



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:35 AM UTC

PDB ID : 4GWF / pdb_00004gwf
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

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

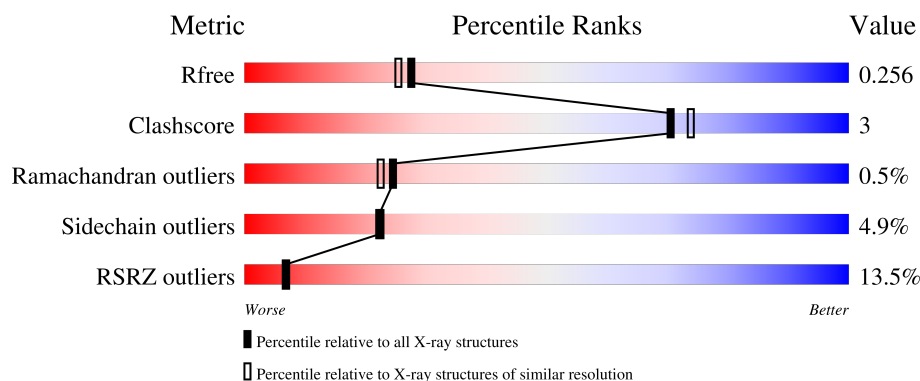
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (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	A	560	13% 77% 10% • 11%
1	B	560	11% 80% 8% 12%

2 Entry composition

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 (CCD ID: EDO) (formula: C₂H₆O₂).



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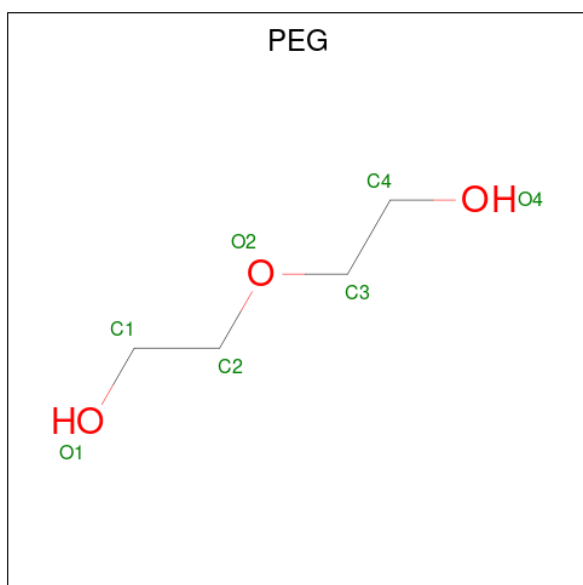
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



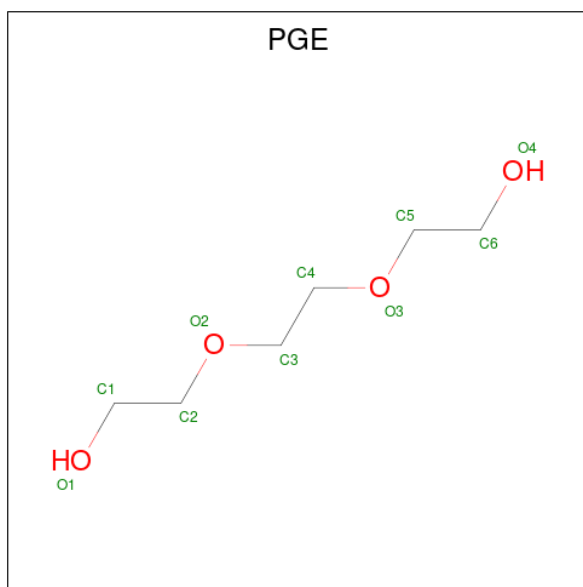
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: 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 (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

