



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:03 AM EDT

PDB ID : 9EMY / pdb_00009emy
Title : P. falciparum FIKK13 in complex with ATPgammaS
Authors : Purkiss, A.G.; Ogradowicz, R.W.; Christodoulou, E.; Kjaer, S.
Deposited on : 2024-03-11
Resolution : 2.81 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

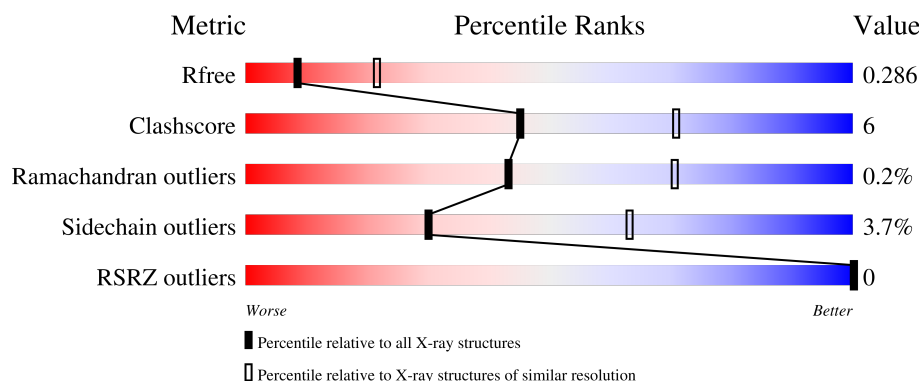
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	413	
1	B	413	
1	G	413	
1	H	413	
2	C	136	

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Mol	Chain	Length	Quality of chain
2	D	136	77% 12% • 10%
2	I	136	78% 14% 8%
2	J	136	76% 12% • 11%
3	E	134	76% 16% • 7%
3	F	134	75% 11% • 13%
3	K	134	72% 19% • 7%
3	L	134	73% 14% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19180 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 non-specific serine/threonine protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			3028	1982	480	547	19			
1	B	379	Total	C	N	O	S	0	0	0
			3007	1957	483	549	18			
1	G	369	Total	C	N	O	S	0	0	0
			2999	1964	476	540	19			
1	H	375	Total	C	N	O	S	0	0	0
			2996	1954	479	545	18			

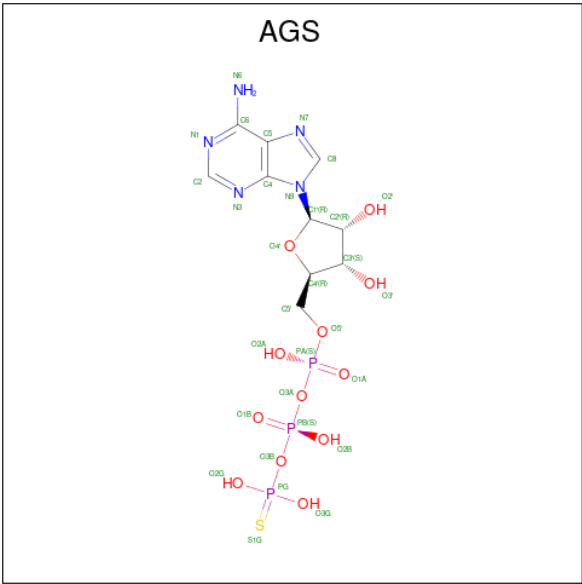
- Molecule 2 is a protein called Nanobody 9F10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	125	Total	C	N	O	S	0	0	0
			905	568	155	178	4			
2	D	122	Total	C	N	O	S	0	0	0
			869	542	147	176	4			
2	I	125	Total	C	N	O	S	0	0	0
			899	563	154	178	4			
2	J	121	Total	C	N	O	S	0	0	0
			863	540	144	175	4			

- Molecule 3 is a protein called Nanobody 2G9.

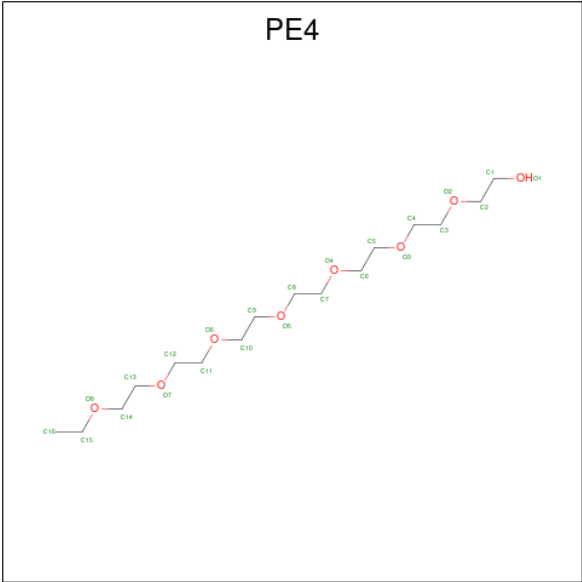
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	125	Total	C	N	O	S	0	0	0
			905	562	157	181	5			
3	F	116	Total	C	N	O	S	0	0	0
			811	503	142	161	5			
3	K	124	Total	C	N	O	S	0	0	0
			904	561	156	182	5			
3	L	117	Total	C	N	O	S	0	0	0
			828	514	144	166	4			

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			24	16	8		

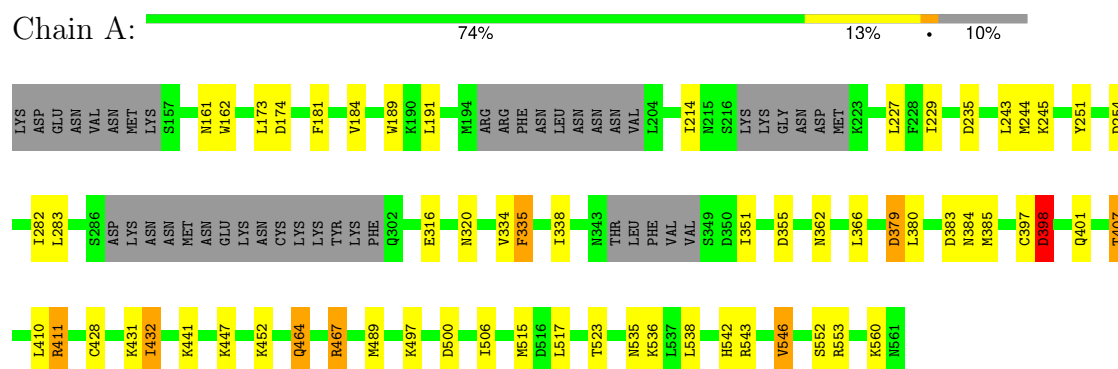
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	4	Total	O	0	0
			4	4		
6	C	1	Total	O	0	0
			1	1		
6	E	1	Total	O	0	0
			1	1		
6	G	2	Total	O	0	0
			2	2		
6	H	6	Total	O	0	0
			6	6		
6	I	2	Total	O	0	0
			2	2		
6	L	1	Total	O	0	0
			1	1		

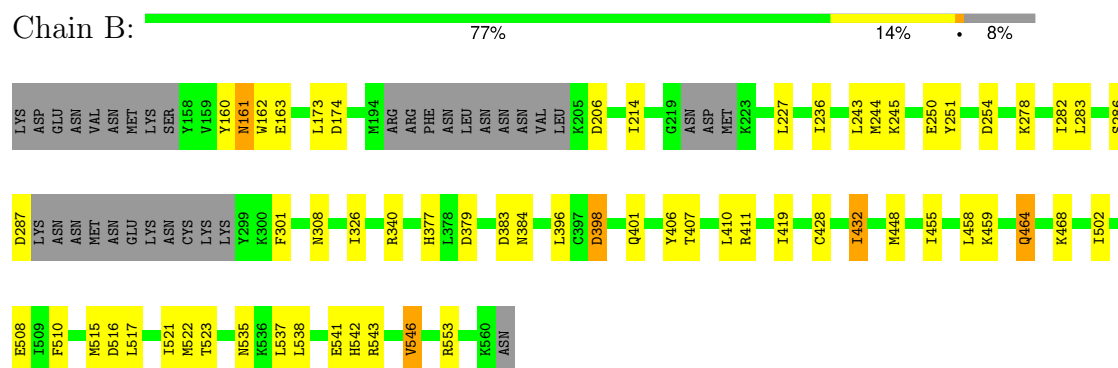
3 Residue-property plots [i](#)

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.

