	0

- Molecule 5 is 3,4-DIHYDROXYBENZOIC ACID (three-letter code: DHB) (formula: $C_7H_6O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	O		0	0
			11	7	4			
5	M	1	Total	C	O		0	0
			11	7	4			
5	N	1	Total	C	O		0	0
			11	7	4			
5	N	1	Total	C	O		0	0
			11	7	4			
5	N	1	Total	C	O		0	0
			11	7	4			
5	O	1	Total	C	O		0	0
			11	7	4			
5	P	1	Total	C	O		0	0
			11	7	4			
5	P	1	Total	C	O		0	0
			11	7	4			
5	Q	1	Total	C	O		0	0
			11	7	4			
5	Q	1	Total	C	O		0	0
			11	7	4			
5	R	1	Total	C	O		0	0
			11	7	4			
5	R	1	Total	C	O		0	0
			11	7	4			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	84	84	84	0	0
			Total	O		
6	M	148	148	148	0	0
			Total	O		
6	B	78	78	78	0	0
			Total	O		
6	N	160	160	160	0	0
			Total	O		
6	C	83	83	83	0	0
			Total	O		
6	O	146	146	146	0	0
			Total	O		
6	D	76	76	76	0	0
			Total	O		
6	P	149	149	149	0	0
			Total	O		
6	E	79	79	79	0	0
			Total	O		
6	Q	156	156	156	0	0
			Total	O		
6	F	81	81	81	0	0
			Total	O		
6	R	152	152	152	0	0

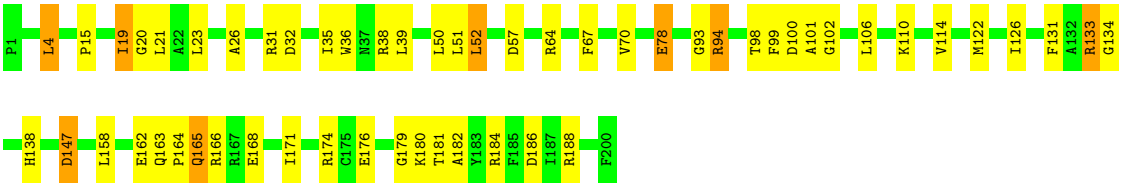
3 Residue-property plots (i)

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 was not executed.

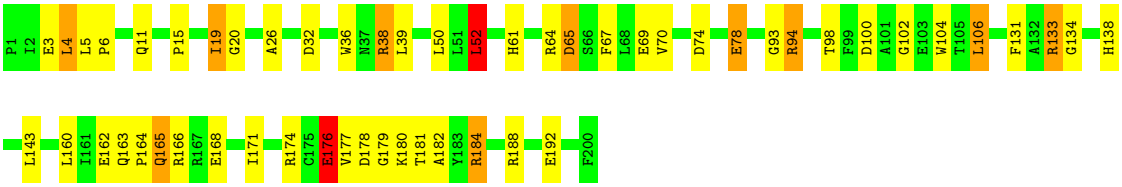
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A:



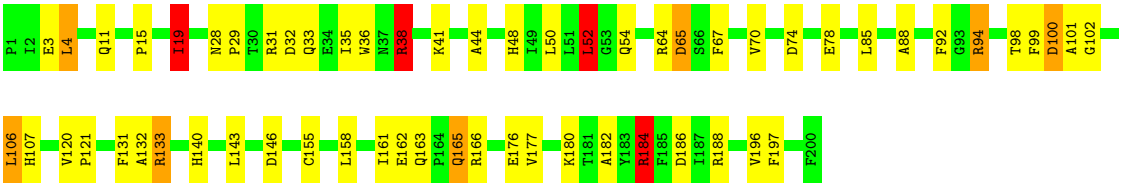
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B:



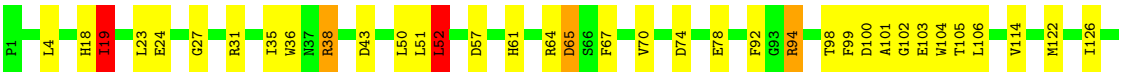
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C:



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D:



F131 A132 R133 H138 L143 Y144 A153 K154 L158 Q165 R166 R167 E168 I171 E176 V177 K180 T181 A182 Y183 R184 F185 D186 I187 R188 G191 E194 F200

• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E: 65% 30% •

P1 L4 T8 P9 P15 I19 G20 L21 A22 L23 E24 A25 A26 G27 N28 P29 T30 R31 I35 W36 N37 R38 L39 A40 K41 A44 H48 I49 L50 L51 L52 D57 H61 R64 D65 S66 F67 A73 D74 E78 N87 A88 F92 G93 R94

