



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2024 – 12:28 AM EST

PDB ID : 1Q0C
Title : Anerobic Substrate Complex of Homoprotocatechuate 2,3-Dioxygenase from *Brevibacterium fuscum*. (Complex with 3,4-Dihydroxyphenylacetate)
Authors : Vetting, M.W.; Wackett, L.P.; Que, L.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 2003-07-15
Resolution : 2.10 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

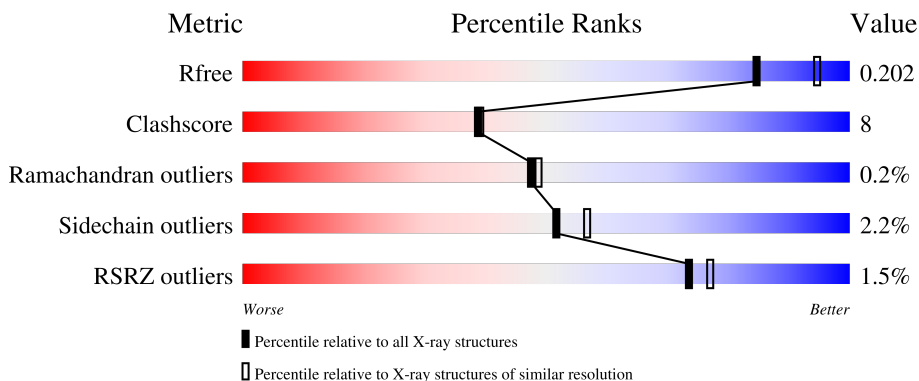
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">71% 15% • 13%</p>
1	B	365	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">70% 16% • 13%</p>
1	C	365	<div style="display: flex; align-items: center;"> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">71% 15% •• 13%</p>
1	D	365	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">75% 12% • 13%</p>

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
3	DHY	A	999	-	X	-	-
3	DHY	B	999	-	X	-	-
3	DHY	C	999	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10829 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.

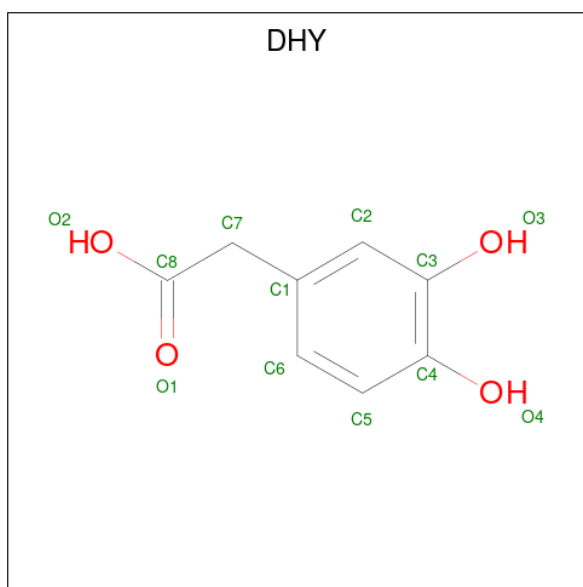
- Molecule 1 is a protein called homoprotocatechuate 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2601	1648	459	487	7	0	0	0
1	B	319	2601	1648	459	487	7	0	0	0
1	C	319	2601	1648	459	487	7	0	0	0
1	D	319	2601	1648	459	487	7	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-(3,4-DIHYDROXYPHENYL)ACETIC ACID (three-letter code: DHY) (formula: C₈H₈O₄).



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

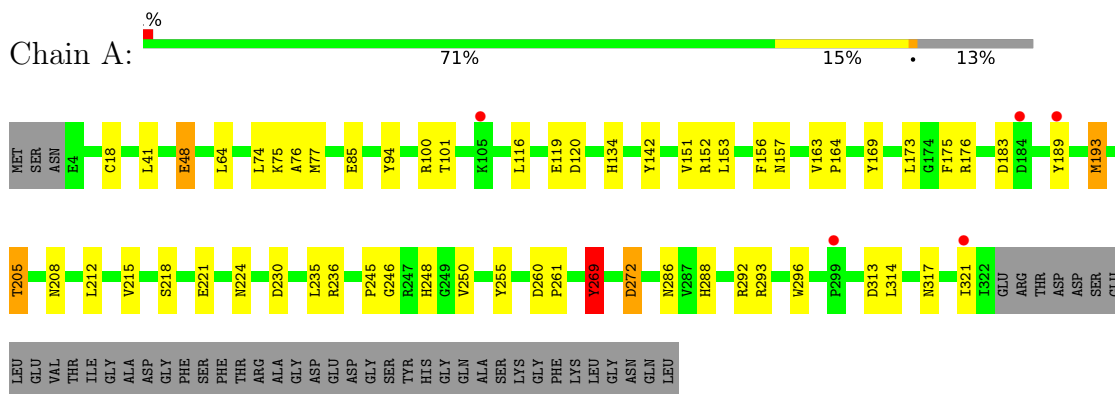
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	84	Total O 84 84	0	0
4	B	67	Total O 67 67	0	0
4	C	107	Total O 107 107	0	0
4	D	115	Total O 115 115	0	0

