



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:13 AM UTC

PDB ID : 5M11 / pdb_00005m11
Title : Structural and functional probing of PorZ, an essential bacterial surface component of the type-IX secretion system of human oral-microbiomic Porphyromonas gingivalis.
Authors : Lasica, A.M.; Goulas, T.; Mizgalska, D.; Zhou, X.; Ksiazek, M.; Madej, M.; Guo, Y.; Guevara, T.; Nowak, M.; Potempa, B.; Goel, A.; Sztukowska, M.; Prabhakar, A.T.; Bzowska, M.; Widziolek, M.; Thogersen, I.B.; Enghild, J.J.; Simonian, M.; Kulczyk, A.W.; Nguyen, K.-A.; Potempa, J.; Gomis-Ruth, F.X.
Deposited on : 2016-10-07
Resolution : 2.90 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)

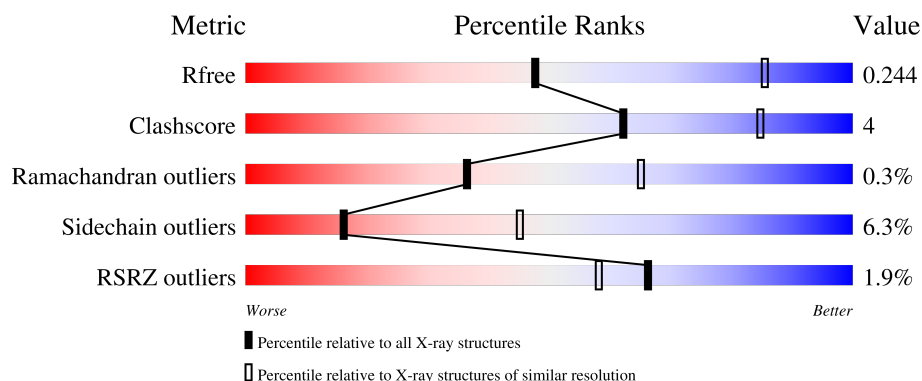
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

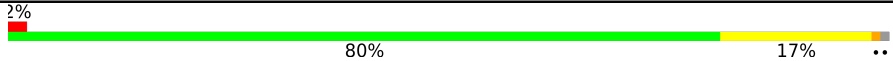
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	758	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5783 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 Immunoreactive 84kD antigen PG93.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	748	Total	C	N	O	S	0	0	0
			5678	3602	956	1103	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP Q9S3Q8
A	20	PRO	-	expression tag	UNP Q9S3Q8
A	21	LEU	-	expression tag	UNP Q9S3Q8
A	22	GLY	-	expression tag	UNP Q9S3Q8
A	23	SER	-	expression tag	UNP Q9S3Q8
A	24	PRO	-	expression tag	UNP Q9S3Q8
A	25	GLU	-	expression tag	UNP Q9S3Q8
A	26	PHE	-	expression tag	UNP Q9S3Q8
A	27	PRO	-	expression tag	UNP Q9S3Q8
A	28	GLY	-	expression tag	UNP Q9S3Q8

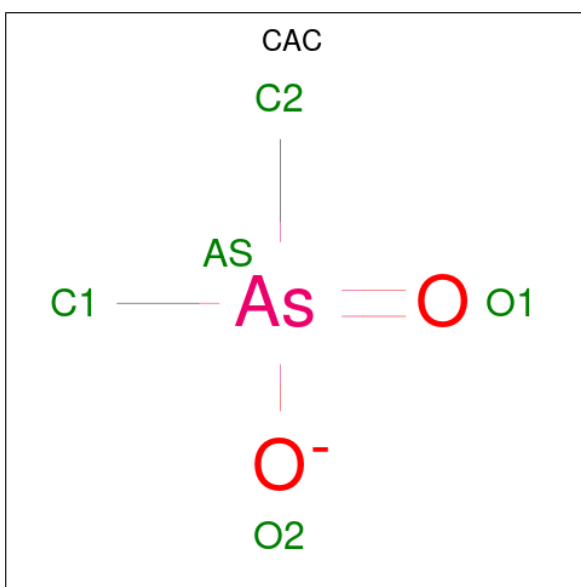
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	Zn	0	0
			8	8		

- Molecule 4 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).

