



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:33 AM UTC

PDB ID : 5F4H / pdb_00005f4h
Title : Archaeal RuvB-like Holiday junction helicase
Authors : Zhai, B.; DuPrez, K.T.; Doukov, T.I.; Shen, Y.; Fan, L.
Deposited on : 2015-12-03
Resolution : 2.70 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	:	4-5-2 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

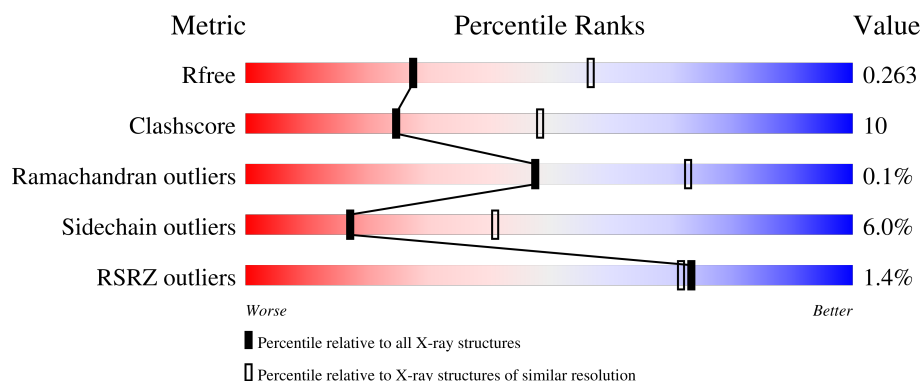
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	505	0.2% 65% 18% 13%
1	B	505	0.2% 65% 18% 14%
1	C	505	2% 66% 18% 14%
1	D	505	2% 66% 18% 14%
1	E	505	0.2% 65% 18% 14%

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Mol	Chain	Length	Quality of chain
1	F	505	% 64% 19% 14%

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
2	GOL	C	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20358 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 Nucleotide binding protein PINc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3329	2118	556	639	16			
1	B	435	Total	C	N	O	S	0	0	0
			3347	2132	556	644	15			
1	C	436	Total	C	N	O	S	0	0	0
			3274	2071	554	635	14			
1	D	436	Total	C	N	O	S	0	0	0
			3324	2110	557	642	15			
1	E	436	Total	C	N	O	S	0	0	0
			3334	2115	561	644	14			
1	F	436	Total	C	N	O	S	0	0	0
			3350	2131	565	638	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ALA	LYS	engineered mutation	UNP C3MQK6
B	261	ALA	LYS	engineered mutation	UNP C3MQK6
C	261	ALA	LYS	engineered mutation	UNP C3MQK6
D	261	ALA	LYS	engineered mutation	UNP C3MQK6
E	261	ALA	LYS	engineered mutation	UNP C3MQK6
F	261	ALA	LYS	engineered mutation	UNP C3MQK6

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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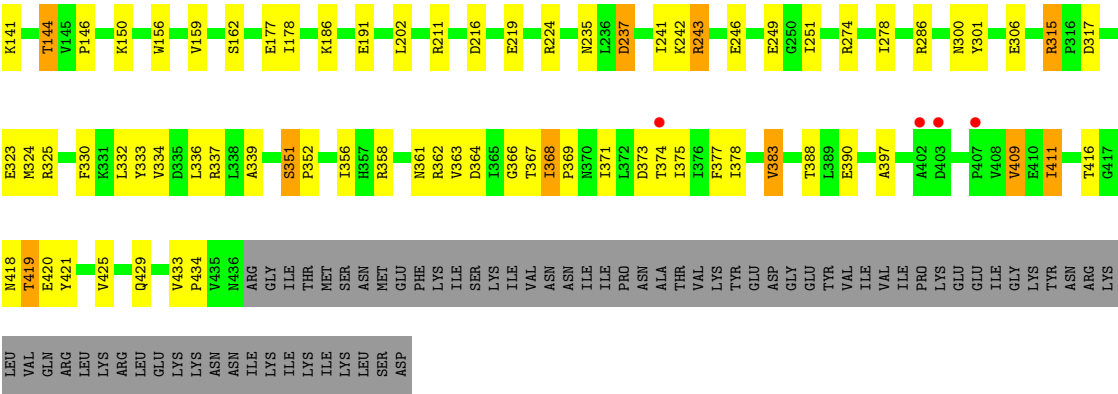
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

