



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 08:18 am GMT

PDB ID : 2Q4R
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

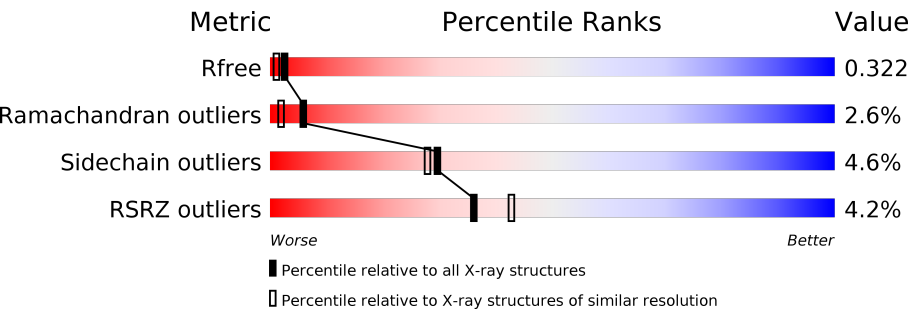
MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	111664	4608 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	10-A	246	
1	11-A	246	
1	12-A	246	
1	13-A	246	
1	14-A	246	
1	15-A	246	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	16-A	246	 91% 6% •
1	2-A	246	 91% 7% •
1	3-A	246	 92% 5% •
1	4-A	246	 93% 5% •
1	5-A	246	 91% 7% •
1	6-A	246	 93% • •
1	7-A	246	 88% 9% •
1	8-A	246	 89% 8% • •
1	9-A	246	 93% • •

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.

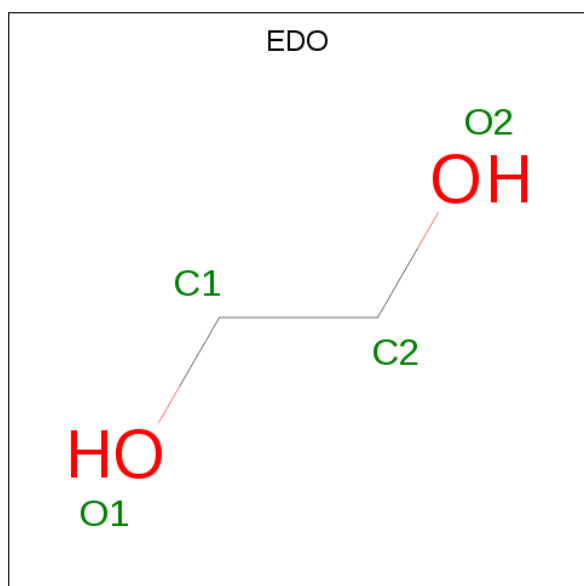
- Molecule 1 is a protein called Phosphomannomutase 2.

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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



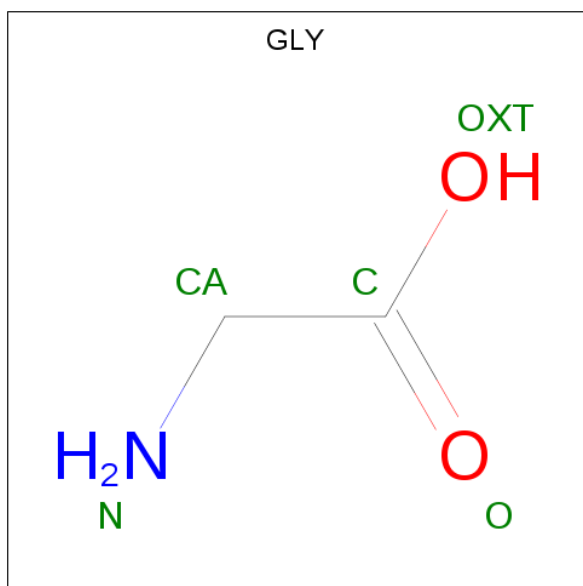
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	1	Total C O 4 2 2	0	0
2	2-A	1	Total C O 4 2 2	0	0
2	3-A	1	Total C O 4 2 2	0	0
2	4-A	1	Total C O 4 2 2	0	0
2	5-A	1	Total C O 4 2 2	0	0
2	6-A	1	Total C O 4 2 2	0	0
2	7-A	1	Total C O 4 2 2	0	0
2	8-A	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