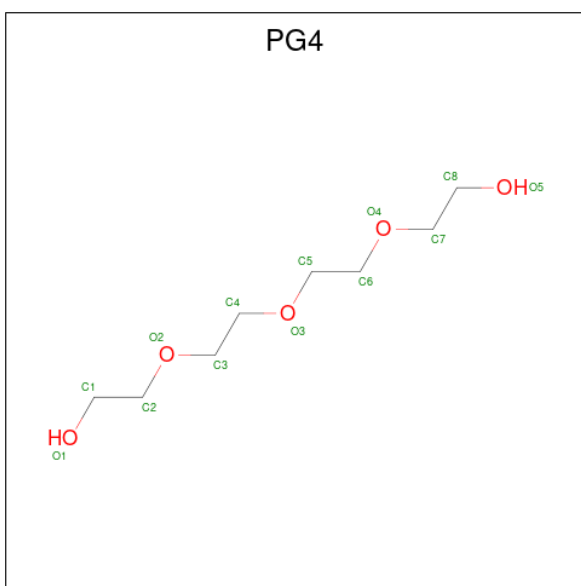


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

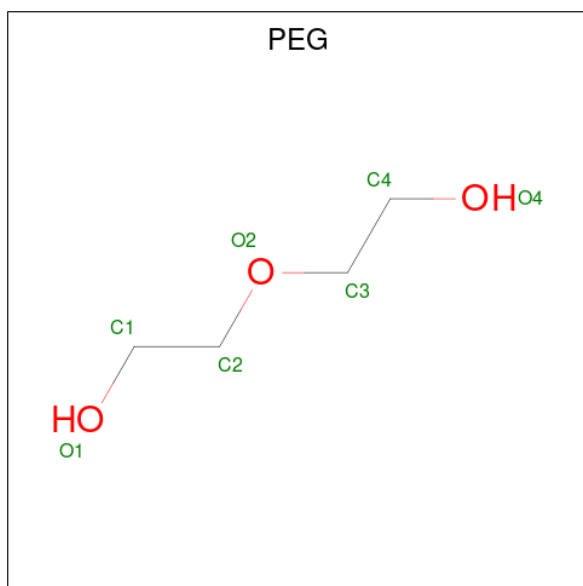
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



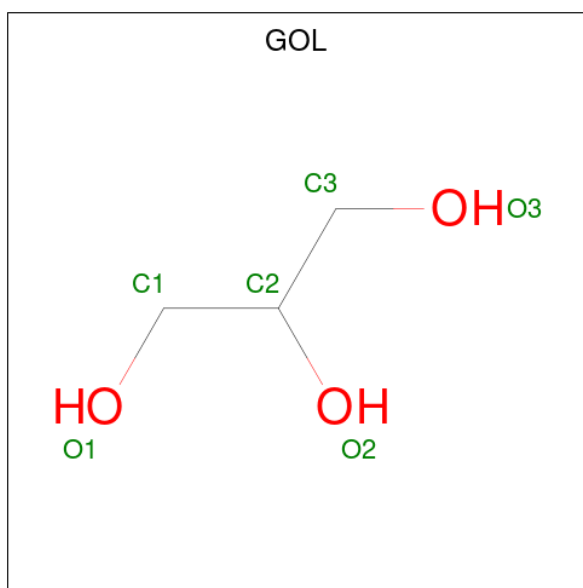
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	43	Total	O	0	0
			43	43		

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: Immunoreactive 84kD antigen PG93



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.52Å 115.52Å 139.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.46 – 2.90 48.46 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.46-2.90) 99.9 (48.46-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.183 , 0.238 0.192 , 0.244	Depositor DCC
R_{free} test set	723 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.6	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	0.94	EDS
Total number of atoms	5783	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: CA, PEG, CL, ZN, CAC, PG4, 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	0.90	2/5793 (0.0%)	1.27	39/7871 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	HIS	CA-C	9.24	1.61	1.52
1	A	554	MET	SD-CE	-5.76	1.65	1.79