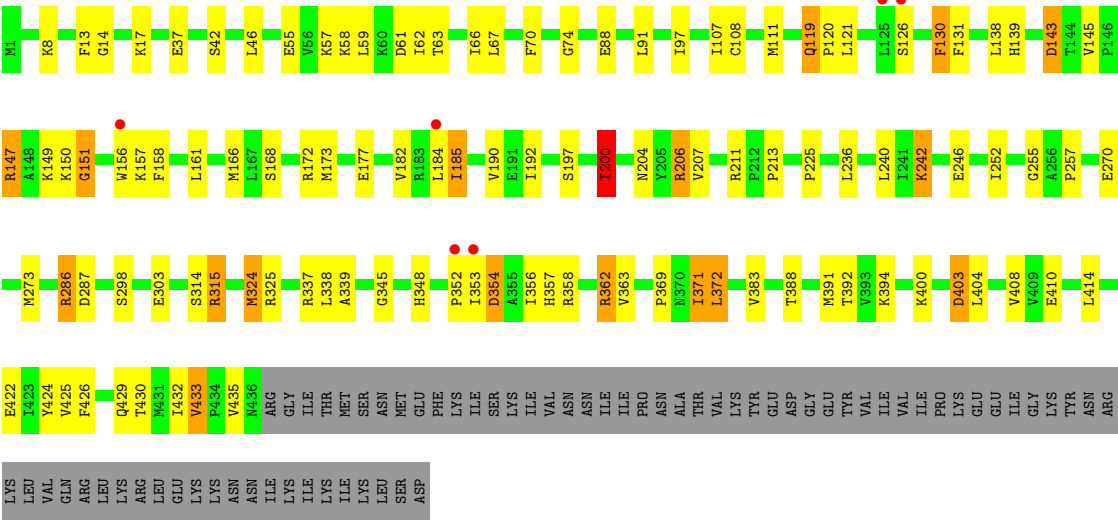
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	49	Total O 49 49	0	0
4	B	28	Total O 28 28	0	0
4	C	19	Total O 19 19	0	0
4	D	38	Total O 38 38	0	0
4	E	56	Total O 56 56	0	0
4	F	40	Total O 40 40	0	0

Y1 M5 L6 D7 E20 K32 L35 E39 V47 D54 K60 D61 T62 T63 L66 L67 V68 N69 F70 F71 F72 I72 I73 V74 G75 D75 D76 D77 S77 K78 K79 E88 E89 Y89 E92 Q104 K105 M111 Y115 L125 S126 F127 E128 D132 T135



● Molecule 1: Nucleotide binding protein PINc



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.72Å 148.98Å 122.13Å 90.00° 104.07° 90.00°	Depositor
Resolution (Å)	39.19 – 2.70 39.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.19-2.70) 97.6 (39.19-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.227 , 0.265 0.227 , 0.263	Depositor DCC
R_{free} test set	4732 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20358	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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	1.29	1/3381 (0.0%)	1.25	20/4585 (0.4%)
1	B	1.22	4/3401 (0.1%)	1.23	18/4610 (0.4%)
1	C	1.21	2/3326 (0.1%)	1.28	26/4515 (0.6%)
1	D	1.22	3/3376 (0.1%)	1.27	17/4577 (0.4%)
1	E	1.30	4/3384 (0.1%)	1.27	21/4587 (0.5%)
1	F	1.32	4/3402 (0.1%)	1.29	24/4604 (0.5%)
All	All	1.26	18/20270 (0.1%)	1.27	126/27478 (0.5%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	224	ARG	CA-C	-6.51	1.47	1.52
1	E	219	GLU	CD-OE1	6.26	1.37	1.25
1	A	38	LEU	N-CA	-6.24	1.38	1.46
1	D	406	ARG	N-CA	6.24	1.50	1.46
1	D	427	GLY	N-CA	6.15	1.54	1.45

