



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:48 pm BST

PDB ID : 2ABJ  
Title : Crystal structure of human branched chain amino acid transaminase in a complex with an inhibitor, C<sub>16</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub>F<sub>3</sub>SCl, and pyridoxal 5' phosphate.  
Authors : Ohren, J.F.; Moreland, D.W.; Rubin, J.R.; Hu, H.L.; McConnell, P.C.; Mistry, A.; Mueller, W.T.; Scholten, J.D.; Hasemann, C.H.  
Deposited on : 2005-07-15  
Resolution : 2.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

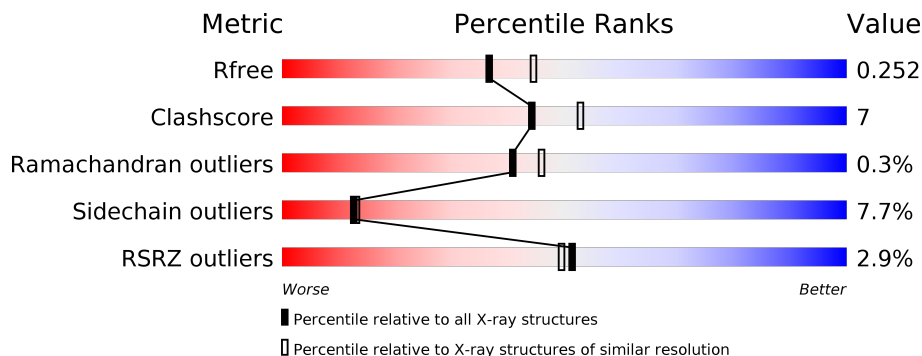
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	366	
1	D	366	
1	G	366	
1	J	366	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13037 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.

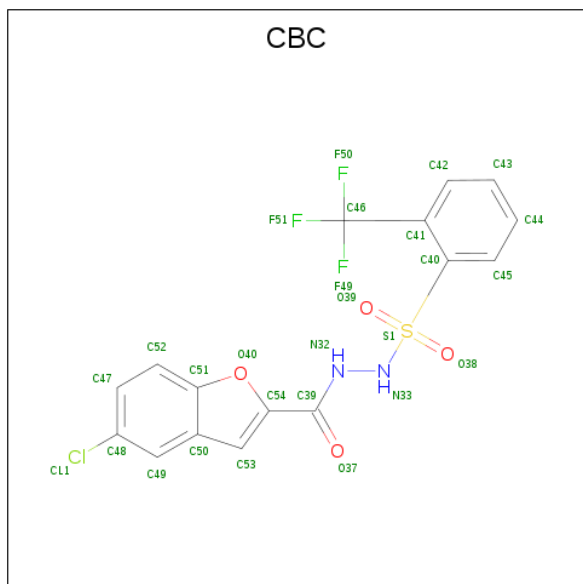
- Molecule 1 is a protein called Branched-chain-amino-acid aminotransferase, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	2892	1859	479	539	15	0	0	0
1	D	359	2840	1826	472	527	15	0	0	0
1	G	358	2832	1819	471	527	15	0	0	0
1	J	366	2892	1859	479	539	15	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	ALA	THR	VARIANT	UNP P54687
A	235	ASP	ALA	VARIANT	UNP P54687
A	249	ARG	GLU	VARIANT	UNP P54687
A	315	THR	SER	VARIANT	UNP P54687
A	328	SER	GLY	VARIANT	UNP P54687
D	163	ALA	THR	VARIANT	UNP P54687
D	235	ASP	ALA	VARIANT	UNP P54687
D	249	ARG	GLU	VARIANT	UNP P54687
D	315	THR	SER	VARIANT	UNP P54687
D	328	SER	GLY	VARIANT	UNP P54687
G	163	ALA	THR	VARIANT	UNP P54687
G	235	ASP	ALA	VARIANT	UNP P54687
G	249	ARG	GLU	VARIANT	UNP P54687
G	315	THR	SER	VARIANT	UNP P54687
G	328	SER	GLY	VARIANT	UNP P54687
J	163	ALA	THR	VARIANT	UNP P54687
J	235	ASP	ALA	VARIANT	UNP P54687
J	249	ARG	GLU	VARIANT	UNP P54687
J	315	THR	SER	VARIANT	UNP P54687
J	328	SER	GLY	VARIANT	UNP P54687

- Molecule 2 is N'-(5-CHLOROBENZOFURAN-2-CARBONYL)-2-(TRIFLUOROMETHYL)BENZENESULFONOHYDRAZIDE (three-letter code: CBC) (formula: C<sub>16</sub>H<sub>10</sub>ClF<sub>3</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	F	N	O	S		
2	A	1	Total	C	Cl	F	N	O	S	0	0
			27	16	1	3	2	4	1		
2	D	1	Total	C	Cl	F	N	O	S	0	0
			27	16	1	3	2	4	1		
2	G	1	Total	C	Cl	F	N	O	S	0	0
			27	16	1	3	2	4	1		
2	J	1	Total	C	Cl	F	N	O	S	0	0
			27	16	1	3	2	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	D	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	G	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	J	1	Total 15	C 8	N 1	O 5	P 1	0	0

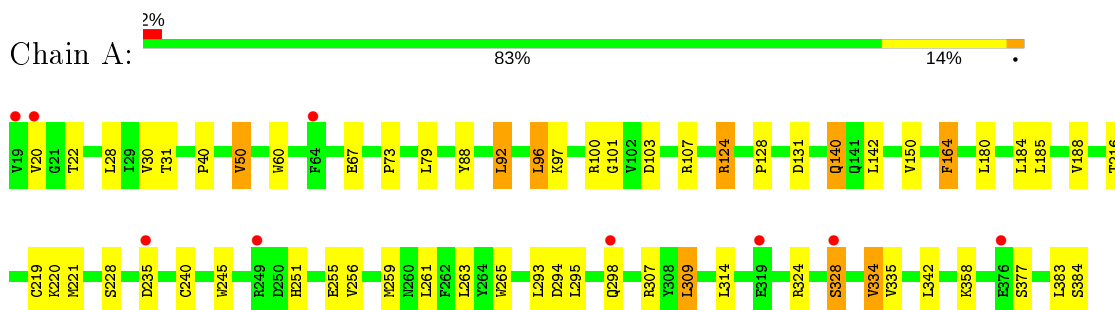
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	356	Total 356	O 356	0	0
4	D	330	Total 330	O 330	0	0
4	G	380	Total 380	O 380	0	0
4	J	347	Total 347	O 347	0	0

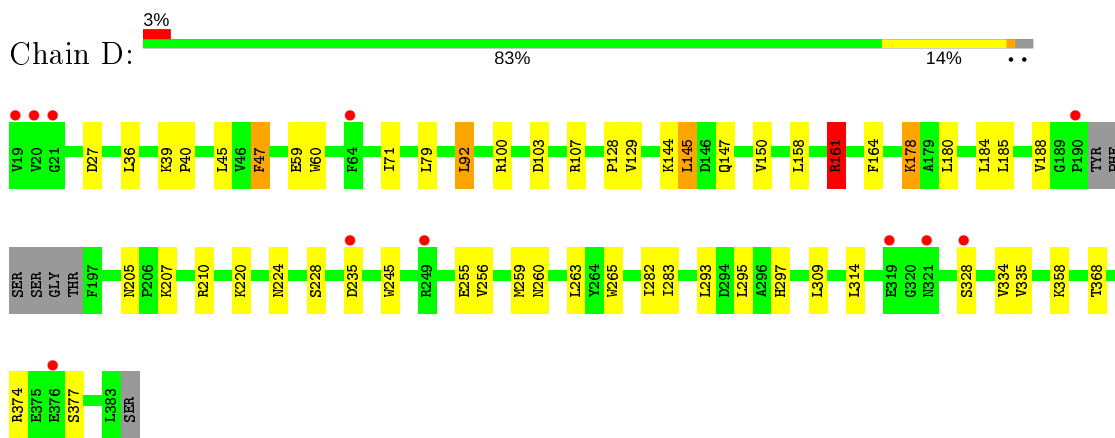
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