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

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: Phosphomannomutase 2



• Molecule 1: Phosphomannomutase 2



• Molecule 1: Phosphomannomutase 2



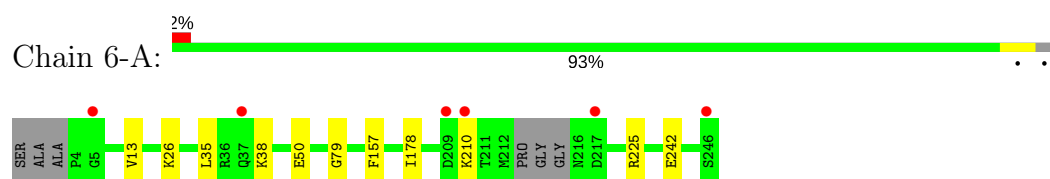
• Molecule 1: Phosphomannomutase 2



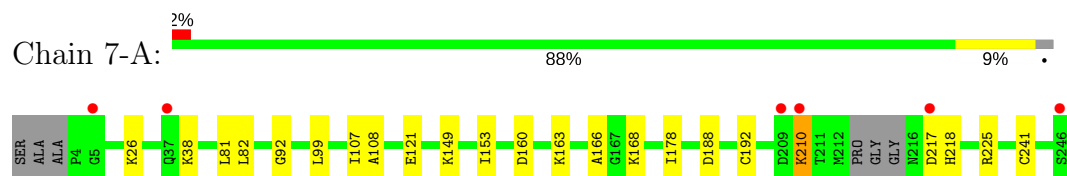
• Molecule 1: Phosphomannomutase 2



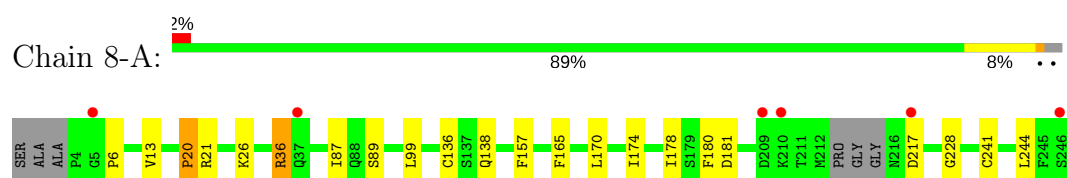
• Molecule 1: Phosphomannomutase 2



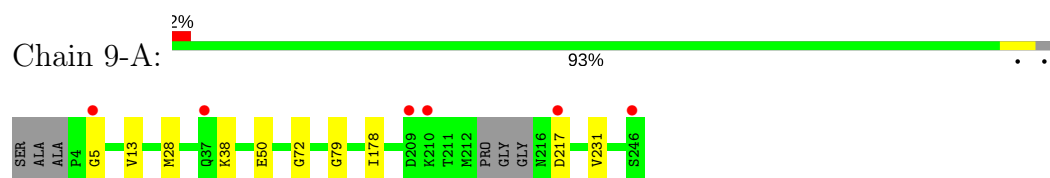
- Molecule 1: Phosphomannomutase 2



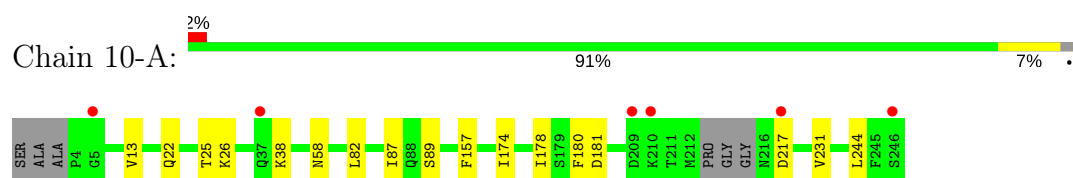
- Molecule 1: Phosphomannomutase 2



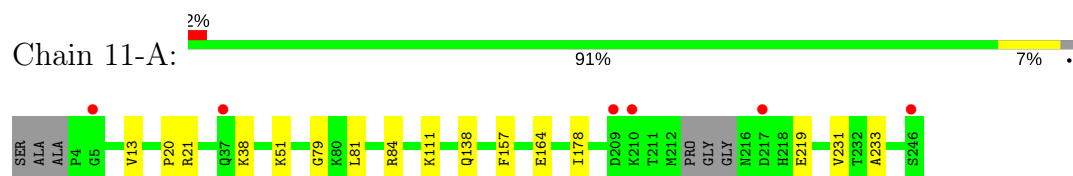
- Molecule 1: Phosphomannomutase 2



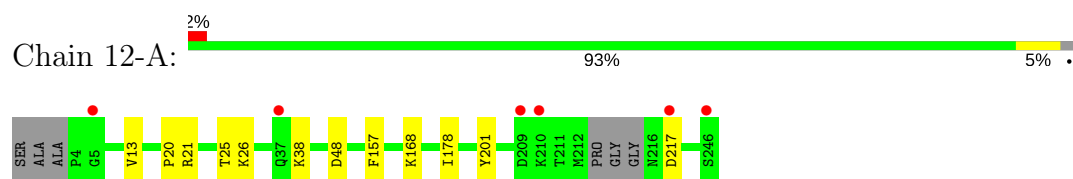
- Molecule 1: Phosphomannomutase 2



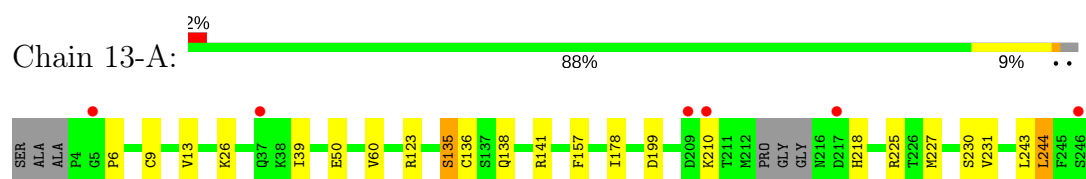
- Molecule 1: Phosphomannomutase 2



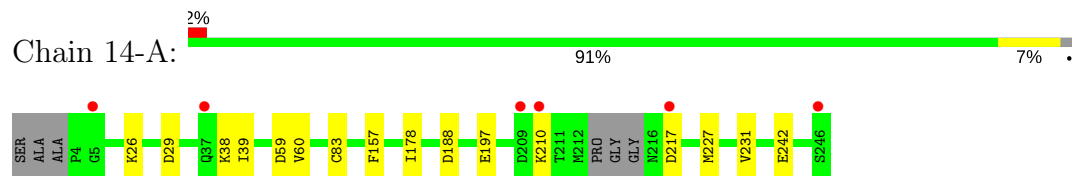
- Molecule 1: Phosphomannomutase 2



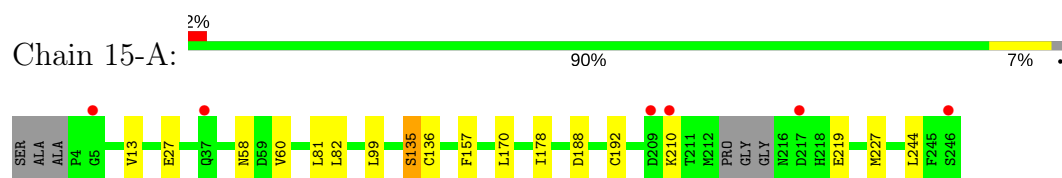
- Molecule 1: Phosphomannomutase 2



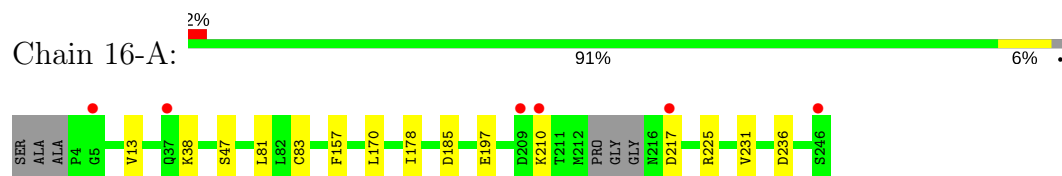
- Molecule 1: Phosphomannomutase 2



- Molecule 1: Phosphomannomutase 2



- Molecule 1: Phosphomannomutase 2



