



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:51 PM UTC

PDB ID : 7YL4 / pdb_00007yl4
Title : Cell surface protein YwfG protein (apo form)
Authors : Tsuchiya, W.; Fujimoto, Z.; Suzuki, C.
Deposited on : 2022-07-25
Resolution : 2.50 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

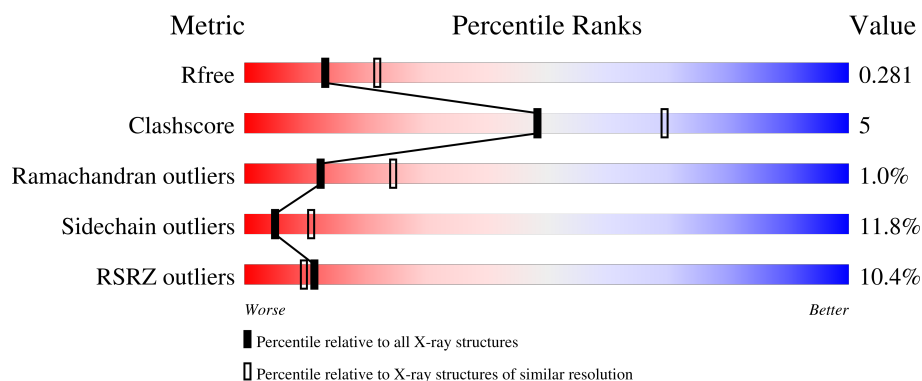
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	505	
1	B	505	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6673 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 GRAM_POS_ANCHORING domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3552	2207	590	750	5			
1	B	397	Total	C	N	O	S	0	0	0
			2975	1849	494	627	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP S6FKX6
A	8	GLY	-	expression tag	UNP S6FKX6
A	9	SER	-	expression tag	UNP S6FKX6
A	10	SER	-	expression tag	UNP S6FKX6
A	11	HIS	-	expression tag	UNP S6FKX6
A	12	HIS	-	expression tag	UNP S6FKX6
A	13	HIS	-	expression tag	UNP S6FKX6
A	14	HIS	-	expression tag	UNP S6FKX6
A	15	HIS	-	expression tag	UNP S6FKX6
A	16	HIS	-	expression tag	UNP S6FKX6
A	17	SER	-	expression tag	UNP S6FKX6
A	18	SER	-	expression tag	UNP S6FKX6
A	19	GLY	-	expression tag	UNP S6FKX6
A	20	LEU	-	expression tag	UNP S6FKX6
A	21	VAL	-	expression tag	UNP S6FKX6
A	22	PRO	-	expression tag	UNP S6FKX6
A	23	ARG	-	expression tag	UNP S6FKX6
A	24	GLY	-	expression tag	UNP S6FKX6
A	25	SER	-	expression tag	UNP S6FKX6
A	26	HIS	-	expression tag	UNP S6FKX6
A	27	MET	-	expression tag	UNP S6FKX6
B	7	MET	-	initiating methionine	UNP S6FKX6
B	8	GLY	-	expression tag	UNP S6FKX6
B	9	SER	-	expression tag	UNP S6FKX6
B	10	SER	-	expression tag	UNP S6FKX6

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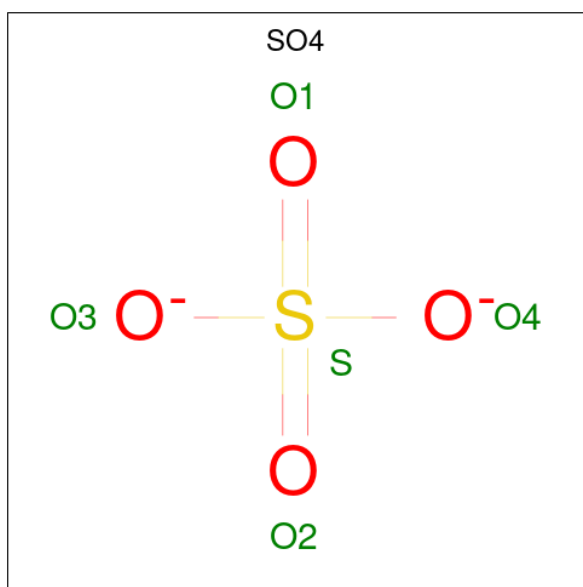
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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	expression tag	UNP S6FKX6
B	12	HIS	-	expression tag	UNP S6FKX6
B	13	HIS	-	expression tag	UNP S6FKX6
B	14	HIS	-	expression tag	UNP S6FKX6
B	15	HIS	-	expression tag	UNP S6FKX6
B	16	HIS	-	expression tag	UNP S6FKX6
B	17	SER	-	expression tag	UNP S6FKX6
B	18	SER	-	expression tag	UNP S6FKX6
B	19	GLY	-	expression tag	UNP S6FKX6
B	20	LEU	-	expression tag	UNP S6FKX6
B	21	VAL	-	expression tag	UNP S6FKX6
B	22	PRO	-	expression tag	UNP S6FKX6
B	23	ARG	-	expression tag	UNP S6FKX6
B	24	GLY	-	expression tag	UNP S6FKX6
B	25	SER	-	expression tag	UNP S6FKX6
B	26	HIS	-	expression tag	UNP S6FKX6
B	27	MET	-	expression tag	UNP S6FKX6

