



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:34 PM UTC

PDB ID : 6SQX / pdb_00006sqx
Title : Insights into a novel NlpC/P60 Endopeptidase from *Photobacterium damsela* subsp. *piscicida*
Authors : Lisboa, J.; Pereira, P.J.B.; dos Santos, N.M.S.
Deposited on : 2019-09-04
Resolution : 1.40 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

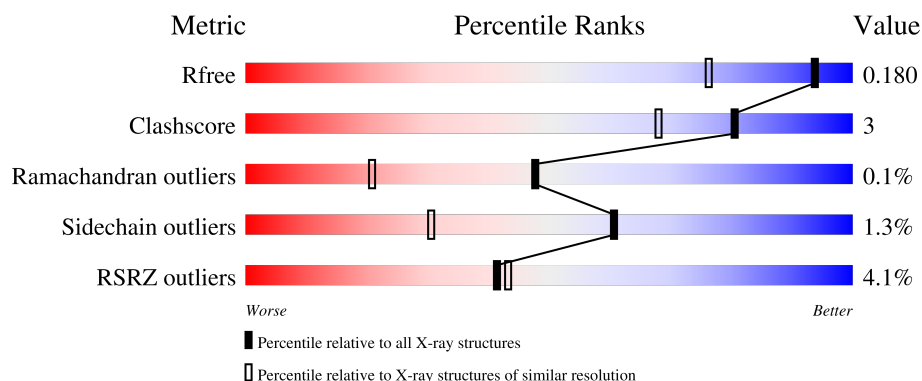
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	499	5% 85% 6% 8%
1	B	499	3% 86% 6% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	518	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8870 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.

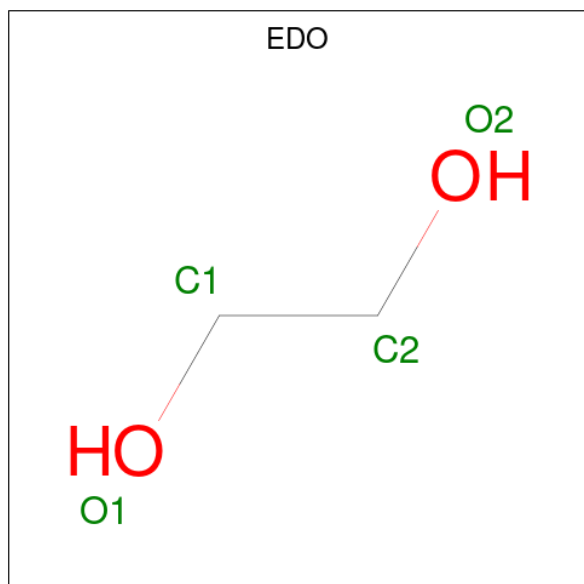
- Molecule 1 is a protein called Peptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	25	0
			3817	2449	627	726	15			
1	B	457	Total	C	N	O	S	0	25	0
			3829	2452	631	730	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cl	0	0
			3	3		
2	B	3	Total	Cl	0	0
			3	3		

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



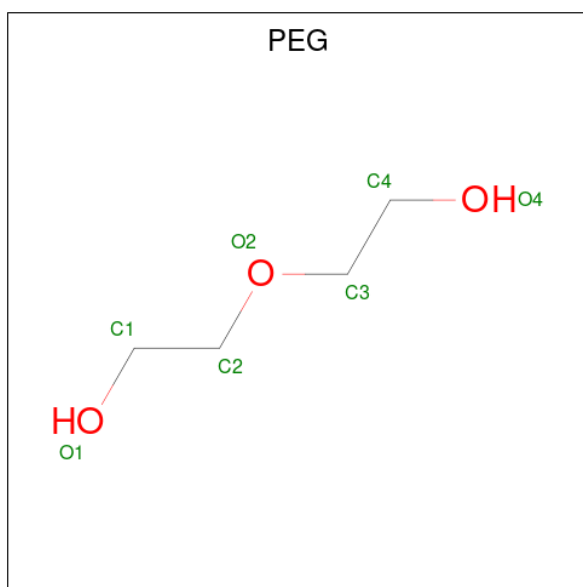
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0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

Continued on next page...

Continued from previous page...