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 38.75 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.58-2.09) 99.5 (38.75-2.09)	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 0.236 , 0.322	Depositor DCC
R_{free} test set	924 reflections (5.28%)	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)	0.24 , 86.5	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	0.93	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 [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	1-A	0.36	0/1977	0.58	0/2646
1	2-A	0.35	0/1977	0.59	0/2646
1	3-A	0.36	0/1977	0.58	0/2646
1	4-A	0.38	0/1977	0.60	0/2646
1	5-A	0.36	0/1977	0.59	0/2646
1	6-A	0.35	0/1977	0.59	0/2646
1	7-A	0.37	0/1977	0.61	0/2646
1	8-A	0.39	0/1977	0.61	0/2646
1	9-A	0.36	0/1977	0.58	0/2646
1	10-A	0.37	0/1977	0.58	0/2646
1	11-A	0.36	0/1977	0.60	0/2646
1	12-A	0.37	0/1977	0.60	0/2646
1	13-A	0.40	0/1977	0.66	0/2646
1	14-A	0.39	0/1977	0.65	0/2646
1	15-A	0.41	0/1977	0.66	0/2646
1	16-A	0.41	0/1977	0.65	0/2646
All	All	0.37	0/31632	0.61	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 [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	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

Continued on next page...

Continued from previous page...

