



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2025 – 04:07 pm BST

PDB ID : 9G7Q / pdb_00009g7q
Title : Structure of the StayRose dimer
Authors : Crow, A.
Deposited on : 2024-07-22
Resolution : 1.65 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

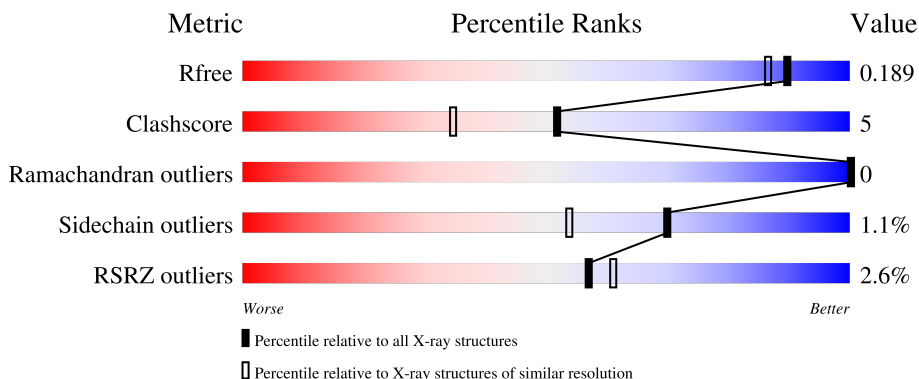
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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	227	
1	B	227	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4155 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 StayRose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	18	0
			1876	1178	326	360	12			
1	B	214	Total	C	N	O	S	0	20	0
			1890	1187	333	358	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	HIS	-	expression tag	UNP A0A8S0GSD4
A	-10	HIS	-	expression tag	UNP A0A8S0GSD4
A	-9	HIS	-	expression tag	UNP A0A8S0GSD4
A	-8	HIS	-	expression tag	UNP A0A8S0GSD4
A	-7	HIS	-	expression tag	UNP A0A8S0GSD4
A	-6	HIS	-	expression tag	UNP A0A8S0GSD4
A	-5	HIS	-	expression tag	UNP A0A8S0GSD4
A	-4	HIS	-	expression tag	UNP A0A8S0GSD4
A	-3	HIS	-	expression tag	UNP A0A8S0GSD4
A	-2	HIS	-	expression tag	UNP A0A8S0GSD4
A	-1	GLY	-	expression tag	UNP A0A8S0GSD4
A	0	SER	-	expression tag	UNP A0A8S0GSD4
A	58	A1IJF	GLY	chromophore	UNP A0A8S0GSD4
A	58	A1IJF	TYR	chromophore	UNP A0A8S0GSD4
A	58	A1IJF	GLY	chromophore	UNP A0A8S0GSD4
A	168	ALA	VAL	engineered mutation	UNP A0A8S0GSD4
B	-11	HIS	-	expression tag	UNP A0A8S0GSD4
B	-10	HIS	-	expression tag	UNP A0A8S0GSD4
B	-9	HIS	-	expression tag	UNP A0A8S0GSD4
B	-8	HIS	-	expression tag	UNP A0A8S0GSD4
B	-7	HIS	-	expression tag	UNP A0A8S0GSD4
B	-6	HIS	-	expression tag	UNP A0A8S0GSD4
B	-5	HIS	-	expression tag	UNP A0A8S0GSD4
B	-4	HIS	-	expression tag	UNP A0A8S0GSD4
B	-3	HIS	-	expression tag	UNP A0A8S0GSD4

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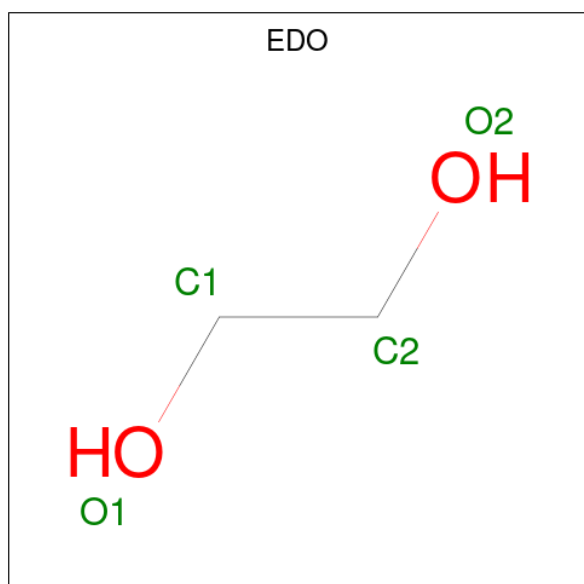
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP A0A8S0GSD4
B	-1	GLY	-	expression tag	UNP A0A8S0GSD4
B	0	SER	-	expression tag	UNP A0A8S0GSD4
B	58	A1IJF	GLY	chromophore	UNP A0A8S0GSD4
B	58	A1IJF	TYR	chromophore	UNP A0A8S0GSD4
B	58	A1IJF	GLY	chromophore	UNP A0A8S0GSD4
B	168	ALA	VAL	engineered mutation	UNP A0A8S0GSD4