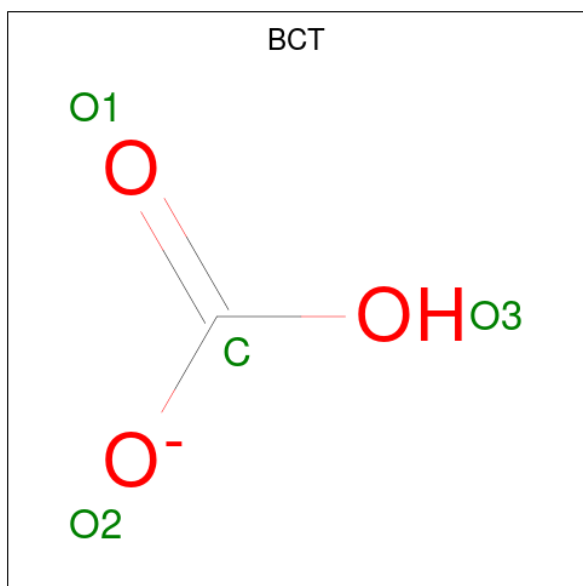
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

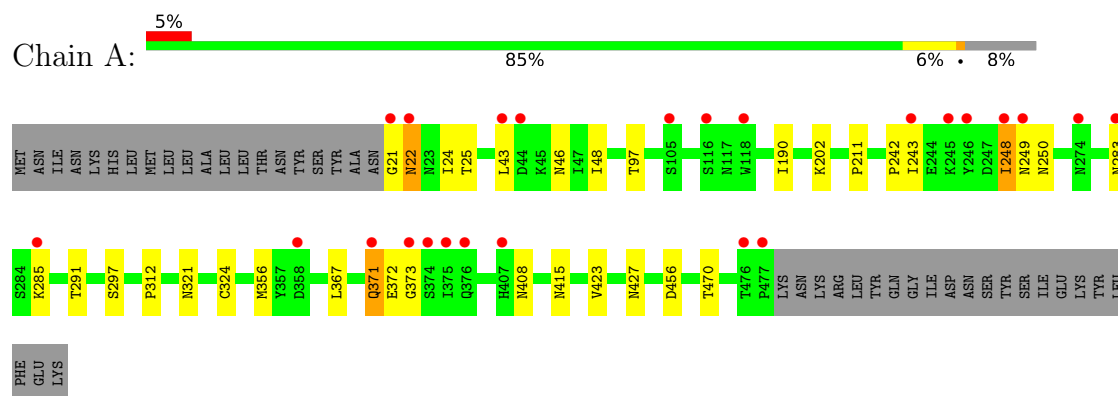
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	507	Total 508	O 508	0	1
6	B	547	Total 547	O 547	0	0

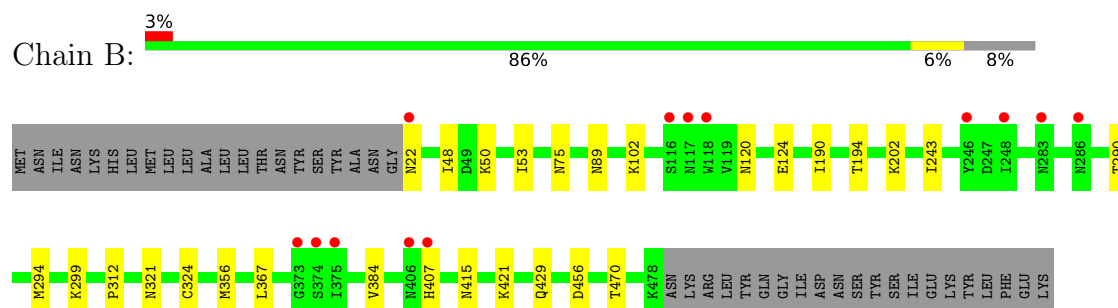
3 Residue-property plots

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: Peptide-binding protein



• Molecule 1: Peptide-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.58Å 109.97Å 130.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.29 – 1.40 38.29 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.29-1.40) 99.9 (38.29-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.147 , 0.175 0.153 , 0.180	Depositor DCC
R_{free} test set	10708 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8870	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, OCS, CL, BCT

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	0.48	0/3960	0.63	2/5387 (0.0%)
1	B	0.48	0/3969	0.62	0/5395
All	All	0.48	0/7929	0.62	2/10782 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	GLY	CA-C-N	6.51	133.98	121.54
1	A	21	GLY	C-N-CA	6.51	133.98	121.54

