



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:30 PM UTC

PDB ID : 9GZK / pdb_00009gzk
Title : Crystal structure of the *L. monocytogenes* RmlT in complex with 4-RboP-(CH₂)₆NH₂
Authors : Cereija, T.B.; Morais-Cabral, J.H.
Deposited on : 2024-10-04
Resolution : 2.52 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

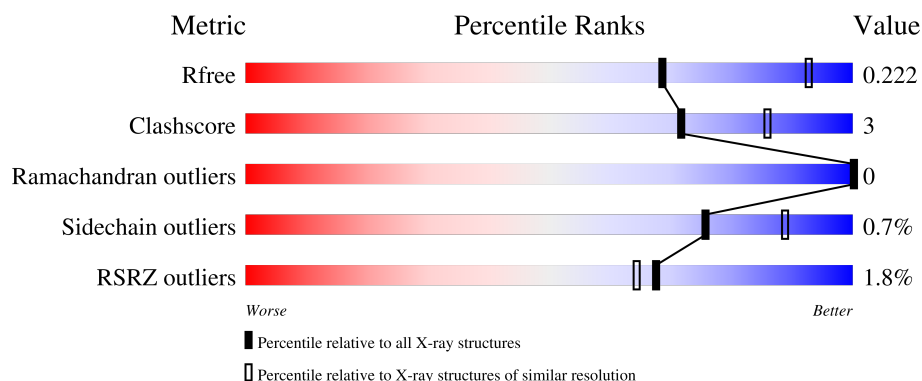
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	624	% 89% 7% .
1	B	624	2% 88% 8% .
1	C	624	88% 8% .
1	D	624	88% 8% .
1	E	624	% 86% 10% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	624	6% 75% 12% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29352 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.

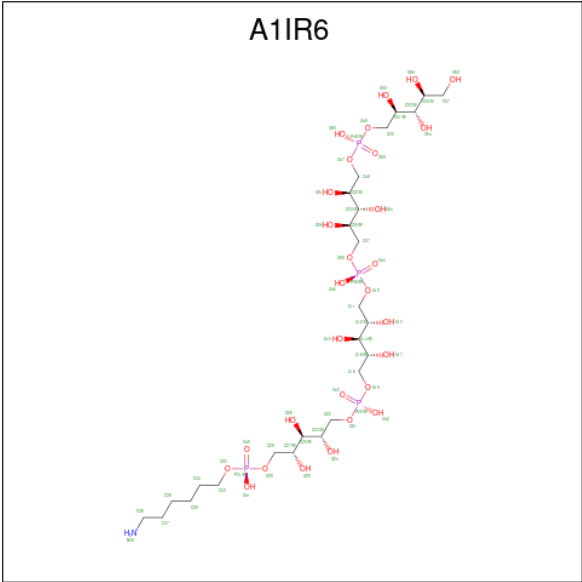
- Molecule 1 is a protein called Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	4	1	0
			4870	3107	809	942	12			
1	B	601	Total	C	N	O	S	38	2	0
			4887	3118	810	947	12			
1	C	599	Total	C	N	O	S	0	2	0
			4881	3115	809	945	12			
1	D	599	Total	C	N	O	S	4	0	0
			4863	3105	807	939	12			
1	E	597	Total	C	N	O	S	0	1	0
			4848	3094	803	939	12			
1	F	544	Total	C	N	O	S	14	1	0
			4433	2830	740	851	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A401AAP7
B	0	GLY	-	expression tag	UNP A0A401AAP7
C	0	GLY	-	expression tag	UNP A0A401AAP7
D	0	GLY	-	expression tag	UNP A0A401AAP7
E	0	GLY	-	expression tag	UNP A0A401AAP7
F	0	GLY	-	expression tag	UNP A0A401AAP7

- Molecule 2 is (Ribitol-phosphate)4-(CH₂)₆-NH₂ (CCD ID: A1IR6) (formula: C₂₆H₅₉NO₂₉P₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	O	P	0	0	
			31	10	18	3			
2	B	1	Total	C	O	P	0	0	
			27	10	15	2			
2	B	1	Total	C	N	O	P	0	0
			34	16	1	15	2		
2	C	1	Total	C	O	P	0	0	
			27	10	15	2			
2	D	1	Total	C	O	P	0	0	
			31	10	18	3			
2	E	1	Total	C	N	O	P	0	0
			38	16	1	18	3		
2	F	1	Total	C	O	P	0	0	
			27	10	15	2			
2	F	1	Total	C	O	P	0	0	
			14	5	8	1			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Mg	0	0
			2	2		

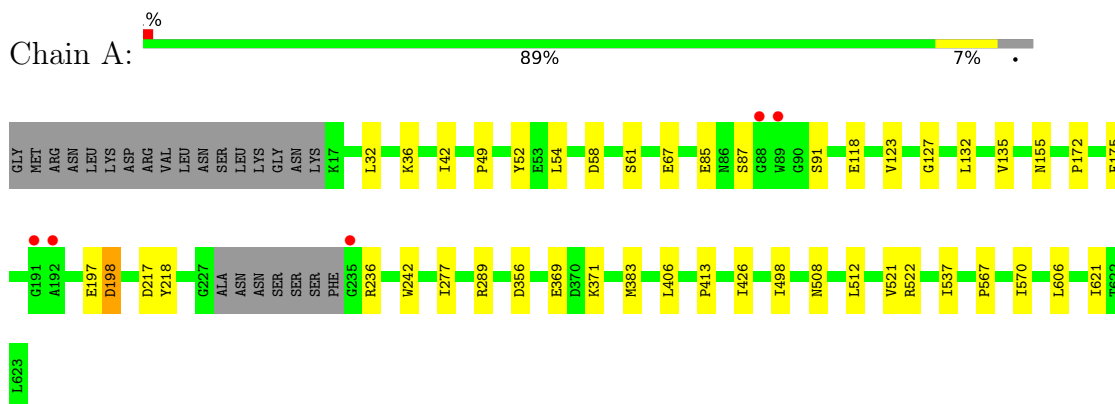
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	57	Total	O	0	0
			57	57		
4	C	54	Total	O	0	0
			54	54		
4	D	51	Total	O	0	0
			51	51		
4	E	66	Total	O	0	0
			66	66		
4	F	21	Total	O	0	0
			21	21		

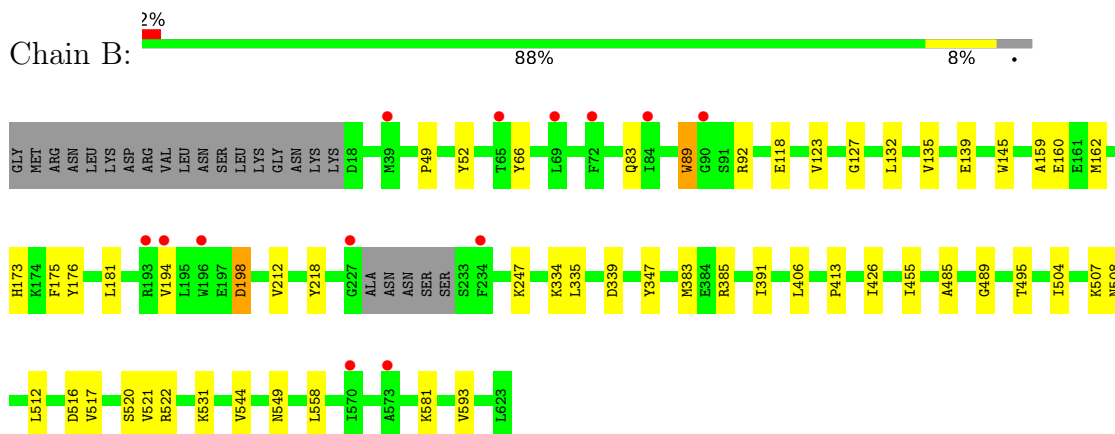
3 Residue-property plots [i](#)

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.

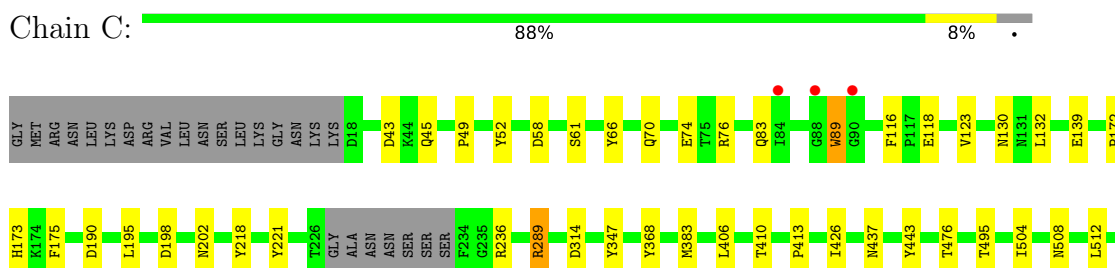
• Molecule 1: Glycosyltransferase



• Molecule 1: Glycosyltransferase



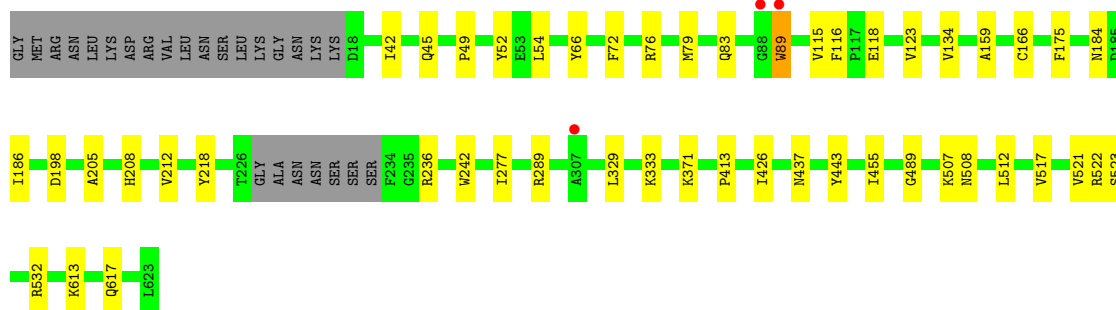
• Molecule 1: Glycosyltransferase





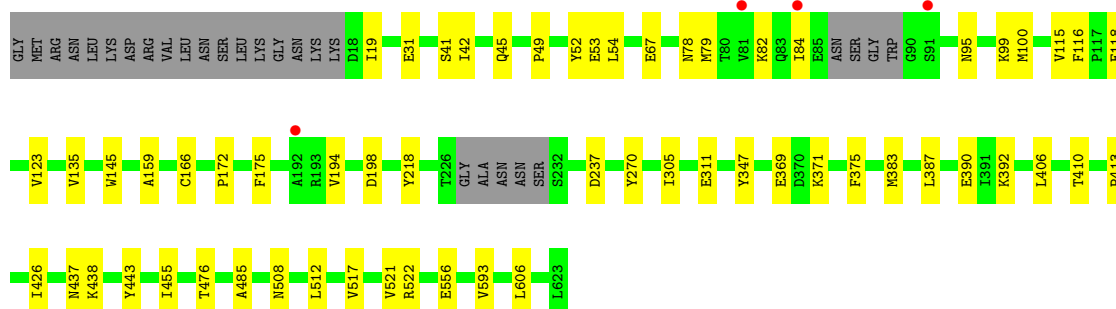
• Molecule 1: Glycosyltransferase

Chain D: 88% 8% .



