

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6E0V
Title	:	Apo crystal structure of the colanidase tailspike protein gp150 of Phage Phi92
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Deposited on	:	2018-07-07
Resolution	:	1.75 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 (i) 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 (1)) 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	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.75 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	А	626	90%	6%	•
1	В	626	90%	7%	•
1	С	626	92%	•	•



 $\mathbf{2}$

Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 30024 atoms, of which 13426 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.

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace
1	Δ	602	Total	С	Η	Ν	0	\mathbf{S}	0	9	0
	I A	002	9052	2895	4438	782	912	25	0		
1	D	602	Total	С	Н	Ν	0	S	0	11	0
	ГВ	002	9067	2902	4443	781	916	25	0	11	0
1	1 0	602	Total	С	Н	Ν	0	S	0	10	0
	602	9057	2898	4433	782	919	25	0	10		

• Molecule 1 is a protein called Bacteriophage Phi92 gp150.

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	179	SER	-	expression tag	UNP 17I026
В	179	SER	-	expression tag	UNP 17I026
С	179	SER	-	expression tag	UNP 17I026

• Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	7	Total Sr 7 7	0	0
2	В	9	Total Sr 9 9	0	0
2	С	8	Total Sr 8 8	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	3	Total Cl 3 3	0	0
3	В	3	Total Cl 3 3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	3	Total Cl 3 3	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Δ	1	Total C H O	0	0
4	A	T	14 3 8 3	0	0
1	Δ	1	Total C H O	0	Ο
4	Π	1	14 3 8 3	0	0
1	Δ	1	Total C H O	0	0
T	11	1	14 3 8 3	0	0
1	В	1	Total C H O	0	0
	D	I	14 3 8 3	0	0
4	В	1	Total C H O	0	0
	D	I	14 3 8 3	0	0
4	В	1	Total C H O	0	0
	D	I	14 3 8 3	0	0
4	С	1	Total C H O	0	0
T		1	14 3 8 3		0
4	C	1	Total C H O	0	0
T		1	14 3 8 3	0	0

• Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
Б	Λ	1	Total	С	Η	Ο	0	0
0	A	1	10	2	6	2	0	0
5	Λ	1	Total	С	Η	Ο	0	0
0	Л	1	10	2	6	2	0	0
5	В	1	Total	С	Η	0	0	0
0	D	1	10	2	6	2	0	0
5	В	1	Total	С	Η	0	0	0
0	D	1	10	2	6	2	0	0
5	В	1	Total	С	Η	0	0	0
0	D	1	10	2	6	2	0	0
5	C	1	Total	С	Η	0	0	0
0	U	1	10	2	6	2	0	0
5	С	1	Total	С	Η	Ο	0	0
0			10	2	6	2	0	0
5	С	1	Total	С	Η	Ο	0	0
0			10	2	6	2	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	977	Total O 977 977	0	0
6	В	908	Total O 908 908	0	0
6	С	738	Total O 738 738	0	0



3 Residue-property plots (i)

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: Bacteriophage Phi92 gp150







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants	118.40Å 118.40Å 140.17Å	Deneriten
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	48.15 - 1.75	Depositor
Resolution (A)	48.15 - 1.75	EDS
% Data completeness	99.7 (48.15-1.75)	Depositor
(in resolution range)	99.8 (48.15 - 1.75)	EDS
R _{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.74 (at 1.75 \text{\AA})$	Xtriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
B B.	0.134 , 0.163	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.131 , 0.159	DCC
R_{free} test set	4441 reflections (2.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	19.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39 , 60.9	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
	0.010 for -h,-k,l	
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
	0.016 for -k,-h,-l	
F_o, F_c correlation	0.98	EDS
Total number of atoms	30024	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: SR, EDO, CL, GOL