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

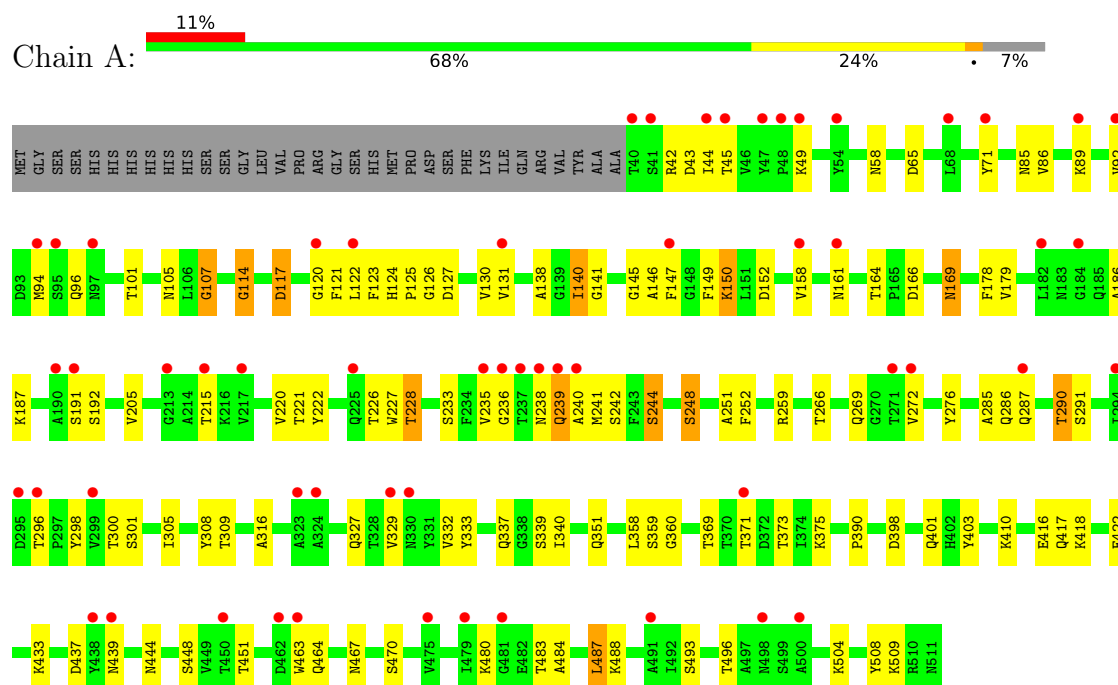
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	61	Total 61	O 61	0	0