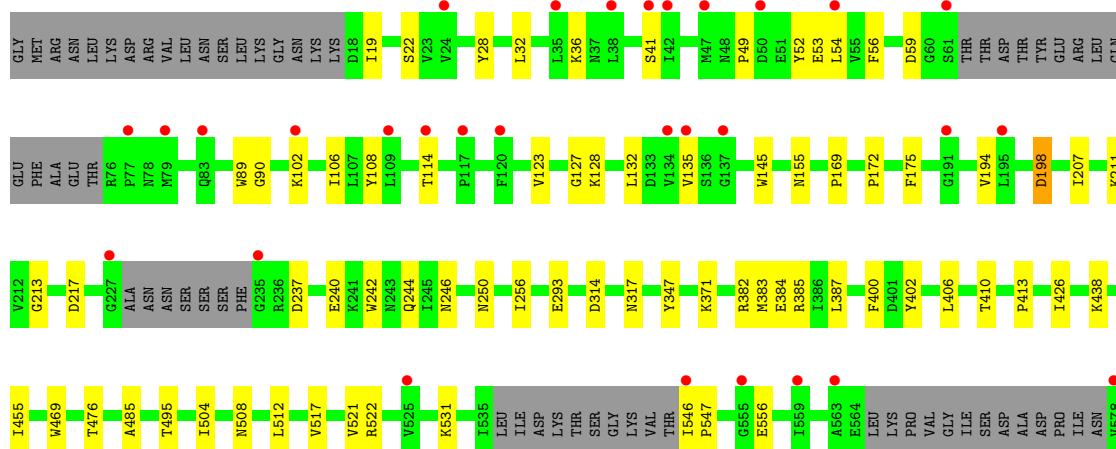
• Molecule 1: Glycosyltransferase

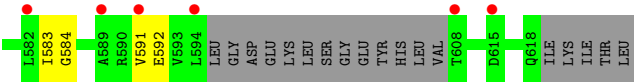
Chain E: 86% 10% .



• Molecule 1: Glycosyltransferase

Chain F: 75% 12% 13%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.32Å 290.76Å 91.03Å 90.00° 100.25° 90.00°	Depositor
Resolution (Å)	42.89 – 2.52 42.89 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.89-2.52) 99.5 (42.89-2.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.199 , 0.232 (Not available) , 0.222	Depositor DCC
R_{free} test set	7276 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29352	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: MG, A1IR6

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	0.08	0/4972	0.25	0/6712
1	B	0.08	0/4990	0.24	0/6737
1	C	0.08	0/4981	0.23	0/6725
1	D	0.08	0/4963	0.24	0/6701
1	E	0.08	0/4948	0.25	0/6678
1	F	0.08	0/4525	0.25	0/6101
All	All	0.08	0/29379	0.24	0/39654

There are no bond length outliers.

There are no bond angle outliers.

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	4870	0	4819	27	0
1	B	4887	0	4826	32	0
1	C	4881	0	4818	31	0
1	D	4863	0	4808	28	0
1	E	4848	0	4797	32	0
1	F	4433	0	4367	46	0
2	A	31	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	61	0	0	0	0
2	C	27	0	0	0	0
2	D	31	0	0	1	0
2	E	38	0	0	1	0
2	F	41	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
4	A	85	0	0	0	0
4	B	57	0	0	0	0
4	C	54	0	0	0	0
4	D	51	0	0	0	0
4	E	66	0	0	0	0
4	F	21	0	0	0	0
All	All	29352	0	28435	191	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 3.

