



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:33 PM UTC

PDB ID : 3OBI / pdb_00003obi
Title : Crystal structure of a formyltetrahydrofolate deformylase (NP_949368) from RHODOPSEUDOMONAS PALUSTRIS CGA009 at 1.95 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2010-08-06
Resolution : 1.95 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

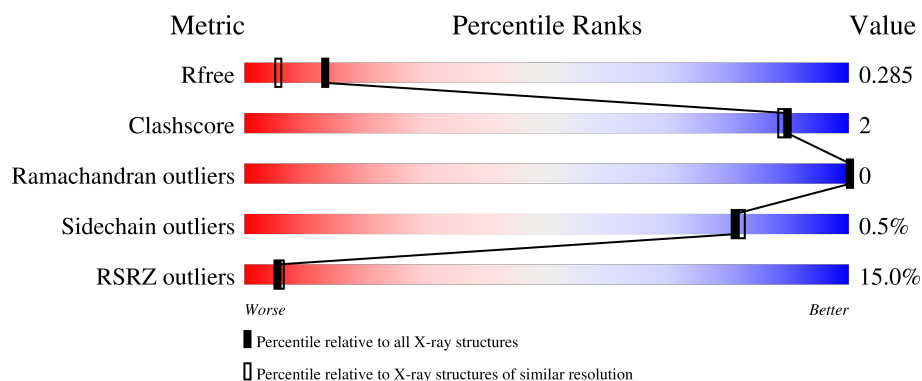
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	288	22% 91% 8% .
1	B	288	14% 92% 7% .
1	C	288	9% 94% . .
1	D	288	12% 95% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10515 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 Formyltetrahydrofolate deformylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	Se	0	14	0
			2366	1502	436	417	3	8			
1	B	285	Total	C	N	O	S	Se	0	16	0
			2374	1509	441	413	3	8			
1	C	284	Total	C	N	O	S	Se	0	8	0
			2316	1470	431	405	3	7			
1	D	284	Total	C	N	O	S	Se	0	11	0
			2330	1478	432	409	3	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q6N2L8
B	0	GLY	-	expression tag	UNP Q6N2L8
C	0	GLY	-	expression tag	UNP Q6N2L8
D	0	GLY	-	expression tag	UNP Q6N2L8

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

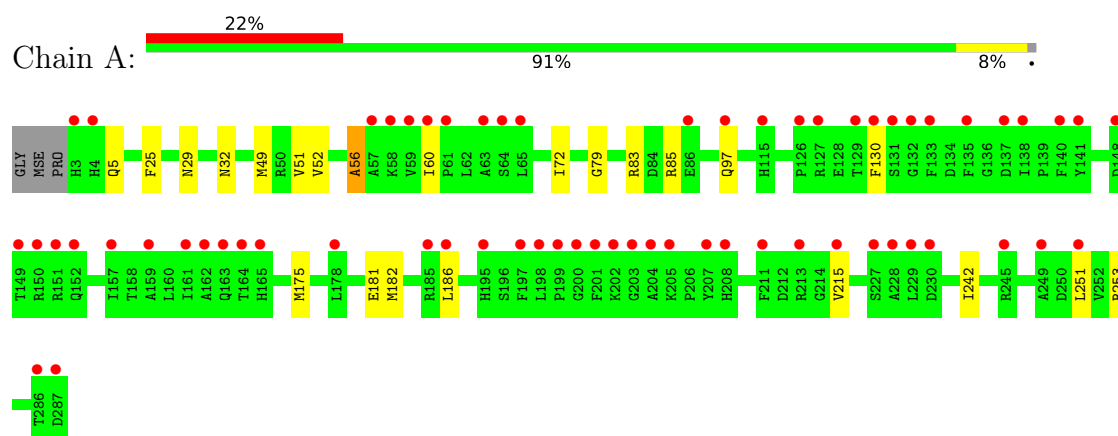
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	259	Total O 261 261	0	2
3	B	266	Total O 272 272	0	6
3	C	263	Total O 264 264	0	1
3	D	213	Total O 216 216	0	3