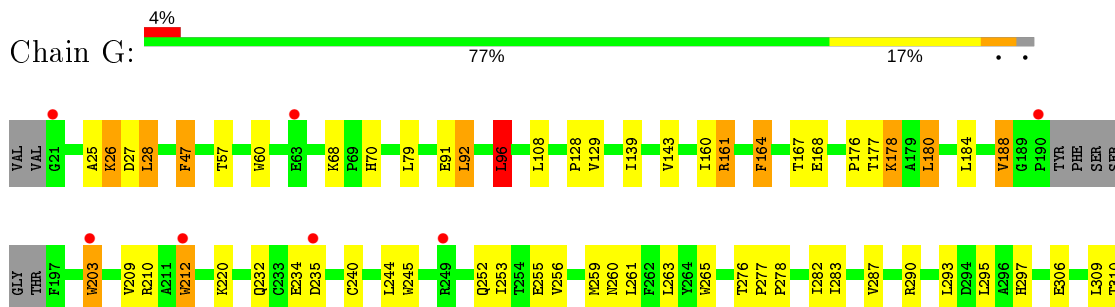
- Molecule 1: Branched-chain-amino-acid aminotransferase, cytosolic



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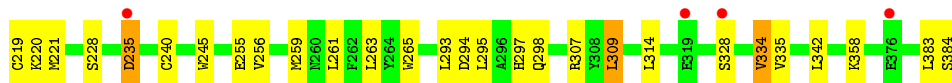
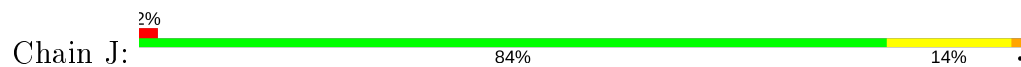


- Molecule 1: Branched-chain-amino-acid aminotransferase, cytosolic





- Molecule 1: Branched-chain-amino-acid aminotransferase, cytosolic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.33Å 114.52Å 148.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.91 – 2.20 49.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (90.91-2.20) 98.1 (49.70-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.04 (at 2.20Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.205 , 0.257 0.202 , 0.252	Depositor DCC
$R_{free}$ test set	4719 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.56$ , $\langle L^2 \rangle = 0.40$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1313e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CBC, PLP

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	0.43	0/2966	0.61	3/4034 (0.1%)
1	D	0.44	0/2911	0.64	2/3958 (0.1%)
1	G	0.44	0/2903	0.66	5/3946 (0.1%)
1	J	0.45	0/2966	0.62	3/4034 (0.1%)
All	All	0.44	0/11746	0.63	13/15972 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	LEU	CA-CB-CG	7.14	131.73	115.30
1	G	96	LEU	CA-CB-CG	6.91	131.18	115.30
1	J	96	LEU	CA-CB-CG	6.74	130.80	115.30
1	G	161	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	92	LEU	CA-CB-CG	6.10	129.33	115.30
1	D	92	LEU	CA-CB-CG	5.89	128.86	115.30
1	J	309	LEU	CA-CB-CG	5.74	128.51	115.30
1	J	92	LEU	CA-CB-CG	5.65	128.30	115.30
1	G	28	LEU	CA-CB-CG	5.64	128.28	115.30
1	G	92	LEU	CA-CB-CG	5.63	128.26	115.30
1	D	161	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	309	LEU	CA-CB-CG	5.35	127.60	115.30
1	G	383	LEU	CA-CB-CG	5.25	127.37	115.30

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	2892	0	2869	31	0
1	D	2840	0	2825	31	0
1	G	2832	0	2812	56	0
1	J	2892	0	2869	32	0
2	A	27	0	10	1	0
2	D	27	0	10	0	0
2	G	27	0	10	0	0
2	J	27	0	10	0	0
3	A	15	0	7	4	0
3	D	15	0	7	3	0
3	G	15	0	7	3	0
3	J	15	0	7	3	0
4	A	356	0	0	3	0
4	D	330	0	0	7	0
4	G	380	0	0	8	0
4	J	347	0	0	2	0
All	All	13037	0	11443	147	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 7.

