



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 09:29 AM EDT

PDB ID : 7WOI / pdb_00007woi
Title : Structure of the shaft pilin Spa2 from *Corynebacterium glutamicum*
Authors : Wu, Y.F.; Wang, L.T.; Huang, Y.Y.; Zhong, C.; Zhou, J.
Deposited on : 2022-01-21
Resolution : 2.73 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

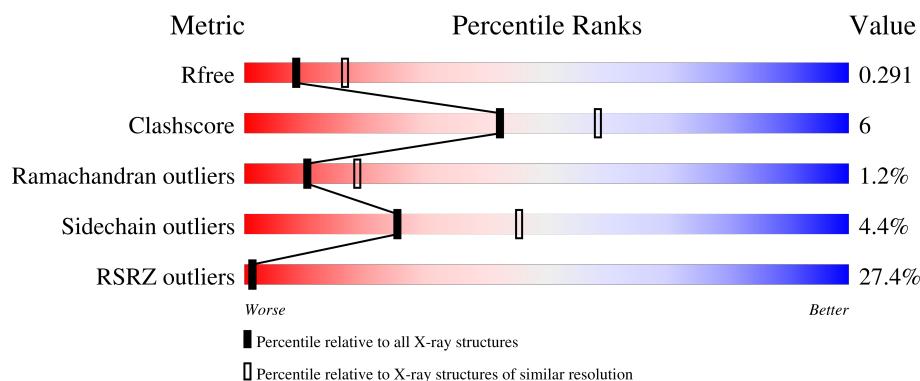
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	509	19% 68% 15% • 16%
1	B	509	28% 71% 12% • 16%

2 Entry composition [i](#)

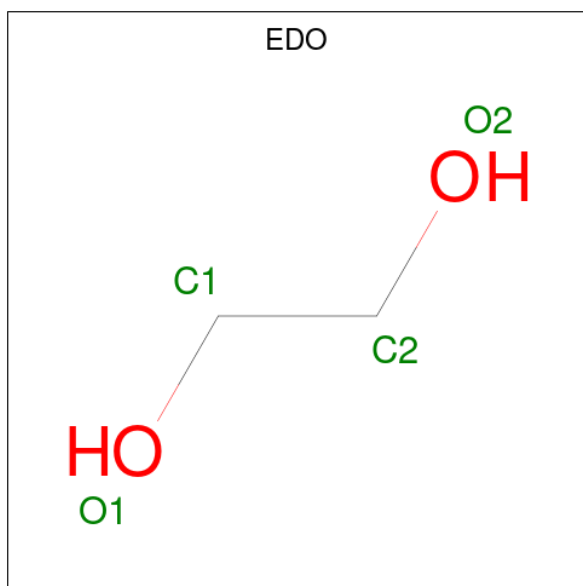
There are 4 unique types of molecules in this entry. The entry contains 6454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Spa2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3176	1987	518	666	5			
1	B	429	Total	C	N	O	S	0	1	0
			3179	1987	520	667	5			

