Full wwPDB X-ray Structure Validation Report (i)

Dec 14, 2023 – 02:51 pm 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 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 (i) 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 (i)) were used in the production of this report:

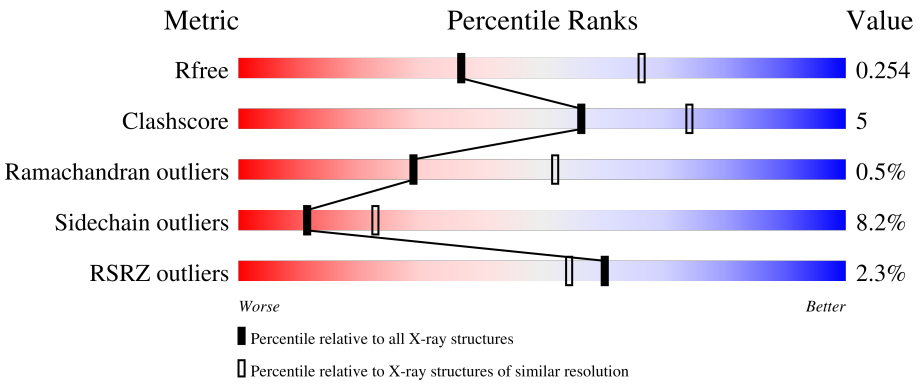
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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 <=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	266	2% 78% 19% •
1	E	266	2% 84% 14% • •
2	B	68	4% 84% 15% •
2	D	68	% 81% 10% • 6%
2	F	68	3% 74% 25% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	266	2% 81% 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	C	301	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 8424 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 INLC PROTEIN.

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

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
			Total	C	N	O			
2	B	68	571	369	96	106	0	4	1
2	D	64	533	346	91	96	0	2	1
2	F	68	556	358	92	106	0	2	1

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

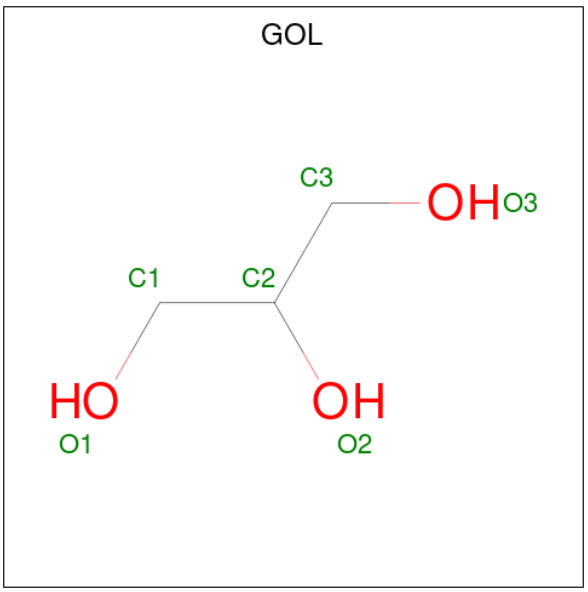
- Molecule 3 is a protein called INLC PROTEIN.

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

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: $C_3H_8O_3$).

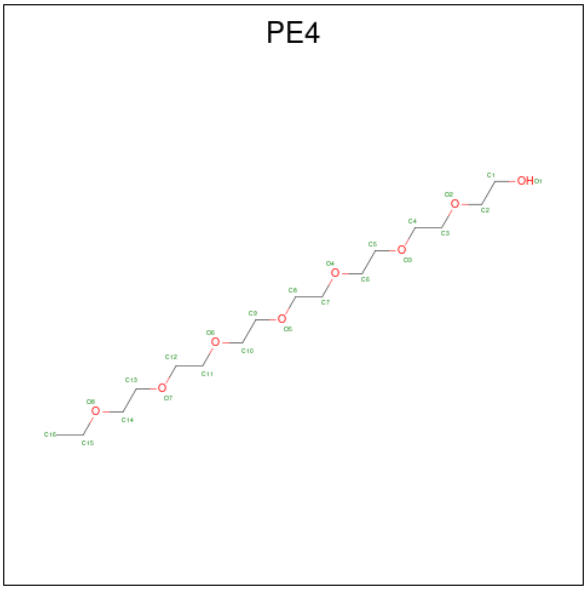


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	C	1	6	3	3	0	0
4	D	1	6	3	3	0	0
4	F	1	6	3	3	0	0