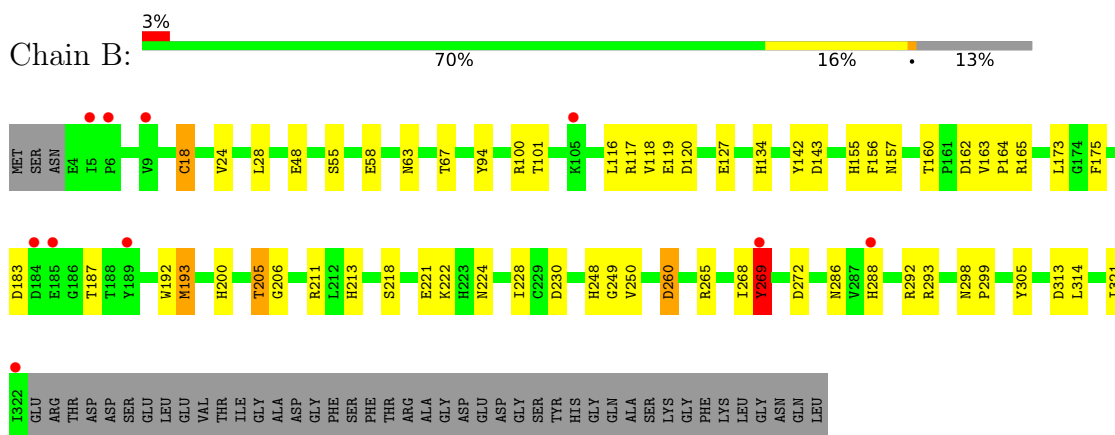
3 Residue-property plots [i](#)

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 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 ($RSRZ > 2$). 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.

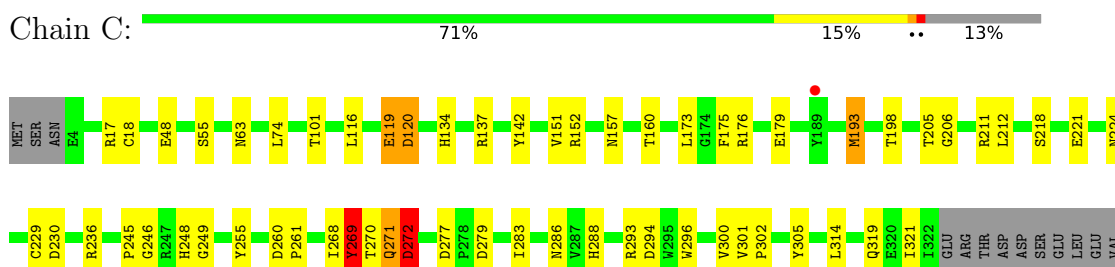
- Molecule 1: homoprotocatechuate 2,3-dioxygenase



- Molecule 1: homoprotocatechuate 2,3-dioxygenase



- Molecule 1: homoprotocatechuate 2,3-dioxygenase



THR
ILE
GLY
ALA
ASP
GLY
PHE
SER
PHE
THR
ARG
ALA
GLY
ASP
GLU
ASP
GLY
SER
TYR
HIS
GLY
GLN
ALA
SER
LYS
GLY
PHE
LYS
LEU
GLY
ASN
GLN
LEU

• Molecule 1: homoprotocatechuate 2,3-dioxygenase

Chain D: %
75% 12% 13%

MET SER ASN E4 V9 R32 Y45 E46 D47 E48 I51 S55 N63 Y94 K110 D120 H134 R137 Y142 V151 R152 M157 D162 Y163 P164 Y169 L173 G174 F175 M193 H194 R195 T205 L212 V215 S218 E221

N224 I225 D230 G246 R247 H248 D262 N263 E267 I268 Y269 T270 Q271 D272 N286 V287 H288 D289 N290 W296 G297 N298 P299 V300 I322

SER
TYR
HIS
GLY
GLN
ALA
SER
LYS
GLY
PHE
LYS
LEU
GLY
ASN
GLN
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	157.00Å 157.00Å 122.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 41.02 – 2.11	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.10) 97.4 (41.02-2.11)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.10Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.170 , 0.234 0.161 , 0.202	Depositor DCC
R_{free} test set	4152 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtrriage
Anisotropy	0.066	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.004 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10829	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: DHY, 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	0.73	1/2672 (0.0%)	0.90	4/3634 (0.1%)
1	B	0.73	2/2672 (0.1%)	0.93	7/3634 (0.2%)
1	C	0.84	2/2672 (0.1%)	0.97	10/3634 (0.3%)
1	D	0.81	0/2672	0.93	5/3634 (0.1%)
All	All	0.78	5/10688 (0.0%)	0.93	26/14536 (0.2%)

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	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	CYS	CB-SG	-6.18	1.71	1.82
1	B	269	TYR	CE1-CZ	5.78	1.46	1.38
1	B	18	CYS	CB-SG	-5.52	1.72	1.81
1	C	229	CYS	CB-SG	-5.18	1.73	1.81
1	A	269	TYR	CE1-CZ	5.04	1.45	1.38

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	D	269	TYR	CA-CB-CG	6.50	125.75	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	TYR	N-CA-CB	-6.37	99.13	110.60
1	D	272	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	A	272	ASP	CB-CG-OD1	-6.18	112.74	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	TYR	Sidechain
1	C	269	TYR	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	2601	0	2485	38	0
1	B	2601	0	2485	45	0
1	C	2601	0	2485	44	0
1	D	2601	0	2485	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	5	0	0
3	B	12	0	5	1	0
3	C	12	0	5	2	0
3	D	12	0	5	1	0
4	A	84	0	0	2	0
4	B	67	0	0	1	0
4	C	107	0	0	1	0
4	D	115	0	0	2	0
All	All	10829	0	9960	154	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 8.