All (147) 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:D:220:LYS:HZ3	3:D:420:PLP:C4A	1.45	1.30
1:J:220:LYS:HZ1	3:J:420:PLP:C4A	1.53	1.21
1:A:220:LYS:HZ1	3:A:420:PLP:C4A	1.57	1.17
1:G:220:LYS:HZ1	3:G:420:PLP:C4A	1.49	1.17
1:G:256:VAL:CG2	1:G:328:SER:HB3	1.76	1.15
1:G:256:VAL:HG21	1:G:328:SER:HB3	1.15	1.13
1:G:220:LYS:HZ3	3:G:420:PLP:C4A	1.69	1.03
1:G:26:LYS:HD2	1:G:26:LYS:H	1.26	0.99
1:J:100:ARG:NH1	1:J:150:VAL:O	1.93	0.99
1:A:100:ARG:NH1	1:A:150:VAL:O	1.97	0.97
1:D:220:LYS:HZ1	3:D:420:PLP:C4A	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:LYS:HZ3	3:J:420:PLP:C4A	1.78	0.94
1:G:244:LEU:HD11	1:G:253:ILE:HG23	1.49	0.92
1:A:220:LYS:HZ3	3:A:420:PLP:C4A	1.86	0.84
1:D:47:PHE:O	1:D:188:VAL:HG12	1.77	0.83
1:G:26:LYS:HD2	1:G:26:LYS:N	1.97	0.80
1:A:256:VAL:HG23	1:A:261:LEU:HD23	1.66	0.76
1:J:294:ASP:O	1:J:298:GLN:HG2	1.86	0.74
1:G:256:VAL:CG2	1:G:328:SER:CB	2.63	0.74
1:G:57:THR:HG22	4:G:3778:HOH:O	1.89	0.71
1:A:256:VAL:CG2	1:A:261:LEU:HD23	2.25	0.66
1:D:259:MET:CB	1:D:328:SER:HB2	2.25	0.66
1:D:178:LYS:HD3	4:D:2465:HOH:O	1.95	0.65
1:G:259:MET:CB	1:G:328:SER:HB2	2.26	0.65
1:D:59:GLU:HG3	4:D:2465:HOH:O	1.97	0.65
1:J:256:VAL:CG2	1:J:261:LEU:HD23	2.27	0.65
1:A:259:MET:SD	1:A:328:SER:HB2	2.38	0.64
1:J:256:VAL:HG23	1:J:261:LEU:HD23	1.79	0.62
1:A:255:GLU:OE1	3:A:420:PLP:N1	2.32	0.62
1:J:140:GLN:NE2	1:J:384:SER:H	1.98	0.61
1:J:259:MET:SD	1:J:328:SER:HB2	2.40	0.61
1:D:259:MET:HB3	1:D:328:SER:HB2	1.83	0.61
1:A:251:HIS:HD2	4:A:1406:HOH:O	1.82	0.61
1:J:67:GLU:HG3	4:J:4519:HOH:O	1.99	0.61
1:G:312:ASP:O	1:G:316:THR:HG23	2.01	0.60
1:A:235:ASP:OD2	1:A:240:CYS:HB2	2.00	0.60
1:A:294:ASP:O	1:A:298:GLN:HG2	2.03	0.59
1:G:259:MET:HB3	1:G:328:SER:HB2	1.85	0.58
1:G:27:ASP:HB2	1:G:68:LYS:HD3	1.85	0.58
1:G:203:TRP:HZ3	1:G:234:GLU:OE1	1.87	0.57
1:G:167:THR:O	1:G:167:THR:HG22	2.03	0.57
1:G:167:THR:HG21	4:G:3423:HOH:O	2.03	0.57
1:A:40:PRO:HG3	1:A:50:VAL:HG21	1.87	0.57
1:G:328:SER:OG	1:G:336:CYS:HB3	2.05	0.56
1:G:232:GLN:O	1:G:235:ASP:HB3	2.05	0.56
1:G:57:THR:HG23	1:G:180:LEU:HD21	1.87	0.56
1:G:203:TRP:CZ3	1:G:234:GLU:OE1	2.59	0.56
1:G:256:VAL:HG23	1:G:256:VAL:O	2.07	0.55
1:D:282:ILE:HG13	1:D:283:ILE:HD12	1.89	0.55
1:G:256:VAL:CG1	1:G:261:LEU:HD23	2.38	0.54
1:A:67:GLU:HG3	4:A:1498:HOH:O	2.07	0.54
1:J:40:PRO:HG3	1:J:50:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:PHE:O	1:G:188:VAL:HG22	2.07	0.54
1:G:255:GLU:OE2	3:G:420:PLP:N1	2.41	0.54
1:J:96:LEU:HD13	1:J:160:ILE:HB	1.90	0.54
1:D:60:TRP:CD2	1:D:128:PRO:HG3	2.44	0.53
1:G:168:GLU:HG3	1:G:176:PRO:HA	1.90	0.53
1:J:255:GLU:OE1	3:J:420:PLP:N1	2.42	0.52
1:A:101:GLY:HA3	1:A:107:ARG:HH21	1.75	0.51
1:J:219:CYS:HB2	1:J:221:MET:CE	2.40	0.51
1:D:256:VAL:HB	1:D:328:SER:HB3	1.92	0.51
1:A:219:CYS:HB2	1:A:221:MET:HE3	1.93	0.51
1:D:100:ARG:NH1	1:D:150:VAL:O	2.44	0.50
1:G:384:SER:HB2	4:G:3546:HOH:O	2.12	0.49
1:G:96:LEU:HD13	1:G:160:ILE:HB	1.94	0.49
1:J:31:THR:O	1:J:73:PRO:HD3	2.13	0.49
1:A:142:LEU:HG	1:A:185:LEU:HD11	1.95	0.49
1:G:244:LEU:HD11	1:G:253:ILE:CG2	2.33	0.49
1:J:219:CYS:CB	1:J:221:MET:HE2	2.43	0.48
1:G:167:THR:CG2	1:G:167:THR:O	2.62	0.48
1:G:240:CYS:SG	1:G:342:LEU:HG	2.54	0.48
1:A:235:ASP:OD2	1:A:240:CYS:CB	2.62	0.47
1:J:235:ASP:OD2	1:J:240:CYS:HB2	2.14	0.47
1:J:167:THR:OG1	1:J:178:LYS:HG2	2.14	0.47
1:G:168:GLU:HG2	1:G:177:THR:H	1.80	0.47
1:A:31:THR:HG23	1:J:207:LYS:HE2	1.96	0.47
1:J:97:LYS:HE2	1:J:188:VAL:HG11	1.97	0.47
1:A:124:ARG:HG2	1:A:221:MET:CE	2.46	0.46
1:D:224:ASN:ND2	4:D:2407:HOH:O	2.48	0.46
1:D:297:HIS:HD2	4:D:2493:HOH:O	1.98	0.46
1:G:259:MET:HB2	1:G:328:SER:HB2	1.98	0.46
1:J:228:SER:HB2	1:J:245:TRP:CZ2	2.50	0.46
1:J:259:MET:CB	1:J:328:SER:HB3	2.46	0.46
1:J:210:ARG:HB2	1:J:245:TRP:CD2	2.51	0.46
1:A:88:TYR:OH	1:D:161:ARG:NH2	2.37	0.46
1:D:255:GLU:OE2	3:D:420:PLP:N1	2.48	0.46
1:J:101:GLY:HA3	1:J:107:ARG:HH21	1.82	0.45
1:D:283:ILE:HD13	4:D:2410:HOH:O	2.16	0.45
1:G:139:ILE:O	1:G:143:VAL:HG12	2.15	0.45
1:G:47:PHE:O	1:G:188:VAL:CG2	2.65	0.45
1:D:158:LEU:HD21	1:D:185:LEU:HD13	1.97	0.45
1:G:70:HIS:HE1	4:G:3487:HOH:O	2.00	0.45
2:A:1401:CBC:H45	3:A:420:PLP:C4A	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:CYS:HB2	1:J:221:MET:HE3	1.98	0.45
1:G:161:ARG:NH2	1:J:88:TYR:CZ	2.83	0.45
1:G:282:ILE:HG13	1:G:283:ILE:HD12	1.97	0.45
1:G:60:TRP:CD2	1:G:128:PRO:HG3	2.52	0.45
1:D:144:LYS:O	1:D:147:GLN:HG3	2.17	0.44
1:D:71:ILE:HG21	1:D:145:LEU:HD12	1.98	0.44
1:G:210:ARG:HB2	1:G:245:TRP:CD2	2.52	0.44
1:G:328:SER:HG	1:G:336:CYS:HB3	1.81	0.44
1:J:259:MET:HB2	1:J:328:SER:HB3	2.00	0.44
1:A:228:SER:HB2	1:A:245:TRP:CZ2	2.53	0.44
1:D:259:MET:HB2	1:D:328:SER:HB2	1.99	0.44
1:G:297:HIS:HD2	4:G:3512:HOH:O	2.00	0.44
1:D:205:ASN:ND2	1:D:207:LYS:HE2	2.33	0.44
1:G:256:VAL:HG11	1:G:261:LEU:HD23	1.99	0.44
1:G:283:ILE:HD13	4:G:3469:HOH:O	2.18	0.44
1:D:260:ASN:O	1:D:328:SER:HA	2.18	0.43
1:A:88:TYR:CZ	1:D:161:ARG:NH2	2.87	0.43
1:G:178:LYS:HD3	4:G:3480:HOH:O	2.19	0.43
1:A:103:ASP:OD2	1:A:107:ARG:NH2	2.47	0.43
1:D:40:PRO:HG2	1:D:45:LEU:HD21	2.00	0.43
1:G:168:GLU:CG	1:G:177:THR:H	2.31	0.43
1:A:31:THR:O	1:A:73:PRO:HD3	2.19	0.43
1:G:368:THR:HG22	1:G:374:ARG:HH21	1.82	0.43
1:G:277:PRO:HA	1:G:278:PRO:HD3	1.83	0.43
1:D:39:LYS:NZ	4:D:2464:HOH:O	2.52	0.42
1:A:140:GLN:NE2	1:A:384:SER:H	2.16	0.42
1:A:22:THR:HG21	1:A:131:ASP:HB2	2.01	0.42
1:D:228:SER:HB2	1:D:245:TRP:CZ2	2.54	0.42
1:D:210:ARG:HB2	1:D:245:TRP:CD2	2.55	0.42
1:J:235:ASP:OD2	1:J:240:CYS:CB	2.68	0.42
1:D:368:THR:HG22	1:D:374:ARG:HH21	1.85	0.42
1:G:203:TRP:CD1	1:G:342:LEU:HB2	2.55	0.42
1:J:297:HIS:HD2	4:J:4620:HOH:O	2.01	0.42
1:D:103:ASP:OD2	1:D:107:ARG:NH2	2.48	0.41
1:G:276:THR:O	1:G:306:GLU:HA	2.21	0.41
1:G:283:ILE:CD1	4:G:3469:HOH:O	2.68	0.41
1:D:39:LYS:HG3	4:D:2726:HOH:O	2.19	0.41
1:A:216:THR:HB	1:A:221:MET:CE	2.50	0.41
1:G:25:ALA:O	1:G:28:LEU:HB2	2.19	0.41
1:J:103:ASP:OD2	1:J:107:ARG:NH2	2.48	0.41
1:J:216:THR:HB	1:J:221:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:SER:HB2	1:D:245:TRP:HZ2	1.86	0.41
1:G:252:GLN:HA	1:G:310:THR:HA	2.03	0.41
1:G:209:VAL:HG11	1:G:212:TRP:CD1	2.56	0.41
1:G:260:ASN:O	1:G:328:SER:HA	2.21	0.41
1:A:60:TRP:CD2	1:A:128:PRO:HG3	2.56	0.41
1:A:128:PRO:HG2	1:A:164:PHE:HZ	1.85	0.41
1:A:358:LYS:HE3	4:A:1499:HOH:O	2.20	0.41
1:A:97:LYS:HE2	1:A:188:VAL:HG11	2.03	0.41
1:G:91:GLU:HA	1:G:164:PHE:O	2.20	0.41
1:J:25:ALA:O	1:J:28:LEU:HB2	2.21	0.41
1:J:45:LEU:HD22	1:J:187:PRO:HB2	2.03	0.40
1:A:324:ARG:HE	1:A:324:ARG:HB3	1.63	0.40
1:G:256:VAL:HG13	1:G:261:LEU:HD23	2.02	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	364/366 (100%)	353 (97%)	10 (3%)	1 (0%)	41	46
1	D	355/366 (97%)	338 (95%)	16 (4%)	1 (0%)	41	46
1	G	354/366 (97%)	340 (96%)	13 (4%)	1 (0%)	41	46
1	J	364/366 (100%)	356 (98%)	7 (2%)	1 (0%)	41	46
All	All	1437/1464 (98%)	1387 (96%)	46 (3%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	47	PHE
1	G	47	PHE