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

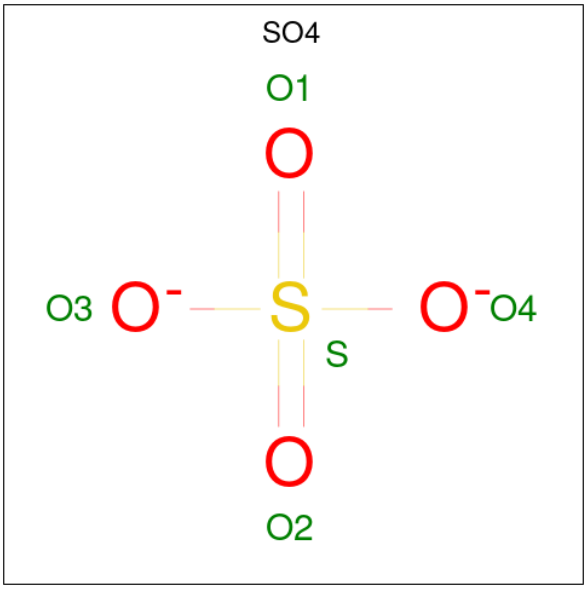
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0
5	C	2	2	2	0	0
5	D	1	1	1	0	0
5	F	2	2	2	0	0

- Molecule 6 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



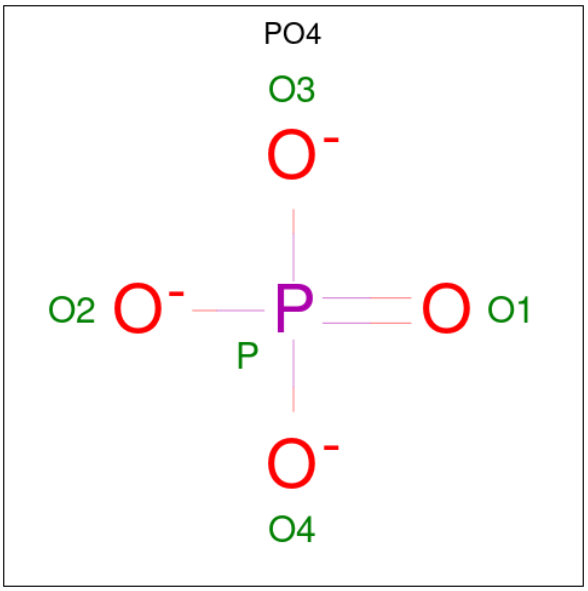
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	C	1	19	12	7	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 9 is water.

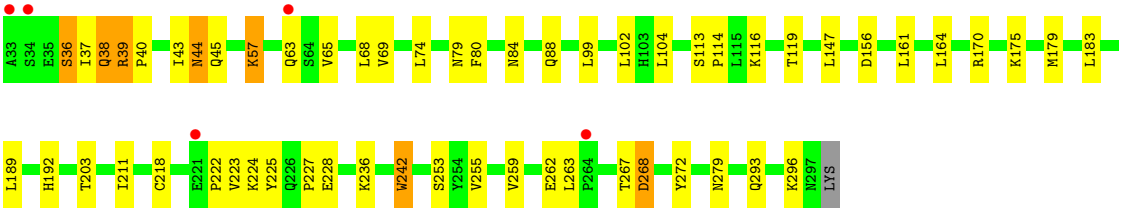
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	115	115	115	0	0
			Total	O		
9	B	19	19	19	0	0
			Total	O		
9	C	56	56	56	0	0
			Total	O		
9	D	24	24	24	0	0
			Total	O		
9	E	52	52	52	0	0
			Total	O		
9	F	14	14	14	0	0

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.

