



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:41 AM GMT

PDB ID : 4CC4
Title : Complex of InlC of *Listeria monocytogenes* and human Tuba C-terminal SH3 domain
Authors : Polle, L.; Rigano, L.; Julian, R.; Ireton, K.; Schubert, W.-D.
Deposited on : 2013-10-17
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

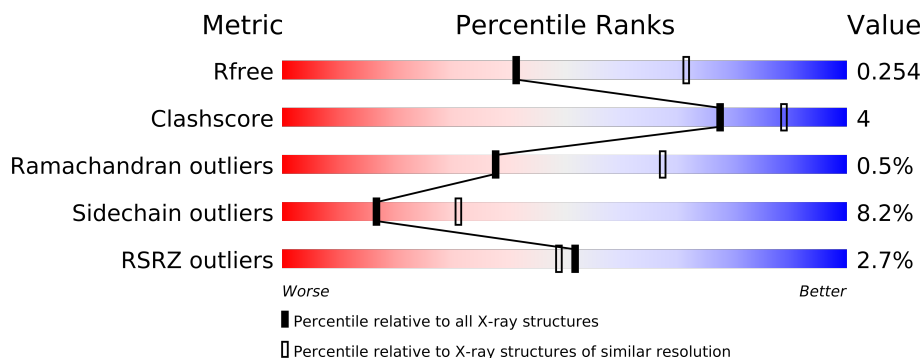
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	266	
1	E	266	
2	B	68	
2	D	68	
2	F	68	
3	C	266	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	1298	-	X
4	GOL	C	1299	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	D	2578	-	X
5	CL	F	2579	-	X
6	PE4	C	1300	-	X
7	SO4	C	1301	-	X
8	PO4	E	1298	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8424 atoms, of which 0 are hydrogen and 0 are deuterium.

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 INLC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	9	0
			2132	1348	365	414	5			
1	E	263	Total	C	N	O	S	0	9	0
			2120	1337	362	416	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ALA	-	EXPRESSION TAG	UNP P71451
A	34	SER	-	EXPRESSION TAG	UNP P71451
A	246	ALA	TYR	ENGINEERED MUTATION	UNP P71451
A	247	ALA	TYR	ENGINEERED MUTATION	UNP P71451
A	298	LYS	-	EXPRESSION TAG	UNP P71451
E	33	ALA	-	EXPRESSION TAG	UNP P71451
E	34	SER	-	EXPRESSION TAG	UNP P71451
E	246	ALA	TYR	ENGINEERED MUTATION	UNP P71451
E	247	ALA	TYR	ENGINEERED MUTATION	UNP P71451
E	298	LYS	-	EXPRESSION TAG	UNP P71451

- Molecule 2 is a protein called DYNAMIN-BINDING PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	68	Total	C	N	O	0	4	1
			571	369	96	106			
2	D	63	Total	C	N	O	0	2	0
			533	346	90	97			
2	F	67	Total	C	N	O	0	2	0
			556	358	91	107			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1511	GLY	-	EXPRESSION TAG	UNP Q6XZF7
B	1512	PRO	-	EXPRESSION TAG	UNP Q6XZF7
B	1578	ALA	-	EXPRESSION TAG	UNP Q6XZF7
D	1511	GLY	-	EXPRESSION TAG	UNP Q6XZF7
D	1512	PRO	-	EXPRESSION TAG	UNP Q6XZF7
D	1578	ALA	-	EXPRESSION TAG	UNP Q6XZF7
F	1511	GLY	-	EXPRESSION TAG	UNP Q6XZF7
F	1512	PRO	-	EXPRESSION TAG	UNP Q6XZF7
F	1578	ALA	-	EXPRESSION TAG	UNP Q6XZF7