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	
1VIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.54	0/4739	0.67	1/6443~(0.0%)
1	В	0.50	0/4755	0.63	0/6464
1	С	0.44	0/4731	0.61	0/6435
All	All	0.50	0/14225	0.64	1/19342~(0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	A	642	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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	А	4614	4438	4436	25	0
1	В	4624	4443	4431	26	0
1	С	4624	4433	4430	23	0
2	А	7	0	0	0	0
2	В	9	0	0	0	0
2	С	8	0	0	0	0
3	А	3	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	3	0	0	0	0
3	С	3	0	0	0	0
4	А	18	24	24	0	0
4	В	18	24	24	0	0
4	С	12	16	16	0	0
5	А	8	12	12	0	0
5	В	12	18	17	1	0
5	С	12	18	18	0	0
6	А	977	0	0	4	7
6	В	908	0	0	7	4
6	С	738	0	0	10	4
All	All	16598	13426	13408	$\overline{74}$	13

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

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:544[B]:ASP:OD1	6:B:1001:HOH:O	1.82	0.94
1:C:544[B]:ASP:OD1	6:C:1001:HOH:O	1.84	0.94
1:C:544[B]:ASP:OD2	6:C:1002:HOH:O	1.86	0.94
1:C:630[A]:GLU:O	6:C:1003:HOH:O	1.95	0.83
1:A:544[B]:ASP:OD1	6:A:1001:HOH:O	2.01	0.78
1:B:756:ASP:OD1	6:B:1002:HOH:O	2.04	0.75
1:B:629:ASP:OD2	6:B:1004:HOH:O	2.08	0.70
1:B:544[B]:ASP:OD2	6:B:1005:HOH:O	2.08	0.70
1:B:561[B]:GLU:OE2	6:B:1006:HOH:O	2.13	0.67
1:C:586:ASN:HB2	6:C:1525:HOH:O	1.95	0.66
1:C:352:TYR:OH	6:C:1005:HOH:O	2.10	0.66
1:C:298:SER:OG	6:C:1004:HOH:O	2.05	0.65
1:A:629:ASP:OD2	6:A:1002:HOH:O	2.14	0.64
1:C:629[B]:ASP:N	1:C:629[B]:ASP:OD1	2.31	0.60
1:C:629[B]:ASP:HB2	6:C:1168:HOH:O	2.03	0.58
1:A:272:ARG:NH2	1:A:292:ASN:OD1	2.31	0.58
1:B:586:ASN:HB2	6:B:1635:HOH:O	2.03	0.57
1:A:251:ILE:HG21	1:A:277:ILE:HD13	1.87	0.57
1:C:296:MET:CE	1:C:298:SER:HB3	2.38	0.54
1:C:392:ASN:O	1:C:393:VAL:HG22	2.11	0.50
1:A:251:ILE:CG2	1:A:277:ILE:HD13	2.42	0.49
1:C:456:CYS:O	1:C:477:PRO:HA	2.14	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:405:GLU:HA	1:B:449:VAL:O	2.14	0.48
1:B:456:CYS:O	1:B:477:PRO:HA	2.15	0.47
1:A:405[A]:GLU:HA	1:A:449:VAL:O	2.14	0.47
1:B:436[B]:ASP:OD1	5:B:916:EDO:O2	2.30	0.46
1:A:405[B]:GLU:HA	1:A:449:VAL:O	2.14	0.46
1:A:467[A]:ASN:HA	1:A:499:ASP:O	2.15	0.46
1:B:714:LYS:NZ	6:B:1017:HOH:O	2.43	0.46
1:A:444:ARG:HA	1:A:466:LYS:O	2.15	0.46
1:A:518:ARG:HE	1:A:551[B]:GLU:CD	2.19	0.46
1:A:518:ARG:NE	1:A:551[B]:GLU:OE2	2.48	0.45
1:B:466:LYS:HA	1:B:498:GLN:O	2.15	0.45
1:C:296:MET:HE3	1:C:298:SER:HB3	1.99	0.45
1:C:296:MET:HE2	1:C:298:SER:HB3	1.98	0.45
1:A:456:CYS:O	1:A:477:PRO:HA	2.16	0.45
1:A:519:MET:HB2	1:A:548:SER:HB3	1.98	0.45
1:C:519:MET:HB2	1:C:548:SER:HB3	1.99	0.45
1:A:670:SER:HA	6:A:1109:HOH:O	2.17	0.45
1:A:467[B]:ASN:HA	1:A:499:ASP:O	2.17	0.44
1:B:370:VAL:HA	1:B:397:HIS:CE1	2.52	0.44
1:A:618:MET:O	1:A:643:CYS:HA	2.18	0.44
1:B:382:HIS:HA	1:B:410:ALA:O	2.18	0.44
1:A:381:ILE:O	1:A:409:ILE:HA	2.18	0.44
1:C:244:VAL:HG23	1:C:245:THR:N	2.33	0.43
1:B:501:GLU:OE2	1:B:541:LYS:CE	2.66	0.43
1:C:620:TRP:O	1:C:645:GLN:HA	2.17	0.43
1:A:382:HIS:HA	1:A:410:ALA:O	2.19	0.43
1:B:497:CYS:O	1:B:535:PRO:HA	2.19	0.43
1:B:591:ARG:N	1:B:591:ARG:HD2	2.34	0.43
1:B:541:LYS:HA	1:B:567:SER:O	2.19	0.43
1:C:444:ARG:HA	1:C:466:LYS:O	2.19	0.43
1:B:618:MET:O	1:B:643:CYS:HA	2.19	0.42
1:C:633[A]:VAL:HG22	6:C:1100:HOH:O	2.19	0.42
1:C:370:VAL:HA	1:C:397:HIS:CE1	2.55	0.42
1:A:497:CYS:O	1:A:535:PRO:HA	2.20	0.42
1:B:519:MET:HB2	1:B:548:SER:HB3	2.00	0.42
1:B:398:TYR:CG	1:B:402:LEU:HB2	2.55	0.42
1:B:467:ASN:HA	1:B:499:ASP:O	2.19	0.42
1:C:405:GLU:HA	1:C:449:VAL:O	2.20	0.42
1:C:308:ARG:NH1	6:C:1027:HOH:O	2.52	0.41
1:B:351:SER:HA	1:B:377:SER:O	2.20	0.41
1:A:591:ARG:N	1:A:591:ARG:HD2	2.36	0.41