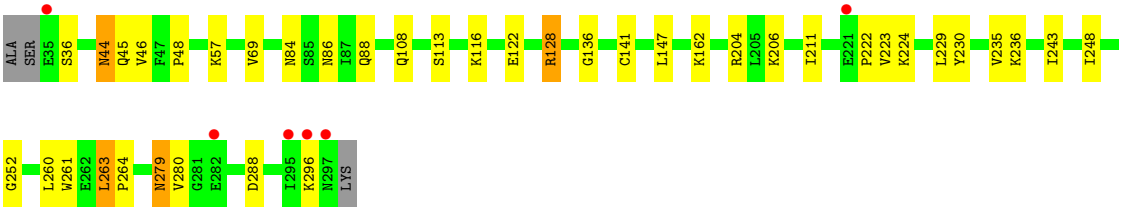
• Molecule 1: INLC PROTEIN

Chain A:



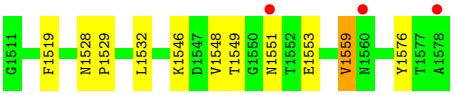
• Molecule 1: INLC PROTEIN

Chain E:



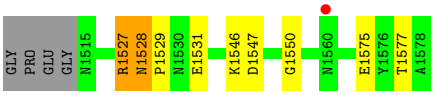
• Molecule 2: DYNAMIN-BINDING PROTEIN

Chain B:



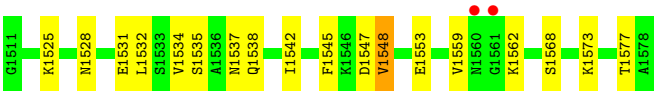
• Molecule 2: DYNAMIN-BINDING PROTEIN

Chain D:



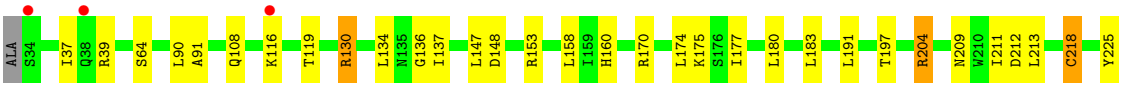
• Molecule 2: DYNAMIN-BINDING PROTEIN

Chain F:



• Molecule 3: INLC PROTEIN

Chain C:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.57 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.196 , 0.262 0.196 , 0.254	Depositor DCC
R_{free} test set	1806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PO4, PE4, SO4, CSX, 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	0.70	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	0.80	1/552 (0.2%)	0.88	1/746 (0.1%)
2	F	0.75	1/576 (0.2%)	0.77	0/781
3	C	0.68	0/2214	0.82	4/2999 (0.1%)
All	All	0.71	2/8268 (0.0%)	0.84	7/11195 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1577	THR	C-N	-5.79	1.20	1.34
2	D	1577	THR	C-N	-5.09	1.22	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2132	0	2176	24	0
1	E	2120	0	2144	15	0
2	B	571	0	568	3	0
2	D	533	0	534	6	0
2	F	556	0	543	7	0
3	C	2157	0	2193	28	0
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	2	0
7	C	10	0	0	1	0
8	E	10	0	0	0	0
9	A	115	0	0	1	0
9	B	19	0	0	0	1
9	C	56	0	0	5	0
9	D	24	0	0	0	0
9	E	52	0	0	1	1
9	F	14	0	0	0	0
All	All	8424	0	8223	82	1

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 5.