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



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

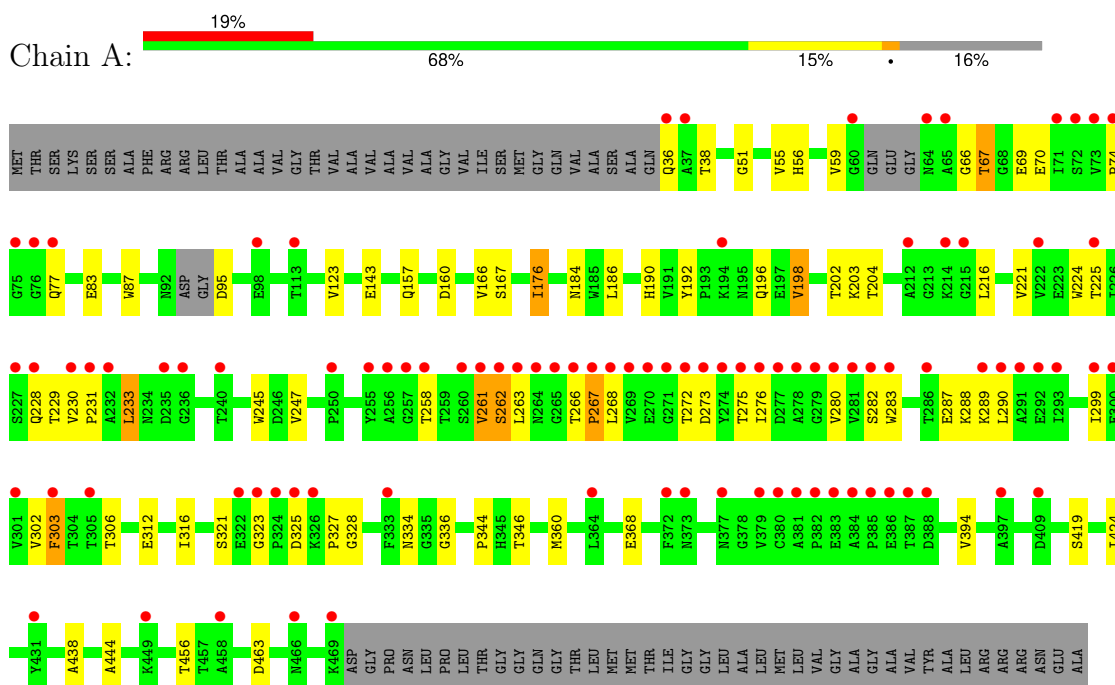
- Molecule 4 is water.

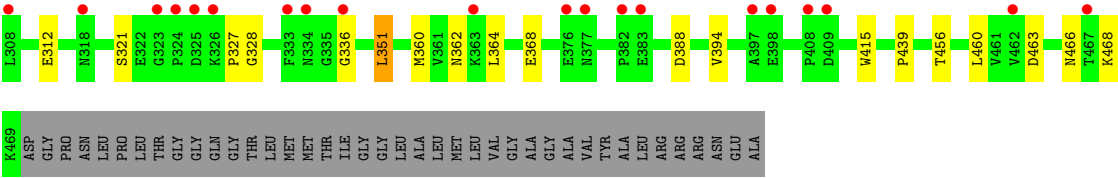
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	46	Total	O	0	0
			46	46		

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: Spa2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.65Å 64.09Å 441.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.43 – 2.73 63.43 – 2.73	Depositor EDS
% Data completeness (in resolution range)	73.7 (63.43-2.73) 73.7 (63.43-2.73)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.266 , 0.293 0.266 , 0.291	Depositor DCC
R_{free} test set	1320 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6454	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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, 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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/3250	0.52	2/4465 (0.0%)
1	B	0.24	0/3253	0.43	3/4469 (0.1%)
All	All	0.28	0/6503	0.48	5/8934 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	ASN	CA-CB-CG	9.64	122.24	112.60
1	B	466	ASN	CA-C-O	-6.11	113.77	120.24
1	B	466	ASN	CB-CA-C	6.02	119.77	110.14
1	A	216	LEU	N-CA-CB	-5.65	102.38	110.80
1	A	176	ILE	CA-C-O	-5.65	113.73	119.89

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	3176	0	2981	41	0
1	B	3179	0	2972	37	0
2	A	8	0	12	0	0
2	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
4	A	35	0	0	0	0
4	B	46	0	0	0	0
All	All	6454	0	5979	78	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 6.

