



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:09 AM UTC

PDB ID : 5D3M / pdb_00005d3m
Title : Folate ECF transporter: AMPPNP bound state
Authors : Guskov, A.; Swier, L.J.Y.M.; Slotboom, D.J.
Deposited on : 2015-08-06
Resolution : 3.30 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:

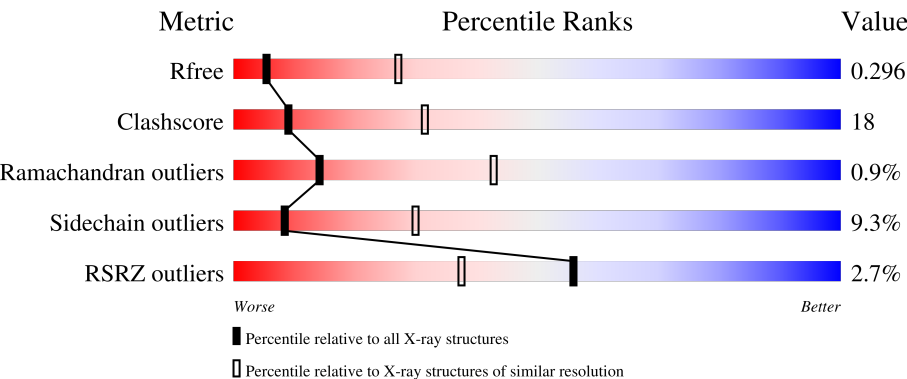
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	298	2% 61% 29% • • 6%
1	E	298	4% 63% 27% • 6%
2	B	287	% 69% 26% • •
2	F	287	3% 66% 28% • •
3	C	184	3% 44% 36% 10% • 9%

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Mol	Chain	Length	Quality of chain
3	G	184	3% 43% 38% 10% 9%
4	D	265	2% 55% 34% 8%
4	H	265	3% 48% 39% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15554 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 Energy-coupling factor transporter ATP-binding protein EcfA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2147	1354	359	430	4			
1	E	280	Total	C	N	O	S	0	0	0
			2147	1354	359	430	4			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q1GBJ0
A	-16	HIS	-	expression tag	UNP Q1GBJ0
A	-15	HIS	-	expression tag	UNP Q1GBJ0
A	-14	HIS	-	expression tag	UNP Q1GBJ0
A	-13	HIS	-	expression tag	UNP Q1GBJ0
A	-12	HIS	-	expression tag	UNP Q1GBJ0
A	-11	HIS	-	expression tag	UNP Q1GBJ0
A	-10	HIS	-	expression tag	UNP Q1GBJ0
A	-9	HIS	-	expression tag	UNP Q1GBJ0
A	-8	HIS	-	expression tag	UNP Q1GBJ0
A	-7	HIS	-	expression tag	UNP Q1GBJ0
A	-6	GLY	-	expression tag	UNP Q1GBJ0
A	-5	GLU	-	expression tag	UNP Q1GBJ0
A	-4	ASN	-	expression tag	UNP Q1GBJ0
A	-3	LEU	-	expression tag	UNP Q1GBJ0
A	-2	TYR	-	expression tag	UNP Q1GBJ0
A	-1	PHE	-	expression tag	UNP Q1GBJ0
A	0	GLN	-	expression tag	UNP Q1GBJ0
A	1	GLY	-	expression tag	UNP Q1GBJ0
E	-17	MET	-	initiating methionine	UNP Q1GBJ0
E	-16	HIS	-	expression tag	UNP Q1GBJ0
E	-15	HIS	-	expression tag	UNP Q1GBJ0
E	-14	HIS	-	expression tag	UNP Q1GBJ0
E	-13	HIS	-	expression tag	UNP Q1GBJ0
E	-12	HIS	-	expression tag	UNP Q1GBJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	HIS	-	expression tag	UNP Q1GBJ0
E	-10	HIS	-	expression tag	UNP Q1GBJ0
E	-9	HIS	-	expression tag	UNP Q1GBJ0
E	-8	HIS	-	expression tag	UNP Q1GBJ0
E	-7	HIS	-	expression tag	UNP Q1GBJ0
E	-6	GLY	-	expression tag	UNP Q1GBJ0
E	-5	GLU	-	expression tag	UNP Q1GBJ0
E	-4	ASN	-	expression tag	UNP Q1GBJ0
E	-3	LEU	-	expression tag	UNP Q1GBJ0
E	-2	TYR	-	expression tag	UNP Q1GBJ0
E	-1	PHE	-	expression tag	UNP Q1GBJ0
E	0	GLN	-	expression tag	UNP Q1GBJ0
E	1	GLY	-	expression tag	UNP Q1GBJ0

- Molecule 2 is a protein called Energy-coupling factor transporter ATP-binding protein EcfA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	281	Total	C	N	O	S	0	0	0
			2183	1394	370	411	8			
2	F	281	Total	C	N	O	S	0	0	0
			2183	1394	370	411	8			

- Molecule 3 is a protein called S-component for folate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	168	Total	C	N	O	S	0	0	0
			1302	876	206	210	10			
3	G	168	Total	C	N	O	S	0	0	0
			1302	876	206	210	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	177	TRP	-	expression tag	UNP Q1G929
C	178	SER	-	expression tag	UNP Q1G929
C	179	HIS	-	expression tag	UNP Q1G929
C	180	PRO	-	expression tag	UNP Q1G929
C	181	GLN	-	expression tag	UNP Q1G929
C	182	PHE	-	expression tag	UNP Q1G929
C	183	GLU	-	expression tag	UNP Q1G929
C	184	LYS	-	expression tag	UNP Q1G929
G	177	TRP	-	expression tag	UNP Q1G929

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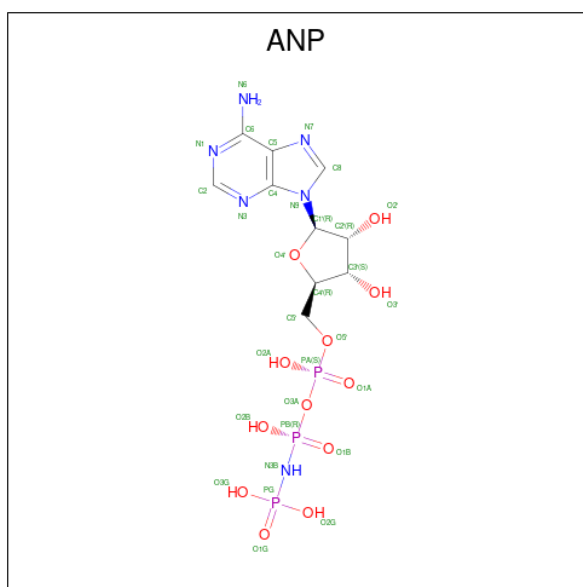
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Chain	Residue	Modelled	Actual	Comment	Reference
G	178	SER	-	expression tag	UNP Q1G929
G	179	HIS	-	expression tag	UNP Q1G929
G	180	PRO	-	expression tag	UNP Q1G929
G	181	GLN	-	expression tag	UNP Q1G929
G	182	PHE	-	expression tag	UNP Q1G929
G	183	GLU	-	expression tag	UNP Q1G929
G	184	LYS	-	expression tag	UNP Q1G929

- Molecule 4 is a protein called Energy-coupling factor transporter transmembrane protein EcfT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	259	Total	C	N	O	S	0	0	0
			2083	1391	333	345	14			
4	H	259	Total	C	N	O	S	0	0	0
			2083	1391	333	345	14			

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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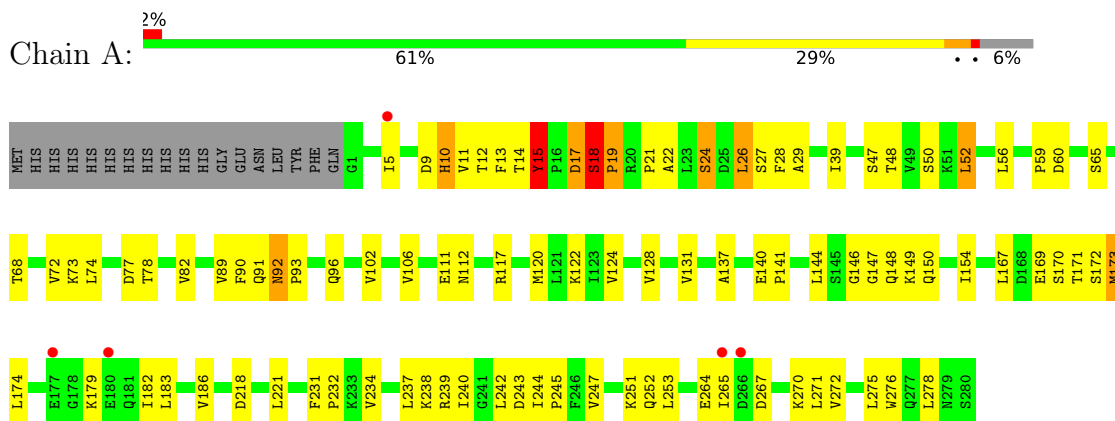
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

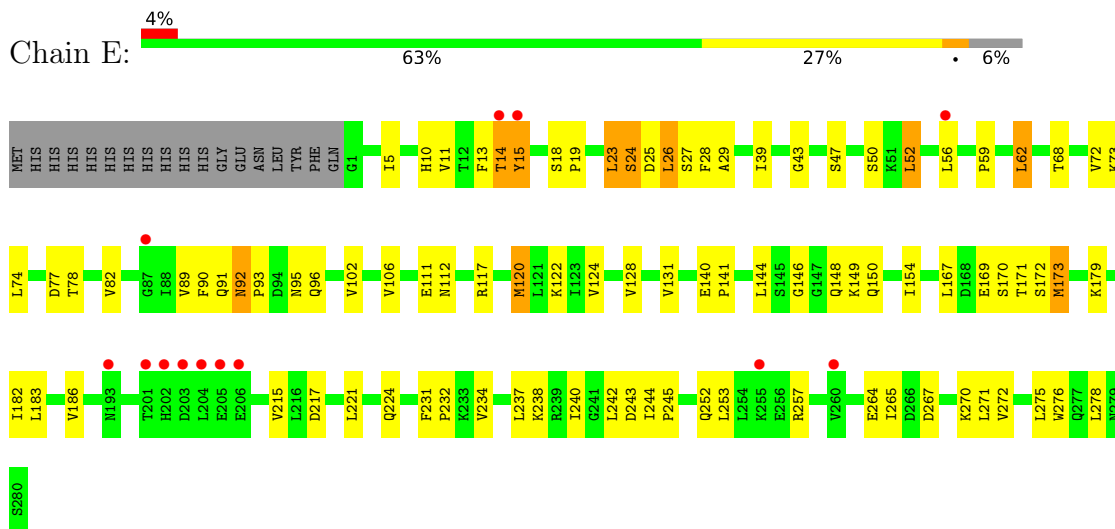
3 Residue-property plots [i](#)

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.

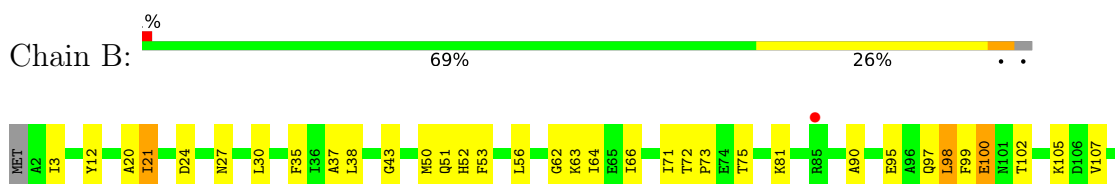
- Molecule 1: Energy-coupling factor transporter ATP-binding protein EcfA1

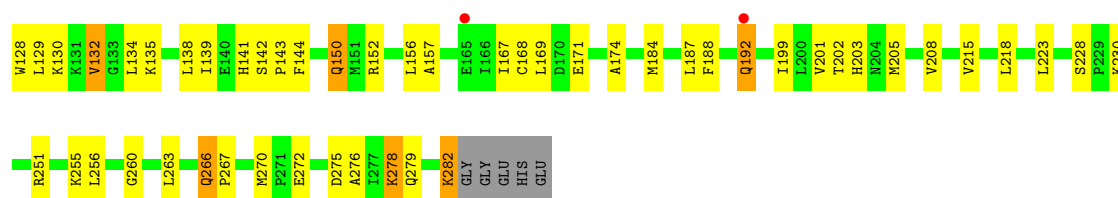


- Molecule 1: Energy-coupling factor transporter ATP-binding protein EcfA1

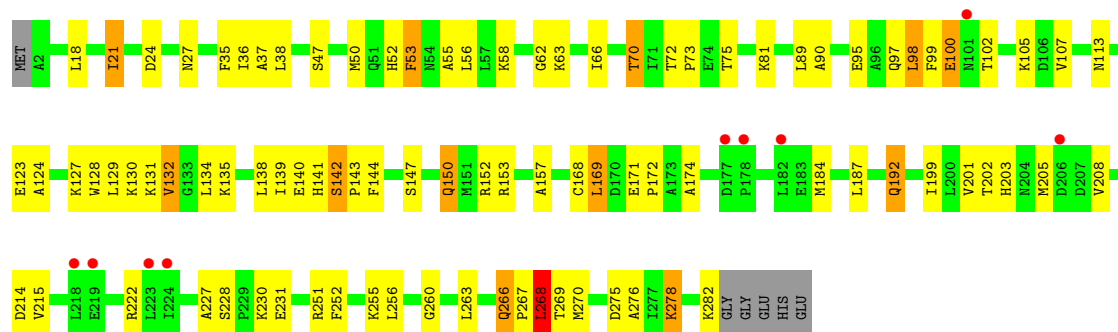


- Molecule 2: Energy-coupling factor transporter ATP-binding protein EcfA2

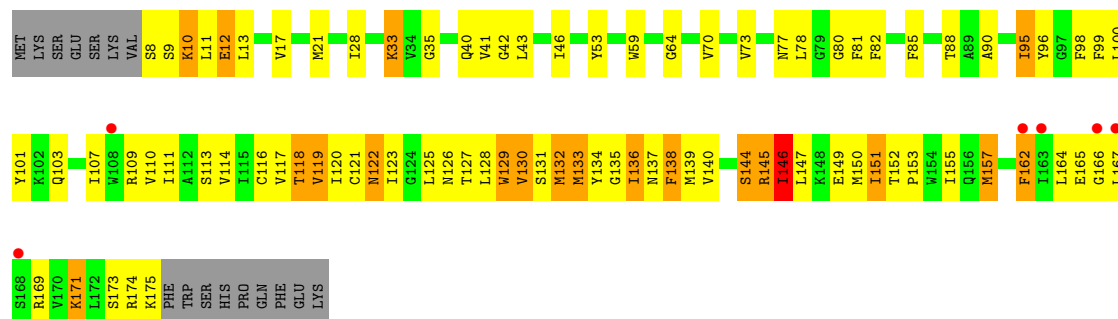




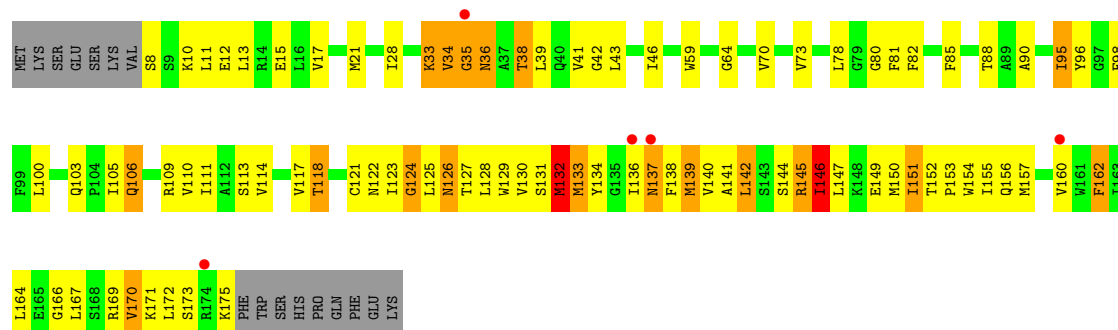
• Molecule 2: Energy-coupling factor transporter ATP-binding protein EcfA2