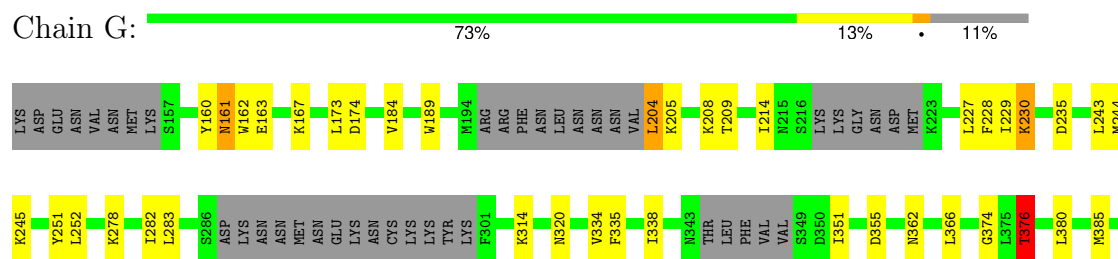
- Molecule 1: non-specific serine/threonine protein kinase



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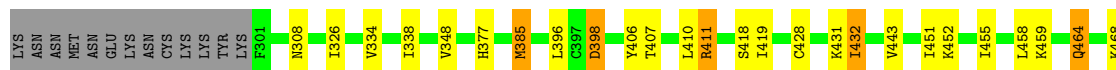
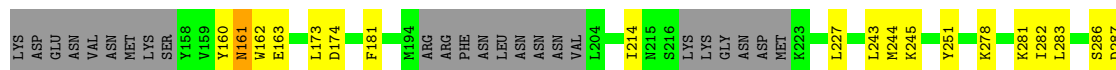
- Molecule 1: non-specific serine/threonine protein kinase





- Molecule 1: non-specific serine/threonine protein kinase

Chain H: 76% 13% 9%



- Molecule 2: Nanobody 9F10

Chain C: 82% 10% 8%



- Molecule 2: Nanobody 9F10

Chain D: 77% 12% 10%



- Molecule 2: Nanobody 9F10

Chain I: 78% 14% 8%



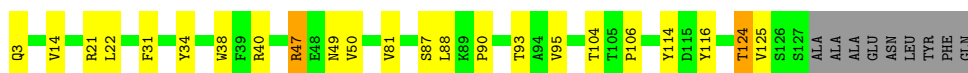
- Molecule 2: Nanobody 9F10

Chain J: 76% 12% 11%



- Molecule 3: Nanobody 2G9

Chain E: 76% 16% 7%



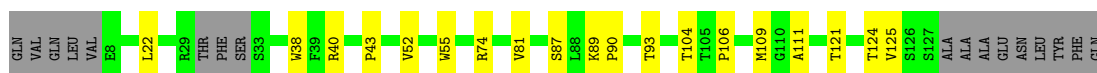
- Molecule 3: Nanobody 2G9



- Molecule 3: Nanobody 2G9



- Molecule 3: Nanobody 2G9



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.40Å 121.66Å 151.06Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	64.17 – 2.81 64.17 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.7 (64.17-2.81) 99.7 (64.17-2.81)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.242 , 0.286 0.242 , 0.286	Depositor DCC
R_{free} test set	3702 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.419 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19180	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, PE4

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	0.57	0/3107	1.14	9/4206 (0.2%)
1	B	0.55	0/3086	1.14	7/4198 (0.2%)
1	G	0.55	0/3076	1.15	7/4167 (0.2%)
1	H	0.56	0/3075	1.14	6/4183 (0.1%)
2	C	0.56	0/929	1.03	1/1268 (0.1%)
2	D	0.55	0/890	1.04	1/1214 (0.1%)
2	I	0.55	0/922	1.02	1/1258 (0.1%)
2	J	0.56	0/884	1.01	0/1206
3	E	0.61	0/924	1.19	5/1258 (0.4%)
3	F	0.62	0/827	1.16	2/1127 (0.2%)
3	K	0.62	0/923	1.13	4/1256 (0.3%)
3	L	0.63	0/845	1.17	1/1151 (0.1%)
All	All	0.57	0/19488	1.13	44/26492 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	G	0	1
1	H	0	1
2	D	0	2
2	J	0	2
3	E	0	2
3	F	0	1
3	K	0	3
3	L	0	2
All	All	0	19

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	ASP	CA-CB-CG	7.75	120.36	112.60
1	H	398	ASP	CB-CA-C	7.13	124.61	110.42
1	B	398	ASP	CB-CA-C	7.08	124.51	110.42
1	A	398	ASP	CB-CA-C	6.54	123.42	110.42
3	F	40	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	B	541	GLU	N-CA-CB	6.18	118.97	110.01
1	B	301	PHE	CB-CA-C	5.98	118.77	110.16
3	F	43	PRO	CB-CA-C	5.89	119.06	111.46
3	E	124	THR	CA-CB-OG1	-5.88	100.78	109.60
1	H	541	GLU	N-CA-CB	5.85	118.49	110.01
1	B	250	GLU	CB-CG-CD	5.72	122.33	112.60
2	D	49	PHE	CA-CB-CG	5.72	119.52	113.80
1	A	379	ASP	N-CA-CB	5.68	120.61	110.79
1	A	383	ASP	CA-CB-CG	5.68	118.28	112.60
3	L	43	PRO	CB-CA-C	5.44	118.48	111.46
1	G	376	THR	OG1-CB-CG2	-5.42	98.46	109.30
1	A	235	ASP	CA-CB-CG	5.39	117.99	112.60
1	H	418	SER	CA-C-N	5.35	127.79	120.35
1	H	418	SER	C-N-CA	5.35	127.79	120.35
1	A	335	PHE	CA-CB-CG	-5.34	108.46	113.80
3	K	70	PHE	CA-CB-CG	5.32	119.11	113.80
3	K	47	ARG	CG-CD-NE	5.28	123.62	112.00
1	G	235	ASP	CA-CB-CG	5.26	117.86	112.60
1	G	167	LYS	CB-CG-CD	5.26	123.40	111.30
3	E	21	ARG	CG-CD-NE	5.24	123.53	112.00
1	H	160	TYR	N-CA-CB	5.24	117.78	109.51
1	B	160	TYR	N-CA-CB	5.19	117.71	109.51
1	G	407	THR	CA-CB-OG1	-5.17	101.84	109.60
1	A	398	ASP	CA-CB-CG	5.17	117.77	112.60
3	E	34	TYR	CB-CA-C	5.15	117.75	110.24
3	E	47	ARG	NE-CZ-NH2	5.14	123.83	119.20
3	K	40	ARG	NE-CZ-NH1	-5.13	116.37	121.50
2	C	70	PHE	CA-CB-CG	5.13	118.93	113.80
1	G	431	LYS	CG-CD-CE	5.12	123.08	111.30
1	G	541	GLU	N-CA-CB	5.11	117.42	110.01
3	E	47	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	B	379	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	407	THR	CA-CB-OG1	-5.10	101.95	109.60
1	H	443	VAL	N-CA-CB	5.09	115.97	110.62
3	K	34	TYR	CB-CA-C	5.09	117.67	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	398	ASP	CB-CA-C	5.08	120.53	110.42
2	I	70	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	560	LYS	CB-CA-C	5.06	117.89	109.53
1	B	383	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	411	ARG	Sidechain
1	A	467	ARG	Sidechain
1	A	553	ARG	Sidechain
1	B	340	ARG	Sidechain
1	B	411	ARG	Sidechain
2	D	102	ARG	Sidechain
2	D	40	ARG	Sidechain
3	E	40	ARG	Sidechain
3	E	47	ARG	Sidechain
3	F	40	ARG	Sidechain
1	G	553	ARG	Sidechain
1	H	411	ARG	Sidechain
2	J	102	ARG	Sidechain
2	J	40	ARG	Sidechain
3	K	103	ARG	Sidechain
3	K	21	ARG	Sidechain
3	K	40	ARG	Sidechain
3	L	40	ARG	Sidechain
3	L	74	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3028	0	2888	38	0
1	B	3007	0	2762	33	0
1	G	2999	0	2858	41	0
1	H	2996	0	2778	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	905	0	794	8	0
2	D	869	0	736	7	0
2	I	899	0	787	10	0
2	J	863	0	736	9	0
3	E	905	0	829	13	0
3	F	811	0	721	11	0
3	K	904	0	831	16	0
3	L	828	0	739	11	0
4	A	31	0	12	4	0
4	B	31	0	12	5	0
4	G	31	0	12	2	0
4	H	31	0	12	4	0
5	A	24	0	34	2	0
6	A	1	0	0	0	0
6	B	4	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	2	0	0	0	0
6	H	6	0	0	1	0
6	I	2	0	0	1	0
6	L	1	0	0	0	0
All	All	19180	0	17541	218	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 6.

