



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:02 AM UTC

PDB ID : 2Q4R / pdb_00002q4r
Title : Ensemble refinement of the protein crystal structure of human phosphomannomutase 2 (PMM2)
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 2.09 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

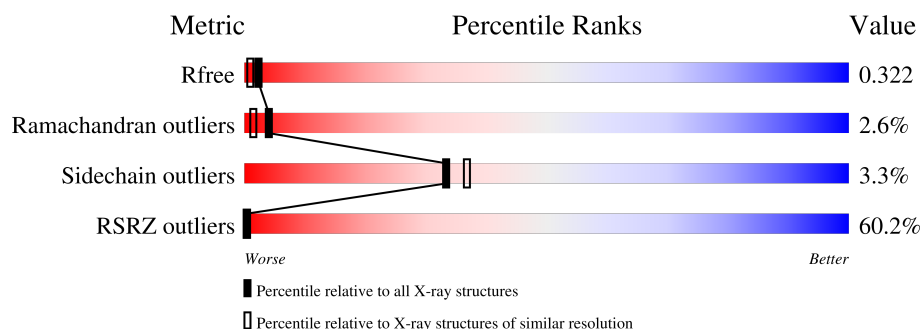
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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.



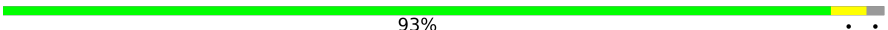
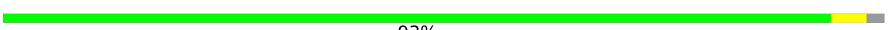
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	1-A	246	58% 93% 6% • •
1	10-A	246	92% 6% •
1	11-A	246	93% 5% •
1	12-A	246	93% 5% •
1	13-A	246	91% 7% •
1	14-A	246	93% 5% •
1	15-A	246	92% 6% •

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Mol	Chain	Length	Quality of chain
1	16-A	246	 93% . .
1	2-A	246	 92% 6% .
1	3-A	246	 93% . .
1	4-A	246	 93% . .
1	5-A	246	 91% 7% .
1	6-A	246	 93% . .
1	7-A	246	 91% 7% .
1	8-A	246	 90% 8% .
1	9-A	246	 93% 5% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33616 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.

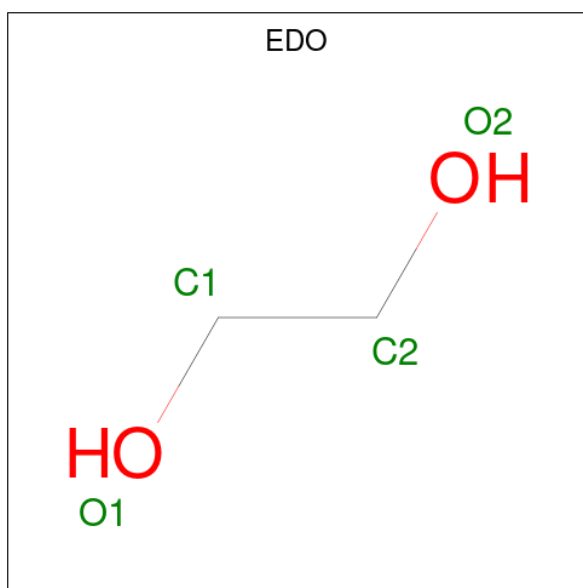
- Molecule 1 is a protein called Phosphomannomutase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	2-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	3-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	4-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	5-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	6-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	7-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	8-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	9-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	10-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	11-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	12-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	13-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	14-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	15-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0
1	16-A	240	Total 1943	C 1239	N 330	O 364	S 6	Se 4	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP O15305
A	28	MSE	MET	modified residue	UNP O15305
A	126	MSE	MET	modified residue	UNP O15305
A	212	MSE	MET	modified residue	UNP O15305
A	227	MSE	MET	modified residue	UNP O15305

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



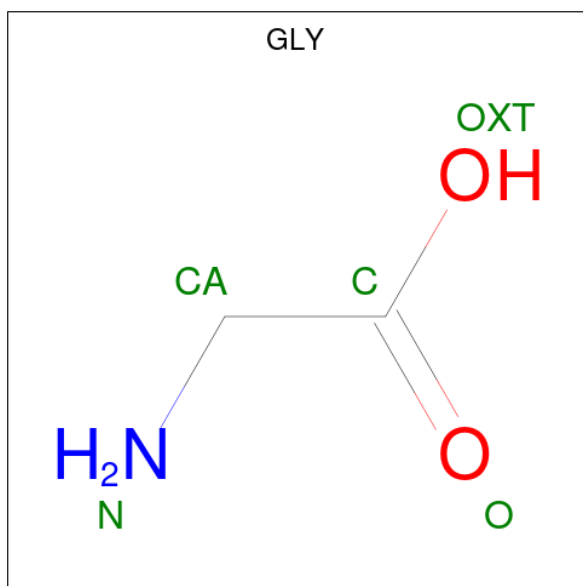
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	1	Total C O 4 2 2	0	0
2	2-A	1	Total C O 4 2 2	0	0
2	3-A	1	Total C O 4 2 2	0	0
2	4-A	1	Total C O 4 2 2	0	0
2	5-A	1	Total C O 4 2 2	0	0
2	6-A	1	Total C O 4 2 2	0	0
2	7-A	1	Total C O 4 2 2	0	0
2	8-A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	9-A	1	Total C O 4 2 2	0	0
2	10-A	1	Total C O 4 2 2	0	0
2	11-A	1	Total C O 4 2 2	0	0
2	12-A	1	Total C O 4 2 2	0	0
2	13-A	1	Total C O 4 2 2	0	0
2	14-A	1	Total C O 4 2 2	0	0
2	15-A	1	Total C O 4 2 2	0	0
2	16-A	1	Total C O 4 2 2	0	0