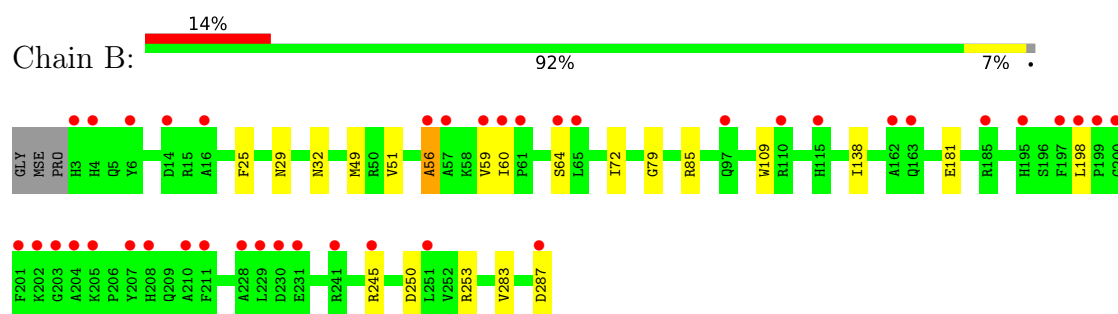
3 Residue-property plots [i](#)

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.

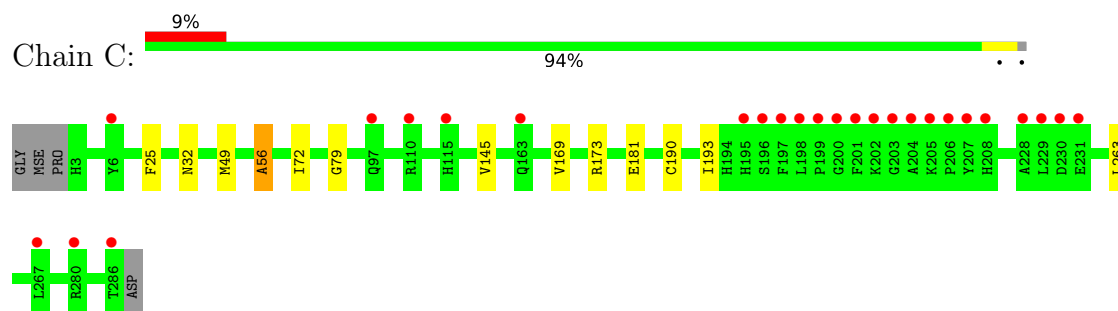
- Molecule 1: Formyltetrahydrofolate deformylase



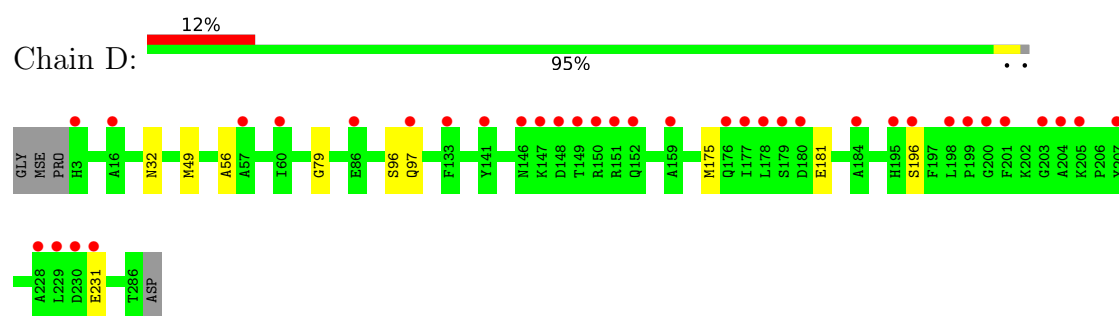
- Molecule 1: Formyltetrahydrofolate deformylase



