



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:39 AM UTC

PDB ID : 5AKB / pdb_00005akb
Title : MutS in complex with the N-terminal domain of MutL - crystal form 1
Authors : Groothuizen, F.S.; Winkler, I.; Cristovao, M.; Fish, A.; Winterwerp, H.H.K.;
Reumer, A.; Marx, A.D.; Hermans, N.; Nicholls, R.A.; Murshudov, G.N.;
Lebbink, J.H.G.; Friedhoff, P.; Sixma, T.K.
Deposited on : 2015-03-03
Resolution : 4.71 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

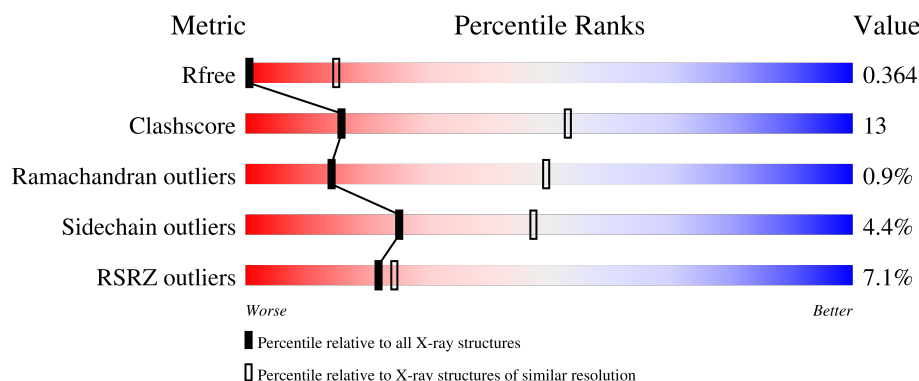
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.71 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	1011 (5.50-3.94)
Clashscore	190562	1009 (5.48-3.96)
Ramachandran outliers	187476	1098 (5.54-3.90)
Sidechain outliers	187428	1079 (5.54-3.90)
RSRZ outliers	180081	1006 (5.50-3.94)

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	800	
1	B	800	
1	E	800	
2	C	369	

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Mol	Chain	Length	Quality of chain
2	D	369	10% 56% 19% •• 23%
2	F	369	7% 54% 20% • 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21906 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 DNA MISMATCH REPAIR PROTEIN MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	B	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	E	588	Total	C	N	O	S	0	0	0
			4605	2894	825	867	19			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ALA	CYS	engineered mutation	UNP P23909
A	235	SER	CYS	engineered mutation	UNP P23909
A	239	ALA	CYS	engineered mutation	UNP P23909
A	246	CYS	ASP	engineered mutation	UNP P23909
A	297	SER	CYS	engineered mutation	UNP P23909
A	569	SER	CYS	engineered mutation	UNP P23909
A	711	VAL	CYS	engineered mutation	UNP P23909
B	93	ALA	CYS	engineered mutation	UNP P23909
B	235	SER	CYS	engineered mutation	UNP P23909
B	239	ALA	CYS	engineered mutation	UNP P23909
B	246	CYS	ASP	engineered mutation	UNP P23909
B	297	SER	CYS	engineered mutation	UNP P23909
B	569	SER	CYS	engineered mutation	UNP P23909
B	711	VAL	CYS	engineered mutation	UNP P23909
E	93	ALA	CYS	engineered mutation	UNP P23909
E	235	SER	CYS	engineered mutation	UNP P23909
E	239	ALA	CYS	engineered mutation	UNP P23909
E	246	CYS	ASP	engineered mutation	UNP P23909
E	297	SER	CYS	engineered mutation	UNP P23909
E	569	SER	CYS	engineered mutation	UNP P23909
E	711	VAL	CYS	engineered mutation	UNP P23909

- Molecule 2 is a protein called DNA MISMATCH REPAIR PROTEIN MUTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	285	Total 2252	C 1423	N 409	O 418	S 2	0	0	0
2	D	285	Total 2252	C 1423	N 409	O 418	S 2	0	0	0
2	F	285	Total 2252	C 1423	N 409	O 418	S 2	0	0	0

There are 75 discrepancies between the modelled and reference sequences:

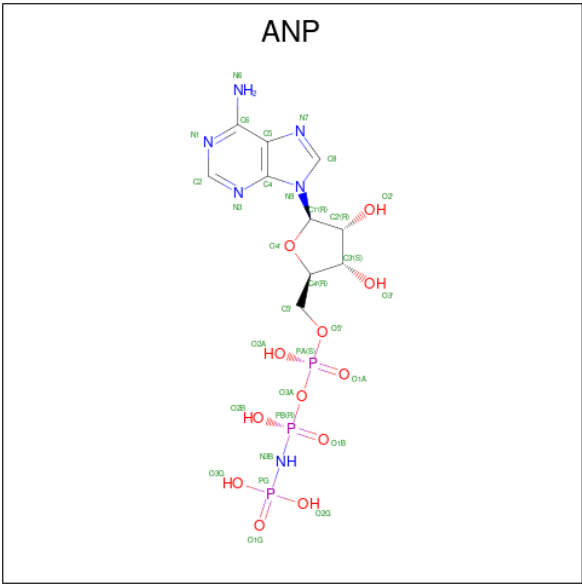
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP P23367
C	-18	GLY	-	expression tag	UNP P23367
C	-17	SER	-	expression tag	UNP P23367
C	-16	SER	-	expression tag	UNP P23367
C	-15	HIS	-	expression tag	UNP P23367
C	-14	HIS	-	expression tag	UNP P23367
C	-13	HIS	-	expression tag	UNP P23367
C	-12	HIS	-	expression tag	UNP P23367
C	-11	HIS	-	expression tag	UNP P23367
C	-10	HIS	-	expression tag	UNP P23367
C	-9	SER	-	expression tag	UNP P23367
C	-8	SER	-	expression tag	UNP P23367
C	-7	GLY	-	expression tag	UNP P23367
C	-6	LEU	-	expression tag	UNP P23367
C	-5	VAL	-	expression tag	UNP P23367
C	-4	PRO	-	expression tag	UNP P23367
C	-3	ARG	-	expression tag	UNP P23367
C	-2	GLY	-	expression tag	UNP P23367
C	-1	SER	-	expression tag	UNP P23367
C	0	HIS	-	expression tag	UNP P23367
C	61	SER	CYS	engineered mutation	UNP P23367
C	131	CYS	ASN	engineered mutation	UNP P23367
C	216	LEU	CYS	engineered mutation	UNP P23367
C	256	PHE	CYS	engineered mutation	UNP P23367
C	276	TYR	CYS	engineered mutation	UNP P23367
D	-19	MET	-	expression tag	UNP P23367
D	-18	GLY	-	expression tag	UNP P23367
D	-17	SER	-	expression tag	UNP P23367
D	-16	SER	-	expression tag	UNP P23367
D	-15	HIS	-	expression tag	UNP P23367
D	-14	HIS	-	expression tag	UNP P23367
D	-13	HIS	-	expression tag	UNP P23367
D	-12	HIS	-	expression tag	UNP P23367

