



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2022 – 06:26 PM JST

PDB ID : 7VW7
Title : Crystal structure of the 2 ADP-AlF₄-bound V1 complex
Authors : Suzuki, K.; Shekhar, M.; Gupta, C.; Singharoy, A.; Murata, T.
Deposited on : 2021-11-09
Resolution : 3.82 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

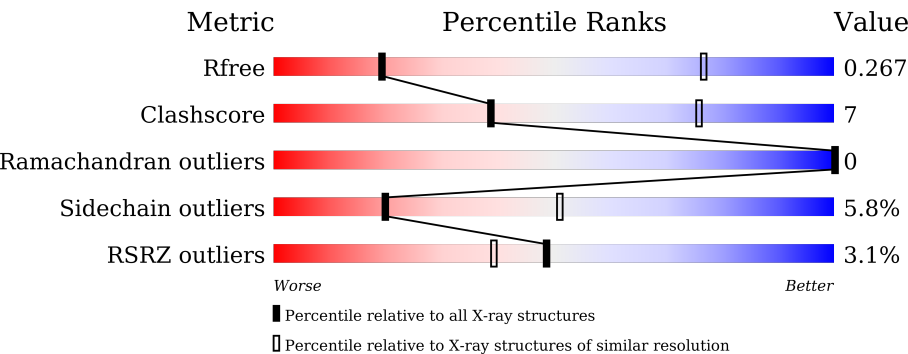
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.82 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	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	600	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>79%17%..</div></div>
1	B	600	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>83%15%..</div></div>
1	C	600	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>80%15%..</div></div>
2	D	465	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>81%15%..</div></div>
2	E	465	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>80%16%..</div></div>
2	F	465	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>73%22%..</div></div>

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Mol	Chain	Length	Quality of chain
3	G	217	
4	H	115	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ALF	B	603	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25072 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	Se	0	0	0
			4320	2718	724	852	3	23			
1	B	593	Total	C	N	O	S	Se	0	0	0
			4370	2732	740	872	3	23			
1	C	579	Total	C	N	O	S	Se	0	0	0
			4220	2604	729	861	3	23			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP A0A1V8WY35
A	-5	SER	-	expression tag	UNP A0A1V8WY35
A	-4	SER	-	expression tag	UNP A0A1V8WY35
A	-3	GLY	-	expression tag	UNP A0A1V8WY35
A	-2	SER	-	expression tag	UNP A0A1V8WY35
A	-1	SER	-	expression tag	UNP A0A1V8WY35
A	0	GLY	-	expression tag	UNP A0A1V8WY35
B	-6	GLY	-	expression tag	UNP A0A1V8WY35
B	-5	SER	-	expression tag	UNP A0A1V8WY35
B	-4	SER	-	expression tag	UNP A0A1V8WY35
B	-3	GLY	-	expression tag	UNP A0A1V8WY35
B	-2	SER	-	expression tag	UNP A0A1V8WY35
B	-1	SER	-	expression tag	UNP A0A1V8WY35
B	0	GLY	-	expression tag	UNP A0A1V8WY35
C	-6	GLY	-	expression tag	UNP A0A1V8WY35
C	-5	SER	-	expression tag	UNP A0A1V8WY35
C	-4	SER	-	expression tag	UNP A0A1V8WY35
C	-3	GLY	-	expression tag	UNP A0A1V8WY35
C	-2	SER	-	expression tag	UNP A0A1V8WY35
C	-1	SER	-	expression tag	UNP A0A1V8WY35
C	0	GLY	-	expression tag	UNP A0A1V8WY35

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	452	Total	C	N	O	Se	0	0	0
			3375	2121	587	653	14			
2	E	452	Total	C	N	O	Se	0	0	0
			3423	2153	587	669	14			
2	F	453	Total	C	N	O	Se	0	0	0
			3445	2181	589	661	14			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP A0A1V8XC32
D	-5	SER	-	expression tag	UNP A0A1V8XC32
D	-4	SER	-	expression tag	UNP A0A1V8XC32
D	-3	GLY	-	expression tag	UNP A0A1V8XC32
D	-2	SER	-	expression tag	UNP A0A1V8XC32
D	-1	SER	-	expression tag	UNP A0A1V8XC32
D	0	GLY	-	expression tag	UNP A0A1V8XC32
E	-6	GLY	-	expression tag	UNP A0A1V8XC32
E	-5	SER	-	expression tag	UNP A0A1V8XC32
E	-4	SER	-	expression tag	UNP A0A1V8XC32
E	-3	GLY	-	expression tag	UNP A0A1V8XC32
E	-2	SER	-	expression tag	UNP A0A1V8XC32
E	-1	SER	-	expression tag	UNP A0A1V8XC32
E	0	GLY	-	expression tag	UNP A0A1V8XC32
F	-6	GLY	-	expression tag	UNP A0A1V8XC32
F	-5	SER	-	expression tag	UNP A0A1V8XC32
F	-4	SER	-	expression tag	UNP A0A1V8XC32
F	-3	GLY	-	expression tag	UNP A0A1V8XC32
F	-2	SER	-	expression tag	UNP A0A1V8XC32
F	-1	SER	-	expression tag	UNP A0A1V8XC32
F	0	GLY	-	expression tag	UNP A0A1V8XC32

- Molecule 3 is a protein called V-type sodium ATPase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	165	Total	C	N	O	S Se	0	0	0
			1207	750	219	230	1 7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	GLY	-	expression tag	UNP A0A7Z9AX30
G	-5	SER	-	expression tag	UNP A0A7Z9AX30

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	SER	-	expression tag	UNP A0A7Z9AX30
G	-3	GLY	-	expression tag	UNP A0A7Z9AX30
G	-2	SER	-	expression tag	UNP A0A7Z9AX30
G	-1	SER	-	expression tag	UNP A0A7Z9AX30
G	0	GLY	-	expression tag	UNP A0A7Z9AX30

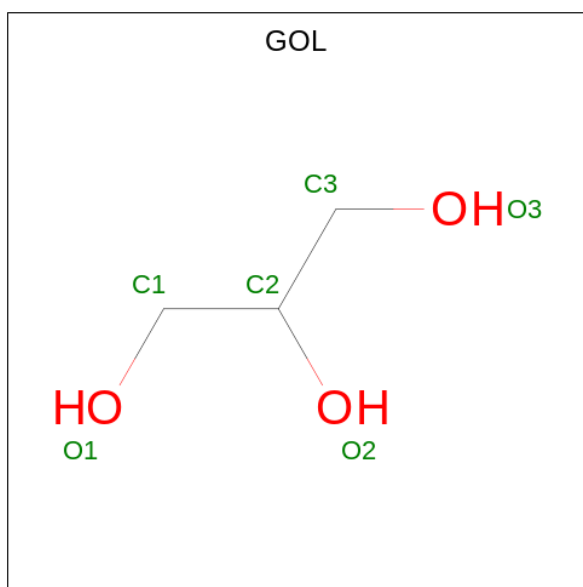
- Molecule 4 is a protein called V-type sodium ATPase subunit NtpG (F).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	H	99	Total	C	N	O	S	Se	0	0	0
			639	402	107	128	1	1			

There are 12 discrepancies between the modelled and reference sequences:

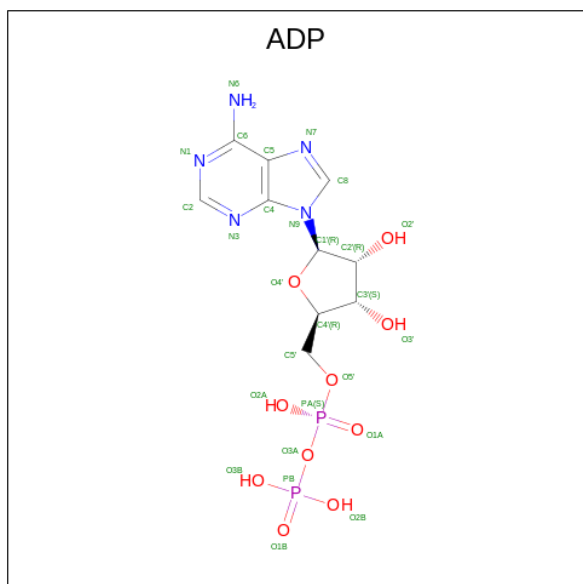
Chain	Residue	Modelled	Actual	Comment	Reference
H	104	SER	-	expression tag	UNP A0A1V8XC17
H	105	GLY	-	expression tag	UNP A0A1V8XC17
H	106	PRO	-	expression tag	UNP A0A1V8XC17
H	107	SER	-	expression tag	UNP A0A1V8XC17
H	108	SER	-	expression tag	UNP A0A1V8XC17
H	109	GLY	-	expression tag	UNP A0A1V8XC17
H	110	GLU	-	expression tag	UNP A0A1V8XC17
H	111	ASN	-	expression tag	UNP A0A1V8XC17
H	112	LEU	-	expression tag	UNP A0A1V8XC17
H	113	TYR	-	expression tag	UNP A0A1V8XC17
H	114	PHE	-	expression tag	UNP A0A1V8XC17
H	115	GLN	-	expression tag	UNP A0A1V8XC17

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

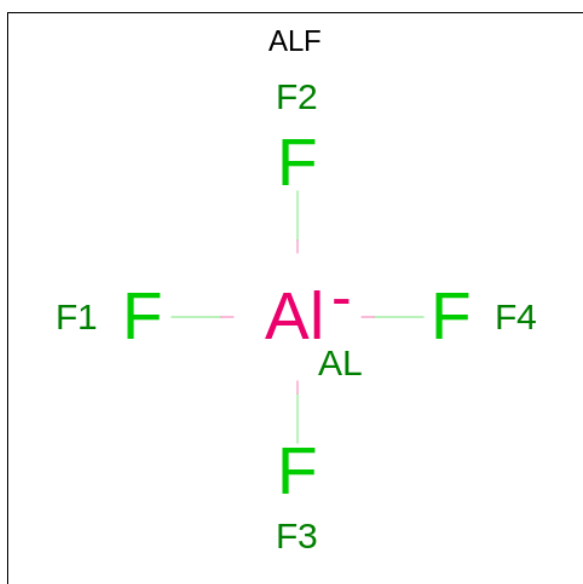


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
6	C	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Al	F	0	0
			5	1	4		
8	C	1	Total	Al	F	0	0
			5	1	4		

