



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:02 pm BST

PDB ID : 6H7R
Title : Sulfolobus solfataricus 2-keto-3-deoxygluconate aldolase T157V/A198L variant
Authors : Crennell, S.J.; Danson, M.J.; Royer, S.
Deposited on : 2018-07-31
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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 : 2.11
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) : 2.11

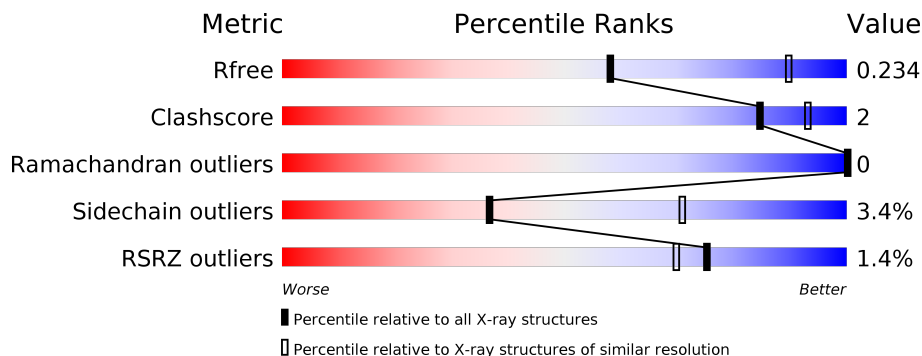
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	293	 2% 89% 10%
1	B	293	 2% 92% 6% •
1	C	293	 % 91% 9% •
1	D	293	 % 92% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19055 atoms, of which 9647 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 2-dehydro-3-deoxy-phosphogluconate/2-dehydro-3-deoxy-6-phosphogalactonate aldolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	293	4730	1507	2401	379	437	6	0	0	0
1	B	293	4731	1507	2402	379	437	6	0	1	0
1	C	293	4731	1507	2402	379	437	6	0	1	0
1	D	293	4752	1513	2414	381	438	6	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

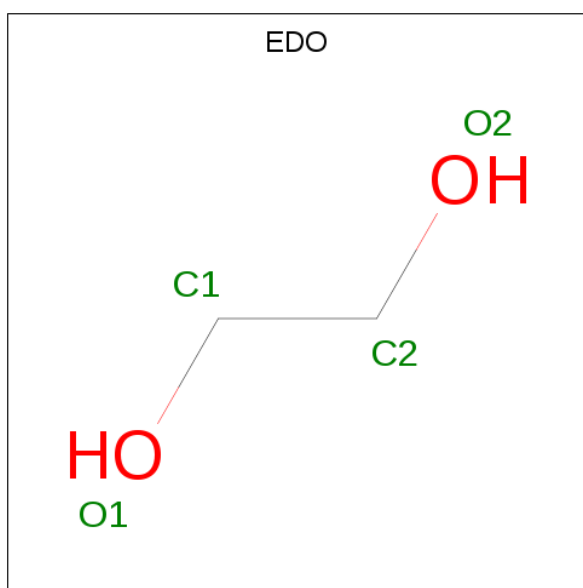
Chain	Residue	Modelled	Actual	Comment	Reference
A	157	VAL	THR	engineered mutation	UNP O54288
A	198	LEU	ALA	engineered mutation	UNP O54288
B	157	VAL	THR	engineered mutation	UNP O54288
B	198	LEU	ALA	engineered mutation	UNP O54288
C	157	VAL	THR	engineered mutation	UNP O54288
C	198	LEU	ALA	engineered mutation	UNP O54288
D	157	VAL	THR	engineered mutation	UNP O54288
D	198	LEU	ALA	engineered mutation	UNP O54288