All (218) 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:G:411:ARG:CD	1:G:467:ARG:HB2	1.84	1.07
1:G:411:ARG:CD	1:G:467:ARG:CB	2.39	0.99
1:G:411:ARG:CD	1:G:467:ARG:HB3	2.18	0.72
1:G:448:MET:HE3	3:K:49:ASN:HB3	1.71	0.71
1:B:508:GLU:OE2	3:F:55:TRP:HB3	1.94	0.68
3:L:38:TRP:HE1	3:L:81:VAL:HG12	1.58	0.67
1:H:432:ILE:HG22	3:L:106:PRO:HG3	1.75	0.67
2:J:22:LEU:HD13	2:J:85:MET:HE2	1.76	0.67
2:D:22:LEU:HD13	2:D:85:MET:HE2	1.76	0.66
1:B:243:LEU:HD13	1:B:251:TYR:CE1	2.32	0.65
1:G:411:ARG:CD	1:G:467:ARG:HE	2.10	0.65
3:K:38:TRP:HE1	3:K:81:VAL:HG12	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:HIS:O	1:A:546:VAL:HG12	1.97	0.64
1:B:542:HIS:O	1:B:546:VAL:HG12	1.98	0.63
1:H:542:HIS:O	1:H:546:VAL:HG12	1.98	0.63
1:A:384:ASN:OD1	4:A:601:AGS:O2B	2.16	0.63
3:E:38:TRP:HE1	3:E:81:VAL:HG12	1.62	0.63
1:G:432:ILE:HG22	3:K:106:PRO:HG3	1.80	0.63
1:A:410:LEU:HG	1:A:464:GLN:NE2	2.14	0.62
1:G:410:LEU:HG	1:G:464:GLN:NE2	2.15	0.61
1:B:432:ILE:HG22	3:F:106:PRO:HG3	1.82	0.61
3:K:49:ASN:ND2	3:K:114:TYR:OH	2.34	0.61
1:H:410:LEU:HG	1:H:464:GLN:NE2	2.15	0.61
1:B:410:LEU:HG	1:B:464:GLN:NE2	2.15	0.60
1:G:448:MET:HE3	3:K:49:ASN:CB	2.30	0.60
4:B:601:AGS:O5'	4:B:601:AGS:H8	2.02	0.60
1:A:447:LYS:NZ	3:E:104:THR:HB	2.17	0.59
1:G:243:LEU:HD13	1:G:251:TYR:CZ	2.38	0.59
4:H:601:AGS:O2B	4:H:601:AGS:H5'2	2.04	0.58
4:H:601:AGS:O5'	4:H:601:AGS:H8	2.03	0.58
1:A:243:LEU:HD13	1:A:251:TYR:CZ	2.38	0.58
2:I:29:GLY:HA3	6:I:201:HOH:O	2.02	0.58
3:E:3:GLN:N	3:E:116:TYR:HH	2.00	0.58
1:A:173:LEU:HA	1:A:282:ILE:HG23	1.86	0.57
1:H:161:ASN:HD21	1:H:163:GLU:HB2	1.69	0.57
1:A:432:ILE:HG22	3:E:106:PRO:HG3	1.86	0.57
1:G:173:LEU:HA	1:G:282:ILE:HG23	1.86	0.57
1:B:161:ASN:HD21	1:B:163:GLU:HB2	1.70	0.56
1:A:191:LEU:HD22	1:A:229:ILE:CD1	2.35	0.56
1:A:447:LYS:HZ1	3:E:104:THR:HB	1.70	0.56
3:F:38:TRP:HE1	3:F:81:VAL:HG12	1.69	0.56
1:G:184:VAL:HG21	1:G:214:ILE:HG23	1.87	0.55
1:A:184:VAL:HG21	1:A:214:ILE:HG23	1.87	0.55
1:H:243:LEU:HD13	1:H:251:TYR:CZ	2.42	0.55
3:F:93:THR:HG22	3:F:125:VAL:H	1.71	0.55
1:A:316:GLU:OE2	1:H:281:LYS:NZ	2.40	0.55
3:K:15:GLN:NE2	3:K:126:SER:HB2	2.22	0.55
3:L:93:THR:HG22	3:L:125:VAL:H	1.72	0.55
1:A:411:ARG:HG2	1:A:464:GLN:HE21	1.71	0.54
1:B:521:ILE:O	1:B:522:MET:HB2	2.08	0.54
1:G:376:THR:HG22	1:G:478:ASP:OD2	2.07	0.54
1:H:521:ILE:O	1:H:522:MET:HB2	2.09	0.53
2:C:21:THR:HG22	2:C:84:GLN:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ASP:O	1:B:401:GLN:NE2	2.41	0.53
1:A:379:ASP:OD2	1:A:398:ASP:OD2	2.27	0.52
1:A:254:ASP:O	1:A:401:GLN:NE2	2.42	0.52
1:H:517:LEU:HD22	1:H:523:THR:HG21	1.92	0.52
2:I:21:THR:HG22	2:I:84:GLN:HA	1.92	0.52
1:A:397:CYS:SG	4:A:601:AGS:C8	2.98	0.52
2:D:21:THR:HG22	2:D:84:GLN:HA	1.90	0.52
2:C:21:THR:HG21	2:C:84:GLN:OE1	2.10	0.52
1:H:508:GLU:OE2	3:L:55:TRP:HB3	2.08	0.52
4:B:601:AGS:O2B	4:B:601:AGS:H5'2	2.10	0.52
3:E:93:THR:HG22	3:E:125:VAL:H	1.74	0.52
1:B:517:LEU:HD22	1:B:523:THR:HG21	1.92	0.52
1:A:244:MET:SD	1:A:251:TYR:HB3	2.50	0.52
2:I:21:THR:HG21	2:I:84:GLN:OE1	2.10	0.52
1:H:173:LEU:HA	1:H:282:ILE:HG23	1.93	0.51
1:B:173:LEU:HA	1:B:282:ILE:HG23	1.93	0.51
1:G:244:MET:SD	1:G:251:TYR:HB3	2.50	0.51
2:J:21:THR:HG22	2:J:84:GLN:HA	1.91	0.51
3:K:7:VAL:CG2	3:K:25:ALA:HB3	2.40	0.51
1:B:243:LEU:HD13	1:B:251:TYR:CZ	2.46	0.51
3:K:84:GLN:HG3	3:K:86:ASN:HD21	1.76	0.51
1:G:162:TRP:CH2	1:G:245:LYS:HA	2.45	0.50
1:B:162:TRP:CH2	1:B:245:LYS:HA	2.47	0.50
1:G:351:ILE:HG23	1:G:355:ASP:HB2	1.94	0.50
1:A:162:TRP:CH2	1:A:245:LYS:HA	2.46	0.50
1:A:351:ILE:HG23	1:A:355:ASP:HB2	1.94	0.50
1:B:244:MET:SD	1:B:251:TYR:HB3	2.51	0.50
1:H:162:TRP:CH2	1:H:245:LYS:HA	2.47	0.49
1:A:517:LEU:HD23	1:A:523:THR:HG21	1.93	0.49
1:G:517:LEU:HD23	1:G:523:THR:HG21	1.93	0.49
1:H:244:MET:SD	1:H:251:TYR:HB3	2.52	0.49
1:B:428:CYS:SG	3:F:106:PRO:HB2	2.53	0.49
1:A:184:VAL:CG2	1:A:214:ILE:HG23	2.43	0.49
1:G:380:LEU:HD22	1:G:385:MET:HE3	1.95	0.48
1:G:174:ASP:O	1:G:283:LEU:HA	2.13	0.48
1:B:448:MET:HE3	3:F:49:ASN:HB3	1.95	0.48
1:G:184:VAL:CG2	1:G:214:ILE:HG23	2.43	0.48
1:A:174:ASP:O	1:A:283:LEU:HA	2.14	0.48
3:F:90:PRO:O	3:F:93:THR:HG23	2.14	0.48
3:L:93:THR:HG22	3:L:125:VAL:N	2.30	0.47
3:F:93:THR:HG22	3:F:125:VAL:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LYS:HB3	1:A:546:VAL:HG11	1.97	0.47
3:E:93:THR:HG22	3:E:125:VAL:N	2.30	0.47
3:E:31:PHE:HZ	3:E:81:VAL:HG23	1.79	0.47
1:A:338:ILE:HG12	1:A:351:ILE:HD12	1.97	0.47
2:C:22:LEU:HD13	2:C:85:MET:CE	2.45	0.47
1:H:515:MET:O	1:H:535:ASN:ND2	2.48	0.47
1:B:515:MET:O	1:B:535:ASN:ND2	2.48	0.46
1:G:411:ARG:CD	1:G:467:ARG:NE	2.78	0.46
2:J:6:LEU:HD13	2:J:98:CYS:SG	2.56	0.46
3:K:93:THR:HG22	3:K:125:VAL:H	1.79	0.46
2:D:8:GLU:HB2	2:D:123:THR:HG23	1.97	0.46
1:G:334:VAL:HG11	1:G:489:MET:HE1	1.98	0.46
1:G:397:CYS:SG	4:G:601:AGS:C8	3.04	0.46
1:G:161:ASN:OD1	1:G:163:GLU:N	2.48	0.46
3:K:15:GLN:NE2	3:K:127:SER:O	2.49	0.46
1:B:174:ASP:O	1:B:283:LEU:HA	2.16	0.46
1:A:362:ASN:O	1:A:366:LEU:HG	2.16	0.46
1:G:161:ASN:OD1	1:G:161:ASN:C	2.59	0.46
2:J:8:GLU:HB2	2:J:123:THR:HG23	1.98	0.46
1:G:335:PHE:CZ	2:I:55:TRP:CZ3	3.03	0.46
1:G:338:ILE:HG12	1:G:351:ILE:HD12	1.98	0.46
1:H:174:ASP:O	1:H:283:LEU:HA	2.16	0.46
1:G:497:LYS:NZ	2:I:101:ASP:OD1	2.39	0.46