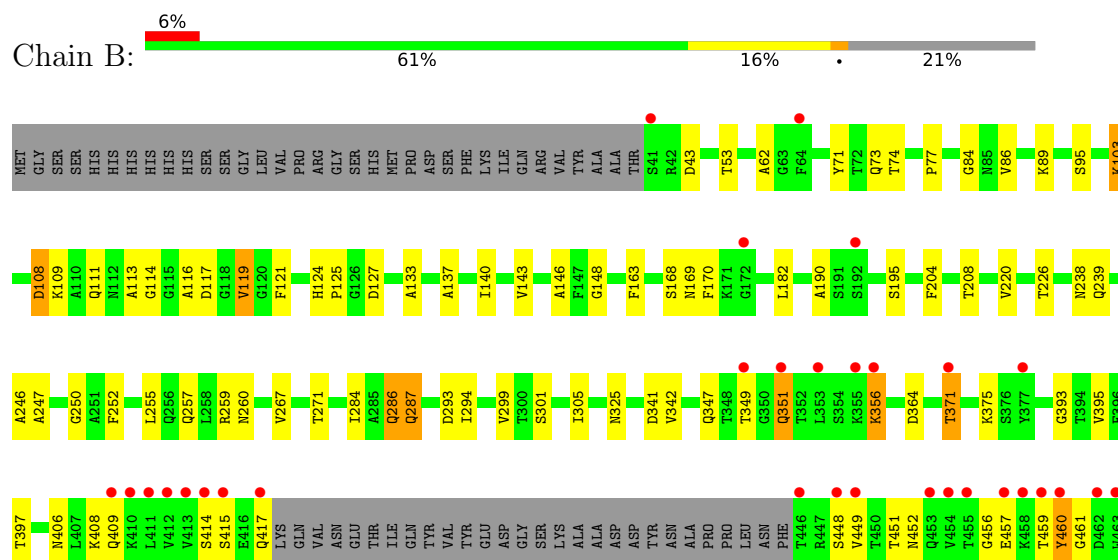
3 Residue-property plots

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: GRAM_POS_ANCHORING domain-containing protein



• Molecule 1: GRAM_POS_ANCHORING domain-containing protein



Q464	A465	GLN	GLY	ASN	ASP	SER	PHE	GLY	GLU	VAL	VAL	SER	PRO	THR	ILE	LYS	GLY	GLU	THR	ALA	ASP	GLN	LEU	LYS	ILE	ASP	ALA	ILE	SER	GLY	ILE	THR	ALA	ASN	SER	ALA	ASP	ILE	GLN	LYS	VAL	VAL	TYR	LYS	ARG	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	43.22Å 272.93Å 320.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.53 – 2.50 45.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.53-2.50) 100.0 (45.53-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.245 , 0.280 0.252 , 0.281	Depositor DCC
R_{free} test set	3224 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4

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	1.21	2/3620 (0.1%)	1.52	10/4924 (0.2%)
1	B	1.28	8/3033 (0.3%)	1.48	13/4127 (0.3%)
All	All	1.24	10/6653 (0.2%)	1.50	23/9051 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	HIS	CE1-NE2	7.82	1.40	1.32
1	B	119	VAL	C-O	7.23	1.31	1.24
1	B	125	PRO	C-O	-7.22	1.15	1.24
1	A	251	ALA	C-O	6.93	1.32	1.24
1	B	267	VAL	C-O	6.45	1.31	1.24
1	B	246	ALA	C-O	6.15	1.31	1.23
1	A	178	PHE	C-O	5.76	1.30	1.23
1	B	84	GLY	C-O	5.21	1.29	1.23
1	B	73	GLN	C-O	5.15	1.29	1.24
1	B	182	LEU	N-CA	5.01	1.52	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	PHE	CA-CB-CG	7.94	121.74	113.80
1	A	117	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	416	GLU	CB-CA-C	6.35	120.01	109.53
1	A	107	GLY	N-CA-C	6.30	117.92	111.56
1	B	95	SER	N-CA-C	-6.14	105.27	112.89
1	B	190	ALA	CA-C-O	-6.02	114.50	120.82
1	B	287	GLN	CB-CG-CD	-5.98	102.44	112.60
1	B	140	ILE	CA-C-N	5.95	125.75	120.10
1	B	140	ILE	C-N-CA	5.95	125.75	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	PHE	CA-C-O	-5.79	115.08	121.33
1	B	226	THR	CA-CB-OG1	-5.70	101.06	109.60
1	B	53	THR	CA-CB-OG1	-5.50	101.35	109.60
1	A	422	GLU	CB-CA-C	5.49	119.19	110.19
1	A	43	ASP	CA-CB-CG	5.41	118.00	112.60
1	B	364	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	393	GLY	CA-C-O	-5.39	117.61	122.57
1	B	111	GLN	N-CA-C	-5.38	105.31	111.07
1	B	299	VAL	CA-C-O	-5.26	114.21	120.78
1	B	371	THR	CA-CB-OG1	-5.21	101.79	109.60
1	A	228	THR	CA-CB-OG1	-5.11	101.94	109.60
1	A	269	GLN	CB-CA-C	5.01	117.80	109.53
1	A	114	GLY	CA-C-N	5.00	125.98	122.33
1	A	114	GLY	C-N-CA	5.00	125.98	122.33

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	3552	0	3355	41	0
1	B	2975	0	2795	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	0	0	0
3	B	40	0	0	3	0
4	A	13	0	0	1	0
4	B	61	0	0	1	0
All	All	6673	0	6150	70	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 5.