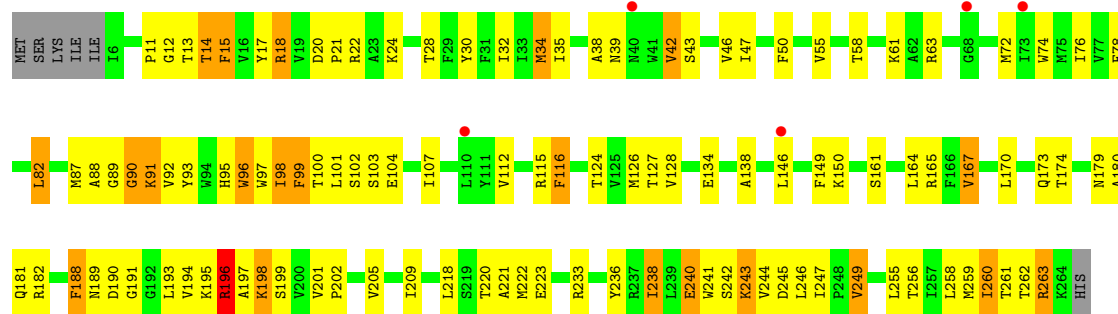
• Molecule 3: S-component for folate



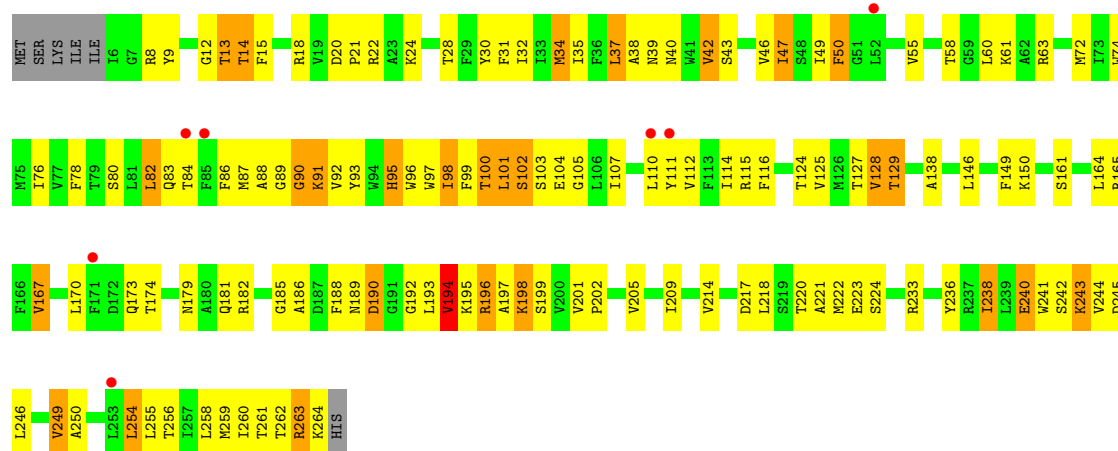
• Molecule 3: S-component for folate



• Molecule 4: Energy-coupling factor transporter transmembrane protein EcfT



• Molecule 4: Energy-coupling factor transporter transmembrane protein EcFt



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.07Å 97.26Å 105.45Å 84.67° 64.78° 62.59°	Depositor
Resolution (Å)	43.86 – 3.30 43.86 – 3.30	Depositor EDS
% Data completeness (in resolution range)	78.8 (43.86-3.30) 78.8 (43.86-3.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.250 , 0.289 0.255 , 0.296	Depositor DCC
R_{free} test set	1709 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	132.9	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 153.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.368 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15554	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: ANP

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	0.44	0/2180	0.94	5/2959 (0.2%)
1	E	0.40	0/2180	0.93	4/2959 (0.1%)
2	B	0.35	0/2229	0.87	2/3009 (0.1%)
2	F	0.36	0/2229	0.87	2/3009 (0.1%)
3	C	0.53	0/1333	1.15	8/1806 (0.4%)
3	G	0.47	0/1333	1.12	7/1806 (0.4%)
4	D	0.46	1/2136 (0.0%)	1.02	12/2901 (0.4%)
4	H	0.46	1/2136 (0.0%)	1.07	18/2901 (0.6%)
All	All	0.43	2/15756 (0.0%)	0.98	58/21350 (0.3%)

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	2
1	E	0	1
2	B	0	1
2	F	0	1
3	G	0	1
4	D	0	1
4	H	0	6
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	201	VAL	CA-CB	5.37	1.57	1.53
4	H	201	VAL	CA-CB	5.04	1.57	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	146	ILE	N-CA-C	9.34	120.15	110.72
3	C	129	TRP	N-CA-C	9.21	125.25	112.45
4	H	98	ILE	CA-C-N	9.19	138.25	121.70
4	H	98	ILE	C-N-CA	9.19	138.25	121.70
3	C	146	ILE	N-CA-C	8.41	121.56	111.05
4	H	196	ARG	N-CA-C	8.23	121.82	111.69
4	H	196	ARG	CA-C-N	8.17	136.40	121.70
4	H	196	ARG	C-N-CA	8.17	136.40	121.70
3	C	135	GLY	N-CA-C	7.65	121.91	112.73
4	H	90	GLY	N-CA-C	7.53	124.97	110.66
4	D	90	GLY	N-CA-C	7.46	124.84	110.66
4	D	98	ILE	CA-C-N	7.27	134.79	121.70
4	D	98	ILE	C-N-CA	7.27	134.79	121.70
3	G	124	GLY	N-CA-C	7.18	120.83	112.50
4	D	196	ARG	CA-C-N	7.12	134.51	121.70
4	D	196	ARG	C-N-CA	7.12	134.51	121.70
4	H	205	VAL	CA-C-N	-7.05	112.44	119.56
4	H	205	VAL	C-N-CA	-7.05	112.44	119.56
4	D	196	ARG	N-CA-C	7.03	119.97	111.40
4	D	205	VAL	CA-C-N	-6.79	112.70	119.56
4	D	205	VAL	C-N-CA	-6.79	112.70	119.56
3	G	132	MET	N-CA-C	-6.67	101.28	110.35
2	B	100	GLU	CB-CA-C	-6.36	107.50	115.89
4	H	98	ILE	N-CA-C	6.30	122.45	109.34
2	F	100	GLU	CB-CA-C	-6.28	107.60	115.89
3	C	119	VAL	N-CA-C	6.24	116.41	110.42
2	F	268	LEU	CA-CB-CG	6.21	138.03	116.30
3	C	128	LEU	N-CA-C	6.16	121.08	113.50
1	A	92	ASN	CA-C-N	6.14	126.32	119.32
1	A	92	ASN	C-N-CA	6.14	126.32	119.32
3	G	145	ARG	N-CA-C	6.10	120.86	113.17
4	H	40	ASN	N-CA-C	6.04	118.35	111.11
4	D	20	ASP	CA-C-N	5.94	125.14	118.97
4	D	20	ASP	C-N-CA	5.94	125.14	118.97
1	E	92	ASN	CA-C-N	5.90	126.04	119.32
1	E	92	ASN	C-N-CA	5.90	126.04	119.32
4	H	20	ASP	CA-C-N	5.82	125.02	118.97
4	H	20	ASP	C-N-CA	5.82	125.02	118.97
1	A	15	TYR	CA-C-N	-5.61	112.83	119.84
1	A	15	TYR	C-N-CA	-5.61	112.83	119.84
4	D	15	PHE	N-CA-C	5.47	117.94	110.55
4	H	14	THR	N-CA-C	5.41	122.33	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	98	ILE	CA-C-O	-5.32	114.13	120.78
4	H	86	PHE	N-CA-C	-5.29	102.37	110.30
3	C	100	LEU	N-CA-C	5.26	120.56	113.72
1	E	243	ASP	N-CA-C	5.25	115.21	108.34
3	C	138	PHE	N-CA-C	5.21	116.77	111.14
4	D	14	THR	N-CA-C	5.21	121.90	110.80
3	C	133	MET	N-CA-C	-5.15	99.83	110.80
3	G	100	LEU	N-CA-C	5.14	120.41	113.72
3	G	11	LEU	CB-CA-C	-5.13	109.11	115.89
4	H	101	LEU	N-CA-C	5.10	116.88	110.24
3	G	35	GLY	N-CA-C	5.04	127.93	113.30
2	B	100	GLU	N-CA-C	5.04	117.49	109.02
1	E	217	ASP	N-CA-C	5.02	116.60	108.26
1	A	243	ASP	N-CA-C	5.02	114.92	108.34
4	H	201	VAL	CA-C-N	-5.00	114.51	119.56
4	H	201	VAL	C-N-CA	-5.00	114.51	119.56

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	SER	Peptide
1	A	26	LEU	Peptide
2	B	132	VAL	Peptide
4	D	196	ARG	Peptide
1	E	26	LEU	Peptide
2	F	132	VAL	Peptide
3	G	132	MET	Peptide
4	H	13	THR	Peptide
4	H	14	THR	Peptide
4	H	15	PHE	Peptide
4	H	192	GLY	Peptide
4	H	197	ALA	Peptide
4	H	97	TRP	Peptide

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	2147	0	2159	63	0
1	E	2147	0	2159	63	0
2	B	2183	0	2187	68	0
2	F	2183	0	2187	68	0
3	C	1302	0	1380	90	0
3	G	1302	0	1380	96	0
4	D	2083	0	2185	91	0
4	H	2083	0	2185	106	0
5	A	31	0	13	4	0
5	B	31	0	13	1	0
5	E	31	0	13	5	0
5	F	31	0	13	1	0
All	All	15554	0	15874	579	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 18.

