wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2023 – 07:58 PM EDT

PDB ID	:	4DFE
Title	:	Crystal structure of 3-oxoacyl-[acyl-carrier-protein] synthase III from Burkholderia xenovorans
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2012-01-23
Resolution	:	2.35 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:

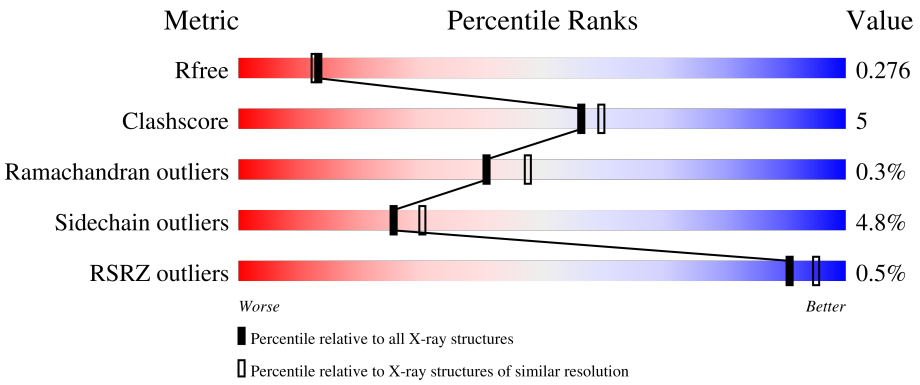
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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% 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	333	86% 10% •
1	B	333	% 86% 10% • •
1	C	333	% 83% 12% • •
1	D	333	84% 11% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9719 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.

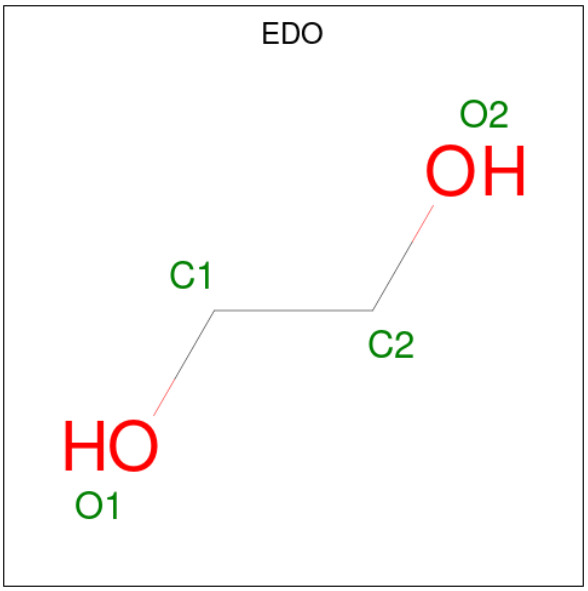
- Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein] synthase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	2346	1473	419	446	8	0	0	0
1	B	324	2352	1481	421	442	8	0	2	0
1	C	322	2342	1471	416	447	8	0	0	0
1	D	323	2385	1495	429	453	8	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q13VL5
A	-2	PRO	-	expression tag	UNP Q13VL5
A	-1	GLY	-	expression tag	UNP Q13VL5
A	0	SER	-	expression tag	UNP Q13VL5
B	-3	GLY	-	expression tag	UNP Q13VL5
B	-2	PRO	-	expression tag	UNP Q13VL5
B	-1	GLY	-	expression tag	UNP Q13VL5
B	0	SER	-	expression tag	UNP Q13VL5
C	-3	GLY	-	expression tag	UNP Q13VL5
C	-2	PRO	-	expression tag	UNP Q13VL5
C	-1	GLY	-	expression tag	UNP Q13VL5
C	0	SER	-	expression tag	UNP Q13VL5
D	-3	GLY	-	expression tag	UNP Q13VL5
D	-2	PRO	-	expression tag	UNP Q13VL5
D	-1	GLY	-	expression tag	UNP Q13VL5
D	0	SER	-	expression tag	UNP Q13VL5

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	4	2	2	0	0

- Molecule 3 is water.