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	A	3817	0	3754	21	0
1	B	3829	0	3757	20	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	68	0	102	3	0
3	B	84	0	126	8	0
4	A	7	0	10	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	1	0	0
6	A	508	0	0	3	0
6	B	547	0	0	3	0
All	All	8870	0	7750	41	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 (41) 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:243[A]:ILE:HD11	1:A:250:ASN:HA	1.56	0.88
1:B:75:ASN:HB3	3:B:518:EDO:H22	1.58	0.84
1:B:356:MET:HE1	1:B:470:THR:HG23	1.65	0.77
1:A:367:LEU:HD13	1:A:373:GLY:HA3	1.67	0.76
1:B:89:ASN:HD21	3:B:518:EDO:H21	1.55	0.70
1:A:243[A]:ILE:HD11	1:A:250:ASN:CA	2.22	0.70
1:A:291[B]:THR:HG21	6:A:911:HOH:O	1.97	0.65
1:B:89:ASN:ND2	3:B:518:EDO:H21	2.13	0.64
1:A:356:MET:HE1	1:A:470:THR:HG23	1.80	0.64
1:B:290:THR:HG21	1:B:294:MET:HE2	1.81	0.63
1:B:194:THR:HB	3:B:522:EDO:H22	1.82	0.61
1:B:356:MET:CE	1:B:470:THR:HG23	2.34	0.56
1:A:456:ASP:HB3	3:A:515:EDO:H21	1.89	0.54
1:A:427:ASN:HD21	4:A:521:PEG:H21	1.73	0.54
1:A:285:LYS:HD3	1:A:285:LYS:H	1.74	0.53
1:B:421:LYS:NZ	1:B:429[A]:GLN:HE21	2.08	0.52
1:B:102:LYS:NZ	6:B:604:HOH:O	2.41	0.52
6:A:750:HOH:O	3:B:516:EDO:H21	2.09	0.51
1:B:384[B]:VAL:HG12	1:B:470:THR:HG22	1.93	0.50
1:B:299:LYS:HD3	6:B:862:HOH:O	2.11	0.50
1:A:371:GLN:HB3	6:A:709:HOH:O	2.12	0.49
1:A:97:THR:HA	3:A:520:EDO:H22	1.94	0.49
1:A:46:ASN:HA	1:A:297:SER:HA	1.94	0.48
1:B:190[B]:ILE:HD11	1:B:202:LYS:HE3	1.95	0.48
1:A:423:VAL:HG21	4:A:521:PEG:H12	1.95	0.48
1:B:48:ILE:HD11	1:B:53:ILE:HD13	1.94	0.48
1:B:367:LEU:HB2	6:B:982:HOH:O	2.15	0.46
1:A:242:PRO:HG2	1:A:283:ASN:O	2.16	0.46
1:A:243[B]:ILE:HD13	3:B:521:EDO:H11	1.99	0.45
1:B:89:ASN:HD21	3:B:518:EDO:C2	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190[B]:ILE:HD11	1:A:202:LYS:HE3	1.99	0.44
1:A:24[B]:ILE:HG22	1:A:25:THR:O	2.19	0.43
1:B:456:ASP:OD1	3:B:511:EDO:H12	2.18	0.43
1:A:43:LEU:HD11	1:B:243:ILE:HG21	2.00	0.43
1:A:243[A]:ILE:HD13	1:A:243[A]:ILE:HA	1.70	0.43
1:B:312:PRO:O	1:B:321:ASN:HB3	2.18	0.43
1:A:312:PRO:O	1:A:321:ASN:HB3	2.18	0.43
1:A:248:ILE:O	1:A:249:ASN:ND2	2.53	0.42
1:B:421:LYS:HE3	1:B:429[A]:GLN:HG2	2.02	0.41
1:A:211:PRO:HG3	3:A:511:EDO:H22	2.04	0.40
1:B:120:ASN:O	1:B:124[A]:GLU:HG3	2.21	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	479/499 (96%)	474 (99%)	4 (1%)	1 (0%)	43	19
1	B	479/499 (96%)	474 (99%)	5 (1%)	0	100	100
All	All	958/998 (96%)	948 (99%)	9 (1%)	1 (0%)	48	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ASN

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	433/447 (97%)	426 (98%)	7 (2%)	55	23
1	B	434/447 (97%)	430 (99%)	4 (1%)	70	44
All	All	867/894 (97%)	856 (99%)	11 (1%)	61	30

