



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:15 AM UTC

PDB ID : 7WSS / pdb_00007wss
Title : Collagenase from Grimontia (Vibrio) hollisae 1706B
Authors : Ikeuchi, T.; Yasumoto, M.; Takita, T.; Mizutani, K.; Mikami, B.; Tanaka, K.;
Hattori, S.; Yasukawa, K.
Deposited on : 2022-02-01
Resolution : 2.19 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

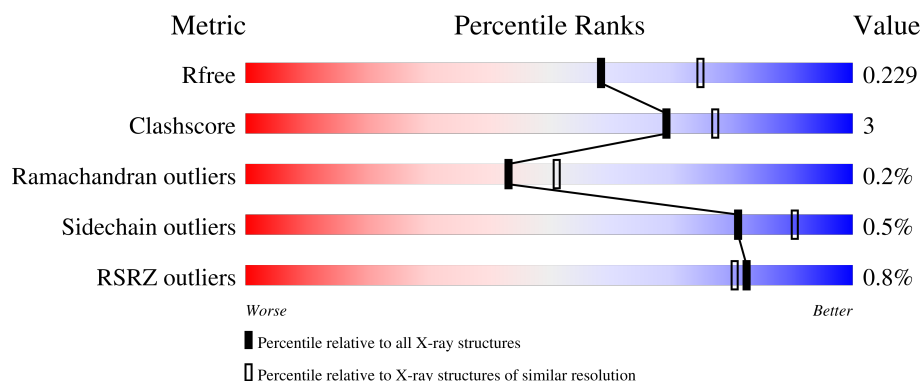
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

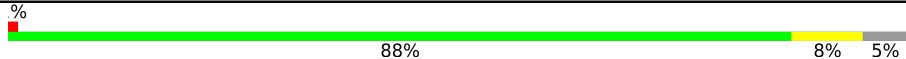
The reported resolution of this entry is 2.19 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	559	
1	B	559	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9236 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 Microbial collagenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	8	0
			4275	2704	721	833	17			
1	B	533	Total	C	N	O	S	0	7	0
			4268	2700	721	828	19			

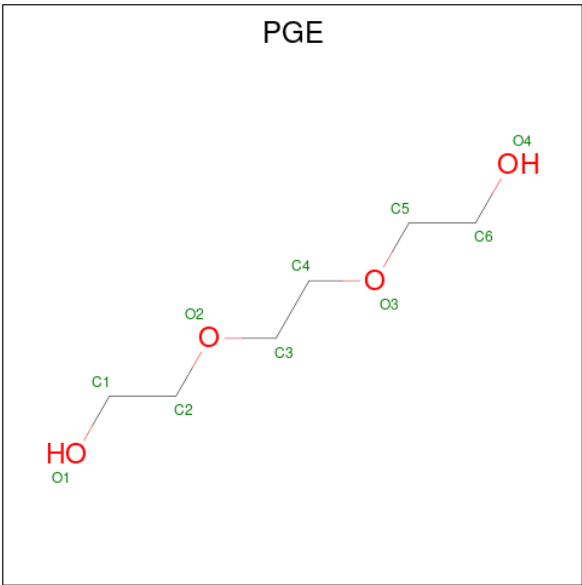
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

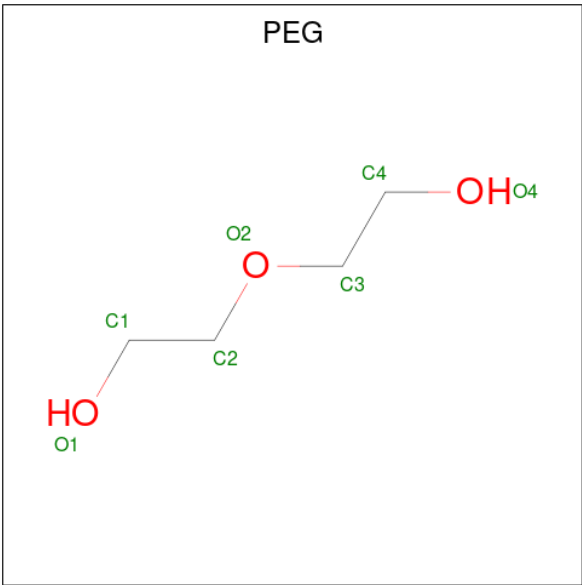
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	B	4	Total	Ca	0	0
			4	4		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	1
			20	12	8		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			14	8	6		
5	A	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