All (78) 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:262:SER:HA	1:A:267:PRO:HA	1.62	0.80
1:A:261:VAL:HG13	1:A:268:LEU:HB3	1.65	0.79
1:B:294:LYS:HD3	1:B:295:ALA:H	1.49	0.78
1:B:283:TRP:CZ3	1:B:301:VAL:HB	2.23	0.74
1:B:82:ALA:H	1:B:138:THR:HG22	1.53	0.73
1:A:247:VAL:HB	1:A:327:PRO:HA	1.70	0.71
1:B:261:VAL:HG12	1:B:301:VAL:HG12	1.71	0.71
1:A:312:GLU:HA	1:A:456:THR:HG22	1.74	0.70
1:B:247:VAL:HB	1:B:327:PRO:HA	1.77	0.66
1:B:312:GLU:HA	1:B:456:THR:HG22	1.76	0.66
1:A:261:VAL:HG13	1:A:268:LEU:CB	2.29	0.62
1:A:83:GLU:HB3	1:A:160:ASP:HB3	1.82	0.61
1:A:261:VAL:CG1	1:A:268:LEU:HD13	2.31	0.60
1:B:166:VAL:HG12	1:B:336:GLY:HA3	1.83	0.60
1:B:83:GLU:HB2	1:B:137:THR:HG22	1.84	0.58
1:B:247:VAL:HG22	1:B:280:VAL:HG13	1.88	0.56
1:A:368:GLU:HG2	1:A:394:VAL:HG12	1.88	0.55
1:B:283:TRP:CD1	1:B:283:TRP:N	2.74	0.55
1:B:280:VAL:HG12	1:B:280:VAL:O	2.05	0.55
1:B:269:VAL:HG12	1:B:270:GLU:H	1.73	0.53
1:B:67:THR:HB	1:B:69:GLU:OE1	2.08	0.53
1:B:228:GLN:HE21	1:B:229:THR:N	2.08	0.52
1:A:263:LEU:N	1:A:266:THR:O	2.33	0.51
1:A:247:VAL:HG22	1:A:280:VAL:HG13	1.92	0.50
1:B:283:TRP:CH2	1:B:301:VAL:HB	2.45	0.50
1:A:56:HIS:HB2	1:A:192:TYR:CD1	2.47	0.50
1:B:87:TRP:HZ3	1:B:157:GLN:HG2	1.77	0.49
1:B:368:GLU:HG2	1:B:394:VAL:HG12	1.93	0.49
1:B:54:THR:HG22	1:B:145:THR:HG23	1.93	0.49
1:B:321:SER:HB2	1:B:328:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLN:HE21	1:A:229:THR:N	2.11	0.49
1:B:56:HIS:HB2	1:B:192:TYR:CD1	2.47	0.48
1:A:275:THR:HA	1:A:283:TRP:HD1	1.78	0.48
1:A:419:SER:HB2	1:A:424:ILE:HD11	1.96	0.48
1:B:287:GLU:HA	1:B:290:LEU:HD12	1.96	0.47
1:A:59:VAL:HB	1:A:77:GLN:HG2	1.95	0.47
1:B:83:GLU:HA	1:B:137:THR:HA	1.95	0.47
1:A:166:VAL:HG12	1:A:336:GLY:HA3	1.97	0.47
1:B:282:SER:C	1:B:283:TRP:CD1	2.93	0.47
1:A:56:HIS:HB2	1:A:192:TYR:HD1	1.79	0.47
1:B:151:LEU:HD22	1:B:177:PRO:HD3	1.96	0.46
1:A:316:ILE:HB	1:A:346:THR:HG23	1.97	0.46
1:A:55:VAL:O	1:A:143:GLU:HA	2.16	0.46
1:B:360:MET:HE3	1:B:463:ASP:HB3	1.96	0.46
1:B:364:LEU:HD23	1:B:439:PRO:HG2	1.96	0.46
1:A:167:SER:HB3	1:A:196:GLN:HB2	1.98	0.46
1:A:198:VAL:HA	1:A:231:PRO:HB3	1.98	0.46
1:A:221:VAL:HG12	1:A:306:THR:HA	1.98	0.45
1:A:225:THR:HG22	1:A:302:VAL:HG22	1.98	0.45
1:B:351:LEU:HD12	1:B:460:LEU:HD23	1.98	0.45
1:A:272:THR:HG21	1:A:288:LYS:HD2	1.97	0.45
1:B:262:SER:HA	1:B:267:PRO:HA	1.99	0.45
1:A:268:LEU:H	1:A:268:LEU:HD23	1.82	0.44
1:A:70:GLU:HB2	1:A:190:HIS:CG	2.52	0.44
1:B:198:VAL:HA	1:B:231:PRO:HB3	1.99	0.44
1:A:245:TRP:HA	1:A:282:SER:HA	1.99	0.44
1:A:87:TRP:HZ3	1:A:157:GLN:HG2	1.82	0.44
1:A:321:SER:HB2	1:A:328:GLY:HA3	2.00	0.44
1:A:51:GLY:HA3	1:A:176:ILE:HG21	2.00	0.43
1:B:71:ILE:HG13	1:B:73:VAL:H	1.83	0.43
1:B:211:GLN:HG2	1:B:415:TRP:CE2	2.54	0.42
1:B:102:LEU:HG	1:B:152:GLY:HA2	2.00	0.42
1:B:468:LYS:HE2	1:B:468:LYS:HB3	1.84	0.42
1:A:323:GLY:C	1:A:325:ASP:H	2.28	0.42
1:B:201:PRO:HB3	1:B:228:GLN:HB2	2.01	0.42
1:A:203:LYS:HG2	1:A:344:PRO:HG3	2.01	0.42
1:A:258:THR:HA	1:A:303:PHE:HA	2.01	0.42
1:A:272:THR:HG22	1:A:289:LYS:HG2	2.01	0.42
1:A:438:ALA:HB2	1:A:444:ALA:HB2	2.02	0.42
1:B:280:VAL:O	1:B:281:VAL:C	2.62	0.42
1:A:66:GLY:O	1:A:67:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLU:HA	1:A:290:LEU:HD12	2.01	0.41
1:A:360:MET:HE3	1:A:463:ASP:HB3	2.03	0.41
1:A:233:LEU:HD21	1:A:334:ASN:HD21	1.86	0.41
1:B:83:GLU:HB3	1:B:160:ASP:HB3	2.02	0.41
1:A:268:LEU:HB2	1:A:273:ASP:OD2	2.20	0.40
1:B:69:GLU:H	1:B:69:GLU:HG3	1.61	0.40
1:A:287:GLU:HA	1:A:290:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/509 (83%)	391 (92%)	27 (6%)	5 (1%)	10	19
1	B	424/509 (83%)	397 (94%)	22 (5%)	5 (1%)	10	19
All	All	847/1018 (83%)	788 (93%)	49 (6%)	10 (1%)	10	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	184	ASN
1	A	74	PRO
1	B	267	PRO
1	A	267	PRO
1	A	276	ILE
1	B	277	ASP
1	B	74	PRO
1	B	276	ILE
1	B	280	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	339/397 (85%)	323 (95%)	16 (5%)	23	43
1	B	338/397 (85%)	323 (96%)	15 (4%)	25	45
All	All	677/794 (85%)	646 (95%)	31 (5%)	25	43