All (70) 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:94:MET:HG3	1:A:241:MET:HG3	1.81	0.61
1:B:286:GLN:N	3:B:606:SO4:O3	2.34	0.61
1:A:390:PRO:HD3	1:A:403:TYR:CE1	2.37	0.59
1:A:117:ASP:HB2	1:A:248:SER:O	2.02	0.59
1:B:74:THR:HA	1:B:257:GLN:HG2	1.88	0.56
1:B:127:ASP:HA	1:B:325:ASN:OD1	2.06	0.55
1:A:444:ASN:HB2	1:A:467:ASN:OD1	2.08	0.54
1:A:308:TYR:HB3	1:A:333:TYR:HB3	1.89	0.54
1:A:122:LEU:HD13	1:A:140:ILE:HA	1.91	0.53
1:A:96:GLN:HG3	1:A:266:THR:HG21	1.89	0.53
1:A:125:PRO:HD3	1:A:145:GLY:O	2.09	0.53
1:A:150:LYS:HD2	1:A:152:ASP:HB2	1.89	0.53
1:B:452:ASN:O	1:B:456:GLY:HA2	2.08	0.52
1:A:127:ASP:HB3	1:A:130:VAL:HG23	1.91	0.52
1:A:114:GLY:HA2	1:A:252:PHE:CD2	2.44	0.52
1:B:103:LYS:HB3	1:B:204:PHE:HB3	1.92	0.52
1:A:205:VAL:HB	1:A:222:TYR:CE1	2.45	0.51
1:A:272:VAL:HG21	1:A:298:TYR:CG	2.45	0.51
1:B:133:ALA:O	1:B:137:ALA:HB3	2.10	0.51
1:B:349:THR:HG22	1:B:351:GLN:HB2	1.92	0.51
1:A:114:GLY:HA2	1:A:252:PHE:CG	2.47	0.50
1:B:409:GLN:HB3	1:B:452:ASN:HD21	1.77	0.49
1:A:105:ASN:OD1	1:A:105:ASN:C	2.55	0.49
1:A:221:THR:HG22	1:A:226:THR:HG23	1.95	0.49
1:A:309:THR:HA	4:A:712:HOH:O	2.12	0.49
1:A:316:ALA:HB3	1:A:329:VAL:HG22	1.94	0.49
1:B:238:ASN:O	1:B:239:GLN:HB3	2.11	0.49
1:A:120:GLY:HA3	1:A:138:ALA:O	2.13	0.48
1:A:124:HIS:O	1:A:242:SER:N	2.40	0.48
1:A:149:PHE:CD2	1:A:220:VAL:HG11	2.49	0.48
1:B:250:GLY:N	3:B:609:SO4:O2	2.43	0.47
1:B:448:SER:O	1:B:461:GLY:N	2.47	0.47
1:B:397:THR:HB	3:B:608:SO4:O1	2.16	0.46
1:B:341:ASP:HA	1:B:356:LYS:O	2.16	0.46
1:A:122:LEU:HB3	1:A:244:SER:OG	2.16	0.46
1:A:152:ASP:OD2	1:A:166:ASP:OD2	2.33	0.46
1:A:121:PHE:O	1:A:140:ILE:HD11	2.16	0.46
1:A:141:GLY:CA	1:A:186:ALA:HB2	2.45	0.46
1:B:449:VAL:HA	1:B:460:TYR:HA	1.97	0.46
1:A:340:ILE:HG12	1:A:401:GLN:HB2	1.97	0.45
1:B:108:ASP:OD1	1:B:109:LYS:HG3	2.16	0.45
1:B:116:ALA:HB1	1:B:117:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLN:HB2	4:B:746:HOH:O	2.16	0.45
1:B:89:LYS:HD3	1:B:89:LYS:HA	1.83	0.45
1:A:58:ASN:HB2	1:A:85:ASN:OD1	2.17	0.44
1:A:337:GLN:HA	1:A:360:GLY:O	2.16	0.44
1:B:71:TYR:O	1:B:259:ARG:HA	2.18	0.44
1:B:114:GLY:HA2	1:B:252:PHE:CG	2.52	0.44
1:B:143:VAL:HB	1:B:146:ALA:HB2	2.00	0.43
1:A:92:VAL:O	1:A:240:ALA:HA	2.18	0.43
1:A:290:THR:OG1	1:A:291:SER:N	2.51	0.43
1:B:119:VAL:HG22	1:B:247:ALA:HB2	2.00	0.43
1:A:149:PHE:CE2	1:A:220:VAL:HG11	2.54	0.43
1:A:369:THR:HG22	1:A:371:THR:H	1.82	0.43
1:B:121:PHE:O	1:B:148:GLY:HA3	2.19	0.43
1:B:349:THR:CG2	1:B:351:GLN:HB2	2.49	0.43
1:A:192:SER:O	1:A:227:TRP:CD1	2.72	0.42
1:B:284:ILE:HG13	1:B:305:ILE:HD13	2.01	0.42
1:A:71:TYR:O	1:A:259:ARG:HA	2.19	0.42
1:B:168:SER:C	1:B:170:PHE:H	2.26	0.42
1:B:293:ASP:O	1:B:294:ILE:C	2.63	0.42
1:A:276:TYR:HB2	1:A:285:ALA:HB3	2.02	0.42
1:A:470:SER:HA	1:A:493:SER:HA	2.02	0.41
1:A:484:ALA:HB2	1:A:508:TYR:CE2	2.55	0.41
1:B:208:THR:O	1:B:220:VAL:HA	2.20	0.41
1:A:123:PHE:O	1:A:146:ALA:HA	2.21	0.41
1:B:77:PRO:HA	1:B:255:LEU:HD12	2.03	0.40
1:A:105:ASN:OD1	1:A:107:GLY:N	2.51	0.40
1:A:220:VAL:O	1:A:227:TRP:HE3	2.04	0.40
1:A:487:LEU:HD12	1:A:487:LEU:HA	1.81	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	470/505 (93%)	434 (92%)	30 (6%)	6 (1%)	9	18
1	B	393/505 (78%)	373 (95%)	17 (4%)	3 (1%)	16	31
All	All	863/1010 (85%)	807 (94%)	47 (5%)	9 (1%)	12	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	TRP
1	B	113	ALA
1	A	236	GLY
1	A	239	GLN
1	A	169	ASN
1	B	62	ALA
1	B	169	ASN
1	A	235	VAL
1	A	126	GLY