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	4-A	1	Total 4	C 2	N 1	O 1	0	0
3	5-A	1	Total 4	C 2	N 1	O 1	0	0
3	6-A	1	Total 4	C 2	N 1	O 1	0	0
3	7-A	1	Total 4	C 2	N 1	O 1	0	0
3	8-A	1	Total 4	C 2	N 1	O 1	0	0
3	9-A	1	Total 4	C 2	N 1	O 1	0	0
3	10-A	1	Total 4	C 2	N 1	O 1	0	0
3	11-A	1	Total 4	C 2	N 1	O 1	0	0
3	12-A	1	Total 4	C 2	N 1	O 1	0	0
3	13-A	1	Total 4	C 2	N 1	O 1	0	0
3	14-A	1	Total 4	C 2	N 1	O 1	0	0
3	15-A	1	Total 4	C 2	N 1	O 1	0	0
3	16-A	1	Total 4	C 2	N 1	O 1	0	0
3	1-A	1	Total 4	C 2	N 1	O 1	0	0
3	2-A	1	Total 4	C 2	N 1	O 1	0	0
3	3-A	1	Total 4	C 2	N 1	O 1	0	0
3	4-A	1	Total 4	C 2	N 1	O 1	0	0
3	5-A	1	Total 4	C 2	N 1	O 1	0	0
3	6-A	1	Total 4	C 2	N 1	O 1	0	0
3	7-A	1	Total 4	C 2	N 1	O 1	0	0
3	8-A	1	Total 4	C 2	N 1	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	9-A	1	Total 4	C 2	N 1	O 1	0	0
3	10-A	1	Total 4	C 2	N 1	O 1	0	0
3	11-A	1	Total 4	C 2	N 1	O 1	0	0
3	12-A	1	Total 4	C 2	N 1	O 1	0	0
3	13-A	1	Total 4	C 2	N 1	O 1	0	0
3	14-A	1	Total 4	C 2	N 1	O 1	0	0
3	15-A	1	Total 4	C 2	N 1	O 1	0	0
3	16-A	1	Total 4	C 2	N 1	O 1	0	0
3	1-A	1	Total 4	C 2	N 1	O 1	0	0
3	2-A	1	Total 4	C 2	N 1	O 1	0	0
3	3-A	1	Total 4	C 2	N 1	O 1	0	0
3	4-A	1	Total 4	C 2	N 1	O 1	0	0
3	5-A	1	Total 4	C 2	N 1	O 1	0	0
3	6-A	1	Total 4	C 2	N 1	O 1	0	0
3	7-A	1	Total 4	C 2	N 1	O 1	0	0
3	8-A	1	Total 4	C 2	N 1	O 1	0	0
3	9-A	1	Total 4	C 2	N 1	O 1	0	0
3	10-A	1	Total 4	C 2	N 1	O 1	0	0
3	11-A	1	Total 4	C 2	N 1	O 1	0	0
3	12-A	1	Total 4	C 2	N 1	O 1	0	0
3	13-A	1	Total 4	C 2	N 1	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	14-A	1	Total 4	C 2	N 1	O 1	0	0
3	15-A	1	Total 4	C 2	N 1	O 1	0	0
3	16-A	1	Total 4	C 2	N 1	O 1	0	0

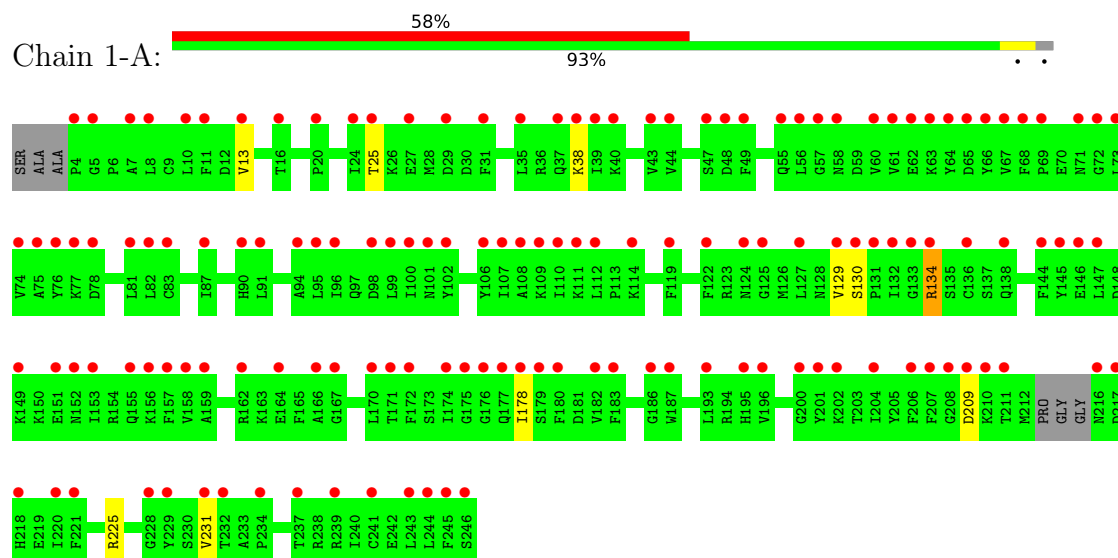
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	142	Total 142	O 142	0	0
4	2-A	142	Total 142	O 142	0	0
4	3-A	142	Total 142	O 142	0	0
4	4-A	142	Total 142	O 142	0	0
4	5-A	142	Total 142	O 142	0	0
4	6-A	142	Total 142	O 142	0	0
4	7-A	142	Total 142	O 142	0	0
4	8-A	142	Total 142	O 142	0	0
4	9-A	142	Total 142	O 142	0	0
4	10-A	142	Total 142	O 142	0	0
4	11-A	142	Total 142	O 142	0	0
4	12-A	142	Total 142	O 142	0	0
4	13-A	142	Total 142	O 142	0	0
4	14-A	142	Total 142	O 142	0	0
4	15-A	142	Total 142	O 142	0	0
4	16-A	142	Total 142	O 142	0	0

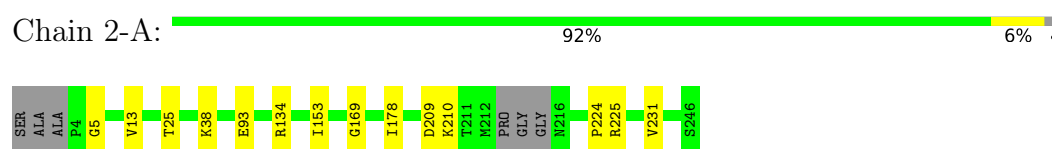
3 Residue-property plots

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.