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	38	THR
1	A	69	GLU
1	A	95	ASP
1	A	123	VAL
1	A	186	LEU
1	A	198	VAL
1	A	202	THR
1	A	204	THR
1	A	224	TRP
1	A	230	VAL
1	A	233	LEU
1	A	261	VAL
1	A	262	SER
1	A	299	ILE
1	A	303	PHE
1	B	54	THR
1	B	69	GLU
1	B	120	LEU
1	B	186	LEU
1	B	230	VAL
1	B	233	LEU
1	B	261	VAL
1	B	269	VAL
1	B	276	ILE
1	B	283	TRP
1	B	303	PHE

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Mol	Chain	Res	Type
1	B	351	LEU
1	B	362[A]	ASN
1	B	362[B]	ASN
1	B	388	ASP

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

Mol	Chain	Res	Type
1	A	106	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	601	-	3,3,3	0.43	0	2,2,2	0.34	0
2	EDO	B	601	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	A	602	-	3,3,3	0.44	0	2,2,2	0.31	0
3	GOL	B	602	-	5,5,5	0.94	0	5,5,5	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	A	602	-	-	0/1/1/1	-
3	GOL	B	602	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	429/509 (84%)	1.20	95 (22%) 2 2	16, 49, 96, 130	0
1	B	429/509 (84%)	1.64	140 (32%) 1 1	18, 62, 121, 165	1 (0%)
All	All	858/1018 (84%)	1.42	235 (27%) 1 1	16, 54, 110, 165	1 (0%)

