



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:54 pm BST

PDB ID : 4GWF  
Title : Crystal structure of the tyrosine phosphatase SHP-2 with Y279C mutation  
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Deposited on : 2012-09-03  
Resolution : 2.10 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

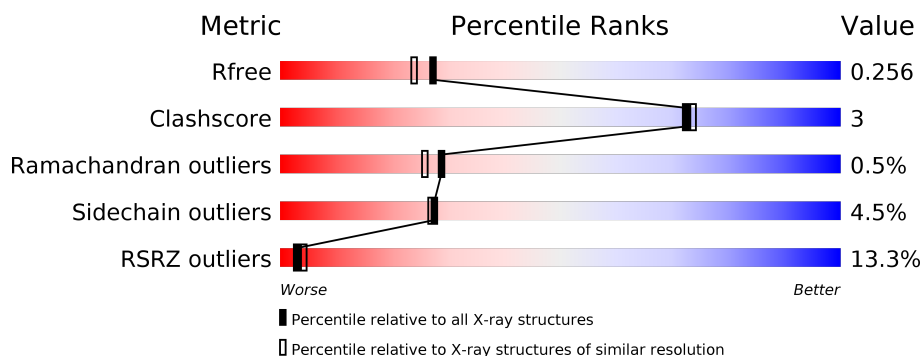
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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  $\geq 3$ , 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	560	<div> <div>13%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>11%</div> </div> </div>
1	B	560	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>12%</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8367 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 Tyrosine-protein phosphatase non-receptor type 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	1	0
			4025	2530	717	758	20			
1	B	493	Total	C	N	O	S	0	0	0
			3991	2509	715	748	19			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q06124
A	-19	GLY	-	EXPRESSION TAG	UNP Q06124
A	-18	SER	-	EXPRESSION TAG	UNP Q06124
A	-17	SER	-	EXPRESSION TAG	UNP Q06124
A	-16	HIS	-	EXPRESSION TAG	UNP Q06124
A	-15	HIS	-	EXPRESSION TAG	UNP Q06124
A	-14	HIS	-	EXPRESSION TAG	UNP Q06124
A	-13	HIS	-	EXPRESSION TAG	UNP Q06124
A	-12	HIS	-	EXPRESSION TAG	UNP Q06124
A	-11	HIS	-	EXPRESSION TAG	UNP Q06124
A	-10	SER	-	EXPRESSION TAG	UNP Q06124
A	-9	SER	-	EXPRESSION TAG	UNP Q06124
A	-8	GLY	-	EXPRESSION TAG	UNP Q06124
A	-7	ARG	-	EXPRESSION TAG	UNP Q06124
A	-6	GLU	-	EXPRESSION TAG	UNP Q06124
A	-5	ASN	-	EXPRESSION TAG	UNP Q06124
A	-4	LEU	-	EXPRESSION TAG	UNP Q06124
A	-3	TYR	-	EXPRESSION TAG	UNP Q06124
A	-2	PHE	-	EXPRESSION TAG	UNP Q06124
A	-1	GLN	-	EXPRESSION TAG	UNP Q06124
A	0	GLY	-	EXPRESSION TAG	UNP Q06124
A	279	CYS	TYR	ENGINEERED MUTATION	UNP Q06124
A	?	-	GLN	DELETION	UNP Q06124
A	?	-	ALA	DELETION	UNP Q06124
A	?	-	LEU	DELETION	UNP Q06124