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	HIS	-	expression tag	UNP P23367
D	-10	HIS	-	expression tag	UNP P23367
D	-9	SER	-	expression tag	UNP P23367
D	-8	SER	-	expression tag	UNP P23367
D	-7	GLY	-	expression tag	UNP P23367
D	-6	LEU	-	expression tag	UNP P23367
D	-5	VAL	-	expression tag	UNP P23367
D	-4	PRO	-	expression tag	UNP P23367
D	-3	ARG	-	expression tag	UNP P23367
D	-2	GLY	-	expression tag	UNP P23367
D	-1	SER	-	expression tag	UNP P23367
D	0	HIS	-	expression tag	UNP P23367
D	61	SER	CYS	engineered mutation	UNP P23367
D	131	CYS	ASN	engineered mutation	UNP P23367
D	216	LEU	CYS	engineered mutation	UNP P23367
D	256	PHE	CYS	engineered mutation	UNP P23367
D	276	TYR	CYS	engineered mutation	UNP P23367
F	-19	MET	-	expression tag	UNP P23367
F	-18	GLY	-	expression tag	UNP P23367
F	-17	SER	-	expression tag	UNP P23367
F	-16	SER	-	expression tag	UNP P23367
F	-15	HIS	-	expression tag	UNP P23367
F	-14	HIS	-	expression tag	UNP P23367
F	-13	HIS	-	expression tag	UNP P23367
F	-12	HIS	-	expression tag	UNP P23367
F	-11	HIS	-	expression tag	UNP P23367
F	-10	HIS	-	expression tag	UNP P23367
F	-9	SER	-	expression tag	UNP P23367
F	-8	SER	-	expression tag	UNP P23367
F	-7	GLY	-	expression tag	UNP P23367
F	-6	LEU	-	expression tag	UNP P23367
F	-5	VAL	-	expression tag	UNP P23367
F	-4	PRO	-	expression tag	UNP P23367
F	-3	ARG	-	expression tag	UNP P23367
F	-2	GLY	-	expression tag	UNP P23367
F	-1	SER	-	expression tag	UNP P23367
F	0	HIS	-	expression tag	UNP P23367
F	61	SER	CYS	engineered mutation	UNP P23367
F	131	CYS	ASN	engineered mutation	UNP P23367
F	216	LEU	CYS	engineered mutation	UNP P23367
F	256	PHE	CYS	engineered mutation	UNP P23367
F	276	TYR	CYS	engineered mutation	UNP P23367