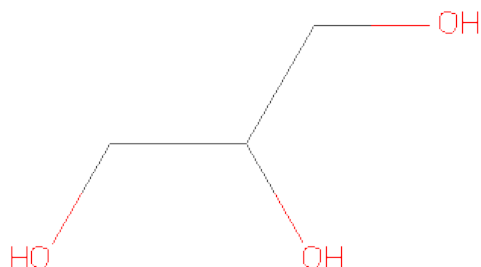
- Molecule 3 is a protein called INLC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	12	0
			2157	1365	368	419	5			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	33	ALA	-	EXPRESSION TAG	UNP P71451
C	34	SER	-	EXPRESSION TAG	UNP P71451
C	246	ALA	TYR	ENGINEERED MUTATION	UNP P71451
C	247	ALA	TYR	ENGINEERED MUTATION	UNP P71451
C	298	LYS	-	EXPRESSION TAG	UNP P71451

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

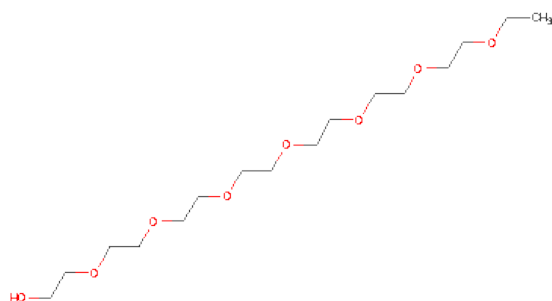


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

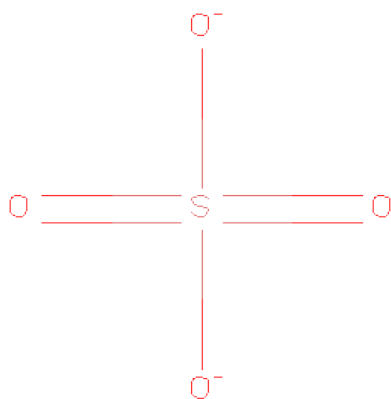
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	C	2	Total Cl 2 2	0	0
5	F	2	Total Cl 2 2	0	0

- Molecule 6 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



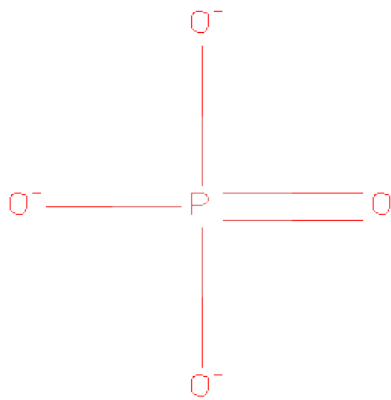
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			19	12	7		

- Molecule 7 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 8 is PHOSPHATE ION (three-letter code: PO₄) (formula: O₄P).

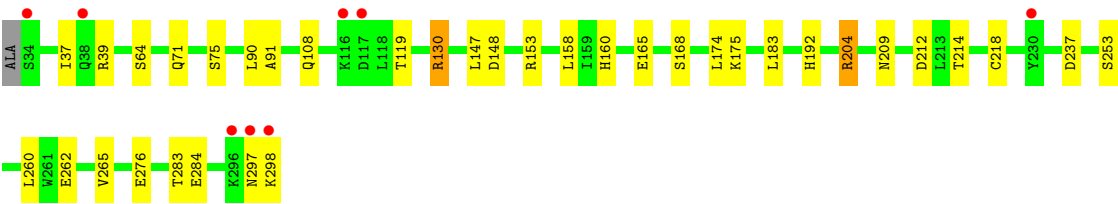


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	O	P	0	0
			5	4	1		
8	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	124	Total	O	0	0
			124	124		
9	B	19	Total	O	0	0
			19	19		
9	C	55	Total	O	0	0
			55	55		
9	D	20	Total	O	0	0
			20	20		
9	E	51	Total	O	0	0
			51	51		
9	F	11	Total	O	0	0
			11	11		