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	DELETION	UNP Q06124
B	-20	MET	-	EXPRESSION TAG	UNP Q06124
B	-19	GLY	-	EXPRESSION TAG	UNP Q06124
B	-18	SER	-	EXPRESSION TAG	UNP Q06124
B	-17	SER	-	EXPRESSION TAG	UNP Q06124
B	-16	HIS	-	EXPRESSION TAG	UNP Q06124
B	-15	HIS	-	EXPRESSION TAG	UNP Q06124
B	-14	HIS	-	EXPRESSION TAG	UNP Q06124
B	-13	HIS	-	EXPRESSION TAG	UNP Q06124
B	-12	HIS	-	EXPRESSION TAG	UNP Q06124
B	-11	HIS	-	EXPRESSION TAG	UNP Q06124
B	-10	SER	-	EXPRESSION TAG	UNP Q06124
B	-9	SER	-	EXPRESSION TAG	UNP Q06124
B	-8	GLY	-	EXPRESSION TAG	UNP Q06124
B	-7	ARG	-	EXPRESSION TAG	UNP Q06124
B	-6	GLU	-	EXPRESSION TAG	UNP Q06124
B	-5	ASN	-	EXPRESSION TAG	UNP Q06124
B	-4	LEU	-	EXPRESSION TAG	UNP Q06124
B	-3	TYR	-	EXPRESSION TAG	UNP Q06124
B	-2	PHE	-	EXPRESSION TAG	UNP Q06124
B	-1	GLN	-	EXPRESSION TAG	UNP Q06124
B	0	GLY	-	EXPRESSION TAG	UNP Q06124
B	279	CYS	TYR	ENGINEERED MUTATION	UNP Q06124
B	?	-	GLN	DELETION	UNP Q06124
B	?	-	ALA	DELETION	UNP Q06124
B	?	-	LEU	DELETION	UNP Q06124
B	?	-	LEU	DELETION	UNP Q06124

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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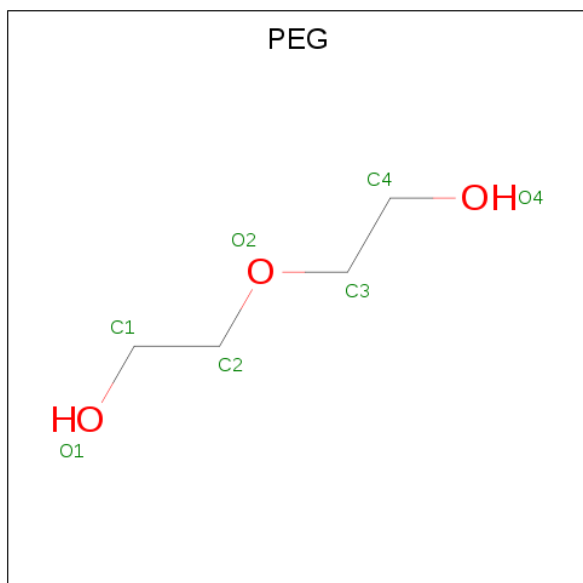
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



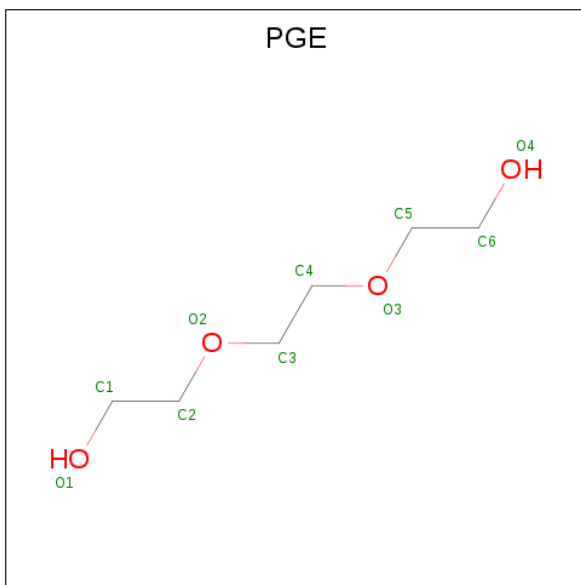
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