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%)	10 5

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	207 (98%)	5 (2%)	52	56
1	2-A	212/210 (101%)	203 (96%)	9 (4%)	32	32
1	3-A	212/210 (101%)	203 (96%)	9 (4%)	32	32
1	4-A	212/210 (101%)	204 (96%)	8 (4%)	36	36
1	5-A	212/210 (101%)	206 (97%)	6 (3%)	47	50
1	6-A	212/210 (101%)	204 (96%)	8 (4%)	36	36
1	7-A	212/210 (101%)	197 (93%)	15 (7%)	16	13
1	8-A	212/210 (101%)	200 (94%)	12 (6%)	23	20
1	9-A	212/210 (101%)	207 (98%)	5 (2%)	52	56
1	10-A	212/210 (101%)	202 (95%)	10 (5%)	29	27
1	11-A	212/210 (101%)	201 (95%)	11 (5%)	25	23
1	12-A	212/210 (101%)	205 (97%)	7 (3%)	41	43
1	13-A	212/210 (101%)	196 (92%)	16 (8%)	15	11
1	14-A	212/210 (101%)	201 (95%)	11 (5%)	25	23
1	15-A	212/210 (101%)	200 (94%)	12 (6%)	23	20
1	16-A	212/210 (101%)	200 (94%)	12 (6%)	23	20
All	All	3392/3360 (101%)	3236 (95%)	156 (5%)	29	28