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	383/411 (93%)	326 (85%)	57 (15%)	3	6
1	B	320/411 (78%)	294 (92%)	26 (8%)	11	23
All	All	703/822 (86%)	620 (88%)	83 (12%)	5	11

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	44	ILE
1	A	45	THR
1	A	49	LYS
1	A	65	ASP
1	A	86	VAL
1	A	89	LYS

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Mol	Chain	Res	Type
1	A	101	THR
1	A	131	VAL
1	A	140	ILE
1	A	150	LYS
1	A	158	VAL
1	A	161	ASN
1	A	164	THR
1	A	169	ASN
1	A	179	VAL
1	A	187	LYS
1	A	191	SER
1	A	215	THR
1	A	228	THR
1	A	233	SER
1	A	238	ASN
1	A	239	GLN
1	A	244	SER
1	A	248	SER
1	A	286	GLN
1	A	287	GLN
1	A	290	THR
1	A	296	THR
1	A	300	THR
1	A	301	SER
1	A	305	ILE
1	A	327	GLN
1	A	332	VAL
1	A	339	SER
1	A	351	GLN
1	A	358	LEU
1	A	359	SER
1	A	373	THR
1	A	375	LYS
1	A	398	ASP
1	A	410	LYS
1	A	417	GLN
1	A	418	LYS
1	A	433	LYS
1	A	437	ASP
1	A	439	ASN
1	A	448	SER
1	A	451	THR

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Mol	Chain	Res	Type
1	A	464	GLN
1	A	480	LYS
1	A	483	THR
1	A	487	LEU
1	A	488	LYS
1	A	496	THR
1	A	504	LYS
1	A	509	LYS
1	B	43	ASP
1	B	86	VAL
1	B	103	LYS
1	B	108	ASP
1	B	195	SER
1	B	260	ASN
1	B	271	THR
1	B	286	GLN
1	B	301	SER
1	B	342	VAL
1	B	347	GLN
1	B	351	GLN
1	B	356	LYS
1	B	371	THR
1	B	375	LYS
1	B	395	VAL
1	B	406	ASN
1	B	408	LYS
1	B	414	SER
1	B	415	SER
1	B	417	GLN
1	B	451	THR
1	B	457	GLU
1	B	459	THR
1	B	460	TYR
1	B	464	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	78	ASN
1	A	201	ASN
1	A	269	GLN

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Mol	Chain	Res	Type
1	A	282	ASN
1	A	321	ASN
1	A	337	GLN
1	A	409	GLN
1	A	417	GLN
1	B	201	ASN
1	B	286	GLN
1	B	347	GLN
1	B	406	ASN
1	B	453	GLN