Atom-1	Atom-2	Interatomic	Clash
	1100111 2	distance $(Å)$	overlap (Å)
1:A:436[B]:ASP:OD2	6:A:1003:HOH:O	2.21	0.41
1:C:551:GLU:OE1	6:C:1006:HOH:O	2.22	0.41
1:A:351:SER:HA	1:A:377:SER:O	2.20	0.41
1:A:398:TYR:CG	1:A:402:LEU:HB2	2.56	0.41
1:A:620:TRP:O	1:A:645:GLN:HA	2.21	0.41
1:B:377:SER:HA	1:B:405:GLU:O	2.21	0.41
1:C:541:LYS:HA	1:C:567:SER:O	2.21	0.40
1:B:471:ARG:HA	1:B:503:ASP:O	2.22	0.40
1:B:305:GLU:HA	1:B:324:TYR:O	2.21	0.40
1:B:381:ILE:O	1:B:409:ILE:HA	2.21	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
6:A:1069:HOH:O	6:A:1607:HOH:O[3_655]	1.84	0.36
6:B:1488:HOH:O	6:B:1510:HOH:O[3_555]	1.95	0.25
6:C:1432:HOH:O	6:C:1563:HOH:O[2_655]	1.96	0.24
6:A:1501:HOH:O	6:A:1703:HOH:O[3_655]	2.00	0.20
6:A:1438:HOH:O	6:A:1684:HOH:O[3_655]	2.01	0.19
6:C:1560:HOH:O	6:C:1664:HOH:O[2_655]	2.03	0.17
6:A:1264:HOH:O	6:A:1746:HOH:O[2_545]	2.08	0.12
6:B:1649:HOH:O	6:B:1777:HOH:O[2_555]	2.09	0.11
6:C:1229:HOH:O	6:C:1519:HOH:O[3_665]	2.09	0.11
6:B:1749:HOH:O	6:B:1837:HOH:O[3_555]	2.13	0.07
6:A:1397:HOH:O	6:B:1571:HOH:O[2_656]	2.15	0.05
6:A:1241:HOH:O	6:A:1241:HOH:O[2_545]	2.19	0.01
6:A:1661:HOH:O	6:C:1574:HOH:O[2_655]	2.19	0.01