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

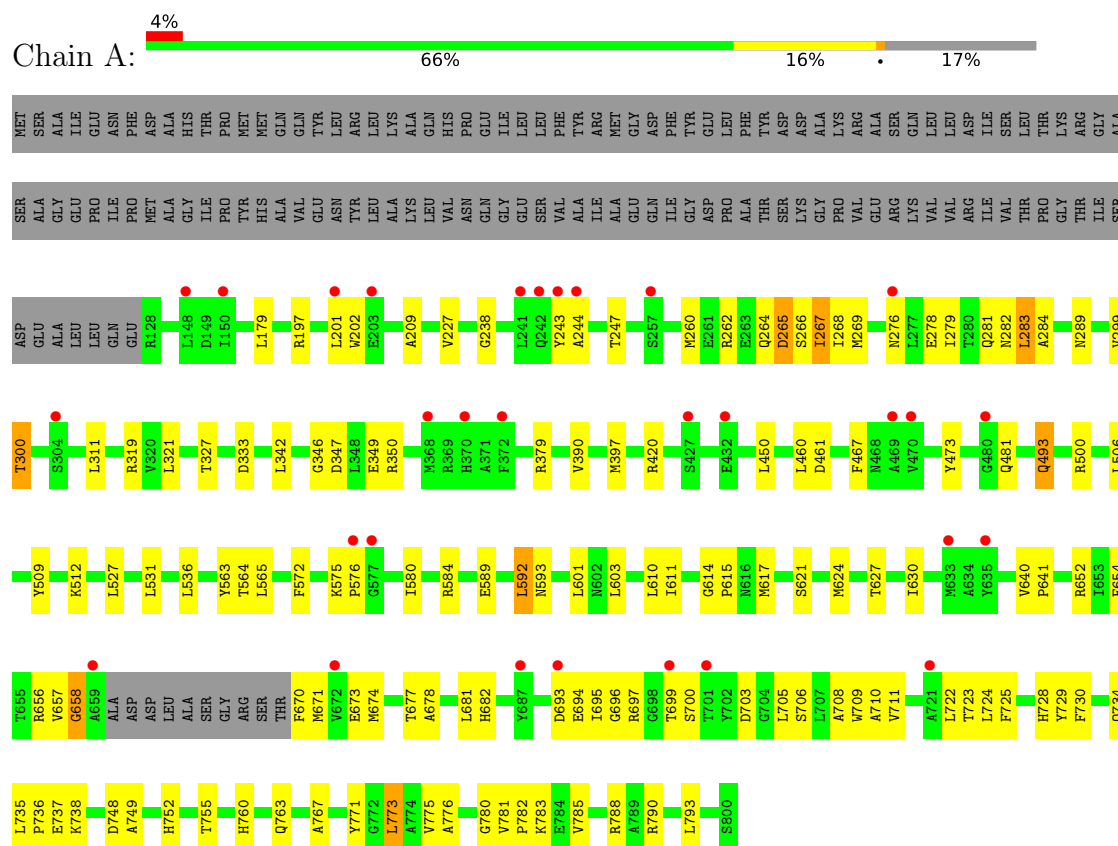


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

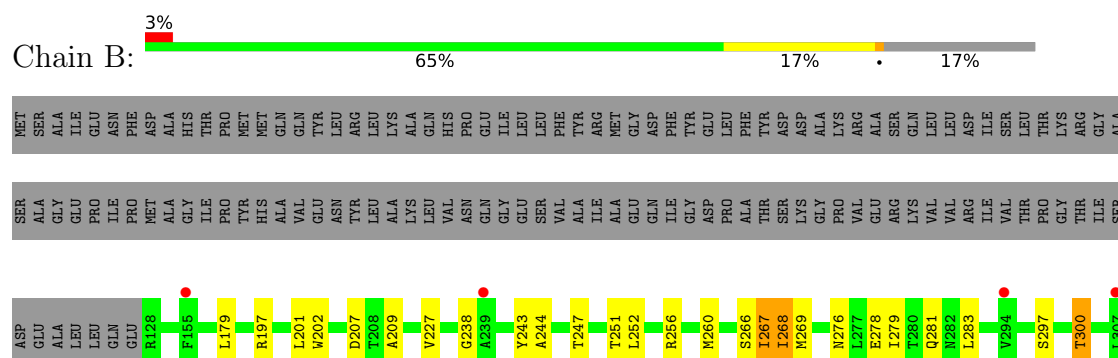
3 Residue-property plots

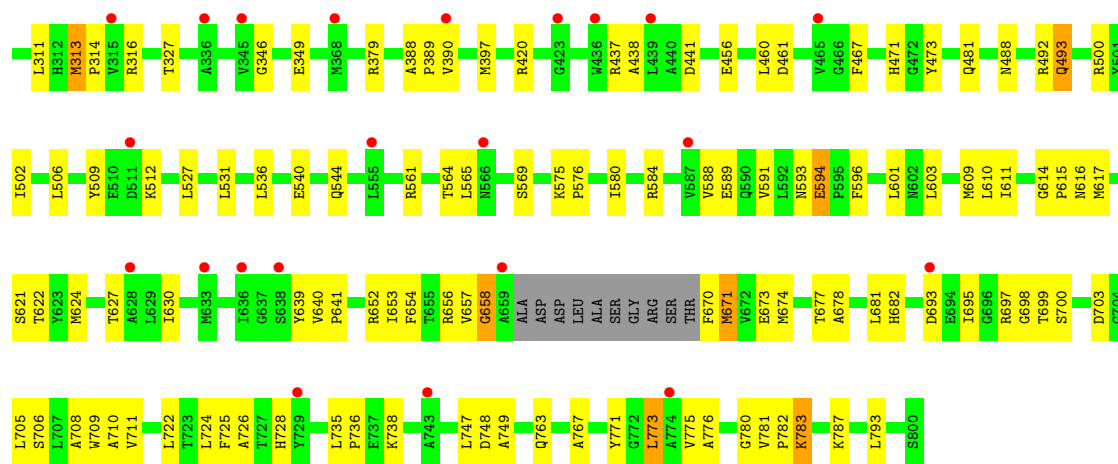
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