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Mol	Chain	Res	Type
1	A	334	VAL
1	J	334	VAL

### 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	320/320 (100%)	295 (92%)	25 (8%)	12	13
1	D	314/320 (98%)	292 (93%)	22 (7%)	15	16
1	G	313/320 (98%)	285 (91%)	28 (9%)	9	9
1	J	320/320 (100%)	298 (93%)	22 (7%)	15	16
All	All	1267/1280 (99%)	1170 (92%)	97 (8%)	13	13

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	28	LEU
1	A	30	VAL
1	A	50	VAL
1	A	79	LEU
1	A	92	LEU
1	A	96	LEU
1	A	124	ARG
1	A	140	GLN
1	A	164	PHE
1	A	180	LEU
1	A	184	LEU
1	A	263	LEU
1	A	265	TRP
1	A	293	LEU
1	A	295	LEU
1	A	307	ARG
1	A	309	LEU
1	A	314	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	328	SER
1	A	334	VAL
1	A	335	VAL
1	A	342	LEU
1	A	377	SER
1	A	383	LEU
1	D	27	ASP
1	D	36	LEU
1	D	79	LEU
1	D	92	LEU
1	D	129	VAL
1	D	145	LEU
1	D	161	ARG
1	D	164	PHE
1	D	178	LYS
1	D	180	LEU
1	D	184	LEU
1	D	235	ASP
1	D	263	LEU
1	D	265	TRP
1	D	293	LEU
1	D	295	LEU
1	D	309	LEU
1	D	314	LEU
1	D	334	VAL
1	D	335	VAL
1	D	358	LYS
1	D	377	SER
1	G	26	LYS
1	G	79	LEU
1	G	92	LEU
1	G	96	LEU
1	G	108	LEU
1	G	129	VAL
1	G	164	PHE
1	G	178	LYS
1	G	180	LEU
1	G	184	LEU
1	G	188	VAL
1	G	203	TRP
1	G	212	TRP
1	G	263	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	265	TRP
1	G	287	VAL
1	G	290	ARG
1	G	293	LEU
1	G	295	LEU
1	G	309	LEU
1	G	314	LEU
1	G	315	THR
1	G	316	THR
1	G	335	VAL
1	G	354	GLU
1	G	364	LEU
1	G	377	SER
1	G	383	LEU
1	J	28	LEU
1	J	30	VAL
1	J	50	VAL
1	J	79	LEU
1	J	92	LEU
1	J	96	LEU
1	J	140	GLN
1	J	164	PHE
1	J	180	LEU
1	J	235	ASP
1	J	263	LEU
1	J	265	TRP
1	J	293	LEU
1	J	295	LEU
1	J	307	ARG
1	J	309	LEU
1	J	314	LEU
1	J	334	VAL
1	J	335	VAL
1	J	342	LEU
1	J	358	LYS
1	J	383	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	140	GLN
1	A	198	ASN