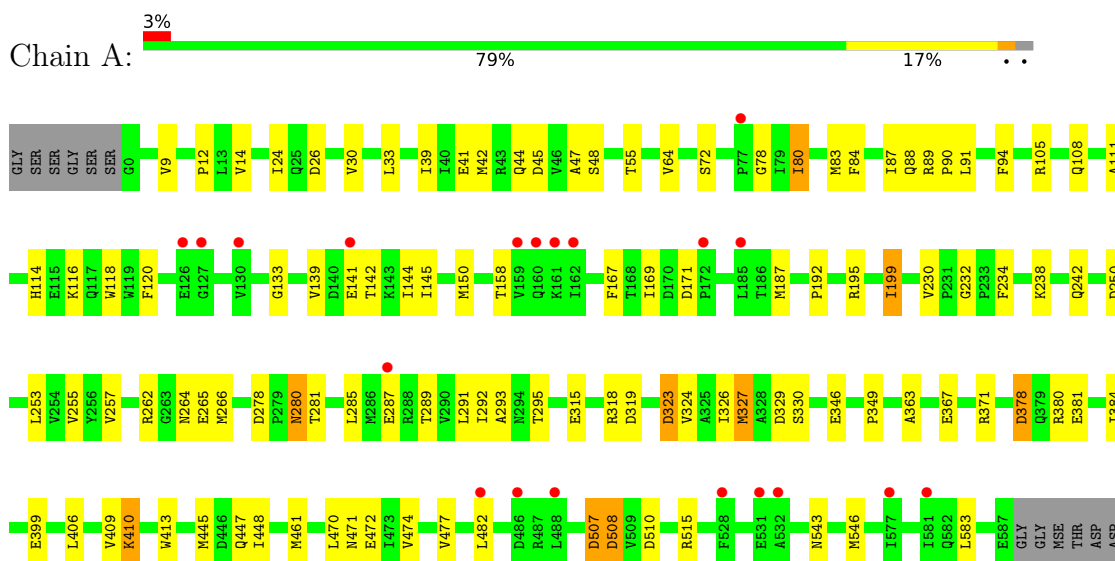
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	O	0	0
			1	1		

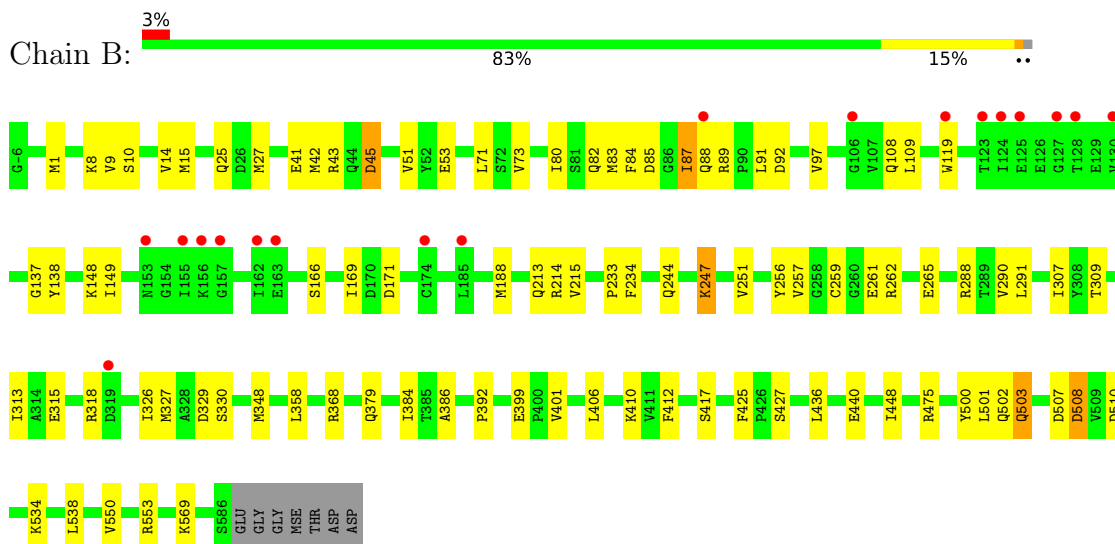
3 Residue-property plots

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.

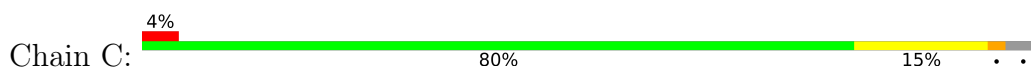
• Molecule 1: V-type sodium ATPase catalytic subunit A

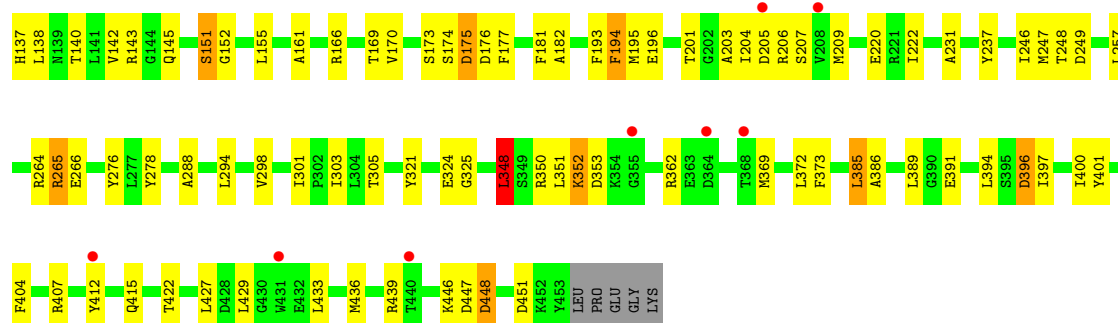


• Molecule 1: V-type sodium ATPase catalytic subunit A

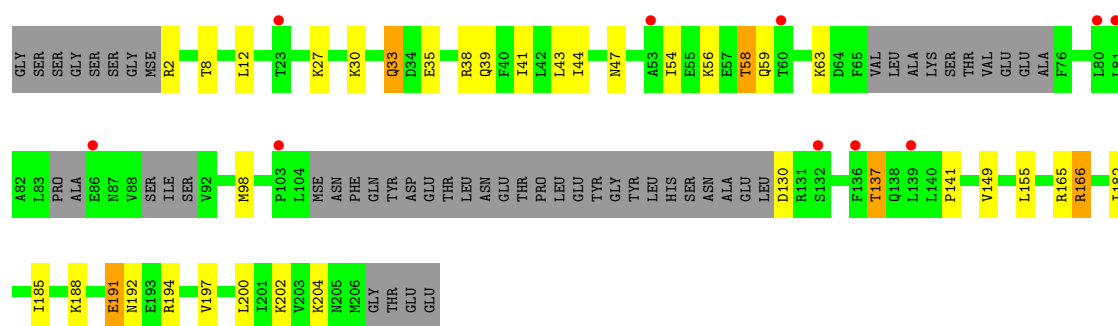


• Molecule 1: V-type sodium ATPase catalytic subunit A

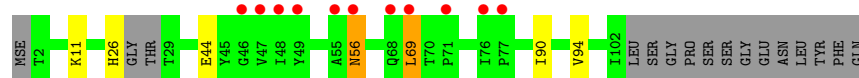
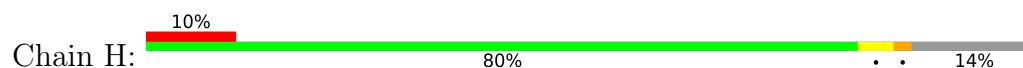




• Molecule 3: V-type sodium ATPase subunit D



• Molecule 4: V-type sodium ATPase subunit NtpG (F)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.74Å 128.87Å 231.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.13 – 3.82 46.13 – 3.82	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.13-3.82) 99.5 (46.13-3.82)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.226 , 0.267 0.226 , 0.267	Depositor DCC
R_{free} test set	1884 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	120.1	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 107.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.048 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25072	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: ALF, GOL, ADP, MG