2:J:94:ALA:HB3	2:J:96:TYR:HE1	1.80	0.46
1:G:362:ASN:O	1:G:366:LEU:HG	2.16	0.46
1:B:538:LEU:O	1:B:543:ARG:HD3	2.16	0.45
1:G:204:LEU:HB3	1:G:205:LYS:H	1.65	0.45
2:I:22:LEU:HD13	2:I:85:MET:CE	2.46	0.45
3:L:90:PRO:O	3:L:93:THR:HG23	2.16	0.45
2:D:6:LEU:HD13	2:D:98:CYS:SG	2.57	0.45
1:H:538:LEU:O	1:H:543:ARG:HD3	2.17	0.45
1:B:553:ARG:NH1	3:E:87:SER:OG	2.50	0.45
1:H:428:CYS:SG	3:L:106:PRO:HB2	2.56	0.45
3:K:31:PHE:HZ	3:K:81:VAL:HG23	1.81	0.45
1:A:506:ILE:HG12	2:C:111:TYR:CE1	2.52	0.45
1:G:553:ARG:NH1	3:L:87:SER:OG	2.48	0.45
2:I:93:THR:HG23	2:I:127:VAL:HB	1.99	0.45
4:B:601:AGS:H8	4:B:601:AGS:PA	2.56	0.44
1:G:515:MET:O	1:G:535:ASN:ND2	2.51	0.44
1:B:502:ILE:HD12	3:F:52:VAL:HG12	1.99	0.44
2:C:6:LEU:HD13	2:C:98:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:LEU:HD12	1:H:326:ILE:HD11	1.99	0.44
1:G:252:LEU:HD12	1:G:252:LEU:N	2.33	0.44
1:G:538:LEU:O	1:G:543:ARG:HD3	2.17	0.44
3:K:93:THR:HG22	3:K:125:VAL:N	2.33	0.44
1:B:455:ILE:HD12	1:B:455:ILE:H	1.82	0.44
2:D:22:LEU:HD13	2:D:85:MET:CE	2.46	0.44
1:H:553:ARG:HG2	6:H:706:HOH:O	2.16	0.44
2:I:6:LEU:HD13	2:I:98:CYS:SG	2.57	0.44
1:A:538:LEU:O	1:A:543:ARG:HD3	2.17	0.44
1:G:517:LEU:HD12	1:G:535:ASN:ND2	2.33	0.44
1:H:510:PHE:HE1	1:H:517:LEU:HD23	1.82	0.44
5:A:602:PE4:H62	5:A:602:PE4:H41	1.66	0.44
1:G:209:THR:HG22	1:G:230:LYS:HG3	2.00	0.44
1:B:214:ILE:HD12	1:B:227:LEU:HD11	1.99	0.43
1:B:286:SER:OG	1:B:287:ASP:N	2.51	0.43
1:B:510:PHE:HE1	1:B:517:LEU:HD23	1.83	0.43
1:H:377:HIS:HD2	1:H:396:LEU:HD13	1.83	0.43
1:A:335:PHE:CZ	2:C:55:TRP:CZ3	3.06	0.43
1:H:502:ILE:HD12	3:L:52:VAL:HG12	2.00	0.43
3:K:90:PRO:O	3:K:93:THR:HG23	2.18	0.43
1:A:515:MET:O	1:A:535:ASN:ND2	2.52	0.43
2:C:93:THR:HG23	2:C:127:VAL:HB	2.00	0.43
3:K:15:GLN:CD	3:K:126:SER:HB2	2.44	0.43
1:B:283:LEU:HD12	1:B:326:ILE:HD11	2.00	0.43
3:E:49:ASN:ND2	3:E:114:TYR:OH	2.51	0.43
2:J:22:LEU:HD13	2:J:85:MET:CE	2.47	0.43
4:A:601:AGS:O5'	4:A:601:AGS:H8	2.19	0.43
1:H:411:ARG:HG2	1:H:464:GLN:HE21	1.83	0.43
5:A:602:PE4:H121	5:A:602:PE4:H102	1.60	0.43
2:D:93:THR:HG23	2:D:126:THR:HA	1.99	0.43
1:H:406:TYR:HB3	1:H:419:ILE:HG23	2.00	0.43
3:F:55:TRP:CE3	3:F:56:SER:HB3	2.54	0.43
1:G:214:ILE:HD12	1:G:227:LEU:HD11	2.01	0.43
3:K:104:THR:HG22	3:K:111:ALA:O	2.19	0.43
1:H:286:SER:OG	1:H:287:ASP:N	2.50	0.43
1:H:452:LYS:HB3	3:L:109:MET:SD	2.59	0.43
1:A:214:ILE:HD12	1:A:227:LEU:HD11	2.01	0.42
3:E:90:PRO:O	3:E:93:THR:HG23	2.19	0.42
4:H:601:AGS:H8	4:H:601:AGS:PA	2.59	0.42
2:J:93:THR:HG23	2:J:126:THR:HA	2.00	0.42
1:A:189:TRP:CE2	1:A:214:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ASN:OD1	4:B:601:AGS:O1B	2.37	0.42
1:B:521:ILE:O	1:B:522:MET:CB	2.67	0.42
1:G:228:PHE:CZ	4:G:601:AGS:C8	3.02	0.42
1:H:214:ILE:HD12	1:H:227:LEU:HD11	2.01	0.42
2:I:8:GLU:HB2	2:I:123:THR:HG23	2.02	0.42
1:B:206:ASP:HB3	1:B:236:ILE:CD1	2.50	0.42
2:D:35:ALA:N	2:D:101:ASP:O	2.47	0.42
1:B:406:TYR:HB3	1:B:419:ILE:HG23	2.01	0.42
1:H:521:ILE:O	1:H:522:MET:CB	2.67	0.42
1:A:181:PHE:HB3	1:A:214:ILE:HD13	2.01	0.42
1:A:380:LEU:HD22	1:A:385:MET:HE3	2.02	0.42
1:A:517:LEU:HD12	1:A:535:ASN:ND2	2.35	0.42
3:K:55:TRP:CD1	3:K:55:TRP:H	2.38	0.42
4:A:601:AGS:H3'	4:A:601:AGS:O1B	2.20	0.41
1:H:385:MET:HE2	1:H:385:MET:HB2	1.99	0.41
1:B:458:LEU:O	1:B:459:LYS:C	2.63	0.41
1:H:455:ILE:HD12	1:H:455:ILE:H	1.85	0.41
1:G:189:TRP:CE2	1:G:214:ILE:HD11	2.56	0.41
1:A:334:VAL:HG11	1:A:489:MET:HE1	2.03	0.41
1:B:377:HIS:HD2	1:B:396:LEU:HD13	1.86	0.41
3:F:36:MET:HG3	3:F:81:VAL:CG2	2.51	0.41
1:A:500:ASP:OD1	1:A:500:ASP:C	2.64	0.41
1:H:181:PHE:HB3	1:H:214:ILE:HD13	2.02	0.41
1:H:458:LEU:O	1:H:459:LYS:C	2.64	0.41
4:H:601:AGS:H8	4:H:601:AGS:O2A	2.20	0.41
1:A:497:LYS:NZ	2:C:101:ASP:OD1	2.53	0.41
3:E:14:VAL:HG21	3:E:88:LEU:HD13	2.03	0.41
1:A:428:CYS:SG	3:E:106:PRO:HB2	2.60	0.41
1:H:334:VAL:O	1:H:338:ILE:HG13	2.20	0.41
1:G:500:ASP:OD1	1:G:500:ASP:C	2.64	0.41
2:I:14:VAL:HG11	2:I:19:SER:O	2.21	0.41
1:B:516:ASP:HA	1:B:535:ASN:HD21	1.86	0.40
1:G:537:LEU:O	1:G:543:ARG:HD2	2.21	0.40
1:H:537:LEU:O	1:H:543:ARG:HD2	2.21	0.40
1:H:542:HIS:C	1:H:546:VAL:HG12	2.45	0.40
2:J:35:ALA:N	2:J:101:ASP:O	2.48	0.40
1:A:467:ARG:HH21	1:A:467:ARG:HG2	1.86	0.40
2:J:40:ARG:HG2	2:J:50:ALA:HB2	2.04	0.40
3:L:104:THR:HG22	3:L:111:ALA:O	2.21	0.40
1:B:537:LEU:O	1:B:543:ARG:HD2	2.22	0.40
4:B:601:AGS:H8	4:B:601:AGS:O2A	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:TYR:HB3	1:G:374:GLY:O	2.22	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	360/413 (87%)	334 (93%)	25 (7%)	1 (0%)	36	64
1	B	371/413 (90%)	344 (93%)	26 (7%)	1 (0%)	36	64
1	G	359/413 (87%)	334 (93%)	24 (7%)	1 (0%)	36	64
1	H	367/413 (89%)	342 (93%)	24 (6%)	1 (0%)	36	64
2	C	123/136 (90%)	119 (97%)	4 (3%)	0	100	100
2	D	116/136 (85%)	112 (97%)	4 (3%)	0	100	100
2	I	123/136 (90%)	114 (93%)	9 (7%)	0	100	100
2	J	115/136 (85%)	110 (96%)	5 (4%)	0	100	100
3	E	123/134 (92%)	113 (92%)	10 (8%)	0	100	100
3	F	112/134 (84%)	98 (88%)	14 (12%)	0	100	100
3	K	122/134 (91%)	113 (93%)	9 (7%)	0	100	100
3	L	113/134 (84%)	100 (88%)	13 (12%)	0	100	100
All	All	2404/2732 (88%)	2233 (93%)	167 (7%)	4 (0%)	43	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ASP
1	B	398	ASP
1	G	398	ASP