All (579) 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)
3:C:147:LEU:HG	3:G:147:LEU:H	1.34	0.92
1:E:43:GLY:HA2	5:E:301:ANP:H4'	1.53	0.91
3:G:150:MET:HE2	3:G:151:ILE:HG12	1.56	0.84
4:D:98:ILE:HB	4:D:99:PHE:HB2	1.60	0.84
4:D:38:ALA:HB1	4:D:39:ASN:HB2	1.61	0.83
3:C:174:ARG:HG3	3:C:175:LYS:HB2	1.63	0.80
4:H:92:VAL:HG22	4:H:104:GLU:HB2	1.62	0.80
1:A:90:PHE:HB2	1:A:96:GLN:HG2	1.65	0.78
3:C:150:MET:HE2	3:C:151:ILE:HG12	1.66	0.77
4:D:196:ARG:N	4:D:197:ALA:HB3	2.00	0.76
3:G:140:VAL:HG21	4:H:82:LEU:HD22	1.65	0.76
4:D:39:ASN:ND2	4:D:263:ARG:O	2.17	0.76
3:G:121:CYS:O	3:G:126:ASN:ND2	2.19	0.76
4:H:39:ASN:HD21	4:H:264:LYS:HE3	1.48	0.76
1:E:173:MET:SD	1:E:173:MET:N	2.59	0.75
3:C:133:MET:HE3	3:C:134:TYR:H	1.51	0.75
1:A:141:PRO:O	1:A:149:LYS:NZ	2.20	0.75
3:C:121:CYS:HA	3:C:125:LEU:HD23	1.69	0.75
4:H:193:LEU:HA	4:H:196:ARG:HB2	1.69	0.75
3:G:125:LEU:HA	3:G:128:LEU:HG	1.68	0.74
2:F:107:VAL:HG11	2:F:129:LEU:HD21	1.70	0.73
1:E:90:PHE:HB2	1:E:96:GLN:HG2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:196:ARG:H	4:D:197:ALA:HB3	1.55	0.72
1:E:91:GLN:NE2	5:E:301:ANP:O3G	2.23	0.71
3:G:121:CYS:HA	3:G:125:LEU:HD23	1.71	0.71
4:D:100:THR:HG22	4:D:101:LEU:H	1.57	0.70
2:B:107:VAL:HG11	2:B:129:LEU:HD21	1.72	0.70
1:E:238:LYS:HE2	1:E:244:ILE:HD11	1.74	0.70
4:D:98:ILE:CB	4:D:99:PHE:HB2	2.22	0.70
3:C:116:CYS:HB2	3:C:120:ILE:HD11	1.74	0.69
4:H:193:LEU:C	4:H:195:LYS:H	2.00	0.69
4:H:89:GLY:O	4:H:91:LYS:NZ	2.23	0.69
1:A:238:LYS:HE2	1:A:244:ILE:HD11	1.74	0.69
1:E:141:PRO:O	1:E:149:LYS:NZ	2.26	0.68
3:G:140:VAL:HG11	4:H:82:LEU:HD13	1.74	0.68
1:A:106:VAL:HG23	1:A:124:VAL:HG23	1.73	0.68
4:D:39:ASN:N	4:D:43:SER:OG	2.27	0.68
2:F:171:GLU:HB3	2:F:174:ALA:HB2	1.76	0.68
1:E:106:VAL:HG23	1:E:124:VAL:HG23	1.74	0.67
4:H:39:ASN:N	4:H:43:SER:OG	2.26	0.67
4:D:88:ALA:HB2	4:D:98:ILE:HG23	1.78	0.66
3:C:132:MET:O	4:D:115:ARG:NH1	2.28	0.66
1:A:14:THR:HG22	5:A:301:ANP:HN61	1.61	0.66
2:B:171:GLU:HB3	2:B:174:ALA:HB2	1.78	0.66
3:C:88:THR:CG2	3:C:129:TRP:HE1	2.08	0.66
2:B:53:PHE:HB2	2:B:66:ILE:HD13	1.78	0.66
4:H:125:VAL:O	4:H:129:THR:OG1	2.14	0.66
3:C:131:SER:O	3:C:133:MET:HB2	1.95	0.66
3:G:154:TRP:HA	3:G:157:MET:HG3	1.78	0.65
4:H:263:ARG:HD2	4:H:264:LYS:HG2	1.78	0.65
2:F:134:LEU:HD12	2:F:135:LYS:HB2	1.77	0.65
1:A:14:THR:HG22	5:A:301:ANP:N6	2.11	0.65
5:E:301:ANP:O2A	5:E:301:ANP:N3B	2.29	0.65
3:C:118:THR:HG21	3:C:153:PRO:HG3	1.78	0.65
3:C:145:ARG:HA	3:G:147:LEU:HD21	1.79	0.65
4:D:92:VAL:HG22	4:D:104:GLU:HB2	1.79	0.65
4:H:190:ASP:O	4:H:196:ARG:NH1	2.30	0.64
2:B:63:LYS:HD3	2:F:70:THR:HG21	1.78	0.64
2:F:138:LEU:HA	2:F:141:HIS:CD2	2.31	0.64
3:G:128:LEU:HA	3:G:131:SER:HB3	1.78	0.64
3:G:139:MET:HA	3:G:142:LEU:HD23	1.78	0.64
3:G:164:LEU:O	3:G:169:ARG:HB3	1.98	0.64
2:B:138:LEU:HA	2:B:141:HIS:CD2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:GLU:HA	3:G:167:LEU:HD13	1.80	0.63
1:A:17:ASP:OD2	1:A:17:ASP:N	2.31	0.63
2:B:134:LEU:HD12	2:B:135:LYS:HB2	1.79	0.63
3:G:155:ILE:HD13	4:H:193:LEU:HD11	1.78	0.63
3:C:147:LEU:HG	3:G:147:LEU:HB2	1.81	0.63
3:C:147:LEU:HB2	3:G:147:LEU:HB2	1.80	0.63
1:E:252:GLN:HG3	1:E:253:LEU:HD12	1.81	0.63
1:E:77:ASP:O	1:E:78:THR:HG22	1.98	0.63
1:A:112:ASN:OD1	4:D:233:ARG:NH1	2.32	0.63
1:A:252:GLN:HG3	1:A:253:LEU:HD12	1.81	0.63
2:B:90:ALA:HB3	2:B:169:LEU:HD22	1.81	0.63
1:A:11:VAL:HG22	1:A:59:PRO:HA	1.79	0.62
3:G:127:THR:O	3:G:138:PHE:HB2	1.99	0.62
1:A:77:ASP:O	1:A:78:THR:HG22	1.98	0.62
2:F:168:CYS:HB3	2:F:199:ILE:HB	1.80	0.62
1:A:11:VAL:O	1:A:22:ALA:HA	1.99	0.62
3:G:118:THR:HA	3:G:122:ASN:HB3	1.80	0.61
3:G:113:SER:O	3:G:117:VAL:HG23	2.00	0.61
3:G:162:PHE:O	3:G:166:GLY:HA3	2.01	0.61
4:H:39:ASN:ND2	4:H:263:ARG:O	2.32	0.61
3:C:162:PHE:O	3:C:166:GLY:HA3	2.01	0.61
2:B:168:CYS:HB3	2:B:199:ILE:HB	1.81	0.61
2:B:75:THR:HA	2:F:75:THR:HA	1.82	0.61
1:E:112:ASN:OD1	4:H:233:ARG:NH1	2.34	0.61
3:C:110:VAL:O	3:C:113:SER:OG	2.15	0.61
4:D:161:SER:O	4:D:165:ARG:NH1	2.34	0.61
4:H:92:VAL:HG23	4:H:93:TYR:CD1	2.35	0.61
1:A:171:THR:HB	1:A:179:LYS:HG3	1.81	0.60
1:E:272:VAL:HG21	2:F:255:LYS:HD2	1.83	0.60
4:H:38:ALA:HB1	4:H:39:ASN:HB2	1.83	0.60
3:C:147:LEU:HB2	3:G:147:LEU:HD12	1.82	0.60
4:H:50:PHE:HD2	4:H:255:LEU:HD13	1.65	0.60
4:D:194:VAL:O	4:D:195:LYS:HB3	2.02	0.60
1:A:74:LEU:HD12	1:A:82:VAL:HG11	1.84	0.60
4:H:112:VAL:HA	4:H:115:ARG:HG2	1.84	0.59
4:H:161:SER:O	4:H:165:ARG:NH1	2.35	0.59
1:E:74:LEU:HD12	1:E:82:VAL:HG11	1.85	0.59
2:F:98:LEU:HD13	2:F:143:PRO:HB2	1.84	0.59
4:H:43:SER:HB2	4:H:259:MET:HE2	1.83	0.59
4:H:190:ASP:O	4:H:196:ARG:HG3	2.02	0.59
2:F:53:PHE:HB2	2:F:66:ILE:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:HA	1:A:27:SER:HB2	1.85	0.59
4:H:195:LYS:HA	4:H:198:LYS:HB3	1.85	0.59
3:C:81:PHE:N	3:C:82:PHE:HA	2.18	0.59
3:G:81:PHE:N	3:G:82:PHE:HA	2.17	0.59
4:D:91:LYS:HB3	4:D:104:GLU:HB3	1.85	0.58
2:B:37:ALA:HB3	2:B:215:VAL:HG22	1.85	0.58
4:D:30:TYR:HE2	4:D:256:THR:HG21	1.68	0.58
4:H:34:MET:HA	4:H:37:LEU:HD23	1.84	0.58
4:H:96:TRP:HB3	4:H:100:THR:HB	1.85	0.58
1:E:144:LEU:HB3	1:E:148:GLN:HG3	1.85	0.58
2:B:128:TRP:O	2:B:132:VAL:HG12	2.04	0.58
2:B:97:GLN:O	4:D:181:GLN:NE2	2.37	0.58
4:D:95:HIS:N	4:D:96:TRP:HA	2.18	0.58
3:G:136:ILE:O	3:G:139:MET:HG3	2.03	0.58
3:C:96:TYR:CZ	3:C:117:VAL:HG21	2.38	0.57
3:G:136:ILE:HD12	3:G:139:MET:HG2	1.85	0.57
4:H:170:LEU:O	4:H:174:THR:OG1	2.21	0.57
4:H:189:ASN:HB3	4:H:196:ARG:HG2	1.86	0.57
2:B:167:ILE:HD11	2:B:169:LEU:HD21	1.87	0.57
3:C:130:VAL:HG22	3:C:138:PHE:CE1	2.40	0.57
3:G:167:LEU:HA	3:G:170:VAL:HG22	1.85	0.57
4:D:170:LEU:O	4:D:174:THR:OG1	2.21	0.57
2:F:268:LEU:HD13	2:F:269:THR:HG22	1.87	0.57
3:C:131:SER:O	3:C:133:MET:N	2.37	0.57
1:A:11:VAL:HG21	1:A:52:LEU:HD21	1.87	0.56
1:A:272:VAL:HG21	2:B:255:LYS:HD2	1.87	0.56
2:B:134:LEU:HD21	2:B:150:GLN:HB3	1.86	0.56
3:C:10:LYS:HE2	3:C:59:TRP:HE1	1.70	0.56
4:D:195:LYS:HA	4:D:198:LYS:HG2	1.87	0.56
4:D:28:THR:HG21	4:D:126:MET:HB2	1.87	0.56
4:D:96:TRP:HD1	4:D:97:TRP:CD1	2.24	0.56
3:G:127:THR:HG22	3:G:145:ARG:HH22	1.69	0.56
3:G:128:LEU:O	3:G:131:SER:OG	2.21	0.56
3:C:119:VAL:O	3:C:123:ILE:HB	2.05	0.56
3:G:126:ASN:O	3:G:130:VAL:HG23	2.06	0.56
1:A:169:GLU:HG2	1:A:172:SER:HB3	1.87	0.56
3:C:116:CYS:HB2	3:C:120:ILE:CD1	2.35	0.56
2:F:134:LEU:HD21	2:F:150:GLN:HB3	1.88	0.56
4:H:30:TYR:CE2	4:H:256:THR:HG21	2.41	0.56
4:H:124:THR:O	4:H:128:VAL:HG22	2.05	0.55
3:C:95:ILE:HD11	3:C:117:VAL:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:82:PHE:HB3	3:G:85:PHE:H	1.71	0.55
3:G:28:ILE:HD11	4:H:167:VAL:HG13	1.87	0.55
3:G:39:LEU:HD12	3:G:151:ILE:HD12	1.88	0.55
2:F:135:LYS:HB3	2:F:138:LEU:HG	1.89	0.55
3:G:36:ASN:N	3:G:36:ASN:HD22	2.03	0.55
1:A:102:VAL:O	1:A:106:VAL:HG22	2.07	0.55
3:C:53:TYR:HE1	3:C:169:ARG:HD3	1.71	0.55
3:G:95:ILE:HD11	3:G:117:VAL:HG22	1.89	0.55
3:G:172:LEU:O	3:G:175:LYS:N	2.31	0.55
4:H:91:LYS:HB3	4:H:104:GLU:HB3	1.88	0.55
4:H:21:PRO:HB2	4:H:138:ALA:HB2	1.89	0.55
1:A:231:PHE:N	1:A:232:PRO:HD2	2.22	0.55
3:C:11:LEU:C	3:C:12:GLU:HG2	2.31	0.55
2:F:37:ALA:HB3	2:F:215:VAL:HG22	1.89	0.55
3:C:99:PHE:O	3:C:109:ARG:HD3	2.06	0.55
4:D:88:ALA:CB	4:D:98:ILE:HG23	2.36	0.55
1:A:10:HIS:O	1:A:60:ASP:N	2.32	0.54
1:A:14:THR:O	1:A:14:THR:OG1	2.23	0.54
4:D:89:GLY:O	4:D:91:LYS:NZ	2.32	0.54
3:G:126:ASN:ND2	3:G:126:ASN:H	2.04	0.54
3:C:130:VAL:HG13	3:C:138:PHE:CZ	2.42	0.54
1:A:68:THR:HA	1:A:72:VAL:O	2.07	0.54
1:A:237:LEU:HA	1:A:240:ILE:HD12	1.90	0.54
1:E:167:LEU:HD11	1:E:186:VAL:HG21	1.90	0.54
3:G:34:VAL:HG13	3:G:35:GLY:HA2	1.89	0.54
1:E:26:LEU:HD12	1:E:221:LEU:HD23	1.90	0.54
1:E:231:PHE:N	1:E:232:PRO:HD2	2.22	0.54
5:A:301:ANP:N3B	5:A:301:ANP:O1A	2.40	0.54
2:B:98:LEU:HD13	2:B:143:PRO:HB2	1.90	0.54
4:H:115:ARG:HG3	4:H:116:PHE:N	2.23	0.54
3:C:129:TRP:C	3:C:131:SER:H	2.14	0.54
4:H:199:SER:O	4:H:202:PRO:HD2	2.08	0.54
1:A:167:LEU:HD11	1:A:186:VAL:HG21	1.89	0.53
3:C:130:VAL:HG13	3:C:138:PHE:HZ	1.73	0.53
3:C:126:ASN:O	3:C:138:PHE:CZ	2.62	0.53
4:H:196:ARG:O	4:H:199:SER:OG	2.19	0.53
1:A:144:LEU:HB3	1:A:148:GLN:HG3	1.90	0.53
3:C:118:THR:OG1	3:C:119:VAL:N	2.42	0.53
2:F:102:THR:HA	2:F:142:SER:HA	1.91	0.53
4:H:193:LEU:O	4:H:195:LYS:N	2.33	0.53
3:C:147:LEU:CG	3:G:147:LEU:HB2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:LEU:HD12	2:B:135:LYS:HE3	1.90	0.53
4:D:21:PRO:HB2	4:D:138:ALA:HB2	1.91	0.53
1:E:172:SER:OG	1:E:173:MET:SD	2.59	0.53
1:E:102:VAL:O	1:E:106:VAL:HG22	2.09	0.53
1:E:237:LEU:HA	1:E:240:ILE:HD12	1.91	0.53
3:G:129:TRP:O	3:G:132:MET:HG3	2.09	0.53
3:G:150:MET:CE	3:G:151:ILE:HG12	2.34	0.53
3:C:118:THR:HA	3:C:122:ASN:HD22	1.75	0.52
4:D:72:MET:O	4:D:76:ILE:HG12	2.09	0.52