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	0.24	0/4373	0.42	0/5921
1	B	0.25	0/4422	0.43	0/5974
1	C	0.25	0/4271	0.42	0/5774
2	D	0.25	0/3423	0.43	0/4628
2	E	0.26	0/3472	0.44	0/4693
2	F	0.26	0/3492	0.46	1/4715 (0.0%)
3	G	0.24	0/1204	0.41	0/1612
4	H	0.25	0/645	0.45	0/887
All	All	0.25	0/25302	0.43	1/34204 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	348	LEU	CA-CB-CG	5.09	127.02	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	4320	0	4062	68	0
1	B	4370	0	4075	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4220	0	3737	58	0
2	D	3375	0	3136	50	0
2	E	3423	0	3194	52	0
2	F	3445	0	3355	83	0
3	G	1207	0	1119	23	0
4	H	639	0	539	6	0
5	A	6	0	8	0	0
6	B	27	0	12	2	0
6	C	27	0	12	3	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	5	0	0	3	0
8	C	5	0	0	0	0
9	B	1	0	0	0	0
All	All	25072	0	23249	360	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 (360) 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:42:MSE:HG2	2:E:65:LEU:HD21	1.49	0.93
1:C:509:VAL:HG11	1:C:561:TYR:HA	1.53	0.88
2:F:195:MSE:HA	2:F:195:MSE:HE2	1.57	0.87
2:F:385:LEU:HB3	2:F:394:LEU:HD21	1.65	0.79
1:B:214:ARG:NH1	1:B:510:ASP:OD1	2.16	0.78
2:D:277:LEU:HD23	2:D:318:LEU:HD12	1.66	0.77
2:F:175:ASP:N	2:F:175:ASP:OD1	2.17	0.76
2:F:195:MSE:HE1	2:F:209:MSE:SE	2.35	0.76
3:G:54:ILE:O	3:G:58:THR:OG1	2.04	0.76
2:F:448:ASP:OD1	2:F:448:ASP:N	2.15	0.76
2:E:124:PRO:HG2	2:E:351:LEU:HD13	1.67	0.75
2:F:176:ASP:HB2	2:F:206:ARG:NH1	2.03	0.73
1:A:278:ASP:OD2	1:A:280:ASN:ND2	2.21	0.72
1:B:503:GLN:NE2	1:B:510:ASP:O	2.22	0.72
2:F:140:THR:HB	2:F:352:LYS:HB2	1.70	0.71
1:C:478:GLY:HA3	3:G:166:ARG:HH12	1.55	0.71
2:D:32:VAL:HG22	2:D:70:VAL:HG22	1.73	0.71
2:D:386:ALA:HB2	2:D:394:LEU:HD11	1.73	0.71
1:C:561:TYR:HE1	2:F:446:LYS:HE3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.74	0.68
1:C:208:PRO:HA	1:C:223:THR:HA	1.75	0.68
1:B:80:ILE:HA	1:B:290:VAL:HG22	1.76	0.68
3:G:47:ASN:HD22	3:G:149:VAL:HG12	1.59	0.67
1:A:378:ASP:OD1	1:A:378:ASP:N	2.27	0.67
2:E:7:THR:OG1	2:E:19:GLU:O	2.13	0.66
1:B:358:LEU:HD21	1:B:401:VAL:HG12	1.79	0.65
1:C:41:GLU:HG3	1:C:48:SER:HB2	1.79	0.64
2:D:8:ILE:HG22	2:D:65:LEU:HD13	1.78	0.64
1:A:266:MSE:HE2	1:A:293:ALA:HA	1.79	0.64
2:D:356:THR:HB	2:D:365:HIS:CG	2.33	0.64
2:E:112:ASN:O	2:E:287:ARG:NH1	2.30	0.64
1:C:249:SER:O	1:C:288:ARG:NH2	2.31	0.64
1:C:201:GLN:HB3	1:C:373:ILE:HD12	1.80	0.64
2:D:376:TYR:OH	2:D:409:GLU:OE2	2.13	0.63
2:F:325:GLY:H	2:F:350:ARG:HE	1.44	0.63
3:G:137:THR:O	3:G:141:PRO:HD2	1.97	0.63
1:B:87:ILE:HG13	1:B:89:ARG:HG3	1.81	0.63
2:F:142:VAL:HG22	2:F:145:GLN:HB2	1.79	0.63
2:F:173:SER:HB3	2:F:175:ASP:OD1	1.98	0.63
1:C:20:SER:HB2	2:D:66:LYS:HE3	1.80	0.62
1:A:255:VAL:HB	1:A:326:ILE:HG13	1.81	0.62
2:E:356:THR:HA	2:E:361:THR:OG1	2.00	0.62
1:A:118:TRP:HB3	1:A:139:VAL:HG11	1.82	0.62
2:E:364:ASP:OD2	2:E:431:TRP:NE1	2.32	0.62
1:C:42:MSE:HG2	2:D:65:LEU:HG	1.82	0.61
1:A:280:ASN:HD22	1:A:281:THR:N	1.98	0.61
1:A:371:ARG:NH1	1:A:381:GLU:OE2	2.33	0.61
2:D:88:ARG:HG3	2:D:103:ILE:HD11	1.83	0.61
2:D:267:VAL:HG23	3:G:204:LYS:HD2	1.81	0.61
1:A:42:MSE:SE	1:A:47:ALA:HB2	2.51	0.61
2:F:389:LEU:HD22	3:G:166:ARG:HD2	1.82	0.61
3:G:44:ILE:HD11	4:H:90:ILE:HG23	1.83	0.60
1:A:12:PRO:HA	1:A:55:THR:HG21	1.83	0.60
1:A:9:VAL:HG22	1:A:14:VAL:HG22	1.83	0.60
1:A:133:GLY:O	1:A:380:ARG:NH2	2.34	0.60
2:E:44:VAL:HA	2:E:54:VAL:HG12	1.84	0.59
2:E:57:PHE:HA	2:E:219:ILE:HD12	1.85	0.59
2:E:106:GLU:OE1	2:E:234:TYR:OH	2.19	0.59
2:E:229:LEU:HD13	2:E:287:ARG:HG3	1.84	0.59
1:A:150:MSE:HE1	1:A:319:ASP:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:170:VAL:HG13	2:F:173:SER:HB2	1.84	0.59
1:B:41:GLU:OE1	1:B:43:ARG:NH2	2.35	0.58
1:A:192:PRO:HG2	1:A:195:ARG:HG2	1.84	0.58
1:C:214:ARG:HD3	1:C:521:MSE:HE1	1.85	0.58
2:F:176:ASP:HB2	2:F:206:ARG:HH11	1.67	0.58
3:G:59:GLN:O	3:G:63:LYS:N	2.33	0.58
1:B:85:ASP:OD1	1:B:89:ARG:N	2.29	0.58
1:B:425:PHE:HB3	6:B:601:ADP:C6	2.39	0.58
1:C:349:PRO:HB2	1:C:353:GLY:HA2	1.85	0.58
2:D:248:THR:HB	2:D:303:ILE:HB	1.86	0.58
1:C:421:GLN:O	1:C:423:ARG:NH1	2.37	0.58
1:A:232:GLY:HA3	1:A:238:LYS:HD3	1.86	0.57
1:B:215:VAL:HG23	1:B:501:LEU:HD22	1.84	0.57
1:C:498:GLU:HA	1:C:502:GLN:HE21	1.69	0.57
2:F:91:ASP:OD1	2:F:95:ARG:N	2.37	0.57
1:C:479:ILE:HD13	1:C:479:ILE:H	1.69	0.57
2:F:195:MSE:HA	2:F:195:MSE:CE	2.33	0.57
2:F:161:ALA:HB3	2:F:194:PHE:HZ	1.69	0.57
3:G:41:ILE:HA	3:G:44:ILE:HG22	1.87	0.57
1:C:262:ARG:NH2	1:C:265:GLU:OE2	2.33	0.57
2:E:182:ALA:HB3	2:E:247:MSE:HG2	1.87	0.56
1:A:280:ASN:HD22	1:A:281:THR:H	1.53	0.56
1:C:561:TYR:CE1	2:F:446:LYS:HE3	2.37	0.56
1:A:78:GLY:N	1:A:141:GLU:OE2	2.39	0.56
1:B:45:ASP:OD1	1:B:45:ASP:N	2.35	0.56
1:C:375:LEU:O	1:C:380:ARG:NH2	2.38	0.55
1:C:41:GLU:HB3	2:D:12:VAL:HA	1.88	0.55
2:E:145:GLN:HG3	2:E:351:LEU:HD12	1.88	0.55
1:C:81:SER:HA	1:C:286:MSE:HE2	1.89	0.55
2:E:248:THR:HB	2:E:303:ILE:HB	1.86	0.55
1:B:213:GLN:HA	1:B:503:GLN:OE1	2.06	0.55
2:D:288:ALA:HA	2:D:298:VAL:HB	1.87	0.55
1:C:236:ALA:O	1:C:427:SER:OG	2.24	0.55
1:B:259:CYS:N	1:B:329:ASP:O	2.40	0.55
2:E:122:ASP:HA	2:E:292:ARG:NH1	2.22	0.55
1:A:349:PRO:HG3	3:G:197:VAL:HG11	1.88	0.54
1:B:8:LYS:HD3	1:B:15:MSE:HE2	1.89	0.54
2:E:384:GLU:O	2:E:388:VAL:HG22	2.07	0.54
2:F:124:PRO:HB3	2:F:143:ARG:O	2.07	0.54
2:F:129:GLN:NE2	2:F:422:THR:HA	2.22	0.54
1:A:116:LYS:HD3	1:A:118:TRP:CZ2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:GLU:HG3	2:F:276:TYR:HB3	1.89	0.54
2:F:166:ARG:HG3	2:F:201:THR:HG23	1.89	0.54
1:C:233:PRO:HG3	1:C:417:SER:HB2	1.89	0.54
2:F:325:GLY:N	2:F:350:ARG:HE	2.05	0.54
1:A:507:ASP:OD1	1:A:510:ASP:N	2.28	0.54
2:F:134:ALA:HA	2:F:138:LEU:HD12	1.89	0.54
2:F:246:ILE:HG12	2:F:301:ILE:HB	1.89	0.54
1:A:230:VAL:HG22	1:A:413:TRP:HB2	1.90	0.54
2:D:11:VAL:HG22	2:D:16:MSE:HB2	1.90	0.53
2:E:151:SER:HB2	2:E:329:LEU:HD12	1.90	0.53
3:G:44:ILE:HG12	4:H:94:VAL:HG22	1.89	0.53
1:C:517:LYS:HG2	1:C:521:MSE:HE2	1.91	0.53
1:A:118:TRP:HB2	1:A:187:MSE:HE1	1.91	0.53
1:A:323:ASP:OD1	1:A:323:ASP:N	2.41	0.53
2:D:150:PHE:N	2:D:327:ILE:O	2.41	0.52
2:E:176:ASP:OD1	2:E:176:ASP:N	2.41	0.52
2:F:126:GLU:O	2:F:142:VAL:HB	2.08	0.52
1:B:119:TRP:HA	1:B:166:SER:HA	1.91	0.52
2:D:44:VAL:HA	2:D:54:VAL:HG12	1.92	0.52
2:D:163:GLN:HA	2:D:166:ARG:NH2	2.24	0.52
1:A:257:VAL:HA	1:A:292:ILE:HB	1.90	0.52
1:A:142:THR:HG23	1:A:144:ILE:H	1.74	0.52
2:D:233:GLU:HG2	2:D:237:TYR:CD2	2.45	0.52
2:D:30:ILE:HG21	2:D:54:VAL:HG11	1.92	0.52
2:E:7:THR:OG1	2:E:7:THR:O	2.27	0.52
3:G:155:LEU:HD13	4:H:69:LEU:HD12	1.92	0.52
2:E:360:LYS:O	2:E:361:THR:HG23	2.09	0.52
1:A:242:GLN:NE2	1:A:329:ASP:OD2	2.42	0.51
1:B:51:VAL:HG12	1:B:53:GLU:H	1.75	0.51
1:C:478:GLY:HA3	3:G:166:ARG:NH1	2.24	0.51
1:A:471:ASN:OD1	1:A:472:GLU:N	2.42	0.51
1:C:102:PHE:HB3	2:F:114:GLU:HB3	1.91	0.51
2:E:454:LEU:HD12	2:E:455:PRO:HD2	1.92	0.51
2:F:396:ASP:OD1	2:F:396:ASP:N	2.42	0.51
1:C:51:VAL:HG12	1:C:53:GLU:H	1.75	0.51
1:B:534:LYS:O	1:B:538:LEU:HG	2.11	0.51
2:F:386:ALA:HB2	2:F:394:LEU:HD11	1.93	0.51
1:A:83:MSE:HG2	1:A:291:LEU:HB3	1.93	0.51
1:B:318:ARG:HD3	1:B:384:ILE:HG13	1.93	0.50
1:A:72:SER:HA	1:A:192:PRO:HA	1.93	0.50
1:B:42:MSE:HG2	2:F:65:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:MSE:HB2	2:D:304:LEU:HB3	1.93	0.50
2:E:16:MSE:SE	2:E:56:ILE:HD11	2.61	0.50
2:E:126:GLU:O	2:E:355:GLY:HA2	2.11	0.50
2:E:272:GLY:HA2	3:G:194:ARG:HD3	1.93	0.50
1:B:550:VAL:HG22	1:B:553:ARG:NH2	2.27	0.50
6:B:601:ADP:O1B	8:B:603:ALF:F3	2.20	0.50
1:A:406:LEU:HA	1:A:409:VAL:HG22	1.92	0.50
1:B:508:ASP:N	1:B:508:ASP:OD1	2.44	0.50
1:A:142:THR:HG21	1:A:287:GLU:O	2.12	0.49
1:A:262:ARG:HB2	1:A:265:GLU:HB2	1.93	0.49
2:E:151:SER:OG	2:E:152:GLY:N	2.44	0.49
1:B:88:GLN:HE21	1:B:313:ILE:HD11	1.77	0.49
2:F:93:LEU:HD21	2:F:220:GLU:HB2	1.94	0.49
2:F:137:HIS:CD2	2:F:427:LEU:HD23	2.47	0.49
3:G:188:LYS:O	3:G:192:ASN:ND2	2.43	0.49
1:A:474:VAL:HG22	1:A:482:LEU:HD11	1.95	0.49
2:F:369:MSE:HG2	2:F:373:PHE:HE2	1.76	0.49
2:E:126:GLU:HA	2:E:360:LYS:HB3	1.95	0.49
2:F:44:VAL:HA	2:F:54:VAL:HG12	1.95	0.49
3:G:47:ASN:ND2	3:G:149:VAL:HG12	2.26	0.49
1:C:391:SER:HB3	2:F:321:TYR:CE1	2.48	0.48
2:E:122:ASP:HA	2:E:292:ARG:HH11	1.77	0.48
1:B:73:VAL:HG11	1:B:309:THR:HG23	1.96	0.48
2:E:91:ASP:OD1	2:E:95:ARG:N	2.39	0.48
1:B:410:LYS:HB3	1:B:436:LEU:HB2	1.95	0.48
1:B:392:PRO:O	2:E:321:TYR:OH	2.22	0.48
2:E:123:TYR:CD2	2:E:124:PRO:HD2	2.49	0.48
2:E:129:GLN:O	2:E:168:ALA:HA	2.13	0.48
2:F:145:GLN:HG3	2:F:351:LEU:HD12	1.94	0.48
1:C:558:ARG:NH2	2:F:447:ASP:OD1	2.46	0.48
1:A:445:MSE:HA	1:A:448:ILE:HG22	1.96	0.48
2:F:142:VAL:CG2	2:F:145:GLN:HB2	2.44	0.48
2:E:132:ILE:HA	2:E:415:GLN:HE22	1.79	0.48
2:F:372:LEU:HD13	2:F:412:TYR:HE1	1.79	0.48
1:A:87:ILE:HG13	1:A:89:ARG:HG3	1.96	0.48
1:B:244:GLN:HA	1:B:247:LYS:HD3	1.95	0.48
1:B:97:VAL:HG21	1:B:109:LEU:HD21	1.96	0.48
1:A:41:GLU:HG2	1:A:48:SER:HB2	1.96	0.47
