



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:23 PM GMT

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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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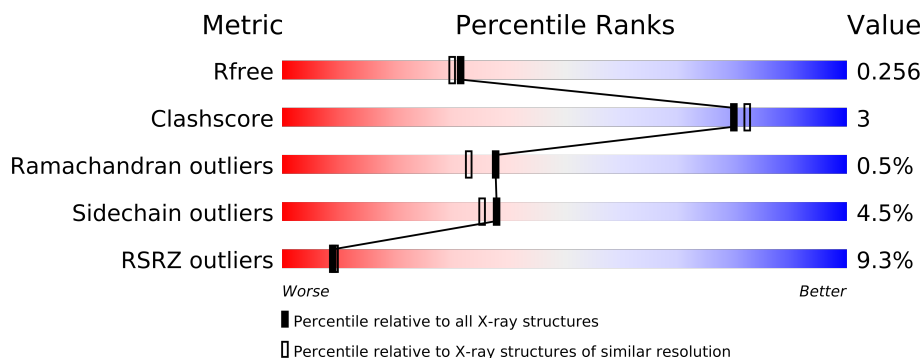
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	EDO	A	603	-	X
2	EDO	A	604	-	X
2	EDO	B	601	-	X
2	EDO	B	605	-	X
3	GOL	A	606	-	X
5	PGE	A	609	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8367 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

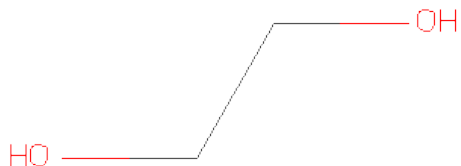
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q06124
A	-19	GLY	-	EXPRESSION TAG	UNP Q06124
A	-18	SER	-	EXPRESSION TAG	UNP Q06124
A	-17	SER	-	EXPRESSION TAG	UNP Q06124
A	-16	HIS	-	EXPRESSION TAG	UNP Q06124
A	-15	HIS	-	EXPRESSION TAG	UNP Q06124
A	-14	HIS	-	EXPRESSION TAG	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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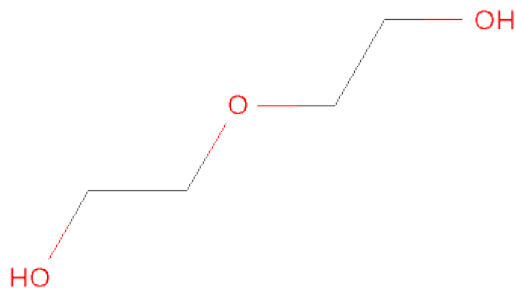
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	4	2	2	0	0

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



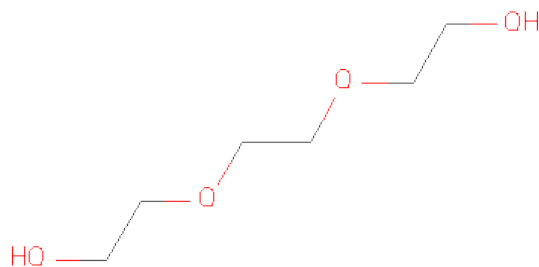
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0