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	38	LYS
1	1-A	106	TYR
1	1-A	134	ARG
1	1-A	178	ILE
1	1-A	225	ARG
1	2-A	26	LYS
1	2-A	38	LYS
1	2-A	83	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-A	98	ASP
1	2-A	106	TYR
1	2-A	111	LYS
1	2-A	157	PHE
1	2-A	178	ILE
1	2-A	227	MSE
1	3-A	25	THR
1	3-A	38	LYS
1	3-A	106	TYR
1	3-A	146	GLU
1	3-A	157	PHE
1	3-A	168	LYS
1	3-A	178	ILE
1	3-A	188	ASP
1	3-A	242	GLU
1	4-A	26	LYS
1	4-A	27	GLU
1	4-A	83	CYS
1	4-A	136	CYS
1	4-A	139	GLU
1	4-A	146	GLU
1	4-A	178	ILE
1	4-A	244	LEU
1	5-A	50	GLU
1	5-A	157	PHE
1	5-A	178	ILE
1	5-A	225	ARG
1	5-A	231	VAL
1	5-A	241	CYS
1	6-A	26	LYS
1	6-A	35	LEU
1	6-A	38	LYS
1	6-A	50	GLU
1	6-A	157	PHE
1	6-A	178	ILE
1	6-A	225	ARG
1	6-A	242	GLU
1	7-A	26	LYS
1	7-A	38	LYS
1	7-A	81	LEU
1	7-A	99	LEU
1	7-A	121	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-A	149	LYS
1	7-A	160	ASP
1	7-A	168	LYS
1	7-A	178	ILE
1	7-A	188	ASP
1	7-A	192	CYS
1	7-A	210	LYS
1	7-A	218	HIS
1	7-A	225	ARG
1	7-A	241	CYS
1	8-A	20	PRO
1	8-A	26	LYS
1	8-A	36	ARG
1	8-A	87	ILE
1	8-A	99	LEU
1	8-A	138	GLN
1	8-A	157	PHE
1	8-A	170	LEU
1	8-A	178	ILE
1	8-A	181	ASP
1	8-A	241	CYS
1	8-A	244	LEU
1	9-A	28	MSE
1	9-A	38	LYS
1	9-A	50	GLU
1	9-A	178	ILE
1	9-A	231	VAL
1	10-A	22	GLN
1	10-A	25	THR
1	10-A	26	LYS
1	10-A	38	LYS
1	10-A	87	ILE
1	10-A	157	PHE
1	10-A	178	ILE
1	10-A	181	ASP
1	10-A	231	VAL
1	10-A	244	LEU
1	11-A	38	LYS
1	11-A	51	LYS
1	11-A	81	LEU
1	11-A	84	ARG
1	11-A	111	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	11-A	138	GLN
1	11-A	157	PHE
1	11-A	164	GLU
1	11-A	178	ILE
1	11-A	219	GLU
1	11-A	231	VAL
1	12-A	25	THR
1	12-A	26	LYS
1	12-A	38	LYS
1	12-A	48	ASP
1	12-A	157	PHE
1	12-A	168	LYS
1	12-A	178	ILE
1	13-A	9	CYS
1	13-A	26	LYS
1	13-A	39	ILE
1	13-A	50	GLU
1	13-A	123	ARG
1	13-A	135	SER
1	13-A	141	ARG
1	13-A	157	PHE
1	13-A	178	ILE
1	13-A	210	LYS
1	13-A	218	HIS
1	13-A	225	ARG
1	13-A	227	MSE
1	13-A	230	SER
1	13-A	231	VAL
1	13-A	244	LEU
1	14-A	26	LYS
1	14-A	29	ASP
1	14-A	38	LYS
1	14-A	59	ASP
1	14-A	83	CYS
1	14-A	157	PHE
1	14-A	178	ILE
1	14-A	188	ASP
1	14-A	227	MSE
1	14-A	231	VAL
1	14-A	242	GLU
1	15-A	27	GLU
1	15-A	81	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	15-A	99	LEU
1	15-A	135	SER
1	15-A	157	PHE
1	15-A	170	LEU
1	15-A	178	ILE
1	15-A	188	ASP
1	15-A	192	CYS
1	15-A	219	GLU
1	15-A	227	MSE
1	15-A	244	LEU
1	16-A	38	LYS
1	16-A	47	SER
1	16-A	81	LEU
1	16-A	83	CYS
1	16-A	157	PHE
1	16-A	170	LEU
1	16-A	178	ILE
1	16-A	185	ASP
1	16-A	210	LYS
1	16-A	225	ARG
1	16-A	231	VAL
1	16-A	236	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	2-A	138	GLN
1	2-A	152	ASN
1	3-A	55	GLN
1	3-A	138	GLN
1	3-A	218	HIS
1	4-A	138	GLN
1	5-A	138	GLN
1	5-A	198	ASN
1	5-A	218	HIS
1	6-A	138	GLN
1	6-A	152	ASN
1	7-A	37	GLN
1	7-A	55	GLN
1	7-A	97	GLN
1	7-A	101	ASN
1	7-A	152	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-A	177	GLN
1	8-A	37	GLN
1	8-A	55	GLN
1	8-A	97	GLN
1	8-A	101	ASN
1	8-A	138	GLN
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	11-A	97	GLN
1	11-A	101	ASN
1	11-A	138	GLN
1	11-A	216	ASN
1	12-A	71	ASN
1	12-A	152	ASN
1	12-A	218	HIS
1	13-A	198	ASN
1	14-A	138	GLN
1	15-A	22	GLN
1	15-A	55	GLN
1	15-A	90	HIS
1	16-A	90	HIS
1	16-A	138	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 carbohydrates in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
2	EDO	1-A	300	-	3,3,3	0.49	0	2,2,2	0.34	0
3	GLY	1-A	400	-	3,3,4	0.65	0	1,2,4	0.99	0
3	GLY	1-A	401	-	3,3,4	0.54	0	1,2,4	1.17	0
3	GLY	1-A	402	-	3,3,4	0.67	0	1,2,4	0.94	0
2	EDO	10-A	300	-	3,3,3	0.50	0	2,2,2	0.36	0
3	GLY	10-A	400	-	3,3,4	0.69	0	1,2,4	0.98	0