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

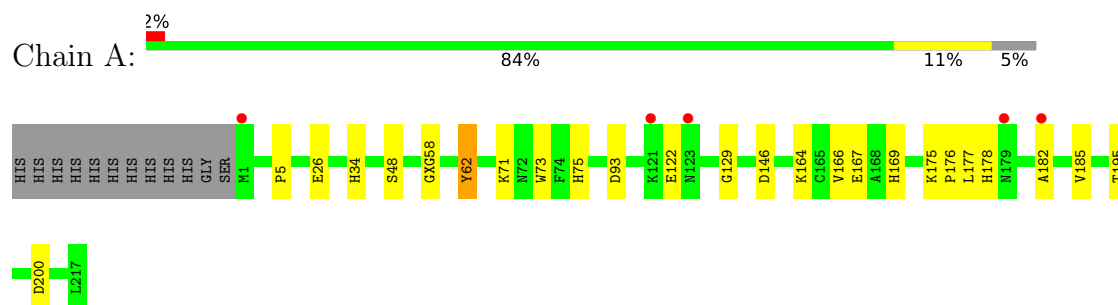
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	179	Total O 179 179	0	0
4	B	160	Total O 160 160	0	0

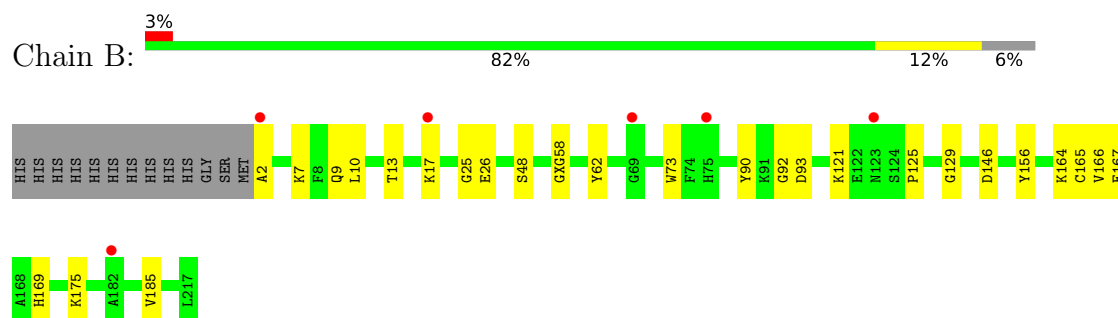
3 Residue-property plots [i](#)

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: StayRose



- Molecule 1: StayRose



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	133.31Å 133.31Å 58.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.63 – 1.65 43.63 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.63-1.65) 98.5 (43.63-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.154 , 0.178 0.167 , 0.189	Depositor DCC
R_{free} test set	3537 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4155	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: CL, EDO, A1IJF

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	0.70	0/1909	1.04	4/2579 (0.2%)
1	B	0.69	0/1923	1.03	1/2594 (0.0%)
All	All	0.70	0/3832	1.04	5/5173 (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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	93	ASP	CA-CB-CG	7.44	120.04	112.60
1	A	93	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	200	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	178	HIS	CA-CB-CG	5.30	119.10	113.80
1	A	34	HIS	CA-CB-CG	5.28	119.08	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	B	164	LYS	Mainchain

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	1876	0	1743	17	0
1	B	1890	0	1769	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	40	0	58	2	0
3	B	8	0	12	0	0
4	A	179	0	0	1	0
4	B	160	0	0	4	0
All	All	4155	0	3582	37	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 5.