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	Perce	ntiles
1	А	609/626~(97%)	584 (96%)	24 (4%)	1 (0%)	47	29
1	В	611/626~(98%)	585~(96%)	26 (4%)	0	100	100
1	С	610/626~(97%)	581 (95%)	29~(5%)	0	100	100
All	All	1830/1878~(97%)	1750 (96%)	79 (4%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	597	GLY

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	Percer	ntiles
1	А	499/509~(98%)	499 (100%)	0	100	100
1	В	501/509~(98%)	498 (99%)	3 (1%)	86	79
1	С	499/509~(98%)	499 (100%)	0	100	100
All	All	1499/1527~(98%)	1496 (100%)	3 (0%)	93	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	201	SER
1	В	786[A]	GLU
1	В	786[B]	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
1	С	236	GLN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 49 ligands modelled in this entry, 33 are monoatomic - leaving 16 for Mogul analysis.

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	Bos	Link	B	Bond leng		E	Bond ang	gles
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	GOL	С	912	-	5,5,5	1.08	0	$5,\!5,\!5$	0.93	0
4	GOL	С	913	-	5,5,5	0.94	0	$5,\!5,\!5$	0.93	0
4	GOL	В	914	-	5,5,5	0.90	0	$5,\!5,\!5$	0.82	0
5	EDO	В	918	-	3,3,3	0.61	0	2,2,2	0.17	0
4	GOL	В	913	-	5,5,5	0.69	0	$5,\!5,\!5$	1.05	0
4	GOL	А	911	-	5,5,5	0.63	0	$5,\!5,\!5$	0.92	0
5	EDO	В	917	-	3,3,3	0.49	0	2,2,2	0.54	0
4	GOL	А	912	-	5,5,5	0.75	0	$5,\!5,\!5$	1.01	0
5	EDO	А	914	-	3,3,3	0.54	0	2,2,2	0.26	0
5	EDO	В	916	2	3,3,3	0.48	0	2,2,2	0.31	0
4	GOL	В	915	-	5,5,5	1.00	0	$5,\!5,\!5$	1.26	0
5	EDO	С	914	-	3,3,3	0.47	0	2,2,2	0.37	0
5	EDO	С	916	-	3,3,3	0.43	0	2,2,2	0.51	0
5	EDO	А	915	-	3,3,3	0.32	0	2,2,2	0.46	0
4	GOL	A	913	-	5,5,5	1.16	1 (20%)	$5,\!5,\!5$	1.04	0
5	EDO	С	915	-	3,3,3	0.45	0	2,2,2	0.32	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
4	GOL	С	912	-	-	0/4/4/4	-
4	GOL	С	913	-	-	2/4/4/4	-
4	GOL	В	914	-	-	0/4/4/4	-
5	EDO	В	918	-	-	1/1/1/1	-
4	GOL	В	913	-	-	0/4/4/4	-
4	GOL	А	911	-	-	2/4/4/4	-
5	EDO	В	917	-	-	1/1/1/1	-
4	GOL	А	912	-	-	2/4/4/4	-
5	EDO	А	914	-	-	0/1/1/1	-
5	EDO	В	916	2	-	0/1/1/1	-
4	GOL	В	915	-	-	0/4/4/4	-
5	EDO	С	914	-	-	0/1/1/1	-
5	EDO	С	916	-	-	0/1/1/1	-
5	EDO	A	915	-	-	1/1/1/1	-
4	GOL	A	913	-	-	0/4/4/4	-
5	EDO	С	915	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
4	А	913	GOL	C3-C2	2.05	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	911	GOL	C1-C2-C3-O3
4	А	912	GOL	C1-C2-C3-O3
4	С	913	GOL	O1-C1-C2-C3
4	С	913	GOL	O1-C1-C2-O2
5	А	915	EDO	O1-C1-C2-O2
5	В	917	EDO	O1-C1-C2-O2
4	А	911	GOL	O2-C2-C3-O3
4	А	912	GOL	O2-C2-C3-O3
5	В	918	EDO	O1-C1-C2-O2