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Mol	Chain	Res	Type
1	H	398	ASP

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	320/397 (81%)	310 (97%)	10 (3%)	35	69
1	B	305/397 (77%)	297 (97%)	8 (3%)	40	73
1	G	316/397 (80%)	299 (95%)	17 (5%)	20	50
1	H	308/397 (78%)	295 (96%)	13 (4%)	26	59
2	C	83/104 (80%)	81 (98%)	2 (2%)	43	75
2	D	79/104 (76%)	76 (96%)	3 (4%)	29	62
2	I	82/104 (79%)	79 (96%)	3 (4%)	30	63
2	J	79/104 (76%)	78 (99%)	1 (1%)	61	85
3	E	89/105 (85%)	85 (96%)	4 (4%)	24	57
3	F	74/105 (70%)	71 (96%)	3 (4%)	27	60
3	K	90/105 (86%)	87 (97%)	3 (3%)	33	67
3	L	77/105 (73%)	73 (95%)	4 (5%)	21	51
All	All	1902/2424 (78%)	1831 (96%)	71 (4%)	30	63

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	320	ASN
1	A	407	THR
1	A	431	LYS
1	A	432	ILE
1	A	441	LYS
1	A	452	LYS
1	A	464	GLN
1	A	546	VAL

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Mol	Chain	Res	Type
1	A	552	SER
1	B	161	ASN
1	B	278	LYS
1	B	308	ASN
1	B	407	THR
1	B	432	ILE
1	B	464	GLN
1	B	468	LYS
1	B	546	VAL
2	C	106	SER
2	C	114	ASP
2	D	40	ARG
2	D	41	GLN
2	D	47	ARG
3	E	22	LEU
3	E	50	VAL
3	E	95	VAL
3	E	124	THR
3	F	22	LEU
3	F	107	GLN
3	F	124	THR
1	G	161	ASN
1	G	204	LEU
1	G	208	LYS
1	G	229	ILE
1	G	230	LYS
1	G	278	LYS
1	G	314	LYS
1	G	320	ASN
1	G	376	THR
1	G	397	CYS
1	G	407	THR
1	G	431	LYS
1	G	432	ILE
1	G	441	LYS
1	G	464	GLN
1	G	521	ILE
1	G	522	MET
1	H	161	ASN
1	H	278	LYS
1	H	308	ASN
1	H	348	VAL

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Mol	Chain	Res	Type
1	H	385	MET
1	H	407	THR
1	H	431	LYS
1	H	432	ILE
1	H	451	ILE
1	H	464	GLN
1	H	468	LYS
1	H	546	VAL
1	H	558	SER
2	I	91	GLU
2	I	106	SER
2	I	114	ASP
2	J	40	ARG
3	K	22	LEU
3	K	103	ARG
3	K	124	THR
3	L	22	LEU
3	L	89	LYS
3	L	121	THR
3	L	124	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	322	ASN
1	A	362	ASN
1	A	365	ASN
1	A	377	HIS
1	A	384	ASN
1	A	417	ASN
1	A	532	ASN
1	A	535	ASN
1	B	161	ASN
1	B	166	GLN
1	B	362	ASN
1	B	365	ASN
1	B	384	ASN
1	B	463	ASN
1	B	528	HIS
1	B	532	ASN
1	B	535	ASN

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Mol	Chain	Res	Type
2	D	86	ASN
3	E	41	GLN
3	E	49	ASN
3	E	84	GLN
3	E	86	ASN
1	G	166	GLN
1	G	322	ASN
1	G	362	ASN
1	G	365	ASN
1	G	417	ASN
1	G	532	ASN
1	G	535	ASN
1	H	161	ASN
1	H	166	GLN
1	H	322	ASN
1	H	365	ASN
1	H	417	ASN
1	H	463	ASN
1	H	492	ASN
1	H	528	HIS
1	H	532	ASN
1	H	535	ASN
2	J	61	HIS
3	K	41	GLN
3	K	49	ASN
3	K	84	GLN
3	K	86	ASN
3	L	107	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

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AGS	A	601	-	32,33,33	0.73	1 (3%)	45,52,52	0.71	2 (4%)
4	AGS	H	601	-	32,33,33	0.89	3 (9%)	45,52,52	0.61	0
4	AGS	B	601	-	32,33,33	0.78	1 (3%)	45,52,52	0.61	0
4	AGS	G	601	-	32,33,33	0.78	1 (3%)	45,52,52	0.58	0
5	PE4	A	602	-	23,23,23	0.28	0	22,22,22	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	A	601	-	-	3/21/38/38	0/3/3/3
4	AGS	H	601	-	-	6/21/38/38	0/3/3/3
4	AGS	B	601	-	-	7/21/38/38	0/3/3/3
4	AGS	G	601	-	-	8/21/38/38	0/3/3/3
5	PE4	A	602	-	-	10/21/21/21	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	601	AGS	PA-O3A	2.70	1.62	1.59
4	G	601	AGS	PG-S1G	2.54	1.96	1.90
4	H	601	AGS	PG-S1G	2.37	1.95	1.90
4	B	601	AGS	PA-O3A	2.29	1.62	1.59
4	A	601	AGS	PA-O3A	2.24	1.61	1.59
4	H	601	AGS	PB-O3A	2.00	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	AGS	O3G-PG-O3B	-2.65	95.81	104.64
4	A	601	AGS	O2B-PB-O3A	2.02	112.72	107.27

There are no chirality outliers.

All (34) torsion outliers are listed below:

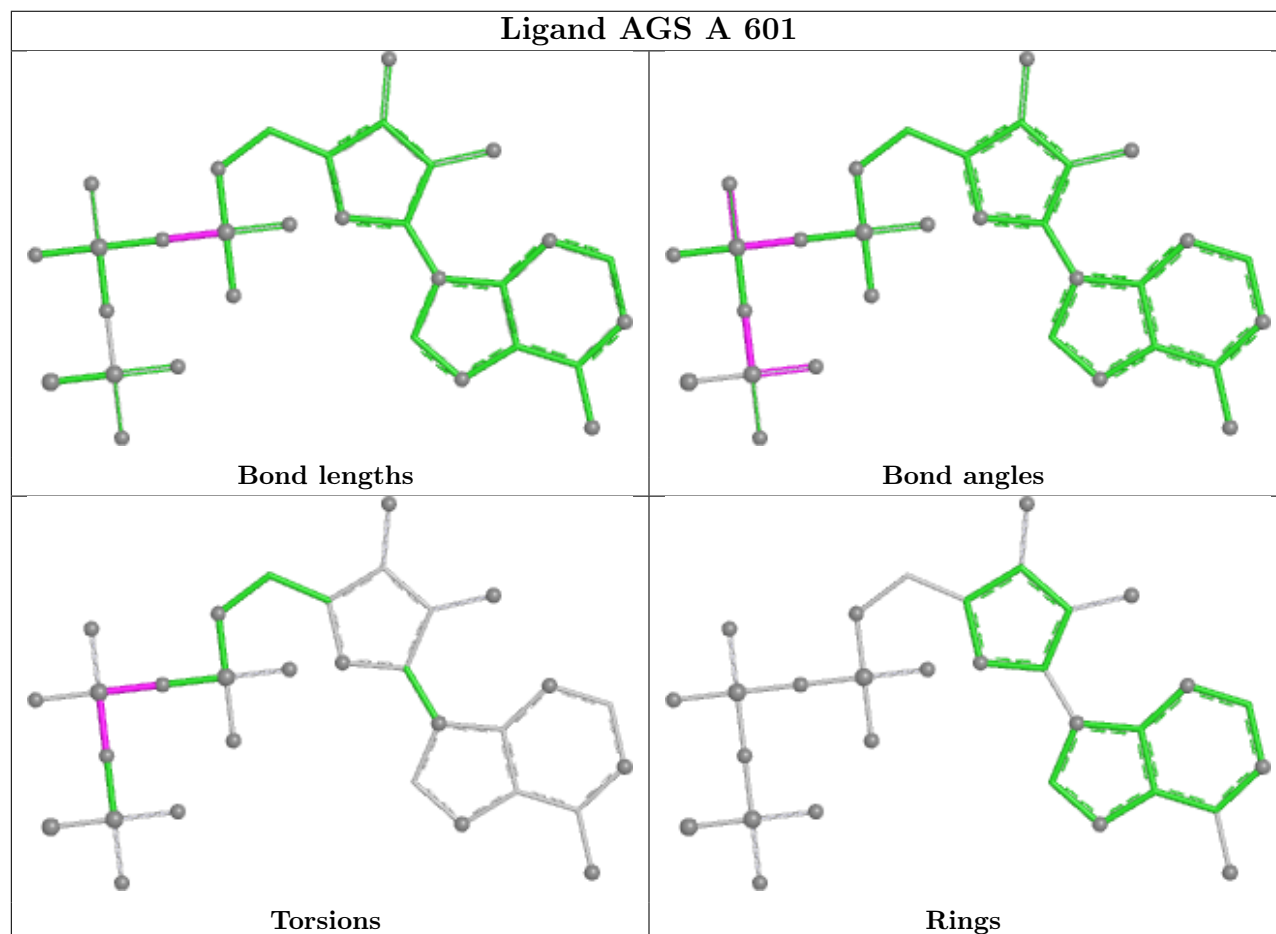
Mol	Chain	Res	Type	Atoms
4	B	601	AGS	C5'-O5'-PA-O1A
4	B	601	AGS	C5'-O5'-PA-O3A
4	G	601	AGS	PB-O3B-PG-O2G
4	G	601	AGS	PB-O3B-PG-O3G
4	G	601	AGS	C5'-O5'-PA-O1A
4	G	601	AGS	C5'-O5'-PA-O2A
4	G	601	AGS	C5'-O5'-PA-O3A
4	H	601	AGS	C5'-O5'-PA-O1A
5	A	602	PE4	C12-C11-O6-C10
5	A	602	PE4	O6-C11-C12-O7
4	B	601	AGS	PG-O3B-PB-O1B
5	A	602	PE4	C6-C5-O3-C4
5	A	602	PE4	C9-C10-O6-C11
4	B	601	AGS	C5'-O5'-PA-O2A
4	H	601	AGS	C5'-O5'-PA-O2A
4	H	601	AGS	C5'-O5'-PA-O3A
4	H	601	AGS	PG-O3B-PB-O2B
5	A	602	PE4	O2-C3-C4-O3
5	A	602	PE4	O6-C10-C9-O5
5	A	602	PE4	C11-C12-O7-C13
5	A	602	PE4	C16-C15-O8-C14
4	H	601	AGS	C4'-C5'-O5'-PA
4	B	601	AGS	PG-O3B-PB-O2B
5	A	602	PE4	C14-C13-O7-C12
4	B	601	AGS	PA-O3A-PB-O1B
4	H	601	AGS	PA-O3A-PB-O1B
4	B	601	AGS	C4'-C5'-O5'-PA
4	A	601	AGS	PG-O3B-PB-O1B
4	A	601	AGS	PG-O3B-PB-O2B
4	G	601	AGS	PG-O3B-PB-O2B
4	A	601	AGS	PA-O3A-PB-O2B
5	A	602	PE4	C8-C7-O4-C6
4	G	601	AGS	O4'-C4'-C5'-O5'
4	G	601	AGS	C3'-C4'-C5'-O5'

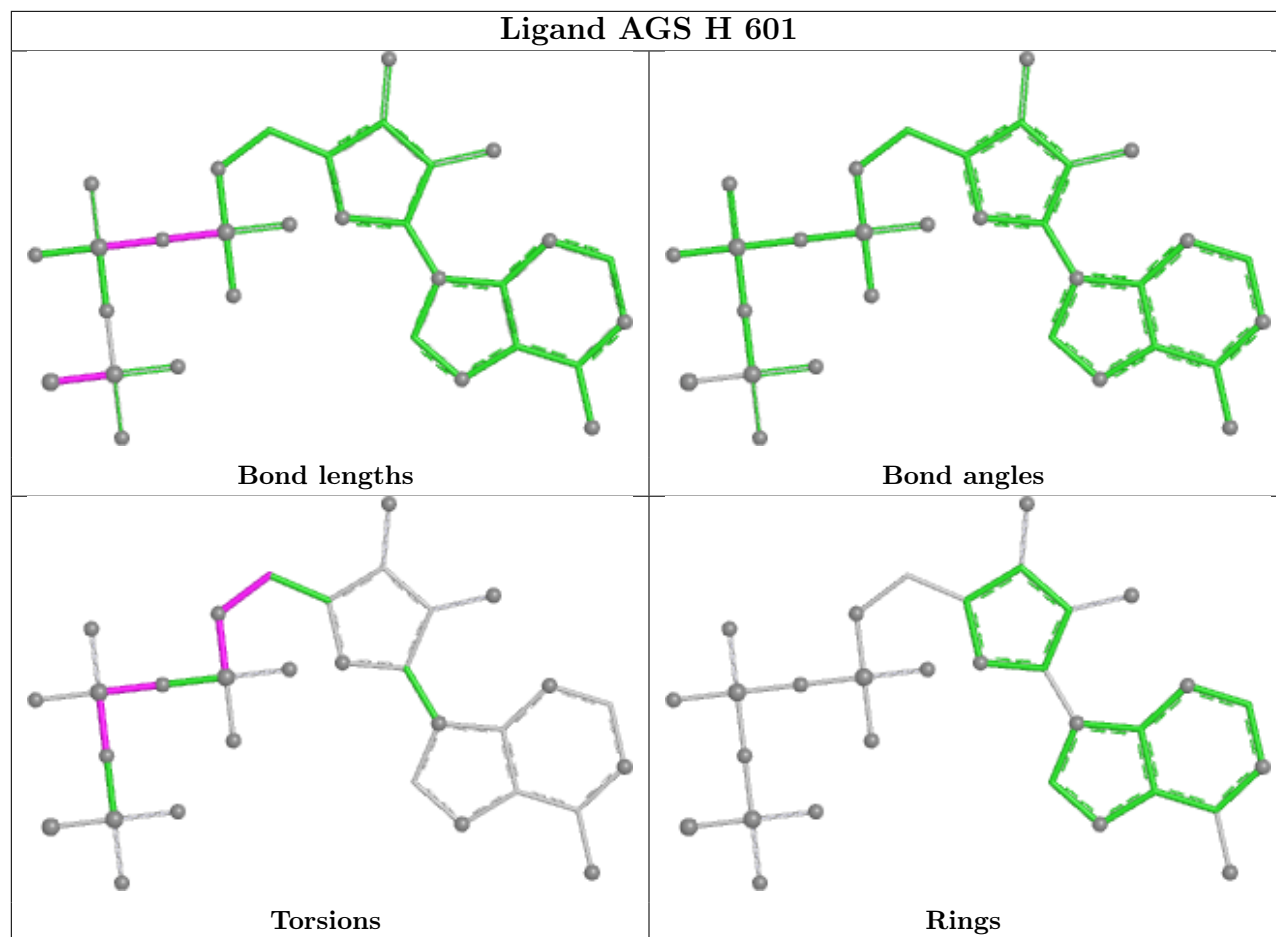
There are no ring outliers.