4:D:91:LYS:N	4:D:102:SER:OG	2.41	0.52
3:G:43:LEU:HB2	3:G:46:ILE:HD11	1.91	0.52
4:D:34:MET:HE2	4:D:256:THR:HB	1.92	0.52
2:B:102:THR:HA	2:B:142:SER:HA	1.91	0.52
3:C:88:THR:HG21	3:C:129:TRP:HE1	1.74	0.52
4:D:43:SER:HB2	4:D:259:MET:HE2	1.90	0.52
4:D:11:PRO:HD2	4:D:128:VAL:HG13	1.91	0.52
4:D:149:PHE:CG	4:D:150:LYS:N	2.78	0.52
3:G:126:ASN:H	3:G:126:ASN:HD22	1.57	0.52
3:C:28:ILE:HD11	4:D:167:VAL:HG13	1.90	0.52
4:D:12:GLY:HA2	4:D:18:ARG:NH1	2.24	0.52
4:D:30:TYR:CE2	4:D:256:THR:HG21	2.44	0.52
1:E:13:PHE:HB2	5:E:301:ANP:C2	2.39	0.52
1:E:89:VAL:HG21	1:E:154:ILE:HD13	1.90	0.52
2:B:100:GLU:HA	3:C:167:LEU:HD13	1.91	0.52
2:B:21:ILE:HD12	2:B:24:ASP:OD2	2.09	0.52
3:C:113:SER:O	3:C:117:VAL:HG23	2.10	0.52
4:D:190:ASP:O	4:D:196:ARG:NH1	2.42	0.52
2:B:99:PHE:HD1	2:B:100:GLU:HG3	1.75	0.52
2:B:279:GLN:HA	2:B:282:LYS:HB2	1.91	0.52
4:H:149:PHE:CG	4:H:150:LYS:N	2.76	0.52
2:F:99:PHE:HD1	2:F:100:GLU:HG3	1.75	0.51
2:F:171:GLU:HA	2:F:202:THR:HG22	1.91	0.51
3:G:137:ASN:OD1	3:G:137:ASN:N	2.25	0.51
4:H:43:SER:O	4:H:47:ILE:HG23	2.09	0.51
3:G:96:TYR:CZ	3:G:117:VAL:HG21	2.46	0.51
4:H:28:THR:O	4:H:32:ILE:HG12	2.10	0.51
1:A:24:SER:OG	1:A:26:LEU:HD13	2.10	0.51
3:C:110:VAL:O	3:C:114:VAL:HG23	2.10	0.51
4:D:28:THR:O	4:D:32:ILE:HG12	2.10	0.51
4:H:30:TYR:HE2	4:H:256:THR:HG21	1.74	0.51
1:A:12:THR:HG22	1:A:21:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:SER:OG	3:G:150:MET:SD	2.53	0.51
3:G:129:TRP:O	3:G:132:MET:HE3	2.10	0.51
3:G:141:ALA:O	3:G:144:SER:HB2	2.10	0.51
3:C:129:TRP:CE3	3:C:129:TRP:HA	2.45	0.51
3:G:82:PHE:CD1	3:G:132:MET:HE2	2.45	0.51
1:A:89:VAL:HG21	1:A:154:ILE:HD13	1.91	0.51
3:C:132:MET:HB2	4:D:115:ARG:HH12	1.75	0.51
3:C:136:ILE:HD13	3:C:136:ILE:H	1.75	0.51
3:G:111:ILE:HG13	3:G:157:MET:SD	2.51	0.50
2:B:51:GLN:HB2	2:B:56:LEU:HB2	1.93	0.50
3:C:77:ASN:O	3:C:78:LEU:HG	2.11	0.50
4:D:92:VAL:HG23	4:D:93:TYR:CD1	2.46	0.50
2:F:50:MET:HE1	2:F:199:ILE:HG21	1.93	0.50
4:H:263:ARG:HG3	4:H:264:LYS:N	2.26	0.50
4:D:38:ALA:HB1	4:D:39:ASN:CB	2.35	0.50
2:F:134:LEU:HD12	2:F:135:LYS:HE3	1.93	0.50
2:B:72:THR:H	2:B:75:THR:HG23	1.77	0.50
3:C:147:LEU:HD21	3:G:146:ILE:N	2.26	0.50
3:G:129:TRP:HA	3:G:129:TRP:CE3	2.47	0.50
2:B:152:ARG:O	2:B:152:ARG:HG2	2.11	0.50
2:B:266:GLN:N	2:B:267:PRO:HD3	2.27	0.50
1:E:267:ASP:HB2	1:E:270:LYS:HB2	1.93	0.50
2:B:38:LEU:HB3	2:B:201:VAL:HG22	1.92	0.50
1:E:171:THR:HB	1:E:179:LYS:HG3	1.93	0.50
2:F:256:LEU:O	2:F:260:GLY:HA3	2.10	0.50
1:A:147:GLY:HA2	1:A:174:LEU:HD22	1.94	0.50
3:C:43:LEU:HB2	3:C:46:ILE:HD11	1.93	0.50
1:E:68:THR:HA	1:E:72:VAL:O	2.12	0.50
4:H:38:ALA:HB1	4:H:39:ASN:CB	2.42	0.50
2:B:171:GLU:HA	2:B:202:THR:HG22	1.93	0.49
4:D:190:ASP:O	4:D:196:ARG:HG3	2.12	0.49
3:G:118:THR:HG21	3:G:153:PRO:HG3	1.94	0.49
3:C:70:VAL:HG13	4:D:164:LEU:HD23	1.93	0.49
2:F:152:ARG:HG2	2:F:152:ARG:O	2.12	0.49
2:F:169:LEU:HD13	2:F:172:PRO:HG3	1.94	0.49
2:F:275:ASP:O	2:F:278:LYS:HG3	2.12	0.49
1:E:96:GLN:HG3	4:H:221:ALA:HB2	1.94	0.49
2:F:278:LYS:HE3	2:F:282:LYS:HG3	1.93	0.49
2:B:256:LEU:O	2:B:260:GLY:HA3	2.11	0.49
1:A:124:VAL:HG11	4:D:236:TYR:CE1	2.48	0.49
2:B:138:LEU:HA	2:B:141:HIS:CG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:260:ILE:O	4:D:263:ARG:HB3	2.12	0.49
2:F:95:GLU:HG3	2:F:152:ARG:HB2	1.94	0.49
2:F:266:GLN:N	2:F:267:PRO:HD3	2.27	0.49
4:H:242:SER:O	4:H:244:VAL:N	2.41	0.49
2:B:50:MET:HE1	2:B:199:ILE:HG21	1.95	0.49
2:F:97:GLN:O	4:H:181:GLN:NE2	2.46	0.49
3:G:70:VAL:HG13	4:H:164:LEU:HD23	1.93	0.49
2:B:134:LEU:CD2	2:B:150:GLN:HB3	2.42	0.49
3:C:145:ARG:HA	3:G:147:LEU:CD2	2.41	0.49
4:H:74:TRP:O	4:H:78:PHE:HB2	2.13	0.49
1:E:10:HIS:HE1	1:E:25:ASP:OD1	1.96	0.48
1:E:11:VAL:HG22	1:E:59:PRO:HA	1.95	0.48
2:F:138:LEU:HA	2:F:141:HIS:CG	2.48	0.48
3:G:103:GLN:HB3	3:G:109:ARG:CZ	2.43	0.48
2:B:95:GLU:HG3	2:B:152:ARG:HB2	1.95	0.48
2:F:56:LEU:HD13	4:H:179:ASN:HB3	1.96	0.48
1:E:117:ARG:HD3	4:H:238:ILE:HG13	1.94	0.48
3:G:17:VAL:O	3:G:21:MET:HG2	2.14	0.48
1:E:5:ILE:HG13	1:E:29:ALA:HB2	1.96	0.48
2:F:144:PHE:CE2	4:H:209:ILE:HG21	2.48	0.48
3:G:152:THR:HA	3:G:155:ILE:HG22	1.94	0.48
1:A:150:GLN:O	1:A:154:ILE:HG12	2.13	0.48
4:D:198:LYS:O	4:D:198:LYS:NZ	2.45	0.48
3:G:82:PHE:CE1	3:G:132:MET:HE2	2.49	0.48
3:C:17:VAL:O	3:C:21:MET:HG2	2.14	0.48
3:C:95:ILE:HA	3:C:98:PHE:HD2	1.79	0.48
3:C:131:SER:HB3	3:C:138:PHE:CD2	2.48	0.48
2:B:102:THR:HG23	2:B:105:LYS:H	1.78	0.48
2:B:132:VAL:HG11	2:B:157:ALA:HB2	1.96	0.48
2:B:135:LYS:HB3	2:B:138:LEU:HG	1.96	0.48
1:E:124:VAL:HG11	4:H:236:TYR:CE1	2.49	0.48
2:F:90:ALA:HB3	2:F:169:LEU:HB3	1.95	0.48
3:C:82:PHE:HB3	3:C:85:PHE:H	1.79	0.47
3:C:147:LEU:CB	3:G:147:LEU:HB2	2.43	0.47
3:C:33:LYS:HA	3:C:42:GLY:HA2	1.97	0.47
3:C:132:MET:HG3	4:D:115:ARG:HH22	1.79	0.47
4:D:188:PHE:HB2	4:D:189:ASN:HA	1.95	0.47
3:C:88:THR:HG21	3:C:129:TRP:NE1	2.30	0.47
2:F:47:SER:OG	5:F:301:ANP:O3G	2.32	0.47
2:B:168:CYS:O	2:B:169:LEU:HD23	2.14	0.47
3:C:121:CYS:O	3:C:125:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:GLN:HA	1:E:170:SER:HA	1.95	0.47
1:A:96:GLN:HG3	4:D:221:ALA:HB2	1.96	0.47
4:D:74:TRP:O	4:D:78:PHE:HB2	2.14	0.47
3:C:123:ILE:O	3:C:127:THR:HG23	2.15	0.47
3:C:147:LEU:HG	3:G:147:LEU:N	2.16	0.47
4:D:13:THR:O	4:D:14:THR:HG22	2.14	0.47
1:E:150:GLN:O	1:E:154:ILE:HG12	2.14	0.47
2:F:129:LEU:HD13	2:F:139:ILE:HG13	1.96	0.47
3:C:147:LEU:HD21	3:G:146:ILE:H	1.80	0.47
4:D:246:LEU:O	4:D:249:VAL:HG22	2.15	0.47
3:G:153:PRO:O	3:G:156:GLN:HB2	2.14	0.47
4:H:93:TYR:HD2	4:H:95:HIS:CE1	2.33	0.47
2:B:99:PHE:CZ	4:D:202:PRO:HB3	2.50	0.47
4:D:242:SER:C	4:D:244:VAL:H	2.22	0.47
4:H:88:ALA:HB2	4:H:98:ILE:O	2.15	0.47
4:H:46:VAL:O	4:H:49:ILE:HG13	2.14	0.47
1:A:117:ARG:HA	1:A:120:MET:HB2	1.97	0.47
3:G:46:ILE:HD12	3:G:46:ILE:H	1.80	0.47
4:H:195:LYS:C	4:H:198:LYS:H	2.23	0.47
1:A:117:ARG:HD3	4:D:238:ILE:HG13	1.96	0.46
3:C:127:THR:O	3:C:138:PHE:CD2	2.68	0.46
3:C:130:VAL:C	3:C:132:MET:HG2	2.40	0.46
4:D:14:THR:HG23	4:D:15:PHE:HD2	1.78	0.46
3:G:110:VAL:O	3:G:113:SER:OG	2.26	0.46
2:B:144:PHE:CE2	4:D:209:ILE:HG21	2.50	0.46
4:D:90:GLY:HA3	4:D:91:LYS:HD2	1.96	0.46
2:F:35:PHE:HB2	2:F:192:GLN:HE21	1.80	0.46
1:A:267:ASP:HB2	1:A:270:LYS:HB2	1.97	0.46
4:D:38:ALA:HB2	4:D:263:ARG:HE	1.80	0.46
2:F:38:LEU:HB3	2:F:201:VAL:HG22	1.96	0.46
1:A:47:SER:O	1:A:50:SER:OG	2.30	0.46
3:C:122:ASN:O	3:C:126:ASN:ND2	2.48	0.46
4:D:258:LEU:O	4:D:262:THR:HG22	2.15	0.46
1:E:146:GLY:HA2	1:E:149:LYS:HD2	1.97	0.46
2:F:102:THR:HG23	2:F:105:LYS:H	1.79	0.46
3:G:36:ASN:HD22	3:G:36:ASN:H	1.62	0.46
3:C:111:ILE:HG23	3:C:157:MET:SD	2.56	0.46
2:F:72:THR:H	2:F:75:THR:HG23	1.79	0.46
1:E:39:ILE:HG12	1:E:242:LEU:HD22	1.98	0.46
2:F:99:PHE:CD1	2:F:100:GLU:HG3	2.51	0.46
3:G:36:ASN:OD1	3:G:38:THR:OG1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HD12	3:C:46:ILE:H	1.81	0.46
4:D:199:SER:O	4:D:202:PRO:HD2	2.16	0.46
4:H:246:LEU:O	4:H:249:VAL:HG22	2.16	0.46
2:B:169:LEU:HD12	2:B:188:PHE:CZ	2.50	0.46
1:E:271:LEU:O	1:E:275:LEU:HG	2.15	0.46
2:B:267:PRO:HA	2:B:272:GLU:OE1	2.17	0.45
4:D:96:TRP:CD1	4:D:100:THR:HG21	2.51	0.45
1:E:11:VAL:HG21	1:E:52:LEU:HD21	1.99	0.45
3:G:41:VAL:HB	3:G:152:THR:HG22	1.98	0.45
4:H:90:GLY:HA3	4:H:91:LYS:HD2	1.97	0.45
3:C:147:LEU:HD11	3:G:145:ARG:C	2.40	0.45
1:E:244:ILE:HG22	1:E:245:PRO:O	2.16	0.45
2:F:171:GLU:OE2	2:F:203:HIS:ND1	2.48	0.45
1:A:183:LEU:HA	1:A:186:VAL:HG22	1.99	0.45
3:G:121:CYS:SG	3:G:122:ASN:N	2.89	0.45
4:D:245:ASP:O	4:D:249:VAL:HG13	2.16	0.45
4:H:193:LEU:C	4:H:195:LYS:N	2.68	0.45
2:B:275:ASP:O	2:B:278:LYS:HG3	2.17	0.45
3:C:43:LEU:O	3:C:43:LEU:HD12	2.17	0.45
2:F:124:ALA:HA	2:F:127:LYS:HD2	1.98	0.45
1:A:18:SER:C	1:A:19:PRO:O	2.59	0.45
2:F:128:TRP:O	2:F:132:VAL:HG12	2.15	0.45
1:A:146:GLY:HA2	1:A:149:LYS:HD2	1.99	0.45
3:C:8:SER:N	3:C:9:SER:HA	2.31	0.45
3:C:140:VAL:O	3:C:144:SER:HB3	2.16	0.45
3:C:150:MET:HE1	4:H:74:TRP:HE1	1.81	0.45
3:C:174:ARG:CG	3:C:175:LYS:HB2	2.40	0.45
3:C:167:LEU:HB3	3:C:171:LYS:HZ2	1.81	0.45
1:E:93:PRO:HB3	1:E:150:GLN:OE1	2.17	0.45
4:H:12:GLY:HA2	4:H:18:ARG:NH1	2.32	0.45
4:H:245:ASP:O	4:H:249:VAL:HG13	2.17	0.45
1:A:271:LEU:O	1:A:275:LEU:HG	2.16	0.45
2:B:168:CYS:C	2:B:169:LEU:HD23	2.42	0.45
3:C:116:CYS:O	3:C:120:ILE:HG13	2.17	0.45
3:G:133:MET:HE2	4:H:83:GLN:HE21	1.82	0.45
4:D:50:PHE:CD2	4:D:255:LEU:HD13	2.51	0.45
2:B:184:MET:O	2:B:187:LEU:HG	2.17	0.44
4:D:104:GLU:O	4:D:107:ILE:HG13	2.16	0.44
4:H:39:ASN:HD22	4:H:263:ARG:C	2.25	0.44
1:A:111:GLU:HG3	4:D:233:ARG:NH2	2.32	0.44
1:A:244:ILE:HG22	1:A:245:PRO:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:ILE:HB	2:B:71:ILE:HB	1.98	0.44