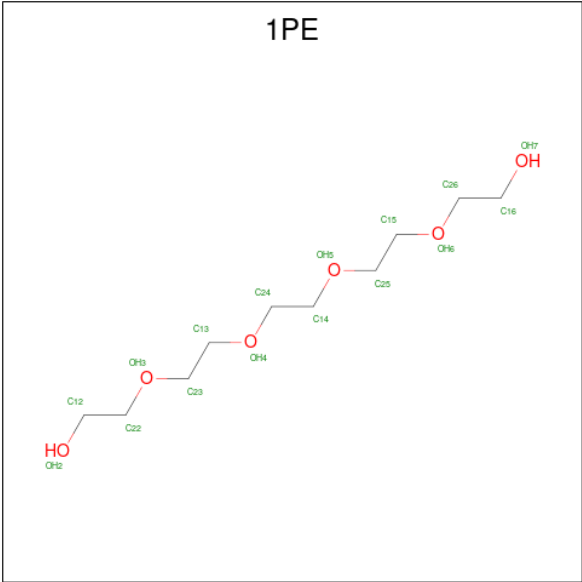
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	1
			8	4	4		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	1
			8	4	4		
6	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	1
			8	4	4		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	1
			8	4	4		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	1
			8	4	4		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	1
			8	4	4		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	1
			8	4	4		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	C	O	0
			16	10	6	

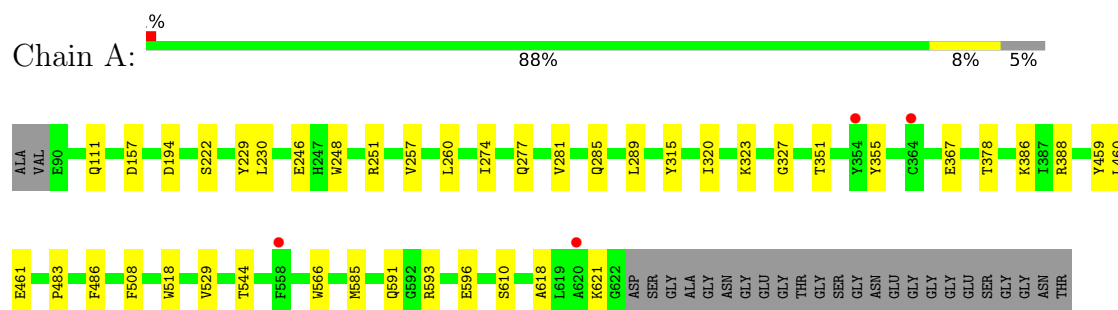
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	214	Total	O	0	0
			214	214		
8	B	264	Total	O	0	0
			264	264		

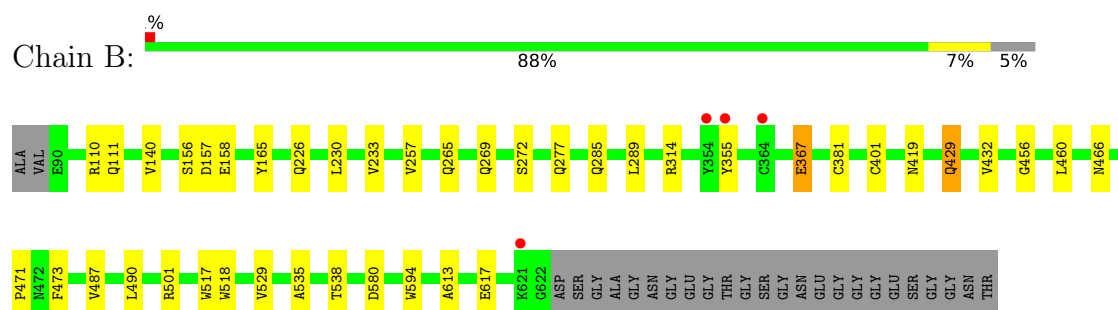
3 Residue-property plots [i](#)