All (82) 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)
3:C:276[A]:GLU:CD	9:C:401:HOH:O	1.72	1.25
3:C:276[A]:GLU:OE2	9:C:401:HOH:O	1.76	0.92
3:C:108[A]:GLN:HG2	3:C:130[A]:ARG:NH2	1.98	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39[B]:ARG:NH2	9:C:402:HOH:O	2.17	0.77
1:E:211:ILE:HD13	1:E:280:VAL:HG11	1.68	0.76
3:C:108[A]:GLN:HG2	3:C:130[A]:ARG:HH22	1.54	0.72
3:C:175:LYS:NZ	3:C:218:CSX:OD	2.23	0.71
2:D:1528:ASN:HB2	2:D:1529:PRO:CD	2.30	0.62
1:A:39:ARG:HD3	1:A:39:ARG:C	2.20	0.62
2:D:1546:LYS:HD2	2:D:1550:GLY:HA2	1.82	0.61
1:E:222:PRO:HB2	1:E:296:LYS:HE3	1.84	0.60
2:F:1553[B]:GLU:HA	2:F:1568:SER:OG	2.01	0.59
1:A:236:LYS:HE2	1:A:242:TRP:CD2	2.37	0.59
3:C:108[A]:GLN:CG	3:C:130[A]:ARG:NH2	2.65	0.58
1:A:170[B]:ARG:HG2	1:A:192:HIS:HB3	1.85	0.57
1:E:211:ILE:CD1	1:E:280:VAL:HG11	2.34	0.56
3:C:170:ARG:HE	6:C:302:PE4:H92	1.72	0.55
3:C:148:ASP:HB2	6:C:302:PE4:H122	1.89	0.54
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.73	0.54
3:C:177:ILE:HB	3:C:180[B]:LEU:HD22	1.91	0.53
2:D:1527[A]:ARG:HG2	2:D:1531:GLU:OE1	2.08	0.53
1:A:38:GLN:HE21	1:A:38:GLN:N	2.07	0.52
2:F:1559:VAL:O	2:F:1562:LYS:HG2	2.09	0.52
1:A:80:PHE:HB2	1:A:99:LEU:HD11	1.92	0.50
3:C:211:ILE:HD13	3:C:280:VAL:HG11	1.94	0.50
1:E:261:TRP:HB3	1:E:263:LEU:HD21	1.94	0.50
1:E:113:SER:HA	1:E:136:GLY:HA3	1.93	0.49
1:E:223:VAL:HG11	1:E:229:LEU:HD11	1.94	0.49
1:A:57:LYS:HE2	1:A:63:GLN:O	2.13	0.49
2:B:1528:ASN:HB3	2:B:1529:PRO:HD2	1.95	0.48
2:F:1553[A]:GLU:HA	2:F:1568:SER:OG	2.12	0.48
3:C:297:ASN:ND2	3:C:297:ASN:H	2.11	0.48
1:A:267:THR:OG1	1:A:268:ASP:N	2.46	0.48
1:A:236:LYS:HE2	1:A:242:TRP:CE3	2.48	0.48
1:E:236[A]:LYS:HD3	9:E:413:HOH:O	2.13	0.48
2:D:1528:ASN:HD22	2:D:1528:ASN:N	2.11	0.48
1:A:39:ARG:HD3	1:A:40:PRO:O	2.14	0.48
3:C:236:LYS:HE2	3:C:242[B]:TRP:CE2	2.49	0.48
1:E:86:ASN:HA	1:E:108:GLN:HE22	1.78	0.47