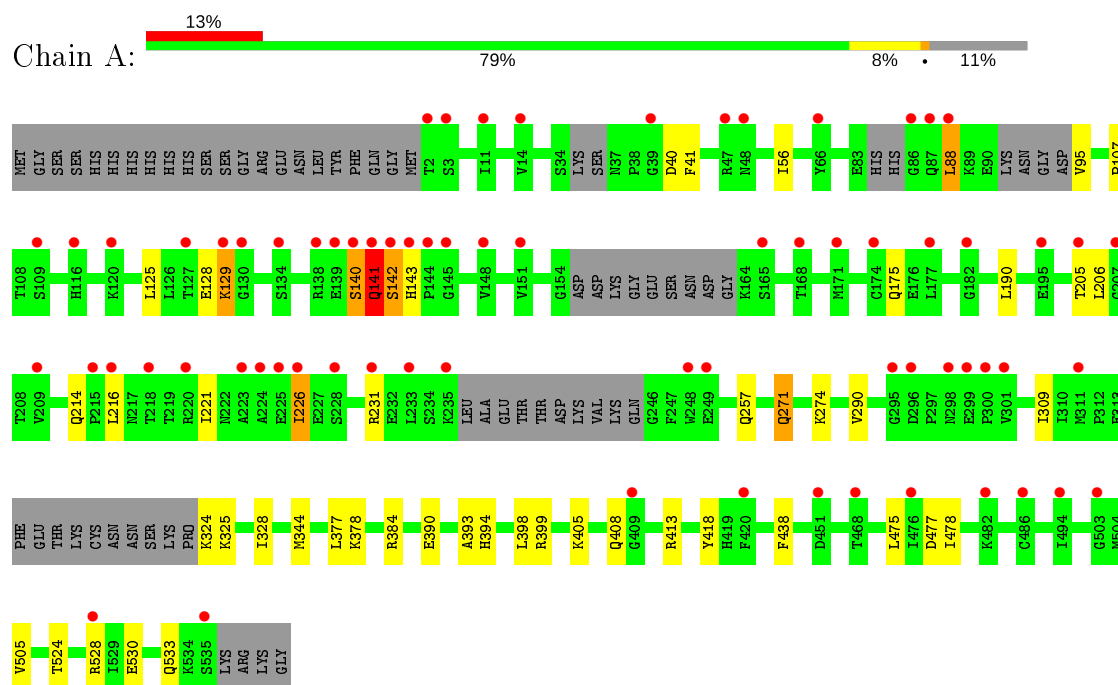
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	134	Total	O	0	0
			134	134		
6	B	127	Total	O	0	0
			127	127		

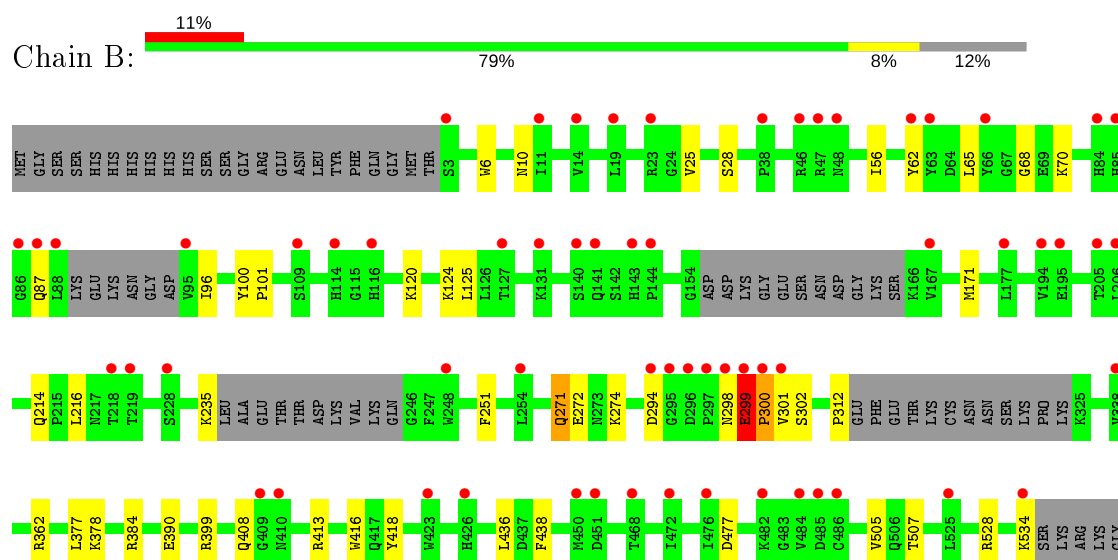
### 3 Residue-property plots [i](#)

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: Tyrosine-protein phosphatase non-receptor type 11