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	48	ILE
1	A	248	ILE
1	A	371	GLN
1	A	372	GLU
1	A	408	ASN
1	A	415	ASN
1	B	22	ASN
1	B	50	LYS
1	B	407	HIS
1	B	415	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	36	HIS
1	A	225	GLN
1	A	249	ASN
1	A	262	HIS
1	A	376	GLN
1	A	406	ASN
1	B	22	ASN
1	B	147	ASN
1	B	406	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	OCS	A	324	1	6,8,9	1.30	1 (16%)	7,11,13	1.44	1 (14%)
1	OCS	B	324	1	6,8,9	0.98	0	7,11,13	1.10	1 (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	OCS	A	324	1	-	1/4/7/9	-
1	OCS	B	324	1	-	1/4/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	OCS	CB-CA	2.64	1.55	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	OCS	OD2-SG-CB	2.72	111.23	105.97
1	B	324	OCS	OD3-SG-CB	2.38	110.31	106.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	324	OCS	N-CA-CB-SG
1	B	324	OCS	N-CA-CB-SG

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 46 ligands modelled in this entry, 6 are monoatomic - leaving 40 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	508	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	B	512	-	3,3,3	0.43	0	2,2,2	0.50	0
3	EDO	B	506	-	3,3,3	0.68	0	2,2,2	0.40	0
3	EDO	B	523	-	3,3,3	0.49	0	2,2,2	0.33	0
3	EDO	B	522	-	3,3,3	0.38	0	2,2,2	0.28	0
3	EDO	A	506	-	3,3,3	0.56	0	2,2,2	0.43	0
3	EDO	B	516	-	3,3,3	0.59	0	2,2,2	0.11	0
5	BCT	B	525	-	3,3,3	1.06	0	2,3,3	4.18	1 (50%)
3	EDO	A	509	-	3,3,3	0.46	0	2,2,2	0.60	0
3	EDO	B	505	-	3,3,3	0.19	0	2,2,2	0.38	0
3	EDO	B	517	-	3,3,3	0.35	0	2,2,2	0.52	0
3	EDO	A	520	-	3,3,3	0.47	0	2,2,2	0.34	0
3	EDO	B	508	-	3,3,3	0.70	0	2,2,2	0.34	0
3	EDO	B	515	-	3,3,3	0.70	0	2,2,2	0.07	0
3	EDO	B	514	-	3,3,3	0.49	0	2,2,2	0.25	0
3	EDO	B	520	-	3,3,3	0.42	0	2,2,2	0.27	0
3	EDO	B	521	-	3,3,3	0.39	0	2,2,2	0.84	0
3	EDO	B	509	-	3,3,3	0.37	0	2,2,2	0.53	0
3	EDO	A	511	-	3,3,3	0.47	0	2,2,2	0.41	0
3	EDO	B	507	-	3,3,3	0.46	0	2,2,2	0.07	0
3	EDO	A	513	-	3,3,3	0.37	0	2,2,2	0.65	0
3	EDO	A	510	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	A	504	-	3,3,3	0.42	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	507	-	3,3,3	0.40	0	2,2,2	0.64	0
3	EDO	A	514	-	3,3,3	0.34	0	2,2,2	0.74	0
3	EDO	B	524	-	3,3,3	0.50	0	2,2,2	0.39	0
3	EDO	A	519	-	3,3,3	0.39	0	2,2,2	0.44	0
3	EDO	A	518	-	3,3,3	0.56	0	2,2,2	0.28	0
3	EDO	B	511	-	3,3,3	0.46	0	2,2,2	0.36	0
4	PEG	A	521	-	6,6,6	0.11	0	5,5,5	0.09	0
3	EDO	A	515	-	3,3,3	0.43	0	2,2,2	0.41	0
3	EDO	B	519	-	3,3,3	0.42	0	2,2,2	0.39	0
3	EDO	B	513	-	3,3,3	0.52	0	2,2,2	0.07	0
3	EDO	B	518	-	3,3,3	0.55	0	2,2,2	0.25	0
3	EDO	A	516	-	3,3,3	0.40	0	2,2,2	0.76	0
3	EDO	B	510	-	3,3,3	0.47	0	2,2,2	0.60	0
3	EDO	B	504	-	3,3,3	0.58	0	2,2,2	0.25	0
3	EDO	A	512	-	3,3,3	0.39	0	2,2,2	0.45	0
3	EDO	A	517	-	3,3,3	0.43	0	2,2,2	0.55	0
3	EDO	A	505	-	3,3,3	0.46	0	2,2,2	0.21	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	508	-	-	0/1/1/1	-
3	EDO	B	512	-	-	0/1/1/1	-
3	EDO	B	506	-	-	0/1/1/1	-
3	EDO	B	523	-	-	1/1/1/1	-
3	EDO	B	522	-	-	0/1/1/1	-
3	EDO	A	506	-	-	0/1/1/1	-
3	EDO	B	516	-	-	0/1/1/1	-
3	EDO	A	509	-	-	0/1/1/1	-
3	EDO	B	505	-	-	0/1/1/1	-
3	EDO	B	517	-	-	0/1/1/1	-
3	EDO	A	520	-	-	0/1/1/1	-
3	EDO	B	508	-	-	0/1/1/1	-
3	EDO	B	515	-	-	0/1/1/1	-
3	EDO	B	514	-	-	0/1/1/1	-
3	EDO	B	520	-	-	1/1/1/1	-
3	EDO	B	521	-	-	1/1/1/1	-
3	EDO	B	509	-	-	0/1/1/1	-
3	EDO	A	511	-	-	0/1/1/1	-
3	EDO	B	507	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	513	-	-	1/1/1/1	-
3	EDO	A	510	-	-	0/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	507	-	-	1/1/1/1	-
3	EDO	A	514	-	-	0/1/1/1	-
3	EDO	B	524	-	-	0/1/1/1	-
3	EDO	A	519	-	-	1/1/1/1	-
3	EDO	A	518	-	-	1/1/1/1	-
3	EDO	B	511	-	-	0/1/1/1	-
4	PEG	A	521	-	-	1/4/4/4	-
3	EDO	A	515	-	-	0/1/1/1	-
3	EDO	B	519	-	-	0/1/1/1	-
3	EDO	B	513	-	-	1/1/1/1	-
3	EDO	B	518	-	-	1/1/1/1	-
3	EDO	A	516	-	-	1/1/1/1	-
3	EDO	B	510	-	-	0/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
3	EDO	A	512	-	-	0/1/1/1	-
3	EDO	A	517	-	-	0/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	525	BCT	O2-C-O1	5.65	134.12	119.68