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	362	ARG	N-CA-C	10.78	123.03	111.28
1	F	74	GLY	N-CA-C	-9.82	102.03	112.04
1	A	80	GLY	N-CA-C	-9.72	96.56	110.75
1	E	80	GLY	N-CA-C	-9.62	99.36	112.25
1	F	131	PHE	N-CA-C	9.46	121.60	111.28

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	3329	0	3283	69	0
1	B	3347	0	3303	67	0
1	C	3274	0	3126	64	0
1	D	3324	0	3234	66	1
1	E	3334	0	3295	77	0
1	F	3350	0	3334	70	1
2	A	18	0	24	2	0
2	B	12	0	16	2	0
2	C	6	0	8	6	0
2	D	36	0	48	3	0
2	E	30	0	40	0	0
2	F	24	0	32	0	0
3	A	8	0	12	3	0
3	B	16	0	24	1	0
3	C	4	0	6	0	0
3	D	8	0	12	0	0
3	F	8	0	12	1	0
4	A	49	0	0	0	0
4	B	28	0	0	0	0
4	C	19	0	0	0	0
4	D	38	0	0	0	0
4	E	56	0	0	0	0
4	F	40	0	0	0	0
All	All	20358	0	19809	390	1

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 10.

The worst 5 of 390 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:191:GLU:OE1	1:A:206:ARG:NH1	1.63	1.32
1:F:394:LYS:NZ	1:F:422:GLU:OE2	1.65	1.29
1:B:325:ARG:O	1:B:358:ARG:NH2	1.76	1.18
1:D:206:ARG:NH1	1:D:287:ASP:OD2	1.78	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ARG:HH12	1:A:388:THR:HB	0.97	1.13

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:GLY:O	1:F:121:LEU:O[2_356]	2.17	0.03

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	435/505 (86%)	426 (98%)	9 (2%)	0	100	100
1	B	433/505 (86%)	423 (98%)	9 (2%)	1 (0%)	43	68
1	C	434/505 (86%)	428 (99%)	6 (1%)	0	100	100
1	D	434/505 (86%)	423 (98%)	11 (2%)	0	100	100
1	E	434/505 (86%)	426 (98%)	7 (2%)	1 (0%)	43	68
1	F	434/505 (86%)	425 (98%)	9 (2%)	0	100	100
All	All	2604/3030 (86%)	2551 (98%)	51 (2%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	75	ASP
1	B	407	PRO

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	348/447 (78%)	325 (93%)	23 (7%)	15	36
1	B	351/447 (78%)	328 (93%)	23 (7%)	15	36
1	C	328/447 (73%)	306 (93%)	22 (7%)	15	36
1	D	340/447 (76%)	322 (95%)	18 (5%)	20	46
1	E	350/447 (78%)	334 (95%)	16 (5%)	24	51
1	F	352/447 (79%)	329 (94%)	23 (6%)	15	37
All	All	2069/2682 (77%)	1944 (94%)	125 (6%)	17	41