- Molecule 1: Tyrosine-protein phosphatase non-receptor type 11





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.97Å 211.95Å 55.69Å 90.00° 96.63° 90.00°	Depositor
Resolution (Å)	42.00 – 2.10 41.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.00-2.10) 99.5 (41.94-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.210 , 0.243 0.228 , 0.256	Depositor DCC
$R_{free}$ test set	1241 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PEG, PGE, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	0/4106	0.64	1/5533 (0.0%)
1	B	0.39	0/4073	0.61	0/5494
All	All	0.40	0/8179	0.63	1/11027 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	143	HIS	N-CA-C	-7.42	90.97	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	GLN	Peptide

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4025	0	3969	27	0
1	B	3991	0	3923	28	0
2	A	20	0	30	0	0
2	B	40	0	60	6	0
3	A	6	0	8	0	0
4	A	14	0	20	3	0
5	A	10	0	14	1	0
6	A	134	0	0	0	0
6	B	127	0	0	1	0
All	All	8367	0	8024	55	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLU:HB2	1:B:300:PRO:CD	1.85	1.05
1:A:140:SER:HA	1:A:141:GLN:HB3	1.35	1.03
1:B:298:ASN:O	1:B:299:GLU:HG2	1.69	0.91
1:A:140:SER:HA	1:A:141:GLN:CB	2.05	0.86
1:B:298:ASN:O	1:B:299:GLU:CG	2.30	0.79
1:A:141:GLN:CG	1:A:141:GLN:O	2.30	0.79
1:A:257:GLN:HG3	5:A:609:PGE:H3	1.65	0.78
1:B:299:GLU:HB2	1:B:300:PRO:HD3	1.70	0.74
1:B:299:GLU:CB	1:B:300:PRO:HD3	2.19	0.72
1:B:299:GLU:CB	1:B:300:PRO:CD	2.60	0.71
1:B:298:ASN:O	1:B:299:GLU:CB	2.39	0.70
1:B:299:GLU:HB2	1:B:300:PRO:HD2	1.72	0.69
1:A:141:GLN:O	1:A:141:GLN:HG2	1.91	0.68
1:B:298:ASN:C	1:B:299:GLU:CG	2.58	0.67
1:A:141:GLN:NE2	1:A:141:GLN:O	2.29	0.65
1:B:312:PRO:HG2	2:B:602:EDO:H11	1.79	0.64
1:A:141:GLN:N	1:A:142:SER:HA	2.16	0.61
1:A:140:SER:CA	1:A:141:GLN:HB3	2.23	0.61
1:B:272:GLU:HG3	1:B:301:VAL:HG23	1.82	0.60
2:B:608:EDO:H22	6:B:737:HOH:O	2.01	0.59
1:A:394:HIS:H	4:A:608:PEG:H42	1.69	0.57
1:B:298:ASN:C	1:B:299:GLU:HG2	2.24	0.55
1:B:390:GLU:HG2	1:B:399:ARG:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:TRP:HZ3	2:B:608:EDO:H21	1.72	0.52
1:A:141:GLN:O	1:A:141:GLN:CD	2.48	0.51
1:A:175:GLN:HB3	1:B:25:VAL:HG11	1.92	0.50
1:B:299:GLU:OE2	1:B:302:SER:HB3	2.13	0.49
1:B:436:LEU:HB3	2:B:603:EDO:H21	1.96	0.48
1:A:390:GLU:HG2	1:A:399:ARG:HG2	1.96	0.48
1:A:290:VAL:HG11	1:A:344:MET:HG3	1.97	0.47
1:B:251:PHE:HE2	2:B:609:EDO:H22	1.79	0.47
1:A:271:GLN:HA	1:A:274:LYS:HE2	1.97	0.46
1:B:507:THR:HA	2:B:609:EDO:H11	1.98	0.46
1:B:271:GLN:HA	1:B:274:LYS:HE2	1.99	0.45
1:B:65:LEU:HD12	1:B:68:GLY:HA3	1.97	0.45
1:B:125:LEU:HB3	1:B:216:LEU:HD21	1.98	0.44
1:B:418:TYR:HB3	1:B:438:PHE:CE1	2.52	0.44
1:A:377:LEU:HD11	1:A:384:ARG:HD3	1.98	0.44
1:A:88:LEU:HD12	1:A:95:VAL:HG22	1.98	0.44
1:A:221:ILE:HD11	1:A:226:ILE:HD12	1.98	0.44
1:B:28:SER:HA	1:B:100:TYR:O	2.18	0.43
1:A:475:LEU:HA	1:A:478:ILE:HD12	2.00	0.43
1:A:393:ALA:HB2	4:A:607:PEG:H11	2.00	0.43
1:A:398:LEU:HD22	4:A:607:PEG:H32	2.01	0.43
1:A:418:TYR:HB3	1:A:438:PHE:CE1	2.54	0.43
1:A:309:ILE:HD13	1:A:328:ILE:HG12	2.01	0.42
1:B:56:ILE:HG12	1:B:65:LEU:HD23	2.02	0.42
1:A:107:PRO:HG3	1:A:190:LEU:HD12	2.02	0.42
1:A:41:PHE:HB2	1:A:56:ILE:HB	2.01	0.42
1:A:125:LEU:HB3	1:A:216:LEU:HD21	2.02	0.42
1:A:405:LYS:HB3	1:A:408:GLN:HB2	2.02	0.42
1:B:377:LEU:HD21	1:B:384:ARG:HD3	2.01	0.42
1:B:65:LEU:HD11	1:B:87:GLN:HE22	1.85	0.41
1:B:6:TRP:HB3	1:B:101:PRO:HB3	2.02	0.40
1:A:128:GLU:HG3	1:A:129:LYS:HG2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	484/560 (86%)	467 (96%)	15 (3%)	2 (0%)	34	32
1	B	483/560 (86%)	465 (96%)	15 (3%)	3 (1%)	25	21
All	All	967/1120 (86%)	932 (96%)	30 (3%)	5 (0%)	29	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	B	299	GLU
1	B	300	PRO
1	A	505	VAL
1	B	505	VAL