3:C:88:THR:CG2	3:C:129:TRP:NE1	2.79	0.44
3:G:95:ILE:HA	3:G:98:PHE:HD2	1.81	0.44
2:B:99:PHE:CD1	2:B:100:GLU:HG3	2.52	0.44
3:C:70:VAL:O	3:C:73:VAL:HG22	2.18	0.44
1:E:117:ARG:HA	1:E:120:MET:HB2	1.99	0.44
2:F:267:PRO:O	2:F:268:LEU:HD12	2.17	0.44
3:G:33:LYS:HA	3:G:42:GLY:HA2	1.98	0.44
3:G:125:LEU:O	3:G:129:TRP:N	2.47	0.44
4:H:72:MET:O	4:H:76:ILE:HG12	2.17	0.44
3:C:80:GLY:HA3	3:C:81:PHE:HA	1.82	0.44
1:E:264:GLU:N	1:E:265:ILE:HB	2.33	0.44
2:F:38:LEU:HD23	2:F:50:MET:HE3	1.99	0.44
4:H:31:PHE:O	4:H:35:ILE:HG13	2.17	0.44
1:A:11:VAL:HG21	1:A:52:LEU:HD11	1.99	0.44
1:A:26:LEU:HD11	1:A:221:LEU:H	1.83	0.44
1:A:264:GLU:N	1:A:265:ILE:HB	2.33	0.44
1:E:257:ARG:NH1	2:F:275:ASP:OD1	2.51	0.44
3:C:152:THR:HA	3:C:155:ILE:HG22	1.99	0.44
3:G:110:VAL:O	3:G:114:VAL:HG23	2.17	0.44
3:G:136:ILE:HD13	3:G:136:ILE:HA	1.83	0.44
4:H:91:LYS:N	4:H:102:SER:OG	2.39	0.44
1:A:5:ILE:HG13	1:A:29:ALA:HB2	2.00	0.44
2:B:38:LEU:HD23	2:B:50:MET:HE3	2.00	0.44
4:D:55:VAL:O	4:D:58:THR:OG1	2.34	0.44
4:D:188:PHE:HA	4:D:189:ASN:C	2.43	0.44
3:G:39:LEU:HD23	3:G:39:LEU:HA	1.86	0.44
3:G:80:GLY:HA3	3:G:81:PHE:HA	1.82	0.44
2:B:35:PHE:HB2	2:B:192:GLN:HE21	1.83	0.44
4:D:78:PHE:O	4:D:82:LEU:HB2	2.18	0.44
4:D:88:ALA:HA	4:D:89:GLY:HA3	1.55	0.44
1:E:62:LEU:HD22	1:E:62:LEU:O	2.18	0.44
1:E:95:ASN:ND2	4:H:214:VAL:HG12	2.32	0.44
2:F:134:LEU:HD22	2:F:153:ARG:CZ	2.48	0.44
3:G:124:GLY:O	3:G:127:THR:OG1	2.26	0.44
3:C:10:LYS:HE2	3:C:10:LYS:HB3	1.56	0.43
1:E:128:VAL:HA	1:E:131:VAL:HG22	2.00	0.43
3:G:88:THR:CG2	3:G:129:TRP:HE1	2.31	0.43
1:A:39:ILE:HG12	1:A:242:LEU:HD22	2.00	0.43
1:A:47:SER:HB3	5:A:301:ANP:O2G	2.18	0.43
3:C:131:SER:HB3	3:C:138:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:LEU:O	4:D:222:MET:HB2	2.17	0.43
3:G:123:ILE:O	3:G:127:THR:HG23	2.18	0.43
4:H:92:VAL:CG2	4:H:104:GLU:HB2	2.43	0.43
3:G:43:LEU:HD12	3:G:43:LEU:O	2.18	0.43
3:G:64:GLY:HA3	3:G:90:ALA:HA	2.01	0.43
3:C:101:TYR:O	3:C:103:GLN:HG2	2.18	0.43
4:D:242:SER:O	4:D:244:VAL:N	2.37	0.43
1:E:47:SER:O	1:E:50:SER:OG	2.33	0.43
2:F:62:GLY:O	2:F:73:PRO:HD3	2.18	0.43
4:H:55:VAL:O	4:H:58:THR:OG1	2.34	0.43
1:A:93:PRO:HB2	1:A:149:LYS:HB3	2.00	0.43
2:B:97:GLN:HG3	4:D:180:ALA:HB1	1.99	0.43
4:D:78:PHE:CZ	3:G:150:MET:HG2	2.53	0.43
2:F:139:ILE:HG23	2:F:140:GLU:HG3	2.01	0.43
4:H:50:PHE:CD2	4:H:255:LEU:HD13	2.50	0.43
3:C:64:GLY:HA3	3:C:90:ALA:HA	2.01	0.43
4:D:21:PRO:HG3	4:D:134:GLU:HB3	2.00	0.43
4:D:90:GLY:HA2	4:D:91:LYS:NZ	2.34	0.43
1:E:89:VAL:HG12	1:E:170:SER:HB3	1.99	0.43
2:F:21:ILE:HD12	2:F:24:ASP:OD2	2.19	0.43
3:G:118:THR:HA	3:G:122:ASN:CB	2.49	0.43
2:B:43:GLY:N	5:B:301:ANP:O1B	2.52	0.43
2:B:56:LEU:HD13	4:D:179:ASN:HB3	2.01	0.43
2:B:62:GLY:O	2:B:73:PRO:HD3	2.18	0.43
2:B:72:THR:OG1	2:B:75:THR:HG23	2.19	0.43
3:C:164:LEU:O	3:C:169:ARG:HB3	2.19	0.43
1:A:48:THR:HG22	1:A:52:LEU:HD13	2.01	0.43
2:B:129:LEU:HD13	2:B:139:ILE:HG13	2.00	0.43
1:E:13:PHE:CD1	1:E:14:THR:N	2.87	0.43
2:F:113:ASN:HD22	4:H:185:GLY:C	2.27	0.43
1:A:56:LEU:HD13	4:D:220:THR:HG23	2.00	0.42
3:C:129:TRP:C	3:C:131:SER:N	2.74	0.42
1:E:56:LEU:HD11	4:H:224:SER:HB3	2.01	0.42
3:G:10:LYS:HB3	3:G:59:TRP:HE1	1.84	0.42
3:G:127:THR:CG2	3:G:145:ARG:HH22	2.32	0.42
3:G:133:MET:O	3:G:134:TYR:CG	2.71	0.42
1:E:96:GLN:HE22	4:H:217:ASP:HB3	1.84	0.42
1:E:140:GLU:HB3	1:E:141:PRO:HD2	2.01	0.42
2:F:263:LEU:HD13	2:F:276:ALA:HB1	2.01	0.42
3:G:36:ASN:HB3	4:H:196:ARG:CZ	2.49	0.42
4:H:43:SER:HA	4:H:46:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:MET:SD	1:A:173:MET:N	2.90	0.42
3:C:146:ILE:HG22	3:G:146:ILE:HG22	2.00	0.42
4:D:17:TYR:C	4:D:18:ARG:HG3	2.44	0.42
4:D:103:SER:O	4:D:107:ILE:HG23	2.18	0.42
4:D:190:ASP:CG	4:D:191:GLY:H	2.27	0.42
1:E:183:LEU:HA	1:E:186:VAL:HG22	2.01	0.42
2:F:24:ASP:HB2	2:F:222:ARG:HD2	2.00	0.42
2:F:131:LYS:HB2	2:F:131:LYS:HE3	1.72	0.42
3:G:157:MET:HA	3:G:160:VAL:HG12	2.00	0.42
4:H:218:LEU:O	4:H:222:MET:HB2	2.19	0.42
3:C:136:ILE:O	3:C:140:VAL:HG22	2.20	0.42
4:D:258:LEU:O	4:D:261:THR:HG22	2.19	0.42
1:E:56:LEU:HD13	4:H:220:THR:HG23	2.02	0.42
3:G:133:MET:H	4:H:115:ARG:CZ	2.32	0.42
4:H:50:PHE:CE2	4:H:255:LEU:HB2	2.54	0.42
4:H:98:ILE:HB	4:H:99:PHE:HB2	2.01	0.42
4:H:250:ALA:O	4:H:254:LEU:HB3	2.19	0.42
4:D:17:TYR:OH	4:D:247:ILE:HD13	2.20	0.42
1:E:215:VAL:HG13	1:E:242:LEU:HD21	2.02	0.42
2:F:99:PHE:CZ	4:H:202:PRO:HB3	2.54	0.42
2:F:135:LYS:HB2	2:F:135:LYS:HE3	1.75	0.42
2:F:147:SER:H	2:F:150:GLN:NE2	2.17	0.42
3:G:128:LEU:HA	3:G:131:SER:CB	2.47	0.42
4:H:243:LYS:HE2	4:H:243:LYS:HB3	1.85	0.42
1:A:9:ASP:HB3	1:A:65:SER:HA	2.01	0.42
2:B:156:LEU:HD13	2:B:184:MET:HE2	2.01	0.42
4:D:35:ILE:HG12	4:D:47:ILE:HG21	2.02	0.42
2:F:55:ALA:O	2:F:58:LYS:NZ	2.53	0.42
2:B:72:THR:HG22	2:F:70:THR:HG23	2.00	0.42
4:D:240:GLU:HG3	4:D:241:TRP:N	2.34	0.42
4:H:90:GLY:HA2	4:H:91:LYS:HA	1.73	0.42
4:H:104:GLU:O	4:H:107:ILE:HG13	2.19	0.42
1:A:91:GLN:HA	1:A:170:SER:HA	2.02	0.42
3:G:43:LEU:HB2	3:G:46:ILE:CD1	2.49	0.42
4:D:100:THR:HG22	4:D:101:LEU:N	2.29	0.41
1:E:26:LEU:HA	1:E:27:SER:HB2	2.01	0.41
2:F:89:LEU:HA	2:F:168:CYS:O	2.20	0.41
2:F:205:MET:O	2:F:208:VAL:HG12	2.20	0.41
4:H:124:THR:HA	4:H:127:THR:HG22	2.01	0.41
2:B:171:GLU:OE2	2:B:203:HIS:ND1	2.50	0.41
4:D:22:ARG:HB3	4:D:138:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:184:MET:O	2:F:187:LEU:HG	2.20	0.41
3:G:106:GLN:HB3	3:G:109:ARG:HG3	2.01	0.41
4:H:193:LEU:HD23	4:H:194:VAL:H	1.84	0.41
2:B:218:LEU:HD23	2:B:223:LEU:HA	2.02	0.41
4:D:124:THR:HA	4:D:127:THR:HG22	2.01	0.41
4:H:84:THR:HG23	4:H:105:GLY:C	2.46	0.41
2:B:3:ILE:HB	2:B:30:LEU:HB2	2.01	0.41
2:B:72:THR:H	2:B:75:THR:CG2	2.33	0.41
2:B:205:MET:O	2:B:208:VAL:HG12	2.21	0.41
2:B:278:LYS:HE3	2:B:278:LYS:HB2	1.84	0.41
4:H:242:SER:C	4:H:244:VAL:H	2.27	0.41
2:B:263:LEU:HD13	2:B:276:ALA:HB1	2.02	0.41
3:C:121:CYS:SG	3:C:122:ASN:N	2.93	0.41
4:D:42:VAL:O	4:D:46:VAL:HG13	2.19	0.41
4:D:182:ARG:HE	4:D:188:PHE:HE1	1.68	0.41
1:E:253:LEU:HD22	2:F:270:MET:HB3	2.02	0.41
2:F:228:SER:C	2:F:230:LYS:H	2.28	0.41
4:H:76:ILE:O	4:H:80:SER:OG	2.29	0.41
4:H:240:GLU:HG3	4:H:241:TRP:N	2.35	0.41
1:A:173:MET:O	1:A:174:LEU:HD23	2.21	0.41
3:C:134:TYR:N	3:C:134:TYR:CD1	2.88	0.41
1:E:169:GLU:OE1	1:E:172:SER:HB3	2.21	0.41
3:G:70:VAL:O	3:G:73:VAL:HG22	2.21	0.41
4:H:22:ARG:HB3	4:H:138:ALA:HA	2.02	0.41
4:D:112:VAL:O	4:D:116:PHE:HB2	2.20	0.41
1:E:111:GLU:HG3	4:H:233:ARG:NH2	2.35	0.41
1:E:96:GLN:OE1	1:E:96:GLN:N	2.54	0.41
1:A:128:VAL:HA	1:A:131:VAL:HG22	2.03	0.41
1:A:140:GLU:HB3	1:A:141:PRO:HD2	2.02	0.41
2:B:12:TYR:N	2:B:20:ALA:O	2.45	0.41
3:C:13:LEU:HD23	4:D:223:GLU:HG3	2.03	0.41
3:C:173:SER:HA	3:C:174:ARG:HA	1.84	0.41
4:H:258:LEU:O	4:H:261:THR:HG22	2.20	0.41
2:F:36:ILE:HA	2:F:214:ASP:HB2	2.03	0.41
2:F:147:SER:N	2:F:150:GLN:HG3	2.36	0.41
2:F:227:ALA:HB1	2:F:231:GLU:OE1	2.21	0.41
3:G:13:LEU:HD23	4:H:223:GLU:HG3	2.03	0.41
4:H:111:TYR:HA	4:H:114:ILE:HG12	2.03	0.41
4:H:182:ARG:HA	4:H:186:ALA:O	2.21	0.41
1:E:23:LEU:HB2	1:E:24:SER:H	1.78	0.40
3:G:12:GLU:HB3	3:G:15:GLU:OE1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:8:ARG:HA	4:H:9:TYR:HA	1.85	0.40
4:H:101:LEU:HD22	4:H:102:SER:H	1.86	0.40
4:H:258:LEU:O	4:H:262:THR:HG22	2.21	0.40
1:A:92:ASN:HA	1:A:93:PRO:HD2	1.79	0.40
3:C:35:GLY:HA2	3:C:40:GLN:HA	2.03	0.40
1:E:124:VAL:HG11	4:H:236:TYR:HE1	1.86	0.40
4:H:101:LEU:HD22	4:H:102:SER:N	2.35	0.40
1:A:102:VAL:CG2	1:A:137:ALA:HA	2.52	0.40
1:A:124:VAL:HG11	4:D:236:TYR:HE1	1.86	0.40
1:A:247:VAL:O	1:A:251:LYS:HG2	2.20	0.40
1:E:13:PHE:CD1	5:E:301:ANP:C5	3.05	0.40
2:F:123:GLU:HB2	2:F:127:LYS:NZ	2.37	0.40
4:H:42:VAL:O	4:H:46:VAL:HG13	2.21	0.40
4:H:103:SER:O	4:H:107:ILE:HG23	2.21	0.40
2:B:134:LEU:HG	2:B:138:LEU:HD21	2.03	0.40
1:E:92:ASN:HA	1:E:93:PRO:HD2	1.84	0.40
4:H:88:ALA:HA	4:H:89:GLY:HA3	1.63	0.40
4:H:91:LYS:HB3	4:H:104:GLU:CB	2.51	0.40
1:A:253:LEU:HD22	2:B:270:MET:HB3	2.02	0.40
2:B:205:MET:HE2	2:B:205:MET:HA	2.03	0.40
2:B:228:SER:C	2:B:230:LYS:H	2.29	0.40
1:E:215:VAL:O	1:E:221:LEU:HA	2.21	0.40
2:F:153:ARG:O	2:F:157:ALA:N	2.53	0.40
4:H:112:VAL:O	4:H:116:PHE:HB2	2.21	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	278/298 (93%)	243 (87%)	30 (11%)	5 (2%)	6 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	278/298 (93%)	242 (87%)	32 (12%)	4 (1%)	9	33
2	B	279/287 (97%)	264 (95%)	15 (5%)	0	100	100
2	F	279/287 (97%)	261 (94%)	18 (6%)	0	100	100
3	C	166/184 (90%)	149 (90%)	15 (9%)	2 (1%)	10	37
3	G	166/184 (90%)	150 (90%)	16 (10%)	0	100	100
4	D	257/265 (97%)	231 (90%)	23 (9%)	3 (1%)	10	37
4	H	257/265 (97%)	230 (90%)	24 (9%)	3 (1%)	10	37
All	All	1960/2068 (95%)	1770 (90%)	173 (9%)	17 (1%)	14	43