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	513	EDO	O1-C1-C2-O2
3	A	518	EDO	O1-C1-C2-O2
4	A	521	PEG	C4-C3-O2-C2
3	A	519	EDO	O1-C1-C2-O2
3	B	518	EDO	O1-C1-C2-O2
3	A	516	EDO	O1-C1-C2-O2
3	B	513	EDO	O1-C1-C2-O2
3	B	520	EDO	O1-C1-C2-O2
3	B	523	EDO	O1-C1-C2-O2
3	A	507	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	521	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	522	EDO	1	0
3	B	516	EDO	1	0
3	A	520	EDO	1	0
3	B	521	EDO	1	0
3	A	511	EDO	1	0
3	B	511	EDO	1	0
4	A	521	PEG	2	0
3	A	515	EDO	1	0
3	B	518	EDO	4	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	456/499 (91%)	-0.11	24 (5%) 32 34	9, 23, 50, 95	25 (5%)
1	B	456/499 (91%)	-0.22	13 (2%) 53 56	9, 22, 45, 81	25 (5%)
All	All	912/998 (91%)	-0.17	37 (4%) 41 43	9, 23, 47, 95	50 (5%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	GLY	5.4
1	A	248	ILE	5.1
1	A	246	TYR	4.6
1	A	243[A]	ILE	4.4
1	A	373	GLY	4.4
1	A	375	ILE	4.1
1	A	477	PRO	3.6
1	A	22	ASN	3.6
1	B	246	TYR	3.3
1	B	407	HIS	3.3
1	B	22	ASN	3.2
1	B	117	ASN	3.2
1	B	375	ILE	3.2
1	A	374	SER	3.1
1	A	249	ASN	2.9
1	A	407	HIS	2.9
1	B	116	SER	2.9
1	A	358	ASP	2.7
1	B	373	GLY	2.6
1	A	371	GLN	2.6
1	B	118	TRP	2.6
1	B	406	ASN	2.5
1	A	476	THR	2.4
1	A	116	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	283	ASN	2.4
1	A	118	TRP	2.3
1	B	374	SER	2.3
1	B	248	ILE	2.2
1	A	274	ASN	2.2
1	B	286	ASN	2.2
1	A	376	GLN	2.2
1	A	44	ASP	2.1
1	A	43	LEU	2.1
1	A	105[A]	SER	2.1
1	B	283	ASN	2.1
1	A	245	LYS	2.0
1	A	285	LYS	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	OCS	A	324	9/10	0.99	0.04	16,17,23,25	0
1	OCS	B	324	9/10	0.99	0.04	14,16,20,23	0