The worst 5 of 154 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:C:271:GLN:O	1:C:271:GLN:HG2	1.73	0.88
1:D:271:GLN:HG2	1:D:271:GLN:O	1.74	0.86
1:C:286:ASN:ND2	1:C:288:HIS:H	1.73	0.85
1:D:286:ASN:ND2	1:D:288:HIS:H	1.78	0.81
1:D:48:GLU:H	1:D:48:GLU:CD	1.84	0.80

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	317/365 (87%)	305 (96%)	12 (4%)	0	100	100
1	B	317/365 (87%)	303 (96%)	14 (4%)	0	100	100
1	C	317/365 (87%)	305 (96%)	11 (4%)	1 (0%)	41	41
1	D	317/365 (87%)	307 (97%)	9 (3%)	1 (0%)	41	41
All	All	1268/1460 (87%)	1220 (96%)	46 (4%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	271	GLN
1	D	271	GLN

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	277/313 (88%)	270 (98%)	7 (2%)	47	52
1	B	277/313 (88%)	270 (98%)	7 (2%)	47	52
1	C	277/313 (88%)	272 (98%)	5 (2%)	59	65
1	D	277/313 (88%)	272 (98%)	5 (2%)	59	65
All	All	1108/1252 (88%)	1084 (98%)	24 (2%)	52	57

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	120	ASP
1	C	193	MET
1	C	173	LEU
1	C	272	ASP
1	A	272	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	224	ASN
1	C	291	GLN
1	C	288	HIS
1	D	63	ASN
1	B	63	ASN

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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	DHY	C	999	2	12,12,12	2.32	7 (58%)	16,16,16	2.38	8 (50%)
3	DHY	A	999	2	12,12,12	2.00	6 (50%)	16,16,16	2.47	8 (50%)
3	DHY	D	999	2	12,12,12	1.71	5 (41%)	16,16,16	2.41	8 (50%)
3	DHY	B	999	2	12,12,12	2.02	5 (41%)	16,16,16	2.75	9 (56%)

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
3	DHY	C	999	2	-	0/4/4/4	0/1/1/1
3	DHY	A	999	2	-	0/4/4/4	0/1/1/1
3	DHY	D	999	2	-	0/4/4/4	0/1/1/1
3	DHY	B	999	2	-	0/4/4/4	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	999	DHY	C4-C3	3.65	1.46	1.40
3	B	999	DHY	C6-C5	3.19	1.44	1.38
3	C	999	DHY	C2-C1	3.17	1.44	1.39
3	B	999	DHY	C4-C3	3.09	1.45	1.40
3	B	999	DHY	C6-C1	2.99	1.45	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	DHY	C7-C1-C2	-4.66	113.00	120.38
3	A	999	DHY	O3-C3-C2	4.02	130.23	119.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	DHY	O2-C8-O1	-4.00	113.32	123.30
3	B	999	DHY	C7-C1-C6	3.98	126.59	120.89
3	D	999	DHY	O3-C3-C2	3.81	129.67	119.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	999	DHY	2	0
3	D	999	DHY	1	0
3	B	999	DHY	1	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	319/365 (87%)	-0.22	5 (1%) 72 75	28, 41, 59, 76	0
1	B	319/365 (87%)	-0.17	10 (3%) 49 55	27, 40, 60, 75	0
1	C	319/365 (87%)	-0.40	1 (0%) 94 94	23, 32, 49, 62	0
1	D	319/365 (87%)	-0.30	3 (0%) 84 86	25, 33, 53, 69	0
All	All	1276/1460 (87%)	-0.28	19 (1%) 73 77	23, 37, 57, 76	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	ILE	3.4
1	B	184	ASP	3.3
1	A	321	ILE	3.3
1	B	6	PRO	2.9
1	C	189	TYR	2.9

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	B-factors(\AA^2)	Q<0.9
3	DHY	C	999	12/12	0.88	0.11	43,45,46,47	0
3	DHY	B	999	12/12	0.89	0.12	40,43,51,52	0
3	DHY	A	999	12/12	0.94	0.11	45,46,50,50	0
3	DHY	D	999	12/12	0.95	0.11	42,44,49,50	0
2	FE	A	500	1/1	0.98	0.05	43,43,43,43	0
2	FE	B	500	1/1	0.99	0.06	42,42,42,42	0
2	FE	C	500	1/1	0.99	0.05	34,34,34,34	0
2	FE	D	500	1/1	1.00	0.06	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.