T98 F99 D100 A101 G102 E103 W104 T105 L106 K110 P111 V114 V120 P121 M122 F131 A132 R133 H138 L143 D147 I161 E162 Q163 P164 Q165 R166 R167 E168 I171 R174 C175 E176 G179 K180 T181 A182 Y183 R184 F185 D186 I187 R188 V196 F200

• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F: 68% 26% 6%

P1 I2 E3 L4 T8 P9 P15 Y16 V17 H18 I19 R31 D32 Q33 E34 I35 W36 N37 R38 L39 A40 K41 H48 I49 L50 L51 L52 D57 R64 D65 S66 F67 D74 G77 E78 Y79 Q80 D81 L85 A88 F89 R94 T98 F99 D100 A101 G102

H107 V114 V120 P121 F131 A132 R133 G134 I135 H138 R142 L143 Y144 F145 D146 K154 Q163 P164 Q165 R166 R174 C175 E176 V177 D178 G179 K180 T181 A182 Y183 R188 F200

• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M: 69% 25% • •

P301 R307 I310 R311 D312 R313 N314 W315 H316 P317 K318 D323 T326 R330 N350 F351 S352 F356 H359 D360 H361 D362 L363 L364 I365 N366 F367 ASN ASN GLY G371 L372 R377 R383 Q387 K390 T395 M399 W400 G405 G406 R407 Y408 R409 H410

K411 L416 D420 G425 V426 G427 R428 D432 R440 P446 Y447 P448 G452 P453 R457 H462 P468 I475 L478 C489 P490 N497 P498 E499 Q503 K507 L508 D509 Y521 R522 F523 D524 R528 T533 H534 F535 E536 ASN CYS

• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain N: 73% 21% • •

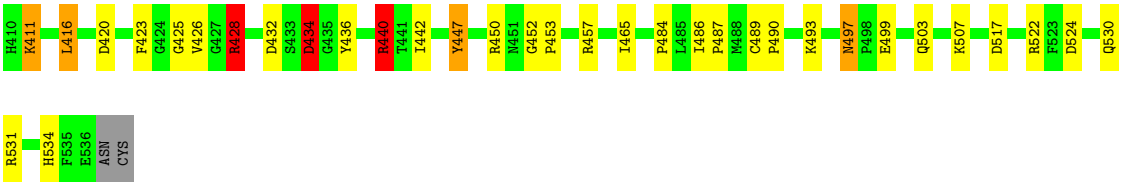
P301 D304 R307 R311 D312 R313 N314 W315 T326 S327 I328 A329 R330 R333 F356 H359 D360 H361 L364 I365 N366 F367 ASN ASN GLY G371 L372 P373 E376 R383 D386 Q387 T395 M399 W400 G406 R407 Y408 R409 H410 D413 R414 Y415 L416

F423 G424 G425 V426 G427 R428 C429 L430 S433 D434 G435 Y436 R440 T441 I442 Y447 R450 R457 H462 L478 I486 P487 N488 C489 P490 N497 P498 E499 Q503 K507 R522 F523 D524 L527 R528 T533 H534 F535 E536 ASN CYS

• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

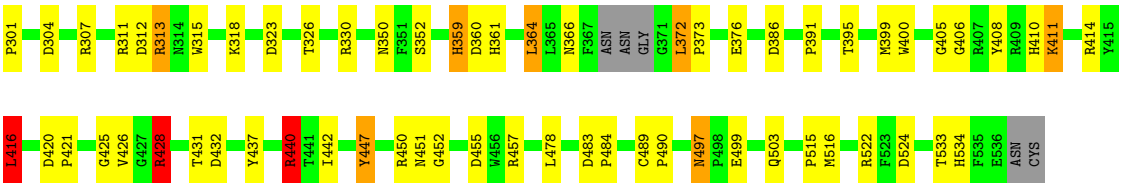
Chain O: 70% 24% • • •

P301 F308 R313 N314 W315 D323 T326 R330 A335 H353 F356 H359 D360 H361 D362 L363 L364 I365 N366 F367 ASN ASN GLY G371 L372 P373 E376 A381 G382 R383 Q387 K390 P391 V392 P393 N394 T395 M399 W400 N403 G406 R407 Y408 R409



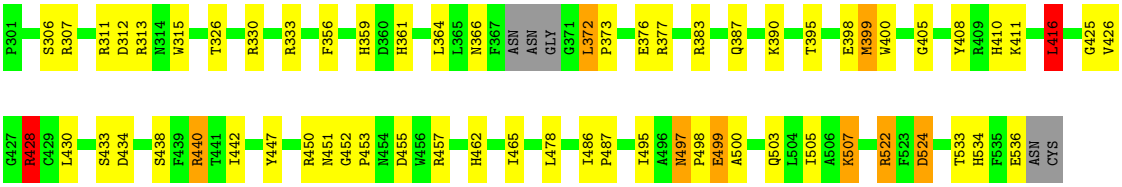
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:



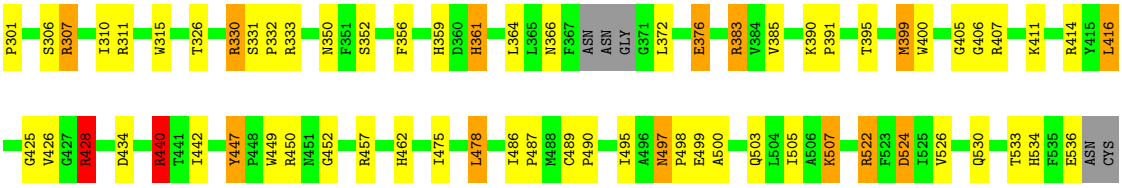
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q:



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R:



4 Data and refinement statistics (i)

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	196.30Å 127.20Å 133.80Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	96.0 (6.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22020	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

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: BME, 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	0.90	0/1611	1.56	26/2195 (1.2%)
1	B	0.92	0/1611	1.56	24/2195 (1.1%)
1	C	0.94	0/1611	1.58	22/2195 (1.0%)
1	D	0.93	1/1611 (0.1%)	1.59	25/2195 (1.1%)
1	E	0.94	0/1611	1.48	17/2195 (0.8%)
1	F	0.94	0/1611	1.57	23/2195 (1.0%)
2	M	0.97	0/1895	1.51	28/2580 (1.1%)
2	N	0.94	0/1895	1.55	19/2580 (0.7%)
2	O	0.94	0/1895	1.50	27/2580 (1.0%)
2	P	0.95	0/1895	1.54	24/2580 (0.9%)
2	Q	0.97	1/1895 (0.1%)	1.53	27/2580 (1.0%)
2	R	0.96	0/1895	1.49	24/2580 (0.9%)
All	All	0.94	2/21036 (0.0%)	1.54	286/28650 (1.0%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	ARG	CD-NE	-6.46	1.35	1.46
2	Q	433	SER	CB-OG	5.26	1.49	1.42

The worst 5 of 286 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	94	ARG	NE-CZ-NH2	-18.94	110.83	120.30
2	R	440	ARG	NE-CZ-NH2	-18.52	111.04	120.30
2	P	440	ARG	NE-CZ-NH2	-17.63	111.49	120.30
2	N	440	ARG	NE-CZ-NH2	-17.33	111.63	120.30
2	Q	440	ARG	NE-CZ-NH2	-16.98	111.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	184	ARG	Sidechain

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	1571	0	1499	43	0
1	B	1571	0	1499	44	0
1	C	1571	0	1499	51	0
1	D	1571	0	1499	48	0
1	E	1571	0	1499	52	0
1	F	1571	0	1499	64	0
2	M	1840	0	1793	49	0
2	N	1840	0	1793	42	0
2	O	1840	0	1793	48	0
2	P	1840	0	1793	49	0
2	Q	1840	0	1793	52	0
2	R	1840	0	1793	56	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	4	0	5	0	0
4	N	4	0	5	0	0
4	O	4	0	5	0	0
4	P	4	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	4	0	5	2	0
4	R	4	0	5	0	0
5	M	22	0	8	1	0
5	N	33	0	13	0	0
5	O	11	0	3	1	0
5	P	22	0	8	0	0
5	Q	22	0	9	0	0
5	R	22	0	9	0	0
6	A	84	0	0	0	0
6	B	78	0	0	0	0
6	C	83	0	0	0	0
6	D	76	0	0	0	0
6	E	79	0	0	1	0
6	F	81	0	0	1	0
6	M	148	0	0	4	0
6	N	160	0	0	1	0
6	O	146	0	0	6	0
6	P	149	0	0	3	0
6	Q	156	0	0	5	0
6	R	152	0	0	5	0
All	All	22020	0	19832	530	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 13.

The worst 5 of 530 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:HE21	1:E:165:GLN:N	1.38	1.19
1:E:165:GLN:H	1:E:165:GLN:NE2	1.37	1.19
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.43	1.00
1:B:165:GLN:H	1:B:165:GLN:NE2	1.61	0.98
1:F:64:ARG:NH1	1:F:100:ASP:O	1.96	0.98