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: Microbial collagenase



- Molecule 1: Microbial collagenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.94Å 75.12Å 135.15Å 90.00° 128.18° 90.00°	Depositor
Resolution (Å)	44.48 – 2.19 44.48 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.3 (44.48-2.19) 98.3 (44.48-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.186 , 0.227 0.192 , 0.229	Depositor DCC
R_{free} test set	3647 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.0	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	0.96	EDS
Total number of atoms	9236	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: EDO, CA, PGE, PEG, 1PE, ZN

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	0.30	0/4401	0.48	0/5996
1	B	0.31	0/4391	0.48	0/5982
All	All	0.31	0/8792	0.48	0/11978

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4275	0	3959	31	0
1	B	4268	0	3956	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	10	0	14	2	0
4	B	20	0	28	1	0
5	A	21	0	30	4	0
5	B	14	0	20	2	0
6	A	44	0	66	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	80	0	120	8	0
7	B	16	0	22	1	0
8	A	214	0	0	0	0
8	B	264	0	0	0	0
All	All	9236	0	8215	59	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 (59) 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:285[A]:GLN:HG3	1:A:289:LEU:HD12	1.68	0.73
1:B:157:ASP:H	6:B:718[A]:EDO:H21	1.56	0.69
1:B:156:SER:HA	6:B:718[B]:EDO:H22	1.83	0.61
1:B:269:GLN:HG2	7:B:707:1PE:H252	1.83	0.60
1:A:285[B]:GLN:NE2	1:A:323:LYS:O	2.37	0.58
1:A:230:LEU:HD13	1:A:277:GLN:HG3	1.85	0.57
1:B:230:LEU:HD13	1:B:277:GLN:HG3	1.86	0.56
1:A:460:LEU:HA	5:A:708:PEG:H22	1.88	0.56
1:B:594:TRP:CD1	4:B:706[B]:PGE:H6	2.42	0.55
1:A:508:PHE:HB2	5:A:708:PEG:H42	1.87	0.55
1:A:483:PRO:HB3	1:A:486:PHE:CZ	2.42	0.54
1:A:461:GLU:HB2	5:A:708:PEG:H41	1.90	0.54
1:B:367:GLU:H	1:B:367:GLU:CD	2.16	0.53
1:A:281:VAL:O	1:A:285[B]:GLN:HG3	2.09	0.53
1:A:246:GLU:HG3	6:A:715:EDO:O1	2.09	0.52
1:B:157:ASP:H	6:B:718[B]:EDO:H11	1.75	0.52
1:A:388:ARG:HH11	1:A:388:ARG:HG2	1.73	0.52
1:B:233:VAL:HG13	1:B:257:VAL:HB	1.93	0.50
1:B:501:ARG:HH21	6:B:714[B]:EDO:H22	1.76	0.50
1:B:517:TRP:CG	1:B:518:TRP:N	2.81	0.49
1:B:226:GLN:HE22	5:B:708:PEG:H11	1.76	0.49
1:B:110:ARG:HB2	1:B:158:GLU:HG3	1.95	0.49