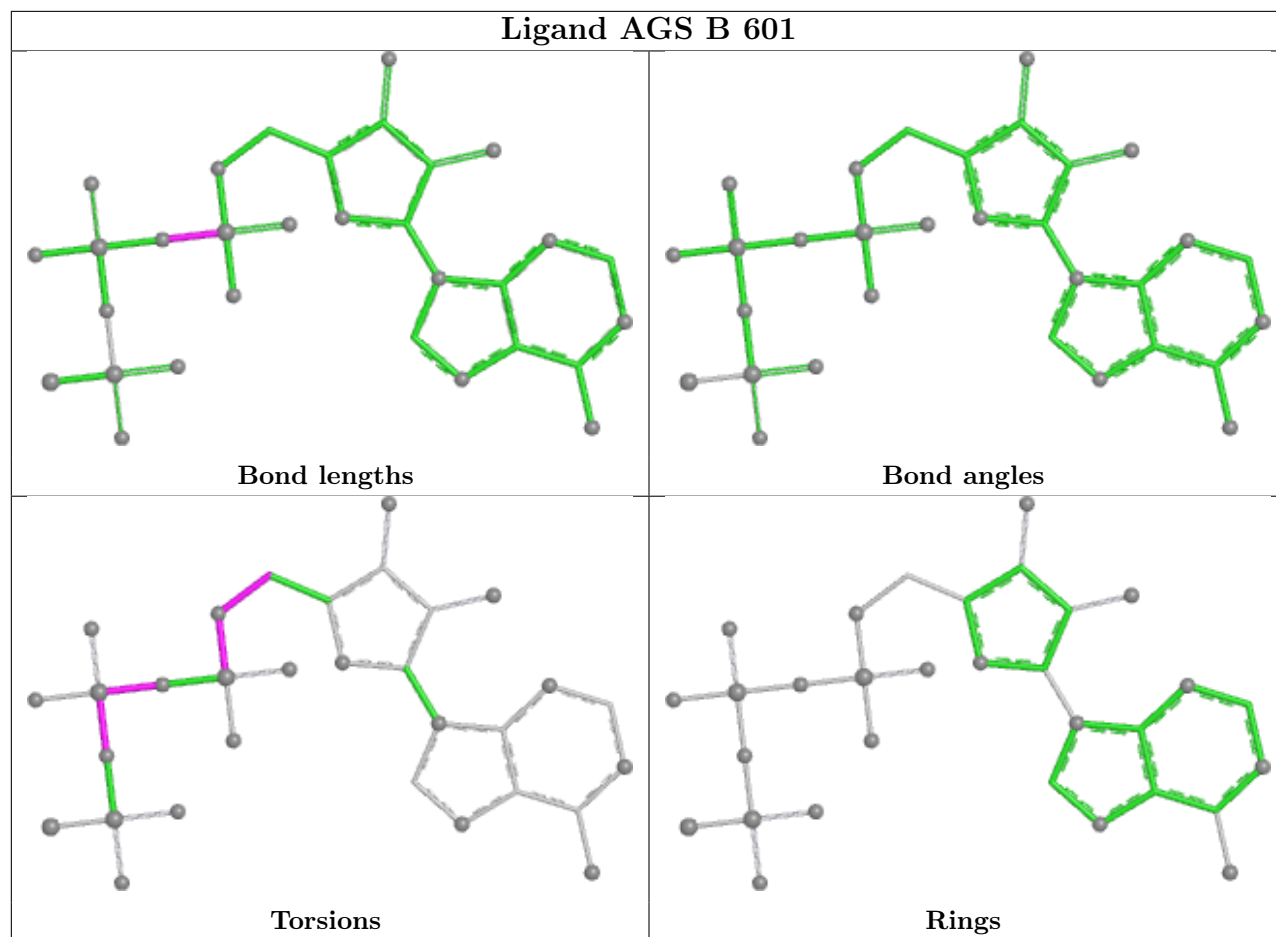
5 monomers are involved in 17 short contacts:

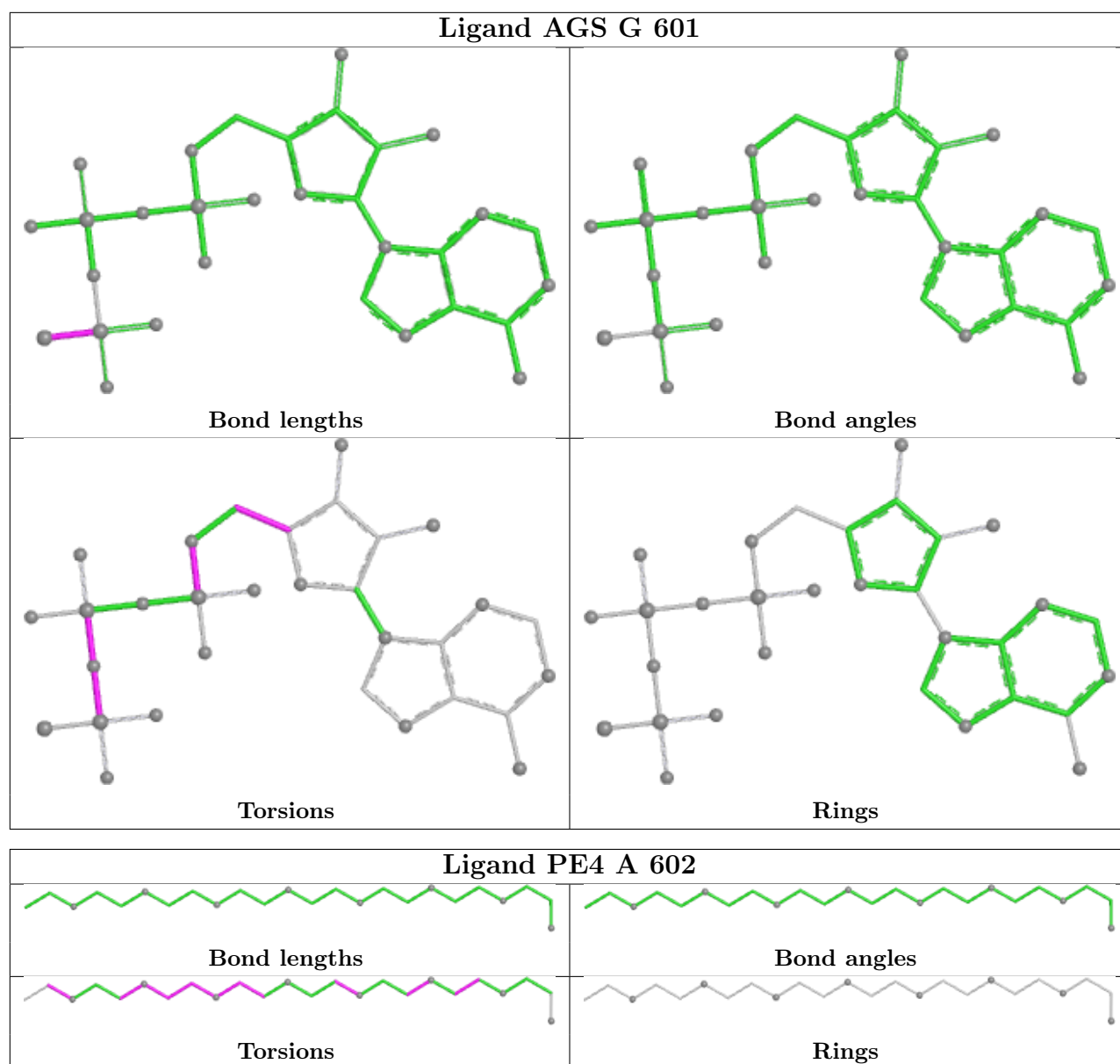
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	AGS	4	0
4	H	601	AGS	4	0
4	B	601	AGS	5	0
4	G	601	AGS	2	0
5	A	602	PE4	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	370/413 (89%)	-0.84	0 100 100	47, 65, 94, 128	0
1	B	379/413 (91%)	-0.87	0 100 100	53, 71, 98, 130	0
1	G	369/413 (89%)	-0.85	0 100 100	46, 65, 92, 125	0
1	H	375/413 (90%)	-0.87	0 100 100	52, 70, 96, 112	0
2	C	125/136 (91%)	-0.92	0 100 100	53, 77, 97, 108	0
2	D	122/136 (89%)	-0.62	0 100 100	68, 93, 135, 157	0
2	I	125/136 (91%)	-0.93	0 100 100	54, 77, 100, 110	0
2	J	121/136 (88%)	-0.66	0 100 100	66, 92, 134, 154	0
3	E	125/134 (93%)	-0.78	0 100 100	52, 78, 101, 128	0
3	F	116/134 (86%)	-0.85	0 100 100	54, 73, 104, 126	0
3	K	124/134 (92%)	-0.86	0 100 100	52, 77, 100, 135	0
3	L	117/134 (87%)	-0.81	0 100 100	57, 73, 102, 114	0
All	All	2468/2732 (90%)	-0.84	0 100 100	46, 72, 105, 157	0

There are no RSRZ outliers to report.