2:E:184:ILE:HG21	2:E:253:TYR:HB2	1.95	0.47
2:F:33:ARG:HG3	2:F:39:ILE:CD1	2.45	0.47
2:F:132:ILE:HA	2:F:415:GLN:HE22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:151:SER:O	2:F:305:THR:HA	2.14	0.47
1:A:474:VAL:HG22	1:A:482:LEU:HD21	1.96	0.47
1:B:348:MSE:HE1	3:G:202:LYS:HD3	1.96	0.47
1:A:410:LYS:HE3	1:A:410:LYS:HB3	1.54	0.47
2:F:264:ARG:O	2:F:265:ARG:HG2	2.15	0.47
2:E:356:THR:HA	2:E:361:THR:HG1	1.79	0.47
2:D:166:ARG:NH1	2:D:197:ASP:OD2	2.48	0.47
2:D:324:GLU:HB3	2:D:350:ARG:HB2	1.97	0.47
2:E:113:GLY:HA3	2:E:287:ARG:HH12	1.80	0.47
1:C:38:GLU:O	1:C:50:GLN:N	2.47	0.47
2:D:307:PRO:O	2:D:308:GLU:HG2	2.15	0.47
2:F:161:ALA:HB2	2:F:303:ILE:HD11	1.97	0.46
1:A:33:LEU:HD21	1:A:105:ARG:HB2	1.98	0.46
1:B:326:ILE:HG23	1:B:386:ALA:HA	1.96	0.46
2:F:182:ALA:HB3	2:F:247:MSE:HG2	1.96	0.46
1:A:30:VAL:HA	1:A:64:VAL:HG22	1.96	0.46
2:E:131:GLY:O	2:E:415:GLN:NE2	2.44	0.46
1:C:333:ARG:HD2	2:F:278:TYR:CE1	2.50	0.46
2:E:13:GLY:O	2:E:60:THR:OG1	2.24	0.46
1:A:167:PHE:HB3	1:A:171:ASP:HB2	1.98	0.46
1:C:425:PHE:HB3	6:C:601:ADP:C6	2.50	0.46
2:D:145:GLN:HG3	2:D:351:LEU:HD12	1.97	0.46
1:B:256:TYR:HA	1:B:327:MSE:HB2	1.97	0.46
2:F:34:MSE:SE	2:F:63:ILE:HG12	2.66	0.46
1:B:92:ASP:OD1	1:B:92:ASP:N	2.47	0.45
2:F:40:ARG:HH12	2:F:61:SER:H	1.62	0.45
1:C:167:PHE:HB3	1:C:171:ASP:HB2	1.98	0.45
1:B:137:GLY:O	1:B:149:ILE:N	2.50	0.45
2:F:237:TYR:HB3	2:F:294:LEU:HD13	1.99	0.45
1:C:378:ASP:HB2	1:C:380:ARG:HH11	1.81	0.45
2:E:250:MSE:HB2	2:E:304:LEU:HB3	1.98	0.45
2:D:268:PRO:HD2	3:G:200:LEU:HD13	1.99	0.45
2:D:137:HIS:ND1	2:D:412:TYR:OH	2.45	0.45
1:C:471:ASN:HA	1:C:474:VAL:HG12	1.98	0.45
1:C:558:ARG:HH12	2:F:446:LYS:HA	1.82	0.45
2:D:44:VAL:HG11	2:D:47:VAL:CG2	2.47	0.45
6:C:601:ADP:H4'	2:F:348:LEU:HD11	1.98	0.45
2:E:249:ASP:OD1	2:E:250:MSE:N	2.50	0.45
2:E:370:ASN:HB3	2:E:444:ARG:HD3	1.98	0.45
1:A:84:PHE:HB3	1:A:88:GLN:HA	1.98	0.45
1:C:555:ARG:NH2	1:C:572:SER:OG	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:433:LEU:HA	2:F:436:MSE:HE3	1.99	0.45
1:B:251:VAL:HG23	1:B:288:ARG:HH12	1.82	0.44
2:E:126:GLU:O	2:E:142:VAL:HG13	2.16	0.44
1:A:90:PRO:HD3	1:A:111:ALA:HA	1.99	0.44
1:B:83:MSE:HG3	1:B:91:LEU:HD12	1.99	0.44
2:F:248:THR:HB	2:F:303:ILE:HB	1.99	0.44
3:G:30:LYS:HA	3:G:33:GLN:HB3	1.99	0.44
1:C:332:SER:HG	1:C:391:SER:H	1.60	0.44
1:A:26:ASP:HB2	1:A:39:ILE:HD12	2.00	0.44
1:A:250:ASP:OD1	1:A:250:ASP:N	2.49	0.44
2:E:130:THR:O	2:E:132:ILE:HD12	2.18	0.44
2:F:8:ILE:HD13	2:F:18:VAL:HG22	2.00	0.44
2:D:324:GLU:HA	2:D:350:ARG:HD2	2.00	0.44
4:H:11:LYS:HA	4:H:26:HIS:CE1	2.53	0.44
2:F:369:MSE:HG2	2:F:373:PHE:CE2	2.52	0.44
1:A:295:THR:HG23	2:D:118:PRO:HB3	2.00	0.44
2:F:151:SER:OG	2:F:152:GLY:N	2.51	0.44
1:B:257:VAL:HG11	1:B:307:ILE:HD13	1.99	0.44
2:F:79:LEU:HD21	2:F:231:ALA:HB2	2.00	0.44
1:A:508:ASP:OD1	1:A:508:ASP:N	2.50	0.44
2:F:138:LEU:HB3	2:F:373:PHE:CZ	2.53	0.44
1:C:351:ASP:HB2	1:C:400:PRO:HG3	2.00	0.43
1:A:329:ASP:HA	1:A:330:SER:HA	1.57	0.43
1:B:214:ARG:HD2	1:B:500:TYR:CE1	2.53	0.43
2:F:194:PHE:HD1	2:F:194:PHE:HA	1.69	0.43
1:A:324:VAL:O	1:A:384:ILE:HA	2.18	0.43
2:D:91:ASP:OD1	2:D:95:ARG:N	2.51	0.43
2:F:352:LYS:HG2	2:F:353:ASP:N	2.33	0.43
2:F:396:ASP:O	2:F:400:ILE:HG12	2.18	0.43
1:A:42:MSE:HE3	2:E:65:LEU:HD11	1.99	0.43
2:F:288:ALA:HA	2:F:298:VAL:HB	2.00	0.43
1:B:233:PRO:HG3	1:B:417:SER:HB2	1.99	0.43
1:B:315:GLU:OE2	1:B:368:ARG:HB3	2.19	0.43
1:C:262:ARG:NE	2:F:324:GLU:HG3	2.34	0.43
2:E:186:ILE:O	2:E:214:ALA:N	2.52	0.43
1:C:24:ILE:HG22	1:C:25:GLN:HG2	2.00	0.43
1:C:371:ARG:NH1	1:C:381:GLU:OE2	2.48	0.43
1:B:27:MSE:SE	1:B:71:LEU:HA	2.69	0.43
2:D:137:HIS:HA	2:D:365:HIS:HE2	1.84	0.43
2:F:40:ARG:NH1	2:F:61:SER:H	2.16	0.43
2:F:174:SER:O	2:F:174:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:TYR:HA	1:B:148:LYS:HA	2.00	0.42
1:B:9:VAL:HG22	1:B:14:VAL:HG22	2.01	0.42
1:B:214:ARG:NH2	1:B:502:GLN:O	2.52	0.42
2:F:45:LEU:HD13	2:F:264:ARG:HD2	2.01	0.42
1:A:114:HIS:HA	1:A:169:ILE:HG12	2.01	0.42
1:A:234:PHE:CE1	2:D:350:ARG:HA	2.54	0.42
1:C:329:ASP:HA	1:C:330:SER:HA	1.66	0.42
1:B:1:MSE:HE2	1:B:1:MSE:HB2	1.88	0.42
2:F:140:THR:HB	2:F:352:LYS:CB	2.46	0.42
2:F:195:MSE:CE	2:F:209:MSE:SE	3.14	0.42
2:F:222:ILE:HG12	2:F:257:LEU:HD12	2.01	0.42
1:A:120:PHE:HA	1:A:139:VAL:HG22	2.01	0.42
1:C:218:THR:HG23	1:C:453:TRP:CZ2	2.53	0.42
1:C:453:TRP:HZ3	1:C:519:PHE:HA	1.85	0.42
2:D:233:GLU:HG2	2:D:237:TYR:HD2	1.84	0.42
2:F:152:GLY:H	2:F:155:LEU:HD12	1.84	0.42
3:G:35:GLU:OE2	3:G:98:MSE:HE1	2.20	0.42
4:H:56:ASN:O	4:H:56:ASN:ND2	2.44	0.42
1:B:262:ARG:HB2	1:B:265:GLU:HG3	2.01	0.42
2:D:162:ALA:O	2:D:166:ARG:NH1	2.51	0.42
2:D:407:ARG:HD3	2:D:436:MSE:SE	2.69	0.42
2:E:34:MSE:HE3	2:E:38:GLU:HB3	2.01	0.42
1:A:234:PHE:CD2	2:D:348:LEU:HD13	2.54	0.42
1:B:410:LYS:HG2	1:B:436:LEU:HD12	2.01	0.42
1:C:41:GLU:OE1	2:D:12:VAL:HG13	2.20	0.42
1:C:213:GLN:HA	1:C:503:GLN:HE22	1.85	0.42
1:B:329:ASP:HA	1:B:330:SER:HA	1.80	0.42
2:E:447:ASP:OD1	2:E:447:ASP:N	2.48	0.42
3:G:191:GLU:HG3	3:G:192:ASN:N	2.34	0.42
1:A:142:THR:CG2	1:A:145:ILE:H	2.33	0.42
1:C:92:ASP:OD1	1:C:92:ASP:N	2.53	0.42
1:C:453:TRP:HA	1:C:456:MSE:SE	2.70	0.42
1:B:108:GLN:H	1:B:108:GLN:CD	2.21	0.42
1:C:524:VAL:HG11	1:C:556:ILE:HG12	2.02	0.42
2:D:110:ASP:N	2:D:110:ASP:OD1	2.51	0.42
2:D:288:ALA:HB2	2:D:300:GLN:HG3	2.02	0.42
2:F:125:ASP:OD1	2:F:125:ASP:N	2.53	0.42
2:F:181:PHE:HB3	2:F:209:MSE:HG2	2.02	0.42
2:F:407:ARG:HD3	2:F:436:MSE:HE1	2.02	0.42
1:A:80:ILE:HG13	1:A:141:GLU:CD	2.40	0.41
1:B:261:GLU:HG2	1:B:329:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:TYR:O	2:F:404:PHE:HB3	2.20	0.41
1:A:242:GLN:O	1:A:327:MSE:HE1	2.20	0.41
1:A:363:ALA:O	1:A:367:GLU:HB2	2.20	0.41
1:C:240:VAL:HG21	6:C:601:ADP:C8	2.55	0.41
2:D:89:VAL:HG22	2:D:209:MSE:HB2	2.02	0.41
2:D:232:ALA:HB1	2:D:243:VAL:HG11	2.02	0.41
2:F:248:THR:HA	2:F:249:ASP:HA	1.77	0.41
1:B:262:ARG:NH2	8:B:603:ALF:F3	2.43	0.41
2:D:11:VAL:HG22	2:D:16:MSE:CB	2.50	0.41
2:D:127:PHE:HD2	2:D:171:LEU:HD23	1.86	0.41
1:A:118:TRP:CH2	1:A:141:GLU:HG3	2.56	0.41
1:A:199:ILE:H	1:A:199:ILE:HD13	1.85	0.41
1:A:315:GLU:HA	1:A:384:ILE:HD11	2.03	0.41
1:A:24:ILE:HG12	2:E:63:ILE:O	2.21	0.41
1:A:264:ASN:ND2	2:D:145:GLN:HA	2.36	0.41
2:F:129:GLN:HE21	2:F:422:THR:HA	1.85	0.41
2:F:133:SER:HB3	2:F:412:TYR:HE2	1.85	0.41
1:B:234:PHE:HA	8:B:603:ALF:F1	2.11	0.41
1:B:315:GLU:HA	1:B:384:ILE:HD11	2.03	0.41
1:A:477:VAL:HG22	3:G:38:ARG:HH12	1.85	0.41
2:D:44:VAL:HG11	2:D:47:VAL:HG22	2.01	0.41
1:A:44:GLN:HB3	1:A:45:ASP:H	1.77	0.41
1:C:90:PRO:HD3	1:C:111:ALA:HA	2.02	0.41
1:C:287:GLU:H	1:C:287:GLU:HG2	1.49	0.41
1:C:430:TRP:O	1:C:461:MSE:HE1	2.21	0.41
1:C:463:ILE:HG21	1:C:492:VAL:HG12	2.02	0.41
1:C:550:VAL:HG12	1:C:553:ARG:HH22	1.86	0.41
2:D:28:GLU:H	2:D:44:VAL:HB	1.86	0.41
2:E:56:ILE:HD13	2:E:60:THR:HG22	2.03	0.41
2:E:221:ARG:HE	2:E:256:ALA:HB2	1.85	0.41
2:E:248:THR:HA	2:E:249:ASP:HA	1.75	0.41
2:F:439:ARG:NH2	2:F:451:ASP:OD1	2.53	0.41
1:A:470:LEU:O	1:A:474:VAL:HG23	2.21	0.41
1:C:412:PHE:CD2	1:C:433:SER:HA	2.56	0.41
2:D:354:LYS:HD2	2:D:354:LYS:HA	1.90	0.41
2:E:339:GLN:HA	2:E:340:PRO:HA	1.93	0.41
2:F:203:ALA:CB	2:F:206:ARG:HH21	2.33	0.41
2:D:84:ASP:N	2:D:84:ASP:OD1	2.54	0.40
2:D:182:ALA:HB3	2:D:247:MSE:HG2	2.02	0.40
2:E:251:THR:O	2:E:255:GLU:HG2	2.22	0.40
2:D:394:LEU:HD22	2:D:398:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:130:THR:H	2:E:130:THR:HG1	1.65	0.40
2:F:28:GLU:OE2	2:F:72:PHE:HB3	2.21	0.40
2:F:264:ARG:NH1	2:F:266:GLU:OE2	2.54	0.40
1:A:445:MSE:HE1	1:A:515:ARG:HG3	2.02	0.40
1:B:169:ILE:HB	1:B:188:MSE:HB2	2.04	0.40
1:B:406:LEU:HD21	1:B:412:PHE:CD1	2.57	0.40
1:C:140:ASP:N	1:C:140:ASP:OD1	2.55	0.40
3:G:12:LEU:HB2	3:G:185:ILE:HG21	2.02	0.40
4:H:90:ILE:O	4:H:94:VAL:HG23	2.20	0.40
1:A:318:ARG:HD3	1:A:384:ILE:HG13	2.02	0.40
1:C:470:LEU:O	1:C:474:VAL:HB	2.21	0.40
2:F:369:MSE:HE2	2:F:369:MSE:HB3	1.96	0.40
2:F:385:LEU:HD23	2:F:385:LEU:HA	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	586/600 (98%)	568 (97%)	18 (3%)	0	100	100
1	B	591/600 (98%)	575 (97%)	16 (3%)	0	100	100
1	C	577/600 (96%)	560 (97%)	17 (3%)	0	100	100
2	D	450/465 (97%)	438 (97%)	12 (3%)	0	100	100
2	E	450/465 (97%)	438 (97%)	12 (3%)	0	100	100
2	F	451/465 (97%)	441 (98%)	10 (2%)	0	100	100
3	G	155/217 (71%)	153 (99%)	2 (1%)	0	100	100
4	H	95/115 (83%)	89 (94%)	6 (6%)	0	100	100
All	All	3355/3527 (95%)	3262 (97%)	93 (3%)	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	437/487 (90%)	414 (95%)	23 (5%)	22	54
1	B	437/487 (90%)	419 (96%)	18 (4%)	30	59
1	C	394/487 (81%)	366 (93%)	28 (7%)	14	45
2	D	313/372 (84%)	299 (96%)	14 (4%)	27	57
2	E	324/372 (87%)	307 (95%)	17 (5%)	23	54
2	F	349/372 (94%)	326 (93%)	23 (7%)	16	47
3	G	111/188 (59%)	97 (87%)	14 (13%)	4	23
4	H	53/97 (55%)	50 (94%)	3 (6%)	20	52
All	All	2418/2862 (84%)	2278 (94%)	140 (6%)	20	51