### 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	444/498 (89%)	423 (95%)	21 (5%)	26	25
1	B	438/498 (88%)	419 (96%)	19 (4%)	29	29
All	All	882/996 (89%)	842 (96%)	40 (4%)	27	27

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	88	LEU
1	A	129	LYS
1	A	140	SER
1	A	141	GLN
1	A	142	SER
1	A	205	THR

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Mol	Chain	Res	Type
1	A	206	LEU
1	A	214	GLN
1	A	226	ILE
1	A	231	ARG
1	A	271	GLN
1	A	324	LYS
1	A	325	LYS
1	A	378	LYS
1	A	413	ARG
1	A	477	ASP
1	A	524	THR
1	A	528	ARG
1	A	530	GLU
1	A	533	GLN
1	B	10	ASN
1	B	62	TYR
1	B	70	LYS
1	B	96	ILE
1	B	120	LYS
1	B	124	LYS
1	B	171	MET
1	B	214	GLN
1	B	235	LYS
1	B	271	GLN
1	B	294	ASP
1	B	299	GLU
1	B	362	ARG
1	B	378	LYS
1	B	408	GLN
1	B	413	ARG
1	B	477	ASP
1	B	528	ARG
1	B	534	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	222	ASN
1	A	281	ASN
1	B	169	HIS