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	PRO
4	H	194	VAL
3	C	132	MET
4	D	42	VAL
1	A	18	SER
1	A	234	VAL
1	E	234	VAL
1	A	15	TYR
1	A	24	SER
4	D	243	LYS
1	E	24	SER
4	H	95	HIS
4	D	238	ILE
4	H	238	ILE
1	E	15	TYR
3	C	41	VAL
1	E	19	PRO

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	240/257 (93%)	226 (94%)	14 (6%)	18	47
1	E	240/257 (93%)	225 (94%)	15 (6%)	16	44
2	B	230/234 (98%)	218 (95%)	12 (5%)	21	49
2	F	230/234 (98%)	211 (92%)	19 (8%)	10	34
3	C	139/155 (90%)	119 (86%)	20 (14%)	3	14
3	G	139/155 (90%)	116 (84%)	23 (16%)	2	11
4	D	227/233 (97%)	205 (90%)	22 (10%)	8	28
4	H	227/233 (97%)	196 (86%)	31 (14%)	3	16
All	All	1672/1758 (95%)	1516 (91%)	156 (9%)	8	30

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	13	PHE
1	A	15	TYR
1	A	17	ASP
1	A	28	PHE
1	A	52	LEU
1	A	73	LYS
1	A	122	LYS
1	A	173	MET
1	A	182	ILE
1	A	218	ASP
1	A	239	ARG
1	A	276	TRP
1	A	278	LEU
2	B	21	ILE
2	B	27	ASN
2	B	52	HIS
2	B	81	LYS
2	B	98	LEU
2	B	130	LYS
2	B	150	GLN
2	B	192	GLN
2	B	251	ARG
2	B	266	GLN
2	B	278	LYS
2	B	282	LYS
3	C	10	LYS

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Mol	Chain	Res	Type
3	C	12	GLU
3	C	33	LYS
3	C	95	ILE
3	C	107	ILE
3	C	118	THR
3	C	122	ASN
3	C	130	VAL
3	C	136	ILE
3	C	137	ASN
3	C	139	MET
3	C	144	SER
3	C	145	ARG
3	C	146	ILE
3	C	149	GLU
3	C	151	ILE
3	C	157	MET
3	C	162	PHE
3	C	165	GLU
3	C	171	LYS
4	D	18	ARG
4	D	24	LYS
4	D	34	MET
4	D	61	LYS
4	D	63	ARG
4	D	82	LEU
4	D	87	MET
4	D	91	LYS
4	D	96	TRP
4	D	99	PHE
4	D	116	PHE
4	D	146	LEU
4	D	167	VAL
4	D	173	GLN
4	D	188	PHE
4	D	193	LEU
4	D	198	LYS
4	D	240	GLU
4	D	243	LYS
4	D	249	VAL
4	D	260	ILE
4	D	263	ARG
1	E	14	THR

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Mol	Chain	Res	Type
1	E	15	TYR
1	E	18	SER
1	E	23	LEU
1	E	28	PHE
1	E	52	LEU
1	E	62	LEU
1	E	73	LYS
1	E	120	MET
1	E	122	LYS
1	E	173	MET
1	E	182	ILE
1	E	224	GLN
1	E	276	TRP
1	E	278	LEU
2	F	18	LEU
2	F	21	ILE
2	F	27	ASN
2	F	52	HIS
2	F	53	PHE
2	F	63	LYS
2	F	70	THR
2	F	81	LYS
2	F	98	LEU
2	F	130	LYS
2	F	142	SER
2	F	150	GLN
2	F	169	LEU
2	F	192	GLN
2	F	251	ARG
2	F	252	PHE
2	F	266	GLN
2	F	268	LEU
2	F	278	LYS
3	G	8	SER
3	G	33	LYS
3	G	34	VAL
3	G	36	ASN
3	G	38	THR
3	G	78	LEU
3	G	95	ILE
3	G	105	ILE
3	G	106	GLN

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Mol	Chain	Res	Type
3	G	118	THR
3	G	126	ASN
3	G	132	MET
3	G	133	MET
3	G	137	ASN
3	G	139	MET
3	G	142	LEU
3	G	146	ILE
3	G	149	GLU
3	G	151	ILE
3	G	162	PHE
3	G	170	VAL
3	G	171	LYS
3	G	173	SER
4	H	13	THR
4	H	24	LYS
4	H	34	MET
4	H	37	LEU
4	H	42	VAL
4	H	47	ILE
4	H	50	PHE
4	H	60	LEU
4	H	61	LYS
4	H	63	ARG
4	H	82	LEU
4	H	87	MET
4	H	91	LYS
4	H	100	THR
4	H	102	SER
4	H	110	LEU
4	H	128	VAL
4	H	129	THR
4	H	146	LEU
4	H	167	VAL
4	H	173	GLN
4	H	188	PHE
4	H	190	ASP
4	H	194	VAL
4	H	198	LYS
4	H	240	GLU
4	H	243	LYS
4	H	249	VAL

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Mol	Chain	Res	Type
4	H	254	LEU
4	H	260	ILE
4	H	263	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	252	GLN
2	B	54	ASN
2	B	141	HIS
2	B	150	GLN
2	B	196	HIS
2	B	243	HIS
3	C	77	ASN
3	C	122	ASN
3	C	126	ASN
1	E	252	GLN
2	F	113	ASN
2	F	150	GLN
2	F	192	GLN
2	F	196	HIS
2	F	243	HIS
3	G	77	ASN
3	G	126	ASN

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

4 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
5	ANP	F	301	-	33,33,33	0.96	4 (12%)	45,52,52	0.57	0
5	ANP	E	301	-	33,33,33	0.93	4 (12%)	45,52,52	0.64	0
5	ANP	A	301	-	33,33,33	2.07	6 (18%)	45,52,52	0.80	1 (2%)
5	ANP	B	301	-	33,33,33	2.01	6 (18%)	45,52,52	0.69	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
5	ANP	F	301	-	-	6/18/38/38	0/3/3/3
5	ANP	E	301	-	-	12/18/38/38	0/3/3/3
5	ANP	A	301	-	-	6/18/38/38	0/3/3/3
5	ANP	B	301	-	-	7/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	ANP	PG-O1G	8.25	1.58	1.46
5	B	301	ANP	PG-O1G	7.91	1.58	1.46
5	A	301	ANP	PB-O1B	6.52	1.56	1.46
5	B	301	ANP	PB-O1B	6.43	1.55	1.46
5	B	301	ANP	PB-O2B	-2.64	1.49	1.56
5	A	301	ANP	PG-N3B	2.63	1.70	1.63
5	A	301	ANP	PB-O2B	-2.62	1.49	1.56
5	A	301	ANP	PG-O3G	-2.59	1.49	1.56
5	B	301	ANP	PG-O2G	-2.56	1.50	1.56
5	F	301	ANP	PG-O1G	2.56	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	301	ANP	PG-N3B	2.56	1.70	1.63
5	E	301	ANP	PG-O1G	2.50	1.50	1.46
5	F	301	ANP	PG-N3B	2.47	1.69	1.63
5	B	301	ANP	PG-N3B	2.46	1.69	1.63
5	F	301	ANP	PB-O1B	2.44	1.49	1.46
5	E	301	ANP	PB-O1B	2.31	1.49	1.46
5	B	301	ANP	PB-O3A	-2.22	1.56	1.59
5	F	301	ANP	PB-O3A	-2.10	1.56	1.59
5	E	301	ANP	PB-O3A	-2.06	1.56	1.59
5	A	301	ANP	PB-N3B	2.01	1.68	1.63

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	ANP	O1B-PB-N3B	-2.43	108.19	111.77
5	A	301	ANP	O1B-PB-N3B	-2.18	108.56	111.77

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	ANP	PB-N3B-PG-O1G
5	A	301	ANP	PA-O3A-PB-O2B
5	A	301	ANP	O4'-C1'-N9-C8
5	A	301	ANP	O4'-C1'-N9-C4
5	B	301	ANP	PB-N3B-PG-O1G
5	B	301	ANP	PG-N3B-PB-O1B
5	E	301	ANP	PB-N3B-PG-O1G
5	E	301	ANP	PG-N3B-PB-O3A
5	E	301	ANP	PA-O3A-PB-O2B
5	E	301	ANP	C5'-O5'-PA-O1A
5	E	301	ANP	C5'-O5'-PA-O2A
5	E	301	ANP	C5'-O5'-PA-O3A
5	E	301	ANP	O4'-C4'-C5'-O5'
5	F	301	ANP	PB-N3B-PG-O1G
5	F	301	ANP	PG-N3B-PB-O3A
5	E	301	ANP	C3'-C4'-C5'-O5'
5	B	301	ANP	O4'-C4'-C5'-O5'
5	F	301	ANP	O4'-C4'-C5'-O5'
5	B	301	ANP	C3'-C4'-C5'-O5'
5	F	301	ANP	C3'-C4'-C5'-O5'
5	E	301	ANP	C2'-C1'-N9-C8