All (37) 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:A:177[B]:LEU:O	1:A:177[B]:LEU:HD23	1.82	0.79
1:A:177[B]:LEU:HD23	1:A:177[B]:LEU:C	2.14	0.73
1:B:7:LYS:HE2	1:B:9[B]:GLN:HE21	1.61	0.66
1:B:7:LYS:HE2	1:B:9[B]:GLN:NE2	2.13	0.64
1:A:62:TYR:O	1:A:75[B]:HIS:CE1	2.52	0.63
1:B:146:ASP:OD2	1:B:175:LYS:NZ	2.31	0.62
1:A:62:TYR:O	1:A:75[B]:HIS:HE1	1.81	0.62
1:A:146:ASP:OD2	1:A:175:LYS:HE2	2.00	0.61
1:B:121[A]:LYS:NZ	4:B:403:HOH:O	2.37	0.58
1:B:166[A]:VAL:HG23	4:B:435:HOH:O	2.06	0.56
1:B:167:GLU:OE2	1:B:169[B]:HIS:HE1	1.90	0.55
1:A:176:PRO:HG2	1:A:182:ALA:HB2	1.90	0.53
1:B:48[B]:SER:OG	1:B:129:GLY:HA2	2.09	0.53
1:A:176:PRO:CG	1:A:182:ALA:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:GLU:OE2	1:B:169[B]:HIS:CE1	2.67	0.48
1:A:71:LYS:O	1:A:71:LYS:HG3	2.13	0.47
1:A:48[B]:SER:OG	1:A:129:GLY:HA2	2.14	0.47
1:A:177[B]:LEU:C	1:A:177[B]:LEU:CD2	2.85	0.47
1:B:156:TYR:HB2	1:B:166[A]:VAL:HG12	1.96	0.46
1:A:167:GLU:OE2	1:A:169[B]:HIS:CE1	2.68	0.46
1:A:195:THR:HG23	3:A:305:EDO:H21	1.96	0.46
1:B:2:ALA:O	4:B:401:HOH:O	2.21	0.45
1:A:75[B]:HIS:CE1	4:A:456:HOH:O	2.70	0.44
1:B:7:LYS:CE	1:B:9[B]:GLN:HE21	2.28	0.44
1:A:73:TRP:CG	1:A:185:VAL:HG22	2.52	0.44
1:B:25:GLY:O	1:B:26[B]:GLU:HG3	2.17	0.43
1:B:73:TRP:CG	1:B:185:VAL:HG22	2.54	0.43
1:B:92:GLY:O	1:B:121[A]:LYS:HE2	2.19	0.42
1:A:167:GLU:OE2	1:A:169[B]:HIS:HE1	2.02	0.42
1:B:165[B]:CYS:SG	4:B:535:HOH:O	2.18	0.42
1:B:7:LYS:CE	1:B:9[B]:GLN:NE2	2.82	0.42
1:B:13[A]:THR:HA	1:B:17[A]:LYS:O	2.20	0.42
1:B:125:PRO:HG2	1:B:166[B]:VAL:HG21	2.01	0.41
1:B:10:LEU:HD23	1:B:10:LEU:C	2.46	0.41
1:A:5:PRO:HA	1:A:26[B]:GLU:HG2	2.01	0.41
1:B:90:TYR:HD2	1:B:166[A]:VAL:HG22	1.85	0.40
1:A:195:THR:OG1	3:A:309:EDO:C1	2.70	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	228/227 (100%)	223 (98%)	5 (2%)	0	100	100
1	B	229/227 (101%)	225 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	457/454 (101%)	448 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	208/201 (104%)	204 (98%)	4 (2%)	52	30
1	B	209/201 (104%)	208 (100%)	1 (0%)	86	80
All	All	417/402 (104%)	412 (99%)	5 (1%)	70	50

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	TYR
1	A	122	GLU
1	A	166[A]	VAL
1	A	166[B]	VAL
1	B	62	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	106	ASN
1	A	170	GLN
1	B	170	GLN
1	B	179	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	A1IJF	B	58	1	21,21,22	0.80	0	27,29,31	1.17	3 (11%)
1	A1IJF	A	58	1	21,21,22	0.94	1 (4%)	27,29,31	1.33	4 (14%)