3	GLY	10-A	401	-	3,3,4	0.53	0	1,2,4	1.21	0
3	GLY	10-A	402	-	3,3,4	0.66	0	1,2,4	0.91	0
2	EDO	11-A	300	-	3,3,3	0.50	0	2,2,2	0.35	0
3	GLY	11-A	400	-	3,3,4	0.66	0	1,2,4	1.00	0
3	GLY	11-A	401	-	3,3,4	0.55	0	1,2,4	1.17	0
3	GLY	11-A	402	-	3,3,4	0.65	0	1,2,4	0.92	0
2	EDO	12-A	300	-	3,3,3	0.50	0	2,2,2	0.36	0
3	GLY	12-A	400	-	3,3,4	0.66	0	1,2,4	1.00	0
3	GLY	12-A	401	-	3,3,4	0.54	0	1,2,4	1.20	0
3	GLY	12-A	402	-	3,3,4	0.65	0	1,2,4	0.92	0
2	EDO	13-A	300	-	3,3,3	0.50	0	2,2,2	0.35	0
3	GLY	13-A	400	-	3,3,4	0.66	0	1,2,4	0.99	0
3	GLY	13-A	401	-	3,3,4	0.51	0	1,2,4	1.25	0
3	GLY	13-A	402	-	3,3,4	0.65	0	1,2,4	0.93	0
2	EDO	14-A	300	-	3,3,3	0.50	0	2,2,2	0.35	0
3	GLY	14-A	400	-	3,3,4	0.67	0	1,2,4	1.00	0
3	GLY	14-A	401	-	3,3,4	0.52	0	1,2,4	1.26	0
3	GLY	14-A	402	-	3,3,4	0.66	0	1,2,4	0.93	0
2	EDO	15-A	300	-	3,3,3	0.51	0	2,2,2	0.36	0
3	GLY	15-A	400	-	3,3,4	0.67	0	1,2,4	1.01	0
3	GLY	15-A	401	-	3,3,4	0.53	0	1,2,4	1.20	0
3	GLY	15-A	402	-	3,3,4	0.67	0	1,2,4	0.94	0
2	EDO	16-A	300	-	3,3,3	0.50	0	2,2,2	0.35	0
3	GLY	16-A	400	-	3,3,4	0.66	0	1,2,4	0.99	0
3	GLY	16-A	401	-	3,3,4	0.53	0	1,2,4	1.21	0
3	GLY	16-A	402	-	3,3,4	0.67	0	1,2,4	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	2-A	300	-	3,3,3	0.50	0	2,2,2	0.35	0
3	GLY	2-A	400	-	3,3,4	0.65	0	1,2,4	1.00	0
3	GLY	2-A	401	-	3,3,4	0.53	0	1,2,4	1.19	0
3	GLY	2-A	402	-	3,3,4	0.65	0	1,2,4	0.94	0
2	EDO	3-A	300	-	3,3,3	0.50	0	2,2,2	0.35	0
3	GLY	3-A	400	-	3,3,4	0.66	0	1,2,4	1.01	0
3	GLY	3-A	401	-	3,3,4	0.54	0	1,2,4	1.18	0
3	GLY	3-A	402	-	3,3,4	0.65	0	1,2,4	0.93	0
2	EDO	4-A	300	-	3,3,3	0.50	0	2,2,2	0.35	0
3	GLY	4-A	400	-	3,3,4	0.65	0	1,2,4	1.00	0
3	GLY	4-A	401	-	3,3,4	0.54	0	1,2,4	1.20	0
3	GLY	4-A	402	-	3,3,4	0.67	0	1,2,4	0.89	0
2	EDO	5-A	300	-	3,3,3	0.50	0	2,2,2	0.36	0
3	GLY	5-A	400	-	3,3,4	0.67	0	1,2,4	0.99	0
3	GLY	5-A	401	-	3,3,4	0.53	0	1,2,4	1.21	0
3	GLY	5-A	402	-	3,3,4	0.66	0	1,2,4	0.92	0
2	EDO	6-A	300	-	3,3,3	0.50	0	2,2,2	0.35	0
3	GLY	6-A	400	-	3,3,4	0.65	0	1,2,4	0.99	0
3	GLY	6-A	401	-	3,3,4	0.54	0	1,2,4	1.18	0
3	GLY	6-A	402	-	3,3,4	0.66	0	1,2,4	0.93	0
2	EDO	7-A	300	-	3,3,3	0.49	0	2,2,2	0.36	0
3	GLY	7-A	400	-	3,3,4	0.70	0	1,2,4	0.96	0
3	GLY	7-A	401	-	3,3,4	0.53	0	1,2,4	1.21	0
3	GLY	7-A	402	-	3,3,4	0.67	0	1,2,4	0.90	0
2	EDO	8-A	300	-	3,3,3	0.50	0	2,2,2	0.36	0
3	GLY	8-A	400	-	3,3,4	0.66	0	1,2,4	1.00	0
3	GLY	8-A	401	-	3,3,4	0.55	0	1,2,4	1.18	0
3	GLY	8-A	402	-	3,3,4	0.66	0	1,2,4	0.91	0
2	EDO	9-A	300	-	3,3,3	0.50	0	2,2,2	0.36	0
3	GLY	9-A	400	-	3,3,4	0.65	0	1,2,4	0.97	0
3	GLY	9-A	401	-	3,3,4	0.54	0	1,2,4	1.15	0
3	GLY	9-A	402	-	3,3,4	0.65	0	1,2,4	0.93	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	1-A	300	-	-	0/1/1/1	0/0/0/0
3	GLY	1-A	400	-	-	0/0/1/2	0/0/0/0
3	GLY	1-A	401	-	-	0/0/1/2	0/0/0/0
3	GLY	1-A	402	-	-	0/0/1/2	0/0/0/0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	5-A	401	-	-	0/0/1/2	0/0/0/0
3	GLY	5-A	402	-	-	0/0/1/2	0/0/0/0
2	EDO	6-A	300	-	-	0/1/1/1	0/0/0/0
3	GLY	6-A	400	-	-	0/0/1/2	0/0/0/0
3	GLY	6-A	401	-	-	0/0/1/2	0/0/0/0
3	GLY	6-A	402	-	-	0/0/1/2	0/0/0/0
2	EDO	7-A	300	-	-	0/1/1/1	0/0/0/0
3	GLY	7-A	400	-	-	0/0/1/2	0/0/0/0
3	GLY	7-A	401	-	-	0/0/1/2	0/0/0/0
3	GLY	7-A	402	-	-	0/0/1/2	0/0/0/0
2	EDO	8-A	300	-	-	0/1/1/1	0/0/0/0
3	GLY	8-A	400	-	-	0/0/1/2	0/0/0/0
3	GLY	8-A	401	-	-	0/0/1/2	0/0/0/0
3	GLY	8-A	402	-	-	0/0/1/2	0/0/0/0
2	EDO	9-A	300	-	-	0/1/1/1	0/0/0/0
3	GLY	9-A	400	-	-	0/0/1/2	0/0/0/0
3	GLY	9-A	401	-	-	0/0/1/2	0/0/0/0
3	GLY	9-A	402	-	-	0/0/1/2	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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 ⓘ