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		

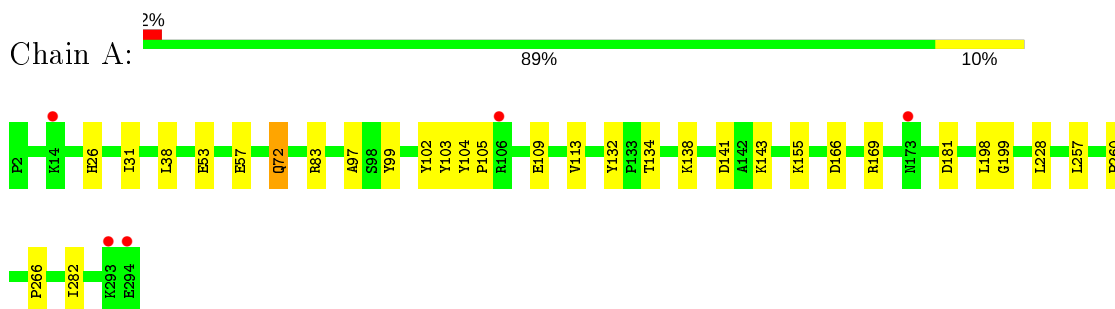
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total 15	O 15	0	0
4	B	13	Total 13	O 13	0	0
4	C	23	Total 23	O 23	0	0
4	D	12	Total 12	O 12	0	0

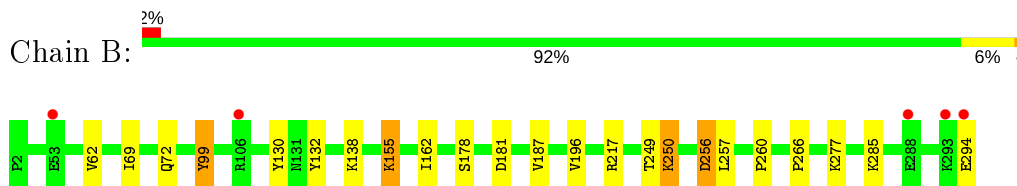
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

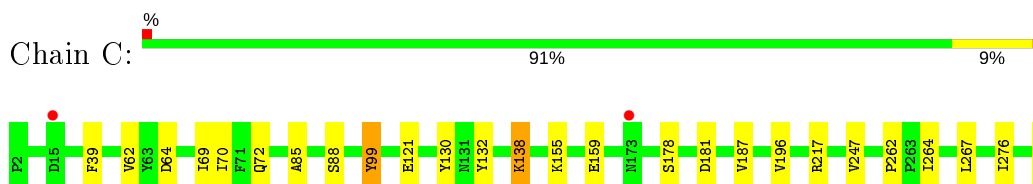
- Molecule 1: 2-dehydro-3-deoxy-phosphogluconate/2-dehydro-3-deoxy-6-phosphogalactonate aldolase



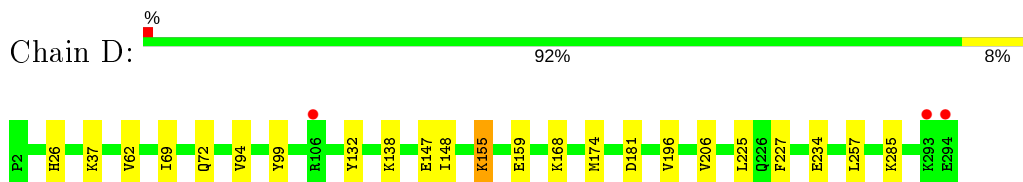
- Molecule 1: 2-dehydro-3-deoxy-phosphogluconate/2-dehydro-3-deoxy-6-phosphogalactonate aldolase



- Molecule 1: 2-dehydro-3-deoxy-phosphogluconate/2-dehydro-3-deoxy-6-phosphogalactonate aldolase



- Molecule 1: 2-dehydro-3-deoxy-phosphogluconate/2-dehydro-3-deoxy-6-phosphogalactonate aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.10Å 126.04Å 126.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.55 – 2.80 23.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.4 (23.55-2.80) 89.4 (23.54-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.80Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.187 , 0.234 0.187 , 0.234	Depositor DCC
R_{free} test set	1523 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtrriage
Anisotropy	0.075	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.034 for -h,l,k	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19055	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: GOL, 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	0.29	0/2375	0.47	0/3212
1	B	0.28	0/2383	0.47	0/3223
1	C	0.29	0/2383	0.47	0/3223
1	D	0.29	0/2384	0.46	0/3223
All	All	0.29	0/9525	0.47	0/12881

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2329	2401	2400	15	0
1	B	2329	2402	2396	9	0
1	C	2329	2402	2396	14	0
1	D	2338	2414	2412	10	0
2	A	6	8	8	0	0
2	B	6	8	8	0	0
3	A	4	6	6	0	0
3	C	4	6	6	0	0
4	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	13	0	0	0	0
4	C	23	0	0	0	0
4	D	12	0	0	0	0
All	All	9408	9647	9632	43	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 2.