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Mol	Chain	Res	Type
1	A	224	ASN
1	A	238	ASN
1	A	251	HIS
1	A	252	GLN
1	A	297	HIS
1	D	110	GLN
1	D	141	GLN
1	D	224	ASN
1	D	260	ASN
1	D	297	HIS
1	G	70	HIS
1	G	112	ASN
1	G	224	ASN
1	G	260	ASN
1	G	297	HIS
1	J	140	GLN
1	J	224	ASN
1	J	238	ASN
1	J	251	HIS
1	J	252	GLN
1	J	260	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CBC	A	1401	-	25,29,29	2.40	4 (16%)	33,44,44	2.29	10 (30%)
2	CBC	G	3401	-	25,29,29	2.39	4 (16%)	33,44,44	2.41	10 (30%)
3	PLP	D	420	1	15,15,16	1.34	3 (20%)	20,22,23	1.28	2 (10%)
3	PLP	G	420	1	15,15,16	1.32	3 (20%)	20,22,23	1.32	4 (20%)
2	CBC	J	4401	-	25,29,29	2.38	4 (16%)	33,44,44	2.49	10 (30%)
3	PLP	J	420	1	15,15,16	1.05	1 (6%)	20,22,23	1.28	1 (5%)
2	CBC	D	2401	-	25,29,29	2.33	3 (12%)	33,44,44	2.57	10 (30%)
3	PLP	A	420	1	15,15,16	1.10	1 (6%)	20,22,23	1.22	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CBC	A	1401	-	-	4/19/22/22	0/3/3/3
2	CBC	G	3401	-	-	5/19/22/22	0/3/3/3
3	PLP	D	420	1	-	0/6/6/8	0/1/1/1
3	PLP	G	420	1	-	0/6/6/8	0/1/1/1
2	CBC	J	4401	-	-	6/19/22/22	0/3/3/3
3	PLP	J	420	1	-	0/6/6/8	0/1/1/1
2	CBC	D	2401	-	-	6/19/22/22	0/3/3/3
3	PLP	A	420	1	-	0/6/6/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	4401	CBC	C40-S1	-10.27	1.62	1.77
2	A	1401	CBC	C40-S1	-10.24	1.62	1.77
2	G	3401	CBC	C40-S1	-9.90	1.63	1.77
2	D	2401	CBC	C40-S1	-9.59	1.63	1.77
2	G	3401	CBC	S1-N33	-3.81	1.60	1.65
2	D	2401	CBC	S1-N33	-3.75	1.60	1.65
2	A	1401	CBC	S1-N33	-3.36	1.61	1.65
2	J	4401	CBC	S1-N33	-3.24	1.61	1.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	420	PLP	C2-N1	3.22	1.39	1.33
3	G	420	PLP	C2-N1	2.99	1.39	1.33
2	J	4401	CBC	C50-C51	-2.73	1.37	1.43
2	A	1401	CBC	C50-C51	-2.68	1.37	1.43
2	G	3401	CBC	C50-C51	-2.68	1.37	1.43
3	A	420	PLP	C2-N1	2.65	1.38	1.33
3	G	420	PLP	C3-C2	-2.64	1.38	1.40
2	D	2401	CBC	C50-C51	-2.64	1.37	1.43
3	J	420	PLP	C2-N1	2.61	1.38	1.33
3	D	420	PLP	C6-N1	2.35	1.39	1.34
3	D	420	PLP	C3-C2	-2.28	1.38	1.40
3	G	420	PLP	C6-N1	2.27	1.39	1.34
2	J	4401	CBC	C48-CL1	2.26	1.79	1.74
2	G	3401	CBC	C48-CL1	2.21	1.79	1.74
2	A	1401	CBC	C48-CL1	2.19	1.79	1.74

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	4401	CBC	O39-S1-O38	-9.03	108.45	119.55
2	D	2401	CBC	O39-S1-O38	-8.85	108.67	119.55
2	G	3401	CBC	O39-S1-O38	-8.70	108.85	119.55
2	A	1401	CBC	O39-S1-O38	-8.44	109.17	119.55
2	D	2401	CBC	C41-C40-S1	5.92	128.19	122.12
2	G	3401	CBC	C41-C40-S1	5.54	127.81	122.12
2	J	4401	CBC	C41-C40-S1	5.26	127.51	122.12
2	D	2401	CBC	C53-C50-C51	4.91	110.56	106.27
2	J	4401	CBC	C53-C50-C51	4.29	110.02	106.27
2	A	1401	CBC	C41-C40-S1	4.27	126.49	122.12
2	G	3401	CBC	C53-C50-C51	4.10	109.85	106.27
2	A	1401	CBC	C53-C50-C51	3.93	109.70	106.27
2	J	4401	CBC	O39-S1-C40	3.67	113.70	107.66
2	D	2401	CBC	C45-C40-C41	-3.37	117.21	121.63
2	J	4401	CBC	C45-C40-C41	-3.27	117.34	121.63
2	G	3401	CBC	C45-C40-C41	-3.19	117.45	121.63
2	A	1401	CBC	O39-S1-C40	3.18	112.90	107.66
2	A	1401	CBC	C45-C40-C41	-3.05	117.64	121.63
2	A	1401	CBC	O39-S1-N33	2.91	111.13	105.57
3	A	420	PLP	C5-C6-N1	-2.80	119.16	123.82
3	J	420	PLP	C5-C6-N1	-2.78	119.19	123.82
2	D	2401	CBC	O39-S1-C40	2.77	112.22	107.66
2	G	3401	CBC	O39-S1-N33	2.68	110.70	105.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3401	CBC	S1-N33-N32	2.63	119.18	114.74
3	D	420	PLP	C5-C6-N1	-2.55	119.57	123.82
2	J	4401	CBC	O39-S1-N33	2.46	110.27	105.57
2	G	3401	CBC	O39-S1-C40	2.41	111.63	107.66
3	G	420	PLP	C5-C6-N1	-2.40	119.81	123.82
2	A	1401	CBC	S1-N33-N32	2.40	118.78	114.74
2	D	2401	CBC	O39-S1-N33	2.37	110.09	105.57
3	A	420	PLP	C3-C4-C5	2.31	121.23	118.74
2	J	4401	CBC	F51-C46-C41	-2.29	108.71	112.70
3	G	420	PLP	C4A-C4-C3	-2.28	116.63	120.50
2	D	2401	CBC	C44-C45-C40	2.28	122.92	118.78
3	G	420	PLP	C2A-C2-N1	2.25	122.06	117.67
2	A	1401	CBC	C42-C41-C40	2.21	119.28	116.59
2	J	4401	CBC	C42-C41-C40	2.21	119.27	116.59
2	J	4401	CBC	C44-C45-C40	2.21	122.80	118.78
2	D	2401	CBC	S1-N33-N32	2.18	118.42	114.74
3	D	420	PLP	C3-C4-C5	2.15	121.06	118.74
2	G	3401	CBC	C44-C45-C40	2.14	122.66	118.78
2	G	3401	CBC	C40-S1-N33	2.11	110.75	107.34
2	D	2401	CBC	C42-C41-C40	2.08	119.12	116.59
2	D	2401	CBC	C45-C40-S1	-2.08	114.60	117.42
2	G	3401	CBC	C42-C41-C40	2.05	119.08	116.59
2	J	4401	CBC	S1-N33-N32	2.05	118.19	114.74
3	G	420	PLP	C4A-C4-C5	-2.04	118.83	120.94
2	A	1401	CBC	C44-C45-C40	2.04	122.49	118.78
2	A	1401	CBC	F51-C46-C41	-2.04	109.15	112.70

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	CBC	C41-C40-S1-N33
2	G	3401	CBC	C41-C40-S1-N33
2	J	4401	CBC	C41-C40-S1-N33
2	D	2401	CBC	C41-C40-S1-N33
2	A	1401	CBC	C41-C40-S1-O38
2	G	3401	CBC	C41-C40-S1-O38
2	J	4401	CBC	C41-C40-S1-O38
2	D	2401	CBC	C41-C40-S1-O38
2	D	2401	CBC	C41-C40-S1-O39
2	D	2401	CBC	C45-C40-S1-O38
2	G	3401	CBC	C45-C40-S1-O38