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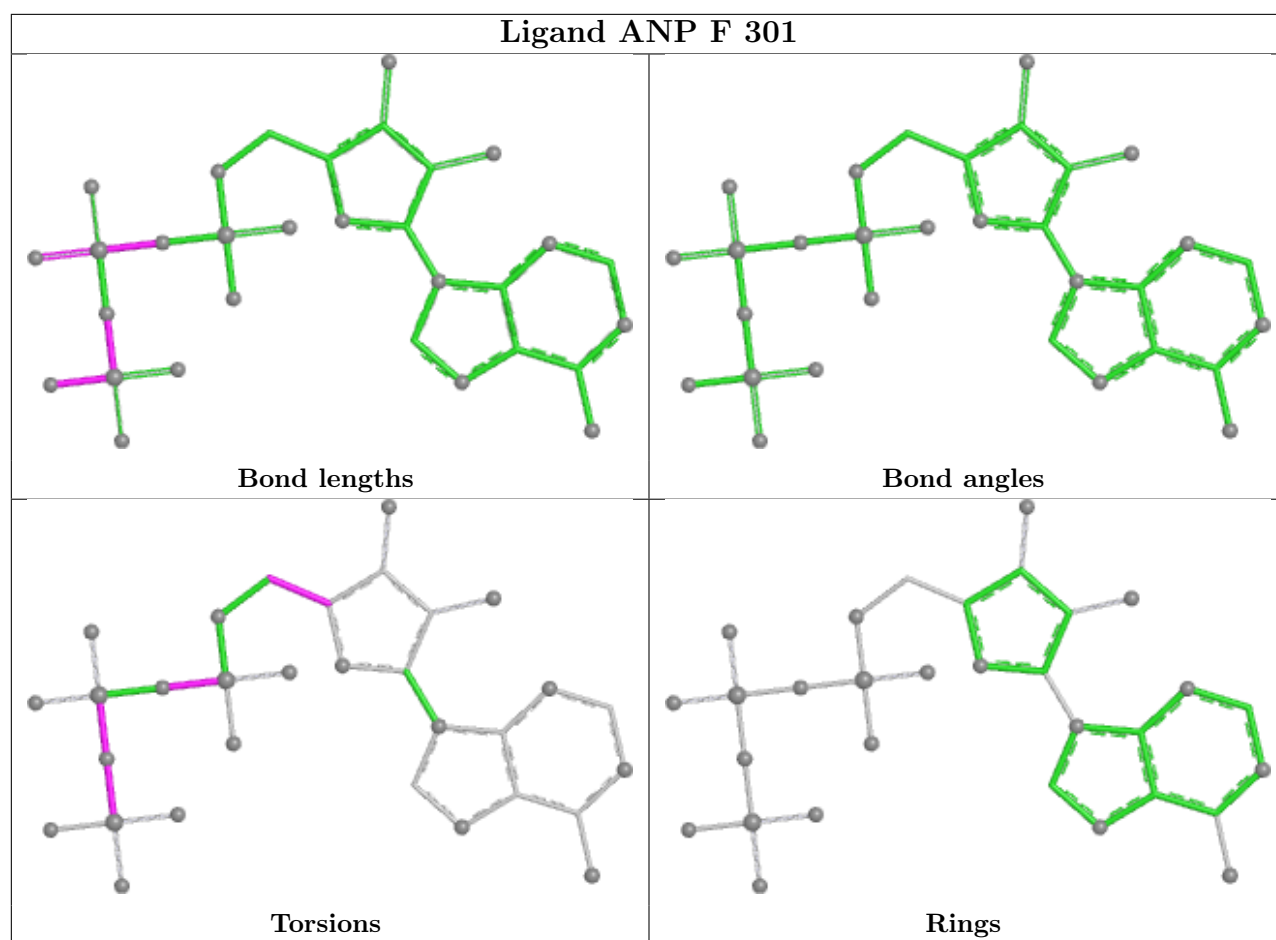
Mol	Chain	Res	Type	Atoms
5	F	301	ANP	PB-O3A-PA-O1A
5	A	301	ANP	PG-N3B-PB-O3A
5	B	301	ANP	PG-N3B-PB-O3A
5	B	301	ANP	PB-O3A-PA-O2A
5	E	301	ANP	C2'-C1'-N9-C4
5	E	301	ANP	PB-O3A-PA-O1A
5	A	301	ANP	O4'-C4'-C5'-O5'
5	F	301	ANP	PB-O3A-PA-O2A
5	E	301	ANP	PA-O3A-PB-O1B
5	B	301	ANP	PB-O3A-PA-O1A

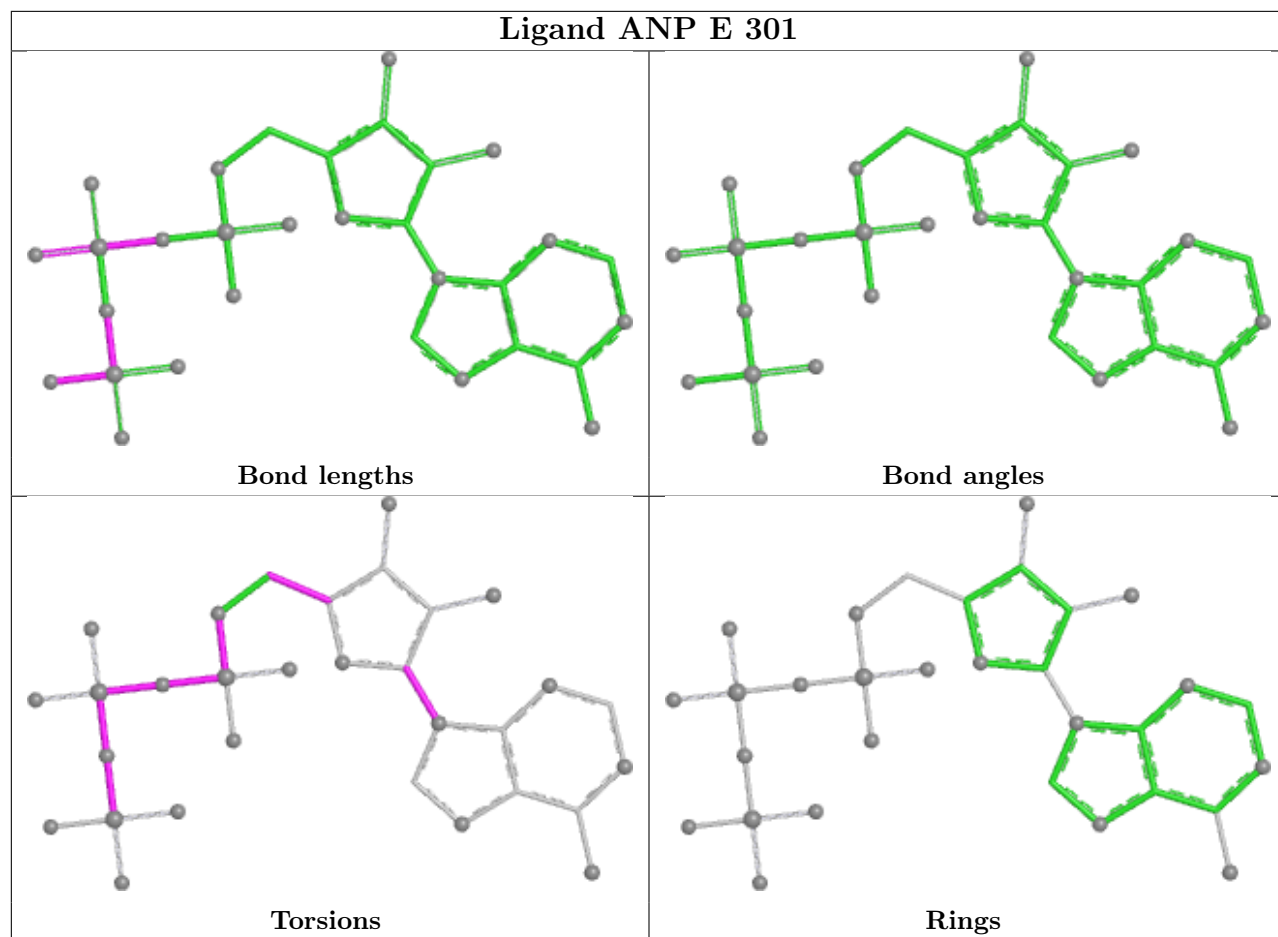
There are no ring outliers.

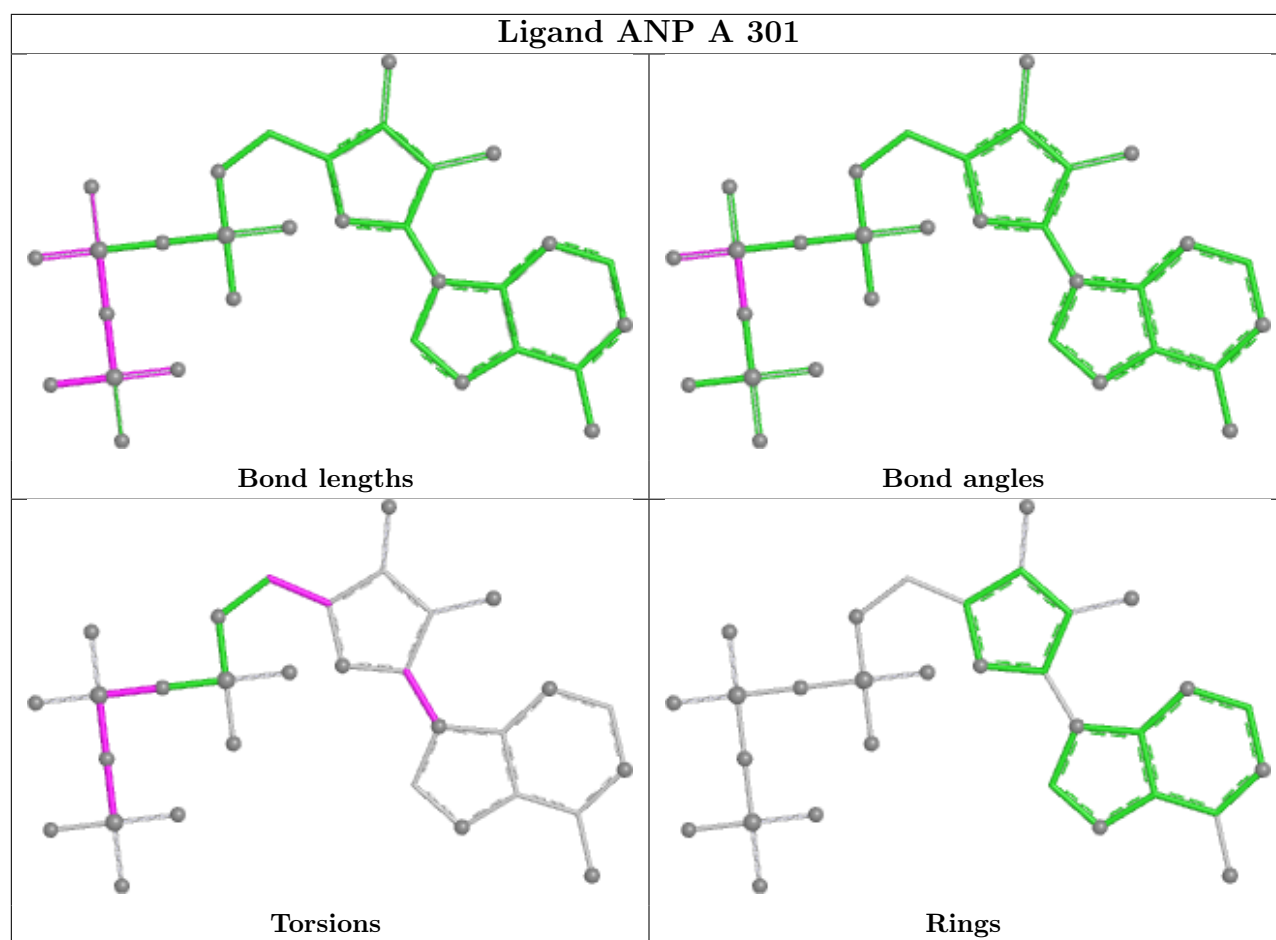
4 monomers are involved in 11 short contacts:

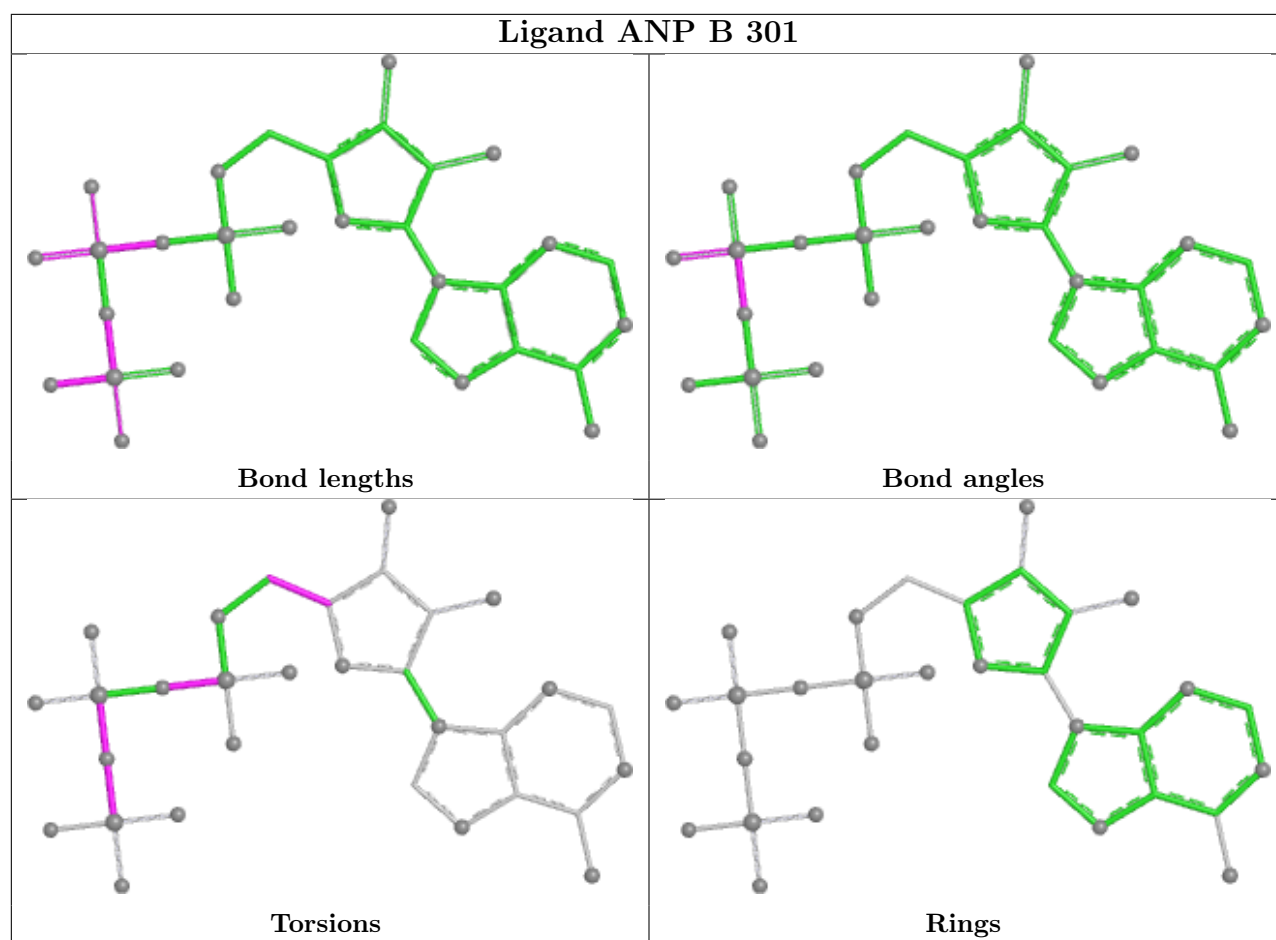
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	301	ANP	1	0
5	E	301	ANP	5	0
5	A	301	ANP	4	0
5	B	301	ANP	1	0

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.