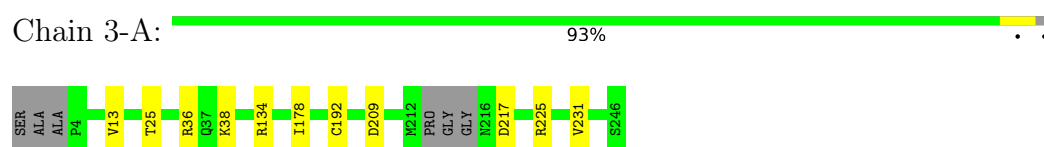
• Molecule 1: Phosphomannomutase 2



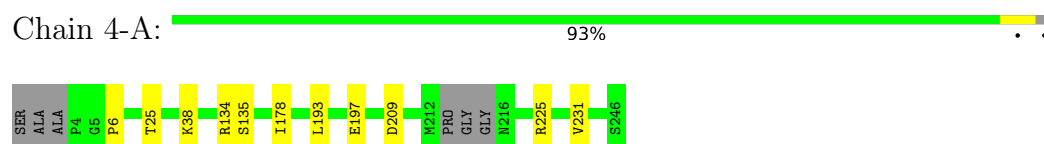
• Molecule 1: Phosphomannomutase 2



• Molecule 1: Phosphomannomutase 2



• Molecule 1: Phosphomannomutase 2

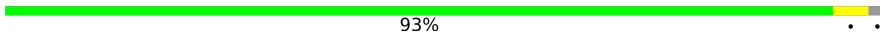


- Molecule 1: Phosphomannomutase 2

Chain 5-A:  91% 7% .



- Molecule 1: Phosphomannomutase 2

Chain 6-A:  93% . .



- Molecule 1: Phosphomannomutase 2

Chain 7-A:  91% 7% .



- Molecule 1: Phosphomannomutase 2

Chain 8-A:  90% 8% .

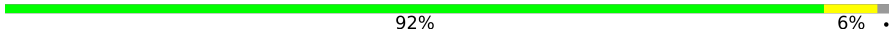


- Molecule 1: Phosphomannomutase 2

Chain 9-A:  93% 5% .



- Molecule 1: Phosphomannomutase 2

Chain 10-A:  92% 6% .



- Molecule 1: Phosphomannomutase 2

Chain 11-A:  93% 5% .



- Molecule 1: Phosphomannomutase 2

Chain 12-A:  93% 5% .



• Molecule 1: Phosphomannomutase 2

Chain 13-A:  91% 7% .



• Molecule 1: Phosphomannomutase 2

Chain 14-A:  93% 5% .

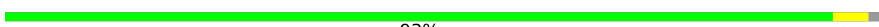


• Molecule 1: Phosphomannomutase 2

Chain 15-A:  92% 6% .



• Molecule 1: Phosphomannomutase 2

Chain 16-A:  93% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.62Å 70.62Å 100.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.58 – 2.09 30.58 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.58-2.09) 99.5 (30.58-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.298 0.237 , 0.322	Depositor DCC
R_{free} test set	924 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	33616	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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

5.1 Standard geometry

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	1-A	0.17	0/1977	0.37	0/2646
1	2-A	0.17	0/1977	0.37	0/2646
1	3-A	0.17	0/1977	0.37	0/2646
1	4-A	0.17	0/1977	0.37	0/2646
1	5-A	0.17	0/1977	0.37	0/2646
1	6-A	0.17	0/1977	0.37	0/2646
1	7-A	0.17	0/1977	0.37	0/2646
1	8-A	0.17	0/1977	0.37	0/2646
1	9-A	0.17	0/1977	0.37	0/2646
1	10-A	0.17	0/1977	0.37	0/2646
1	11-A	0.17	0/1977	0.37	0/2646
1	12-A	0.17	0/1977	0.37	0/2646
1	13-A	0.17	0/1977	0.37	0/2646
1	14-A	0.17	0/1977	0.37	0/2646
1	15-A	0.17	0/1977	0.37	0/2646
1	16-A	0.17	0/1977	0.37	0/2646
All	All	0.17	0/31632	0.37	0/42336

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

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	1-A	1943	0	1930	0	0
1	2-A	1943	0	1930	0	0
1	3-A	1943	0	1930	0	0
1	4-A	1943	0	1930	0	0
1	5-A	1943	0	1930	0	0
1	6-A	1943	0	1930	0	0
1	7-A	1943	0	1930	0	0
1	8-A	1943	0	1930	0	0
1	9-A	1943	0	1930	0	0
1	10-A	1943	0	1930	0	0
1	11-A	1943	0	1930	0	0
1	12-A	1943	0	1930	0	0
1	13-A	1943	0	1930	0	0
1	14-A	1943	0	1930	0	0
1	15-A	1943	0	1930	0	0
1	16-A	1943	0	1930	0	0
2	1-A	4	0	6	0	0
2	2-A	4	0	6	0	0
2	3-A	4	0	6	0	0
2	4-A	4	0	6	0	0
2	5-A	4	0	6	0	0
2	6-A	4	0	6	0	0
2	7-A	4	0	6	0	0
2	8-A	4	0	6	0	0
2	9-A	4	0	6	0	0
2	10-A	4	0	6	0	0
2	11-A	4	0	6	0	0
2	12-A	4	0	6	0	0
2	13-A	4	0	6	0	0
2	14-A	4	0	6	0	0
2	15-A	4	0	6	0	0
2	16-A	4	0	6	0	0
3	1-A	12	0	6	0	0
3	2-A	12	0	6	0	0
3	3-A	12	0	6	0	0
3	4-A	12	0	6	0	0
3	5-A	12	0	6	0	0
3	6-A	12	0	6	0	0
3	7-A	12	0	6	0	0
3	8-A	12	0	6	0	0
3	9-A	12	0	6	0	0
3	10-A	12	0	6	0	0
3	11-A	12	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	12-A	12	0	6	0	0
3	13-A	12	0	6	0	0
3	14-A	12	0	6	0	0
3	15-A	12	0	6	0	0
3	16-A	12	0	6	0	0
4	1-A	142	0	0	0	0
4	2-A	142	0	0	0	0
4	3-A	142	0	0	0	0
4	4-A	142	0	0	0	0
4	5-A	142	0	0	0	0
4	6-A	142	0	0	0	0
4	7-A	142	0	0	0	0
4	8-A	142	0	0	0	0
4	9-A	142	0	0	0	0
4	10-A	142	0	0	0	0
4	11-A	142	0	0	0	0
4	12-A	142	0	0	0	0
4	13-A	142	0	0	0	0
4	14-A	142	0	0	0	0
4	15-A	142	0	0	0	0
4	16-A	142	0	0	0	0
All	All	33616	0	31072	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	236/246 (96%)	208 (88%)	24 (10%)	4 (2%)	7 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-A	236/246 (96%)	210 (89%)	19 (8%)	7 (3%)	3	1
1	3-A	236/246 (96%)	215 (91%)	17 (7%)	4 (2%)	7	3
1	4-A	236/246 (96%)	202 (86%)	30 (13%)	4 (2%)	7	3
1	5-A	236/246 (96%)	200 (85%)	26 (11%)	10 (4%)	2	0
1	6-A	236/246 (96%)	214 (91%)	19 (8%)	3 (1%)	9	6
1	7-A	236/246 (96%)	190 (80%)	37 (16%)	9 (4%)	2	1
1	8-A	236/246 (96%)	193 (82%)	31 (13%)	12 (5%)	1	0
1	9-A	236/246 (96%)	204 (86%)	27 (11%)	5 (2%)	5	2
1	10-A	236/246 (96%)	201 (85%)	28 (12%)	7 (3%)	3	1
1	11-A	236/246 (96%)	204 (86%)	27 (11%)	5 (2%)	5	2
1	12-A	236/246 (96%)	214 (91%)	17 (7%)	5 (2%)	5	2
1	13-A	236/246 (96%)	203 (86%)	24 (10%)	9 (4%)	2	1
1	14-A	236/246 (96%)	205 (87%)	26 (11%)	5 (2%)	5	2
1	15-A	236/246 (96%)	210 (89%)	19 (8%)	7 (3%)	3	1
1	16-A	236/246 (96%)	207 (88%)	26 (11%)	3 (1%)	9	6
All	All	3776/3936 (96%)	3280 (87%)	397 (10%)	99 (3%)	4	1