### 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 ⓘ

19 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	B	609	-	3,3,3	0.52	0	2,2,2	0.45	0
2	EDO	A	604	-	3,3,3	0.53	0	2,2,2	0.43	0
2	EDO	A	603	-	3,3,3	0.54	0	2,2,2	0.33	0
2	EDO	B	603	-	3,3,3	0.54	0	2,2,2	0.37	0
2	EDO	A	601	-	3,3,3	0.40	0	2,2,2	0.43	0
2	EDO	B	607	-	3,3,3	0.59	0	2,2,2	0.29	0
4	PEG	A	608	-	6,6,6	0.10	0	5,5,5	0.07	0
2	EDO	A	605	-	3,3,3	0.61	0	2,2,2	0.19	0
3	GOL	A	606	-	5,5,5	0.06	0	5,5,5	0.16	0
2	EDO	A	602	-	3,3,3	0.62	0	2,2,2	0.27	0
2	EDO	B	602	-	3,3,3	0.57	0	2,2,2	0.20	0
2	EDO	B	608	-	3,3,3	0.59	0	2,2,2	0.29	0
2	EDO	B	610	-	3,3,3	0.60	0	2,2,2	0.18	0
2	EDO	B	606	-	3,3,3	0.61	0	2,2,2	0.24	0
2	EDO	B	601	-	3,3,3	0.43	0	2,2,2	0.49	0
5	PGE	A	609	-	9,9,9	0.09	0	8,8,8	0.13	0
2	EDO	B	605	-	3,3,3	0.50	0	2,2,2	0.31	0
4	PEG	A	607	-	6,6,6	0.09	0	5,5,5	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	B	604	-	3,3,3	0.54	0	2,2,2	0.35	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	B	609	-	-	1/1/1/1	-
2	EDO	A	604	-	-	0/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	B	607	-	-	0/1/1/1	-
4	PEG	A	608	-	-	1/4/4/4	-
2	EDO	A	605	-	-	0/1/1/1	-
3	GOL	A	606	-	-	0/4/4/4	-
2	EDO	A	602	-	-	0/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-
2	EDO	B	608	-	-	0/1/1/1	-
2	EDO	B	610	-	-	0/1/1/1	-
2	EDO	B	606	-	-	0/1/1/1	-
2	EDO	B	601	-	-	1/1/1/1	-
5	PGE	A	609	-	-	4/7/7/7	-
2	EDO	B	605	-	-	0/1/1/1	-
4	PEG	A	607	-	-	2/4/4/4	-
2	EDO	B	604	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	609	PGE	C6-C5-O3-C4
5	A	609	PGE	C1-C2-O2-C3
5	A	609	PGE	C4-C3-O2-C2
4	A	608	PEG	C4-C3-O2-C2
4	A	607	PEG	C4-C3-O2-C2
2	B	609	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	607	PEG	O2-C3-C4-O4
2	B	601	EDO	O1-C1-C2-O2
5	A	609	PGE	O2-C3-C4-O3