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	231	LEU
1	F	200	ILE
1	D	53	LEU
1	F	192	ILE
1	F	357	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	180	ASN
1	E	104	GLN
1	F	348	HIS
1	E	370	ASN
1	F	69	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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	D	603	-	5,5,5	0.62	0	5,5,5	0.81	0
3	EDO	F	605	-	3,3,3	0.78	0	2,2,2	0.13	0
2	GOL	E	603	-	5,5,5	0.74	0	5,5,5	0.33	0
2	GOL	A	603	-	5,5,5	0.82	0	5,5,5	0.64	0
2	GOL	E	601	-	5,5,5	0.57	0	5,5,5	0.39	0
3	EDO	F	606	-	3,3,3	0.65	0	2,2,2	0.19	0
2	GOL	F	602	-	5,5,5	0.88	0	5,5,5	0.81	0
2	GOL	D	601	-	5,5,5	0.28	0	5,5,5	0.41	0
3	EDO	D	608	-	3,3,3	0.74	0	2,2,2	0.31	0
2	GOL	E	604	-	5,5,5	0.88	0	5,5,5	0.97	0
3	EDO	B	605	-	3,3,3	0.58	0	2,2,2	0.72	0
3	EDO	A	605	-	3,3,3	0.69	0	2,2,2	0.10	0
2	GOL	E	602	-	5,5,5	0.44	0	5,5,5	0.58	0
3	EDO	B	603	-	3,3,3	0.58	0	2,2,2	0.32	0
2	GOL	D	605	-	5,5,5	0.45	0	5,5,5	0.32	0
2	GOL	A	602	-	5,5,5	0.73	0	5,5,5	0.63	0
2	GOL	E	605	-	5,5,5	0.80	0	5,5,5	0.78	0
3	EDO	D	607	-	3,3,3	0.50	0	2,2,2	0.31	0
2	GOL	F	603	-	5,5,5	0.77	0	5,5,5	0.52	0
2	GOL	D	606	-	5,5,5	0.73	0	5,5,5	0.27	0
3	EDO	C	602	-	3,3,3	0.58	0	2,2,2	0.34	0
2	GOL	D	602	-	5,5,5	0.86	0	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	604	-	3,3,3	0.63	0	2,2,2	0.16	0
3	EDO	A	604	-	3,3,3	0.62	0	2,2,2	0.30	0
2	GOL	F	604	-	5,5,5	0.83	0	5,5,5	0.58	0
2	GOL	F	601	-	5,5,5	0.53	0	5,5,5	1.05	1 (20%)
2	GOL	B	602	-	5,5,5	0.81	0	5,5,5	0.74	0
2	GOL	B	601	-	5,5,5	0.19	0	5,5,5	1.12	1 (20%)
2	GOL	C	601	-	5,5,5	0.50	0	5,5,5	0.86	0
2	GOL	A	601	-	5,5,5	0.39	0	5,5,5	0.90	0
3	EDO	B	606	-	3,3,3	0.51	0	2,2,2	0.16	0
2	GOL	D	604	-	5,5,5	0.76	0	5,5,5	0.76	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	D	603	-	-	0/4/4/4	-
3	EDO	F	605	-	-	0/1/1/1	-
2	GOL	E	603	-	-	4/4/4/4	-
2	GOL	A	603	-	-	3/4/4/4	-
2	GOL	E	601	-	-	2/4/4/4	-
3	EDO	F	606	-	-	1/1/1/1	-
2	GOL	F	602	-	-	4/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-
3	EDO	D	608	-	-	1/1/1/1	-
2	GOL	E	604	-	-	1/4/4/4	-
3	EDO	B	605	-	-	1/1/1/1	-
3	EDO	A	605	-	-	1/1/1/1	-
2	GOL	E	602	-	-	2/4/4/4	-
3	EDO	B	603	-	-	0/1/1/1	-
2	GOL	D	605	-	-	0/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	E	605	-	-	2/4/4/4	-
3	EDO	D	607	-	-	1/1/1/1	-
2	GOL	F	603	-	-	4/4/4/4	-
2	GOL	D	606	-	-	2/4/4/4	-
3	EDO	C	602	-	-	0/1/1/1	-
2	GOL	D	602	-	-	2/4/4/4	-
3	EDO	B	604	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	604	-	-	1/1/1/1	-
2	GOL	F	604	-	-	1/4/4/4	-
2	GOL	F	601	-	-	2/4/4/4	-
2	GOL	B	602	-	-	2/4/4/4	-
2	GOL	B	601	-	-	4/4/4/4	-
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	A	601	-	-	4/4/4/4	-
3	EDO	B	606	-	-	1/1/1/1	-
2	GOL	D	604	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	GOL	O2-C2-C1	2.15	118.08	109.18
2	B	601	GOL	O3-C3-C2	2.10	119.85	110.38