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	749	ARG	CA-C-N	6.86	129.96	120.49
1	A	749	ARG	C-N-CA	6.86	129.96	120.49
1	A	761	ASP	CA-CB-CG	6.61	119.20	112.60
1	A	336	GLU	CB-CG-CD	6.15	123.05	112.60
1	A	762	PRO	CA-C-N	6.11	128.26	120.56
1	A	762	PRO	C-N-CA	6.11	128.26	120.56
1	A	673	GLY	N-CA-C	6.10	119.50	111.70
1	A	268	ASN	CA-CB-CG	6.03	118.63	112.60
1	A	462	LYS	CA-C-N	6.03	128.61	120.65
1	A	462	LYS	C-N-CA	6.03	128.61	120.65
1	A	557	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	367	GLY	N-CA-C	-5.86	106.94	114.85
1	A	458	GLY	CA-C-N	5.80	130.60	122.36
1	A	458	GLY	C-N-CA	5.80	130.60	122.36
1	A	535	VAL	CA-C-N	5.73	127.96	120.28
1	A	535	VAL	C-N-CA	5.73	127.96	120.28
1	A	365	TYR	CA-C-N	5.67	128.94	120.31
1	A	365	TYR	C-N-CA	5.67	128.94	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	604	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	614	ASP	CA-C-N	5.42	128.54	120.31
1	A	614	ASP	C-N-CA	5.42	128.54	120.31
1	A	527	THR	N-CA-C	-5.39	107.06	113.97
1	A	67	HIS	CA-C-N	5.29	130.07	122.35
1	A	67	HIS	C-N-CA	5.29	130.07	122.35
1	A	29	GLY	CA-C-N	5.16	127.80	120.53
1	A	29	GLY	C-N-CA	5.16	127.80	120.53
1	A	613	VAL	CA-C-N	5.11	130.04	120.95
1	A	613	VAL	C-N-CA	5.11	130.04	120.95
1	A	374	ASP	CA-C-N	5.08	127.40	120.54
1	A	374	ASP	C-N-CA	5.08	127.40	120.54
1	A	427	GLY	CA-C-N	5.02	127.98	120.90
1	A	427	GLY	C-N-CA	5.02	127.98	120.90
1	A	259	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	168	VAL	CA-C-N	5.01	127.00	120.28
1	A	168	VAL	C-N-CA	5.01	127.00	120.28
1	A	602	VAL	CA-C-N	5.00	131.09	121.54
1	A	602	VAL	C-N-CA	5.00	131.09	121.54

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	5678	0	5591	47	0
2	A	4	0	0	0	0
3	A	8	0	0	0	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
6	A	13	0	18	0	0
7	A	7	0	10	0	0
8	A	24	0	28	0	0
9	A	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5783	0	5647	47	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 4.