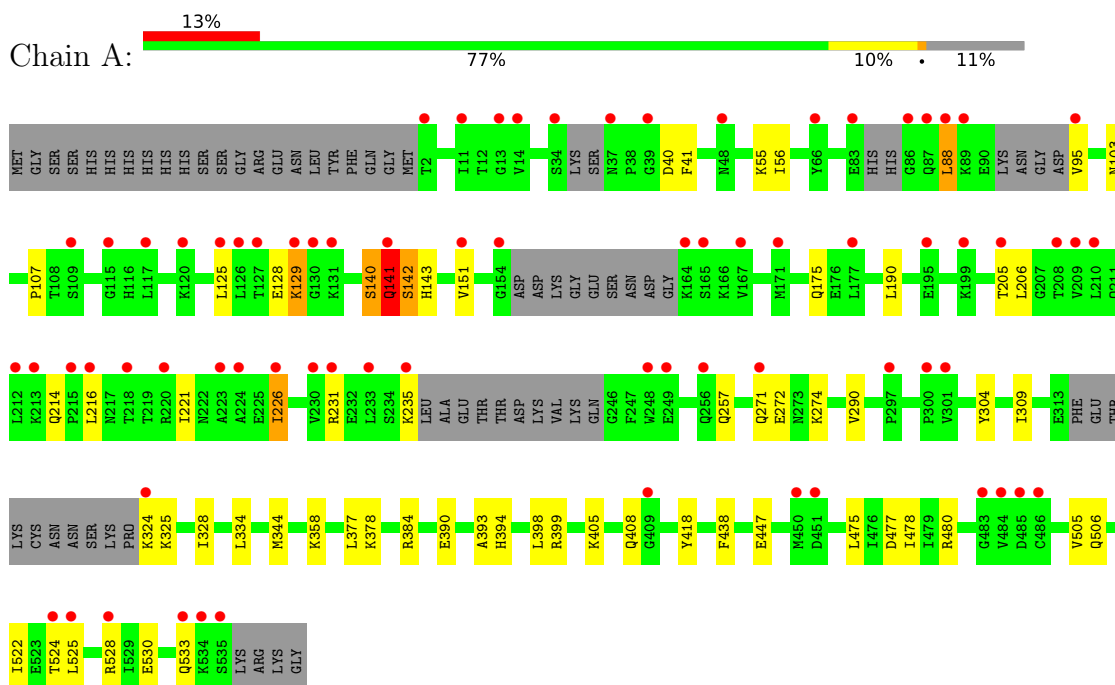
- Molecule 6 is water.

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

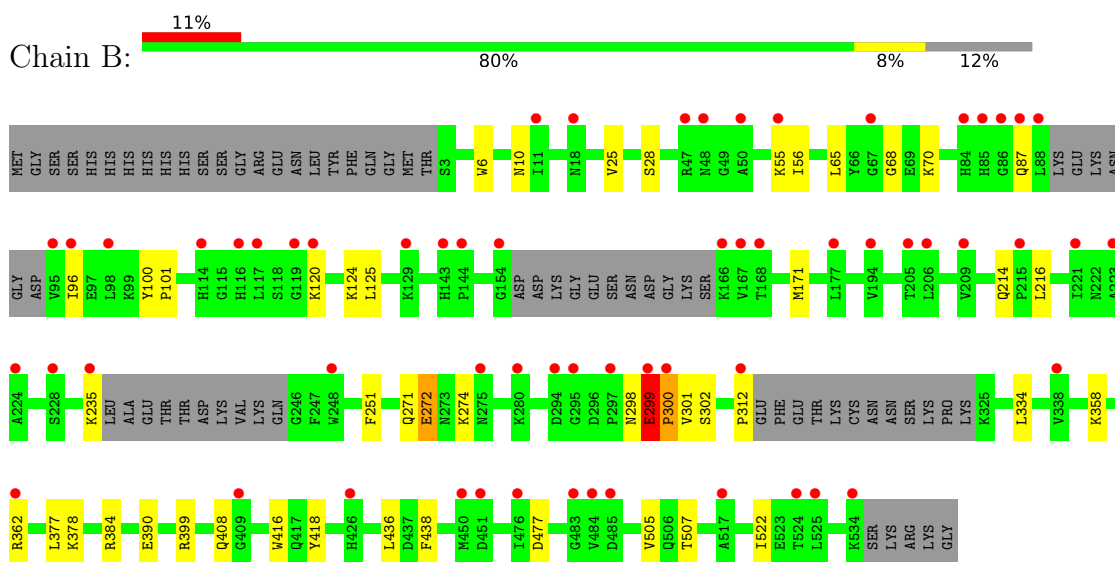
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: 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, α , β , γ	45.97Å 211.95Å 55.69Å 90.00° 96.63° 90.00°	Depositor
Resolution (Å)	42.00 – 2.10 42.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.00-2.10) 99.5 (42.00-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	28.6	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: PGE, EDO, GOL, PEG