All (43) 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:166:ASP:OD1	1:A:169:ARG:NH2	2.26	0.68
1:C:247:VAL:HG21	1:C:267:LEU:HD12	1.75	0.66
1:A:169:ARG:NH1	1:D:234:GLU:OE1	2.30	0.64
1:C:85:ALA:O	1:C:88:SER:OG	2.15	0.62
1:D:37:LYS:HD3	1:D:94:VAL:HG21	1.82	0.62
1:B:155:LYS:HG2	1:B:196:VAL:HG21	1.82	0.61
1:B:249:THR:HG21	1:B:257:LEU:HD11	1.85	0.58
1:D:62:VAL:HG12	1:D:69:ILE:HD11	1.88	0.56
1:A:169:ARG:HG3	1:D:227:PHE:CG	2.40	0.55
1:D:155:LYS:HG2	1:D:196:VAL:HG21	1.89	0.55
1:B:162:ILE:HD12	1:C:159:GLU:HB3	1.89	0.55
1:C:39:PHE:CD1	1:C:155:LYS:HE2	2.42	0.54
1:B:62:VAL:HG12	1:B:69:ILE:HD11	1.91	0.53
1:A:26:HIS:HB2	1:A:257:LEU:HD21	1.92	0.52
1:D:168:LYS:NZ	1:D:174:MET:O	2.22	0.51
1:C:62:VAL:HG12	1:C:69:ILE:HD11	1.92	0.50
1:C:178:SER:HB3	1:C:187:VAL:HG21	1.94	0.49
1:D:26:HIS:HB2	1:D:257:LEU:HD21	1.93	0.49
1:B:178:SER:HB3	1:B:187:VAL:HG21	1.95	0.49
1:C:99:TYR:HA	1:C:130:TYR:O	2.13	0.49
1:A:228:LEU:HD22	1:A:282:ILE:HG23	1.95	0.48
1:B:250:LYS:HD3	1:B:256:ASP:HB2	1.94	0.48
1:B:217:ARG:HD2	1:C:217:ARG:HD2	1.96	0.47
1:A:198:LEU:HD12	1:A:199:GLY:N	2.30	0.47
1:A:31:ILE:HD11	1:A:38:LEU:HG	1.96	0.47
1:A:260:PRO:HD2	1:A:266:PRO:HB3	1.98	0.46
1:C:279:VAL:HA	1:C:282:ILE:HD12	1.98	0.46
1:C:155:LYS:HG2	1:C:196:VAL:HG21	1.98	0.45
1:A:102:TYR:O	1:A:103:TYR:HB3	2.17	0.45
1:A:169:ARG:HH12	1:D:234:GLU:CD	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ILE:HD13	1:C:155:LYS:NZ	2.32	0.44
1:C:262:PRO:HA	1:C:264:ILE:N	2.33	0.44
1:B:99:TYR:HA	1:B:130:TYR:O	2.18	0.43
1:D:206:VAL:HG13	1:D:225:LEU:HD11	2.00	0.43
1:A:141:ASP:OD1	1:A:143:LYS:N	2.52	0.43
1:A:72:GLN:HA	1:A:97:ALA:O	2.18	0.42
1:A:109:GLU:O	1:A:113:VAL:HG23	2.20	0.42
1:A:53:GLU:O	1:A:57:GLU:HG2	2.20	0.41
1:B:260:PRO:HD2	1:B:266:PRO:HB3	2.03	0.41
1:A:104:TYR:HA	1:A:105:PRO:HD3	1.96	0.41
1:C:276:ILE:HA	1:C:279:VAL:HG22	2.02	0.41
1:C:138:LYS:N	1:C:138:LYS:HD2	2.37	0.40
1:D:285[A]:LYS:HB2	1:D:285[A]:LYS:HE2	1.96	0.40