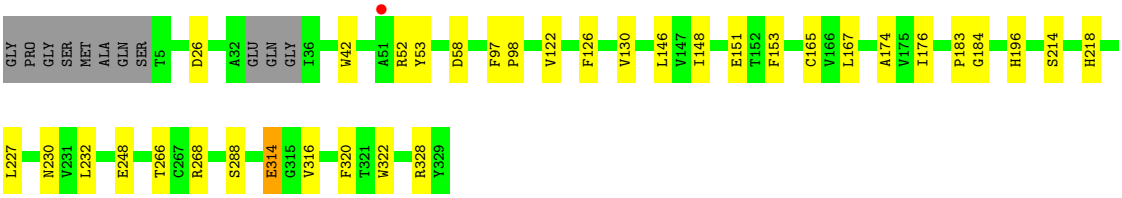
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	67	67	67	0	0
			Total	O		
3	B	75	75	75	0	0
			Total	O		
3	C	65	65	65	0	0
			Total	O		
3	D	83	83	83	0	0

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.

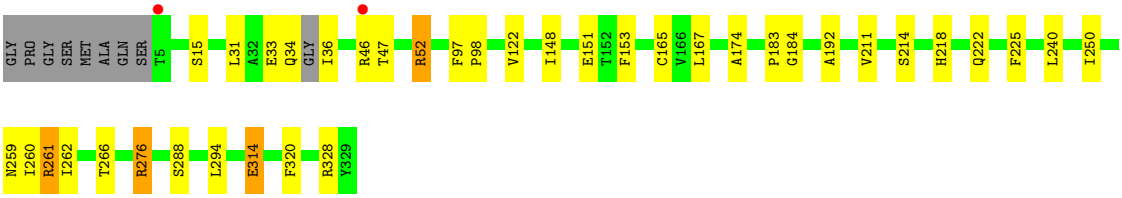
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

Chain A:



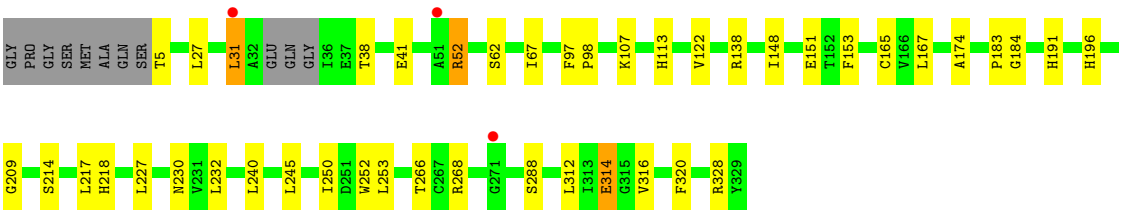
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

Chain B:



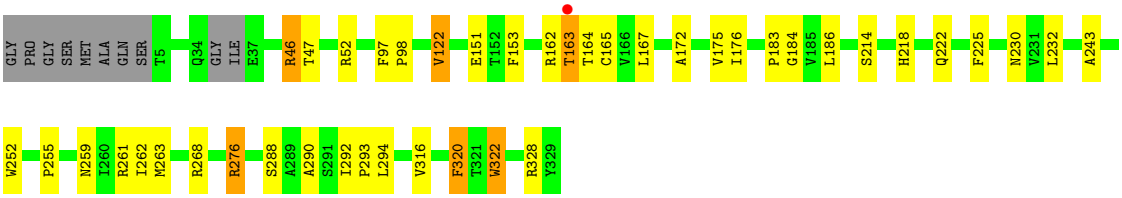
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

Chain C:



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

Chain D:


GLY
PRO
GLY
SER
MET
ALA
GLN
SER
T5
Q34
GLY
ILE
E37
R46
T47
R52
F97
P98
V122
E151
T152
F153
R162
T163
T164
C165
V166
L167
A172
V175
I176
P183
G184
V185
L186
S214
H218
Q222
F225
N230
V231
L232
A243
W252
P255
N259
I260
R261
I262
M263
R268
R276
S288
A289
A290
S291
I292
P293
L294
V316
F320
T321
W322
R328
Y329

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.99Å 67.03Å 89.20Å 113.72° 89.98° 100.25°	Depositor
Resolution (Å)	50.00 – 2.35 48.46 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.35) 98.0 (48.46-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.227 , 0.275 0.227 , 0.276	Depositor DCC
R_{free} test set	2488 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9719	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9826e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CSO, EDO