1:B:460:LEU:HA	6:B:713:EDO:H22	1.96	0.48
1:A:544:THR:HA	1:A:566:TRP:CZ2	2.49	0.48
1:A:281:VAL:HG12	1:A:285[B]:GLN:HE21	1.79	0.47
1:B:265:GLN:OE1	1:B:314[B]:ARG:NH1	2.48	0.47
1:A:593[B]:ARG:NH1	1:A:596[B]:GLU:OE2	2.49	0.46
1:B:419:ASN:HB3	6:B:714[B]:EDO:O1	2.16	0.46
1:B:535:ALA:O	1:B:538:THR:HG22	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:GLN:O	1:B:471:PRO:HD2	2.17	0.45
1:B:381[B]:CYS:HB3	1:B:401[B]:CYS:SG	2.57	0.44
1:A:222:SER:HA	5:A:707[A]:PEG:H31	1.98	0.44
1:A:246:GLU:HG3	6:A:715:EDO:H21	1.98	0.44
1:B:314[B]:ARG:HD3	1:B:355:TYR:CE2	2.52	0.44
1:A:246:GLU:CG	6:A:715:EDO:H21	2.48	0.44
1:B:140:VAL:HG11	1:B:165:TYR:CD2	2.53	0.44
1:A:248:TRP:HA	1:A:251:ARG:NH1	2.32	0.44
1:B:487:VAL:HB	1:B:490:LEU:HB2	2.00	0.44
1:A:591:GLN:HB2	1:A:593[B]:ARG:HG3	2.00	0.43
1:A:367:GLU:H	1:A:367:GLU:CD	2.26	0.43
1:B:613:ALA:O	1:B:617:GLU:HG2	2.19	0.42
1:A:459:TYR:O	4:A:706:PGE:H52	2.20	0.42
1:B:432:VAL:HG13	1:B:473:PHE:CE1	2.54	0.42
1:A:618:ALA:HA	1:A:621:LYS:HE3	2.02	0.42
1:A:111:GLN:HG2	1:B:111:GLN:HG2	2.01	0.42
1:A:157:ASP:H	6:A:716[A]:EDO:C1	2.32	0.42
1:A:378:THR:HG23	1:A:386:LYS:HE3	2.01	0.42
4:A:706:PGE:H42	4:A:706:PGE:H6	1.66	0.42
1:B:272:SER:HA	6:B:717:EDO:H21	2.01	0.42
1:A:194:ASP:OD1	1:A:229:TYR:OH	2.30	0.42
1:A:285[B]:GLN:HG2	1:A:327:GLY:HA3	2.01	0.41
1:A:351:THR:O	1:A:355:TYR:HD1	2.03	0.41
1:A:518:TRP:CE3	1:A:585:MET:HE1	2.55	0.41
1:A:274:ILE:HG21	1:A:315:TYR:CZ	2.56	0.41
1:A:257:VAL:O	1:A:260:LEU:HB3	2.21	0.41
1:A:281:VAL:HG21	1:A:320:ILE:HB	2.03	0.41
1:B:285[A]:GLN:HG2	1:B:289:LEU:HD12	2.04	0.40
1:B:580:ASP:HB2	5:B:709:PEG:O4	2.21	0.40
1:B:456:GLY:H	6:B:712[B]:EDO:H11	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	539/559 (96%)	533 (99%)	5 (1%)	1 (0%)	43	51
1	B	538/559 (96%)	529 (98%)	8 (2%)	1 (0%)	43	51
All	All	1077/1118 (96%)	1062 (99%)	13 (1%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	529	VAL
1	B	529	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	437/442 (99%)	436 (100%)	1 (0%)	87	94
1	B	436/442 (99%)	433 (99%)	3 (1%)	76	87
All	All	873/884 (99%)	869 (100%)	4 (0%)	81	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	610	SER
1	B	367	GLU
1	B	429	GLN
1	B	466	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	142	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	GLN