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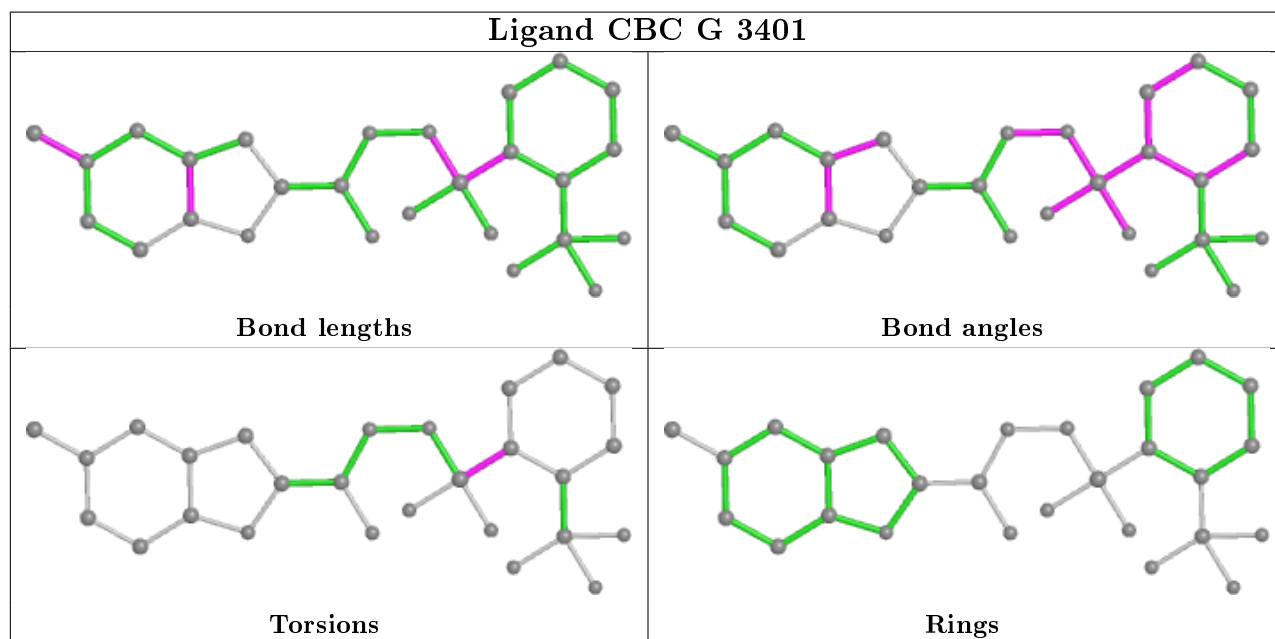
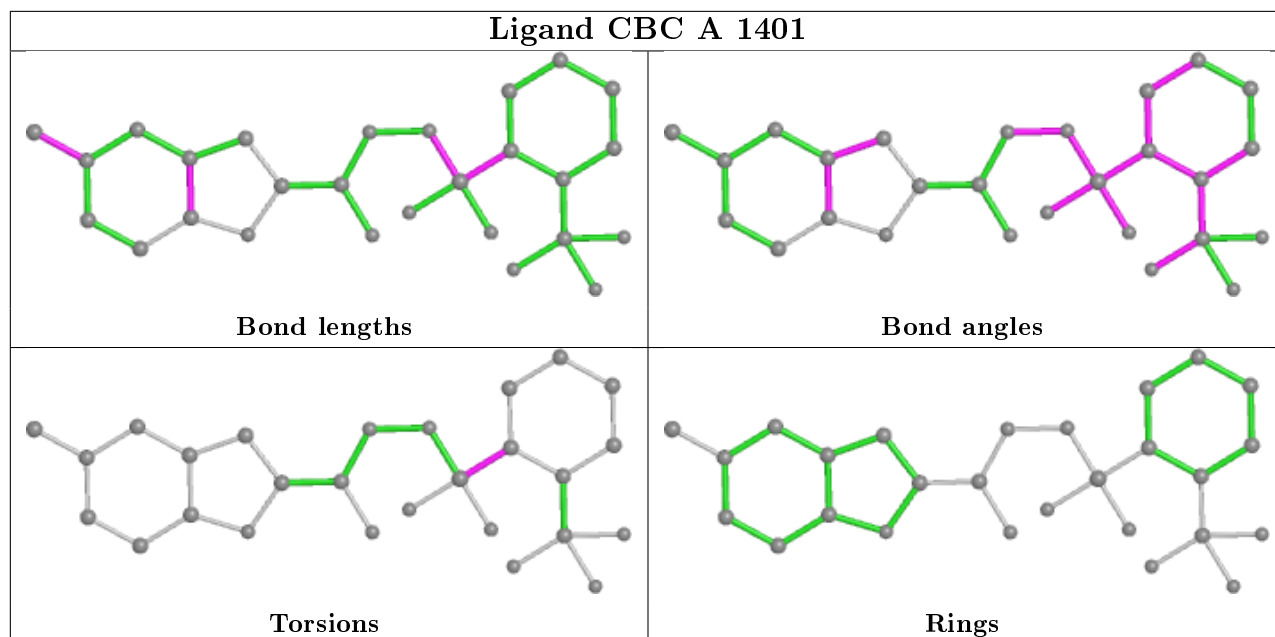
Mol	Chain	Res	Type	Atoms
2	J	4401	CBC	C45-C40-S1-O38
2	A	1401	CBC	C45-C40-S1-O38
2	D	2401	CBC	C45-C40-S1-N33
2	J	4401	CBC	C45-C40-S1-N33
2	G	3401	CBC	C45-C40-S1-N33
2	A	1401	CBC	C45-C40-S1-N33
2	D	2401	CBC	C45-C40-S1-O39
2	J	4401	CBC	C41-C40-S1-O39
2	J	4401	CBC	C45-C40-S1-O39
2	G	3401	CBC	C45-C40-S1-O39