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	C1-C2-C3-O3
2	A	602	GOL	O1-C1-C2-C3
2	A	603	GOL	C1-C2-C3-O3
2	B	601	GOL	O1-C1-C2-C3
2	B	601	GOL	C1-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	605	EDO	1	0
3	B	605	EDO	1	0
3	A	605	EDO	1	0
2	D	605	GOL	1	0
3	A	604	EDO	2	0
2	B	601	GOL	2	0
2	C	601	GOL	6	0
2	A	601	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	604	GOL	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](#)

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	437/505 (86%)	0.01	6 (1%) 73 72	44, 72, 130, 185	0
1	B	435/505 (86%)	0.11	3 (0%) 84 83	47, 81, 147, 192	0
1	C	436/505 (86%)	0.25	9 (2%) 63 61	58, 95, 147, 179	0
1	D	436/505 (86%)	0.09	9 (2%) 63 61	40, 86, 136, 163	0
1	E	436/505 (86%)	-0.05	4 (0%) 81 80	42, 71, 143, 213	0
1	F	436/505 (86%)	-0.01	6 (1%) 73 72	42, 74, 127, 162	0
All	All	2616/3030 (86%)	0.06	37 (1%) 73 72	40, 80, 139, 213	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	374	THR	4.3
1	F	126	SER	3.7
1	B	155	ASN	3.4
1	E	403	ASP	3.3
1	A	184	LEU	3.2

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 ⓘ

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	D	602	6/6	0.51	0.11	107,109,114,119	0
2	GOL	B	601	6/6	0.64	0.17	86,88,91,109	0
3	EDO	C	602	4/4	0.65	0.19	89,96,100,103	0
3	EDO	A	604	4/4	0.68	0.12	83,85,85,89	0
2	GOL	C	601	6/6	0.69	0.19	73,77,86,99	0
3	EDO	B	606	4/4	0.73	0.10	90,97,100,105	0
2	GOL	E	604	6/6	0.74	0.20	96,105,111,114	0
2	GOL	A	603	6/6	0.77	0.13	86,94,102,102	0
2	GOL	F	604	6/6	0.78	0.19	86,104,111,111	0
2	GOL	B	602	6/6	0.78	0.16	85,91,95,98	0
2	GOL	D	601	6/6	0.79	0.17	83,87,90,91	0
2	GOL	F	601	6/6	0.79	0.14	71,80,84,88	0
2	GOL	F	602	6/6	0.80	0.14	74,88,93,95	0
2	GOL	A	601	6/6	0.81	0.17	63,74,82,95	0
2	GOL	F	603	6/6	0.81	0.09	95,101,103,107	0
3	EDO	D	607	4/4	0.81	0.17	92,92,93,94	0
3	EDO	B	604	4/4	0.82	0.09	88,90,91,93	0
2	GOL	E	603	6/6	0.82	0.13	93,95,104,105	0
2	GOL	D	605	6/6	0.83	0.14	97,103,111,111	0
2	GOL	A	602	6/6	0.84	0.10	94,103,108,109	0
2	GOL	D	603	6/6	0.84	0.11	96,101,105,108	0
3	EDO	F	606	4/4	0.84	0.17	78,84,89,90	0
2	GOL	D	604	6/6	0.85	0.12	70,86,94,95	0
2	GOL	D	606	6/6	0.86	0.11	88,101,104,106	0
2	GOL	E	605	6/6	0.86	0.17	78,90,92,97	0
3	EDO	D	608	4/4	0.87	0.12	73,82,84,85	0
2	GOL	E	602	6/6	0.88	0.12	96,102,105,106	0
3	EDO	B	605	4/4	0.89	0.15	67,75,76,76	0
3	EDO	F	605	4/4	0.89	0.16	72,79,81,84	0
2	GOL	E	601	6/6	0.89	0.13	64,79,86,88	0
3	EDO	A	605	4/4	0.90	0.15	68,75,77,81	0
3	EDO	B	603	4/4	0.90	0.15	70,72,75,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.