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	91	LEU
1	A	94	PHE
1	A	108	GLN
1	A	158	THR
1	A	199	ILE
1	A	253	LEU
1	A	280	ASN
1	A	285	LEU
1	A	289	THR
1	A	323	ASP
1	A	327	MSE
1	A	346	GLU
1	A	378	ASP
1	A	399	GLU
1	A	410	LYS

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Mol	Chain	Res	Type
1	A	447	GLN
1	A	461	MSE
1	A	507	ASP
1	A	508	ASP
1	A	543	ASN
1	A	546	MSE
1	A	583	LEU
1	B	10	SER
1	B	25	GLN
1	B	45	ASP
1	B	82	GLN
1	B	87	ILE
1	B	171	ASP
1	B	247	LYS
1	B	291	LEU
1	B	379	GLN
1	B	399	GLU
1	B	427	SER
1	B	440	GLU
1	B	448	ILE
1	B	475	ARG
1	B	503	GLN
1	B	507	ASP
1	B	508	ASP
1	B	569	LYS
1	C	41	GLU
1	C	108	GLN
1	C	140	ASP
1	C	265	GLU
1	C	267	THR
1	C	287	GLU
1	C	288	ARG
1	C	304	GLU
1	C	318	ARG
1	C	452	ASP
1	C	471	ASN
1	C	473	ILE
1	C	474	VAL
1	C	475	ARG
1	C	476	LEU
1	C	479	ILE
1	C	487	ARG

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Mol	Chain	Res	Type
1	C	489	THR
1	C	503	GLN
1	C	507	ASP
1	C	509	VAL
1	C	511	THR
1	C	522	LEU
1	C	541	TYR
1	C	544	GLU
1	C	545	ILE
1	C	546	MSE
1	C	558	ARG
2	D	27	GLU
2	D	41	ARG
2	D	65	LEU
2	D	71	ARG
2	D	95	ARG
2	D	175	ASP
2	D	177	PHE
2	D	238	GLU
2	D	248	THR
2	D	250	MSE
2	D	276	TYR
2	D	348	LEU
2	D	444	ARG
2	D	449	LEU
2	E	6	ARG
2	E	65	LEU
2	E	126	GLU
2	E	127	PHE
2	E	173	SER
2	E	174	SER
2	E	176	ASP
2	E	193	PHE
2	E	345	LEU
2	E	360	LYS
2	E	361	THR
2	E	362	ARG
2	E	380	LYS
2	E	384	GLU
2	E	387	VAL
2	E	396	ASP
2	E	447	ASP

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Mol	Chain	Res	Type
2	F	47	VAL
2	F	97	LYS
2	F	125	ASP
2	F	151	SER
2	F	169	THR
2	F	175	ASP
2	F	177	PHE
2	F	193	PHE
2	F	194	PHE
2	F	196	GLU
2	F	204	ILE
2	F	205	ASP
2	F	207	SER
2	F	265	ARG
2	F	348	LEU
2	F	352	LYS
2	F	362	ARG
2	F	385	LEU
2	F	391	GLU
2	F	396	ASP
2	F	397	ILE
2	F	429	LEU
2	F	448	ASP
3	G	2	ARG
3	G	8	THR
3	G	27	LYS
3	G	33	GLN
3	G	39	GLN
3	G	43	LEU
3	G	56	LYS
3	G	58	THR
3	G	130	ASP
3	G	137	THR
3	G	165	ARG
3	G	166	ARG
3	G	182	ILE
3	G	191	GLU
4	H	44	GLU
4	H	56	ASN
4	H	69	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	280	ASN
2	F	129	GLN
3	G	47	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
6	ADP	B	601	7	24,29,29	0.97	1 (4%)	29,45,45	1.48	5 (17%)
8	ALF	B	603	-	0,4,4	-	-	-		
5	GOL	A	601	-	5,5,5	0.89	0	5,5,5	1.13	0
8	ALF	C	603	-	0,4,4	-	-	-		
6	ADP	C	601	7	24,29,29	0.97	1 (4%)	29,45,45	1.39	4 (13%)

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
6	ADP	B	601	7	-	3/12/32/32	0/3/3/3
5	GOL	A	601	-	-	0/4/4/4	-
6	ADP	C	601	7	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	ADP	C5-C4	2.53	1.47	1.40
6	C	601	ADP	C5-C4	2.51	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601	ADP	C3'-C2'-C1'	3.20	105.79	100.98
6	B	601	ADP	N3-C2-N1	-3.13	123.79	128.68
6	C	601	ADP	N3-C2-N1	-3.09	123.84	128.68
6	B	601	ADP	PA-O3A-PB	-3.07	122.31	132.83
6	C	601	ADP	PA-O3A-PB	-3.04	122.41	132.83
6	C	601	ADP	C4-C5-N7	-2.96	106.32	109.40
6	B	601	ADP	C4-C5-N7	-2.77	106.51	109.40
6	C	601	ADP	C3'-C2'-C1'	2.72	105.07	100.98
6	B	601	ADP	O3A-PB-O1B	-2.29	98.50	111.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