All (191) 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:B:521:VAL:HG23	1:B:522:ARG:HG3	1.76	0.68
1:C:383:MET:HG3	1:C:406:LEU:HD11	1.75	0.67
1:E:42:ILE:HG21	1:E:54:LEU:HD21	1.77	0.67
1:F:198:ASP:OD1	1:F:198:ASP:N	2.26	0.66
1:E:383:MET:HG3	1:E:406:LEU:HD11	1.79	0.65
1:F:155:ASN:ND2	1:F:217:ASP:OD2	2.29	0.63
1:D:508:ASN:HD21	1:D:512:LEU:HB2	1.63	0.63
1:F:413:PRO:HG2	1:F:426:ILE:HB	1.82	0.61
1:C:521:VAL:HG23	1:C:522:ARG:HG3	1.83	0.60
1:A:198:ASP:N	1:A:198:ASP:OD1	2.25	0.60
1:F:383:MET:HG3	1:F:406:LEU:HD11	1.82	0.59
1:B:339:ASP:OD2	1:B:385:ARG:NH2	2.35	0.59
1:D:45:GLN:NE2	1:D:116:PHE:O	2.34	0.59
1:A:413:PRO:HG2	1:A:426:ILE:HB	1.85	0.59
1:D:521:VAL:HG23	1:D:522:ARG:HG3	1.85	0.58
1:B:531:LYS:HE3	1:B:549:ASN:HA	1.85	0.58
1:F:237:ASP:HB3	1:F:240:GLU:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ARG:O	1:D:289:ARG:NH2	2.37	0.57
1:F:455:ILE:HG12	1:F:517:VAL:HG21	1.86	0.57
1:A:606:LEU:HD12	1:A:621:ILE:HD13	1.87	0.57
1:E:413:PRO:HG2	1:E:426:ILE:HB	1.87	0.57
1:D:72:PHE:HB3	1:D:79:MET:HE1	1.86	0.56
1:F:19:ILE:HD12	1:F:102:LYS:HB3	1.85	0.56
1:B:123:VAL:HG13	1:B:135:VAL:HG11	1.88	0.56
1:D:198:ASP:N	1:D:198:ASP:OD1	2.38	0.55
1:D:532:ARG:NH2	1:D:617:GLN:O	2.34	0.55
1:E:508:ASN:HD21	1:E:512:LEU:HB2	1.72	0.55
1:F:521:VAL:HG23	1:F:522:ARG:HG3	1.87	0.55
1:A:508:ASN:HD21	1:A:512:LEU:HB2	1.71	0.55
1:B:335:LEU:HD21	1:B:391:ILE:HG21	1.89	0.54
1:F:123:VAL:HG13	1:F:135:VAL:HG11	1.89	0.54
1:E:387:LEU:HB2	1:E:392:LYS:HG3	1.90	0.54
1:C:413:PRO:HG2	1:C:426:ILE:HB	1.90	0.54
1:D:413:PRO:HG2	1:D:426:ILE:HB	1.90	0.54
1:E:198:ASP:OD1	1:E:198:ASP:N	2.37	0.53
1:F:508:ASN:HD21	1:F:512:LEU:HB2	1.73	0.53
1:A:123:VAL:HG11	1:A:175:PHE:CG	2.44	0.53
1:D:329:LEU:HG	1:D:333:LYS:HD2	1.90	0.53
1:F:531:LYS:HE3	1:F:547:PRO:HB2	1.90	0.53
1:F:127:GLY:HA2	1:F:132:LEU:HD12	1.91	0.53
1:F:385:ARG:HB3	1:F:402:TYR:CE2	2.44	0.53
1:D:123:VAL:HG11	1:D:175:PHE:CG	2.45	0.52
1:B:135:VAL:HB	1:B:175:PHE:HB2	1.92	0.52
1:F:314:ASP:OD1	1:F:317:ASN:ND2	2.43	0.51
1:F:49:PRO:HA	1:F:52:TYR:CZ	2.45	0.51
1:C:49:PRO:HA	1:C:52:TYR:CE2	2.46	0.51
1:C:89:TRP:CD1	1:C:89:TRP:H	2.30	0.50
1:B:123:VAL:HG11	1:B:175:PHE:CG	2.46	0.50
1:E:45:GLN:NE2	1:E:116:PHE:O	2.36	0.50
1:C:89:TRP:H	1:C:89:TRP:HD1	1.58	0.50
1:C:123:VAL:HG11	1:C:175:PHE:CG	2.46	0.49
1:B:127:GLY:HA2	1:B:132:LEU:HD12	1.94	0.49
1:C:118:GLU:HB2	1:C:218:TYR:CZ	2.46	0.49
1:F:22:SER:HB2	1:F:106:ILE:HD13	1.95	0.49
1:F:207:ILE:HD11	1:F:256:ILE:HG12	1.95	0.49
1:A:236:ARG:O	1:A:289:ARG:NH1	2.43	0.48
1:A:198:ASP:OD2	2:A:701:A1IR6:O13	2.30	0.48
1:C:508:ASN:HD21	1:C:512:LEU:HB2	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:ILE:HD13	1:F:53:GLU:HB3	1.96	0.48
1:F:495:THR:HG22	1:F:504:ILE:HG12	1.94	0.48
1:B:558:LEU:HD11	1:B:581:LYS:HD2	1.95	0.48
1:B:194:VAL:HG11	1:B:247:LYS:HE2	1.95	0.48
1:E:123:VAL:HG13	1:E:135:VAL:HG11	1.96	0.48
1:E:455:ILE:HG12	1:E:517:VAL:HG21	1.95	0.48
1:E:270:TYR:CD1	1:E:305:ILE:HG13	2.49	0.48
1:E:198:ASP:OD2	2:E:701:A1IR6:O13	2.32	0.47
1:E:593:VAL:HG21	1:E:606:LEU:HD21	1.95	0.47
1:F:54:LEU:HD23	1:F:56:PHE:HE1	1.79	0.47
1:F:89:TRP:CD1	1:F:90:GLY:H	2.32	0.47
1:F:123:VAL:HG11	1:F:175:PHE:CG	2.49	0.47
1:A:127:GLY:HA2	1:A:132:LEU:HD12	1.96	0.47
1:D:118:GLU:HB2	1:D:218:TYR:CZ	2.50	0.47
1:A:172:PRO:HD3	1:A:198:ASP:OD2	2.15	0.47
1:C:172:PRO:HD3	1:C:198:ASP:OD2	2.14	0.47
1:D:186:ILE:HD13	1:D:205:ALA:HA	1.96	0.47
1:F:28:TYR:HB2	1:F:59:ASP:HB3	1.97	0.47
1:C:236:ARG:O	1:C:289:ARG:NH2	2.45	0.47
1:F:246:ASN:O	1:F:250:ASN:ND2	2.48	0.47
1:A:32:LEU:HG	1:A:36:LYS:HE3	1.97	0.47
1:D:49:PRO:HA	1:D:52:TYR:CE2	2.50	0.47
1:A:67:GLU:OE1	1:A:67:GLU:N	2.47	0.46
1:B:118:GLU:HB2	1:B:218:TYR:CZ	2.51	0.46
1:B:508:ASN:HD21	1:B:512:LEU:HB2	1.79	0.46
1:A:123:VAL:HG13	1:A:135:VAL:HG11	1.97	0.46
1:A:356:ASP:HA	1:A:498:ILE:HD13	1.98	0.46
1:F:41:SER:HB3	1:F:114:THR:HG23	1.98	0.46
1:A:537:ILE:HD11	1:A:621:ILE:HB	1.97	0.46
1:C:58:ASP:OD1	1:C:61:SER:OG	2.29	0.46
1:C:89:TRP:CD1	1:C:89:TRP:N	2.84	0.46
1:B:516:ASP:OD1	1:B:520:SER:OG	2.25	0.46
1:F:385:ARG:HG2	1:F:400:PHE:HB2	1.98	0.46
1:A:87:SER:HB3	1:A:91:SER:O	2.16	0.46
1:A:383:MET:HG3	1:A:406:LEU:HD11	1.97	0.45
1:B:489:GLY:O	1:B:507:LYS:NZ	2.48	0.45
1:C:581:LYS:HE3	1:C:583:ILE:HD11	1.98	0.45
1:E:159:ALA:HB1	1:E:166:CYS:HB2	1.99	0.45
1:F:135:VAL:HB	1:F:175:PHE:HB2	1.98	0.45
1:A:521:VAL:HG23	1:A:522:ARG:HG3	1.99	0.45
1:B:198:ASP:OD1	1:B:198:ASP:N	2.25	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:THR:HG22	1:B:504:ILE:HG12	1.99	0.45
1:A:371:LYS:HA	1:B:347:TYR:CZ	2.51	0.45
1:C:66:TYR:CE1	1:C:83:GLN:HB2	2.52	0.45
1:F:546:ILE:HB	1:F:591:VAL:HB	1.99	0.45
1:B:89:TRP:CD1	1:B:89:TRP:H	2.35	0.45
1:C:130:ASN:HB2	1:C:132:LEU:HG	1.99	0.45
1:F:169:PRO:HG3	2:F:701:A1IR6:O28	2.16	0.45
1:F:194:VAL:HA	1:F:244:GLN:HE22	1.80	0.45
1:F:556:GLU:HA	1:F:584:GLY:O	2.16	0.45
1:D:66:TYR:CE1	1:D:83:GLN:HB2	2.52	0.44
1:E:375:PHE:HZ	1:E:438:LYS:HD3	1.81	0.44
1:D:42:ILE:HG21	1:D:54:LEU:HD21	1.98	0.44
1:F:194:VAL:HA	1:F:244:GLN:NE2	2.33	0.44
1:A:49:PRO:HA	1:A:52:TYR:CE2	2.53	0.44
1:A:118:GLU:HB2	1:A:218:TYR:CZ	2.53	0.44
1:B:92:ARG:HH22	1:C:190:ASP:CG	2.25	0.44
1:B:383:MET:HG3	1:B:406:LEU:HD11	1.99	0.44
1:E:145:TRP:CZ2	1:E:485:ALA:HB2	2.53	0.44
1:D:489:GLY:O	1:D:507:LYS:NZ	2.51	0.44
1:B:160:GLU:HB3	1:B:212:VAL:H	1.81	0.43
1:F:19:ILE:HG21	1:F:53:GLU:HG2	2.00	0.43
1:F:32:LEU:O	1:F:36:LYS:HG3	2.18	0.43
1:E:118:GLU:HB2	1:E:218:TYR:CZ	2.53	0.43
1:E:437:ASN:HB2	1:E:443:TYR:CE2	2.53	0.43
1:E:49:PRO:HA	1:E:52:TYR:CE2	2.54	0.43
1:E:371:LYS:HA	1:F:347:TYR:CZ	2.53	0.43
1:F:410:THR:OG1	1:F:476:THR:OG1	2.25	0.43
1:E:19:ILE:HG21	1:E:53:GLU:HG2	2.00	0.43
1:C:368:TYR:O	1:D:489:GLY:HA3	2.18	0.43
1:E:123:VAL:HG11	1:E:175:PHE:CG	2.54	0.43
1:B:145:TRP:CZ2	1:B:485:ALA:HB2	2.54	0.43
1:F:172:PRO:HD3	1:F:198:ASP:OD2	2.18	0.43
1:C:347:TYR:CZ	1:D:371:LYS:HA	2.54	0.43
1:E:347:TYR:CZ	1:F:371:LYS:HA	2.53	0.43
1:F:455:ILE:HD11	1:F:469:TRP:CE2	2.54	0.43
1:C:495:THR:HG22	1:C:504:ILE:HG12	2.00	0.42
1:E:49:PRO:O	1:E:78:ASN:ND2	2.52	0.42
1:D:134:VAL:HB	1:D:212:VAL:HG22	2.01	0.42
1:E:172:PRO:HD3	1:E:198:ASP:OD2	2.19	0.42
1:F:108:TYR:HB2	1:F:172:PRO:O	2.19	0.42
1:F:145:TRP:CZ2	1:F:485:ALA:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:SER:HB2	1:D:613:LYS:HB3	2.01	0.42
1:E:410:THR:OG1	1:E:476:THR:OG1	2.26	0.42
1:A:42:ILE:HG21	1:A:54:LEU:HD11	2.02	0.42
1:C:45:GLN:NE2	1:C:116:PHE:O	2.46	0.42
1:F:583:ILE:HD11	1:F:592:GLU:CD	2.45	0.42
1:D:89:TRP:N	1:D:89:TRP:CD1	2.87	0.42
2:D:701:A1IR6:O42	2:D:701:A1IR6:O24	2.37	0.42
1:E:41:SER:HB2	1:E:115:VAL:O	2.20	0.42
1:A:567:PRO:HB2	1:A:570:ILE:HD13	2.02	0.42
1:B:49:PRO:HA	1:B:52:TYR:CE2	2.54	0.42
1:B:139:GLU:OE2	1:B:173:HIS:ND1	2.35	0.42
1:D:159:ALA:HB1	1:D:166:CYS:HB2	2.02	0.42
1:B:455:ILE:HD12	1:B:455:ILE:HA	1.94	0.41
1:D:76:ARG:HD2	1:D:79:MET:HE3	2.02	0.41
1:E:82:LYS:HD2	1:E:100:MET:HE1	2.00	0.41
1:E:369:GLU:O	1:E:371:LYS:HG3	2.20	0.41
1:A:242:TRP:HZ2	1:A:277:ILE:HD13	1.84	0.41
1:B:159:ALA:O	1:B:162:MET:HG2	2.19	0.41
1:E:95:ASN:O	1:E:99:LYS:HG2	2.20	0.41
1:E:521:VAL:HG23	1:E:522:ARG:HG3	2.01	0.41
1:A:58:ASP:OD1	1:A:61:SER:OG	2.31	0.41
1:B:455:ILE:HG12	1:B:517:VAL:HG21	2.02	0.41
1:C:139:GLU:HG3	1:C:221:TYR:HB3	2.03	0.41
1:A:369:GLU:O	1:A:371:LYS:HG3	2.20	0.41
1:B:66:TYR:CE1	1:B:83:GLN:HB2	2.56	0.41
1:C:70:GLN:O	1:C:74:GLU:HG3	2.20	0.41
1:C:173:HIS:HB3	1:C:221:TYR:CD2	2.55	0.41
1:E:79:MET:HE3	1:E:79:MET:HB2	1.99	0.41
1:F:242:TRP:HE1	1:F:293:GLU:HB3	1.84	0.41
1:A:155:ASN:HD21	1:A:217:ASP:CG	2.28	0.41
1:C:43:ASP:CG	1:C:76:ARG:HH12	2.29	0.41
1:D:242:TRP:HZ2	1:D:277:ILE:HD13	1.85	0.41
1:C:565:LEU:HB2	1:C:576:ILE:HB	2.03	0.41
1:C:606:LEU:HD12	1:C:621:ILE:HD13	2.03	0.41
1:D:455:ILE:HG12	1:D:517:VAL:HG21	2.03	0.41
1:E:67:GLU:OE1	1:E:67:GLU:N	2.52	0.41
1:F:385:ARG:HG3	1:F:387:LEU:HG	2.03	0.41
1:A:42:ILE:HG21	1:A:54:LEU:HD21	2.03	0.41
1:C:198:ASP:O	1:C:202:ASN:ND2	2.46	0.41
1:D:455:ILE:HD12	1:D:455:ILE:HA	1.96	0.41
1:F:132:LEU:HD13	1:F:213:GLY:HA3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:ARG:NE	1:F:384:GLU:OE2	2.44	0.41
1:B:413:PRO:HG2	1:B:426:ILE:HB	2.03	0.40
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.96	0.40
1:B:176:TYR:HB2	1:B:181:LEU:HD11	2.04	0.40
1:B:544:VAL:HB	1:B:593:VAL:HB	2.02	0.40
1:B:334:LYS:HB3	1:B:391:ILE:HD11	2.03	0.40
1:C:410:THR:OG1	1:C:476:THR:OG1	2.26	0.40
1:C:437:ASN:HB2	1:C:443:TYR:CE2	2.57	0.40
1:D:437:ASN:HB2	1:D:443:TYR:CE2	2.57	0.40
1:D:184:ASN:HB3	1:D:208:HIS:ND1	2.37	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	580/624 (93%)	555 (96%)	25 (4%)	0	100	100
1	B	599/624 (96%)	568 (95%)	31 (5%)	0	100	100
1	C	597/624 (96%)	579 (97%)	18 (3%)	0	100	100
1	D	595/624 (95%)	573 (96%)	22 (4%)	0	100	100
1	E	592/624 (95%)	574 (97%)	18 (3%)	0	100	100
1	F	533/624 (85%)	496 (93%)	37 (7%)	0	100	100
All	All	3496/3744 (93%)	3345 (96%)	151 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	533/553 (96%)	530 (99%)	3 (1%)	78	90
1	B	535/553 (97%)	533 (100%)	2 (0%)	84	92
1	C	534/553 (97%)	530 (99%)	4 (1%)	76	89
1	D	532/553 (96%)	530 (100%)	2 (0%)	84	92
1	E	532/553 (96%)	525 (99%)	7 (1%)	61	81
1	F	483/553 (87%)	479 (99%)	4 (1%)	73	88
All	All	3149/3318 (95%)	3127 (99%)	22 (1%)	76	89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
1	A	197	GLU
1	A	198	ASP
1	B	89	TRP
1	B	198	ASP
1	C	89	TRP
1	C	289	ARG
1	C	314	ASP
1	C	532	ARG
1	D	89	TRP
1	D	115	VAL
1	E	31	GLU
1	E	84	ILE
1	E	194	VAL
1	E	237	ASP
1	E	311	GLU
1	E	390	GLU
1	E	556	GLU
1	F	128	LYS
1	F	198	ASP
1	F	211	LYS
1	F	438	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	286	ASN
1	A	318	GLN
1	A	432	ASN
1	A	587	ASN
1	A	618	GLN
1	B	130	ASN
1	B	158	HIS
1	B	243	ASN
1	B	419	ASN
1	B	587	ASN
1	C	86	ASN
1	C	280	GLN
1	C	432	ASN
1	C	617	GLN
1	D	143	ASN
1	D	250	ASN
1	D	437	ASN
1	E	259	GLN
1	E	280	GLN
1	E	318	GLN
1	E	609	ASN
1	F	255	ASN
1	F	419	ASN
1	F	437	ASN
1	F	617	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 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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
2	A1IR6	F	702	-	13,13,59	1.41	2 (15%)	17,18,82	0.93	0
2	A1IR6	E	701	-	37,37,59	1.25	4 (10%)	48,51,82	0.89	3 (6%)
2	A1IR6	D	701	-	30,30,59	1.47	5 (16%)	41,44,82	0.93	2 (4%)
2	A1IR6	A	701	-	30,30,59	1.46	4 (13%)	41,44,82	0.92	2 (4%)
2	A1IR6	B	702	-	33,33,59	1.18	2 (6%)	42,44,82	0.62	0
2	A1IR6	C	701	-	26,26,59	1.34	3 (11%)	35,37,82	1.04	2 (5%)
2	A1IR6	B	701	-	26,26,59	1.36	3 (11%)	35,37,82	0.88	1 (2%)
2	A1IR6	F	701	-	26,26,59	1.36	3 (11%)	35,37,82	0.86	1 (2%)