- Molecule 1: Formyltetrahydrofolate deformylase



- Molecule 1: Formyltetrahydrofolate deformylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.05Å 141.11Å 77.56Å 90.00° 107.83° 90.00°	Depositor
Resolution (Å)	29.67 – 1.95 29.67 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.67-1.95) 97.0 (29.67-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.234 , 0.278 0.239 , 0.285	Depositor DCC
R_{free} test set	5035 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10515	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 60.25 % 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 1.5648e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.92	2/2450 (0.1%)	1.00	2/3301 (0.1%)
1	B	0.94	1/2467 (0.0%)	1.00	2/3321 (0.1%)
1	C	0.92	3/2385 (0.1%)	0.99	1/3215 (0.0%)
1	D	0.85	1/2409 (0.0%)	0.99	2/3248 (0.1%)
All	All	0.91	7/9711 (0.1%)	1.00	7/13085 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	ALA	CA-C	6.54	1.55	1.52
1	C	49	MSE	SE-CE	-6.25	1.76	1.95
1	D	49	MSE	SE-CE	-5.83	1.77	1.95
1	A	56	ALA	CA-C	5.67	1.55	1.52
1	A	215	VAL	CA-CB	5.44	1.59	1.54
1	C	263	LEU	C-O	-5.39	1.17	1.24
1	C	56	ALA	CA-C	5.03	1.54	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	GLY	N-CA-C	-7.03	98.72	110.95
1	D	79	GLY	N-CA-C	-6.67	99.34	110.95
1	A	79	GLY	N-CA-C	-6.51	99.62	110.95
1	B	79	GLY	N-CA-C	-6.47	98.58	111.34
1	D	231	GLU	N-CA-C	5.70	120.05	112.30
1	B	283	VAL	N-CA-C	-5.43	100.57	108.17
1	A	130	PHE	N-CA-C	5.02	117.68	109.59

There are no chirality outliers.

There are no planarity outliers.

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	2366	0	2364	11	0
1	B	2374	0	2409	13	0
1	C	2316	0	2326	6	0
1	D	2330	0	2330	5	0
2	A	32	0	48	1	0
2	B	36	0	54	0	0
2	C	36	0	54	0	0
2	D	12	0	18	0	0
3	A	261	0	0	1	0
3	B	272	0	0	1	0
3	C	264	0	0	1	0
3	D	216	0	0	0	0
All	All	10515	0	9603	34	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 (34) 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:245[B]:ARG:HH11	1:B:245[B]:ARG:HB3	1.18	1.03
1:B:245[B]:ARG:HB3	1:B:245[B]:ARG:NH1	1.83	0.94
1:B:59:VAL:HG23	3:B:1063:HOH:O	1.89	0.71
1:B:198:LEU:HD11	1:D:196[B]:SER:OG	1.91	0.71
1:A:242:ILE:HD12	1:A:251:LEU:HD23	1.80	0.64
1:C:32:ASN:HB2	1:C:56:ALA:HB2	1.86	0.58
1:D:96:SER:HB3	1:D:175[B]:MSE:HE2	1.90	0.54
1:D:97:GLN:HE21	1:D:175[B]:MSE:HE1	1.72	0.54
1:D:32:ASN:HB2	1:D:56:ALA:HB2	1.91	0.52
1:B:250:ASP:OD1	1:B:253[A]:ARG:NH2	2.43	0.51
1:A:5:GLN:OE1	1:A:85[B]:ARG:NH2	2.44	0.50
1:C:173[A]:ARG:HD3	1:C:193:ILE:HG23	1.95	0.48
1:B:60[B]:ILE:HG22	1:B:64[B]:SER:HB2	1.96	0.47
1:C:173[A]:ARG:HA	1:C:173[A]:ARG:HD2	1.61	0.47
1:A:49:MSE:HE2	1:A:51[A]:VAL:CG2	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:VAL:HG21	3:C:940:HOH:O	2.16	0.45
1:A:32:ASN:HB2	1:A:56:ALA:HB2	1.98	0.45
1:B:25:PHE:HB2	1:B:72:ILE:CD1	2.46	0.45
1:B:32:ASN:HB2	1:B:56:ALA:HB2	1.99	0.44
1:B:85[B]:ARG:HH21	1:B:85[B]:ARG:CB	2.29	0.44
1:B:49:MSE:HE2	1:B:51[B]:VAL:CG2	2.47	0.44
1:A:83:ARG:NH1	3:A:934:HOH:O	2.49	0.44
1:A:253:ARG:NH1	2:A:305:EDO:O1	2.51	0.43
1:C:25:PHE:HB2	1:C:72:ILE:CD1	2.49	0.43
1:D:97:GLN:NE2	1:D:175[B]:MSE:HE1	2.33	0.43
1:A:97:GLN:H	1:A:175[B]:MSE:HE2	1.84	0.42
1:B:109:TRP:CZ3	1:B:138:ILE:HD11	2.55	0.42
1:A:29:ASN:HB3	1:A:60:ILE:HD12	2.02	0.41
1:A:182:MSE:HE3	1:A:186:LEU:HD11	2.02	0.41
1:A:52:VAL:HG11	1:A:85[B]:ARG:NH1	2.35	0.41
1:B:29:ASN:HB3	1:B:60[B]:ILE:HD12	2.02	0.41
1:B:85[B]:ARG:HB3	1:B:85[B]:ARG:NH2	2.35	0.41
1:C:169:VAL:O	1:C:190:CYS:HA	2.21	0.40
1:A:25:PHE:HB2	1:A:72:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