1:A:259:VAL:HG21	1:A:272:TYR:CD1	2.49	0.47
3:C:116[A]:LYS:HA	3:C:136:GLY:O	2.14	0.47
3:C:212:ASP:OD2	2:D:1575:GLU:OE2	2.31	0.47
1:E:279:ASN:HD22	1:E:279:ASN:N	2.11	0.47
3:C:160:HIS:ND1	7:C:303:SO4:O4	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:TYR:OH	1:A:263:LEU:O	2.32	0.46
3:C:283:THR:OG1	3:C:284:GLU:N	2.48	0.46
2:B:1551[B]:ASN:HB3	2:B:1553[B]:GLU:OE1	2.16	0.45
2:D:1528:ASN:HB2	2:D:1529:PRO:HD3	1.98	0.45
3:C:191:LEU:HD12	3:C:213:LEU:HD21	1.99	0.45
3:C:226:GLN:HB2	3:C:228:GLU:O	2.17	0.45
3:C:237:ASP:HB2	3:C:238:PRO:HD2	1.99	0.44
3:C:116[B]:LYS:HA	3:C:136:GLY:O	2.17	0.44
1:A:102:LEU:HD21	1:A:104:LEU:HD11	1.98	0.44
3:C:90:LEU:O	3:C:91:ALA:C	2.56	0.44
2:F:1542:ILE:HG21	2:F:1545:PHE:CE1	2.53	0.44
1:A:43:ILE:HB	1:A:65:VAL:O	2.17	0.43
1:A:189:LEU:O	1:A:211:ILE:HA	2.18	0.43
2:F:1528:ASN:ND2	2:F:1531:GLU:OE2	2.51	0.43
2:F:1547:ASP:OD1	2:F:1547:ASP:C	2.57	0.43
3:C:225:TYR:CE2	3:C:266:TYR:HA	2.53	0.43
3:C:197:THR:O	3:C:235:VAL:HA	2.19	0.43
1:A:36:SER:O	1:A:38:GLN:NE2	2.51	0.43
1:E:46:VAL:O	1:E:48:PRO:HD3	2.19	0.43
1:A:228:GLU:HB3	9:A:447:HOH:O	2.19	0.42
1:A:39:ARG:HG2	1:A:39:ARG:NH1	2.33	0.42
1:A:161:LEU:HB3	1:A:164:LEU:HG	2.02	0.42
2:B:1532:LEU:HD21	2:B:1559:VAL:CG1	2.49	0.42
1:A:37:ILE:C	1:A:38:GLN:HE21	2.23	0.42
1:A:44:ASN:HD22	1:A:45:GLN:N	2.18	0.42
1:A:69[B]:VAL:HG21	1:A:74:LEU:HD21	2.02	0.42
3:C:237:ASP:HB2	3:C:238:PRO:CD	2.50	0.42
3:C:134:LEU:O	3:C:137:ILE:HG22	2.20	0.41
1:A:113:SER:N	1:A:114:PRO:CD	2.83	0.41
3:C:276[A]:GLU:OE1	9:C:401:HOH:O	2.09	0.41
1:E:248:ILE:HG21	1:E:252:GLY:HA3	2.02	0.41
1:A:156:ASP:HA	1:A:179:MET:HG3	2.02	0.41
1:E:122:GLU:HA	1:E:141:CSX:O	2.21	0.41
1:E:116:LYS:HA	1:E:136:GLY:O	2.21	0.40
1:E:235:VAL:HG12	1:E:243:ILE:HD12	2.03	0.40
3:C:204:ARG:NH2	9:C:406:HOH:O	2.50	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
9:B:1714:HOH:O	9:E:450:HOH:O[3_555]	2.13	0.07