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	609	EDO	2	0
2	B	603	EDO	1	0
4	A	608	PEG	1	0
2	B	602	EDO	1	0
2	B	608	EDO	2	0
5	A	609	PGE	1	0
4	A	607	PEG	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	497/560 (88%)	0.90	70 (14%) 2 3	14, 36, 62, 95	0
1	B	493/560 (88%)	0.93	62 (12%) 3 5	17, 36, 62, 85	0
All	All	990/1120 (88%)	0.92	132 (13%) 3 4	14, 36, 62, 95	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	GLN	6.3
1	B	85	HIS	5.3
1	B	248	TRP	5.3
1	B	87	GLN	5.1
1	B	116	HIS	5.0
1	A	486	CYS	4.8
1	B	205	THR	4.7
1	B	294	ASP	4.7
1	B	11	ILE	4.6
1	B	299	GLU	4.6
1	B	450	MET	4.4
1	B	143	HIS	4.4
1	A	48	ASN	4.4
1	B	298	ASN	4.3
1	B	296	ASP	4.2
1	A	301	VAL	4.2
1	B	451	ASP	4.2
1	A	177	LEU	4.1
1	B	409	GLY	4.1
1	A	120	LYS	4.0
1	A	47	ARG	4.0
1	A	66	TYR	3.8
1	A	144	PRO	3.7
1	A	14	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	301	VAL	3.7
1	B	88	LEU	3.7
1	B	338	VAL	3.6
1	A	296	ASP	3.6
1	A	231	ARG	3.5
1	A	130	GLY	3.5
1	A	224	ALA	3.4
1	A	11	ILE	3.3
1	B	47	ARG	3.3
1	B	84	HIS	3.2
1	A	223	ALA	3.1
1	A	300	PRO	3.1
1	A	2	THR	3.0
1	A	209	VAL	3.0
1	A	116	HIS	3.0
1	A	88	LEU	3.0
1	B	297	PRO	3.0
1	B	141	GLN	3.0
1	B	485	ASP	3.0
1	B	48	ASN	2.9
1	A	409	GLY	2.9
1	A	145	GLY	2.9
1	A	482	LYS	2.9
1	B	86	GLY	2.9
1	A	142	SER	2.8
1	B	177	LEU	2.8
1	A	171	MET	2.8
1	A	295	GLY	2.8
1	B	295	GLY	2.8
1	B	144	PRO	2.8
1	B	476	ILE	2.8
1	A	451	ASP	2.7
1	B	228	SER	2.7
1	B	167	VAL	2.7
1	B	3	SER	2.7
1	A	109	SER	2.7
1	B	127	THR	2.6
1	A	129	LYS	2.6
1	B	114	HIS	2.6
1	A	3	SER	2.5
1	B	300	PRO	2.5
1	A	233	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	131	LYS	2.5
1	A	311	MET	2.5
1	A	468	THR	2.5
1	A	298	ASN	2.5
1	A	225	GLU	2.5
1	A	143	HIS	2.5
1	A	299	GLU	2.5
1	B	423	TRP	2.5
1	B	206	LEU	2.4
1	B	218	THR	2.4
1	A	148	VAL	2.4
1	A	218	THR	2.4
1	B	426	HIS	2.4
1	A	228	SER	2.4
1	B	484	VAL	2.4
1	A	86	GLY	2.4
1	A	226	ILE	2.4
1	B	109	SER	2.4
1	A	174	CYS	2.3
1	B	14	VAL	2.3
1	B	472	ILE	2.3
1	A	215	PRO	2.3
1	A	138	ARG	2.3
1	A	528	ARG	2.3
1	B	194	VAL	2.3
1	A	165	SER	2.3
1	A	207	GLY	2.3
1	A	249	GLU	2.3
1	A	139	GLU	2.2
1	A	248	TRP	2.2
1	A	476	ILE	2.2
1	A	535	SER	2.2
1	B	62	TYR	2.2
1	A	420	PHE	2.2
1	A	220	ARG	2.2
1	B	23	ARG	2.2
1	B	46	ARG	2.2
1	B	95	VAL	2.1
1	B	410	ASN	2.1
1	A	494	ILE	2.1
1	A	216	LEU	2.1
1	B	195	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	38	PRO	2.1
1	B	525	LEU	2.1
1	A	39	GLY	2.1
1	A	134	SER	2.1
1	B	63	TYR	2.1
1	A	127	THR	2.1
1	A	205	THR	2.1
1	A	151	VAL	2.1
1	B	482	LYS	2.1
1	B	534	LYS	2.1
1	A	168	THR	2.1
1	B	66	TYR	2.1
1	A	503	GLY	2.1
1	A	140	SER	2.1
1	B	140	SER	2.0
1	B	486	CYS	2.1
1	B	219	THR	2.0
1	A	195	GLU	2.0
1	B	19	LEU	2.0
1	B	254	LEU	2.0
1	A	182	GLY	2.0
1	A	235	LYS	2.0
1	B	468	THR	2.0
1	A	87	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	A	605	4/4	0.33	0.32	78,79,79,79	0
3	GOL	A	606	6/6	0.49	0.34	66,67,67,67	0
2	EDO	B	610	4/4	0.49	0.38	50,50,51,51	0
5	PGE	A	609	10/10	0.59	0.39	58,66,69,70	0
4	PEG	A	608	7/7	0.69	0.24	55,55,56,56	0
2	EDO	A	602	4/4	0.70	0.18	55,56,56,56	0
2	EDO	A	604	4/4	0.73	0.33	48,48,50,50	0
2	EDO	B	607	4/4	0.77	0.19	41,41,42,43	0
4	PEG	A	607	7/7	0.77	0.18	41,46,49,49	0
2	EDO	B	606	4/4	0.78	0.22	40,43,45,46	0
2	EDO	B	605	4/4	0.79	0.23	34,36,37,39	0
2	EDO	B	603	4/4	0.80	0.13	51,52,52,52	0
2	EDO	A	603	4/4	0.80	0.20	55,55,55,55	0
2	EDO	B	601	4/4	0.81	0.28	35,35,35,36	0
2	EDO	B	604	4/4	0.82	0.22	46,46,46,46	0
2	EDO	B	608	4/4	0.84	0.15	35,36,36,37	0
2	EDO	A	601	4/4	0.90	0.25	38,39,41,42	0
2	EDO	B	609	4/4	0.92	0.18	26,28,30,32	0
2	EDO	B	602	4/4	0.92	0.17	29,32,34,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.