There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	916	EDO	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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	602/626~(96%)	-0.46	5 (0%) 86 90	12, 18, 31, 78	0
1	В	602/626~(96%)	-0.13	22 (3%) 41 48	14, 21, 33, 70	0
1	С	602/626~(96%)	-0.02	41 (6%) 17 22	14, 26, 49, 86	0
All	All	1806/1878~(96%)	-0.20	68 (3%) 40 47	12, 21, 44, 86	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	202	TYR	7.6
1	С	781	VAL	5.1
1	С	244	VAL	4.8
1	А	202	TYR	4.8
1	В	202	TYR	4.6
1	С	783	PRO	4.3
1	С	752	ALA	4.3
1	С	206	ASN	4.3
1	С	207	LEU	4.3
1	А	203	VAL	4.2
1	С	753	ASN	4.0
1	С	754	GLY	4.0
1	С	755	GLY	3.9
1	С	201	SER	3.9
1	В	416	GLY	3.9
1	С	751	GLY	3.9
1	В	352	TYR	3.8
1	С	782	THR	3.4
1	С	780	ILE	3.3
1	С	203	VAL	3.2
1	В	419	ALA	3.2
1	А	207	LEU	3.1
1	С	719	VAL	3.0



Mol	Chain	Res	Type	RSRZ
1	В	528	ASN	3.0
1	С	750	ALA	3.0
1	В	324	TYR	3.0
1	С	629[A]	ASP	2.9
1	С	749	GLY	2.8
1	В	449	VAL	2.8
1	В	621	VAL	2.8
1	С	631[A]	THR	2.8
1	С	784	THR	2.7
1	В	646	VAL	2.7
1	С	790	ILE	2.6
1	С	746	VAL	2.6
1	С	204	GLU	2.6
1	В	569	ILE	2.5
1	С	646	VAL	2.5
1	C	757	LEU	2.5
1	В	207	LEU	2.5
1	С	711	ASP	2.5
1	С	621	VAL	2.5
1	С	720	THR	2.4
1	В	790[A]	ILE	2.4
1	С	779	PRO	2.4
1	С	717	ALA	2.4
1	В	647	GLY	2.3
1	A	646	VAL	2.3
1	В	568	ASN	2.3
1	В	303	TRP	2.2
1	C	205	LYS	2.2
1	B	529	GLY	2.2
1	C	748	PRO	2.2
1	В	406	ASN	2.2
1	B	530	ARG	2.1
1	C	274	THR	2.1
1	B	622	GLY	2.1
1	A	205	LYS	2.1
1	B	203	VAL	2.1
1	C	623	CYS	2.1
1	C	208	LEU	2.1
1	C	718	THR	2.0
1	C	216	MET	2.0
1	В	377	SER	2.0
1	B	586	ASN	2.0