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	269/266 (101%)	244 (91%)	22 (8%)	3 (1%)	14	30
1	E	267/266 (100%)	243 (91%)	23 (9%)	1 (0%)	34	57
2	B	70/68 (103%)	66 (94%)	4 (6%)	0	100	100
2	D	64/68 (94%)	59 (92%)	5 (8%)	0	100	100
2	F	68/68 (100%)	63 (93%)	4 (6%)	1 (2%)	10	21
3	C	273/266 (103%)	257 (94%)	16 (6%)	0	100	100
All	All	1011/1002 (101%)	932 (92%)	74 (7%)	5 (0%)	29	52

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	246/238 (103%)	221 (90%)	25 (10%)	7 14
1	E	245/238 (103%)	224 (91%)	21 (9%)	10 20
2	B	62/58 (107%)	56 (90%)	6 (10%)	8 15
2	D	57/58 (98%)	54 (95%)	3 (5%)	22 45
2	F	60/58 (103%)	52 (87%)	8 (13%)	4 7
3	C	250/239 (105%)	233 (93%)	17 (7%)	16 32
All	All	920/889 (104%)	840 (91%)	80 (9%)	11 20

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	44	ASN
1	A	45	GLN
1	A	88	GLN
1	A	250	ASN
1	A	279	ASN
3	C	45	GLN
3	C	58	GLN
3	C	79	ASN
3	C	135	ASN
3	C	149	ASN
3	C	250	ASN
3	C	297	ASN
2	D	1528	ASN
2	D	1538	GLN
2	D	1560	ASN
1	E	44	ASN
1	E	84	ASN
1	E	106	HIS
1	E	108	GLN
1	E	135	ASN
1	E	163	ASN
1	E	250	ASN
1	E	279	ASN
2	F	1551	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)

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	E	258	1	3,6,7	0.87	0	1,6,8	1.99	0
1	CSX	A	258	1	3,6,7	0.97	0	1,6,8	0.78	0
3	CSX	C	141	3	3,6,7	0.90	0	1,6,8	0.40	0
1	CSX	A	218	1	3,6,7	1.03	0	1,6,8	3.96	1 (100%)
1	CSX	E	141	1	3,6,7	0.48	0	1,6,8	0.39	0
3	CSX	C	218	3	3,6,7	0.64	0	1,6,8	3.26	1 (100%)
1	CSX	E	218	1	3,6,7	0.74	0	1,6,8	1.91	0
1	CSX	A	141	1	3,6,7	0.73	0	1,6,8	1.25	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
1	CSX	E	258	1	-	0/1/5/7	-
1	CSX	A	258	1	-	1/1/5/7	-
3	CSX	C	141	3	-	0/1/5/7	-
1	CSX	A	218	1	-	0/1/5/7	-
1	CSX	E	141	1	-	1/1/5/7	-
3	CSX	C	218	3	-	0/1/5/7	-
1	CSX	E	218	1	-	0/1/5/7	-
1	CSX	A	141	1	-	0/1/5/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	218	CSX	CA-CB-SG	-3.96	104.71	113.36
3	C	218	CSX	CA-CB-SG	-3.26	106.23	113.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	258	CSX	N-CA-CB-SG
1	E	141	CSX	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	141	CSX	1	0
3	C	218	CSX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
8	PO4	E	301	-	4,4,4	0.61	0	6,6,6	0.84	0
7	SO4	C	304	-	4,4,4	0.47	0	6,6,6	0.52	0
8	PO4	E	302	-	4,4,4	0.75	0	6,6,6	0.89	0
4	GOL	B	1601	-	5,5,5	0.41	0	5,5,5	0.57	0
4	GOL	F	1601	-	5,5,5	0.65	0	5,5,5	0.60	0
4	GOL	A	301	-	5,5,5	0.75	0	5,5,5	0.89	0
4	GOL	C	301	-	5,5,5	1.06	0	5,5,5	0.76	0
6	PE4	C	302	-	18,18,23	0.66	0	17,17,22	0.58	0
7	SO4	C	303	-	4,4,4	0.61	0	6,6,6	0.38	0
4	GOL	D	1601	-	5,5,5	0.53	0	5,5,5	0.53	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	B	1601	-	-	1/4/4/4	-
4	GOL	F	1601	-	-	0/4/4/4	-
4	GOL	A	301	-	-	3/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-
6	PE4	C	302	-	-	13/16/16/21	-
4	GOL	D	1601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	GOL	C1-C2-C3-O3
4	D	1601	GOL	C1-C2-C3-O3
4	D	1601	GOL	O2-C2-C3-O3
6	C	302	PE4	C3-C4-O3-C5
6	C	302	PE4	C4-C3-O2-C2
6	C	302	PE4	O3-C5-C6-O4
4	C	301	GOL	O2-C2-C3-O3
6	C	302	PE4	O2-C3-C4-O3
6	C	302	PE4	C10-C9-O5-C8
6	C	302	PE4	O1-C1-C2-O2
4	A	301	GOL	O1-C1-C2-C3
4	A	301	GOL	C1-C2-C3-O3
4	A	301	GOL	O1-C1-C2-O2
6	C	302	PE4	O6-C11-C12-O7
6	C	302	PE4	O4-C7-C8-O5
6	C	302	PE4	C8-C7-O4-C6
6	C	302	PE4	C5-C6-O4-C7
6	C	302	PE4	C9-C10-O6-C11
6	C	302	PE4	O6-C10-C9-O5
4	B	1601	GOL	C1-C2-C3-O3
6	C	302	PE4	C1-C2-O2-C3