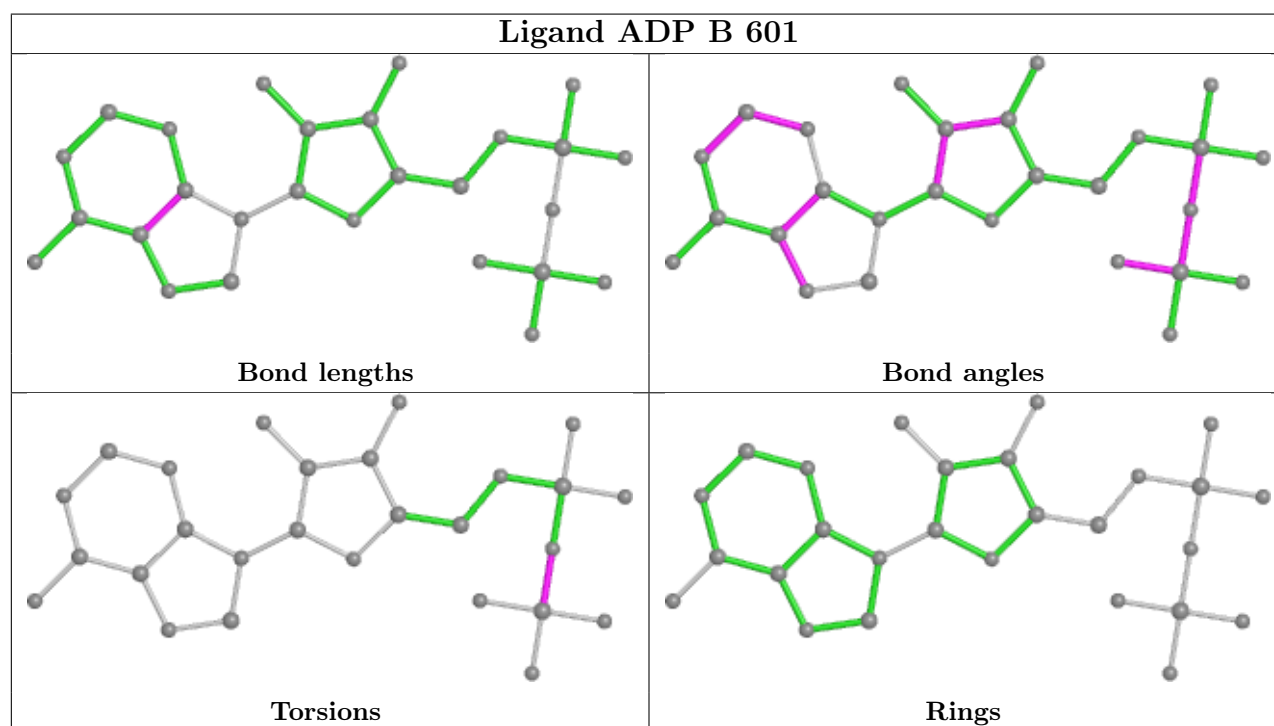
Mol	Chain	Res	Type	Atoms
6	B	601	ADP	PA-O3A-PB-O2B
6	C	601	ADP	PA-O3A-PB-O2B
6	B	601	ADP	PA-O3A-PB-O1B
6	C	601	ADP	PA-O3A-PB-O1B
6	B	601	ADP	PA-O3A-PB-O3B
6	C	601	ADP	PA-O3A-PB-O3B

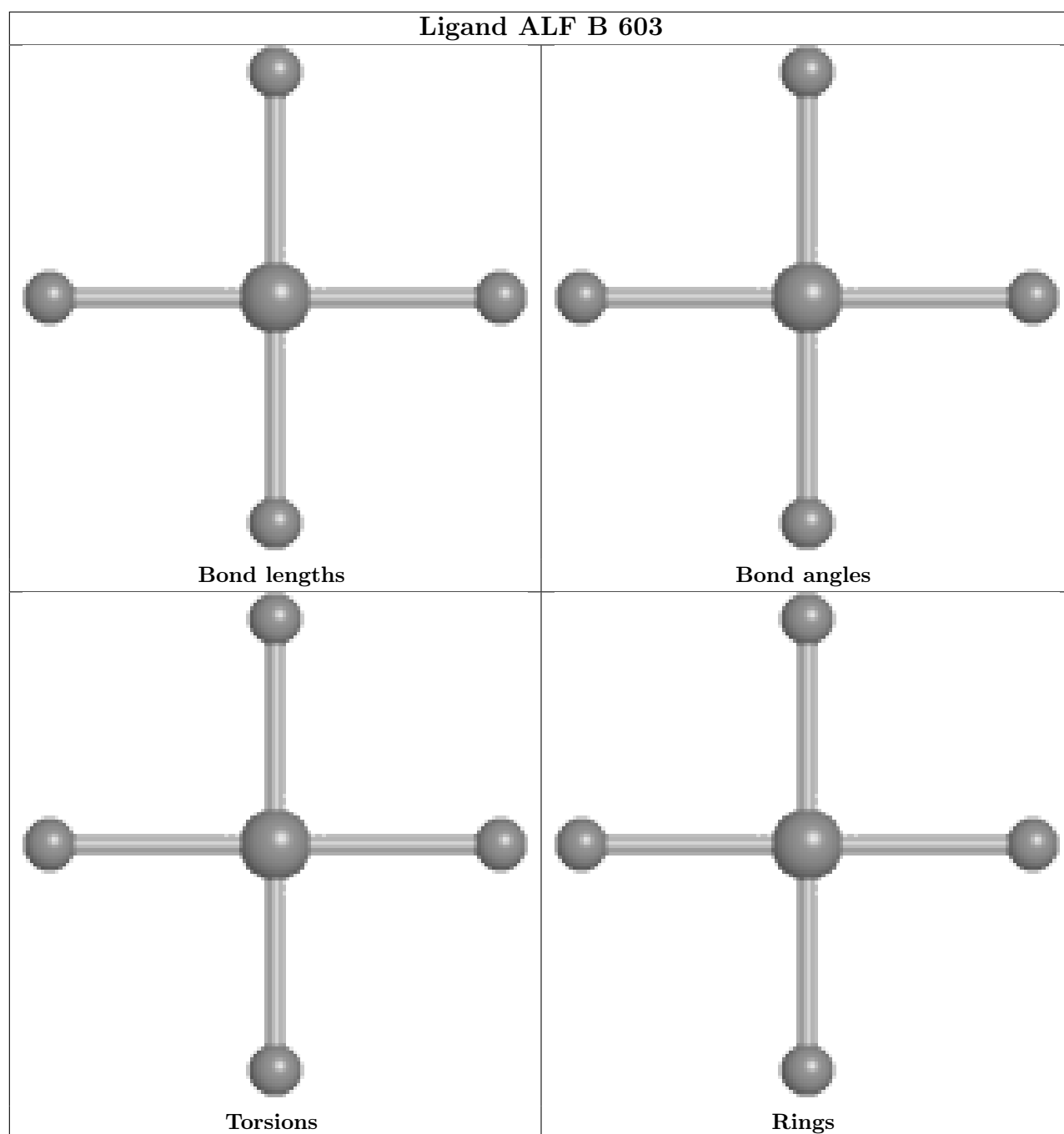
There are no ring outliers.

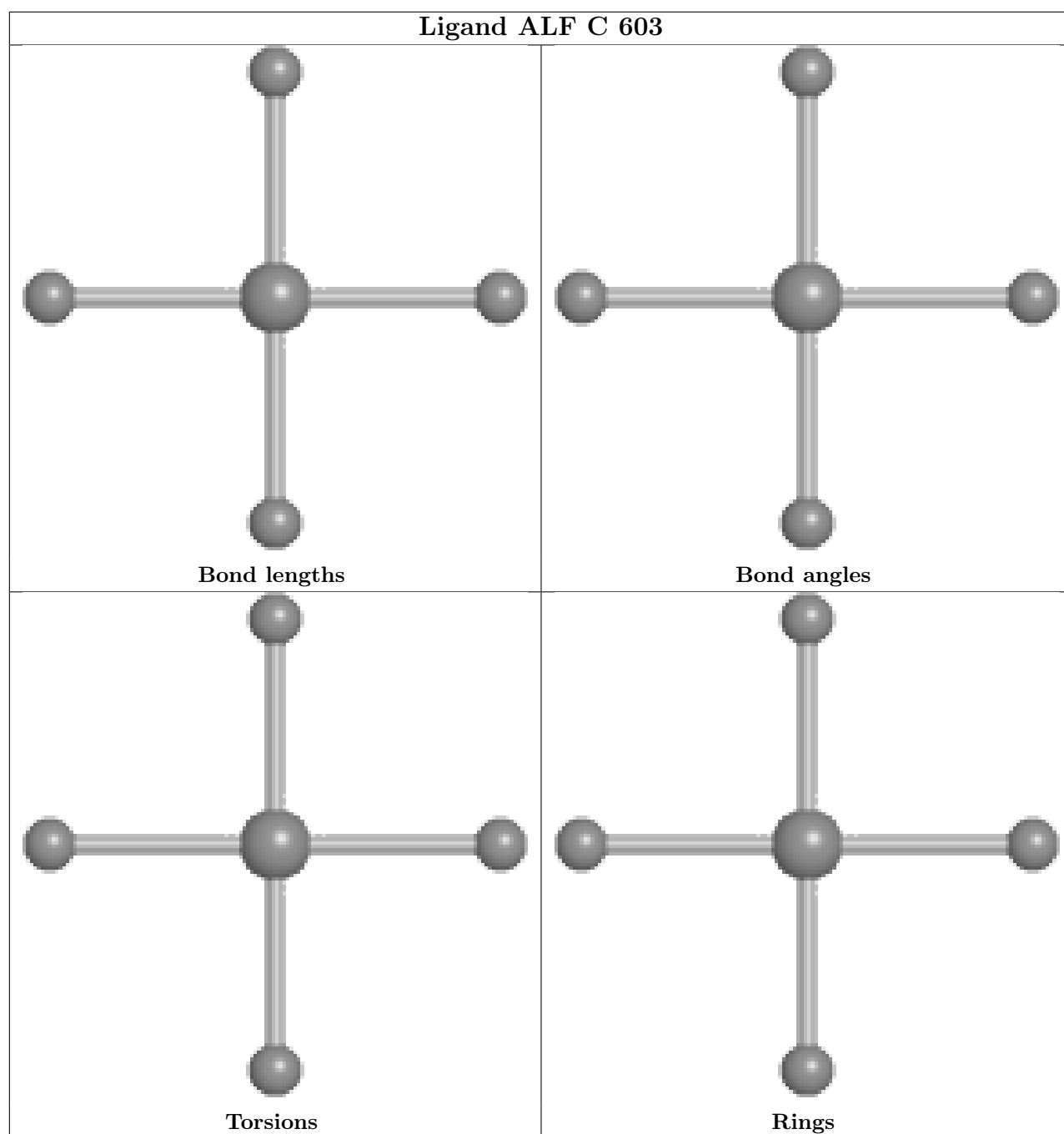
3 monomers are involved in 7 short contacts:

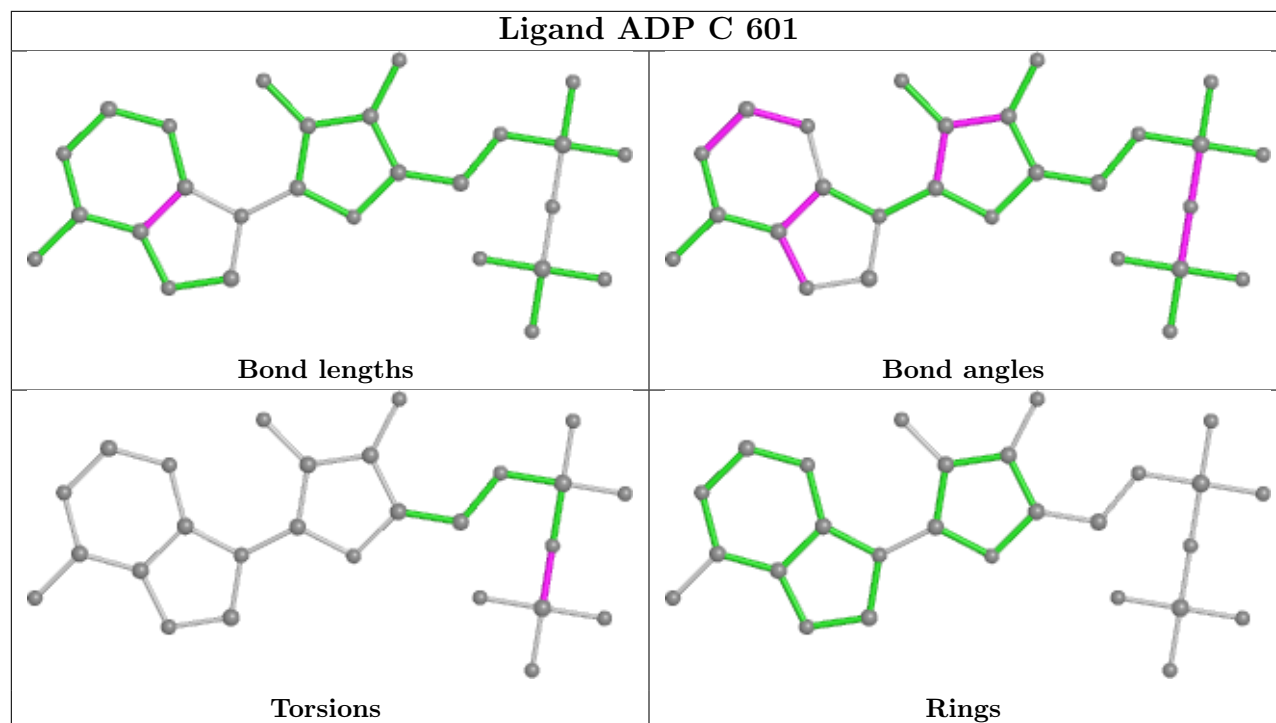
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	ADP	2	0
8	B	603	ALF	3	0
6	C	601	ADP	3	0

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, 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	565/600 (94%)	0.03	20 (3%)	44	35	83, 140, 192, 219	0
1	B	570/600 (95%)	0.10	18 (3%)	47	38	82, 142, 215, 264	0
1	C	556/600 (92%)	0.10	23 (4%)	37	31	99, 150, 229, 266	0
2	D	438/465 (94%)	-0.10	2 (0%)	91	86	84, 138, 201, 228	0
2	E	438/465 (94%)	-0.15	7 (1%)	72	64	70, 122, 169, 218	0
2	F	438/465 (94%)	-0.01	10 (2%)	60	52	87, 151, 218, 240	0
3	G	157/217 (72%)	0.29	10 (6%)	19	14	97, 164, 282, 304	0
4	H	98/115 (85%)	0.62	11 (11%)	5	5	108, 221, 271, 277	0
All	All	3260/3527 (92%)	0.04	101 (3%)	49	39	70, 142, 221, 304	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	ILE	5.9
2	F	364	ASP	5.3
1	B	174	CYS	4.7
1	B	125	GLU	4.5
1	C	174	CYS	4.5
4	H	77	PRO	4.4
1	C	77	PRO	4.1
1	C	562	ILE	3.8
4	H	47	VAL	3.8
2	F	86	ILE	3.7
1	B	156	LYS	3.7
1	B	128	THR	3.6
1	A	160	GLN	3.6
1	B	185	LEU	3.5
1	C	136	ILE	3.5
1	A	162	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	565	GLU	3.4
1	A	581	ILE	3.4
1	A	532	ALA	3.4
1	C	76	GLY	3.3
2	F	368	THR	3.3
4	H	68	GLN	3.3
3	G	80	LEU	3.2
1	B	162	ILE	3.2
1	A	127	GLY	3.1
4	H	48	ILE	3.1
1	B	106	GLY	3.1
1	C	130	VAL	3.1
1	C	160	GLN	3.1
2	F	208	VAL	3.1
1	C	127	GLY	3.1
2	F	133	SER	3.0
1	C	28	CYS	2.9
4	H	49	TYR	2.9
3	G	103	PRO	2.9
2	E	392	SER	2.9
3	G	60	THR	2.8
3	G	132	SER	2.8
1	C	563	PRO	2.7
1	B	127	GLY	2.7
1	C	128	THR	2.7
1	A	482	LEU	2.6
1	C	566	GLU	2.6
4	H	69	LEU	2.6
1	B	119	TRP	2.6
1	C	564	GLU	2.6
1	C	516	GLU	2.6
1	C	552	VAL	2.6
1	A	126	GLU	2.5
3	G	86	GLU	2.5
1	A	161	LYS	2.5
2	E	18	VAL	2.5
2	F	412	TYR	2.5
2	E	5	TYR	2.5
2	E	393	ALA	2.5
1	A	172	PRO	2.4
1	A	577	ILE	2.4
2	F	205	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	70	VAL	2.4
4	H	76	ILE	2.4
1	C	123	THR	2.4
2	F	431	TRP	2.4
1	A	488	LEU	2.3
2	D	355	GLY	2.3
1	B	153	ASN	2.3
4	H	56	ASN	2.3
1	B	319	ASP	2.3
1	C	135	ILE	2.3
2	F	440	THR	2.3
1	A	528	PHE	2.3
2	E	19	GLU	2.2
1	B	123	THR	2.2
1	A	159	VAL	2.2
1	B	130	VAL	2.2
1	C	65	ARG	2.2
1	C	185	LEU	2.2
3	G	139	LEU	2.2
1	A	77	PRO	2.2
3	G	81	LEU	2.2
1	B	88	GLN	2.2
1	B	157	GLY	2.2
4	H	55	ALA	2.2
1	A	130	VAL	2.2
1	C	156	LYS	2.2
4	H	46	GLY	2.2
3	G	23	THR	2.1
3	G	53	ALA	2.1
1	C	112	LEU	2.1
1	B	155	ILE	2.1
1	B	163	GLU	2.1
3	G	136	PHE	2.1
1	A	141	GLU	2.1
1	A	287	GLU	2.1
1	C	535	ALA	2.1
2	D	444	ARG	2.1
2	F	355	GLY	2.1
4	H	71	PRO	2.0
2	E	412	TYR	2.0
1	A	531	GLU	2.0
1	A	185	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	486	ASP	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 monosaccharides in this entry.

6.4 Ligands [i](#)

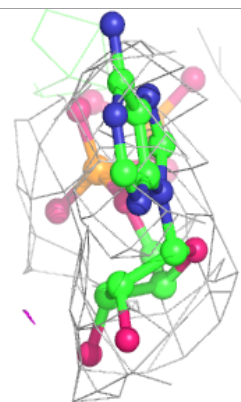
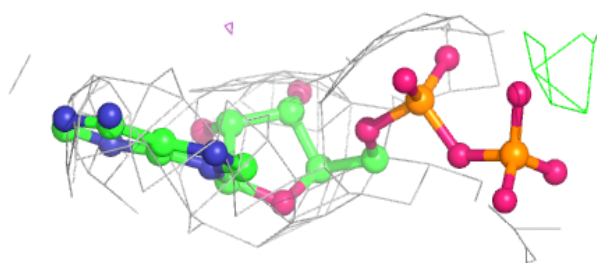
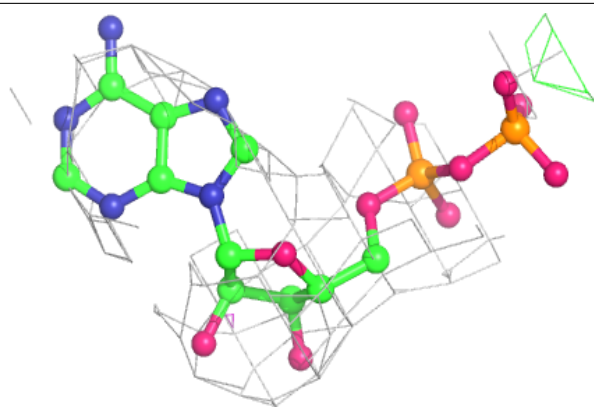
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	601	6/6	0.80	0.57	101,108,117,121	0
6	ADP	B	601	27/27	0.91	0.30	78,107,126,134	0
6	ADP	C	601	27/27	0.91	0.32	95,127,151,162	0
7	MG	C	602	1/1	0.91	0.70	144,144,144,144	0
8	ALF	C	603	5/5	0.91	0.52	101,110,129,135	0
8	ALF	B	603	5/5	0.93	0.41	111,112,155,160	0
7	MG	B	602	1/1	0.98	0.47	76,76,76,76	0

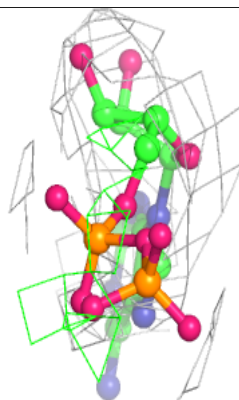
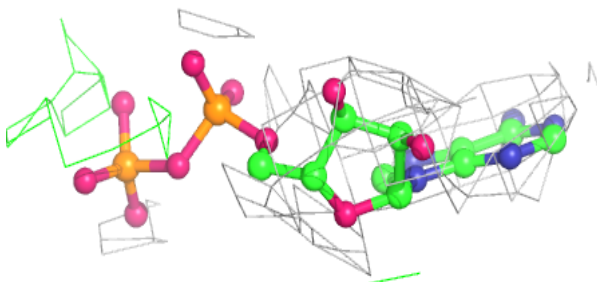
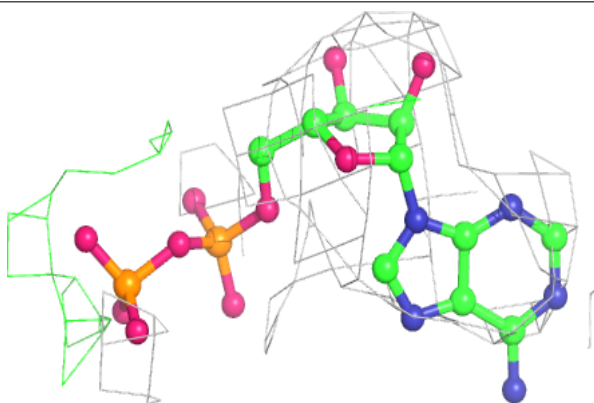
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP 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)