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	A1IR6	F	702	-	-	9/16/16/85	-
2	A1IR6	E	701	-	-	23/49/49/85	-
2	A1IR6	D	701	-	-	1/40/40/85	-
2	A1IR6	A	701	-	-	21/40/40/85	-
2	A1IR6	B	702	-	-	31/45/45/85	-
2	A1IR6	C	701	-	-	8/36/36/85	-
2	A1IR6	B	701	-	-	14/36/36/85	-
2	A1IR6	F	701	-	-	7/36/36/85	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	A1IR6	P31-O32	3.26	1.66	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	A1IR6	P31-O32	3.26	1.66	1.54
2	A	701	A1IR6	P31-O32	3.25	1.66	1.54
2	F	701	A1IR6	P31-O32	3.25	1.66	1.54
2	F	702	A1IR6	P31-O32	3.25	1.66	1.54
2	C	701	A1IR6	P31-O32	3.25	1.66	1.54
2	E	701	A1IR6	P09-O08	3.04	1.66	1.54
2	A	701	A1IR6	P09-O08	3.03	1.66	1.54
2	D	701	A1IR6	P09-O08	3.03	1.66	1.54
2	B	702	A1IR6	P20-O21	2.38	1.68	1.59
2	F	701	A1IR6	P20-O21	2.37	1.68	1.59
2	A	701	A1IR6	P20-O21	2.37	1.68	1.59
2	D	701	A1IR6	P20-O21	2.37	1.68	1.59
2	B	701	A1IR6	P20-O21	2.36	1.68	1.59
2	C	701	A1IR6	P20-O21	2.35	1.68	1.59
2	E	701	A1IR6	P20-O21	2.31	1.68	1.59
2	B	702	A1IR6	P20-O19	2.22	1.68	1.59
2	B	701	A1IR6	P20-O19	2.21	1.68	1.59
2	D	701	A1IR6	P20-O19	2.17	1.67	1.59
2	F	701	A1IR6	P20-O19	2.17	1.67	1.59
2	A	701	A1IR6	P20-O19	2.17	1.67	1.59
2	C	701	A1IR6	P20-O19	2.15	1.67	1.59
2	F	702	A1IR6	P31-O30	2.12	1.67	1.60
2	E	701	A1IR6	P20-O19	2.11	1.67	1.59
2	E	701	A1IR6	P31-O32	2.04	1.67	1.59
2	D	701	A1IR6	P31-O30	2.02	1.66	1.60

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	A1IR6	C27-C25-C23	-2.98	108.62	113.57
2	C	701	A1IR6	C16-C14-C12	-2.98	108.62	113.57
2	D	701	A1IR6	C16-C14-C12	-2.75	109.00	113.57
2	B	701	A1IR6	C27-C25-C23	-2.74	109.01	113.57
2	E	701	A1IR6	C27-C25-C23	-2.69	109.09	113.57
2	A	701	A1IR6	C27-C25-C23	-2.60	109.24	113.57
2	D	701	A1IR6	C27-C25-C23	-2.59	109.25	113.57
2	F	701	A1IR6	C27-C25-C23	-2.39	109.59	113.57
2	A	701	A1IR6	C16-C14-C12	-2.38	109.60	113.57
2	E	701	A1IR6	C16-C14-C12	-2.30	109.75	113.57
2	E	701	A1IR6	C29-C27-C25	-2.05	108.35	112.22

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	A1IR6	C11-O10-P09-O08
2	A	701	A1IR6	C11-O10-P09-O44
2	A	701	A1IR6	C11-O10-P09-O45
2	A	701	A1IR6	C22-C23-C25-O26
2	A	701	A1IR6	C22-C23-C25-C27
2	A	701	A1IR6	O24-C23-C25-O26
2	A	701	A1IR6	C29-O30-P31-O32
2	A	701	A1IR6	C29-O30-P31-O41
2	B	701	A1IR6	C18-O19-P20-O21
2	B	701	A1IR6	C18-O19-P20-O42
2	B	701	A1IR6	C22-O21-P20-O19
2	B	701	A1IR6	C22-O21-P20-O42
2	B	701	A1IR6	C22-O21-P20-O43
2	B	702	A1IR6	C11-C12-C14-O15
2	B	702	A1IR6	C11-C12-C14-C16
2	B	702	A1IR6	O13-C12-C14-O15
2	B	702	A1IR6	O13-C12-C14-C16
2	B	702	A1IR6	C18-O19-P20-O43
2	B	702	A1IR6	C22-O21-P20-O19
2	B	702	A1IR6	C22-O21-P20-O42
2	B	702	A1IR6	C22-O21-P20-O43
2	B	702	A1IR6	O24-C23-C25-O26
2	B	702	A1IR6	O24-C23-C25-C27
2	B	702	A1IR6	C29-O30-P31-O32
2	B	702	A1IR6	C29-O30-P31-O40
2	B	702	A1IR6	C33-O32-P31-O41
2	E	701	A1IR6	C11-O10-P09-O08
2	E	701	A1IR6	C11-O10-P09-O44
2	E	701	A1IR6	C11-O10-P09-O45
2	E	701	A1IR6	C18-O19-P20-O21
2	E	701	A1IR6	C18-O19-P20-O42
2	E	701	A1IR6	C18-O19-P20-O43
2	E	701	A1IR6	O21-C22-C23-O24
2	E	701	A1IR6	O21-C22-C23-C25
2	E	701	A1IR6	C22-C23-C25-O26
2	E	701	A1IR6	C22-C23-C25-C27
2	E	701	A1IR6	O24-C23-C25-O26
2	E	701	A1IR6	O24-C23-C25-C27
2	E	701	A1IR6	C33-O32-P31-O30
2	E	701	A1IR6	C33-O32-P31-O40
2	E	701	A1IR6	C33-O32-P31-O41
2	F	701	A1IR6	C29-O30-P31-O32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	701	A1IR6	C29-O30-P31-O41
2	A	701	A1IR6	O24-C23-C25-C27
2	F	702	A1IR6	C23-C25-C27-O28
2	B	702	A1IR6	C33-C34-C35-C36
2	B	702	A1IR6	C22-C23-C25-O26
2	F	702	A1IR6	O26-C25-C27-C29
2	B	702	A1IR6	C12-C14-C16-C18
2	B	702	A1IR6	C22-C23-C25-C27
2	F	702	A1IR6	C23-C25-C27-C29
2	C	701	A1IR6	O10-C11-C12-O13
2	B	702	A1IR6	O32-C33-C34-C35
2	C	701	A1IR6	O10-C11-C12-C14
2	F	702	A1IR6	C22-C23-C25-O26
2	F	702	A1IR6	O26-C25-C27-O28
2	F	702	A1IR6	C22-C23-C25-C27
2	E	701	A1IR6	O32-C33-C34-C35
2	B	701	A1IR6	O17-C16-C18-O19
2	F	701	A1IR6	O21-C22-C23-O24
2	B	701	A1IR6	C22-C23-C25-O26
2	E	701	A1IR6	O15-C14-C16-C18
2	B	701	A1IR6	O24-C23-C25-O26
2	E	701	A1IR6	C12-C14-C16-O17
2	F	702	A1IR6	O24-C23-C25-C27
2	B	702	A1IR6	C34-C35-C36-C37
2	B	701	A1IR6	O24-C23-C25-C27
2	B	701	A1IR6	C22-C23-C25-C27
2	B	701	A1IR6	C14-C16-C18-O19
2	F	701	A1IR6	O21-C22-C23-C25
2	B	702	A1IR6	O15-C14-C16-O17
2	A	701	A1IR6	C29-O30-P31-O40
2	C	701	A1IR6	C29-O30-P31-O40
2	F	701	A1IR6	C29-O30-P31-O40
2	B	701	A1IR6	C11-C12-C14-C16
2	F	702	A1IR6	O24-C23-C25-O26
2	B	702	A1IR6	O26-C25-C27-C29
2	E	701	A1IR6	C12-C14-C16-C18
2	B	702	A1IR6	C12-C14-C16-O17
2	D	701	A1IR6	C23-C22-O21-P20
2	B	702	A1IR6	O15-C14-C16-C18
2	B	702	A1IR6	C23-C25-C27-C29
2	C	701	A1IR6	C22-C23-C25-C27
2	F	702	A1IR6	C29-O30-P31-O41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	701	A1IR6	O15-C14-C16-O17
2	C	701	A1IR6	O24-C23-C25-C27
2	B	702	A1IR6	C35-C36-C37-C38
2	A	701	A1IR6	O13-C12-C14-C16
2	C	701	A1IR6	O24-C23-C25-O26
2	B	701	A1IR6	C23-C22-O21-P20
2	A	701	A1IR6	C11-C12-C14-C16
2	A	701	A1IR6	C18-O19-P20-O43
2	B	702	A1IR6	C18-O19-P20-O21
2	B	702	A1IR6	C29-O30-P31-O41
2	B	702	A1IR6	C33-O32-P31-O30
2	B	702	A1IR6	C33-O32-P31-O40
2	E	701	A1IR6	C29-O30-P31-O41
2	A	701	A1IR6	C27-C29-O30-P31
2	B	702	A1IR6	O26-C25-C27-O28
2	A	701	A1IR6	O21-C22-C23-C25
2	F	701	A1IR6	C23-C22-O21-P20
2	E	701	A1IR6	O26-C25-C27-C29
2	B	701	A1IR6	C16-C18-O19-P20
2	A	701	A1IR6	O13-C12-C14-O15
2	C	701	A1IR6	C22-C23-C25-O26
2	A	701	A1IR6	O15-C14-C16-C18
2	A	701	A1IR6	O21-C22-C23-O24
2	C	701	A1IR6	C29-O30-P31-O41
2	A	701	A1IR6	C11-C12-C14-O15
2	A	701	A1IR6	C12-C14-C16-O17
2	E	701	A1IR6	C23-C25-C27-O28
2	A	701	A1IR6	O15-C14-C16-O17
2	B	702	A1IR6	C23-C25-C27-O28
2	F	701	A1IR6	C11-C12-C14-C16