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	130	SER
1	5-A	39	ILE
1	5-A	193	LEU
1	7-A	163	LYS
1	8-A	21	ARG
1	8-A	136	CYS
1	10-A	89	SER
1	13-A	60	VAL
1	13-A	138	GLN
1	14-A	39	ILE
1	14-A	60	VAL
1	15-A	82	LEU
1	15-A	135	SER
1	1-A	134	ARG
1	4-A	6	PRO
1	4-A	193	LEU
1	5-A	13	VAL

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Mol	Chain	Res	Type
1	5-A	169	GLY
1	5-A	192	CYS
1	6-A	79	GLY
1	6-A	210	LYS
1	7-A	92	GLY
1	7-A	107	ILE
1	7-A	166	ALA
1	7-A	217	ASP
1	8-A	13	VAL
1	8-A	89	SER
1	8-A	217	ASP
1	8-A	228	GLY
1	9-A	5	GLY
1	10-A	180	PHE
1	11-A	13	VAL
1	11-A	21	ARG
1	12-A	201	TYR
1	13-A	135	SER
1	13-A	244	LEU
1	14-A	197	GLU
1	16-A	13	VAL
1	16-A	197	GLU
1	2-A	5	GLY
1	2-A	210	LYS
1	3-A	217	ASP
1	4-A	135	SER
1	5-A	21	ARG
1	5-A	200	GLY
1	7-A	82	LEU
1	8-A	6	PRO
1	8-A	180	PHE
1	10-A	217	ASP
1	12-A	217	ASP
1	13-A	136	CYS
1	13-A	243	LEU
1	14-A	210	LYS
1	14-A	217	ASP
1	15-A	210	LYS
1	16-A	217	ASP
1	1-A	13	VAL
1	2-A	93	GLU
1	3-A	13	VAL

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Mol	Chain	Res	Type
1	3-A	36	ARG
1	4-A	197	GLU
1	5-A	58	ASN
1	5-A	83	CYS
1	5-A	217	ASP
1	7-A	210	LYS
1	8-A	36	ARG
1	8-A	174	ILE
1	9-A	217	ASP
1	11-A	79	GLY
1	12-A	21	ARG
1	13-A	6	PRO
1	13-A	199	ASP
1	15-A	58	ASN
1	15-A	136	CYS
1	2-A	13	VAL
1	3-A	192	CYS
1	7-A	108	ALA
1	8-A	20	PRO
1	10-A	58	ASN
1	10-A	82	LEU
1	11-A	20	PRO
1	12-A	20	PRO
1	13-A	13	VAL
1	1-A	129	VAL
1	8-A	165	PHE
1	10-A	13	VAL
1	12-A	13	VAL
1	2-A	153	ILE
1	2-A	169	GLY
1	6-A	13	VAL
1	9-A	72	GLY
1	15-A	13	VAL
1	15-A	60	VAL
1	9-A	13	VAL
1	10-A	174	ILE
1	2-A	224	PRO
1	7-A	153	ILE
1	9-A	79	GLY
1	11-A	233	ALA

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	1-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	2-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	3-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	4-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	5-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	6-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	7-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	8-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	9-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	10-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	11-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	12-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	13-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	14-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	15-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
1	16-A	212/210 (101%)	205 (97%)	7 (3%)	33	37
All	All	3392/3360 (101%)	3280 (97%)	112 (3%)	33	37

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	25	THR
1	1-A	38	LYS
1	1-A	134	ARG
1	1-A	178	ILE
1	1-A	209	ASP
1	1-A	225	ARG
1	1-A	231	VAL
1	2-A	25	THR

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Mol	Chain	Res	Type
1	2-A	38	LYS
1	2-A	134	ARG
1	2-A	178	ILE
1	2-A	209	ASP
1	2-A	225	ARG
1	2-A	231	VAL
1	3-A	25	THR
1	3-A	38	LYS
1	3-A	134	ARG
1	3-A	178	ILE
1	3-A	209	ASP
1	3-A	225	ARG
1	3-A	231	VAL
1	4-A	25	THR
1	4-A	38	LYS
1	4-A	134	ARG
1	4-A	178	ILE
1	4-A	209	ASP
1	4-A	225	ARG
1	4-A	231	VAL
1	5-A	25	THR
1	5-A	38	LYS
1	5-A	134	ARG
1	5-A	178	ILE
1	5-A	209	ASP
1	5-A	225	ARG
1	5-A	231	VAL
1	6-A	25	THR
1	6-A	38	LYS
1	6-A	134	ARG
1	6-A	178	ILE
1	6-A	209	ASP
1	6-A	225	ARG
1	6-A	231	VAL
1	7-A	25	THR
1	7-A	38	LYS
1	7-A	134	ARG
1	7-A	178	ILE
1	7-A	209	ASP
1	7-A	225	ARG
1	7-A	231	VAL
1	8-A	25	THR