1	A	178	ASN
1	A	376	ASN
1	A	431	GLN
1	A	433	ASN
1	B	376	ASN
1	B	429	GLN
1	B	466	ASN
1	B	469	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 10 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	$\# Z > 2$
6	EDO	B	720	-	3,3,3	0.54	0	2,2,2	0.22	0
5	PEG	B	708	-	6,6,6	0.25	0	5,5,5	0.10	0
6	EDO	B	721[B]	-	3,3,3	0.46	0	2,2,2	0.28	0
6	EDO	A	713[B]	-	3,3,3	0.48	0	2,2,2	0.28	0
6	EDO	B	718[A]	-	3,3,3	0.44	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	711	-	3,3,3	0.46	0	2,2,2	0.42	0
6	EDO	A	716[B]	-	3,3,3	0.43	0	2,2,2	0.56	0
6	EDO	B	710	-	3,3,3	0.44	0	2,2,2	0.40	0
5	PEG	A	707[B]	-	6,6,6	0.16	0	5,5,5	0.07	0
6	EDO	B	714[B]	-	3,3,3	0.47	0	2,2,2	0.19	0
6	EDO	A	713[A]	-	3,3,3	0.45	0	2,2,2	0.45	0
4	PGE	B	706[B]	-	9,9,9	0.39	0	8,8,8	0.21	0
6	EDO	B	721[A]	-	3,3,3	0.65	0	2,2,2	0.06	0
6	EDO	A	716[A]	-	3,3,3	0.40	0	2,2,2	0.33	0
6	EDO	B	711	-	3,3,3	0.52	0	2,2,2	0.36	0
6	EDO	A	710	-	3,3,3	0.55	0	2,2,2	0.22	0
6	EDO	A	717	-	3,3,3	0.59	0	2,2,2	0.43	0
6	EDO	B	716	-	3,3,3	0.45	0	2,2,2	0.42	0
4	PGE	A	706	-	9,9,9	0.38	0	8,8,8	0.45	0
5	PEG	A	707[A]	-	6,6,6	0.14	0	5,5,5	0.08	0
6	EDO	B	714[A]	-	3,3,3	0.51	0	2,2,2	0.25	0
6	EDO	B	715	-	3,3,3	0.50	0	2,2,2	0.24	0
6	EDO	B	724[B]	-	3,3,3	0.46	0	2,2,2	0.37	0
5	PEG	A	708	-	6,6,6	0.15	0	5,5,5	0.20	0
6	EDO	B	712[B]	-	3,3,3	0.50	0	2,2,2	0.13	0
6	EDO	B	713	-	3,3,3	0.74	0	2,2,2	0.30	0
6	EDO	A	715	-	3,3,3	0.53	0	2,2,2	0.30	0
6	EDO	B	722	-	3,3,3	0.54	0	2,2,2	0.23	0
6	EDO	A	712	-	3,3,3	0.53	0	2,2,2	0.27	0
6	EDO	A	714	-	3,3,3	0.43	0	2,2,2	0.52	0
4	PGE	B	706[A]	-	9,9,9	0.48	0	8,8,8	0.25	0
7	1PE	B	707	-	15,15,15	0.20	0	14,14,14	0.13	0
5	PEG	B	709	-	6,6,6	0.27	0	5,5,5	0.10	0
6	EDO	B	717	-	3,3,3	0.53	0	2,2,2	0.40	0
6	EDO	B	718[B]	-	3,3,3	0.44	0	2,2,2	0.45	0
6	EDO	B	723	-	3,3,3	0.64	0	2,2,2	0.19	0
6	EDO	B	712[A]	-	3,3,3	0.46	0	2,2,2	0.34	0
6	EDO	B	719	-	3,3,3	0.61	0	2,2,2	0.27	0
6	EDO	B	724[A]	-	3,3,3	0.51	0	2,2,2	0.20	0
6	EDO	A	709	-	3,3,3	0.50	0	2,2,2	0.17	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
6	EDO	B	720	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	B	708	-	-	3/4/4/4	-
6	EDO	B	721[B]	-	-	1/1/1/1	-
6	EDO	A	713[B]	-	-	1/1/1/1	-
6	EDO	B	718[A]	-	-	0/1/1/1	-
6	EDO	A	711	-	-	0/1/1/1	-