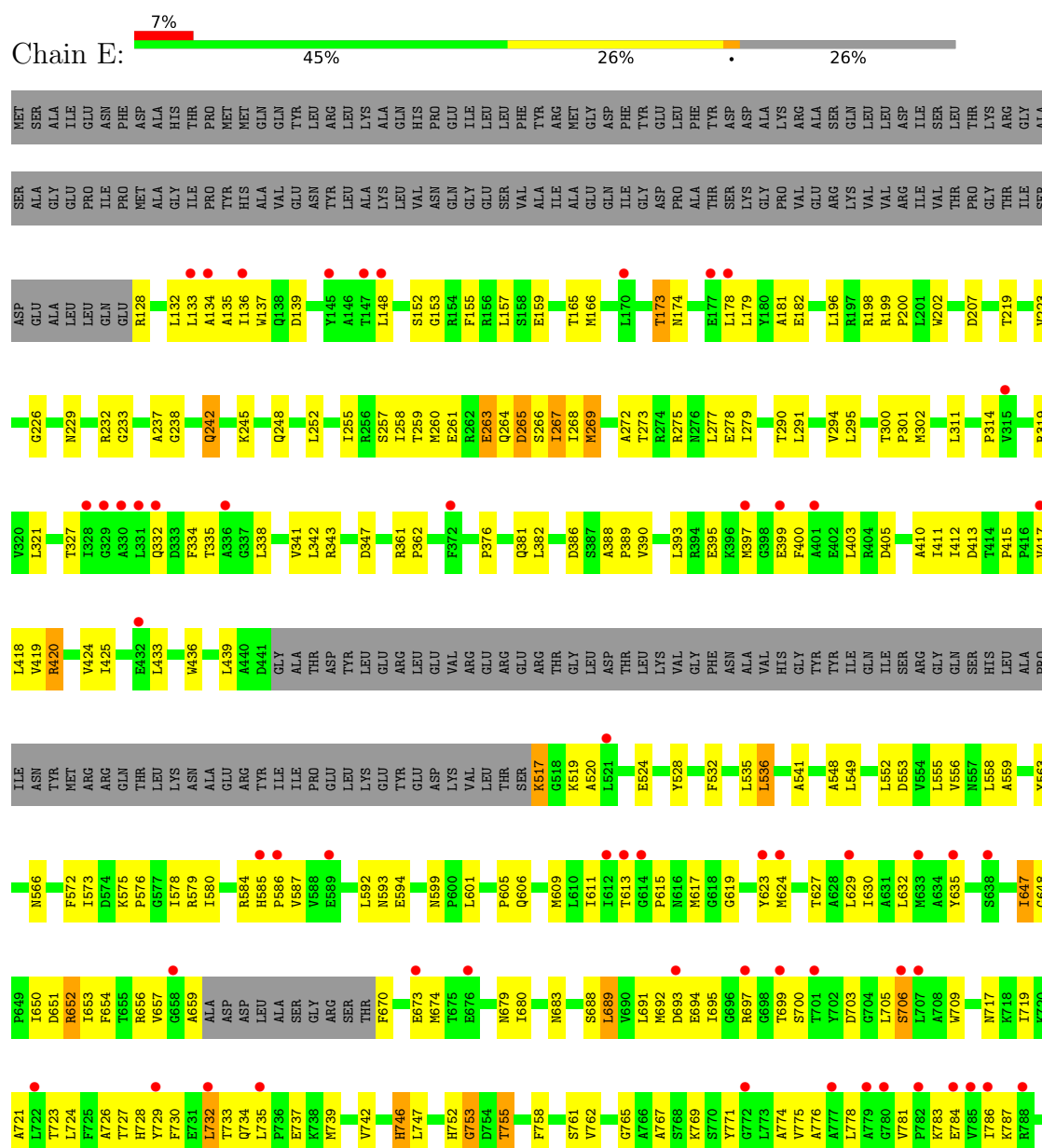


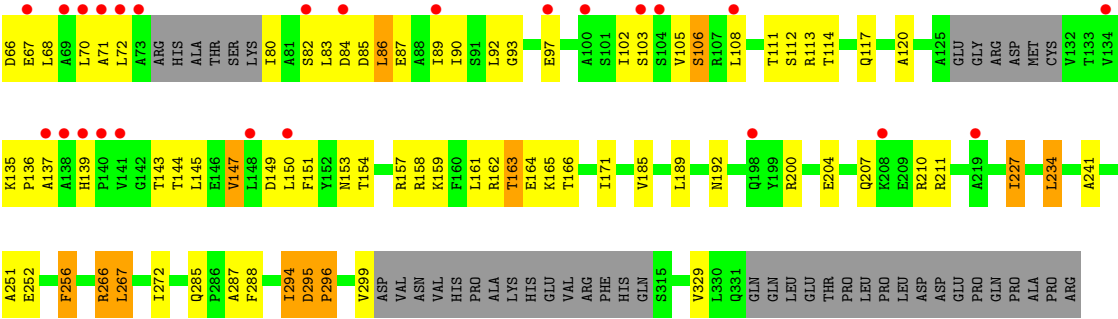
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS





• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.93Å 188.54Å 200.43Å 90.00° 94.77° 90.00°	Depositor
Resolution (Å)	199.73 – 4.71 199.73 – 4.71	Depositor EDS
% Data completeness (in resolution range)	97.2 (199.73-4.71) 97.2 (199.73-4.71)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 4.65Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.319 , 0.349 0.337 , 0.364	Depositor DCC
R_{free} test set	1499 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	172.9	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 440.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	21906	wwPDB-VP
Average B, all atoms (Å ²)	234.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.73	0/5311	0.96	3/7186 (0.0%)
1	B	0.67	0/5311	0.93	3/7186 (0.0%)
1	E	0.80	0/4678	1.03	7/6331 (0.1%)
2	C	0.82	0/2288	1.04	6/3096 (0.2%)
2	D	0.74	2/2288 (0.1%)	1.04	7/3096 (0.2%)
2	F	0.71	0/2288	1.00	9/3096 (0.3%)
All	All	0.74	2/22164 (0.0%)	0.99	35/29991 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	263	MET	N-CA	5.86	1.52	1.45
2	D	118	GLN	CA-C	5.53	1.59	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	118	GLN	N-CA-C	11.52	126.39	108.07
2	F	106	SER	N-CA-C	7.62	118.30	108.24
2	C	106	SER	N-CA-C	6.86	117.64	108.38
2	F	86	LEU	N-CA-C	6.82	118.79	111.36
1	E	776	ALA	N-CA-C	6.75	119.94	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	752	HIS	N-CA-C	6.68	119.35	107.80
2	C	147	VAL	N-CA-C	6.67	117.16	108.35
2	F	103	SER	N-CA-C	6.52	119.38	111.82
2	D	103	SER	N-CA-C	6.50	119.36	111.82
2	D	295	ASP	CA-C-N	6.32	127.74	119.84
2	D	295	ASP	C-N-CA	6.32	127.74	119.84
1	E	647	ILE	N-CA-C	6.24	117.27	108.17
2	C	295	ASP	CA-C-N	6.16	127.54	119.84
2	C	295	ASP	C-N-CA	6.16	127.54	119.84
1	B	267	ILE	N-CA-C	6.08	117.87	108.44
2	D	147	VAL	N-CA-C	6.01	116.28	108.35
1	A	262	ARG	N-CA-C	5.96	118.66	109.07
2	D	106	SER	N-CA-C	5.81	116.23	108.38
1	E	746	HIS	N-CA-C	5.73	117.83	108.55
1	B	609	MET	CB-CG-SD	5.63	129.59	112.70
2	F	256	PHE	CB-CA-C	-5.61	99.45	109.71
2	F	62	GLY	N-CA-C	5.60	120.24	112.57
2	C	103	SER	N-CA-C	5.57	118.28	111.82
1	E	688	SER	N-CA-C	5.57	117.71	110.53
1	E	173	THR	N-CA-C	5.53	118.23	111.82
2	F	295	ASP	CA-C-N	5.52	126.74	119.84
2	F	295	ASP	C-N-CA	5.52	126.74	119.84
2	C	152	TYR	CA-CB-CG	5.46	123.74	113.90
1	E	657	VAL	N-CA-C	5.40	114.57	106.42
1	B	456	GLU	CB-CA-C	-5.39	102.41	110.88
2	F	294	ILE	N-CA-C	5.25	114.93	108.53
2	F	296	PRO	N-CA-C	5.11	123.00	112.47
2	D	296	PRO	N-CA-C	5.05	122.87	112.47
1	A	592	LEU	N-CA-C	5.03	118.41	109.96
1	E	136	ILE	N-CA-C	5.02	115.60	108.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ASP	Peptide
1	A	266	SER	Peptide
1	A	267	ILE	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	5226	0	5283	123	0
1	B	5226	0	5283	131	0
1	E	4605	0	4660	180	1
2	C	2252	0	2272	59	0
2	D	2252	0	2272	45	0
2	F	2252	0	2272	79	0
3	A	31	0	13	3	0
3	B	31	0	13	7	0
3	E	31	0	13	0	0
All	All	21906	0	22081	583	1

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 13.