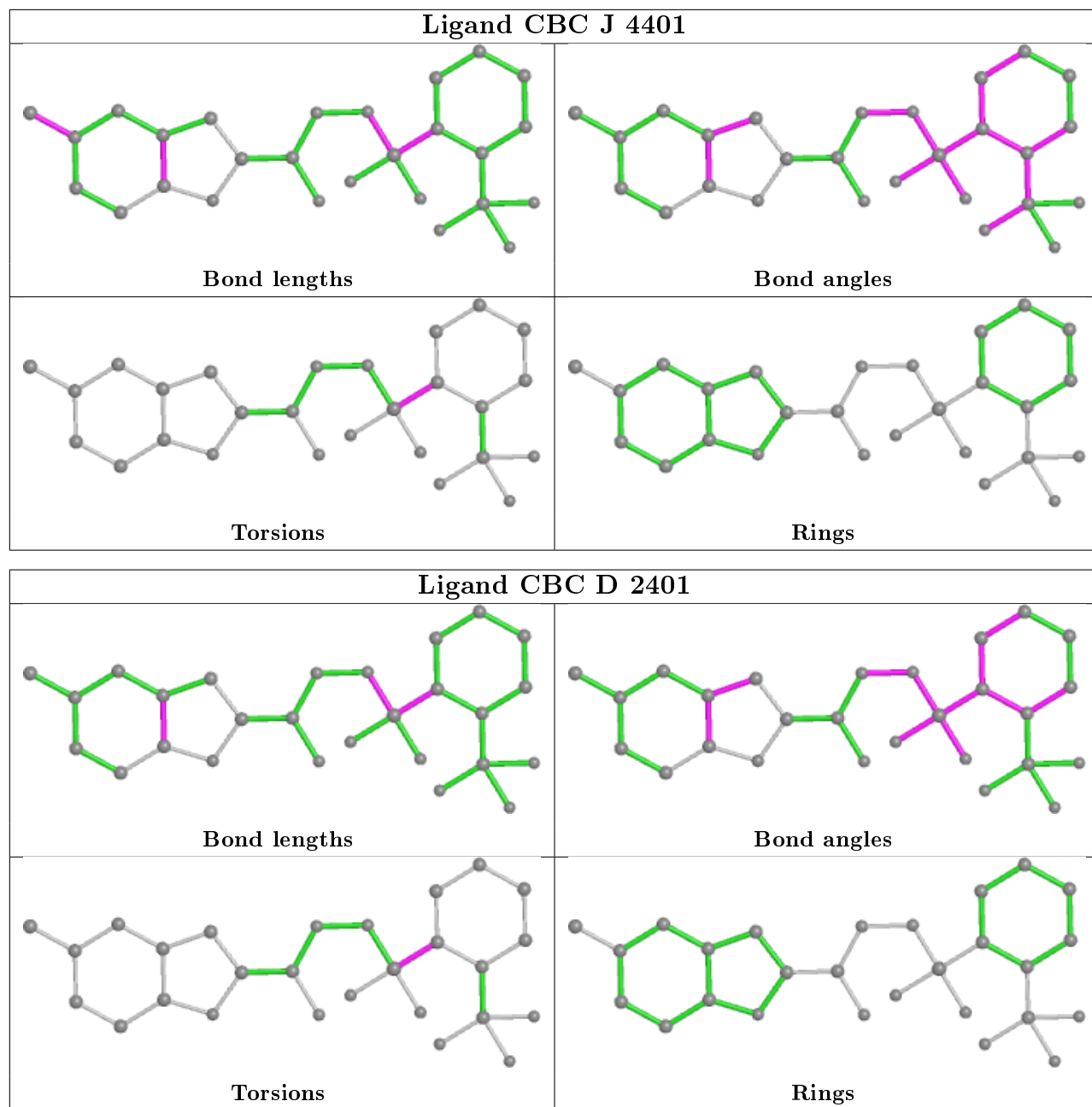
There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	CBC	1	0
3	D	420	PLP	3	0
3	G	420	PLP	3	0
3	J	420	PLP	3	0
3	A	420	PLP	4	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 than 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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	366/366 (100%)	-0.27	9 (2%) 57 55	9, 19, 29, 39	0
1	D	359/366 (98%)	-0.24	11 (3%) 49 47	8, 18, 30, 41	0
1	G	358/366 (97%)	-0.09	15 (4%) 36 34	9, 18, 29, 38	0
1	J	366/366 (100%)	-0.30	7 (1%) 66 65	9, 18, 29, 37	0
All	All	1449/1464 (98%)	-0.23	42 (2%) 51 49	8, 19, 29, 41	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	VAL	8.9
1	A	19	VAL	6.9
1	J	19	VAL	6.1
1	D	20	VAL	5.6
1	A	20	VAL	4.9
1	G	384	SER	4.3
1	J	235	ASP	4.1
1	D	235	ASP	3.9
1	A	235	ASP	3.8
1	J	20	VAL	3.4
1	J	328	SER	3.4
1	D	190	PRO	3.3
1	G	235	ASP	3.1
1	A	319	GLU	3.1
1	G	212	TRP	3.1
1	A	328	SER	2.9
1	G	21	GLY	2.8
1	A	376	GLU	2.8
1	G	321	ASN	2.7
1	G	346	GLU	2.7
1	A	249	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	21	GLY	2.6
1	G	190	PRO	2.6
1	G	383	LEU	2.5
1	A	64	PHE	2.5
1	D	249	ARG	2.4
1	G	249	ARG	2.4
1	G	319	GLU	2.4
1	D	321	ASN	2.4
1	D	376	GLU	2.4
1	G	203	TRP	2.3
1	D	319	GLU	2.3
1	J	319	GLU	2.3
1	D	328	SER	2.2
1	G	315	THR	2.2
1	G	63	GLU	2.1
1	J	44	ASN	2.1
1	D	64	PHE	2.1
1	G	317	ALA	2.1
1	J	376	GLU	2.0
1	G	328	SER	2.0
1	A	298	GLN	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 carbohydrates 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, 95<sup>th</sup> 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.

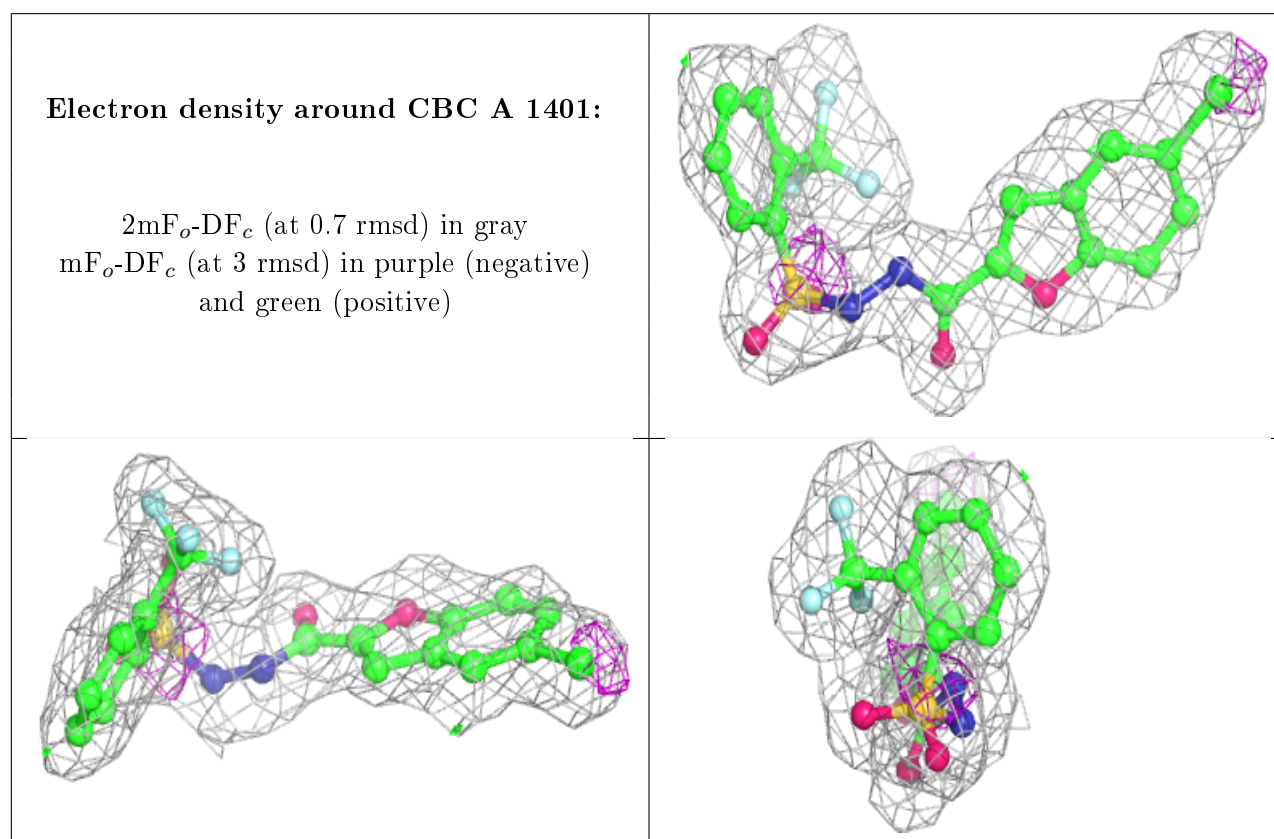
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CBC	A	1401	27/27	0.92	0.12	21,23,25,28	0
2	CBC	D	2401	27/27	0.93	0.12	20,22,26,26	0