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%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	2-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	3-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	4-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	5-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	6-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	7-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	8-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	9-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	10-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	11-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	12-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	13-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	14-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	15-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
1	16-A	236/246 (95%)	0.01	6 (2%)	57	63	26, 40, 52, 74	236 (100%)
All	All	3776/3936 (95%)	0.01	96 (2%)	36	63	26, 40, 52, 74	3776 (100%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	246	SER	7.8
1	2-A	246	SER	7.8
1	3-A	246	SER	7.8
1	4-A	246	SER	7.8
1	5-A	246	SER	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	6-A	246	SER	7.8
1	7-A	246	SER	7.8
1	8-A	246	SER	7.8
1	9-A	246	SER	7.8
1	10-A	246	SER	7.8
1	11-A	246	SER	7.8
1	12-A	246	SER	7.8
1	13-A	246	SER	7.8
1	14-A	246	SER	7.8
1	15-A	246	SER	7.8
1	16-A	246	SER	7.8
1	1-A	209	ASP	4.5
1	2-A	209	ASP	4.5
1	3-A	209	ASP	4.5
1	4-A	209	ASP	4.5
1	5-A	209	ASP	4.5
1	6-A	209	ASP	4.5
1	7-A	209	ASP	4.5
1	8-A	209	ASP	4.5
1	9-A	209	ASP	4.5
1	10-A	209	ASP	4.5
1	11-A	209	ASP	4.5
1	12-A	209	ASP	4.5
1	13-A	209	ASP	4.5
1	14-A	209	ASP	4.5
1	15-A	209	ASP	4.5
1	16-A	209	ASP	4.5
1	1-A	5	GLY	3.1
1	2-A	5	GLY	3.1
1	3-A	5	GLY	3.1
1	4-A	5	GLY	3.1
1	5-A	5	GLY	3.1
1	6-A	5	GLY	3.1
1	7-A	5	GLY	3.1
1	8-A	5	GLY	3.1
1	9-A	5	GLY	3.1
1	10-A	5	GLY	3.1
1	11-A	5	GLY	3.1
1	12-A	5	GLY	3.1
1	13-A	5	GLY	3.1
1	14-A	5	GLY	3.1
1	15-A	5	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	16-A	5	GLY	3.1
1	1-A	217	ASP	2.9
1	2-A	217	ASP	2.9
1	3-A	217	ASP	2.9
1	4-A	217	ASP	2.9
1	5-A	217	ASP	2.9
1	6-A	217	ASP	2.9
1	7-A	217	ASP	2.9
1	8-A	217	ASP	2.9
1	9-A	217	ASP	2.9
1	10-A	217	ASP	2.9
1	11-A	217	ASP	2.9
1	12-A	217	ASP	2.9
1	13-A	217	ASP	2.9
1	14-A	217	ASP	2.9
1	15-A	217	ASP	2.9
1	16-A	217	ASP	2.9
1	1-A	210	LYS	2.3
1	2-A	210	LYS	2.3
1	3-A	210	LYS	2.3
1	4-A	210	LYS	2.3
1	5-A	210	LYS	2.3
1	6-A	210	LYS	2.3
1	7-A	210	LYS	2.3
1	8-A	210	LYS	2.3
1	9-A	210	LYS	2.3
1	10-A	210	LYS	2.3
1	11-A	210	LYS	2.3
1	12-A	210	LYS	2.3
1	13-A	210	LYS	2.3
1	14-A	210	LYS	2.3
1	15-A	210	LYS	2.3
1	16-A	210	LYS	2.3
1	1-A	37	GLN	2.2
1	2-A	37	GLN	2.2
1	3-A	37	GLN	2.2
1	4-A	37	GLN	2.2
1	5-A	37	GLN	2.2
1	6-A	37	GLN	2.2
1	7-A	37	GLN	2.2
1	8-A	37	GLN	2.2
1	9-A	37	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	10-A	37	GLN	2.2
1	11-A	37	GLN	2.2
1	12-A	37	GLN	2.2
1	13-A	37	GLN	2.2
1	14-A	37	GLN	2.2
1	15-A	37	GLN	2.2
1	16-A	37	GLN	2.2