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	0.73	1/4106 (0.0%)	1.22	6/5533 (0.1%)
1	B	0.71	0/4073	1.23	2/5494 (0.0%)
All	All	0.72	1/8179 (0.0%)	1.23	8/11027 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	HIS	N-CA	-6.13	1.40	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	HIS	N-CA-C	-10.46	90.97	108.75
1	A	358	LYS	N-CA-C	-6.57	101.68	110.55
1	A	334	LEU	N-CA-C	-6.33	100.60	110.42
1	B	358	LYS	N-CA-C	-5.88	102.61	110.55
1	B	334	LEU	N-CA-C	-5.84	101.37	110.42
1	A	506	GLN	N-CA-C	5.77	118.79	111.69
1	A	304	TYR	N-CA-C	5.47	118.40	109.59
1	A	103	ASN	N-CA-C	5.27	117.87	110.23

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

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:298:ASN:C	1:B:299:GLU:CG	2.58	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:141:GLN:O	1:A:141:GLN:NE2	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
1:B:298:ASN:C	1:B:299:GLU:HG2	2.24	0.59
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:A:141:GLN:O	1:A:141:GLN:CD	2.48	0.55
1:B:390:GLU:HG2	1:B:399:ARG:HG2	1.89	0.55
1:B:416:TRP:HZ3	2:B:608:EDO:H21	1.72	0.52
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: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:41:PHE:HB2	1:A:56:ILE:HB	2.01	0.42
1:A:107:PRO:HG3	1:A:190:LEU:HD12	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	484/560 (86%)	467 (96%)	15 (3%)	2 (0%)	30	28
1	B	483/560 (86%)	465 (96%)	15 (3%)	3 (1%)	21	18
All	All	967/1120 (86%)	932 (96%)	30 (3%)	5 (0%)	24	22

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 [i](#)

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%)	417 (94%)	27 (6%)	17	15
1	B	438/498 (88%)	422 (96%)	16 (4%)	30	33
All	All	882/996 (89%)	839 (95%)	43 (5%)	22	22

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	55	LYS
1	A	88	LEU
1	A	129	LYS
1	A	140	SER
1	A	141	GLN
1	A	142	SER
1	A	151	VAL
1	A	205	THR
1	A	206	LEU
1	A	214	GLN
1	A	226	ILE
1	A	231	ARG
1	A	235	LYS
1	A	272	GLU
1	A	324	LYS
1	A	325	LYS
1	A	378	LYS
1	A	447	GLU
1	A	477	ASP
1	A	480	ARG
1	A	522	ILE
1	A	524	THR
1	A	525	LEU
1	A	528	ARG
1	A	530	GLU
1	A	533	GLN
1	B	10	ASN
1	B	55	LYS
1	B	70	LYS
1	B	96	ILE
1	B	120	LYS
1	B	124	LYS
1	B	171	MET
1	B	214	GLN

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Mol	Chain	Res	Type
1	B	235	LYS
1	B	272	GLU
1	B	299	GLU
1	B	362	ARG
1	B	378	LYS
1	B	408	GLN
1	B	477	ASP
1	B	522	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	256	GLN
1	A	281	ASN
1	A	298	ASN
1	A	335	GLN
1	A	446	GLN
1	A	526	GLN
1	A	533	GLN
1	B	87	GLN
1	B	200	ASN
1	B	214	GLN
1	B	222	ASN
1	B	271	GLN
1	B	298	ASN
1	B	339	ASN