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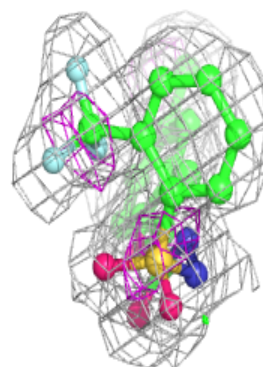
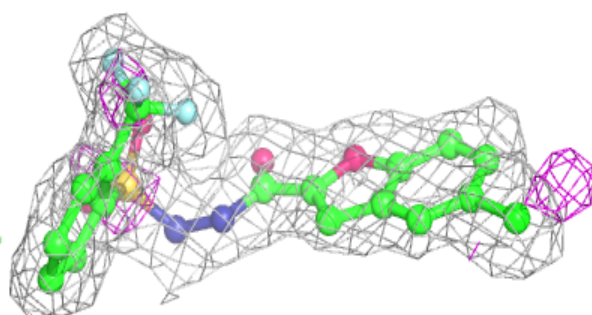
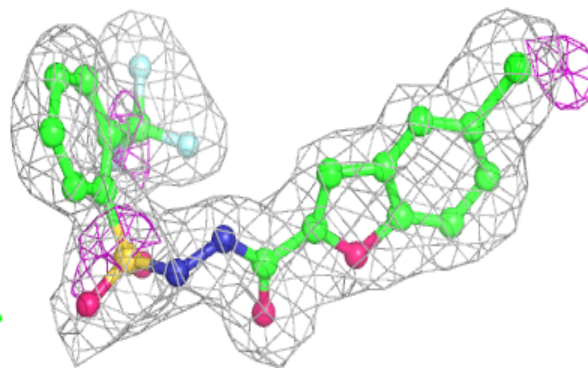
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CBC	J	4401	27/27	0.94	0.10	17,22,25,28	0
2	CBC	G	3401	27/27	0.94	0.12	18,21,25,26	0
3	PLP	G	420	15/16	0.97	0.14	10,11,12,12	0
3	PLP	A	420	15/16	0.97	0.11	10,14,16,17	0
3	PLP	D	420	15/16	0.98	0.11	11,11,12,14	0
3	PLP	J	420	15/16	0.98	0.11	10,12,13,14	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.

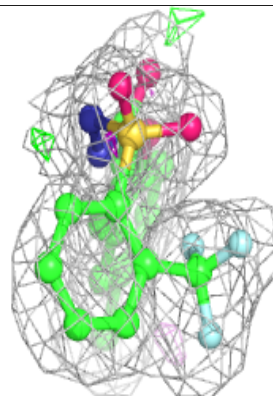
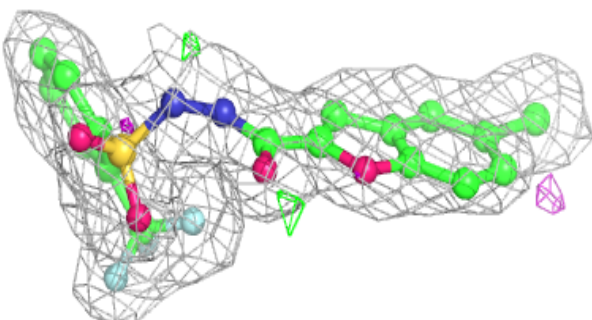
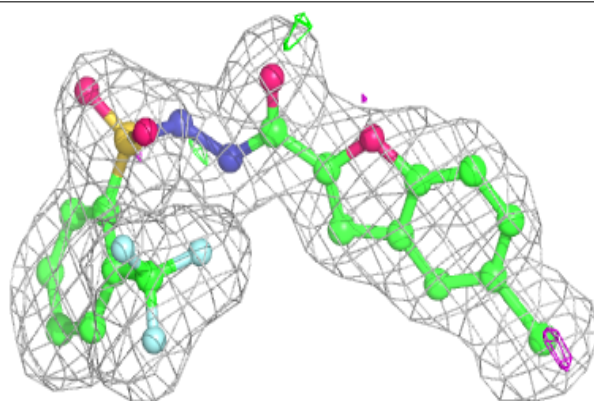


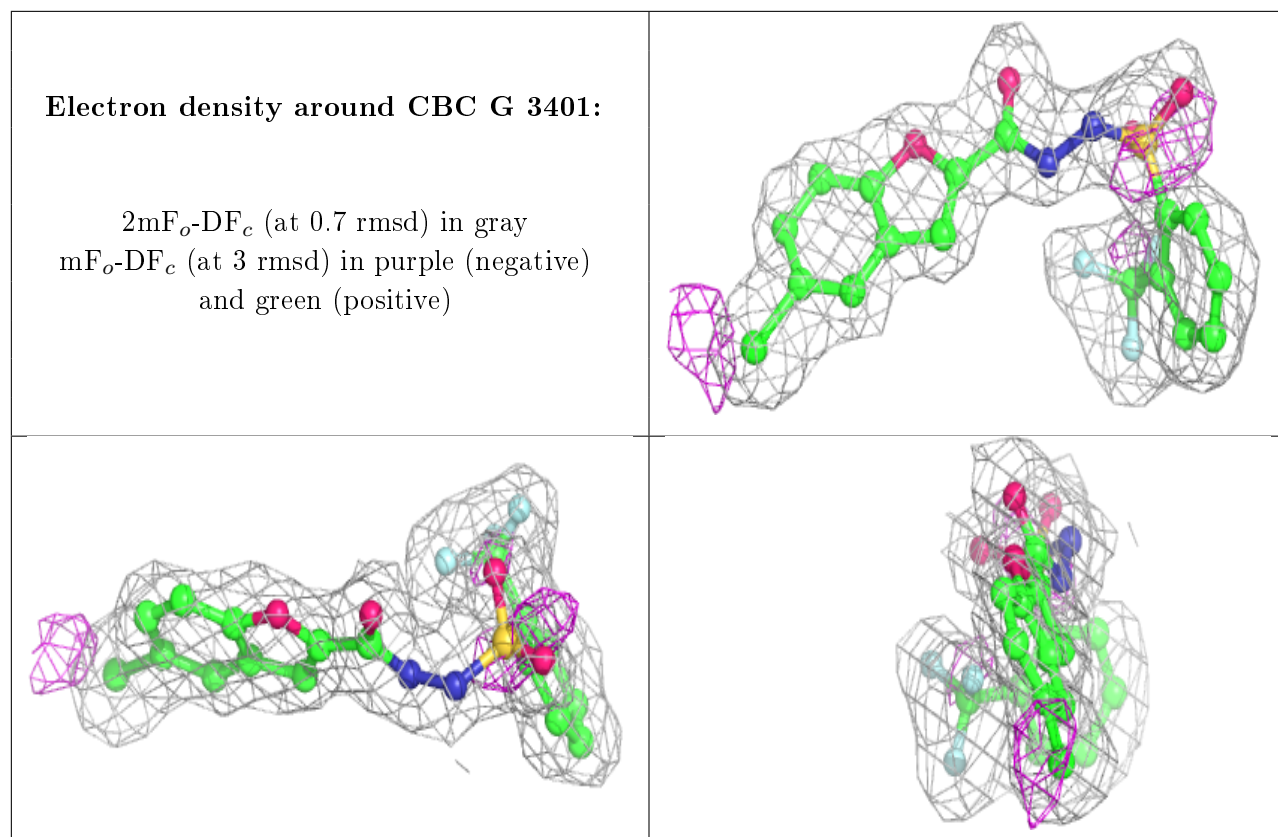
**Electron density around CBC D 2401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CBC J 4401:**

$2mF_o-DF_c$  (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.