All (47) 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:333:ASP:HB2	1:A:348:SER:HB2	1.65	0.78
1:A:270:ILE:HD11	1:A:287:VAL:HG21	1.80	0.64
1:A:493:ILE:HG12	1:A:499:LYS:HG2	1.86	0.57
1:A:735:THR:HG23	1:A:737:GLU:H	1.69	0.57
1:A:502:ASN:HB3	1:A:554:MET:HE3	1.87	0.56
1:A:430:THR:HG22	1:A:432:ILE:H	1.71	0.55
1:A:348:SER:OG	1:A:361:MET:HB3	2.08	0.54
1:A:700:ARG:HG2	1:A:775:ILE:HD11	1.90	0.54
1:A:425:TYR:HB3	1:A:430:THR:HG21	1.90	0.53
1:A:258:THR:HG22	1:A:260:ARG:H	1.75	0.52
1:A:258:THR:HG21	1:A:292:ALA:HB3	1.91	0.52
1:A:375:LYS:HA	1:A:388:PHE:HD2	1.75	0.52
1:A:506:ARG:HG3	1:A:512:ARG:HB2	1.92	0.51
1:A:130:LEU:HD21	1:A:133:LEU:HB2	1.93	0.50
1:A:38:HIS:HE1	1:A:305:GLU:HG3	1.75	0.50
1:A:125:LEU:HG	1:A:146:PHE:HB2	1.94	0.49
1:A:264:ILE:HB	1:A:271:TYR:HB2	1.93	0.49
1:A:37:ILE:HD11	1:A:71:ILE:HD12	1.95	0.49
1:A:742:ALA:O	1:A:750:VAL:HB	2.12	0.49
1:A:620:TRP:CZ2	1:A:679:THR:HG23	2.47	0.49
1:A:443:LYS:HG2	1:A:444:ALA:H	1.78	0.49
1:A:409:TRP:CD2	1:A:441:ARG:HB2	2.48	0.48
1:A:150:VAL:O	1:A:159:PRO:HD2	2.15	0.47
1:A:698:PRO:HB2	1:A:775:ILE:HG12	1.96	0.47
1:A:482:VAL:HG21	1:A:516:LEU:HD22	1.96	0.46
1:A:88:TYR:CE2	1:A:90:GLU:HA	2.51	0.46
1:A:500:TRP:HZ3	1:A:564:MET:HE1	1.80	0.45
1:A:620:TRP:HZ2	1:A:679:THR:HG23	1.82	0.45
1:A:617:ASN:HB3	1:A:633:GLU:HG2	1.98	0.45
1:A:720:ILE:HA	1:A:756:ALA:O	2.17	0.44
1:A:546:ILE:HG22	1:A:568:ILE:HD11	1.99	0.44
1:A:694:VAL:HG13	1:A:709:ILE:HD13	2.00	0.43
1:A:46:THR:HB	1:A:49:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ALA:HB2	1:A:474:TRP:HB3	2.01	0.43
1:A:258:THR:HG22	1:A:261:GLY:H	1.83	0.43
1:A:614:ASP:HB3	1:A:616:LEU:H	1.85	0.42
1:A:347:ALA:HB2	1:A:394:ILE:HD11	2.02	0.42
1:A:174:LEU:HD11	1:A:180:LEU:HD22	2.01	0.42
1:A:409:TRP:CE3	1:A:441:ARG:HB2	2.54	0.42
1:A:454:TRP:CE2	1:A:466:MET:HG3	2.54	0.42
1:A:136:VAL:HG11	1:A:173:LYS:HG2	2.02	0.42
1:A:363:LYS:HB3	1:A:370:TRP:CZ3	2.54	0.42
1:A:651:SER:HB3	1:A:670:THR:HB	2.02	0.41
1:A:40:THR:HG21	1:A:308:LEU:HG	2.01	0.41
1:A:443:LYS:HG2	1:A:444:ALA:N	2.36	0.40
1:A:539:VAL:HA	1:A:544:ALA:O	2.22	0.40
1:A:743:ARG:HD2	1:A:747:GLY:O	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	746/758 (98%)	693 (93%)	51 (7%)	2 (0%)	36 65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	GLY
1	A	704	PRO

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	601/608 (99%)	563 (94%)	38 (6%)	16	45

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	37	ILE
1	A	68	GLU
1	A	75	ILE
1	A	125	LEU
1	A	219	ILE
1	A	224	ILE
1	A	239	GLN
1	A	247	LEU
1	A	258	THR
1	A	296	SER
1	A	305	GLU
1	A	340	SER
1	A	369	ARG
1	A	398	ASN
1	A	402	ASP
1	A	463	ASN
1	A	481	ASP
1	A	494	LEU
1	A	501	VAL
1	A	505	HIS
1	A	526	THR
1	A	583	THR
1	A	603	LEU
1	A	612	VAL
1	A	637	LYS
1	A	646	ASN
1	A	681	THR
1	A	694	VAL
1	A	719	LYS