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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\# Z > 2$
3	SO4	A	606	-	4,4,4	0.23	0	6,6,6	0.23	0
3	SO4	B	606	-	4,4,4	0.34	0	6,6,6	0.19	0
3	SO4	A	604	-	4,4,4	0.29	0	6,6,6	0.17	0
3	SO4	B	607	-	4,4,4	0.27	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	603	-	4,4,4	0.26	0	6,6,6	0.17	0
3	SO4	B	605	-	4,4,4	0.32	0	6,6,6	0.07	0
3	SO4	B	602	-	4,4,4	0.39	0	6,6,6	0.26	0
3	SO4	B	604	-	4,4,4	0.32	0	6,6,6	0.14	0
3	SO4	A	605	-	4,4,4	0.27	0	6,6,6	0.19	0
3	SO4	B	608	-	4,4,4	0.30	0	6,6,6	0.14	0
3	SO4	A	607	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	A	603	-	4,4,4	0.33	0	6,6,6	0.26	0
3	SO4	B	609	-	4,4,4	0.33	0	6,6,6	0.13	0
3	SO4	A	602	-	4,4,4	0.37	0	6,6,6	0.22	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	606	SO4	1	0
3	B	608	SO4	1	0
3	B	609	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	472/505 (93%)	1.10	58 (12%) 8 7	45, 78, 104, 120	0
1	B	397/505 (78%)	0.35	32 (8%) 18 15	32, 52, 120, 153	0
All	All	869/1010 (86%)	0.75	90 (10%) 11 10	32, 69, 107, 153	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	GLY	4.1
1	A	237	THR	4.1
1	B	412	VAL	3.9
1	B	460	TYR	3.8
1	B	172	GLY	3.8
1	A	498	ASN	3.8
1	B	463	TRP	3.8
1	B	449	VAL	3.7
1	A	48	PRO	3.7
1	A	45	THR	3.6
1	A	190	ALA	3.6
1	A	294	ILE	3.6
1	A	191	SER	3.4
1	B	415	SER	3.4
1	A	89	LYS	3.4
1	A	299	VAL	3.4
1	B	453	GLN	3.3
1	B	446	THR	3.3
1	A	44	ILE	3.3
1	A	49	LYS	3.3
1	B	192	SER	3.2
1	B	458	LYS	3.1
1	B	411	LEU	3.1
1	A	147	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	439	ASN	3.0
1	A	296	THR	3.0
1	A	324	ALA	3.0
1	A	120	GLY	3.0
1	A	462	ASP	2.9
1	A	54	TYR	2.9
1	A	238	ASN	2.8
1	A	95	SER	2.7
1	A	94	MET	2.7
1	B	410	LYS	2.7
1	B	417	GLN	2.7
1	A	158	VAL	2.7
1	A	40	THR	2.7
1	A	217	VAL	2.7
1	B	409	GLN	2.7
1	A	92	VAL	2.6
1	B	457	GLU	2.6
1	B	465	ALA	2.6
1	A	41	SER	2.6
1	B	351	GLN	2.6
1	A	47	TYR	2.6
1	B	448	SER	2.5
1	A	479	ILE	2.5
1	B	462	ASP	2.5
1	A	239	GLN	2.5
1	A	97	ASN	2.5
1	A	272	VAL	2.5
1	A	491	ALA	2.5
1	A	450	THR	2.4
1	A	271	THR	2.4
1	B	356	LYS	2.4
1	B	353	LEU	2.4
1	A	323	ALA	2.4
1	B	455	THR	2.4
1	A	68	LEU	2.4
1	A	438	TYR	2.4
1	A	161	ASN	2.4
1	A	213	GLY	2.3
1	A	330	ASN	2.3
1	B	355	LYS	2.3
1	A	371	THR	2.3
1	A	182	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	287	GLN	2.2
1	A	122	LEU	2.2
1	A	295	ASP	2.2
1	A	184	GLY	2.2
1	A	235	VAL	2.2
1	B	413	VAL	2.2
1	A	131	VAL	2.2
1	A	475	VAL	2.2
1	A	225	GLN	2.2
1	B	414	SER	2.2
1	A	500	ALA	2.1
1	A	71	TYR	2.1
1	B	64	PHE	2.1
1	A	215	THR	2.1
1	B	349	THR	2.1
1	B	454	VAL	2.1
1	A	329	VAL	2.1
1	A	481	GLY	2.1
1	B	371	THR	2.1
1	B	459	THR	2.1
1	A	463	TRP	2.0
1	B	377	TYR	2.0
1	B	41	SER	2.0
1	A	240	ALA	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](#)