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	297/288 (103%)	293 (99%)	4 (1%)	0	100	100
1	B	299/288 (104%)	293 (98%)	6 (2%)	0	100	100
1	C	290/288 (101%)	285 (98%)	5 (2%)	0	100	100
1	D	293/288 (102%)	290 (99%)	3 (1%)	0	100	100
All	All	1179/1152 (102%)	1161 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	256/237 (108%)	255 (100%)	1 (0%)	84	85
1	B	258/237 (109%)	256 (99%)	2 (1%)	73	74
1	C	249/237 (105%)	248 (100%)	1 (0%)	84	85
1	D	251/237 (106%)	250 (100%)	1 (0%)	84	85
All	All	1014/948 (107%)	1009 (100%)	5 (0%)	81	82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	GLU
1	B	181	GLU
1	B	287	ASP
1	C	181	GLU
1	D	181	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	HIS
1	A	278	ASN
1	B	192	ASN
1	B	209	GLN
1	B	278	ASN
1	C	29	ASN
1	C	278	ASN
1	D	97	GLN
1	D	209	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

29 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	EDO	A	305	-	3,3,3	0.40	0	2,2,2	0.41	0
2	EDO	C	323	-	3,3,3	0.43	0	2,2,2	0.32	0
2	EDO	A	308	-	3,3,3	0.46	0	2,2,2	0.09	0
2	EDO	B	328	-	3,3,3	0.46	0	2,2,2	0.15	0
2	EDO	A	309	-	3,3,3	0.37	0	2,2,2	0.44	0
2	EDO	C	324	-	3,3,3	0.54	0	2,2,2	0.15	0
2	EDO	B	312	-	3,3,3	0.45	0	2,2,2	0.18	0
2	EDO	B	307	-	3,3,3	0.44	0	2,2,2	0.43	0
2	EDO	C	321	-	3,3,3	0.44	0	2,2,2	0.34	0
2	EDO	C	317	-	3,3,3	0.35	0	2,2,2	0.59	0
2	EDO	B	304	-	3,3,3	0.45	0	2,2,2	0.49	0
2	EDO	A	310	-	3,3,3	0.56	0	2,2,2	0.04	0
2	EDO	A	300	-	3,3,3	0.41	0	2,2,2	0.34	0
2	EDO	B	326	-	3,3,3	0.42	0	2,2,2	0.36	0
2	EDO	B	322	-	3,3,3	0.49	0	2,2,2	0.20	0
2	EDO	A	311	-	3,3,3	0.52	0	2,2,2	0.13	0
2	EDO	D	315	-	3,3,3	0.47	0	2,2,2	0.16	0
2	EDO	A	327	-	3,3,3	0.45	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	316	-	3,3,3	0.46	0	2,2,2	0.21	0