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%)	192 (97%)	6 (3%)	0	100	100
1	B	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	C	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	D	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	F	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
2	M	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	N	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	O	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	P	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	Q	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	R	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
All	All	2562/2628 (98%)	2475 (97%)	87 (3%)	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	162/163 (99%)	155 (96%)	7 (4%)	29	36
1	B	162/163 (99%)	154 (95%)	8 (5%)	25	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	162/163 (99%)	157 (97%)	5 (3%)	40	51
1	D	162/163 (99%)	155 (96%)	7 (4%)	29	36
1	E	162/163 (99%)	156 (96%)	6 (4%)	34	43
1	F	162/163 (99%)	157 (97%)	5 (3%)	40	51
2	M	196/202 (97%)	186 (95%)	10 (5%)	24	29
2	N	196/202 (97%)	186 (95%)	10 (5%)	24	29
2	O	196/202 (97%)	184 (94%)	12 (6%)	18	21
2	P	196/202 (97%)	184 (94%)	12 (6%)	18	21
2	Q	196/202 (97%)	188 (96%)	8 (4%)	30	39
2	R	196/202 (97%)	185 (94%)	11 (6%)	21	25
All	All	2148/2190 (98%)	2047 (95%)	101 (5%)	26	33

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	165	GLN
1	E	19	ILE
2	R	507	LYS
2	P	364	LEU
2	P	416	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	R	361	HIS
2	R	422	ASN
2	R	530	GLN
1	C	165	GLN
1	C	163	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
5	DHB	N	602	-	11,11,11	1.08	0	15,15,15	1.21	2 (13%)
4	BME	M	601	2	3,3,3	0.21	0	1,2,2	0.10	0
5	DHB	O	550	3	11,11,11	1.51	4 (36%)	15,15,15	1.30	2 (13%)
5	DHB	N	551	-	11,11,11	1.19	0	15,15,15	1.15	2 (13%)
5	DHB	N	550	3	11,11,11	1.37	3 (27%)	15,15,15	1.33	2 (13%)
5	DHB	P	551	-	11,11,11	1.26	0	15,15,15	1.33	2 (13%)
5	DHB	P	550	3	11,11,11	1.33	1 (9%)	15,15,15	1.29	2 (13%)
5	DHB	Q	550	3	11,11,11	1.44	2 (18%)	15,15,15	1.15	2 (13%)
5	DHB	M	550	3	11,11,11	1.29	1 (9%)	15,15,15	1.18	2 (13%)
4	BME	N	601	2	3,3,3	0.18	0	1,2,2	0.30	0
5	DHB	Q	551	-	11,11,11	1.25	0	15,15,15	1.27	2 (13%)
5	DHB	R	550	3	11,11,11	1.39	3 (27%)	15,15,15	1.23	2 (13%)
5	DHB	R	551	-	11,11,11	1.20	1 (9%)	15,15,15	1.22	2 (13%)
4	BME	P	601	2	3,3,3	0.40	0	1,2,2	0.75	0
4	BME	R	601	2	3,3,3	0.65	0	1,2,2	0.82	0
4	BME	O	601	2	3,3,3	0.56	0	1,2,2	0.42	0
4	BME	Q	601	2	3,3,3	0.35	0	1,2,2	0.24	0
5	DHB	M	551	-	11,11,11	1.15	0	15,15,15	1.41	3 (20%)

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	DHB	N	602	-	-	0/4/4/4	0/1/1/1
4	BME	M	601	2	-	1/1/1/1	-
5	DHB	O	550	3	-	0/4/4/4	0/1/1/1
5	DHB	N	551	-	-	0/4/4/4	0/1/1/1
5	DHB	N	550	3	-	0/4/4/4	0/1/1/1
5	DHB	P	551	-	-	0/4/4/4	0/1/1/1
5	DHB	P	550	3	-	0/4/4/4	0/1/1/1
5	DHB	Q	550	3	-	0/4/4/4	0/1/1/1
5	DHB	M	550	3	-	0/4/4/4	0/1/1/1
4	BME	N	601	2	-	0/1/1/1	-
5	DHB	Q	551	-	-	0/4/4/4	0/1/1/1
5	DHB	R	550	3	-	0/4/4/4	0/1/1/1
5	DHB	R	551	-	-	0/4/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	-
4	BME	R	601	2	-	0/1/1/1	-
4	BME	O	601	2	-	0/1/1/1	-
4	BME	Q	601	2	-	0/1/1/1	-
5	DHB	M	551	-	-	0/4/4/4	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	550	DHB	O4-C4	3.03	1.42	1.36
5	Q	550	DHB	C2-C1	2.66	1.43	1.39
5	O	550	DHB	O4-C4	2.63	1.41	1.36
5	O	550	DHB	C6-C1	2.54	1.43	1.39
5	N	550	DHB	O4-C4	2.34	1.41	1.36

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	550	DHB	O2-C-O1	-3.51	115.55	123.35
5	R	550	DHB	O2-C-O1	-3.24	116.15	123.35
5	P	550	DHB	O2-C-O1	-3.09	116.49	123.35
5	O	550	DHB	O2-C-C1	3.04	122.75	114.85
5	M	551	DHB	O2-C-C1	2.98	122.59	114.85

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	601	BME	O1-C1-C2-S2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	550	DHB	1	0
5	M	550	DHB	1	0
4	Q	601	BME	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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.