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 ⓘ

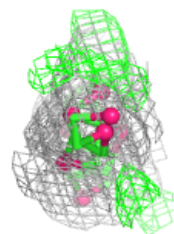
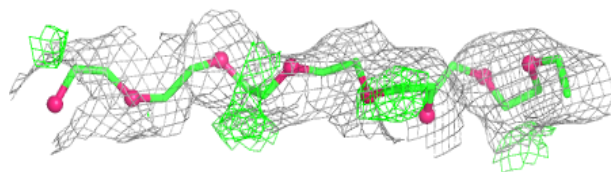
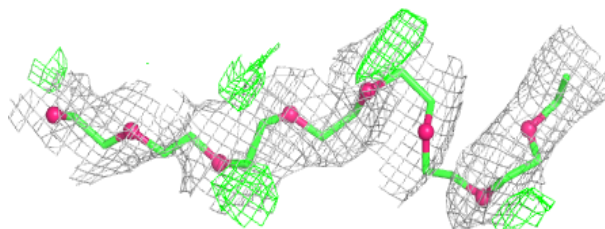
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PE4	A	602	24/24	0.96	0.07	96,128,150,155	0
4	AGS	G	601	31/31	0.98	0.06	80,100,117,123	13
4	AGS	A	601	31/31	0.99	0.05	76,87,110,120	13
4	AGS	H	601	31/31	0.99	0.06	65,89,106,112	12
4	AGS	B	601	31/31	0.99	0.06	66,86,100,105	12

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

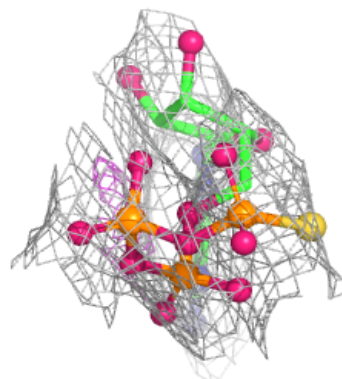
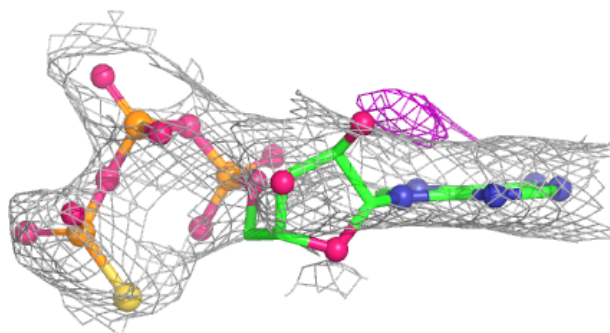
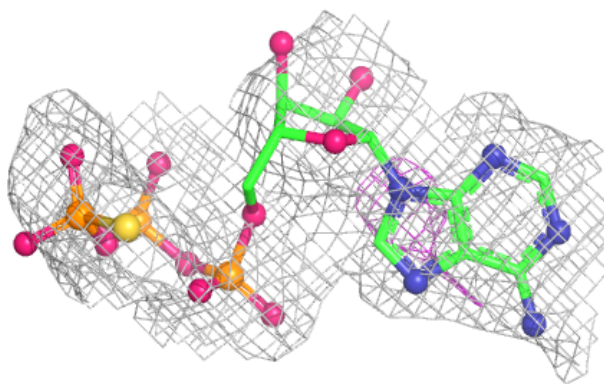
Electron density around PE4 A 602:

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

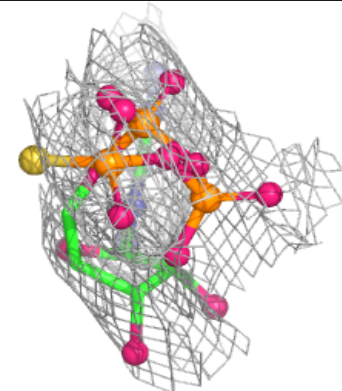
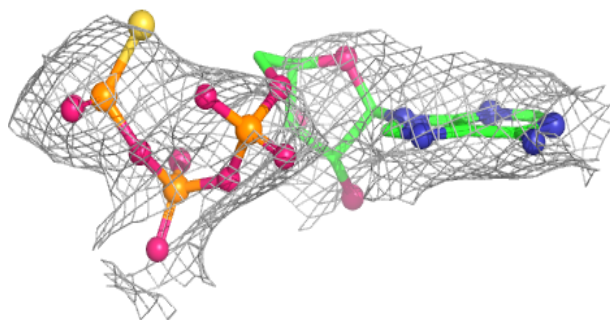
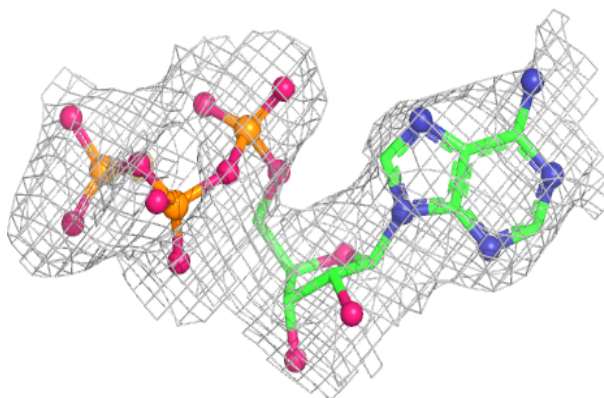


Electron density around AGS G 601:

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

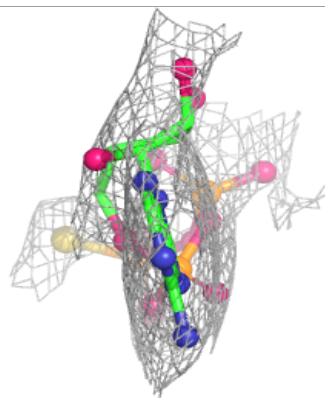
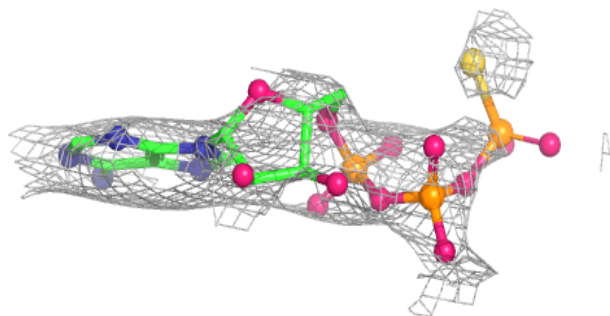
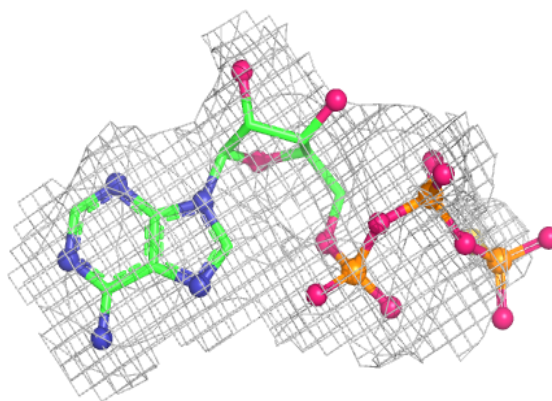
**Electron density around AGS A 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

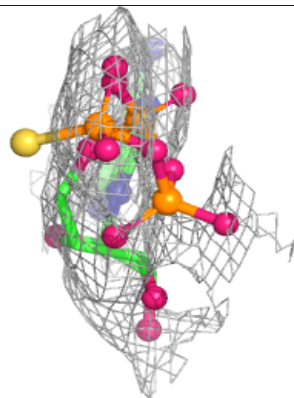
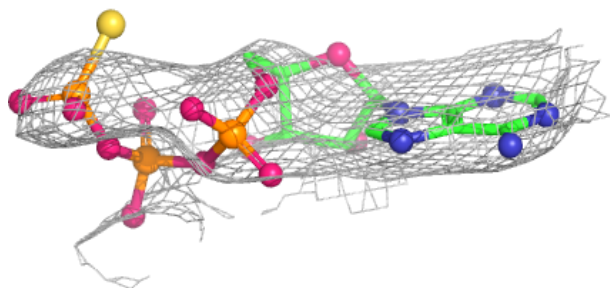
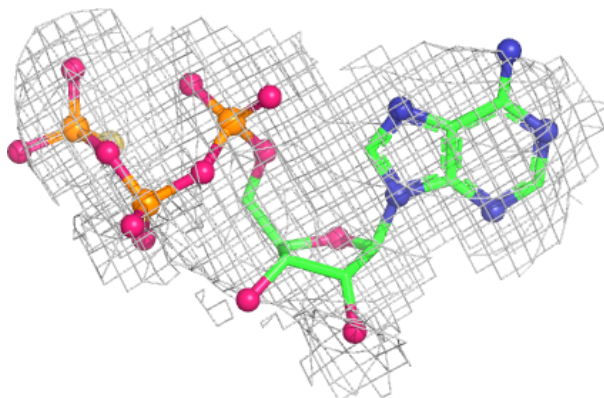


Electron density around AGS H 601:

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

**Electron density around AGS B 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.