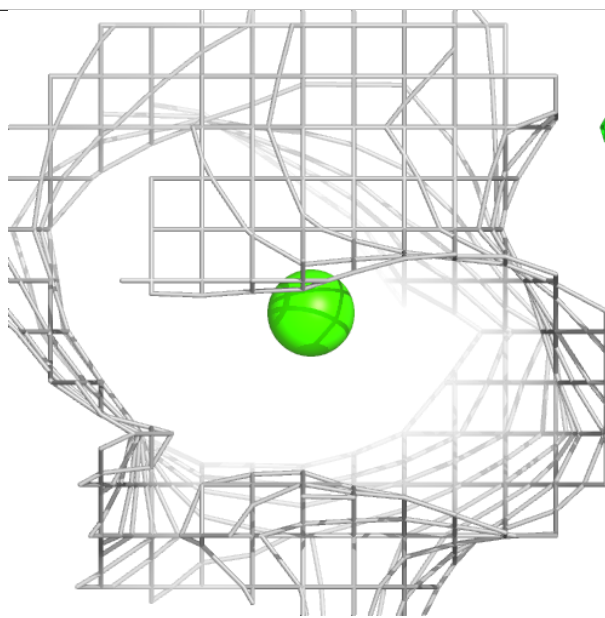
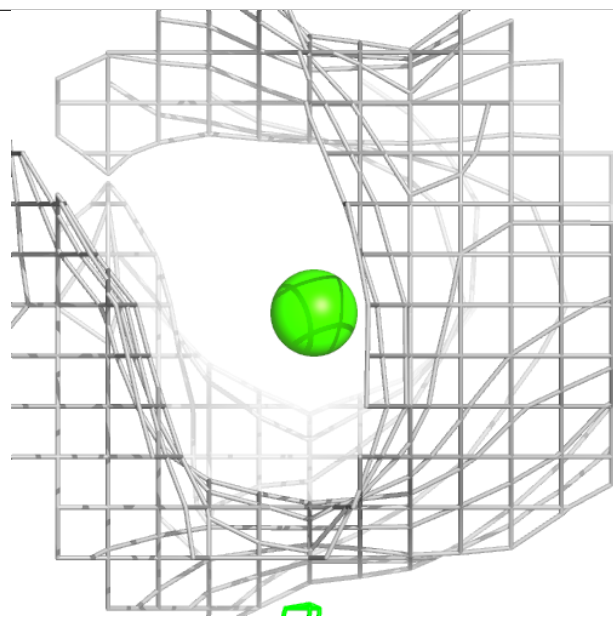
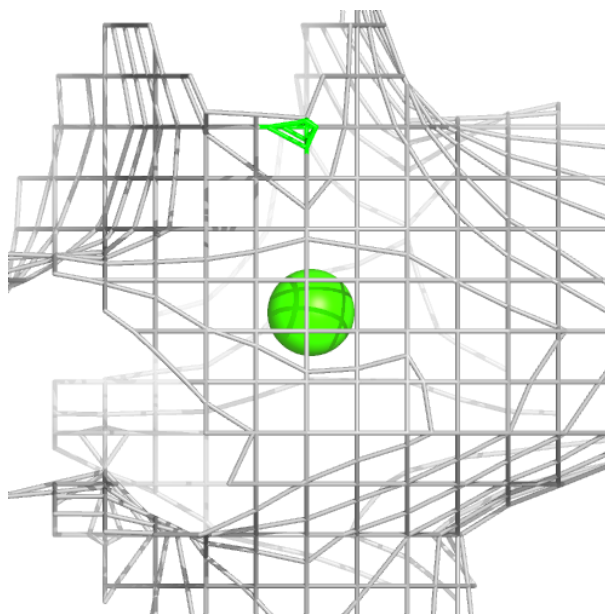
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