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(Å ²)	Q<0.9
5	BCT	B	525	4/4	0.72	0.23	27,36,56,66	0
3	EDO	B	518	4/4	0.74	0.20	41,48,49,60	0
4	PEG	A	521	7/7	0.75	0.27	29,29,30,30	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	B	516	4/4	0.79	0.20	35,41,44,44	0
3	EDO	B	524	4/4	0.81	0.20	35,49,51,52	0
3	EDO	B	523	4/4	0.82	0.19	50,52,61,67	0
3	EDO	B	519	4/4	0.82	0.14	57,58,59,64	0
3	EDO	A	518	4/4	0.84	0.17	40,40,53,55	0
3	EDO	A	517	4/4	0.85	0.17	42,43,48,55	0
3	EDO	A	511	4/4	0.85	0.14	50,52,54,60	0
3	EDO	A	519	4/4	0.85	0.15	42,48,52,66	0
3	EDO	B	504	4/4	0.85	0.16	40,41,42,45	0
3	EDO	B	511	4/4	0.85	0.14	45,47,55,57	0
3	EDO	A	515	4/4	0.85	0.13	48,54,55,59	0
3	EDO	B	521	4/4	0.86	0.14	38,43,44,60	0
3	EDO	B	522	4/4	0.86	0.12	48,53,55,64	0
3	EDO	A	520	4/4	0.87	0.12	50,56,56,62	0
3	EDO	A	516	4/4	0.87	0.18	52,52,55,58	0
3	EDO	B	520	4/4	0.87	0.16	42,43,56,63	0
3	EDO	B	514	4/4	0.88	0.13	45,49,52,67	0
3	EDO	B	512	4/4	0.88	0.13	43,49,53,55	0
3	EDO	B	517	4/4	0.88	0.18	28,33,49,52	0
3	EDO	A	514	4/4	0.89	0.14	37,43,52,54	0
3	EDO	A	509	4/4	0.90	0.14	46,46,49,52	0
3	EDO	B	513	4/4	0.90	0.14	36,37,52,57	0
3	EDO	A	507	4/4	0.91	0.13	28,34,37,46	0
3	EDO	A	513	4/4	0.92	0.13	30,34,37,50	0
3	EDO	A	506	4/4	0.92	0.11	29,30,31,37	0
3	EDO	A	508	4/4	0.92	0.11	34,35,35,39	0
3	EDO	B	515	4/4	0.93	0.12	24,37,43,44	0
3	EDO	A	510	4/4	0.93	0.10	43,50,50,54	0
3	EDO	B	510	4/4	0.93	0.10	31,31,37,38	0
3	EDO	B	505	4/4	0.94	0.09	26,27,27,30	0
3	EDO	B	506	4/4	0.95	0.10	32,33,37,38	0
3	EDO	A	505	4/4	0.95	0.09	29,32,34,36	0
3	EDO	B	507	4/4	0.96	0.10	28,33,40,44	0
3	EDO	A	512	4/4	0.96	0.09	21,31,32,34	0
3	EDO	B	509	4/4	0.97	0.08	23,30,33,37	0
2	CL	A	501	1/1	0.97	0.06	21,21,21,21	0
2	CL	A	502	1/1	0.97	0.08	23,23,23,23	0
2	CL	A	503	1/1	0.97	0.12	29,29,29,29	0
3	EDO	A	504	4/4	0.97	0.08	27,32,34,39	0
3	EDO	B	508	4/4	0.97	0.07	24,27,30,33	0
2	CL	B	503	1/1	0.98	0.07	23,23,23,23	0
2	CL	B	502	1/1	0.99	0.05	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	501	1/1	0.99	0.05	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.