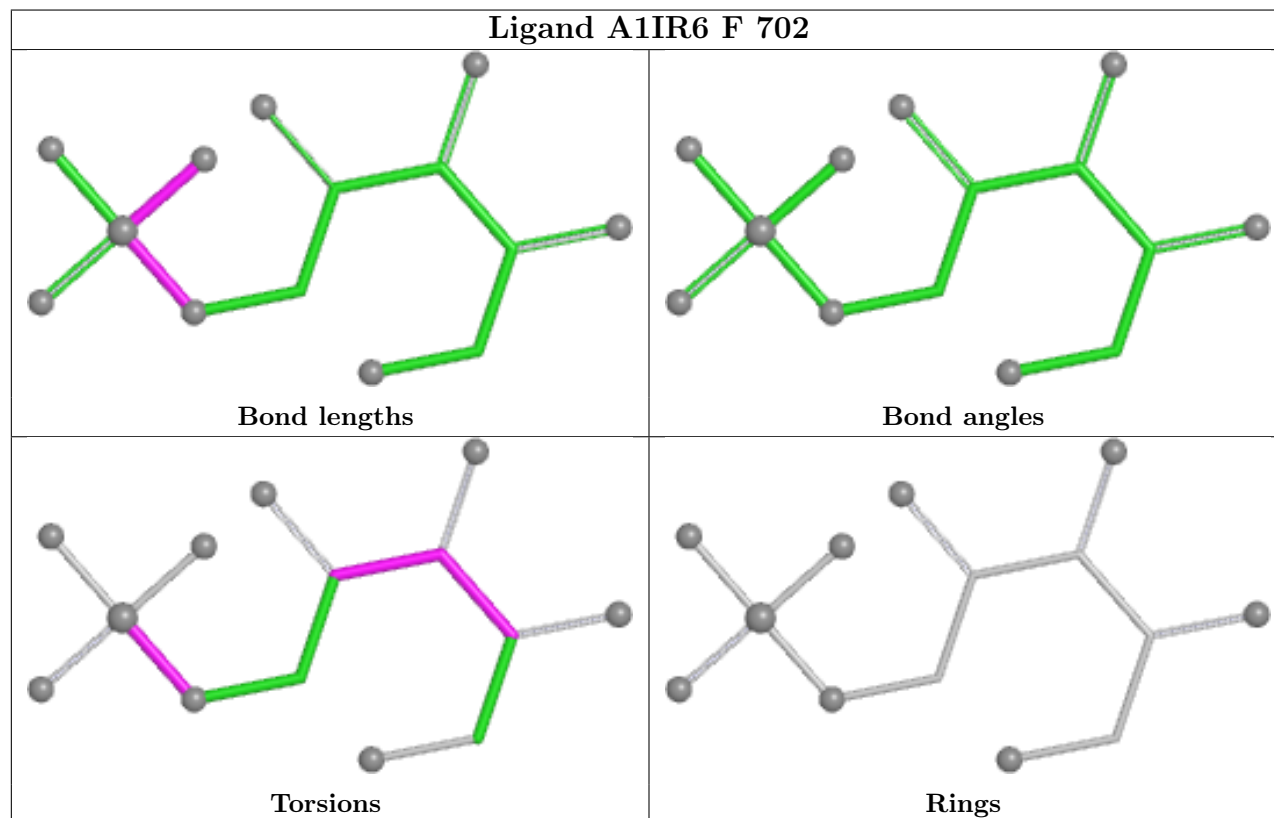
There are no ring outliers.

4 monomers are involved in 4 short contacts:

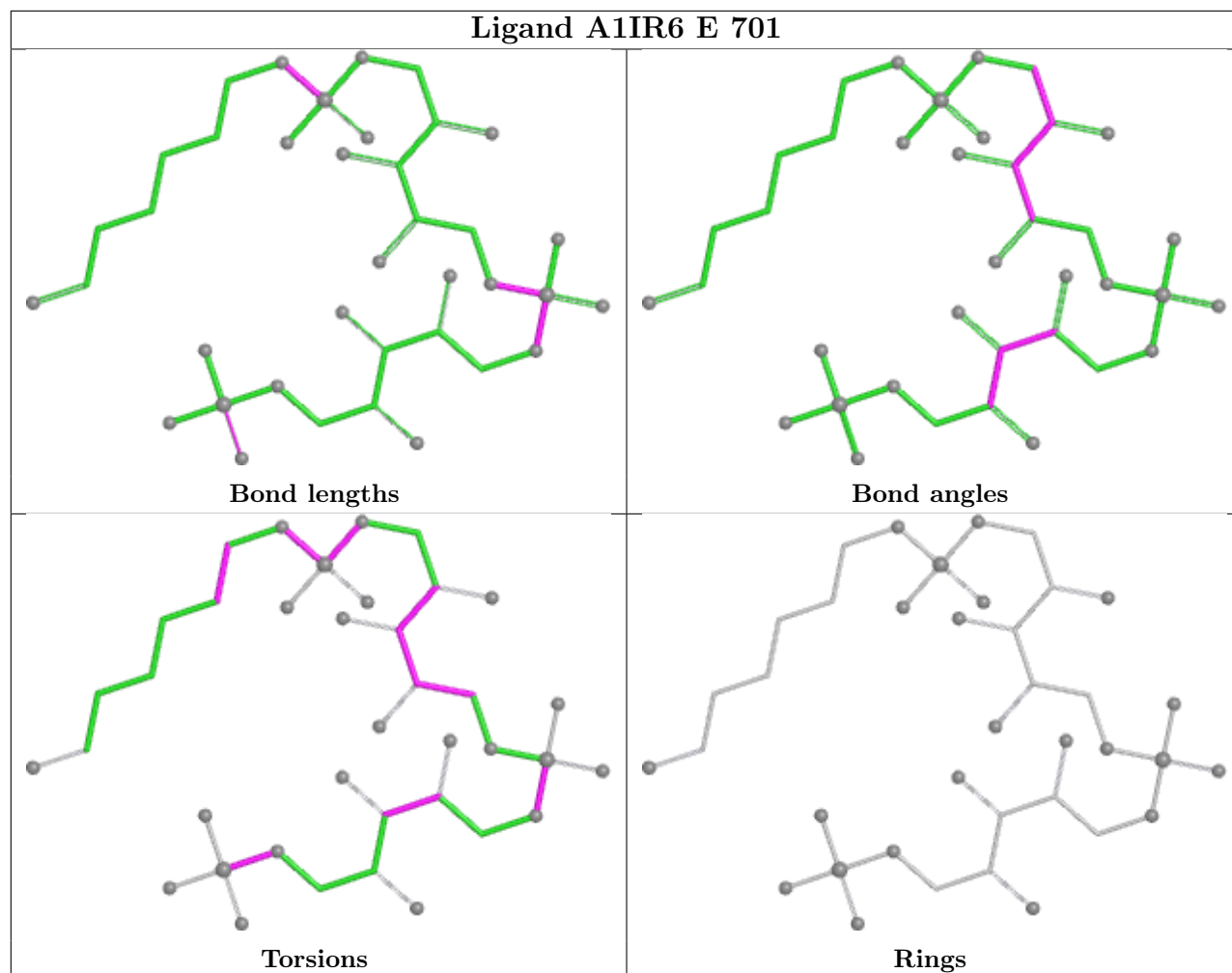
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	701	A1IR6	1	0
2	D	701	A1IR6	1	0
2	A	701	A1IR6	1	0
2	F	701	A1IR6	1	0

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

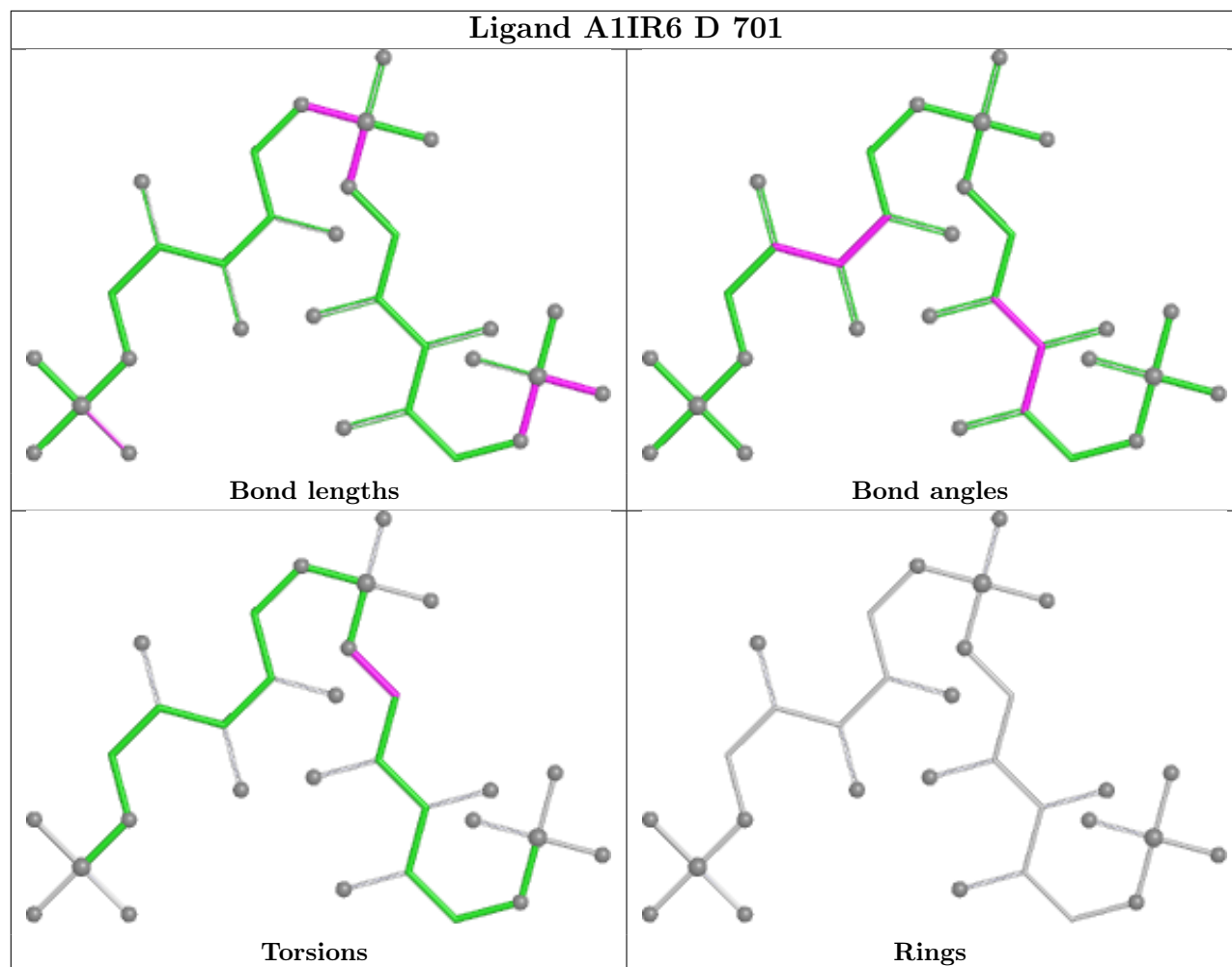
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