- 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		

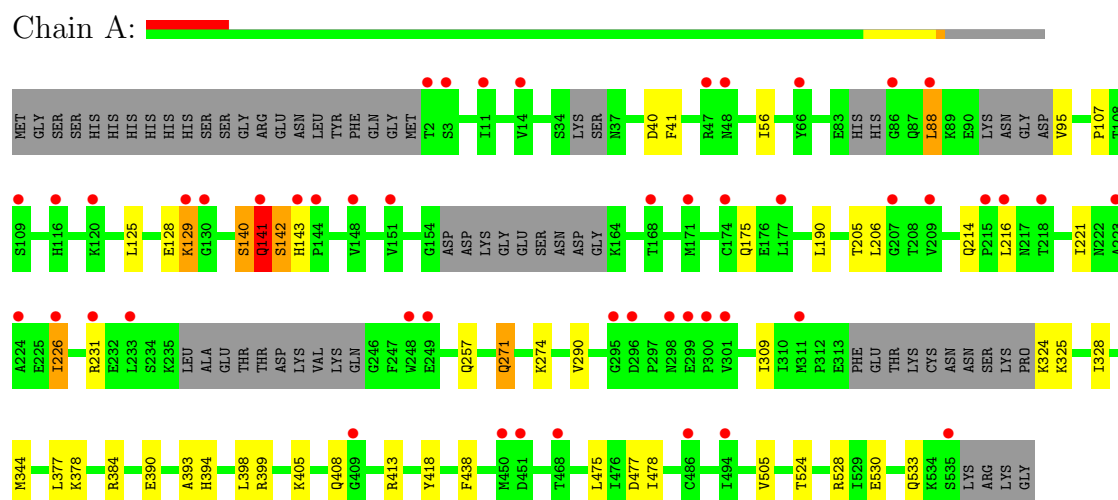
- Molecule 6 is water.

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

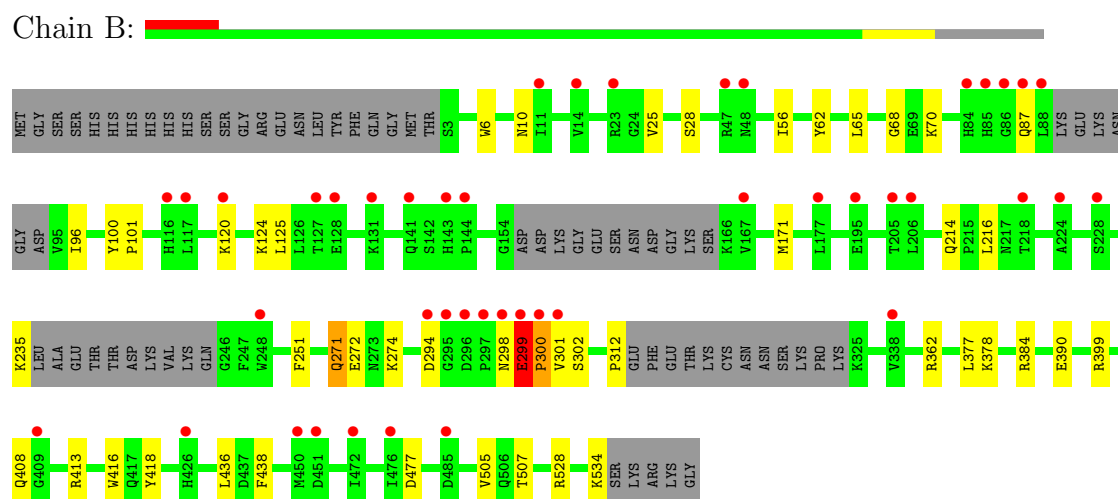
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 0.230 , 0.256	Depositor DCC
$R_{free}$ test set	1241 reflections (2.07%)	DCC
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> )	0.36 , 40.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 61105 reflections	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.

## 5 Model quality

### 5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (55) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:393:ALA:HB2	4:A:607:PEG:H11	2.00	0.43
1:A:475:LEU:HA	1:A:478:ILE:HD12	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:B:56:ILE:HG12	1:B:65:LEU:HD23	2.02	0.42
1:A:309:ILE:HD13	1:A:328:ILE:HG12	2.01	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%)	43	39
1	B	483/560 (86%)	465 (96%)	15 (3%)	3 (1%)	33	28
All	All	967/1120 (86%)	932 (96%)	30 (3%)	5 (0%)	38	33

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%)	36	33
1	B	438/498 (88%)	419 (96%)	19 (4%)	40	37
All	All	882/996 (89%)	842 (96%)	40 (4%)	38	35

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
1	A	206	LEU
1	A	214	GLN
1	A	226	ILE