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Mol	Chain	Res	Type
1	A	723	THR
1	A	724	THR
1	A	727	LEU
1	A	734	VAL
1	A	736	THR
1	A	750	VAL
1	A	763	VAL
1	A	766	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	197	GLN
1	A	268	ASN
1	A	484	ASN
1	A	653	ASN
1	A	741	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 13 are monoatomic - leaving 7 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
8	GOL	A	817	3	5,5,5	0.09	0	5,5,5	0.18	0
8	GOL	A	819	3	5,5,5	0.11	0	5,5,5	0.17	0
4	CAC	A	813	3	2,4,4	2.62	2 (100%)	4,6,6	2.56	1 (25%)
8	GOL	A	820	-	5,5,5	0.10	0	5,5,5	0.37	0
6	PG4	A	815	-	12,12,12	0.51	0	11,11,11	0.29	0
8	GOL	A	818	3	5,5,5	0.10	0	5,5,5	0.16	0
7	PEG	A	816	-	6,6,6	0.19	0	5,5,5	0.14	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
8	GOL	A	817	3	-	2/4/4/4	-
8	GOL	A	819	3	-	1/4/4/4	-
8	GOL	A	820	-	-	1/4/4/4	-
6	PG4	A	815	-	-	7/10/10/10	-
8	GOL	A	818	3	-	1/4/4/4	-
7	PEG	A	816	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	813	CAC	AS-C2	2.67	1.96	1.90
4	A	813	CAC	AS-C1	2.57	1.96	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	813	CAC	O1-AS-C2	-4.95	105.34	111.50

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	817	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	815	PG4	O2-C3-C4-O3
6	A	815	PG4	O3-C5-C6-O4
8	A	817	GOL	O2-C2-C3-O3
6	A	815	PG4	O1-C1-C2-O2
8	A	820	GOL	O2-C2-C3-O3
6	A	815	PG4	C8-C7-O4-C6
7	A	816	PEG	C1-C2-O2-C3
6	A	815	PG4	C1-C2-O2-C3
6	A	815	PG4	C6-C5-O3-C4
7	A	816	PEG	C4-C3-O2-C2
8	A	818	GOL	O1-C1-C2-C3
8	A	819	GOL	O2-C2-C3-O3
6	A	815	PG4	O4-C7-C8-O5

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 [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	748/758 (98%)	-0.07	14 (1%) 66 58	33, 72, 116, 155	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	ALA	3.5
1	A	66	PRO	3.5
1	A	685	SER	3.3
1	A	65	ALA	3.2
1	A	323	PRO	3.1
1	A	684	GLY	2.6
1	A	734	VAL	2.6
1	A	583	THR	2.5
1	A	683	SER	2.4
1	A	686	ALA	2.4
1	A	597	PRO	2.2
1	A	763	VAL	2.2
1	A	326	PHE	2.1
1	A	306	GLU	2.1

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

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
8	GOL	A	820	6/6	0.49	0.15	85,90,91,92	0
7	PEG	A	816	7/7	0.74	0.23	76,79,84,84	0
8	GOL	A	819	6/6	0.75	0.15	98,99,100,100	0
6	PG4	A	815	13/13	0.79	0.17	89,92,95,96	0
8	GOL	A	818	6/6	0.86	0.16	80,84,85,86	0
2	CA	A	811	1/1	0.87	0.18	98,98,98,98	0
2	CA	A	810	1/1	0.90	0.10	87,87,87,87	0
2	CA	A	812	1/1	0.92	0.14	105,105,105,105	0
8	GOL	A	817	6/6	0.93	0.15	88,89,91,94	0
3	ZN	A	802	1/1	0.94	0.08	113,113,113,113	0
3	ZN	A	807	1/1	0.96	0.07	117,117,117,117	0
3	ZN	A	804	1/1	0.97	0.09	88,88,88,88	0
2	CA	A	801	1/1	0.98	0.07	81,81,81,81	0
4	CAC	A	813	5/5	0.98	0.08	103,103,104,105	0
5	CL	A	814	1/1	0.98	0.06	53,53,53,53	0
3	ZN	A	805	1/1	0.99	0.09	88,88,88,88	0
3	ZN	A	806	1/1	0.99	0.09	113,113,113,113	0
3	ZN	A	803	1/1	0.99	0.03	106,106,106,106	0
3	ZN	A	809	1/1	0.99	0.05	80,80,80,80	0
3	ZN	A	808	1/1	1.00	0.01	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.