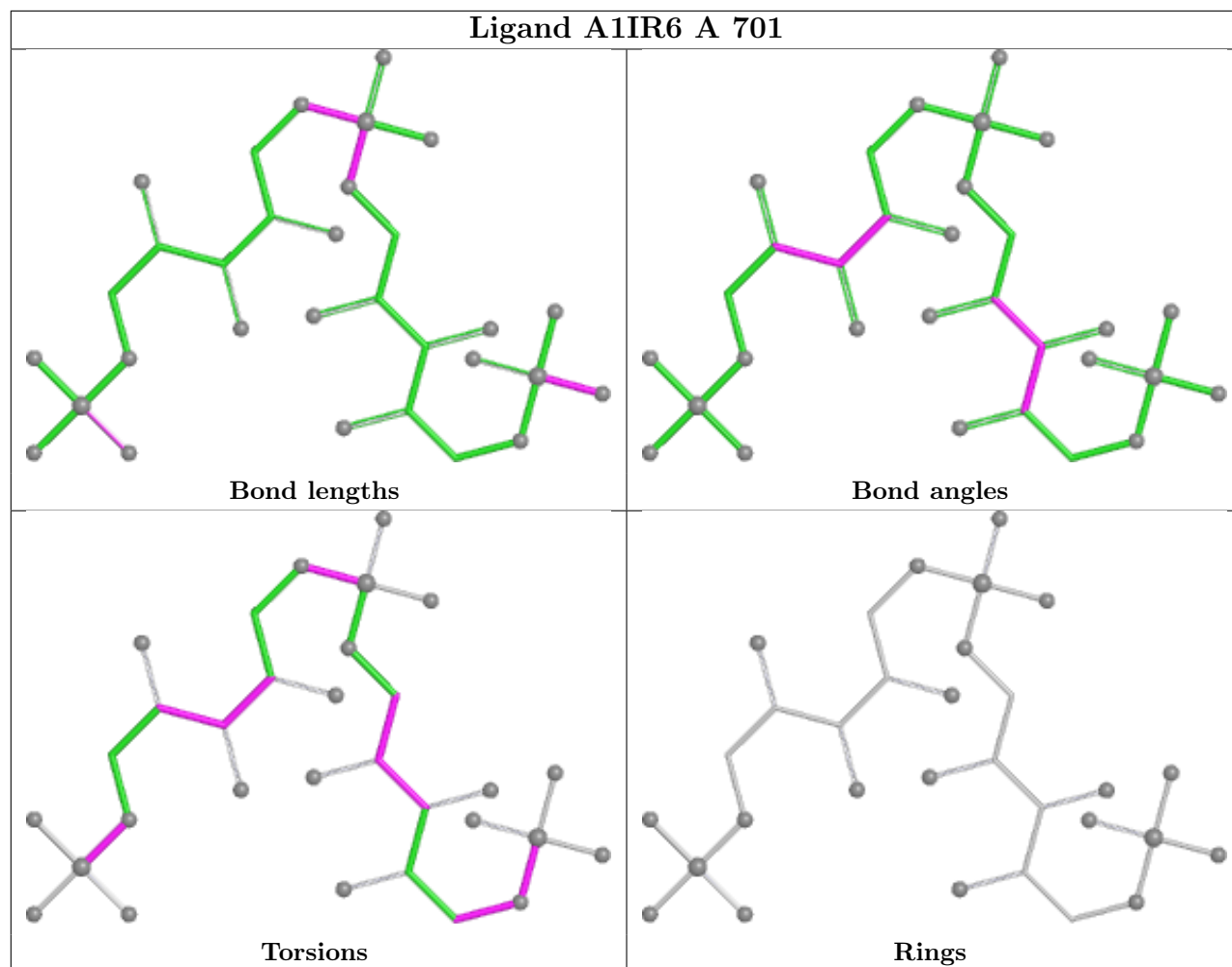
Ligand A1IR6 E 701



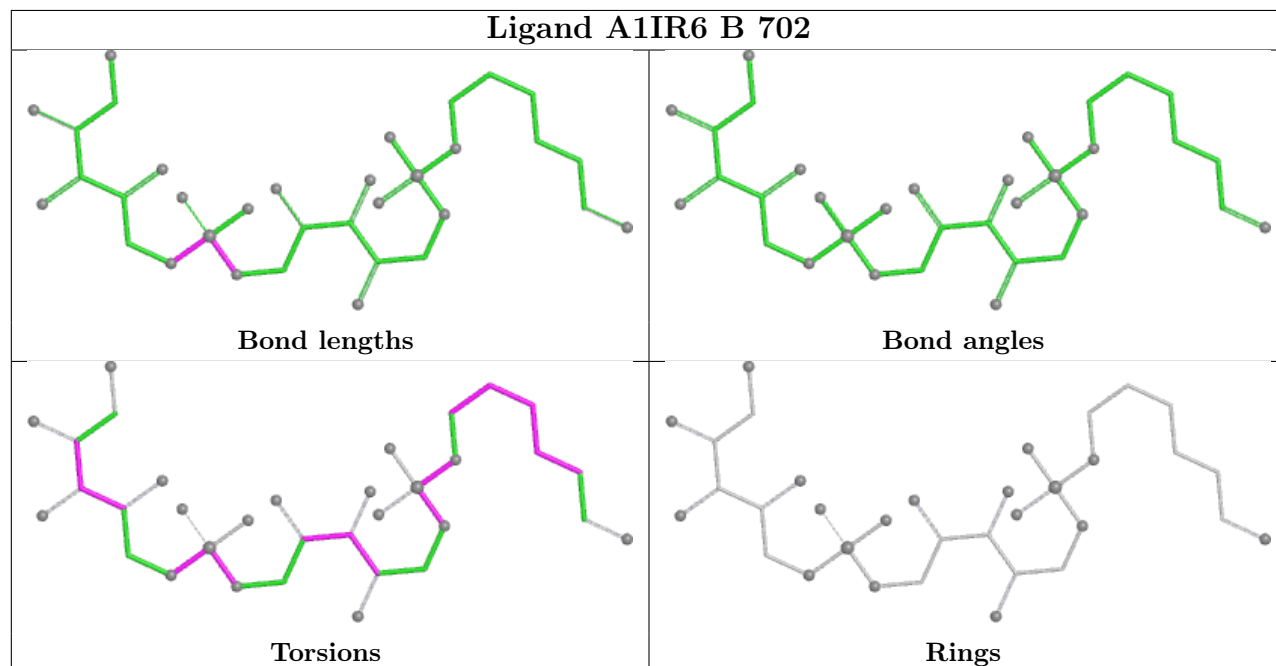
Ligand A1IR6 D 701



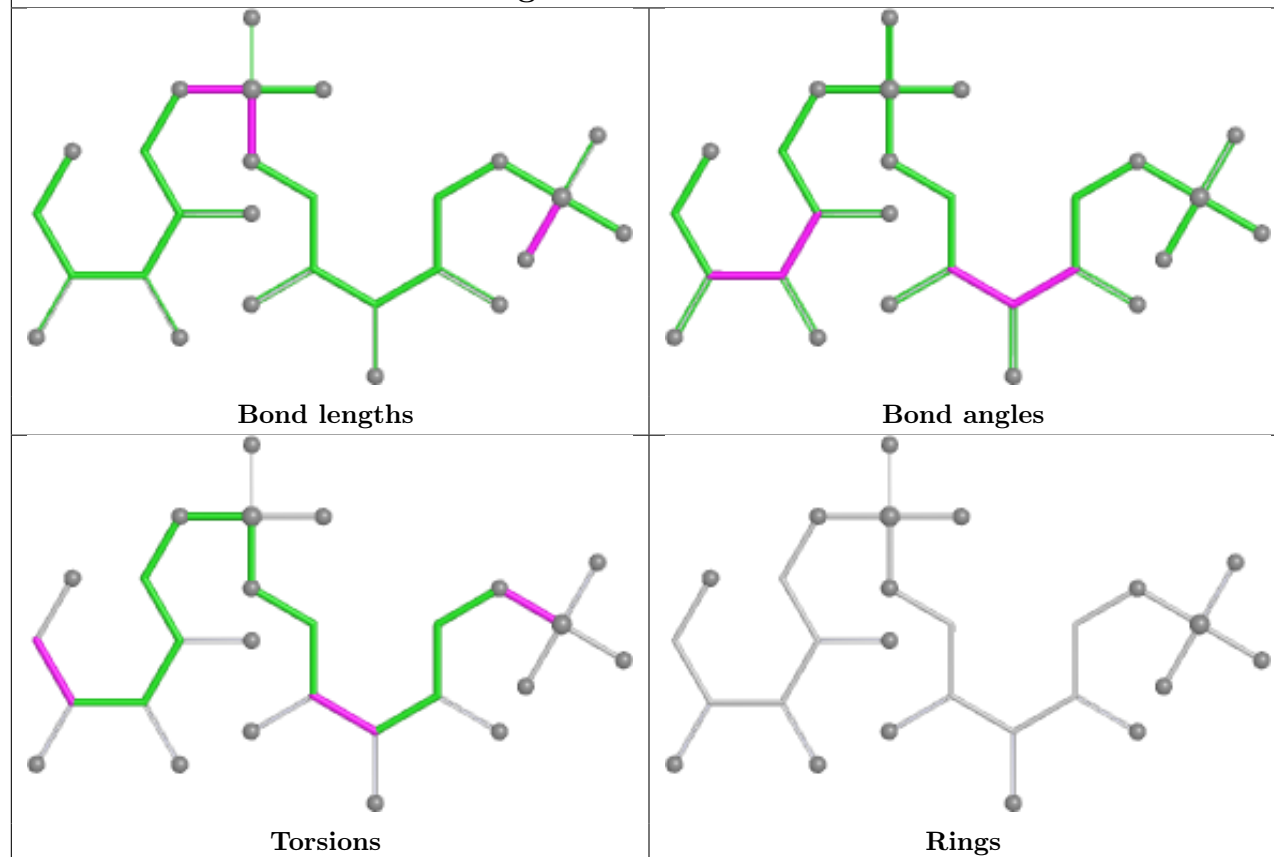
Ligand A1IR6 A 701



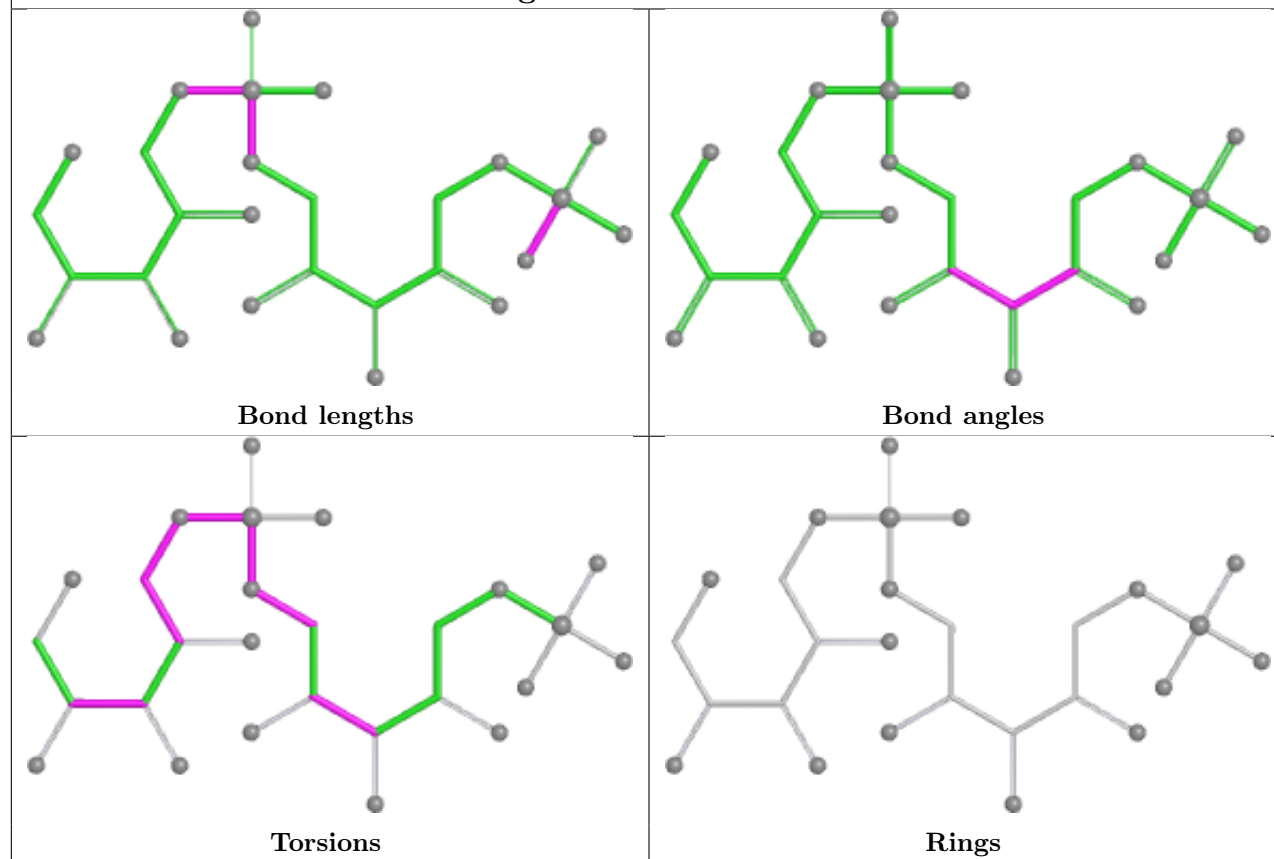
Ligand A1IR6 B 702

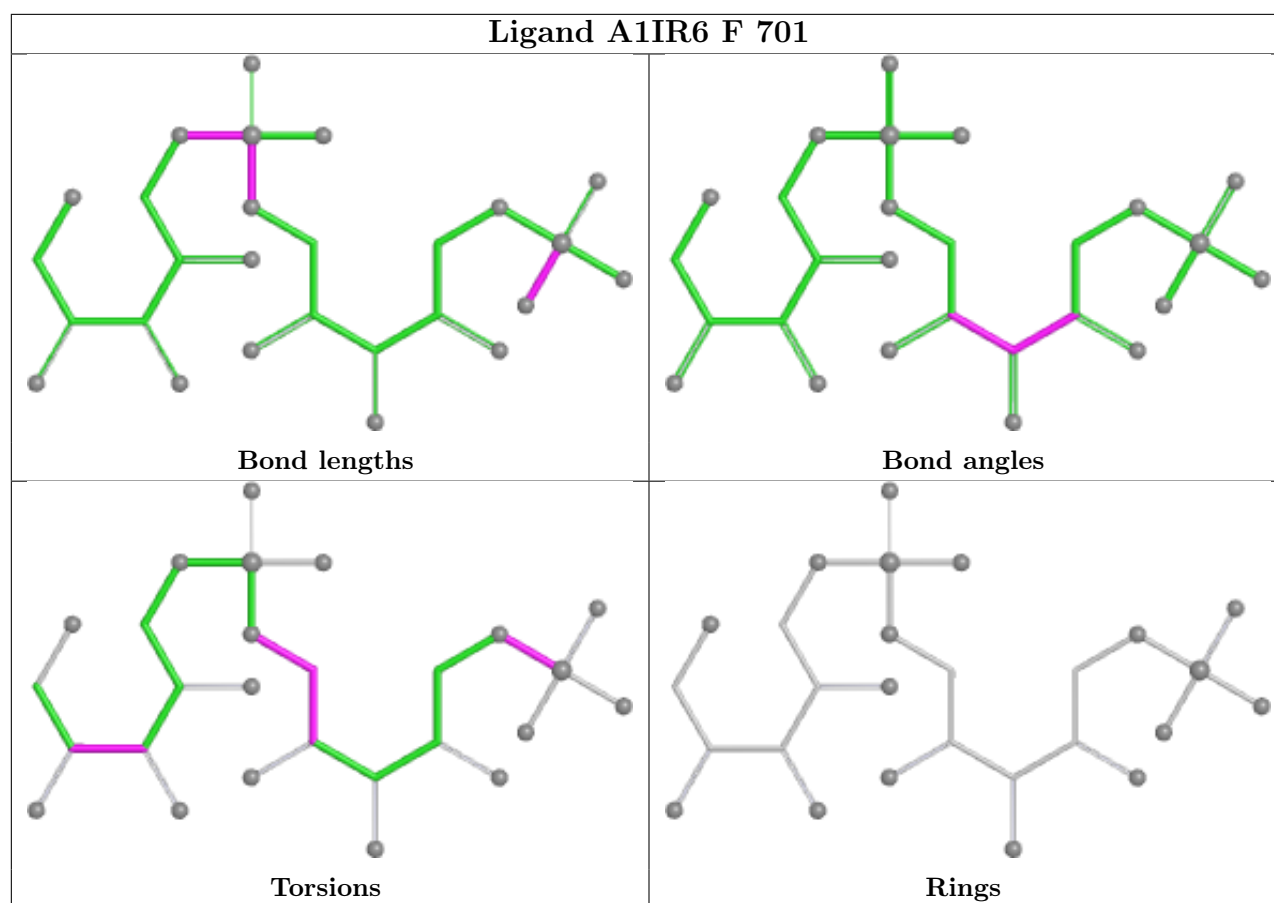


Ligand A1IR6 C 701



Ligand A1IR6 B 701





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	600/624 (96%)	-0.17	5 (0%) 82 80	28, 63, 102, 175	2 (0%)
1	B	601/624 (96%)	0.18	13 (2%) 62 59	25, 81, 142, 183	9 (1%)
1	C	599/624 (95%)	-0.07	3 (0%) 87 85	30, 67, 99, 137	2 (0%)
1	D	599/624 (95%)	0.03	3 (0%) 87 85	44, 75, 109, 140	1 (0%)
1	E	597/624 (95%)	-0.14	4 (0%) 84 82	33, 64, 103, 150	1 (0%)
1	F	544/624 (87%)	0.63	36 (6%) 24 22	30, 98, 149, 197	5 (0%)
All	All	3540/3744 (94%)	0.07	64 (1%) 67 64	25, 72, 131, 197	20 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	591	VAL	4.0
1	A	235	GLY	4.0
1	B	234	PHE	3.8
1	F	525	VAL	3.6
1	F	235	GLY	3.5
1	F	594	LEU	3.5
1	A	192	ALA	3.2
1	F	563	ALA	3.2
1	A	191	GLY	3.1
1	A	89	TRP	3.1
1	D	88	GLY	2.9
1	B	193	ARG	2.8
1	F	35	LEU	2.8
1	F	102	LYS	2.8
1	F	79	MET	2.7
1	C	88	GLY	2.7
1	F	54	LEU	2.7
1	F	546	ILE	2.7
1	F	61	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	582	LEU	2.6
1	F	83	GLN	2.6
1	F	114	THR	2.6
1	B	194	VAL	2.6
1	F	134	VAL	2.6
1	B	65	THR	2.5
1	F	559	ILE	2.5
1	F	191	GLY	2.5
1	F	615	ASP	2.5
1	F	117	PRO	2.4
1	B	570	ILE	2.4
1	F	578	VAL	2.4
1	A	88	GLY	2.3
1	F	41	SER	2.3
1	B	90	GLY	2.3
1	F	195	LEU	2.3
1	F	589	ALA	2.3
1	B	227	GLY	2.3
1	F	135	VAL	2.3