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Mol	Chain	Res	Type
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 chains 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	A	601	-	3,3,3	0.48	0	2,2,2	0.47	0
2	EDO	A	602	-	3,3,3	0.72	0	2,2,2	0.31	0
2	EDO	A	603	-	3,3,3	0.63	0	2,2,2	0.37	0
2	EDO	A	604	-	3,3,3	0.62	0	2,2,2	0.47	0
2	EDO	A	605	-	3,3,3	0.71	0	2,2,2	0.23	0
3	GOL	A	606	-	5,5,5	0.14	0	5,5,5	0.30	0
4	PEG	A	607	-	6,6,6	0.09	0	5,5,5	0.08	0
4	PEG	A	608	-	6,6,6	0.11	0	5,5,5	0.09	0
5	PGE	A	609	-	9,9,9	0.09	0	8,8,8	0.16	0
2	EDO	B	601	-	3,3,3	0.51	0	2,2,2	0.53	0
2	EDO	B	602	-	3,3,3	0.66	0	2,2,2	0.24	0
2	EDO	B	603	-	3,3,3	0.63	0	2,2,2	0.42	0
2	EDO	B	604	-	3,3,3	0.63	0	2,2,2	0.39	0
2	EDO	B	605	-	3,3,3	0.60	0	2,2,2	0.35	0
2	EDO	B	606	-	3,3,3	0.71	0	2,2,2	0.28	0
2	EDO	B	607	-	3,3,3	0.68	0	2,2,2	0.33	0
2	EDO	B	608	-	3,3,3	0.68	0	2,2,2	0.33	0
2	EDO	B	609	-	3,3,3	0.60	0	2,2,2	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EDO	B	610	-	3,3,3	0.69	0	2,2,2	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	601	-	-	0/1/1/1	0/0/0/0
2	EDO	A	602	-	-	0/1/1/1	0/0/0/0
2	EDO	A	603	-	-	0/1/1/1	0/0/0/0
2	EDO	A	604	-	-	0/1/1/1	0/0/0/0
2	EDO	A	605	-	-	0/1/1/1	0/0/0/0
3	GOL	A	606	-	-	0/4/4/4	0/0/0/0
4	PEG	A	607	-	-	0/4/4/4	0/0/0/0
4	PEG	A	608	-	-	0/4/4/4	0/0/0/0
5	PGE	A	609	-	-	0/7/7/7	0/0/0/0
2	EDO	B	601	-	-	0/1/1/1	0/0/0/0
2	EDO	B	602	-	-	0/1/1/1	0/0/0/0
2	EDO	B	603	-	-	0/1/1/1	0/0/0/0
2	EDO	B	604	-	-	0/1/1/1	0/0/0/0
2	EDO	B	605	-	-	0/1/1/1	0/0/0/0
2	EDO	B	606	-	-	0/1/1/1	0/0/0/0
2	EDO	B	607	-	-	0/1/1/1	0/0/0/0
2	EDO	B	608	-	-	0/1/1/1	0/0/0/0
2	EDO	B	609	-	-	0/1/1/1	0/0/0/0
2	EDO	B	610	-	-	0/1/1/1	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.