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Mol	Chain	Res	Type
1	8-A	38	LYS
1	8-A	134	ARG
1	8-A	178	ILE
1	8-A	209	ASP
1	8-A	225	ARG
1	8-A	231	VAL
1	9-A	25	THR
1	9-A	38	LYS
1	9-A	134	ARG
1	9-A	178	ILE
1	9-A	209	ASP
1	9-A	225	ARG
1	9-A	231	VAL
1	10-A	25	THR
1	10-A	38	LYS
1	10-A	134	ARG
1	10-A	178	ILE
1	10-A	209	ASP
1	10-A	225	ARG
1	10-A	231	VAL
1	11-A	25	THR
1	11-A	38	LYS
1	11-A	134	ARG
1	11-A	178	ILE
1	11-A	209	ASP
1	11-A	225	ARG
1	11-A	231	VAL
1	12-A	25	THR
1	12-A	38	LYS
1	12-A	134	ARG
1	12-A	178	ILE
1	12-A	209	ASP
1	12-A	225	ARG
1	12-A	231	VAL
1	13-A	25	THR
1	13-A	38	LYS
1	13-A	134	ARG
1	13-A	178	ILE
1	13-A	209	ASP
1	13-A	225	ARG
1	13-A	231	VAL
1	14-A	25	THR

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Mol	Chain	Res	Type
1	14-A	38	LYS
1	14-A	134	ARG
1	14-A	178	ILE
1	14-A	209	ASP
1	14-A	225	ARG
1	14-A	231	VAL
1	15-A	25	THR
1	15-A	38	LYS
1	15-A	134	ARG
1	15-A	178	ILE
1	15-A	209	ASP
1	15-A	225	ARG
1	15-A	231	VAL
1	16-A	25	THR
1	16-A	38	LYS
1	16-A	134	ARG
1	16-A	178	ILE
1	16-A	209	ASP
1	16-A	225	ARG
1	16-A	231	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	138	GLN
1	2-A	71	ASN
1	2-A	152	ASN
1	3-A	33	GLN
1	3-A	55	GLN
1	3-A	138	GLN
1	3-A	218	HIS
1	4-A	55	GLN
1	4-A	138	GLN
1	5-A	53	GLN
1	5-A	138	GLN
1	5-A	198	ASN
1	5-A	218	HIS
1	6-A	22	GLN
1	6-A	55	GLN
1	6-A	138	GLN
1	6-A	152	ASN
1	7-A	37	GLN

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Mol	Chain	Res	Type
1	7-A	55	GLN
1	7-A	97	GLN
1	7-A	101	ASN
1	7-A	152	ASN
1	7-A	177	GLN
1	8-A	22	GLN
1	8-A	37	GLN
1	8-A	55	GLN
1	8-A	58	ASN
1	8-A	97	GLN
1	8-A	101	ASN
1	8-A	124	ASN
1	8-A	138	GLN
1	8-A	218	HIS
1	9-A	90	HIS
1	9-A	138	GLN
1	9-A	218	HIS
1	10-A	55	GLN
1	10-A	97	GLN
1	10-A	101	ASN
1	10-A	138	GLN
1	10-A	152	ASN
1	10-A	195	HIS
1	11-A	58	ASN
1	11-A	97	GLN
1	11-A	101	ASN
1	11-A	216	ASN
1	12-A	71	ASN
1	12-A	90	HIS
1	12-A	152	ASN
1	12-A	218	HIS
1	13-A	152	ASN
1	13-A	198	ASN
1	14-A	85	GLN
1	14-A	138	GLN
1	15-A	22	GLN
1	15-A	37	GLN
1	15-A	90	HIS
1	15-A	216	ASN
1	16-A	22	GLN
1	16-A	90	HIS
1	16-A	138	GLN

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Mol	Chain	Res	Type
1	16-A	218	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