1	E	91	SER	2.3
1	E	81	VAL	2.3
1	F	24	VAL	2.3
1	B	69	LEU	2.2
1	C	84	ILE	2.2
1	F	50	ASP	2.2
1	B	72	PHE	2.2
1	F	109	LEU	2.1
1	E	84	ILE	2.1
1	F	120	PHE	2.1
1	B	39	MET	2.1
1	B	573	ALA	2.1
1	E	192	ALA	2.1
1	F	137	GLY	2.1
1	F	42	ILE	2.1
1	B	196	TRP	2.1
1	D	307	ALA	2.1
1	D	89	TRP	2.1
1	F	608	THR	2.1
1	F	38	LEU	2.0
1	F	227	GLY	2.0
1	B	84	ILE	2.0
1	F	47	MET	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	90	GLY	2.0
1	F	555	GLY	2.0
1	F	77	PRO	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](#)

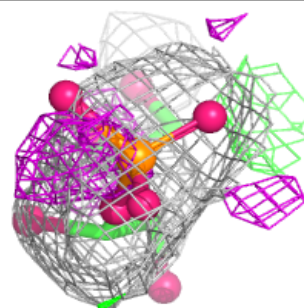
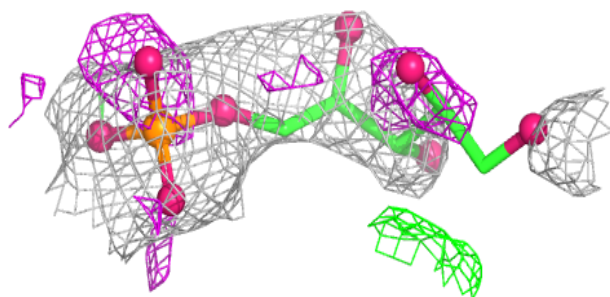
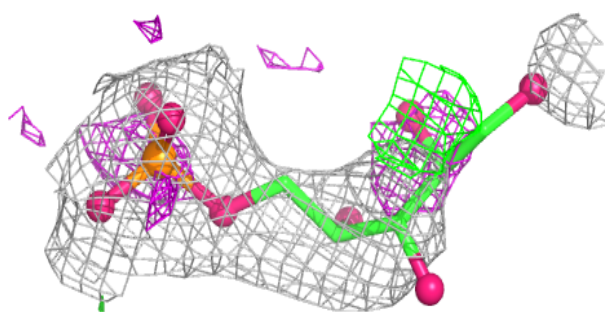
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1IR6	F	702	14/60	0.64	0.15	88,94,99,100	0
2	A1IR6	B	702	34/60	0.76	0.16	63,77,85,92	0
2	A1IR6	F	701	27/60	0.85	0.12	75,88,97,100	0
2	A1IR6	D	701	31/60	0.85	0.11	67,77,93,103	0
2	A1IR6	B	701	27/60	0.88	0.11	63,75,86,90	0
2	A1IR6	E	701	38/60	0.89	0.12	52,65,93,98	0
2	A1IR6	C	701	27/60	0.89	0.10	60,67,73,75	0
2	A1IR6	A	701	31/60	0.89	0.11	55,67,100,105	0
3	MG	D	702	1/1	0.91	0.12	72,72,72,72	0
3	MG	C	702	1/1	0.93	0.07	47,47,47,47	0
3	MG	A	702	1/1	0.96	0.05	58,58,58,58	0
3	MG	E	702	1/1	0.96	0.07	53,53,53,53	0
3	MG	B	703	1/1	0.97	0.03	31,31,31,31	0
3	MG	C	703	1/1	0.97	0.04	56,56,56,56	0
3	MG	E	703	1/1	0.98	0.08	55,55,55,55	0

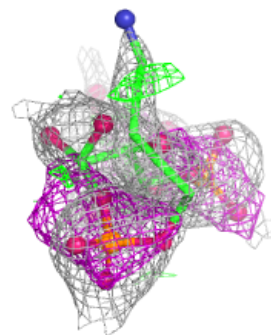
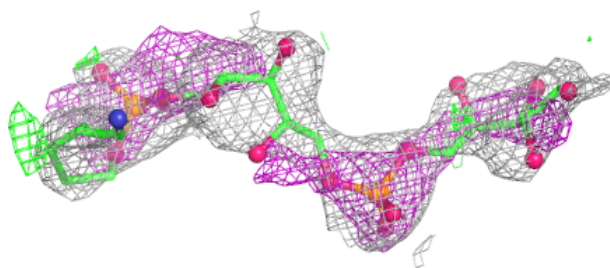
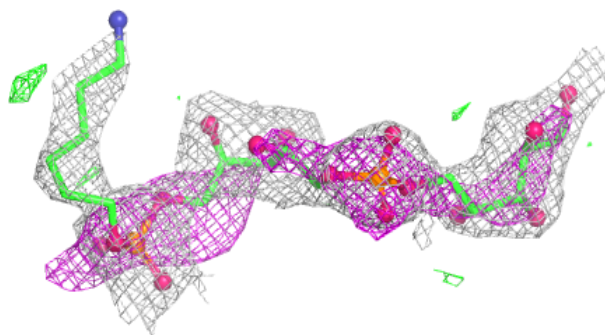
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IR6 F 702:

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

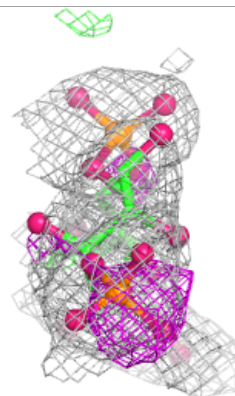
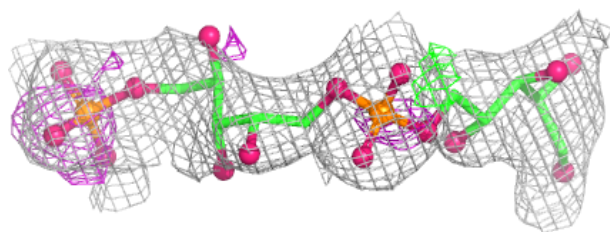
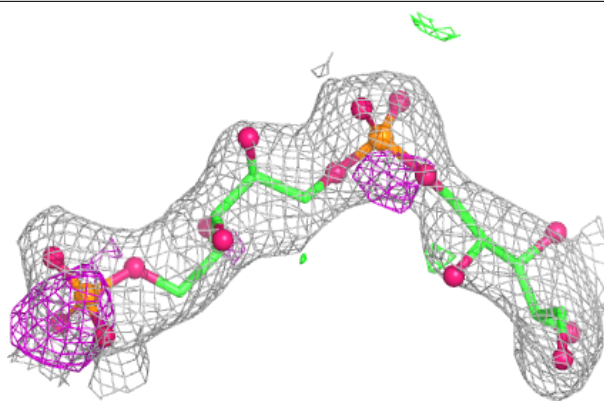
**Electron density around A1IR6 B 702:**

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



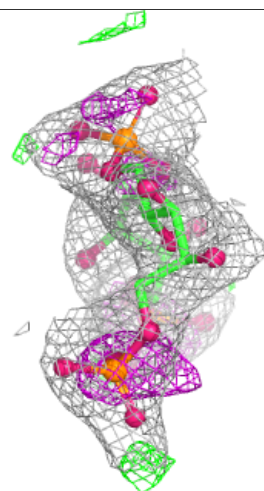
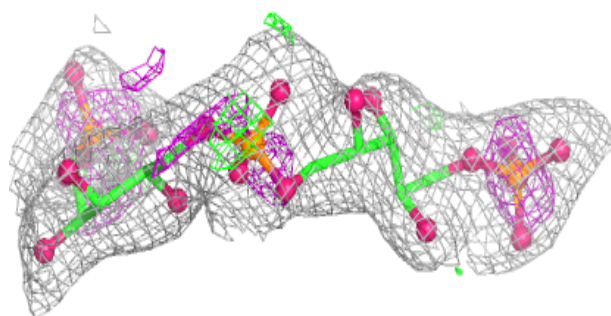
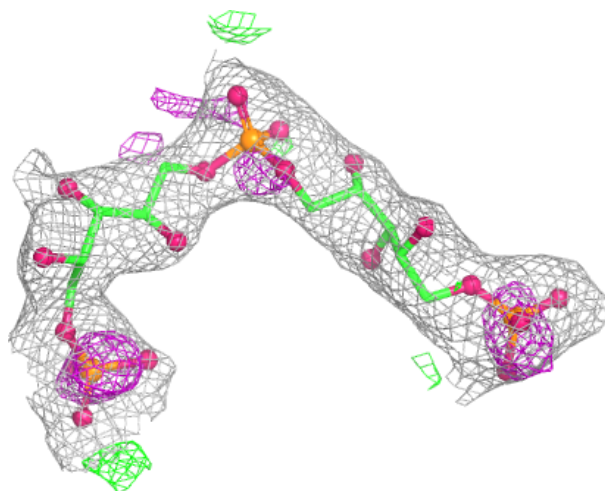
Electron density around A1IR6 F 701:

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



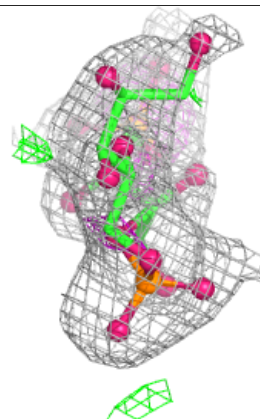
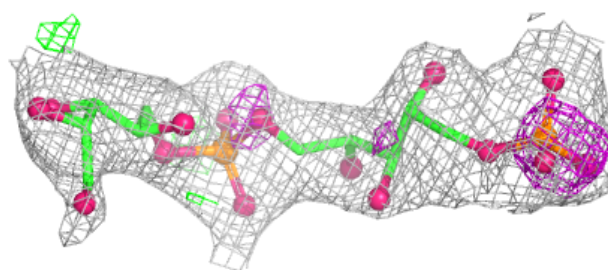
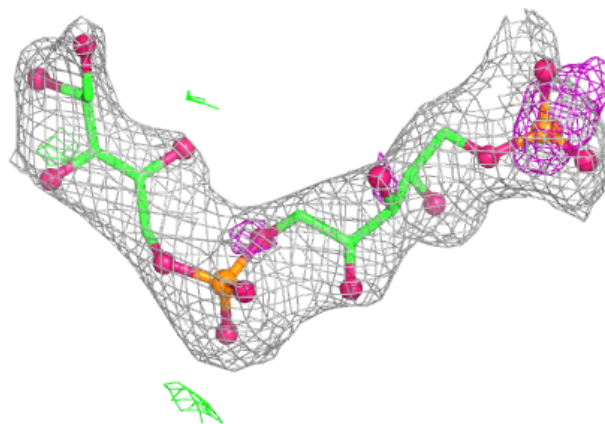
Electron density around A1IR6 D 701:

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



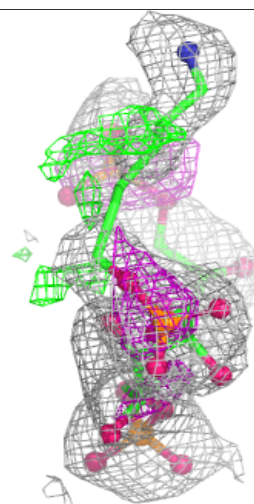
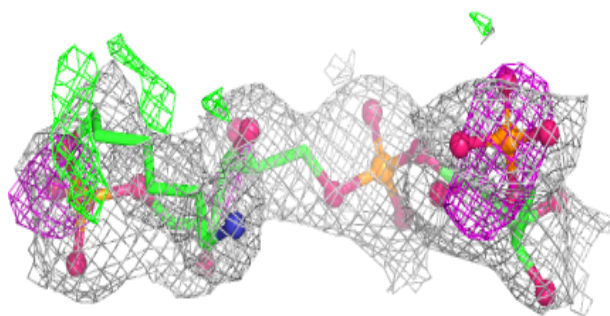
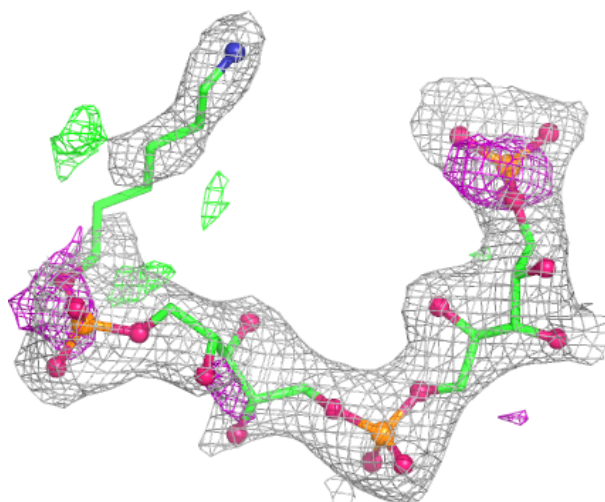
Electron density around A1IR6 B 701:

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



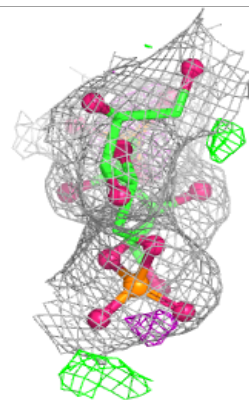
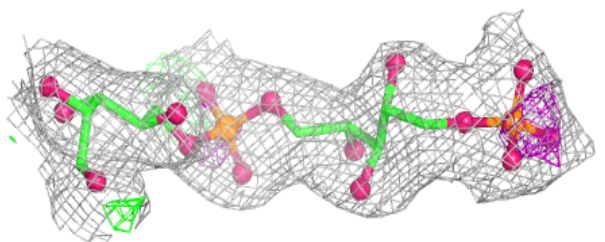
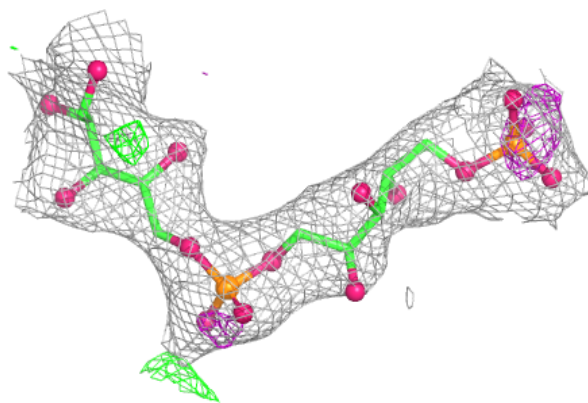
Electron density around A1IR6 E 701:

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

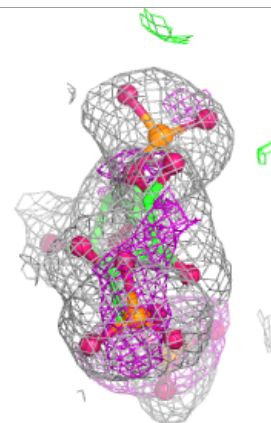
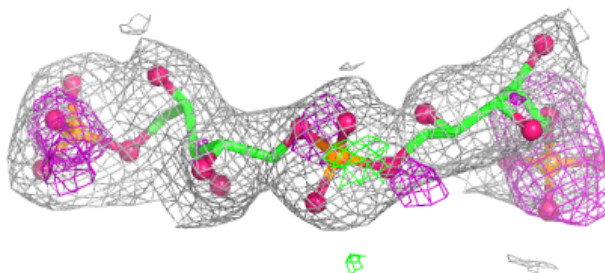
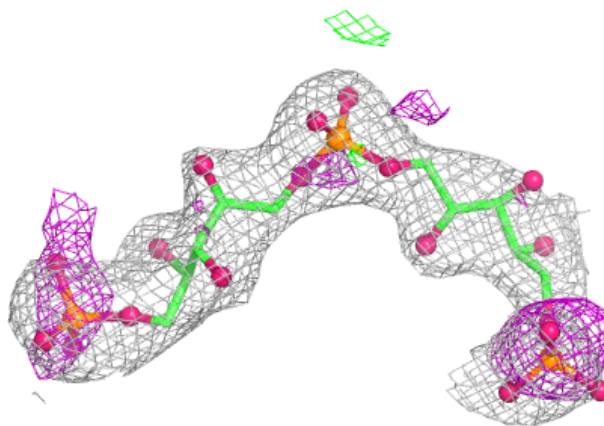


Electron density around A1IR6 C 701:

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

**Electron density around A1IR6 A 701:**

$2mF_o-DF_c$ (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.