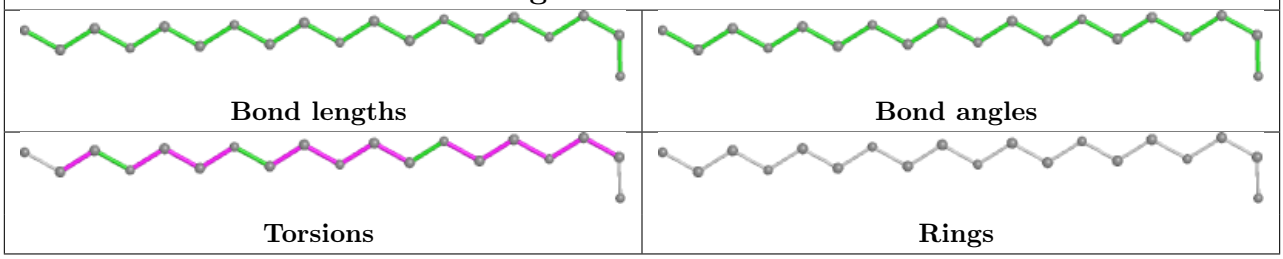
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	302	PE4	2	0
7	C	303	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PE4 C 302



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	262/266 (98%)	-0.34	5 (1%)	66	62	26, 42, 82, 105	0
1	E	260/266 (97%)	-0.20	6 (2%)	60	54	30, 54, 84, 110	0
2	B	68/68 (100%)	-0.36	3 (4%)	34	27	28, 44, 67, 85	0
2	D	64/68 (94%)	-0.41	1 (1%)	72	68	29, 41, 61, 70	0
2	F	68/68 (100%)	-0.12	2 (2%)	51	45	37, 52, 84, 91	0
3	C	263/266 (98%)	-0.29	6 (2%)	60	54	24, 47, 84, 148	0
All	All	985/1002 (98%)	-0.28	23 (2%)	60	54	24, 47, 83, 148	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	38	GLN	4.9
1	A	33	ALA	4.3
2	F	1561	GLY	3.8
1	E	35	GLU	3.6
3	C	34	SER	3.4
3	C	298	LYS	3.2
1	E	296	LYS	2.9
3	C	297	ASN	2.9
1	A	63	GLN	2.6
1	E	282	GLU	2.5
1	E	221	GLU	2.4
1	A	221	GLU	2.4
1	E	295	ILE	2.4
1	E	297	ASN	2.3
2	F	1560	ASN	2.3
1	A	264	PRO	2.2
1	A	34	SER	2.2
2	D	1560	ASN	2.2
2	B	1560	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	1578	ALA	2.1
2	B	1551[A]	ASN	2.0
3	C	116[A]	LYS	2.0
3	C	296	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSX	E	218	7/8	0.79	0.20	49,53,66,68	0
3	CSX	C	141	7/8	0.87	0.15	48,53,64,64	0
3	CSX	C	218	7/8	0.90	0.15	42,44,51,51	1
1	CSX	E	141	7/8	0.92	0.16	54,60,68,71	0
1	CSX	E	258	7/8	0.92	0.13	50,53,63,64	0
1	CSX	A	218	7/8	0.93	0.14	46,47,50,54	1
1	CSX	A	258	7/8	0.94	0.12	48,48,54,54	0
1	CSX	A	141	7/8	0.94	0.13	39,42,48,50	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
4	GOL	C	301	6/6	0.55	0.43	52,59,60,64	0
5	CL	C	306	1/1	0.82	0.09	70,70,70,70	0
4	GOL	A	301	6/6	0.83	0.22	58,61,63,64	0
6	PE4	C	302	19/24	0.83	0.31	42,65,80,83	0
4	GOL	D	1601	6/6	0.85	0.17	54,60,65,66	0
5	CL	D	1602	1/1	0.89	0.14	71,71,71,71	0

Continued on next page...