64 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	$\# Z > 2$
3	GLY	6-A	400	-	3,3,4	0.64	0	1,2,4	0.33	0
3	GLY	10-A	400	-	3,3,4	0.67	0	1,2,4	0.32	0
2	EDO	16-A	300	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	1-A	300	-	3,3,3	0.44	0	2,2,2	0.36	0
2	EDO	15-A	300	-	3,3,3	0.45	0	2,2,2	0.37	0
3	GLY	7-A	402	-	3,3,4	0.65	0	1,2,4	0.23	0
3	GLY	11-A	402	-	3,3,4	0.64	0	1,2,4	0.32	0
2	EDO	13-A	300	-	3,3,3	0.45	0	2,2,2	0.36	0
3	GLY	15-A	402	-	3,3,4	0.66	0	1,2,4	0.29	0
2	EDO	3-A	300	-	3,3,3	0.45	0	2,2,2	0.37	0
3	GLY	16-A	401	-	3,3,4	0.52	0	1,2,4	0.51	0
3	GLY	11-A	401	-	3,3,4	0.54	0	1,2,4	0.48	0
3	GLY	8-A	402	-	3,3,4	0.65	0	1,2,4	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLY	12-A	402	-	3,3,4	0.64	0	1,2,4	0.31	0
3	GLY	1-A	400	-	3,3,4	0.64	0	1,2,4	0.31	0
3	GLY	16-A	402	-	3,3,4	0.65	0	1,2,4	0.30	0
3	GLY	8-A	401	-	3,3,4	0.54	0	1,2,4	0.51	0
3	GLY	9-A	401	-	3,3,4	0.54	0	1,2,4	0.46	0
2	EDO	4-A	300	-	3,3,3	0.45	0	2,2,2	0.37	0
3	GLY	5-A	401	-	3,3,4	0.52	0	1,2,4	0.50	0
3	GLY	5-A	402	-	3,3,4	0.64	0	1,2,4	0.31	0
3	GLY	15-A	400	-	3,3,4	0.66	0	1,2,4	0.32	0
3	GLY	6-A	402	-	3,3,4	0.64	0	1,2,4	0.32	0
3	GLY	12-A	400	-	3,3,4	0.64	0	1,2,4	0.35	0
3	GLY	7-A	401	-	3,3,4	0.52	0	1,2,4	0.52	0
3	GLY	4-A	402	-	3,3,4	0.65	0	1,2,4	0.32	0
2	EDO	14-A	300	-	3,3,3	0.45	0	2,2,2	0.36	0
3	GLY	3-A	401	-	3,3,4	0.53	0	1,2,4	0.49	0
3	GLY	14-A	400	-	3,3,4	0.65	0	1,2,4	0.32	0
3	GLY	3-A	402	-	3,3,4	0.63	0	1,2,4	0.31	0
3	GLY	6-A	401	-	3,3,4	0.53	0	1,2,4	0.49	0
3	GLY	9-A	402	-	3,3,4	0.63	0	1,2,4	0.31	0
3	GLY	2-A	402	-	3,3,4	0.64	0	1,2,4	0.30	0
3	GLY	1-A	401	-	3,3,4	0.52	0	1,2,4	0.45	0
2	EDO	9-A	300	-	3,3,3	0.45	0	2,2,2	0.38	0
3	GLY	1-A	402	-	3,3,4	0.65	0	1,2,4	0.24	0
3	GLY	2-A	401	-	3,3,4	0.53	0	1,2,4	0.50	0
3	GLY	11-A	400	-	3,3,4	0.64	0	1,2,4	0.31	0
3	GLY	15-A	401	-	3,3,4	0.52	0	1,2,4	0.48	0
2	EDO	8-A	300	-	3,3,3	0.45	0	2,2,2	0.37	0
3	GLY	9-A	400	-	3,3,4	0.64	0	1,2,4	0.31	0
2	EDO	5-A	300	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	6-A	300	-	3,3,3	0.45	0	2,2,2	0.36	0
3	GLY	2-A	400	-	3,3,4	0.63	0	1,2,4	0.35	0
3	GLY	5-A	400	-	3,3,4	0.65	0	1,2,4	0.31	0
3	GLY	8-A	400	-	3,3,4	0.64	0	1,2,4	0.31	0
3	GLY	13-A	402	-	3,3,4	0.64	0	1,2,4	0.29	0
3	GLY	16-A	400	-	3,3,4	0.65	0	1,2,4	0.31	0
2	EDO	12-A	300	-	3,3,3	0.45	0	2,2,2	0.37	0
3	GLY	4-A	400	-	3,3,4	0.63	0	1,2,4	0.30	0
3	GLY	13-A	400	-	3,3,4	0.64	0	1,2,4	0.36	0
2	EDO	7-A	300	-	3,3,3	0.44	0	2,2,2	0.37	0
3	GLY	12-A	401	-	3,3,4	0.53	0	1,2,4	0.46	0
3	GLY	3-A	400	-	3,3,4	0.64	0	1,2,4	0.34	0
3	GLY	7-A	400	-	3,3,4	0.68	0	1,2,4	0.30	0
3	GLY	4-A	401	-	3,3,4	0.53	0	1,2,4	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLY	13-A	401	-	3,3,4	0.50	0	1,2,4	0.65	0
2	EDO	10-A	300	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	11-A	300	-	3,3,3	0.45	0	2,2,2	0.37	0
3	GLY	10-A	401	-	3,3,4	0.52	0	1,2,4	0.54	0
3	GLY	14-A	401	-	3,3,4	0.51	0	1,2,4	0.61	0
3	GLY	10-A	402	-	3,3,4	0.64	0	1,2,4	0.31	0
3	GLY	14-A	402	-	3,3,4	0.65	0	1,2,4	0.29	0
2	EDO	2-A	300	-	3,3,3	0.45	0	2,2,2	0.36	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
3	GLY	6-A	400	-	-	0/0/1/2	-
3	GLY	10-A	400	-	-	0/0/1/2	-
2	EDO	16-A	300	-	-	1/1/1/1	-
2	EDO	1-A	300	-	-	1/1/1/1	-
2	EDO	15-A	300	-	-	1/1/1/1	-
3	GLY	7-A	402	-	-	0/0/1/2	-
3	GLY	11-A	402	-	-	0/0/1/2	-
2	EDO	13-A	300	-	-	1/1/1/1	-
3	GLY	15-A	402	-	-	0/0/1/2	-
2	EDO	3-A	300	-	-	1/1/1/1	-
3	GLY	16-A	401	-	-	0/0/1/2	-
3	GLY	11-A	401	-	-	0/0/1/2	-
3	GLY	8-A	402	-	-	0/0/1/2	-
3	GLY	12-A	402	-	-	0/0/1/2	-
3	GLY	1-A	400	-	-	0/0/1/2	-
3	GLY	16-A	402	-	-	0/0/1/2	-
3	GLY	8-A	401	-	-	0/0/1/2	-
3	GLY	9-A	401	-	-	0/0/1/2	-
2	EDO	4-A	300	-	-	1/1/1/1	-
3	GLY	5-A	401	-	-	0/0/1/2	-
3	GLY	5-A	402	-	-	0/0/1/2	-
3	GLY	15-A	400	-	-	0/0/1/2	-
3	GLY	6-A	402	-	-	0/0/1/2	-
3	GLY	12-A	400	-	-	0/0/1/2	-
3	GLY	7-A	401	-	-	0/0/1/2	-
3	GLY	4-A	402	-	-	0/0/1/2	-
2	EDO	14-A	300	-	-	1/1/1/1	-
3	GLY	3-A	401	-	-	0/0/1/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	14-A	400	-	-	0/0/1/2	-
3	GLY	3-A	402	-	-	0/0/1/2	-
3	GLY	6-A	401	-	-	0/0/1/2	-
3	GLY	9-A	402	-	-	0/0/1/2	-
3	GLY	2-A	402	-	-	0/0/1/2	-
3	GLY	1-A	401	-	-	0/0/1/2	-
2	EDO	9-A	300	-	-	1/1/1/1	-
3	GLY	1-A	402	-	-	0/0/1/2	-
3	GLY	2-A	401	-	-	0/0/1/2	-
3	GLY	11-A	400	-	-	0/0/1/2	-
3	GLY	15-A	401	-	-	0/0/1/2	-
2	EDO	8-A	300	-	-	1/1/1/1	-
3	GLY	9-A	400	-	-	0/0/1/2	-
2	EDO	5-A	300	-	-	1/1/1/1	-
2	EDO	6-A	300	-	-	1/1/1/1	-
3	GLY	2-A	400	-	-	0/0/1/2	-
3	GLY	5-A	400	-	-	0/0/1/2	-
3	GLY	8-A	400	-	-	0/0/1/2	-
3	GLY	13-A	402	-	-	0/0/1/2	-
3	GLY	16-A	400	-	-	0/0/1/2	-
2	EDO	12-A	300	-	-	1/1/1/1	-
3	GLY	4-A	400	-	-	0/0/1/2	-
3	GLY	13-A	400	-	-	0/0/1/2	-
2	EDO	7-A	300	-	-	1/1/1/1	-
3	GLY	12-A	401	-	-	0/0/1/2	-
3	GLY	3-A	400	-	-	0/0/1/2	-
3	GLY	7-A	400	-	-	0/0/1/2	-
3	GLY	4-A	401	-	-	0/0/1/2	-
3	GLY	13-A	401	-	-	0/0/1/2	-
2	EDO	10-A	300	-	-	1/1/1/1	-
2	EDO	11-A	300	-	-	1/1/1/1	-
3	GLY	10-A	401	-	-	0/0/1/2	-
3	GLY	14-A	401	-	-	0/0/1/2	-
3	GLY	10-A	402	-	-	0/0/1/2	-
3	GLY	14-A	402	-	-	0/0/1/2	-
2	EDO	2-A	300	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	5-A	300	EDO	O1-C1-C2-O2
2	1-A	300	EDO	O1-C1-C2-O2
2	2-A	300	EDO	O1-C1-C2-O2
2	4-A	300	EDO	O1-C1-C2-O2
2	7-A	300	EDO	O1-C1-C2-O2
2	8-A	300	EDO	O1-C1-C2-O2
2	9-A	300	EDO	O1-C1-C2-O2
2	10-A	300	EDO	O1-C1-C2-O2
2	12-A	300	EDO	O1-C1-C2-O2
2	14-A	300	EDO	O1-C1-C2-O2
2	15-A	300	EDO	O1-C1-C2-O2
2	16-A	300	EDO	O1-C1-C2-O2
2	3-A	300	EDO	O1-C1-C2-O2
2	6-A	300	EDO	O1-C1-C2-O2
2	11-A	300	EDO	O1-C1-C2-O2
2	13-A	300	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 ⓘ