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	280/298 (93%)	-0.74	5 (1%) 67 49	69, 140, 260, 421	0
1	E	280/298 (93%)	-0.52	13 (4%) 37 25	77, 144, 262, 320	0
2	B	281/287 (97%)	-0.79	3 (1%) 78 60	90, 137, 219, 282	0
2	F	281/287 (97%)	-0.79	9 (3%) 50 34	92, 139, 211, 257	0
3	C	168/184 (91%)	-0.41	6 (3%) 46 31	85, 163, 255, 338	0
3	G	168/184 (91%)	-0.55	5 (2%) 52 35	90, 163, 296, 349	0
4	D	259/265 (97%)	-0.79	5 (1%) 66 48	89, 162, 252, 414	0
4	H	259/265 (97%)	-0.74	7 (2%) 56 37	90, 155, 243, 368	0
All	All	1976/2068 (95%)	-0.69	53 (2%) 56 37	69, 148, 250, 421	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	136	ILE	7.5
2	F	223	LEU	7.3
1	E	203	ASP	7.2
2	F	206	ASP	5.5
3	C	162	PHE	5.3
1	E	206	GLU	5.3
1	A	177	GLU	4.6
2	F	101	ASN	4.5
3	C	166	GLY	4.3
1	E	193	ASN	4.0
1	E	205	GLU	4.0
1	E	14	THR	3.9
4	D	40	ASN	3.9
3	G	137	ASN	3.8
2	F	182	LEU	3.7
4	H	85	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	265	ILE	3.5
3	G	35	GLY	3.5
4	H	110	LEU	3.5
2	B	85	ARG	3.5
1	A	266	ASP	3.4
2	F	177	ASP	3.3
4	H	52	LEU	3.2
3	C	168	SER	3.2
1	E	255	LYS	3.2
2	F	224	ILE	3.1
4	H	84	THR	3.1
3	C	167	LEU	3.0
1	E	15	TYR	2.9
1	E	201	THR	2.8
4	D	110	LEU	2.7
4	D	68	GLY	2.7
2	B	165	GLU	2.7
2	F	218	LEU	2.6
2	B	192	GLN	2.5
1	E	204	LEU	2.5
2	F	178	PRO	2.5
1	A	180	GLU	2.5
1	E	260	VAL	2.4
1	E	56	LEU	2.4
4	H	111	TYR	2.4
4	H	171	PHE	2.3
2	F	219	GLU	2.3
4	D	146	LEU	2.3
3	C	163	ILE	2.3
3	G	160	VAL	2.2
3	C	108	TRP	2.2
1	E	202	HIS	2.1
4	D	73	ILE	2.1
1	E	87	GLY	2.0
3	G	174	ARG	2.0
4	H	253	LEU	2.0
1	A	5	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

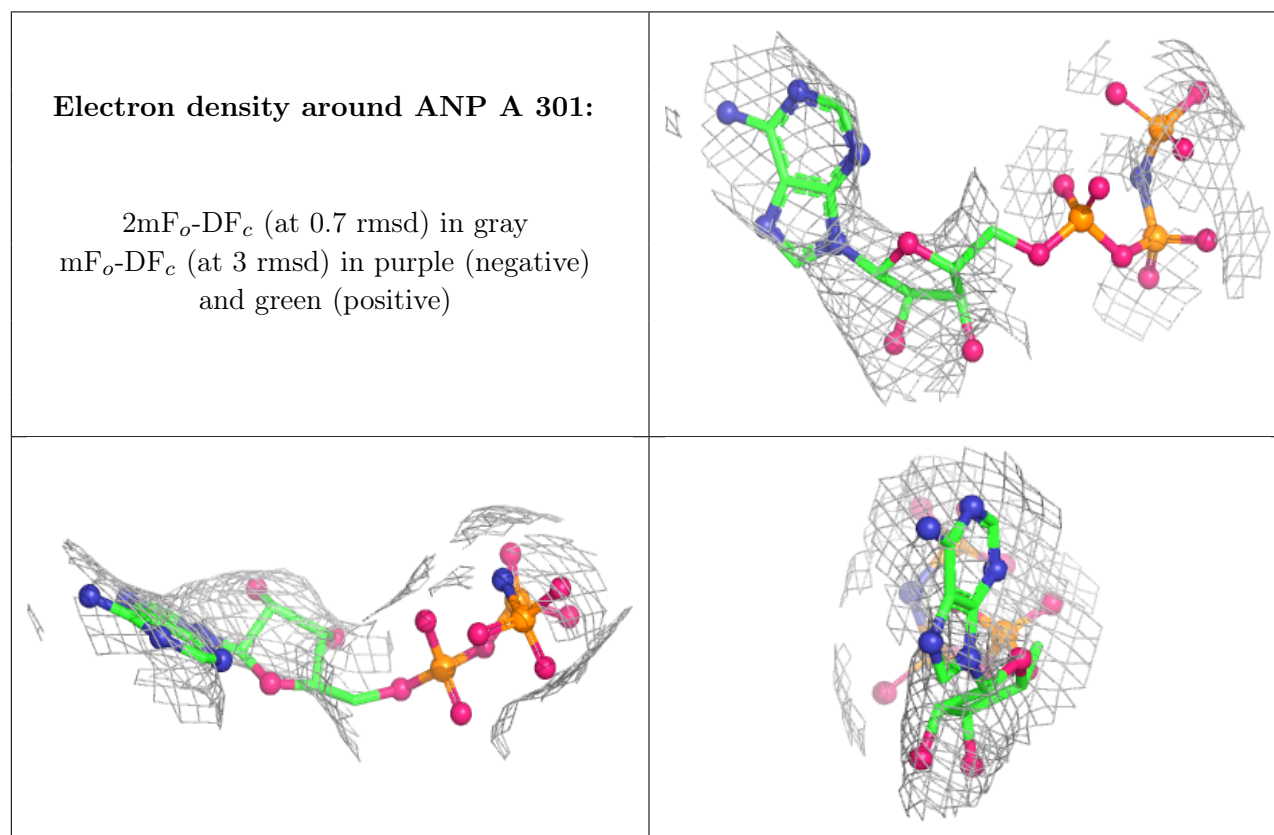
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

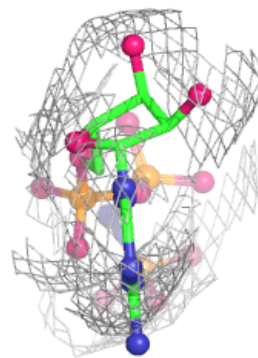
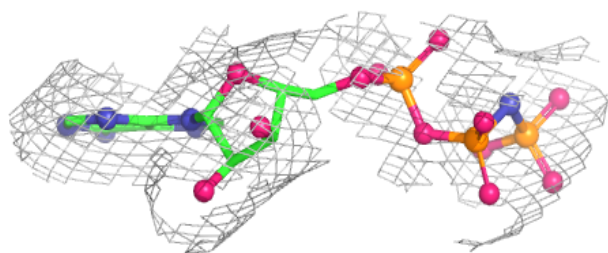
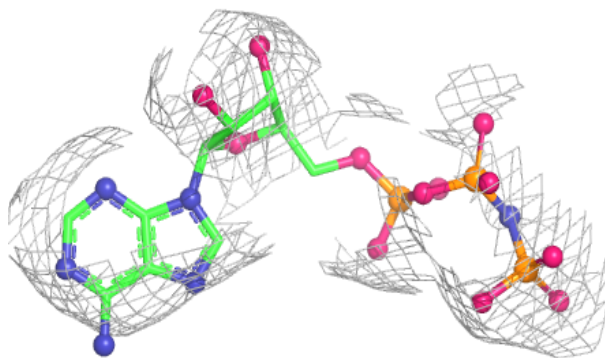
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ANP	A	301	31/31	0.99	0.04	133,177,206,207	0
5	ANP	B	301	31/31	0.99	0.04	133,136,164,222	0
5	ANP	E	301	31/31	0.99	0.04	126,173,203,246	0
5	ANP	F	301	31/31	0.99	0.05	78,130,178,273	0

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.



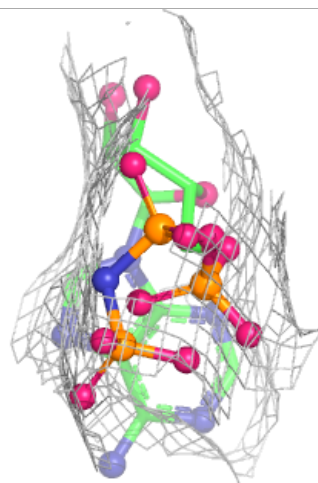
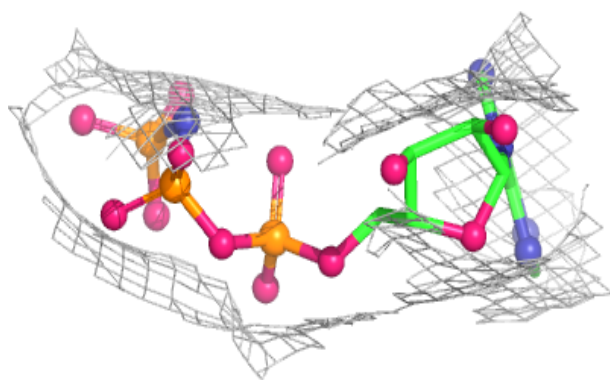
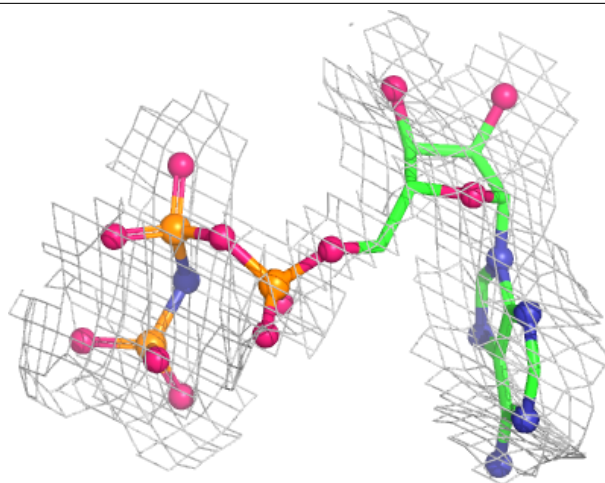
Electron density around ANP B 301:

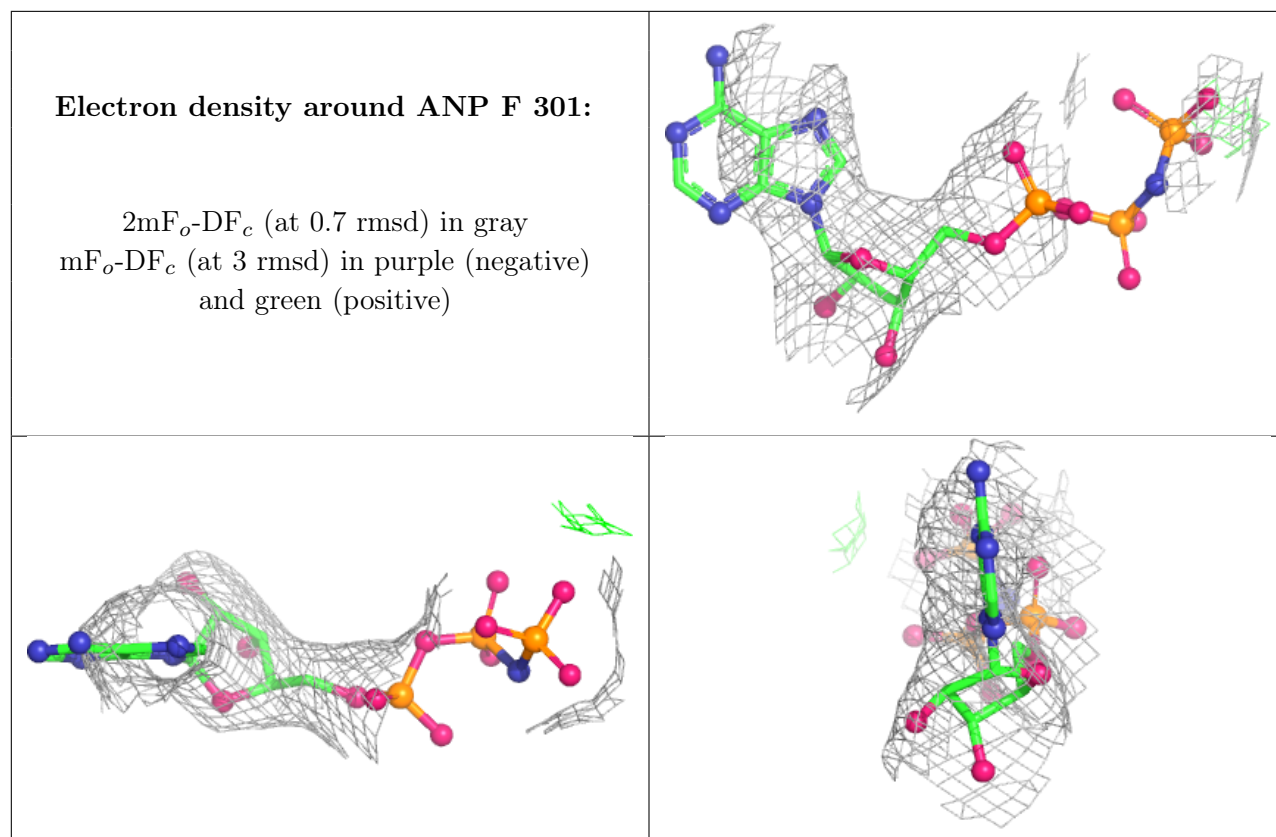
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ANP E 301:

$2mF_o-DF_c$ (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.