## 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, 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%)	0.76	49 (9%)	8 8	14, 36, 62, 95	0
1	B	493/560 (88%)	0.80	44 (8%)	10 10	17, 36, 62, 85	0
All	All	990/1120 (88%)	0.78	93 (9%)	9 9	14, 36, 62, 95	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	GLN	6.3
1	A	48	ASN	5.0
1	B	205	THR	4.8
1	B	87	GLN	4.6
1	A	301	VAL	4.6
1	B	248	TRP	4.5
1	B	409	GLY	4.4
1	B	116	HIS	4.3
1	B	143	HIS	4.3
1	B	450	MET	4.1
1	B	451	ASP	4.1
1	A	486	CYS	4.0
1	A	14	VAL	3.9
1	B	294	ASP	3.8
1	A	120	LYS	3.8
1	B	298	ASN	3.7
1	B	301	VAL	3.7
1	B	85	HIS	3.7
1	B	299	GLU	3.6
1	B	11	ILE	3.5
1	A	300	PRO	3.5
1	A	231	ARG	3.5
1	B	141	GLN	3.4
1	A	296	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	177	LEU	3.3
1	B	88	LEU	3.3
1	B	485	ASP	3.2
1	B	296	ASP	3.2
1	A	66	TYR	3.1
1	B	297	PRO	3.1
1	A	2	THR	3.0
1	A	130	GLY	3.0
1	A	409	GLY	3.0
1	A	11	ILE	3.0
1	A	47	ARG	2.9
1	A	144	PRO	2.8
1	B	300	PRO	2.8
1	A	3	SER	2.8
1	B	48	ASN	2.8
1	A	223	ALA	2.8
1	B	86	GLY	2.8
1	A	86	GLY	2.7
1	B	177	LEU	2.7
1	B	426	HIS	2.7
1	A	451	ASP	2.6
1	A	129	LYS	2.6
1	B	295	GLY	2.6
1	B	117	LEU	2.6
1	B	338	VAL	2.6
1	B	84	HIS	2.6
1	A	298	ASN	2.6
1	B	218	THR	2.6
1	A	171	MET	2.5
1	A	116	HIS	2.5
1	B	228	SER	2.5
1	A	224	ALA	2.5
1	A	233	LEU	2.5
1	A	209	VAL	2.5
1	A	88	LEU	2.4
1	B	167	VAL	2.4
1	B	127	THR	2.4
1	A	535	SER	2.4
1	B	476	ILE	2.3
1	B	47	ARG	2.3
1	B	128	GLU	2.3
1	B	14	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	109	SER	2.3
1	A	218	THR	2.3
1	A	151	VAL	2.2
1	B	472	ILE	2.2
1	A	174	CYS	2.2
1	A	450	MET	2.2
1	B	120	LYS	2.2
1	B	144	PRO	2.2
1	A	299	GLU	2.1
1	B	23	ARG	2.1
1	A	248	TRP	2.1
1	A	311	MET	2.1
1	A	168	THR	2.1
1	A	148	VAL	2.1
1	A	216	LEU	2.1
1	A	143	HIS	2.1
1	A	215	PRO	2.1
1	A	249	GLU	2.1
1	B	224	ALA	2.0
1	A	494	ILE	2.0
1	A	207	GLY	2.0
1	A	468	THR	2.0
1	A	226	ILE	2.0
1	A	295	GLY	2.0
1	B	131	LYS	2.0
1	B	206	LEU	2.0
1	B	195	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	A	603	4/4	0.21	7.25	55,55,55,55	0
5	PGE	A	609	10/10	0.35	7.17	58,66,69,70	0
3	GOL	A	606	6/6	0.31	6.00	66,67,67,67	0
2	EDO	A	604	4/4	0.32	5.31	48,48,50,50	0
2	EDO	B	605	4/4	0.27	3.59	34,36,37,39	0
2	EDO	B	601	4/4	0.26	2.15	35,35,35,36	0
2	EDO	B	606	4/4	0.23	1.93	40,43,45,46	0
2	EDO	A	605	4/4	0.34	1.64	78,79,79,79	0
4	PEG	A	607	7/7	0.19	1.14	41,46,49,49	0
2	EDO	A	602	4/4	0.17	1.06	55,56,56,56	0
2	EDO	A	601	4/4	0.22	0.83	38,39,41,42	0
2	EDO	B	610	4/4	0.32	0.67	50,50,51,51	0
2	EDO	B	604	4/4	0.18	0.49	46,46,46,46	0
4	PEG	A	608	7/7	0.21	0.20	55,55,56,56	0
2	EDO	B	609	4/4	0.16	0.14	26,28,30,32	0
2	EDO	B	608	4/4	0.15	-0.22	35,36,36,37	0
2	EDO	B	607	4/4	0.16	-0.63	41,41,42,43	0
2	EDO	B	602	4/4	0.13	-0.92	29,32,34,36	0
2	EDO	B	603	4/4	0.13	-1.40	51,52,52,52	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.