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	1-A	236/246 (95%)	2.48	142 (60%) 0 0	2, 2, 3, 4	236 (100%)
1	2-A	0/246	-	-	-	-
1	3-A	0/246	-	-	-	-
1	4-A	0/246	-	-	-	-
1	5-A	0/246	-	-	-	-
1	6-A	0/246	-	-	-	-
1	7-A	0/246	-	-	-	-
1	8-A	0/246	-	-	-	-
1	9-A	0/246	-	-	-	-
1	10-A	0/246	-	-	-	-
1	11-A	0/246	-	-	-	-
1	12-A	0/246	-	-	-	-
1	13-A	0/246	-	-	-	-
1	14-A	0/246	-	-	-	-
1	15-A	0/246	-	-	-	-
1	16-A	0/246	-	-	-	-
All	All	236/3936 (5%)	2.48	142 (60%) 0 0	2, 2, 3, 4	236 (100%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	133	GLY	6.7
1	1-A	95	LEU	6.7
1	1-A	196	VAL	6.3
1	1-A	131	PRO	6.1
1	1-A	56	LEU	6.0
1	1-A	76	TYR	5.6
1	1-A	136	CYS	5.3
1	1-A	217	ASP	5.2
1	1-A	158	VAL	5.2
1	1-A	82	LEU	5.0
1	1-A	132	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	1-A	244	LEU	4.9
1	1-A	49	PHE	4.8
1	1-A	90	HIS	4.8
1	1-A	74	VAL	4.7
1	1-A	221	PHE	4.5
1	1-A	156	LYS	4.4
1	1-A	83	CYS	4.4
1	1-A	193	LEU	4.2
1	1-A	60	VAL	4.2
1	1-A	246	SER	4.2
1	1-A	27	GLU	4.1
1	1-A	200	GLY	4.1
1	1-A	25	THR	4.1
1	1-A	69	PRO	4.1
1	1-A	147	LEU	4.1
1	1-A	152	ASN	4.0
1	1-A	167	GLY	4.0
1	1-A	211	THR	3.9
1	1-A	208	GLY	3.9
1	1-A	61	VAL	3.9
1	1-A	47	SER	3.9
1	1-A	73	LEU	3.8
1	1-A	243	LEU	3.8
1	1-A	4	PRO	3.7
1	1-A	157	PHE	3.7
1	1-A	102	TYR	3.7
1	1-A	232	THR	3.7
1	1-A	107	ILE	3.6
1	1-A	159	ALA	3.6
1	1-A	31	PHE	3.6
1	1-A	58	ASN	3.5
1	1-A	218	HIS	3.5
1	1-A	91	LEU	3.5
1	1-A	37	GLN	3.5
1	1-A	178	ILE	3.3
1	1-A	172	PHE	3.3
1	1-A	245	PHE	3.3
1	1-A	129	VAL	3.3
1	1-A	24	ILE	3.3
1	1-A	55	GLN	3.3
1	1-A	228	GLY	3.2
1	1-A	130	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	182	VAL	3.2
1	1-A	110	ILE	3.2
1	1-A	39	ILE	3.1
1	1-A	106	TYR	3.1
1	1-A	78	ASP	3.1
1	1-A	186	GLY	3.1
1	1-A	124	ASN	3.1
1	1-A	75	ALA	3.1
1	1-A	99	LEU	3.1
1	1-A	48	ASP	3.1
1	1-A	145	TYR	3.0
1	1-A	229	TYR	3.0
1	1-A	177	GLN	3.0
1	1-A	216	ASN	3.0
1	1-A	64	TYR	3.0
1	1-A	5	GLY	3.0
1	1-A	166	ALA	2.9
1	1-A	220	ILE	2.9
1	1-A	146	GLU	2.9
1	1-A	179	SER	2.9
1	1-A	29	ASP	2.9
1	1-A	164	GLU	2.9
1	1-A	127	LEU	2.8
1	1-A	155	GLN	2.8
1	1-A	195	HIS	2.8
1	1-A	162	ARG	2.8
1	1-A	68	PHE	2.8
1	1-A	183	PHE	2.8
1	1-A	210	LYS	2.7
1	1-A	7	ALA	2.7
1	1-A	66	TYR	2.7
1	1-A	187	TRP	2.7
1	1-A	171	THR	2.7
1	1-A	62	GLU	2.7
1	1-A	94	ALA	2.6
1	1-A	144	PHE	2.6
1	1-A	98	ASP	2.6
1	1-A	77	LYS	2.6
1	1-A	175	GLY	2.6
1	1-A	67	VAL	2.6
1	1-A	72	GLY	2.6
1	1-A	40	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	1-A	20	PRO	2.6
1	1-A	207	PHE	2.5
1	1-A	100	ILE	2.5
1	1-A	138	GLN	2.5
1	1-A	13	VAL	2.5
1	1-A	87	ILE	2.5
1	1-A	231	VAL	2.5
1	1-A	237	THR	2.5
1	1-A	63	LYS	2.5
1	1-A	96	ILE	2.5
1	1-A	174	ILE	2.5
1	1-A	112	LEU	2.4
1	1-A	202	LYS	2.4
1	1-A	114	LYS	2.4
1	1-A	134	ARG	2.4
1	1-A	57	GLY	2.4
1	1-A	101	ASN	2.4
1	1-A	180	PHE	2.4
1	1-A	10	LEU	2.3
1	1-A	109	LYS	2.3
1	1-A	43	VAL	2.3
1	1-A	176	GLY	2.3
1	1-A	151	GLU	2.3
1	1-A	65	ASP	2.3
1	1-A	201	TYR	2.3
1	1-A	125	GLY	2.2
1	1-A	44	VAL	2.2
1	1-A	234	PRO	2.2
1	1-A	8	LEU	2.2
1	1-A	122	PHE	2.2
1	1-A	204	ILE	2.2
1	1-A	241	CYS	2.2