2	EDO	C	314	-	3,3,3	0.30	0	2,2,2	0.37	0
2	EDO	D	303	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	C	325	-	3,3,3	0.57	0	2,2,2	0.22	0
2	EDO	B	313	-	3,3,3	0.51	0	2,2,2	0.25	0
2	EDO	B	319	-	3,3,3	0.52	0	2,2,2	0.23	0
2	EDO	B	301	-	3,3,3	0.53	0	2,2,2	0.25	0
2	EDO	A	320	-	3,3,3	0.50	0	2,2,2	0.26	0
2	EDO	D	318	-	3,3,3	0.41	0	2,2,2	0.31	0
2	EDO	C	306	-	3,3,3	0.47	0	2,2,2	0.18	0
2	EDO	C	302	-	3,3,3	0.49	0	2,2,2	0.10	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	A	305	-	-	1/1/1/1	-
2	EDO	C	323	-	-	0/1/1/1	-
2	EDO	A	308	-	-	0/1/1/1	-
2	EDO	B	328	-	-	0/1/1/1	-
2	EDO	A	309	-	-	0/1/1/1	-
2	EDO	C	324	-	-	0/1/1/1	-
2	EDO	B	312	-	-	0/1/1/1	-
2	EDO	B	307	-	-	1/1/1/1	-
2	EDO	C	321	-	-	1/1/1/1	-
2	EDO	C	317	-	-	0/1/1/1	-
2	EDO	B	304	-	-	0/1/1/1	-
2	EDO	A	310	-	-	1/1/1/1	-
2	EDO	A	300	-	-	0/1/1/1	-
2	EDO	B	326	-	-	1/1/1/1	-
2	EDO	B	322	-	-	1/1/1/1	-
2	EDO	A	311	-	-	0/1/1/1	-
2	EDO	D	315	-	-	0/1/1/1	-
2	EDO	A	327	-	-	1/1/1/1	-
2	EDO	C	316	-	-	0/1/1/1	-
2	EDO	C	314	-	-	0/1/1/1	-
2	EDO	D	303	-	-	0/1/1/1	-
2	EDO	C	325	-	-	1/1/1/1	-
2	EDO	B	313	-	-	1/1/1/1	-
2	EDO	B	319	-	-	1/1/1/1	-
2	EDO	B	301	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	320	-	-	0/1/1/1	-
2	EDO	D	318	-	-	0/1/1/1	-
2	EDO	C	306	-	-	0/1/1/1	-
2	EDO	C	302	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	327	EDO	O1-C1-C2-O2
2	B	319	EDO	O1-C1-C2-O2
2	C	321	EDO	O1-C1-C2-O2
2	A	305	EDO	O1-C1-C2-O2
2	B	326	EDO	O1-C1-C2-O2
2	B	307	EDO	O1-C1-C2-O2
2	C	325	EDO	O1-C1-C2-O2
2	A	310	EDO	O1-C1-C2-O2
2	B	301	EDO	O1-C1-C2-O2
2	B	322	EDO	O1-C1-C2-O2
2	B	313	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	305	EDO	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