6	EDO	A	716[B]	-	-	1/1/1/1	-
6	EDO	B	710	-	-	0/1/1/1	-
5	PEG	A	707[B]	-	-	0/4/4/4	-
6	EDO	B	714[B]	-	-	1/1/1/1	-
6	EDO	A	713[A]	-	-	1/1/1/1	-
4	PGE	B	706[B]	-	-	7/7/7/7	-
6	EDO	B	721[A]	-	-	1/1/1/1	-
6	EDO	A	716[A]	-	-	0/1/1/1	-
6	EDO	B	711	-	-	1/1/1/1	-
6	EDO	A	710	-	-	0/1/1/1	-
6	EDO	A	717	-	-	1/1/1/1	-
6	EDO	B	716	-	-	0/1/1/1	-
4	PGE	A	706	-	-	5/7/7/7	-
5	PEG	A	707[A]	-	-	2/4/4/4	-
6	EDO	B	714[A]	-	-	0/1/1/1	-
6	EDO	B	715	-	-	1/1/1/1	-
6	EDO	B	724[B]	-	-	0/1/1/1	-
5	PEG	A	708	-	-	1/4/4/4	-
6	EDO	B	712[B]	-	-	0/1/1/1	-
6	EDO	B	713	-	-	0/1/1/1	-
6	EDO	A	715	-	-	0/1/1/1	-
6	EDO	B	722	-	-	1/1/1/1	-
6	EDO	A	712	-	-	1/1/1/1	-
6	EDO	A	714	-	-	0/1/1/1	-
4	PGE	B	706[A]	-	-	6/7/7/7	-
7	1PE	B	707	-	-	6/13/13/13	-
5	PEG	B	709	-	-	3/4/4/4	-
6	EDO	B	717	-	-	0/1/1/1	-
6	EDO	B	718[B]	-	-	0/1/1/1	-
6	EDO	B	723	-	-	0/1/1/1	-
6	EDO	B	712[A]	-	-	1/1/1/1	-
6	EDO	B	719	-	-	0/1/1/1	-
6	EDO	B	724[A]	-	-	1/1/1/1	-
6	EDO	A	709	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	706	PGE	C6-C5-O3-C4
4	B	706[B]	PGE	O2-C3-C4-O3
4	B	706[A]	PGE	O2-C3-C4-O3
4	B	706[A]	PGE	O3-C5-C6-O4
6	A	713[B]	EDO	O1-C1-C2-O2
7	B	707	1PE	OH4-C13-C23-OH3
4	A	706	PGE	O1-C1-C2-O2
4	B	706[B]	PGE	O3-C5-C6-O4
5	B	709	PEG	O1-C1-C2-O2
4	A	706	PGE	O3-C5-C6-O4
5	A	707[A]	PEG	O2-C3-C4-O4
5	B	709	PEG	O2-C3-C4-O4
6	A	712	EDO	O1-C1-C2-O2
4	A	706	PGE	O2-C3-C4-O3
7	B	707	1PE	C12-C22-OH3-C23
4	A	706	PGE	C3-C4-O3-C5
4	B	706[A]	PGE	C3-C4-O3-C5
7	B	707	1PE	OH6-C15-C25-OH5
7	B	707	1PE	C24-C14-OH5-C25
4	B	706[B]	PGE	C6-C5-O3-C4
4	B	706[A]	PGE	O1-C1-C2-O2
4	B	706[B]	PGE	O1-C1-C2-O2
5	B	708	PEG	C1-C2-O2-C3
6	B	711	EDO	O1-C1-C2-O2
6	B	724[A]	EDO	O1-C1-C2-O2
5	B	708	PEG	O1-C1-C2-O2
5	B	708	PEG	O2-C3-C4-O4
4	B	706[B]	PGE	C4-C3-O2-C2
5	B	709	PEG	C4-C3-O2-C2
7	B	707	1PE	C23-C13-OH4-C24
6	A	716[B]	EDO	O1-C1-C2-O2
6	A	717	EDO	O1-C1-C2-O2
6	B	721[B]	EDO	O1-C1-C2-O2
6	B	722	EDO	O1-C1-C2-O2
4	B	706[A]	PGE	C1-C2-O2-C3
5	A	708	PEG	O2-C3-C4-O4
6	B	712[A]	EDO	O1-C1-C2-O2
6	B	721[A]	EDO	O1-C1-C2-O2
7	B	707	1PE	C15-C25-OH5-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	706[B]	PGE	C3-C4-O3-C5
4	B	706[A]	PGE	C4-C3-O2-C2
6	A	713[A]	EDO	O1-C1-C2-O2
4	B	706[B]	PGE	C1-C2-O2-C3
6	B	714[B]	EDO	O1-C1-C2-O2
6	B	715	EDO	O1-C1-C2-O2
5	A	707[A]	PEG	C1-C2-O2-C3