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	0.66	2/2380 (0.1%)	0.68	1/3241 (0.0%)
1	B	0.72	0/2391	0.71	1/3256 (0.0%)
1	C	0.68	1/2375 (0.0%)	0.68	2/3235 (0.1%)
1	D	0.75	2/2419 (0.1%)	0.73	1/3288 (0.0%)
All	All	0.70	5/9565 (0.1%)	0.70	5/13020 (0.0%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	322	TRP	CD2-CE2	5.70	1.48	1.41
1	D	252	TRP	CD2-CE2	5.47	1.48	1.41
1	A	322	TRP	CD2-CE2	5.24	1.47	1.41
1	A	42	TRP	CD2-CE2	5.21	1.47	1.41
1	C	252	TRP	CD2-CE2	5.19	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	58	ASP	N-CA-CB	-5.83	100.11	110.60
1	C	52	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	52	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	138	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	D	46	ARG	NE-CZ-NH2	5.15	122.88	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	PRO	Peptide
1	B	183	PRO	Peptide
1	C	183	PRO	Peptide
1	D	183	PRO	Peptide

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	2346	0	2277	13	0
1	B	2352	0	2298	29	0
1	C	2342	0	2260	24	0
1	D	2385	0	2354	29	0
2	B	4	0	6	0	0
3	A	67	0	0	2	0
3	B	75	0	0	0	0
3	C	65	0	0	2	0
3	D	83	0	0	2	0
All	All	9719	0	9195	93	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 5.

The worst 5 of 93 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:O	1:B:36:ILE:CB	1.93	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ARG:HG3	1:B:261:ARG:HH21	1.35	0.92
1:D:259:ASN:HD21	1:D:262:ILE:HD12	1.37	0.89
1:B:46[B]:ARG:CG	1:B:47:THR:HG23	2.03	0.88
1:D:163:THR:HG22	1:D:164:THR:HG23	1.58	0.85

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	317/333 (95%)	310 (98%)	6 (2%)	1 (0%)	41	47
1	B	321/333 (96%)	316 (98%)	4 (1%)	1 (0%)	41	47
1	C	317/333 (95%)	310 (98%)	6 (2%)	1 (0%)	41	47
1	D	319/333 (96%)	312 (98%)	6 (2%)	1 (0%)	41	47
All	All	1274/1332 (96%)	1248 (98%)	22 (2%)	4 (0%)	41	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	B	122	VAL
1	C	122	VAL
1	D	122	VAL

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	235/260 (90%)	225 (96%)	10 (4%)	29	35
1	B	234/260 (90%)	223 (95%)	11 (5%)	26	31
1	C	232/260 (89%)	220 (95%)	12 (5%)	23	27
1	D	244/260 (94%)	231 (95%)	13 (5%)	22	26
All	All	945/1040 (91%)	899 (95%)	46 (5%)	25	29

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	218	HIS
1	D	153	PHE
1	C	245	LEU
1	C	320	PHE
1	D	162[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	B	222	GLN
1	B	244	ASN
1	B	259	ASN
1	D	259	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)

4 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	$\#\|Z\| > 2$
1	CSO	B	123	1	3,6,7	1.28	0	0,6,8	-	-
1	CSO	A	123	1	4,5,7	0.71	0	1,5,8	0.29	0
1	CSO	C	123	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	D	123	1	3,6,7	0.96	0	0,6,8	-	-

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
1	CSO	B	123	1	-	0/1/5/7	-
1	CSO	A	123	1	-	0/1/4/7	-
1	CSO	C	123	1	-	0/1/5/7	-
1	CSO	D	123	1	-	0/1/5/7	-

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.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	EDO	B	401	-	3,3,3	0.54	0	2,2,2	0.28	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	EDO	B	401	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	321/333 (96%)	-0.05	1 (0%)	94	97	16, 33, 52, 64	0
1	B	323/333 (96%)	-0.13	2 (0%)	89	93	14, 25, 51, 73	0
1	C	321/333 (96%)	-0.09	3 (0%)	84	90	15, 34, 54, 65	0
1	D	322/333 (96%)	-0.08	1 (0%)	94	97	15, 26, 42, 58	0
All	All	1287/1332 (96%)	-0.09	7 (0%)	91	95	14, 29, 51, 73	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	271	GLY	2.7
1	B	5	THR	2.5
1	C	31	LEU	2.4
1	A	51	ALA	2.3
1	C	51	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
1	CSO	D	123	7/8	0.91	0.11	20,21,24,25	0
1	CSO	B	123	7/8	0.92	0.14	17,17,22,23	0
1	CSO	A	123	6/8	0.92	0.13	29,30,33,37	0
1	CSO	C	123	7/8	0.93	0.12	26,27,31,31	0

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(Å^2)	Q<0.9
2	EDO	B	401	4/4	0.98	0.11	24,24,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.