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.70Å 101.75Å 126.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.60 14.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (14.97-2.60) 99.7 (14.96-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.196 , 0.262 0.197 , 0.254	Depositor DCC
R_{free} test set	1806 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 36135 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8424	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, PE4, PO4, SO4, CSX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	0/2170	0.86	0/2937
1	E	0.66	0/2159	0.84	2/2923 (0.1%)
2	B	0.85	0/597	0.88	0/809
2	D	0.77	0/552	0.87	1/744 (0.1%)
2	F	0.71	0/576	0.77	0/779
3	C	0.68	0/2214	0.82	4/2999 (0.1%)
All	All	0.70	0/8268	0.84	7/11191 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	237	ASP	CB-CG-OD2	-6.50	112.45	118.30
3	C	237	ASP	CB-CG-OD1	6.26	123.94	118.30
3	C	204	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	E	128[A]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	E	128[B]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
3	C	153	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	D	1547	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2132	0	0	11	0
1	E	2120	0	0	4	3
2	B	571	0	0	0	0
2	D	533	0	0	2	0
2	F	556	0	0	3	0
3	C	2157	0	0	14	4
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
4	F	6	0	8	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
6	C	19	0	25	0	0
7	C	10	0	0	1	0
8	E	10	0	0	1	0
9	A	124	0	0	4	0
9	B	19	0	0	0	0
9	C	55	0	0	4	0
9	D	20	0	0	0	0
9	E	51	0	0	0	1
9	F	11	0	0	0	0
All	All	8424	0	65	30	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:276[A]:GLU:CD	9:C:2044:HOH:O	1.72	1.25
3:C:276[A]:GLU:OE2	9:C:2044:HOH:O	1.76	0.92
3:C:175:LYS:NZ	3:C:218:CSX:OD	2.23	0.71
3:C:108[A]:GLN:CG	3:C:130[A]:ARG:NH2	2.65	0.59
1:E:153:ARG:NH1	8:E:1299:PO4:O2	2.44	0.50
1:A:279:ASN:N	9:A:2122:HOH:O	2.46	0.49
1:A:267:THR:OG1	1:A:268:ASP:N	2.46	0.48
1:A:225:TYR:OH	1:A:263:LEU:O	2.32	0.47
3:C:212:ASP:OD2	2:D:1575:GLU:OE2	2.31	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:160:HIS:ND1	7:C:1301:SO4:O4	2.48	0.46
3:C:283:THR:OG1	3:C:284:GLU:N	2.48	0.46
3:C:165:GLU:OE1	2:D:1522:TYR:OH	2.34	0.45
3:C:90:LEU:O	3:C:91:ALA:C	2.56	0.44
3:C:204:ARG:NH2	9:C:2034:HOH:O	2.50	0.44
3:C:148:ASP:OD1	3:C:168:SER:OG	2.35	0.44
1:A:64:SER:N	1:A:67:ASP:OD2	2.51	0.43
2:F:1528:ASN:ND2	2:F:1531:GLU:OE2	2.51	0.43
2:F:1547:ASP:C	2:F:1547:ASP:OD1	2.57	0.43
1:A:241:ARG:NH1	9:A:2103:HOH:O	2.50	0.43
1:A:36:SER:O	1:A:38:GLN:NE2	2.51	0.43
9:A:2004:HOH:O	1:E:162:LYS:NZ	2.52	0.43
3:C:192:HIS:ND1	3:C:214:THR:OG1	2.53	0.42
1:A:268:ASP:OD1	1:E:39:ARG:NE	2.53	0.42
1:A:113:SER:N	1:A:114:PRO:CD	2.83	0.41
3:C:276[A]:GLU:OE1	9:C:2044:HOH:O	2.09	0.41
1:E:123:GLU:OE1	2:F:1570:TYR:OH	2.39	0.41
1:A:39:ARG:C	1:A:39:ARG:CD	2.90	0.41
3:C:71[B]:GLN:NE2	3:C:75:SER:OG	2.53	0.40
1:A:75:SER:O	1:A:98:ASN:ND2	2.54	0.40
1:A:250:ASN:ND2	9:A:2110:HOH:O	2.54	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:39[A]:ARG:NH1	1:E:262[A]:GLU:OE2[2_455]	1.67	0.53
3:C:39[A]:ARG:NH2	1:E:262[A]:GLU:OE2[2_455]	2.16	0.04
3:C:39[A]:ARG:CZ	1:E:262[A]:GLU:OE2[2_455]	2.17	0.03
3:C:39[B]:ARG:NH2	9:E:2050:HOH:O[2_455]	2.17	0.03