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Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	756	ASP	2.0
1	С	788	THR	2.0
1	С	721	GLY	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 monosaccharides 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^{th} 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
5	EDO	В	917	4/4	0.75	0.19	$56,\!67,\!67,\!69$	0
5	EDO	В	916	4/4	0.83	0.15	52,62,64,65	0
5	EDO	А	914	4/4	0.83	0.20	44,53,55,56	0
4	GOL	А	911	6/6	0.85	0.13	45,54,56,56	0
5	EDO	С	914	4/4	0.85	0.12	$63,\!75,\!76,\!77$	0
4	GOL	В	913	6/6	0.88	0.33	52,62,65,66	0
5	EDO	А	915	4/4	0.90	0.14	47,56,57,59	0
5	EDO	В	918	4/4	0.90	0.19	$36,\!43,\!51,\!51$	0
2	SR	В	906	1/1	0.90	0.17	62,62,62,62	1
4	GOL	В	914	6/6	0.91	0.23	34,42,46,50	0
4	GOL	В	915	6/6	0.92	0.10	27,38,43,46	0
4	GOL	С	912	6/6	0.92	0.13	38,45,48,51	0
4	GOL	А	913	6/6	0.93	0.10	$23,\!32,\!37,\!39$	0
4	GOL	С	913	6/6	0.93	0.17	$39,\!47,\!53,\!54$	0
4	GOL	А	912	6/6	0.95	0.10	32,44,53,56	0
5	EDO	С	915	4/4	0.95	0.07	36,43,49,52	0
2	SR	А	907	1/1	0.96	0.15	$65,\!65,\!65,\!65$	1
5	EDO	С	916	4/4	0.96	0.12	24,40,48,51	0
2	SR	В	908	1/1	0.98	0.09	36,36,36,36	1
2	SR	В	909	1/1	0.98	0.23	64,64,64,64	1



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
2	SR	С	908	1/1	0.99	0.15	43,43,43,43	1
3	CL	С	910	1/1	0.99	0.07	32,32,32,32	0
2	SR	В	905	1/1	0.99	0.13	$27,\!27,\!27,\!27$	1
2	SR	А	905	1/1	0.99	0.05	27,27,27,27	1
2	SR	В	907	1/1	0.99	0.16	60,60,60,60	1
2	SR	А	904	1/1	0.99	0.05	28,28,28,28	1
2	SR	В	904	1/1	0.99	0.08	40,40,40,40	1
2	SR	С	906	1/1	0.99	0.09	39,39,39,39	1
2	SR	С	907	1/1	0.99	0.16	44,44,44,44	1
3	CL	В	912	1/1	1.00	0.03	23,23,23,23	0
3	CL	С	909	1/1	1.00	0.07	29,29,29,29	1
2	SR	А	906	1/1	1.00	0.06	30,30,30,30	1
3	CL	С	911	1/1	1.00	0.04	28,28,28,28	0
2	SR	А	903	1/1	1.00	0.12	26,26,26,26	1
2	SR	В	901	1/1	1.00	0.06	$17,\!17,\!17,\!17$	1
2	SR	В	902	1/1	1.00	0.07	26,26,26,26	1
2	SR	С	901	1/1	1.00	0.08	$22,\!22,\!22,\!22$	1
2	SR	С	902	1/1	1.00	0.09	23,23,23,23	1
2	SR	С	903	1/1	1.00	0.10	34,34,34,34	1
2	SR	С	904	1/1	1.00	0.06	$27,\!27,\!27,\!27$	1
2	SR	С	905	1/1	1.00	0.04	36, 36, 36, 36	1
2	SR	В	903	1/1	1.00	0.13	$29,\!29,\!29,\!29$	1
2	SR	А	901	1/1	1.00	0.01	$15,\!15,\!15,\!15$	1
2	SR	А	902	1/1	1.00	0.06	$18,\!18,\!18,\!18$	1
3	CL	А	908	1/1	1.00	0.04	$17,\!17,\!17,\!17$	0
3	CL	A	909	1/1	1.00	0.08	$25,\!25,\!25,\!25,\!25$	1
3	CL	A	910	1/1	1.00	0.05	$31,\!31,\!31,\!31$	0
3	CL	В	910	1/1	1.00	0.06	$26,\!26,\!26,\!26$	1
3	CL	В	911	1/1	1.00	0.05	39, 39, 39, 39, 39	0

6.5 Other polymers (i)

There are no such residues in this entry.