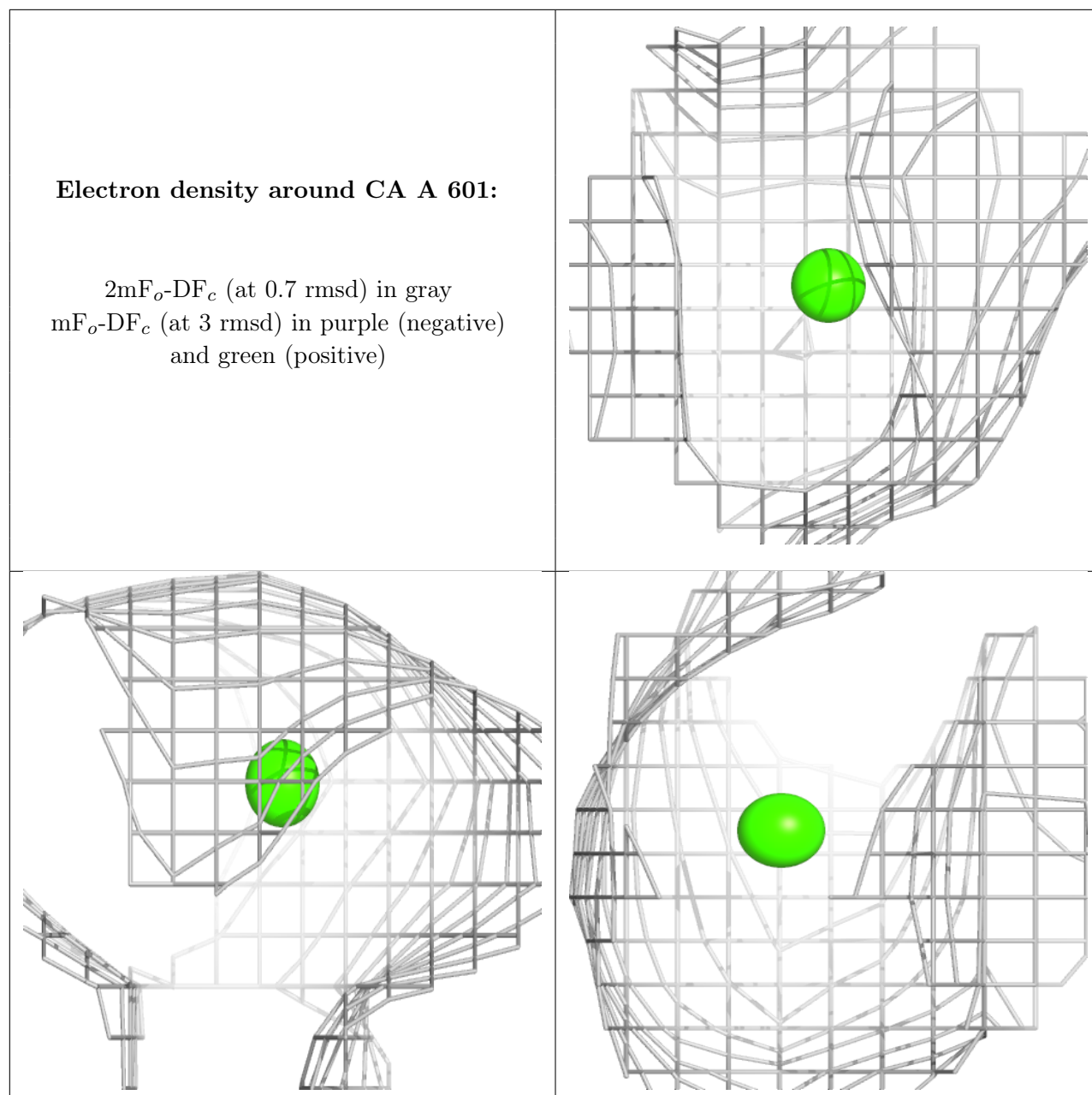
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	604	5/5	0.71	0.16	138,143,165,172	0
3	SO4	B	607	5/5	0.74	0.12	98,100,128,133	0
3	SO4	B	608	5/5	0.78	0.13	104,115,137,154	0
3	SO4	A	607	5/5	0.83	0.12	89,98,113,119	0
3	SO4	B	609	5/5	0.86	0.12	119,122,140,143	0
3	SO4	B	603	5/5	0.87	0.11	79,86,97,104	0
3	SO4	A	605	5/5	0.87	0.09	98,103,107,119	0
3	SO4	B	605	5/5	0.88	0.10	92,99,111,121	0
3	SO4	A	602	5/5	0.88	0.11	66,77,120,120	0
3	SO4	B	606	5/5	0.90	0.08	72,81,97,104	0
3	SO4	A	606	5/5	0.92	0.15	64,78,91,98	0
3	SO4	B	604	5/5	0.94	0.12	74,87,93,99	0
3	SO4	A	603	5/5	0.94	0.09	58,63,83,102	0
3	SO4	B	602	5/5	0.97	0.08	57,61,65,75	0
2	CA	B	601	1/1	0.98	0.04	71,71,71,71	0
2	CA	A	601	1/1	0.99	0.04	74,74,74,74	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 CA B 601:

$2mF_o-DF_c$ (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.