All (583) 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)
2:F:82:SER:O	2:F:85:ASP:OD1	1.56	1.21
2:C:51:ALA:O	2:C:149:ASP:CG	1.90	1.15
2:F:51:ALA:O	2:F:149:ASP:CG	1.90	1.14
2:F:267:LEU:HD12	2:F:299:VAL:HG13	1.28	1.13
2:F:83:LEU:HA	2:F:86:LEU:HB3	1.12	1.12
1:B:267:ILE:HD12	1:B:313:MET:HG2	1.32	1.08
1:E:137:TRP:CH2	1:E:139:ASP:HB3	1.87	1.08
2:C:52:LYS:HA	2:C:149:ASP:OD1	1.55	1.06
1:A:656:ARG:NH2	1:A:673:GLU:HA	1.71	1.03
2:F:83:LEU:HA	2:F:86:LEU:CB	1.89	1.02
2:F:83:LEU:CA	2:F:86:LEU:HB3	1.89	1.01
1:B:473:TYR:HB2	1:B:506:LEU:HD21	1.43	0.98
2:F:52:LYS:HA	2:F:149:ASP:OD1	1.64	0.96
2:F:51:ALA:C	2:F:149:ASP:OD2	2.09	0.95
2:C:51:ALA:C	2:C:149:ASP:OD2	2.09	0.94
1:A:656:ARG:HH21	1:A:673:GLU:HA	1.26	0.92
1:E:266:SER:HA	1:E:651:ASP:HB2	1.50	0.91
1:A:656:ARG:HH21	1:A:673:GLU:CA	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:HIS:CG	1:B:699:THR:HA	2.07	0.90
1:B:267:ILE:HD11	1:B:314:PRO:O	1.72	0.89
2:C:51:ALA:C	2:C:149:ASP:CG	2.40	0.89
2:F:51:ALA:C	2:F:149:ASP:CG	2.40	0.89
1:B:267:ILE:HD13	1:B:314:PRO:CD	2.03	0.89
1:E:269:MET:HG2	1:E:653:ILE:HB	1.55	0.88
1:E:267:ILE:HG22	1:E:268:ILE:HG23	1.56	0.87
1:A:699:THR:HA	1:B:728:HIS:CG	2.11	0.85
2:D:86:LEU:HD21	2:D:89:ILE:HB	1.58	0.85
1:E:730:PHE:CD2	1:E:767:ALA:HB3	2.11	0.85
2:D:111:THR:HG22	2:D:122:GLN:HG3	1.57	0.84
1:B:674:MET:O	1:B:677:THR:OG1	1.96	0.84
2:F:70:LEU:CD2	2:F:86:LEU:HD13	2.06	0.83
1:A:563:TYR:O	2:C:200:ARG:NH2	2.12	0.83
1:A:674:MET:O	1:A:677:THR:OG1	1.97	0.83
1:E:397:MET:HE1	1:E:552:LEU:HD12	1.60	0.82
1:B:565:LEU:O	1:B:584:ARG:NH2	2.13	0.81
2:F:267:LEU:CD1	2:F:299:VAL:HG13	2.09	0.81
1:A:670:PHE:HB3	3:B:1801:ANP:O1G	1.80	0.81
2:F:256:PHE:HE1	2:F:272:ILE:HD12	1.46	0.81
2:C:106:SER:HB3	2:C:150:LEU:HD22	1.63	0.80
1:A:694:GLU:HB2	1:B:697:ARG:HH21	1.47	0.80
1:E:327:THR:HG21	1:E:555:LEU:HD13	1.62	0.80
1:B:267:ILE:HD13	1:B:314:PRO:N	1.95	0.79
1:A:656:ARG:HH21	1:A:673:GLU:CB	1.94	0.79
2:C:86:LEU:HD21	2:C:89:ILE:HB	1.65	0.79
1:E:291:LEU:HD21	1:E:311:LEU:HD22	1.63	0.79
1:B:473:TYR:CB	1:B:506:LEU:HD21	2.12	0.79
2:F:70:LEU:HD22	2:F:86:LEU:HD13	1.64	0.79
1:A:565:LEU:O	1:A:584:ARG:NH2	2.15	0.78
1:E:157:LEU:HD13	1:E:237:ALA:HB2	1.63	0.78
1:E:727:THR:OG1	1:E:729:TYR:CD2	2.36	0.78
1:E:137:TRP:HH2	1:E:139:ASP:HB3	1.42	0.78
1:E:248:GLN:HG3	1:E:252:LEU:HD21	1.66	0.78
1:A:268:ILE:CG2	1:A:269:MET:H	1.96	0.78
2:F:106:SER:HB3	2:F:150:LEU:HD22	1.66	0.78
2:D:150:LEU:HD12	2:D:151:PHE:CD2	2.19	0.78
2:F:51:ALA:HB1	2:F:149:ASP:OD2	1.83	0.78
2:C:51:ALA:HB1	2:C:149:ASP:OD2	1.83	0.77
1:A:682:HIS:CE1	1:B:780:GLY:O	2.38	0.77
1:B:656:ARG:HH22	1:B:673:GLU:CD	1.93	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ARG:NH2	1:B:673:GLU:CD	2.43	0.77
2:C:163:THR:OG1	2:C:166:THR:OG1	2.03	0.76
1:E:576:PRO:O	1:E:605:PRO:HD3	1.87	0.75
2:F:163:THR:OG1	2:F:166:THR:OG1	2.04	0.74
2:D:111:THR:HG22	2:D:122:GLN:CG	2.17	0.73
1:E:295:LEU:CD1	1:E:311:LEU:HD21	2.18	0.73
1:E:755:THR:HG21	2:F:136:PRO:HD2	1.70	0.73
1:A:624:MET:HE1	1:A:724:LEU:HB2	1.71	0.73
1:E:382:LEU:HD11	1:E:552:LEU:HD11	1.71	0.73