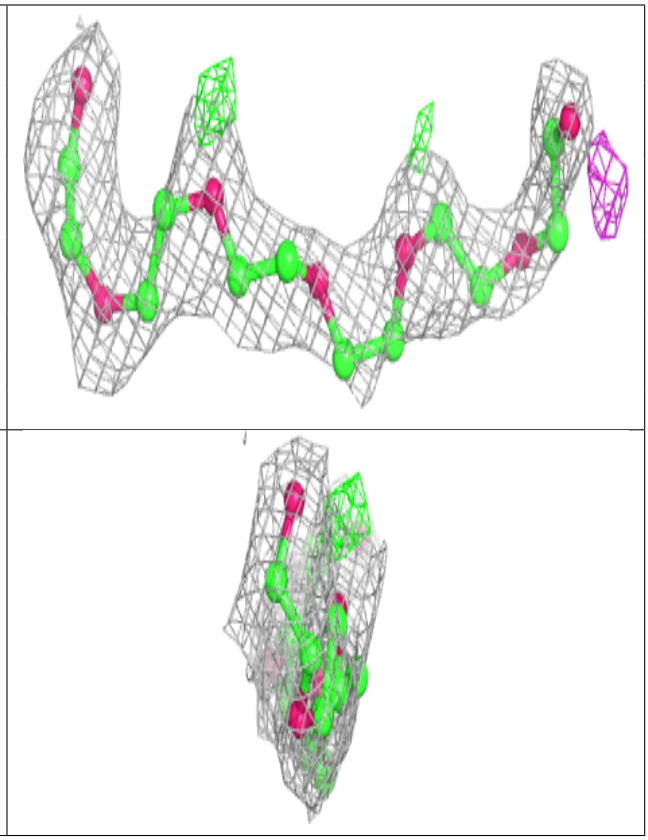
Continued from previous page...

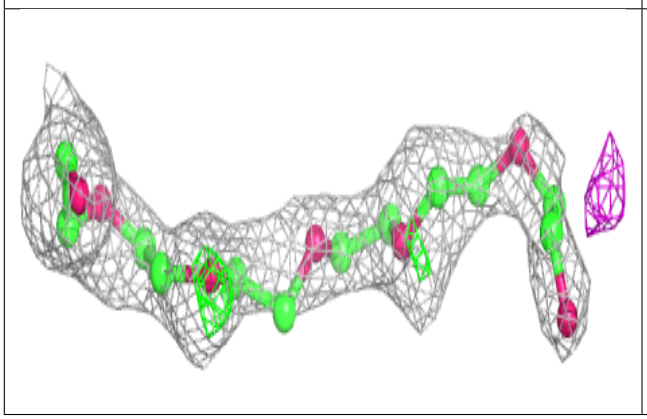
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	C	303	5/5	0.89	0.25	79,80,85,89	0
4	GOL	F	1601	6/6	0.90	0.16	48,48,53,55	0
5	CL	A	302	1/1	0.90	0.09	72,72,72,72	0
5	CL	F	1603	1/1	0.91	0.08	69,69,69,69	0
8	PO4	E	302	5/5	0.92	0.29	72,85,88,91	0
4	GOL	B	1601	6/6	0.93	0.15	59,64,65,69	0
5	CL	F	1602	1/1	0.93	0.23	69,69,69,69	0
8	PO4	E	301	5/5	0.96	0.33	59,62,69,71	0
5	CL	C	305	1/1	0.96	0.08	63,63,63,63	0
7	SO4	C	304	5/5	0.98	0.14	43,46,52,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PE4 C 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.