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	291/293 (99%)	286 (98%)	5 (2%)	0	100	100
1	B	292/293 (100%)	284 (97%)	8 (3%)	0	100	100
1	C	292/293 (100%)	285 (98%)	7 (2%)	0	100	100
1	D	292/293 (100%)	282 (97%)	10 (3%)	0	100	100
All	All	1167/1172 (100%)	1137 (97%)	30 (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	259/259 (100%)	251 (97%)	8 (3%)	40	74
1	B	260/259 (100%)	249 (96%)	11 (4%)	30	63
1	C	260/259 (100%)	253 (97%)	7 (3%)	44	78
1	D	260/259 (100%)	251 (96%)	9 (4%)	36	70
All	All	1039/1036 (100%)	1004 (97%)	35 (3%)	37	71

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	83	ARG
1	A	99	TYR
1	A	132	TYR
1	A	134	THR
1	A	138	LYS
1	A	155	LYS
1	A	181	ASP
1	B	72	GLN
1	B	99	TYR
1	B	132	TYR
1	B	138	LYS
1	B	155	LYS
1	B	181	ASP
1	B	250	LYS
1	B	256	ASP
1	B	277	LYS
1	B	285	LYS
1	B	294	GLU
1	C	64	ASP
1	C	72	GLN
1	C	99	TYR
1	C	121	GLU
1	C	132	TYR

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Mol	Chain	Res	Type
1	C	138	LYS
1	C	181	ASP
1	D	72	GLN
1	D	99	TYR
1	D	132	TYR
1	D	138	LYS
1	D	147	GLU
1	D	148	ILE
1	D	155	LYS
1	D	159	GLU
1	D	181	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	GOL	B	301	-	5,5,5	1.29	1 (20%)	5,5,5	1.01	0
3	EDO	A	402	-	3,3,3	0.44	0	2,2,2	0.44	0
2	GOL	A	401	-	5,5,5	0.88	0	5,5,5	1.03	0
3	EDO	C	301	-	3,3,3	0.45	0	2,2,2	0.43	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	GOL	B	301	-	-	2/4/4/4	-
3	EDO	A	402	-	-	1/1/1/1	-
2	GOL	A	401	-	-	0/4/4/4	-
3	EDO	C	301	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	GOL	C3-C2	2.17	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-O2
3	A	402	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

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	293/293 (100%)	-0.26	5 (1%) 70 63	20, 28, 47, 84	0
1	B	293/293 (100%)	-0.29	5 (1%) 70 63	21, 28, 48, 92	0
1	C	293/293 (100%)	-0.25	3 (1%) 82 77	23, 29, 44, 61	0
1	D	293/293 (100%)	-0.27	3 (1%) 82 77	21, 29, 43, 74	0
All	All	1172/1172 (100%)	-0.27	16 (1%) 75 70	20, 29, 45, 92	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	GLU	3.8
1	B	294	GLU	3.2
1	B	106	ARG	3.2
1	D	106	ARG	2.8
1	B	288	GLU	2.8
1	C	294	GLU	2.7
1	A	293	LYS	2.6
1	D	293	LYS	2.5
1	D	294	GLU	2.4
1	B	53	GLU	2.4
1	B	293	LYS	2.4
1	A	14	LYS	2.3
1	A	173	ASN	2.2
1	A	106	ARG	2.2
1	C	15	ASP	2.1
1	C	173	ASN	2.0

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 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. 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	GOL	B	301	6/6	0.75	0.31	30,39,49,49	0
3	EDO	A	402	4/4	0.85	0.29	38,55,103,116	0
2	GOL	A	401	6/6	0.87	0.27	64,94,132,132	0
3	EDO	C	301	4/4	0.91	0.23	30,37,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.