1:A:624:MET:SD	1:A:724:LEU:HB3	2.29	0.72
1:A:773:LEU:HD12	1:A:793:LEU:HD22	1.71	0.72
1:B:267:ILE:HD13	1:B:314:PRO:HD2	1.69	0.72
1:E:580:ILE:HD12	1:E:601:LEU:HD23	1.70	0.72
1:B:773:LEU:HD12	1:B:793:LEU:HD22	1.72	0.72
2:F:86:LEU:HD21	2:F:90:ILE:HG23	1.72	0.71
2:F:82:SER:C	2:F:85:ASP:OD1	2.33	0.71
2:F:256:PHE:CE1	2:F:272:ILE:HD12	2.26	0.70
1:E:341:VAL:HG21	1:E:381:GLN:HE22	1.56	0.70
1:A:682:HIS:HE1	1:B:780:GLY:O	1.74	0.70
1:B:202:TRP:CZ2	2:C:158:ARG:NH2	2.61	0.69
1:B:267:ILE:CD1	1:B:314:PRO:N	2.55	0.69
1:A:755:THR:HG21	2:C:135:LYS:HB2	1.73	0.69
1:E:632:LEU:O	1:E:632:LEU:HD23	1.93	0.69
2:C:51:ALA:O	2:C:149:ASP:OD1	2.10	0.69
1:A:695:ILE:HD11	1:A:725:PHE:CZ	2.28	0.68
1:B:695:ILE:HD11	1:B:725:PHE:CZ	2.28	0.68
1:E:266:SER:HA	1:E:651:ASP:CB	2.22	0.68
1:A:615:PRO:HG3	1:A:749:ALA:HB2	1.76	0.68
2:C:102:ILE:HG23	2:C:150:LEU:CD2	2.25	0.67
2:F:267:LEU:HD12	2:F:299:VAL:CG1	2.17	0.67
1:E:264:GLN:O	1:E:266:SER:N	2.28	0.67
2:F:51:ALA:O	2:F:149:ASP:OD1	2.12	0.67
2:C:51:ALA:CA	2:C:149:ASP:OD2	2.43	0.67
1:E:272:ALA:HA	1:E:275:ARG:CZ	2.25	0.66
3:A:1801:ANP:O1G	1:B:670:PHE:HB3	1.96	0.66
1:B:267:ILE:CD1	1:B:313:MET:C	2.68	0.66
1:E:268:ILE:HG22	1:E:314:PRO:HD2	1.76	0.66
1:B:615:PRO:HG3	1:B:749:ALA:HB2	1.76	0.66
1:E:735:LEU:HD22	1:E:739:MET:HG3	1.76	0.66
1:B:267:ILE:CD1	1:B:314:PRO:O	2.43	0.66
2:F:70:LEU:HD21	2:F:86:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:83:LEU:N	2:F:86:LEU:HB3	2.11	0.65
2:F:164:GLU:HG3	2:F:165:LYS:H	1.60	0.65
1:A:267:ILE:CG2	1:A:268:ILE:H	2.10	0.65
1:A:267:ILE:HG22	1:A:268:ILE:H	1.60	0.65
2:C:51:ALA:CB	2:C:149:ASP:OD2	2.45	0.65
1:E:269:MET:CG	1:E:653:ILE:HB	2.24	0.65
2:F:51:ALA:CA	2:F:149:ASP:OD2	2.45	0.65
2:C:72:LEU:HD21	2:C:108:LEU:HD22	1.78	0.65
2:F:102:ILE:HG23	2:F:150:LEU:CD2	2.27	0.65
2:F:80:ILE:HG23	2:F:90:ILE:HD13	1.80	0.64
1:A:617:MET:SD	1:B:671:MET:HE3	2.37	0.64
1:E:295:LEU:HD13	1:E:311:LEU:HD21	1.78	0.64
1:E:295:LEU:HD22	1:E:558:LEU:HD23	1.79	0.64
1:B:678:ALA:HA	1:B:681:LEU:HD12	1.80	0.63
1:E:419:VAL:HG12	1:E:524:GLU:HG2	1.80	0.63
2:F:51:ALA:CB	2:F:149:ASP:OD2	2.46	0.63
2:C:102:ILE:HG23	2:C:150:LEU:HD21	1.79	0.63
1:B:267:ILE:HG22	1:B:268:ILE:N	2.14	0.63
1:E:302:MET:HE1	1:E:549:LEU:HD13	1.79	0.63
1:A:785:VAL:HG13	1:B:710:ALA:HB1	1.80	0.63
2:D:150:LEU:CD1	2:D:151:PHE:CE2	2.82	0.63
1:A:773:LEU:CD1	1:A:793:LEU:HD22	2.28	0.63
1:E:419:VAL:HA	1:E:424:VAL:HG21	1.81	0.63
1:B:593:ASN:O	1:B:594:GLU:HB3	1.98	0.62
1:E:700:SER:O	1:E:703:ASP:OD1	2.18	0.62
1:B:266:SER:O	1:B:316:ARG:HD3	1.98	0.62
2:F:102:ILE:HG23	2:F:150:LEU:HD21	1.81	0.62
1:B:773:LEU:CD1	1:B:793:LEU:HD22	2.29	0.62
2:C:106:SER:CB	2:C:150:LEU:HD22	2.29	0.62
2:F:256:PHE:HE1	2:F:272:ILE:CD1	2.10	0.62
2:F:82:SER:O	2:F:86:LEU:N	2.33	0.62
1:E:650:ILE:HD13	1:E:689:LEU:HD22	1.81	0.62
1:E:165:THR:HG21	1:E:263:GLU:HG2	1.82	0.61
1:E:321:LEU:HD13	1:E:572:PHE:CZ	2.35	0.61
2:F:106:SER:CB	2:F:150:LEU:HD22	2.30	0.61
1:E:680:ILE:HD13	1:E:692:MET:HE1	1.83	0.61
2:D:241:ALA:HB3	2:D:287:ALA:HB3	1.83	0.61
1:E:382:LEU:HD22	1:E:390:VAL:CG1	2.31	0.61