1	1-A	119	PHE	2.1
1	1-A	206	PHE	2.1
1	1-A	111	LYS	2.1
1	1-A	149	LYS	2.1
1	1-A	11	PHE	2.1
1	1-A	81	LEU	2.1
1	1-A	209	ASP	2.1
1	1-A	16	THR	2.1
1	1-A	153	ILE	2.1
1	1-A	108	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	35	LEU	2.0
1	1-A	239	ARG	2.0
1	1-A	71	ASN	2.0
1	1-A	170	LEU	2.0
1	1-A	38	LYS	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(Å ²)	Q<0.9
3	GLY	1-A	400	4/5	0.71	0.29	55,56,57,58	4
2	EDO	2-A	300	4/4	-	-	63,64,65,66	4
2	EDO	3-A	300	4/4	-	-	63,65,65,67	4
2	EDO	4-A	300	4/4	-	-	63,65,66,67	4
2	EDO	5-A	300	4/4	-	-	63,64,65,67	4
2	EDO	6-A	300	4/4	-	-	63,64,65,67	4
2	EDO	7-A	300	4/4	-	-	63,64,65,67	4
2	EDO	8-A	300	4/4	-	-	63,64,65,67	4
2	EDO	9-A	300	4/4	-	-	63,64,65,67	4
2	EDO	10-A	300	4/4	-	-	63,64,65,67	4
2	EDO	11-A	300	4/4	-	-	63,65,65,67	4
2	EDO	12-A	300	4/4	-	-	63,65,65,67	4
2	EDO	13-A	300	4/4	-	-	63,64,65,67	4
2	EDO	14-A	300	4/4	-	-	63,64,65,67	4
2	EDO	15-A	300	4/4	-	-	63,64,65,67	4
2	EDO	16-A	300	4/4	-	-	63,64,65,67	4
3	GLY	1-A	401	4/5	0.72	0.21	56,58,58,59	4
3	GLY	2-A	400	4/5	-	-	55,56,57,58	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLY	3-A	400	4/5	-	-	55,56,57,58	4
3	GLY	4-A	400	4/5	-	-	55,56,57,58	4
3	GLY	5-A	400	4/5	-	-	55,56,57,58	4
3	GLY	6-A	400	4/5	-	-	55,56,57,58	4
3	GLY	7-A	400	4/5	-	-	55,56,57,58	4
3	GLY	8-A	400	4/5	-	-	55,56,57,58	4
3	GLY	9-A	400	4/5	-	-	55,56,57,58	4
3	GLY	10-A	400	4/5	-	-	56,56,57,58	4
3	GLY	11-A	400	4/5	-	-	55,56,57,58	4
3	GLY	12-A	400	4/5	-	-	55,56,57,58	4
3	GLY	13-A	400	4/5	-	-	56,56,57,59	4
3	GLY	14-A	400	4/5	-	-	56,56,57,59	4
3	GLY	15-A	400	4/5	-	-	55,56,57,59	4
3	GLY	16-A	400	4/5	-	-	55,56,57,59	4
2	EDO	1-A	300	4/4	0.81	0.20	63,64,65,66	4
3	GLY	2-A	401	4/5	-	-	54,57,57,58	4
3	GLY	3-A	401	4/5	-	-	55,58,58,59	4
3	GLY	4-A	401	4/5	-	-	57,58,58,59	4
3	GLY	5-A	401	4/5	-	-	56,58,58,58	4
3	GLY	6-A	401	4/5	-	-	57,58,59,59	4
3	GLY	7-A	401	4/5	-	-	56,58,58,58	4
3	GLY	8-A	401	4/5	-	-	57,58,59,59	4
3	GLY	9-A	401	4/5	-	-	56,58,58,59	4
3	GLY	10-A	401	4/5	-	-	57,58,59,59	4
3	GLY	11-A	401	4/5	-	-	55,58,58,59	4
3	GLY	12-A	401	4/5	-	-	56,58,59,59	4
3	GLY	13-A	401	4/5	-	-	56,57,57,58	4
3	GLY	14-A	401	4/5	-	-	56,58,58,58	4
3	GLY	15-A	401	4/5	-	-	55,58,58,59	4
3	GLY	16-A	401	4/5	-	-	55,58,58,59	4
3	GLY	1-A	402	4/5	0.81	0.21	64,64,64,65	4
3	GLY	2-A	402	4/5	-	-	63,64,64,64	4
3	GLY	3-A	402	4/5	-	-	63,64,64,64	4
3	GLY	4-A	402	4/5	-	-	64,64,64,65	4
3	GLY	5-A	402	4/5	-	-	63,64,64,64	4
3	GLY	6-A	402	4/5	-	-	63,64,64,64	4
3	GLY	7-A	402	4/5	-	-	65,65,66,66	4
3	GLY	8-A	402	4/5	-	-	64,64,64,65	4
3	GLY	9-A	402	4/5	-	-	63,63,64,64	4
3	GLY	10-A	402	4/5	-	-	64,64,65,65	4
3	GLY	11-A	402	4/5	-	-	63,64,64,64	4
3	GLY	12-A	402	4/5	-	-	63,64,64,64	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLY	13-A	402	4/5	-	-	62,63,63,64	4
3	GLY	14-A	402	4/5	-	-	62,63,63,64	4
3	GLY	15-A	402	4/5	-	-	62,63,63,64	4
3	GLY	16-A	402	4/5	-	-	62,63,63,64	4

6.5 Other polymers [i](#)

There are no such residues in this entry.