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	278/288 (96%)	1.14	64 (23%) 2 2	11, 29, 50, 63	13 (4%)
1	B	278/288 (96%)	0.79	40 (14%) 6 6	11, 25, 46, 59	15 (5%)
1	C	277/288 (96%)	0.64	26 (9%) 14 16	13, 25, 46, 59	8 (2%)
1	D	277/288 (96%)	0.64	36 (12%) 7 8	12, 29, 51, 60	10 (3%)
All	All	1110/1152 (96%)	0.80	166 (14%) 5 6	11, 27, 49, 63	46 (4%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	6.0
1	A	287	ASP	5.9
1	D	133	PHE	5.6
1	A	3	HIS	5.5
1	A	198	LEU	5.3
1	A	133	PHE	5.1
1	B	204	ALA	5.1
1	B	287	ASP	4.7
1	D	229	LEU	4.7
1	A	201	PHE	4.6
1	D	204	ALA	4.5
1	A	199	PRO	4.4
1	A	60	ILE	4.3
1	B	3	HIS	4.2
1	A	228	ALA	4.2
1	C	204	ALA	4.2
1	A	159	ALA	4.1
1	D	148	ASP	4.1
1	D	178	LEU	4.1
1	A	59	VAL	4.0
1	A	207[A]	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	135	PHE	4.0
1	C	228	ALA	4.0
1	B	228	ALA	3.9
1	A	205[A]	LYS	3.9
1	A	245	ARG	3.9
1	A	229	LEU	3.8
1	D	207	TYR	3.8
1	D	198[A]	LEU	3.7
1	C	230	ASP	3.7
1	A	141	TYR	3.7
1	D	3	HIS	3.7
1	C	200	GLY	3.6
1	D	152	GLN	3.6
1	B	4	HIS	3.6
1	D	195	HIS	3.6
1	D	184	ALA	3.6
1	B	199	PRO	3.5
1	A	57	ALA	3.5
1	A	4	HIS	3.5
1	B	207	TYR	3.4
1	A	162	ALA	3.4
1	B	201	PHE	3.3
1	C	229	LEU	3.3
1	B	210	ALA	3.3
1	D	149	THR	3.2
1	B	251	LEU	3.2
1	A	86	GLU	3.2
1	C	202	LYS	3.1
1	C	231	GLU	3.1
1	A	186	LEU	3.1
1	C	201	PHE	3.1
1	A	64[A]	SER	3.1
1	D	179	SER	3.1
1	C	207	TYR	3.1
1	A	163	GLN	3.1
1	A	61	PRO	3.1
1	A	132	GLY	3.0
1	D	57	ALA	3.0
1	D	177	ILE	3.0
1	A	251	LEU	3.0
1	B	163	GLN	3.0
1	A	148	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	63	ALA	3.0
1	D	228	ALA	3.0
1	B	229	LEU	2.9
1	A	150	ARG	2.9
1	A	208	HIS	2.9
1	B	241	ARG	2.9
1	A	200	GLY	2.9
1	A	152	GLN	2.9
1	A	58	LYS	2.9
1	B	202	LYS	2.9
1	D	180	ASP	2.9
1	C	198	LEU	2.9
1	A	197	PHE	2.8
1	B	230	ASP	2.8
1	B	231	GLU	2.8
1	A	164	THR	2.8
1	C	205	LYS	2.8
1	C	206	PRO	2.8
1	A	131[A]	SER	2.8
1	A	65	LEU	2.8
1	D	146	ASN	2.7
1	B	197	PHE	2.7
1	D	201	PHE	2.7
1	A	151	ARG	2.7
1	D	151	ARG	2.7
1	A	286	THR	2.7
1	B	198	LEU	2.6
1	B	200	GLY	2.6
1	C	203	GLY	2.6
1	D	203	GLY	2.6
1	A	130	PHE	2.6
1	B	61	PRO	2.6
1	C	115[A]	HIS	2.6
1	C	196	SER	2.6
1	A	178	LEU	2.5
1	D	230	ASP	2.5
1	C	163	GLN	2.5
1	D	196[A]	SER	2.5
1	A	97	GLN	2.5
1	B	59	VAL	2.5
1	D	150	ARG	2.5
1	A	195[A]	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	115[A]	HIS	2.5
1	B	56	ALA	2.5
1	B	60[A]	ILE	2.4
1	A	202	LYS	2.4