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
1	A1IJF	B	58	1	-	2/6/25/26	0/2/2/2
1	A1IJF	A	58	1	-	1/6/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	A1IJF	C1-N3	2.76	1.41	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	A1IJF	O3-C3-CA3	-3.46	115.95	126.39
1	A	58	A1IJF	O2-C2-CA2	-3.23	129.15	130.96
1	B	58	A1IJF	O3-C3-CA3	-3.04	117.21	126.39
1	B	58	A1IJF	O2-C2-CA2	-2.34	129.65	130.96
1	B	58	A1IJF	C1-CA1-N1	-2.20	107.98	112.85
1	A	58	A1IJF	CG2-CB2-CA2	2.04	132.45	129.94
1	A	58	A1IJF	CD1-CE1-CZ	2.04	121.32	118.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	58	A1IJF	N2-CA2-CB2-CG2
1	A	58	A1IJF	C2-CA2-CB2-CG2
1	B	58	A1IJF	C2-CA2-CB2-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	A	305	-	3,3,3	0.38	0	2,2,2	0.77	0
3	EDO	A	302	-	3,3,3	0.97	0	2,2,2	0.29	0
3	EDO	A	310	-	3,3,3	0.37	0	2,2,2	0.79	0
3	EDO	A	304	-	3,3,3	0.17	0	2,2,2	0.30	0
3	EDO	B	303	-	3,3,3	0.16	0	2,2,2	0.47	0
3	EDO	A	306	-	3,3,3	1.08	0	2,2,2	0.64	0
3	EDO	B	302	-	3,3,3	0.26	0	2,2,2	0.11	0
3	EDO	A	308	-	3,3,3	0.18	0	2,2,2	0.13	0
3	EDO	A	309	-	3,3,3	0.21	0	2,2,2	0.49	0
3	EDO	A	307	-	3,3,3	0.21	0	2,2,2	0.24	0
3	EDO	A	303	-	3,3,3	0.12	0	2,2,2	0.73	0
3	EDO	A	311	-	3,3,3	0.36	0	2,2,2	0.15	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
3	EDO	A	305	-	-	0/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	A	310	-	-	1/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-
3	EDO	B	303	-	-	0/1/1/1	-
3	EDO	A	306	-	-	1/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
3	EDO	A	308	-	-	0/1/1/1	-
3	EDO	A	309	-	-	0/1/1/1	-
3	EDO	A	307	-	-	0/1/1/1	-
3	EDO	A	303	-	-	1/1/1/1	-
3	EDO	A	311	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	306	EDO	O1-C1-C2-O2
3	A	302	EDO	O1-C1-C2-O2
3	A	310	EDO	O1-C1-C2-O2
3	A	303	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	305	EDO	1	0
3	A	309	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, 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	214/227 (94%)	-0.23	5 (2%) 61 65	7, 17, 32, 68	18 (8%)
1	B	213/227 (93%)	-0.26	6 (2%) 55 59	8, 17, 30, 50	20 (9%)
All	All	427/454 (94%)	-0.25	11 (2%) 57 61	7, 17, 32, 68	38 (8%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.2
1	B	2	ALA	4.2
1	A	121[A]	LYS	3.2
1	B	75[A]	HIS	3.1
1	B	182	ALA	3.0
1	A	182	ALA	2.7
1	A	179	ASN	2.2
1	B	17[A]	LYS	2.1
1	B	123[A]	ASN	2.1
1	A	123[A]	ASN	2.0
1	B	69	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	A1IJF	A	58	20/21	0.97	0.06	12,13,17,19	0
1	A1IJF	B	58	20/21	0.98	0.05	12,15,17,18	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	B	303	4/4	0.87	0.14	36,37,44,45	0
3	EDO	A	305	4/4	0.88	0.16	34,35,38,47	0
3	EDO	B	302	4/4	0.89	0.15	36,37,41,47	0
3	EDO	A	307	4/4	0.90	0.14	39,43,44,47	0
3	EDO	A	308	4/4	0.90	0.14	40,42,43,48	0
3	EDO	A	304	4/4	0.91	0.12	34,36,39,39	0
3	EDO	A	310	4/4	0.91	0.20	24,29,33,41	0
3	EDO	A	309	4/4	0.93	0.12	32,35,36,55	0
3	EDO	A	306	4/4	0.93	0.16	25,35,36,40	0
3	EDO	A	302	4/4	0.94	0.14	26,28,28,32	0
3	EDO	A	303	4/4	0.95	0.09	28,30,32,32	0
3	EDO	A	311	4/4	0.96	0.09	22,23,23,24	0
2	CL	A	301	1/1	0.99	0.03	18,18,18,18	0
2	CL	B	301	1/1	0.99	0.03	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.