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	LEU	6.9
1	A	276	ILE	6.2
1	A	283	TRP	5.7
1	A	292	GLU	5.6
1	B	280	VAL	5.4
1	A	269	VAL	5.3
1	B	65	ALA	5.3
1	A	278	ALA	5.1
1	B	275	THR	5.1
1	A	73	VAL	5.1
1	A	397	ALA	5.0
1	A	275	THR	5.0
1	B	273	ASP	5.0
1	B	110	GLN	5.0
1	B	241	SER	4.9
1	B	276	ILE	4.9
1	B	274	TYR	4.8
1	B	74	PRO	4.8
1	A	273	ASP	4.8
1	B	64	ASN	4.7
1	A	230	VAL	4.7
1	B	272	THR	4.7
1	B	73	VAL	4.7
1	A	270	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLY	4.5
1	B	98	GLU	4.5
1	B	292	GLU	4.5
1	B	299	ILE	4.5
1	A	65	ALA	4.5
1	B	286	THR	4.4
1	A	265	GLY	4.4
1	A	281	VAL	4.3
1	B	242	ALA	4.2
1	B	76	GLY	4.2
1	B	383	GLU	4.2
1	B	72	SER	4.2
1	B	269	VAL	4.2
1	B	324	PRO	4.1
1	A	271	GLY	4.1
1	A	71	ILE	4.1
1	A	74	PRO	4.1
1	B	90	GLY	4.0
1	B	257	GLY	4.0
1	B	305	THR	4.0
1	A	381	ALA	3.9
1	A	75	GLY	3.9
1	A	280	VAL	3.9
1	B	281	VAL	3.9
1	B	293	ILE	3.9
1	B	114	GLY	3.9
1	B	398	GLU	3.8
1	A	258	THR	3.8
1	B	71	ILE	3.8
1	B	118	ARG	3.8
1	A	240	THR	3.7
1	B	333	PHE	3.7
1	B	99	PRO	3.7
1	B	266	THR	3.7
1	B	270	GLU	3.7
1	A	212	ALA	3.6
1	B	260	SER	3.6
1	B	75	GLY	3.6
1	A	64	ASN	3.6
1	B	278	ALA	3.6
1	B	283	TRP	3.6
1	A	385	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	260	SER	3.6
1	B	113	THR	3.5
1	B	409	ASP	3.5
1	B	261	VAL	3.5
1	A	279	GLY	3.4
1	B	96	SER	3.4
1	A	300	GLU	3.4
1	B	101	ASP	3.4
1	A	263	LEU	3.4
1	B	37	ALA	3.4
1	A	277	ASP	3.3
1	B	87	TRP	3.3
1	A	37	ALA	3.3
1	A	409	ASP	3.3
1	B	288	LYS	3.2
1	A	291	ALA	3.2
1	A	272	THR	3.2
1	B	66	GLY	3.2
1	B	84	PHE	3.2
1	A	72	SER	3.2
1	B	232	ALA	3.2
1	B	91	THR	3.2
1	A	232	ALA	3.2
1	B	121	SER	3.2
1	B	97	CYS	3.1
1	B	279	GLY	3.1
1	A	379	VAL	3.1
1	A	289	LYS	3.0
1	B	86	ILE	3.0
1	B	137	THR	3.0
1	B	255	TYR	3.0
1	B	70	GLU	2.9
1	B	77	GLN	2.9
1	B	123	VAL	2.9
1	B	289	LYS	2.9
1	A	225	THR	2.9
1	B	181	ALA	2.9
1	B	285	LEU	2.9
1	A	372	PHE	2.9
1	B	308	LEU	2.9
1	A	380	CYS	2.9
1	B	147	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	146	PHE	2.9
1	B	105	THR	2.8
1	B	467	THR	2.8
1	A	431	TYR	2.8
1	B	122	ALA	2.8
1	B	102	LEU	2.8
1	B	325	ASP	2.8
1	B	163	ALA	2.8
1	B	36	GLN	2.8
1	A	449	LYS	2.8
1	B	221	VAL	2.8
1	B	155	TYR	2.8
1	A	267	PRO	2.7
1	B	294	LYS	2.7
1	B	236	GLY	2.7
1	A	261	VAL	2.7