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 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
3	GLY	15-A	400	4/5	0.76	0.20	55,56,57,59	4
3	GLY	7-A	400	4/5	0.76	0.20	55,56,57,58	4
3	GLY	5-A	400	4/5	0.76	0.20	55,56,57,58	4
3	GLY	6-A	400	4/5	0.76	0.20	55,56,57,58	4
3	GLY	14-A	400	4/5	0.76	0.20	56,56,57,59	4
3	GLY	8-A	400	4/5	0.76	0.20	55,56,57,58	4
3	GLY	16-A	400	4/5	0.76	0.20	55,56,57,59	4
3	GLY	2-A	400	4/5	0.76	0.20	55,56,57,58	4
3	GLY	9-A	400	4/5	0.76	0.20	55,56,57,58	4
3	GLY	13-A	400	4/5	0.76	0.20	56,56,57,59	4
3	GLY	3-A	400	4/5	0.76	0.20	55,56,57,58	4
3	GLY	11-A	400	4/5	0.76	0.20	55,56,57,58	4
3	GLY	10-A	400	4/5	0.76	0.20	56,56,57,58	4
3	GLY	4-A	400	4/5	0.76	0.20	55,56,57,58	4
3	GLY	1-A	400	4/5	0.76	0.20	55,56,57,58	4
3	GLY	12-A	400	4/5	0.76	0.20	55,56,57,58	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLY	11-A	401	4/5	0.85	0.20	55,58,58,59	4
2	EDO	3-A	300	4/4	0.85	0.12	63,65,65,67	4
3	GLY	8-A	401	4/5	0.85	0.20	57,58,59,59	4
2	EDO	12-A	300	4/4	0.85	0.12	63,65,65,67	4
3	GLY	1-A	401	4/5	0.85	0.20	56,58,58,59	4
3	GLY	2-A	401	4/5	0.85	0.20	54,57,57,58	4
2	EDO	14-A	300	4/4	0.85	0.12	63,64,65,67	4
3	GLY	13-A	401	4/5	0.85	0.20	56,57,57,58	4
2	EDO	2-A	300	4/4	0.85	0.12	63,64,65,66	4
3	GLY	16-A	401	4/5	0.85	0.20	55,58,58,59	4
2	EDO	9-A	300	4/4	0.85	0.12	63,64,65,67	4
2	EDO	11-A	300	4/4	0.85	0.12	63,65,65,67	4
2	EDO	4-A	300	4/4	0.85	0.12	63,65,66,67	4
3	GLY	7-A	401	4/5	0.85	0.20	56,58,58,58	4
3	GLY	14-A	401	4/5	0.85	0.20	56,58,58,58	4
2	EDO	15-A	300	4/4	0.85	0.12	63,64,65,67	4
2	EDO	5-A	300	4/4	0.85	0.12	63,64,65,67	4
3	GLY	15-A	401	4/5	0.85	0.20	55,58,58,59	4
2	EDO	1-A	300	4/4	0.85	0.12	63,64,65,66	4
3	GLY	6-A	401	4/5	0.85	0.20	57,58,59,59	4
3	GLY	4-A	401	4/5	0.85	0.20	57,58,58,59	4
2	EDO	13-A	300	4/4	0.85	0.12	63,64,65,67	4
2	EDO	16-A	300	4/4	0.85	0.12	63,64,65,67	4
3	GLY	12-A	401	4/5	0.85	0.20	56,58,59,59	4
3	GLY	3-A	401	4/5	0.85	0.20	55,58,58,59	4
2	EDO	6-A	300	4/4	0.85	0.12	63,64,65,67	4
3	GLY	5-A	401	4/5	0.85	0.20	56,58,58,58	4
3	GLY	10-A	401	4/5	0.85	0.20	57,58,59,59	4
3	GLY	9-A	401	4/5	0.85	0.20	56,58,58,59	4
2	EDO	8-A	300	4/4	0.85	0.12	63,64,65,67	4
2	EDO	7-A	300	4/4	0.85	0.12	63,64,65,67	4
2	EDO	10-A	300	4/4	0.85	0.12	63,64,65,67	4
3	GLY	8-A	402	4/5	0.89	0.09	64,64,64,65	4
3	GLY	3-A	402	4/5	0.89	0.09	63,64,64,64	4
3	GLY	12-A	402	4/5	0.89	0.09	63,64,64,64	4
3	GLY	14-A	402	4/5	0.89	0.09	62,63,63,64	4
3	GLY	1-A	402	4/5	0.89	0.09	64,64,64,65	4
3	GLY	13-A	402	4/5	0.89	0.09	62,63,63,64	4
3	GLY	7-A	402	4/5	0.89	0.09	65,65,66,66	4
3	GLY	4-A	402	4/5	0.89	0.09	64,64,64,65	4
3	GLY	9-A	402	4/5	0.89	0.09	63,63,64,64	4
3	GLY	5-A	402	4/5	0.89	0.09	63,64,64,64	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLY	6-A	402	4/5	0.89	0.09	63,64,64,64	4
3	GLY	11-A	402	4/5	0.89	0.09	63,64,64,64	4
3	GLY	15-A	402	4/5	0.89	0.09	62,63,63,64	4
3	GLY	2-A	402	4/5	0.89	0.09	63,64,64,64	4
3	GLY	10-A	402	4/5	0.89	0.09	64,64,65,65	4
3	GLY	16-A	402	4/5	0.89	0.09	62,63,63,64	4

6.5 Other polymers [i](#)

There are no such residues in this entry.