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 oligosaccharides 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	602	-	3,3,3	0.50	0	2,2,2	0.25	0
2	EDO	B	610	-	3,3,3	0.53	0	2,2,2	0.23	0
2	EDO	B	606	-	3,3,3	0.55	0	2,2,2	0.29	0
2	EDO	B	601	-	3,3,3	0.39	0	2,2,2	0.52	0
2	EDO	B	603	-	3,3,3	0.48	0	2,2,2	0.42	0
2	EDO	A	602	-	3,3,3	0.55	0	2,2,2	0.32	0
2	EDO	A	605	-	3,3,3	0.55	0	2,2,2	0.24	0
2	EDO	B	604	-	3,3,3	0.48	0	2,2,2	0.39	0
2	EDO	B	605	-	3,3,3	0.45	0	2,2,2	0.35	0
2	EDO	A	601	-	3,3,3	0.36	0	2,2,2	0.47	0
2	EDO	A	603	-	3,3,3	0.48	0	2,2,2	0.37	0
2	EDO	B	609	-	3,3,3	0.47	0	2,2,2	0.48	0
2	EDO	A	604	-	3,3,3	0.47	0	2,2,2	0.46	0
3	GOL	A	606	-	5,5,5	0.07	0	5,5,5	0.15	0
2	EDO	B	608	-	3,3,3	0.53	0	2,2,2	0.34	0
4	PEG	A	608	-	6,6,6	0.10	0	5,5,5	0.06	0
4	PEG	A	607	-	6,6,6	0.09	0	5,5,5	0.08	0
2	EDO	B	607	-	3,3,3	0.53	0	2,2,2	0.34	0
5	PGE	A	609	-	9,9,9	0.08	0	8,8,8	0.13	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	602	-	-	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	-
2	EDO	B	603	-	-	0/1/1/1	-
2	EDO	A	602	-	-	0/1/1/1	-