1	B	54	THR	2.7
1	B	115	ALA	2.7
1	B	259	THR	2.7
1	B	301	VAL	2.7
1	B	58	TYR	2.7
1	A	36	GLN	2.7
1	A	469	LYS	2.7
1	B	363	LYS	2.7
1	B	224	TRP	2.7
1	A	286	THR	2.7
1	B	326	LYS	2.7
1	B	104	ASN	2.7
1	B	67	THR	2.7
1	B	166	VAL	2.7
1	B	95	ASP	2.7
1	B	117	PRO	2.7
1	A	60	GLY	2.7
1	A	76	GLY	2.7
1	A	214	LYS	2.7
1	B	212	ALA	2.7
1	B	256	ALA	2.7
1	A	377	ASN	2.6
1	B	134	THR	2.6
1	B	182	GLN	2.6
1	B	194	LYS	2.6
1	B	336	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	174	VAL	2.6
1	B	382	PRO	2.6
1	B	129	LEU	2.6
1	A	77	GLN	2.6
1	B	258	THR	2.5
1	B	306	THR	2.5
1	B	235	ASP	2.5
1	B	60	GLY	2.5
1	B	408	PRO	2.5
1	B	124	GLN	2.5
1	A	262	SER	2.5
1	B	377	ASN	2.5
1	A	290	LEU	2.5
1	A	250	PRO	2.5
1	A	228	GLN	2.5
1	A	301	VAL	2.5
1	B	88	ARG	2.4
1	B	106	ASN	2.4
1	B	164	ASN	2.4
1	B	271	GLY	2.4
1	B	187	TYR	2.4
1	A	256	ALA	2.4
1	B	397	ALA	2.4
1	B	303	PHE	2.4
1	A	387	THR	2.4
1	A	323	GLY	2.4
1	A	303	PHE	2.4
1	A	364	LEU	2.4
1	A	322	GLU	2.4
1	B	300	GLU	2.4
1	A	215	GLY	2.4
1	A	274	TYR	2.3
1	A	333	PHE	2.3
1	B	173	TYR	2.3
1	B	287	GLU	2.3
1	A	384	ALA	2.3
1	B	103	ALA	2.3
1	B	334	ASN	2.3
1	B	45	PRO	2.3
1	B	116	ALA	2.3
1	B	243	THR	2.3
1	A	373	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	458	ALA	2.2
1	A	98	GLU	2.2
1	A	466	ASN	2.2
1	B	318	ASN	2.2
1	B	201	PRO	2.2
1	B	189	VAL	2.2
1	A	293	ILE	2.2
1	B	128	CYS	2.2
1	B	78	PRO	2.2
1	A	236	GLY	2.2
1	A	325	ASP	2.2
1	A	383	GLU	2.2
1	B	238	GLN	2.2
1	A	305	THR	2.1
1	A	324	PRO	2.1
1	A	235	ASP	2.1
1	B	462	VAL	2.1
1	B	47	ALA	2.1
1	A	255	TYR	2.1
1	A	386	GLU	2.1
1	B	80	GLU	2.1
1	A	266	THR	2.1
1	B	225	THR	2.1
1	B	298	THR	2.1
1	A	194	LYS	2.1
1	A	382	PRO	2.1
1	B	323	GLY	2.1
1	B	218	VAL	2.1
1	A	227	SER	2.1
1	B	291	ALA	2.1
1	A	231	PRO	2.1
1	B	40	VAL	2.1
1	A	388	ASP	2.0
1	B	150	ASP	2.0
1	A	282	SER	2.0
1	A	264	ASN	2.0
1	A	299	ILE	2.0
1	A	222	VAL	2.0
1	B	107	ASP	2.0
1	B	376	GLU	2.0
1	A	326	LYS	2.0
1	A	113	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	268	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	A	602	4/4	0.73	0.15	36,40,41,44	0
2	EDO	B	601	4/4	0.73	0.18	50,52,53,54	0
3	GOL	B	602	6/6	0.82	0.13	21,39,41,42	0
2	EDO	A	601	4/4	0.84	0.12	27,29,35,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.