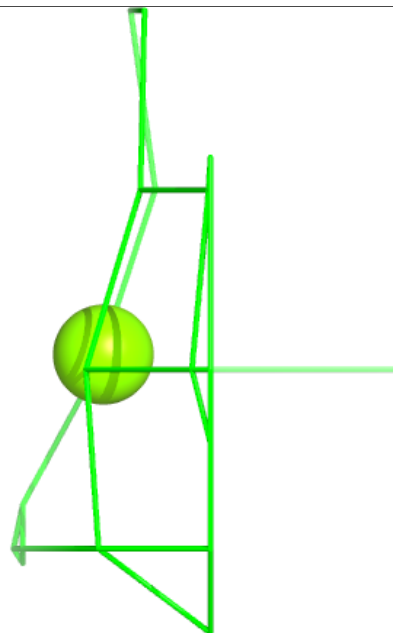
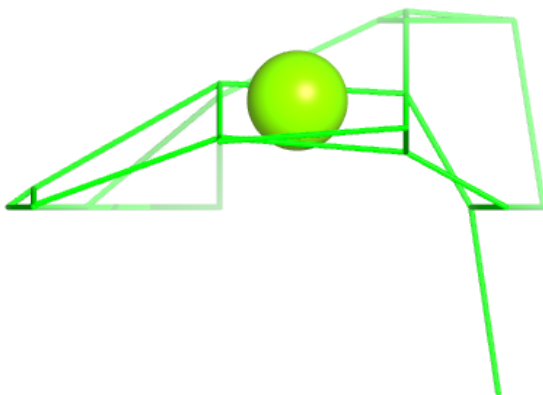
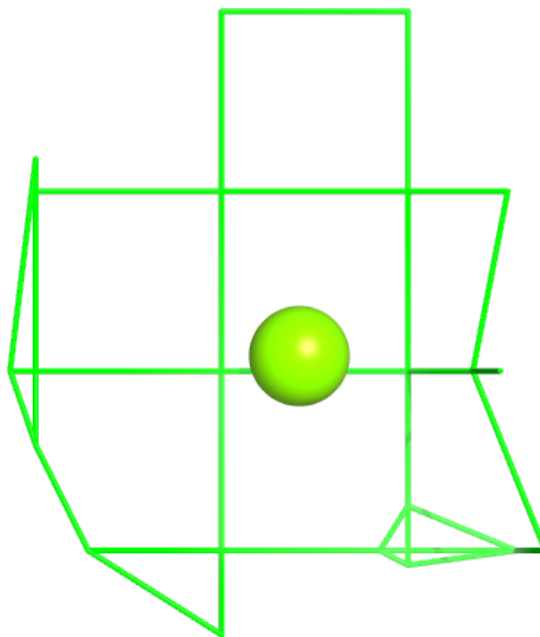
**Electron density around ADP C 601:**

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



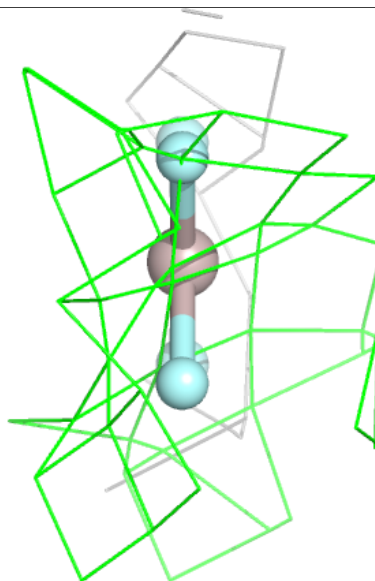
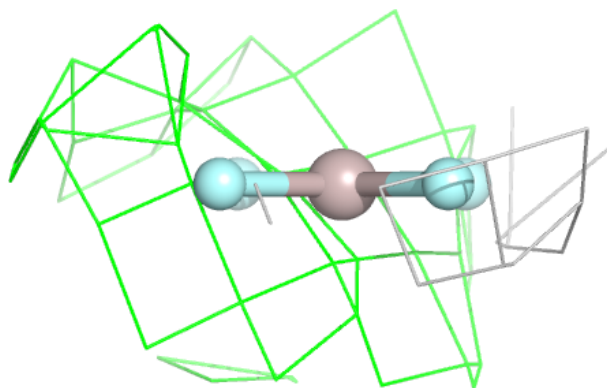
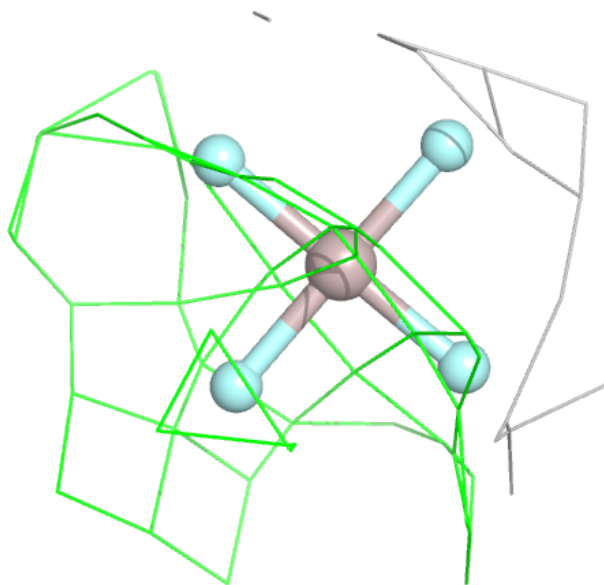
Electron density around MG C 602:

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



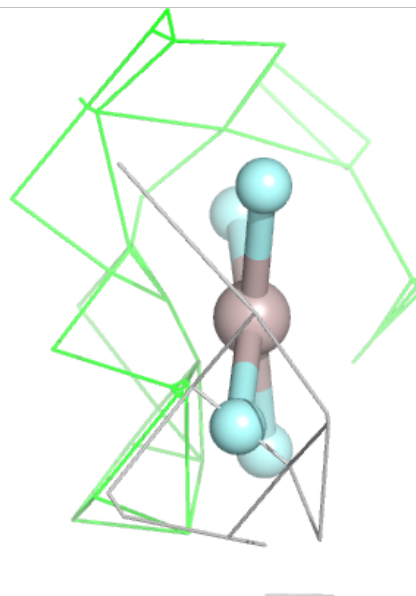
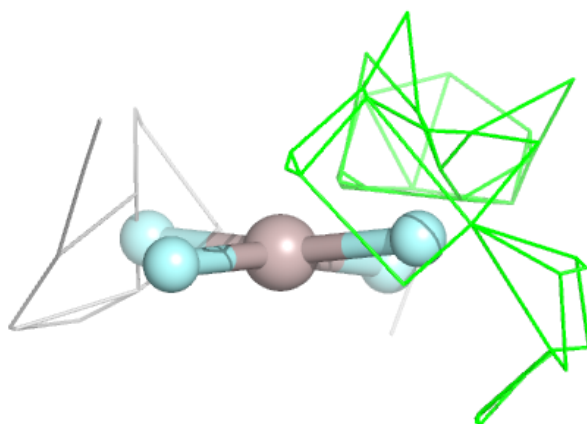
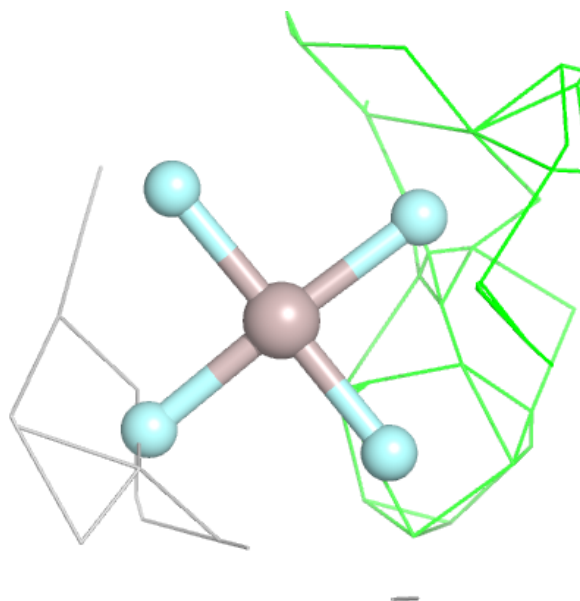
Electron density around ALF C 603:

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



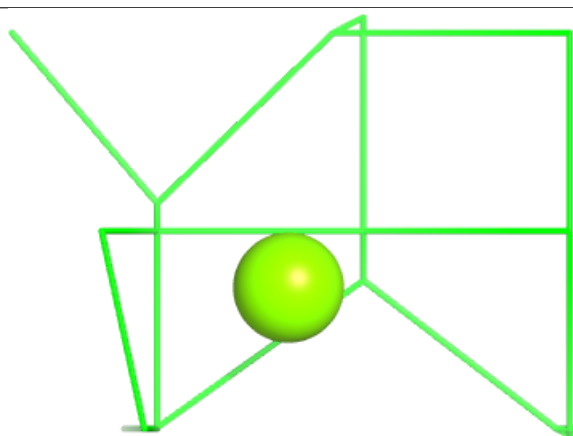
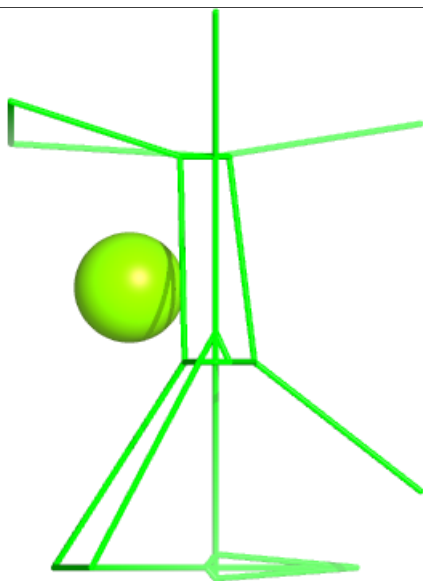
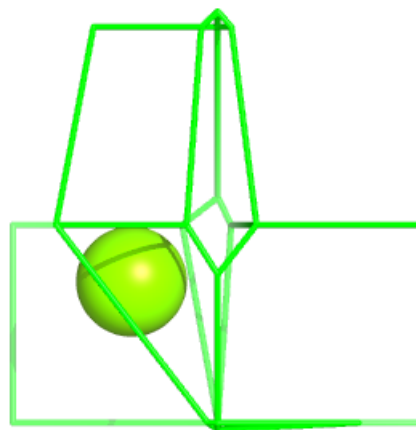
Electron density around ALF B 603:

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



Electron density around MG B 602:

$2mF_o-DF_c$ (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.