1	D	205	LYS	2.4
1	D	86	GLU	2.4
1	D	231	GLU	2.4
1	A	161	ILE	2.4
1	D	16	ALA	2.4
1	C	195	HIS	2.4
1	D	141	TYR	2.4
1	A	185	ARG	2.4
1	A	126	PRO	2.4
1	D	200	GLY	2.4
1	C	280	ARG	2.3
1	C	97	GLN	2.3
1	B	6	TYR	2.3
1	B	211	PHE	2.3
1	B	57	ALA	2.3
1	A	203	GLY	2.3
1	A	127	ARG	2.3
1	C	267	LEU	2.3
1	A	211	PHE	2.3
1	B	16	ALA	2.3
1	B	162	ALA	2.3
1	A	115[A]	HIS	2.3
1	A	165	HIS	2.3
1	B	245[A]	ARG	2.2
1	A	249	ALA	2.2
1	B	64[A]	SER	2.2
1	D	97	GLN	2.2
1	A	129	THR	2.2
1	B	14	ASP	2.2
1	A	230	ASP	2.2
1	C	199	PRO	2.2
1	D	199	PRO	2.2
1	C	6	TYR	2.2
1	B	203	GLY	2.2
1	B	205	LYS	2.2
1	B	208	HIS	2.1
1	C	208	HIS	2.1
1	D	159	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	176[A]	GLN	2.1
1	A	213	ARG	2.1
1	B	110	ARG	2.1
1	B	185	ARG	2.1
1	C	110[A]	ARG	2.1
1	A	140	PHE	2.1
1	A	137	ASP	2.1
1	A	138	ILE	2.0
1	C	197	PHE	2.0
1	A	227	SER	2.0
1	D	60	ILE	2.0
1	D	147	LYS	2.0
1	A	149	THR	2.0
1	A	215	VAL	2.0
1	B	65	LEU	2.0
1	A	157	ILE	2.0
1	B	97[A]	GLN	2.0
1	B	195	HIS	2.0
1	C	286	THR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	EDO	C	321	4/4	0.50	0.26	57,57,58,58	0
2	EDO	B	326	4/4	0.52	0.27	70,70,70,70	0
2	EDO	C	314	4/4	0.61	0.38	58,58,58,58	0
2	EDO	B	307	4/4	0.64	0.28	54,55,56,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	327	4/4	0.65	0.32	66,67,67,67	0
2	EDO	C	325	4/4	0.67	0.21	54,55,56,56	0
2	EDO	C	317	4/4	0.68	0.22	44,45,46,48	0
2	EDO	A	310	4/4	0.71	0.22	57,57,57,57	0
2	EDO	C	323	4/4	0.77	0.17	65,66,66,66	0
2	EDO	B	304	4/4	0.77	0.19	41,45,45,48	0
2	EDO	A	320	4/4	0.78	0.21	49,49,51,51	0
2	EDO	C	306	4/4	0.79	0.19	48,49,50,50	0
2	EDO	A	305	4/4	0.79	0.19	38,40,41,42	0
2	EDO	B	319	4/4	0.80	0.19	42,45,46,46	0
2	EDO	D	318	4/4	0.80	0.17	44,45,45,45	0
2	EDO	B	322	4/4	0.81	0.21	47,47,47,48	0
2	EDO	B	301	4/4	0.82	0.16	41,42,43,44	0
2	EDO	D	303	4/4	0.83	0.16	48,49,49,50	0
2	EDO	C	324	4/4	0.84	0.15	35,38,38,39	0
2	EDO	C	316	4/4	0.85	0.18	33,37,38,41	0
2	EDO	A	309	4/4	0.86	0.25	41,43,44,44	0
2	EDO	B	313	4/4	0.86	0.15	37,38,39,40	0
2	EDO	A	300	4/4	0.86	0.17	47,48,48,48	0
2	EDO	A	308	4/4	0.88	0.15	33,37,37,40	0
2	EDO	B	312	4/4	0.89	0.18	50,51,52,52	0
2	EDO	D	315	4/4	0.91	0.12	31,36,37,40	0
2	EDO	A	311	4/4	0.91	0.14	49,49,49,50	0
2	EDO	C	302	4/4	0.92	0.11	33,37,38,40	0
2	EDO	B	328	4/4	0.93	0.11	33,38,40,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.