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	269/266 (101%)	244 (91%)	22 (8%)	3 (1%)	21	42
1	E	267/266 (100%)	243 (91%)	23 (9%)	1 (0%)	43	72
2	B	70/68 (103%)	66 (94%)	4 (6%)	0	100	100
2	D	63/68 (93%)	58 (92%)	5 (8%)	0	100	100
2	F	67/68 (98%)	62 (92%)	4 (6%)	1 (2%)	15	30
3	C	273/266 (103%)	257 (94%)	16 (6%)	0	100	100
All	All	1009/1002 (101%)	930 (92%)	74 (7%)	5 (0%)	38	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	THR
1	A	222	PRO
2	F	1548	VAL
1	A	227	PRO
1	E	263	LEU

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	246/238 (103%)	221 (90%)	25 (10%)	11	19
1	E	245/238 (103%)	224 (91%)	21 (9%)	15	28
2	B	62/58 (107%)	56 (90%)	6 (10%)	12	22
2	D	57/58 (98%)	54 (95%)	3 (5%)	32	58
2	F	60/58 (103%)	52 (87%)	8 (13%)	6	10
3	C	250/239 (105%)	233 (93%)	17 (7%)	22	43
All	All	920/889 (104%)	840 (91%)	80 (9%)	17	28

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	38	GLN

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Mol	Chain	Res	Type
1	A	39	ARG
1	A	44	ASN
1	A	57	LYS
1	A	68	LEU
1	A	79[A]	ASN
1	A	79[B]	ASN
1	A	84	ASN
1	A	88	GLN
1	A	116	LYS
1	A	147	LEU
1	A	175	LYS
1	A	183	LEU
1	A	203	THR
1	A	223	VAL
1	A	224	LYS
1	A	242	TRP
1	A	253	SER
1	A	255	VAL
1	A	262	GLU
1	A	268	ASP
1	A	279	ASN
1	A	293	GLN
1	A	296	LYS
2	B	1519	PHE
2	B	1546	LYS
2	B	1548	VAL
2	B	1549	THR
2	B	1559	VAL
2	B	1576	TYR
3	C	37	ILE
3	C	64	SER
3	C	119	THR
3	C	130[A]	ARG
3	C	130[B]	ARG
3	C	147	LEU
3	C	158	LEU
3	C	174	LEU
3	C	183	LEU
3	C	209	ASN
3	C	253[A]	SER
3	C	253[B]	SER
3	C	260	LEU

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Mol	Chain	Res	Type
3	C	262	GLU
3	C	265	VAL
3	C	297	ASN
3	C	298	LYS
2	D	1527[A]	ARG
2	D	1527[B]	ARG
2	D	1528	ASN
1	E	36	SER
1	E	44	ASN
1	E	45[A]	GLN
1	E	45[B]	GLN
1	E	57	LYS
1	E	69	VAL
1	E	84	ASN
1	E	88[A]	GLN
1	E	88[B]	GLN
1	E	128[A]	ARG
1	E	128[B]	ARG
1	E	147	LEU
1	E	162	LYS
1	E	204	ARG
1	E	206	LYS
1	E	224	LYS
1	E	230	TYR
1	E	260	LEU
1	E	264	PRO
1	E	279	ASN
1	E	288	ASP
2	F	1525	LYS
2	F	1532	LEU
2	F	1534	VAL
2	F	1535[A]	SER
2	F	1535[B]	SER
2	F	1537	ASN
2	F	1548	VAL
2	F	1573	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