There are no ring outliers.

15 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	708	PEG	1	0
6	B	718[A]	EDO	1	0
6	B	714[B]	EDO	2	0
4	B	706[B]	PGE	1	0
6	A	716[A]	EDO	1	0
4	A	706	PGE	2	0
5	A	707[A]	PEG	1	0
5	A	708	PEG	3	0
6	B	712[B]	EDO	1	0
6	B	713	EDO	1	0
6	A	715	EDO	3	0
7	B	707	1PE	1	0
5	B	709	PEG	1	0
6	B	717	EDO	1	0
6	B	718[B]	EDO	2	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	533/559 (95%)	-0.02	4 (0%) 82 80	17, 43, 67, 98	8 (1%)
1	B	533/559 (95%)	-0.13	4 (0%) 82 80	18, 40, 61, 92	7 (1%)
All	All	1066/1118 (95%)	-0.08	8 (0%) 82 80	17, 42, 63, 98	15 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	TYR	3.1
1	A	364	CYS	2.1
1	A	354	TYR	2.1
1	B	354	TYR	2.1
1	B	621	LYS	2.1
1	A	620	ALA	2.1
1	B	364	CYS	2.0
1	A	558	PHE	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(Å ²)	Q<0.9
6	EDO	B	711	4/4	0.60	0.23	67,69,69,73	0
6	EDO	B	717	4/4	0.66	0.21	46,53,56,63	0
5	PEG	B	708	7/7	0.69	0.19	57,58,65,71	0
4	PGE	B	706[A]	10/10	0.69	0.18	33,50,55,56	10
4	PGE	B	706[B]	10/10	0.69	0.18	36,50,54,54	10
6	EDO	B	724[A]	4/4	0.69	0.29	47,49,51,52	4
6	EDO	B	724[B]	4/4	0.69	0.29	46,48,50,52	4
6	EDO	A	714	4/4	0.71	0.17	62,63,65,67	0
5	PEG	A	708	7/7	0.72	0.19	38,46,53,56	0
6	EDO	B	722	4/4	0.73	0.16	66,66,67,69	0
6	EDO	A	713[A]	4/4	0.74	0.20	45,49,50,52	4
6	EDO	A	713[B]	4/4	0.74	0.20	42,47,51,52	4
4	PGE	A	706	10/10	0.76	0.22	56,63,69,71	0
6	EDO	B	710	4/4	0.77	0.20	60,60,72,78	0
6	EDO	A	710	4/4	0.77	0.19	62,63,63,64	0
6	EDO	A	709	4/4	0.77	0.13	63,65,65,66	0
6	EDO	A	712	4/4	0.78	0.18	46,62,70,71	0
5	PEG	B	709	7/7	0.79	0.20	57,58,66,76	0
6	EDO	B	723	4/4	0.81	0.22	39,52,58,60	0
3	CA	B	705	1/1	0.81	0.15	92,92,92,92	0
6	EDO	B	715	4/4	0.81	0.17	58,62,63,67	0
6	EDO	B	712[B]	4/4	0.82	0.23	46,50,53,54	4
6	EDO	B	713	4/4	0.82	0.23	36,38,48,50	0
6	EDO	B	714[A]	4/4	0.82	0.17	36,46,46,51	4
6	EDO	B	714[B]	4/4	0.82	0.17	43,44,47,49	4
6	EDO	B	712[A]	4/4	0.82	0.23	43,49,51,53	4
6	EDO	A	711	4/4	0.83	0.14	52,56,58,60	0
5	PEG	A	707[B]	7/7	0.84	0.17	45,56,60,63	7
5	PEG	A	707[A]	7/7	0.84	0.17	48,57,61,62	7
6	EDO	A	715	4/4	0.85	0.16	52,52,59,62	0
6	EDO	B	721[A]	4/4	0.86	0.19	45,49,51,61	4
6	EDO	B	721[B]	4/4	0.86	0.19	45,47,49,50	4
6	EDO	B	719	4/4	0.86	0.23	37,39,55,56	0
6	EDO	B	720	4/4	0.87	0.10	54,55,57,62	0
7	1PE	B	707	16/16	0.89	0.12	48,56,63,63	0
6	EDO	A	717	4/4	0.92	0.12	41,46,50,51	0
6	EDO	B	716	4/4	0.92	0.20	51,53,54,59	0
3	CA	A	705	1/1	0.93	0.10	74,74,74,74	0
6	EDO	A	716[A]	4/4	0.95	0.10	39,42,45,45	4
6	EDO	A	716[B]	4/4	0.95	0.10	42,43,47,48	4
6	EDO	B	718[B]	4/4	0.97	0.10	40,41,44,50	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	B	718[A]	4/4	0.97	0.10	31,44,44,44	4
2	ZN	A	701	1/1	0.98	0.05	58,58,58,58	0
3	CA	B	704	1/1	0.99	0.02	52,52,52,52	0
3	CA	A	702	1/1	0.99	0.03	30,30,30,30	0
3	CA	A	704	1/1	0.99	0.03	60,60,60,60	0
2	ZN	B	701	1/1	0.99	0.03	51,51,51,51	0
3	CA	B	702	1/1	0.99	0.06	34,34,34,34	0
3	CA	B	703	1/1	0.99	0.02	42,42,42,42	0
3	CA	A	703	1/1	1.00	0.02	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.