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

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	607	PEG	C4-C3-O2-C2
4	A	608	PEG	C4-C3-O2-C2
2	B	609	EDO	O1-C1-C2-O2
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	602	EDO	1	0
2	B	603	EDO	1	0
2	B	609	EDO	2	0
2	B	608	EDO	2	0
4	A	608	PEG	1	0
4	A	607	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	609	PGE	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	497/560 (88%)	0.83	73 (14%) 6 6	14, 36, 62, 95	1 (0%)
1	B	493/560 (88%)	0.86	61 (12%) 8 8	17, 36, 62, 85	0
All	All	990/1120 (88%)	0.85	134 (13%) 7 7	14, 36, 62, 95	1 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	LEU	7.1
1	B	87	GLN	4.9
1	A	86	GLY	4.9
1	B	534	LYS	4.9
1	B	86	GLY	4.7
1	A	154	GLY	4.0
1	B	167	VAL	3.8
1	A	535	SER	3.8
1	B	154	GLY	3.7
1	A	11	ILE	3.7
1	B	84	HIS	3.7
1	A	87	GLN	3.6
1	B	205	THR	3.6
1	A	2	THR	3.5
1	A	141	GLN	3.4
1	A	233	LEU	3.4
1	A	48	ASN	3.4
1	A	223	ALA	3.4
1	A	120	LYS	3.3
1	B	451	ASP	3.3
1	A	301	VAL	3.3
1	B	248	TRP	3.3
1	A	95	VAL	3.2
1	B	120	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	85	HIS	3.2
1	A	300	PRO	3.1
1	B	484	VAL	3.1
1	B	450	MET	3.1
1	A	235	LYS	3.0
1	B	235	LYS	3.0
1	A	39	GLY	3.0
1	A	486	CYS	3.0
1	B	206	LEU	2.9
1	A	14	VAL	2.9
1	B	166	LYS	2.9
1	B	117	LEU	2.9
1	A	83	GLU	2.9
1	B	143	HIS	2.8
1	A	451	ASP	2.8
1	A	210	LEU	2.8
1	B	95	VAL	2.8
1	A	215	PRO	2.8
1	A	409	GLY	2.8
1	B	517	ALA	2.7
1	A	297	PRO	2.7
1	B	476	ILE	2.7
1	A	34	SER	2.7
1	A	218	THR	2.7
1	B	312	PRO	2.7
1	A	208	THR	2.7
1	A	129	LYS	2.7
1	B	116	HIS	2.6
1	A	66	TYR	2.6
1	A	324	LYS	2.6
1	A	484	VAL	2.6
1	B	426	HIS	2.6
1	A	205	THR	2.6
1	B	177	LEU	2.6
1	A	224	ALA	2.6
1	A	88	LEU	2.6
1	A	216	LEU	2.6
1	A	226	ILE	2.6
1	B	223	ALA	2.6
1	B	300	PRO	2.6
1	A	164	LYS	2.5
1	B	48	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	230	VAL	2.5
1	B	119	GLY	2.5
1	B	114	HIS	2.5
1	A	117	LEU	2.5
1	A	450	MET	2.5
1	A	534	LYS	2.5
1	B	485	ASP	2.5
1	A	195	GLU	2.5
1	A	109	SER	2.5
1	A	151	VAL	2.4
1	B	11	ILE	2.5
1	A	115	GLY	2.4
1	B	483	GLY	2.4
1	A	171	MET	2.4
1	B	280	LYS	2.4
1	A	13	GLY	2.4
1	A	524	THR	2.4
1	B	168	THR	2.4
1	B	409	GLY	2.4
1	A	167	VAL	2.4
1	A	212	LEU	2.3
1	A	483	GLY	2.3
1	A	89	LYS	2.3
1	A	485	ASP	2.3
1	B	294	ASP	2.3
1	B	47	ARG	2.3
1	B	524	THR	2.3
1	A	525	LEU	2.3
1	B	362	ARG	2.3
1	B	209	VAL	2.3
1	B	144	PRO	2.3
1	B	215	PRO	2.3
1	B	297	PRO	2.3
1	A	271	GLN	2.2
1	A	130	GLY	2.2
1	A	248	TRP	2.2
1	A	533	GLN	2.2
1	A	37	ASN	2.2
1	B	275	ASN	2.2
1	A	209	VAL	2.2
1	B	338	VAL	2.2
1	B	295	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	249	GLU	2.2
1	A	127	THR	2.2
1	B	67	GLY	2.2
1	A	165	SER	2.2
1	B	129	LYS	2.2
1	B	96	ILE	2.1
1	B	221	ILE	2.1
1	A	131	LYS	2.1
1	B	299	GLU	2.1
1	B	224	ALA	2.1
1	A	126	LEU	2.1
1	B	98	LEU	2.1
1	A	220	ARG	2.1
1	A	528	ARG	2.1
1	B	50	ALA	2.1
1	B	228	SER	2.1
1	A	125	LEU	2.0
1	B	18	ASN	2.0
1	A	256	GLN	2.0
1	A	231	ARG	2.0
1	A	199	LYS	2.0
1	A	213	LYS	2.0
1	B	55	LYS	2.0
1	B	194	VAL	2.0
1	A	177	LEU	2.0
1	B	525	LEU	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($\text{\AA}^2$)	Q<0.9
2	EDO	A	602	4/4	0.58	0.20	55,56,56,56	0
2	EDO	A	605	4/4	0.64	0.32	78,79,79,79	0
5	PGE	A	609	10/10	0.68	0.25	58,66,69,70	0
2	EDO	B	610	4/4	0.73	0.20	50,50,51,51	0
3	GOL	A	606	6/6	0.75	0.19	66,67,67,67	0
2	EDO	A	603	4/4	0.76	0.16	55,55,55,55	0
2	EDO	A	604	4/4	0.76	0.16	48,48,50,50	0
2	EDO	B	608	4/4	0.78	0.12	35,36,36,37	0
4	PEG	A	608	7/7	0.79	0.15	55,55,56,56	0
2	EDO	B	606	4/4	0.80	0.16	40,43,45,46	0
2	EDO	B	605	4/4	0.80	0.18	34,36,37,39	0
2	EDO	B	601	4/4	0.82	0.15	35,35,35,36	0
4	PEG	A	607	7/7	0.83	0.16	41,46,49,49	0
2	EDO	B	603	4/4	0.84	0.13	51,52,52,52	0
2	EDO	B	604	4/4	0.85	0.12	46,46,46,46	0
2	EDO	B	607	4/4	0.87	0.11	41,41,42,43	0
2	EDO	B	609	4/4	0.89	0.11	26,28,30,32	0
2	EDO	B	602	4/4	0.89	0.10	29,32,34,36	0
2	EDO	A	601	4/4	0.92	0.13	38,39,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.