8 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	CSX	A	141	1	4,6,7	7.32	2 (50%)	3,6,8	1.59	0
1	CSX	A	218	1	4,6,7	7.27	1 (25%)	3,6,8	5.29	2 (66%)
1	CSX	A	258	1	4,6,7	10.73	2 (50%)	3,6,8	1.88	1 (33%)
3	CSX	C	141	3	4,6,7	9.29	1 (25%)	3,6,8	1.03	0
3	CSX	C	218	3	4,6,7	7.42	1 (25%)	3,6,8	5.17	2 (66%)
1	CSX	E	141	1	4,6,7	8.64	2 (50%)	3,6,8	1.88	1 (33%)
1	CSX	E	218	1	4,6,7	8.94	1 (25%)	3,6,8	6.53	3 (100%)
1	CSX	E	258	1	4,6,7	7.96	1 (25%)	3,6,8	2.31	1 (33%)

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	CSX	A	141	1	-	0/2/5/7	0/0/0/0
1	CSX	A	218	1	-	0/2/5/7	0/0/0/0
1	CSX	A	258	1	-	0/2/5/7	0/0/0/0
3	CSX	C	141	3	-	0/2/5/7	0/0/0/0
3	CSX	C	218	3	-	0/2/5/7	0/0/0/0
1	CSX	E	141	1	-	0/2/5/7	0/0/0/0
1	CSX	E	218	1	-	0/2/5/7	0/0/0/0
1	CSX	E	258	1	-	0/2/5/7	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	CSX	O-C	21.31	1.26	1.11
3	C	141	CSX	O-C	18.43	1.24	1.11
1	E	218	CSX	O-C	17.83	1.23	1.11
1	E	141	CSX	O-C	17.14	1.23	1.11
1	E	258	CSX	O-C	15.88	1.22	1.11
3	C	218	CSX	O-C	14.80	1.21	1.11
1	A	141	CSX	O-C	14.49	1.21	1.11
1	A	218	CSX	O-C	14.49	1.21	1.11
1	A	258	CSX	CA-C	2.46	1.52	1.48
1	E	141	CSX	CA-C	2.16	1.52	1.48
1	A	141	CSX	CA-C	2.01	1.52	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	218	CSX	C-CA-N	-9.97	103.87	113.83
3	C	218	CSX	C-CA-N	-8.27	105.57	113.83
1	A	218	CSX	C-CA-N	-8.02	105.82	113.83
1	E	218	CSX	CA-CB-SG	4.86	117.52	110.82
1	A	218	CSX	CA-CB-SG	-4.43	104.71	110.82
1	E	258	CSX	C-CA-N	-3.46	110.38	113.83
3	C	218	CSX	CA-CB-SG	-3.33	106.23	110.82
1	A	258	CSX	CA-CB-SG	3.07	115.05	110.82
1	E	141	CSX	CB-CA-N	-2.66	105.93	110.32
1	E	218	CSX	CB-CA-N	2.18	113.92	110.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	$\# Z > 2$
4	GOL	A	1298	-	5,5,5	0.67	0	5,5,5	0.95	0
4	GOL	B	2579	-	5,5,5	0.34	0	5,5,5	0.59	0
4	GOL	C	1299	-	5,5,5	0.96	0	5,5,5	0.87	0
6	PE4	C	1300	-	18,18,23	0.74	0	17,17,22	0.55	0
7	SO4	C	1301	-	4,4,4	0.91	0	6,6,6	0.38	0
7	SO4	C	1302	-	4,4,4	0.60	0	6,6,6	0.68	0
4	GOL	D	2578	-	5,5,5	0.45	0	5,5,5	0.61	0
8	PO4	E	1298	-	4,4,4	0.21	0	6,6,6	0.32	0
8	PO4	E	1299	-	4,4,4	0.21	0	6,6,6	0.33	0
4	GOL	F	2578	-	5,5,5	0.62	0	5,5,5	0.58	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
4	GOL	A	1298	-	-	0/4/4/4	0/0/0/0
4	GOL	B	2579	-	-	0/4/4/4	0/0/0/0
4	GOL	C	1299	-	-	0/4/4/4	0/0/0/0
6	PE4	C	1300	-	-	0/16/16/21	0/0/0/0