1:E:332:GLN:HG3	1:E:563:TYR:HB2	1.84	0.60
1:B:278:GLU:OE2	1:B:283:LEU:N	2.30	0.60
1:B:630:ILE:HG23	1:B:640:VAL:HG11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:241:ALA:HB3	2:C:287:ALA:HB3	1.83	0.60
1:E:248:GLN:CG	1:E:252:LEU:HD21	2.30	0.60
1:A:268:ILE:HG23	1:A:269:MET:H	1.66	0.60
1:A:782:PRO:HG3	1:B:682:HIS:NE2	2.16	0.60
1:E:566:ASN:O	1:E:584:ARG:NH2	2.35	0.60
1:E:382:LEU:HD22	1:E:390:VAL:HG13	1.82	0.60
1:E:248:GLN:HG3	1:E:252:LEU:HD11	1.83	0.60
1:B:502:ILE:CD1	1:B:506:LEU:HD22	2.32	0.59
1:E:268:ILE:HG22	1:E:314:PRO:HG2	1.82	0.59
2:C:47:GLU:HG3	2:C:53:LEU:HD23	1.83	0.59
2:C:266:ARG:O	2:C:269:ASN:HB2	2.02	0.59
2:F:241:ALA:HB3	2:F:287:ALA:HB3	1.83	0.59
1:E:252:LEU:HD22	1:E:255:ILE:HD12	1.83	0.59
1:A:209:ALA:HB1	1:A:238:GLY:HA3	1.84	0.59
1:E:572:PHE:HA	1:E:647:ILE:O	2.01	0.59
1:A:580:ILE:CD1	1:A:630:ILE:HD13	2.33	0.59
1:E:294:VAL:HG21	1:E:587:VAL:HA	1.85	0.59
2:F:83:LEU:HA	2:F:86:LEU:CA	2.32	0.59
2:D:156:ALA:HB1	2:D:160:PHE:CZ	2.38	0.59
1:E:157:LEU:HD11	1:E:233:GLY:O	2.03	0.59
1:E:403:LEU:HD22	1:E:535:LEU:CD2	2.33	0.59
1:B:266:SER:C	1:B:267:ILE:HG13	2.28	0.58
1:E:332:GLN:OE1	2:F:200:ARG:NH2	2.35	0.58
2:F:164:GLU:HG3	2:F:165:LYS:N	2.19	0.58
2:C:70:LEU:CD2	2:C:86:LEU:HD13	2.34	0.58
1:E:397:MET:HE2	1:E:549:LEU:HG	1.85	0.58
1:E:656:ARG:HG2	1:E:695:ILE:HG22	1.84	0.58
1:A:450:LEU:CD2	1:A:506:LEU:HD21	2.34	0.58
2:C:164:GLU:HG3	2:C:165:LYS:H	1.67	0.58
2:C:80:ILE:O	2:C:83:LEU:HG	2.03	0.58
1:A:630:ILE:HG23	1:A:640:VAL:HG11	1.84	0.58
1:A:734:GLN:O	1:A:737:GLU:HG2	2.04	0.57
1:B:267:ILE:HD11	1:B:314:PRO:C	2.29	0.57
2:C:105:VAL:HG13	2:C:153:ASN:OD1	2.04	0.57
1:E:268:ILE:HD12	1:E:269:MET:O	2.04	0.57
1:E:269:MET:HG2	1:E:653:ILE:CB	2.29	0.57
1:E:652:ARG:NH1	1:E:683:ASN:O	2.37	0.57
1:A:179:LEU:HD23	1:A:197:ARG:HB2	1.86	0.57
1:A:670:PHE:N	3:B:1801:ANP:O2G	2.38	0.57
1:A:708:ALA:O	1:A:709:TRP:C	2.47	0.57
1:E:165:THR:HG21	1:E:263:GLU:CG	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:ALA:O	2:D:80:ILE:HG23	2.03	0.57
1:E:267:ILE:HG22	1:E:268:ILE:CG2	2.32	0.57
1:E:613:THR:O	1:E:746:HIS:HB2	2.05	0.57
2:F:256:PHE:CE1	2:F:288:PHE:CE1	2.92	0.57
1:A:575:LYS:HB3	1:A:576:PRO:HD2	1.86	0.56
1:E:268:ILE:HG22	1:E:314:PRO:CD	2.34	0.56
2:D:70:LEU:CD2	2:D:86:LEU:HD13	2.34	0.56
1:E:264:GLN:HB2	1:E:267:ILE:HG12	1.88	0.56
1:E:735:LEU:HD22	1:E:739:MET:CG	2.35	0.56
1:E:226:GLY:HA3	1:E:683:ASN:HD21	1.71	0.56
2:F:52:LYS:CA	2:F:149:ASP:OD1	2.48	0.56
1:A:268:ILE:CG2	1:A:269:MET:N	2.63	0.56
1:B:576:PRO:HB2	1:B:722:LEU:HD11	1.87	0.56
1:A:678:ALA:HA	1:A:681:LEU:HD12	1.88	0.55
2:D:64:LYS:HG3	2:D:114:THR:HG21	1.87	0.55
1:E:719:ILE:HG22	1:E:721:ALA:HB2	1.88	0.55
1:B:276:ASN:HB2	1:B:657:VAL:HG21	1.89	0.55
1:E:771:TYR:O	1:E:774:ALA:HB3	2.06	0.55
1:A:624:MET:SD	1:A:724:LEU:CB	2.95	0.55
2:D:150:LEU:HD11	2:D:151:PHE:CE2	2.41	0.55
1:E:268:ILE:HG22	1:E:314:PRO:CG	2.36	0.55
1:A:420:ARG:HG3	1:B:420:ARG:NH1	2.22	0.55
1:E:376:PRO:HG3	1:E:399:GLU:CD	2.31	0.55
1:A:760:HIS:HB3	3:A:1801:ANP:C6	2.36	0.55
1:E:135:ALA:HA	1:E:179:LEU:O	2.07	0.55
2:F:47:GLU:HG3	2:F:53:LEU:HD23	1.89	0.55