7	SO4	C	1301	-	-	0/0/0/0	0/0/0/0
7	SO4	C	1302	-	-	0/0/0/0	0/0/0/0
4	GOL	D	2578	-	-	0/4/4/4	0/0/0/0
8	PO4	E	1298	-	-	0/0/0/0	0/0/0/0
8	PO4	E	1299	-	-	0/0/0/0	0/0/0/0
4	GOL	F	2578	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	265/266 (99%)	-0.30	5 (1%) 64 61	26, 42, 82, 105	0
1	E	263/266 (98%)	-0.16	9 (3%) 43 39	30, 54, 83, 110	0
2	B	68/68 (100%)	-0.31	2 (2%) 49 46	28, 44, 67, 85	0
2	D	63/68 (92%)	-0.36	1 (1%) 68 69	29, 40, 61, 70	0
2	F	67/68 (98%)	-0.07	2 (2%) 48 45	37, 52, 84, 91	0
3	C	265/266 (99%)	-0.24	8 (3%) 48 45	24, 47, 84, 148	0
All	All	991/1002 (98%)	-0.23	27 (2%) 52 49	24, 47, 83, 148	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	38	GLN	5.3
2	F	1561	GLY	4.3
1	A	33	ALA	4.3
1	E	35	GLU	3.6
3	C	34	SER	3.5
3	C	298	LYS	3.0
1	E	296	LYS	3.0
3	C	297	ASN	2.9
1	A	63	GLN	2.7
1	A	221	GLU	2.6
1	E	282	GLU	2.4
1	E	221	GLU	2.4
1	A	34	SER	2.3
2	B	1551[A]	ASN	2.3
2	F	1560	ASN	2.2
3	C	296	LYS	2.2
2	B	1560	ASN	2.2
3	C	117	ASP	2.2
1	E	297	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	230	TYR	2.1
1	A	264	PRO	2.1
1	E	61	GLY	2.1
2	D	1560	ASN	2.1
1	E	63	GLN	2.1
1	E	295	ILE	2.1
3	C	116[A]	LYS	2.0
1	E	230	TYR	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSX	E	218	7/8	0.20	1.56	49,53,66,68	0
3	CSX	C	218	7/8	0.15	0.36	42,44,51,51	1
1	CSX	A	218	7/8	0.15	-0.10	46,47,50,54	1
3	CSX	C	141	7/8	0.16	-0.40	48,53,64,64	0
1	CSX	E	141	7/8	0.16	-0.53	54,60,68,71	0
1	CSX	E	258	7/8	0.12	-0.70	50,53,63,64	0
1	CSX	A	258	7/8	0.12	-0.73	48,48,54,54	0
1	CSX	A	141	7/8	0.12	-0.97	39,42,48,50	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	SO4	C	1301	5/5	0.24	3.87	79,80,85,89	0
4	GOL	C	1299	6/6	0.40	3.29	52,59,60,64	0
8	PO4	E	1298	5/5	0.34	3.18	59,62,69,71	0
4	GOL	D	2578	6/6	0.17	3.03	54,60,65,66	0
6	PE4	C	1300	19/24	0.31	2.70	42,65,80,83	0
5	CL	F	2579	1/1	0.21	2.23	69,69,69,69	0
4	GOL	A	1298	6/6	0.20	2.18	58,61,63,64	0
8	PO4	E	1299	5/5	0.28	1.60	72,85,88,91	0
7	SO4	C	1302	5/5	0.16	1.51	43,46,52,53	0
4	GOL	F	2578	6/6	0.18	0.89	48,48,53,55	0
4	GOL	B	2579	6/6	0.16	0.30	59,64,65,69	0
5	CL	D	2579	1/1	0.14	-0.91	71,71,71,71	0
5	CL	C	1304	1/1	0.09	-1.57	70,70,70,70	0
5	CL	C	1303	1/1	0.07	-1.70	63,63,63,63	0
5	CL	A	1299	1/1	0.10	-2.26	72,72,72,72	0
5	CL	F	2580	1/1	0.09	-8.64	69,69,69,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.