1:B:575:LYS:HB3	1:B:576:PRO:HD2	1.87	0.55
2:D:263:MET:SD	2:D:264:ARG:N	2.77	0.55
1:B:708:ALA:O	1:B:709:TRP:C	2.50	0.55
1:A:268:ILE:HG22	1:A:269:MET:H	1.69	0.54
1:B:771:TYR:O	1:B:775:VAL:HG23	2.06	0.54
2:F:70:LEU:HD21	2:F:86:LEU:CD1	2.36	0.54
1:A:738:LYS:HG3	1:E:717:ASN:HD21	1.72	0.54
1:B:580:ILE:HD12	1:B:601:LEU:HB3	1.89	0.54
2:F:82:SER:O	2:F:86:LEU:CB	2.56	0.54
2:D:80:ILE:O	2:D:83:LEU:HG	2.08	0.54
1:A:580:ILE:HD12	1:A:601:LEU:HB3	1.90	0.54
2:C:64:LYS:HG3	2:C:114:THR:HG21	1.89	0.54
1:A:576:PRO:HB2	1:A:722:LEU:HD11	1.89	0.54
1:E:419:VAL:HG21	1:E:528:TYR:CG	2.43	0.53
1:E:599:ASN:HD21	1:E:761:SER:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:GLU:HG3	2:D:53:LEU:HD23	1.89	0.53
2:C:120:ALA:HB3	2:C:137:ALA:O	2.09	0.53
1:E:273:THR:O	1:E:277:LEU:HG	2.07	0.53
1:A:564:THR:HA	2:C:198:GLN:HE22	1.74	0.53
2:C:157:ARG:O	2:C:161:LEU:HG	2.08	0.53
2:F:66:ASP:OD1	2:F:67:GLU:N	2.41	0.53
2:F:82:SER:C	2:F:86:LEU:HB3	2.33	0.53
1:E:635:TYR:OH	1:E:648:GLY:O	2.27	0.53
1:E:656:ARG:NH2	1:E:673:GLU:CG	2.72	0.53
1:B:473:TYR:HB2	1:B:506:LEU:CD2	2.30	0.52
2:C:80:ILE:O	2:C:80:ILE:HG22	2.08	0.52
1:E:403:LEU:HD22	1:E:535:LEU:HD23	1.91	0.52
2:C:52:LYS:CA	2:C:149:ASP:OD1	2.45	0.52
1:E:563:TYR:CE1	2:F:200:ARG:HD2	2.44	0.52
2:F:65:LYS:HA	2:F:68:LEU:HD12	1.92	0.52
1:A:615:PRO:HB3	1:A:771:TYR:CD1	2.44	0.52
2:F:83:LEU:O	2:F:87:GLU:N	2.33	0.52
2:F:120:ALA:HB3	2:F:137:ALA:O	2.09	0.52
1:B:179:LEU:HD23	1:B:197:ARG:HB2	1.90	0.52
1:B:209:ALA:HB1	1:B:238:GLY:HA3	1.90	0.52
1:B:615:PRO:HB3	1:B:771:TYR:CD1	2.45	0.52
2:D:65:LYS:HA	2:D:68:LEU:HD12	1.91	0.52
2:F:105:VAL:HG13	2:F:153:ASN:OD1	2.09	0.52
2:F:157:ARG:O	2:F:161:LEU:HG	2.09	0.52
1:B:700:SER:O	1:B:703:ASP:OD1	2.28	0.52
2:C:185:VAL:O	2:C:211:ARG:NH2	2.43	0.52
2:D:120:ALA:HB3	2:D:137:ALA:O	2.09	0.52
1:E:259:THR:HG22	1:E:260:MET:N	2.25	0.52
1:E:733:THR:HG21	1:E:767:ALA:HB2	1.92	0.52
1:A:728:HIS:CD2	1:B:699:THR:HA	2.43	0.52
1:A:771:TYR:O	1:A:775:VAL:HG23	2.10	0.52
2:C:72:LEU:CD2	2:C:108:LEU:HD22	2.40	0.52
2:C:164:GLU:HG3	2:C:165:LYS:N	2.25	0.52
2:D:116:GLU:HG3	2:D:117:GLN:HG3	1.91	0.52
1:E:341:VAL:HG21	1:E:381:GLN:NE2	2.23	0.52
1:A:268:ILE:HG22	1:A:269:MET:N	2.25	0.51
1:A:700:SER:O	1:A:703:ASP:OD1	2.29	0.51
1:B:580:ILE:CD1	1:B:630:ILE:HD13	2.41	0.51
1:A:592:LEU:HD12	1:A:593:ASN:N	2.25	0.51
2:D:70:LEU:HD21	2:D:86:LEU:HD13	1.91	0.51
1:E:656:ARG:NH2	1:E:673:GLU:HG2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:185:VAL:O	2:F:211:ARG:NH2	2.43	0.51
1:B:588:VAL:HA	1:B:591:VAL:HG12	1.93	0.51
1:E:327:THR:HG23	1:E:390:VAL:HG23	1.92	0.51
1:B:267:ILE:HD13	1:B:313:MET:C	2.33	0.51
1:E:632:LEU:HD23	1:E:632:LEU:C	2.34	0.51
1:A:611:ILE:HD11	1:A:735:LEU:HB2	1.92	0.51
2:C:87:GLU:O	2:C:87:GLU:HG2	2.11	0.51
2:D:113:ARG:HB2	2:D:120:ALA:HB2	1.93	0.51
1:E:264:GLN:O	1:E:267:ILE:HG12	2.11	0.51
1:E:269:MET:HE1	1:E:632:LEU:HD12	1.92	0.51
2:C:70:LEU:HD21	2:C:86:LEU:HD13	1.92	0.51
2:D:80:ILE:O	2:D:80:ILE:HG22	2.11	0.51
1:E:613:THR:HG21	1:E:767:ALA:HA	1.93	0.51
2:D:87:GLU:HG2	2:D:87:GLU:O	2.11	0.51
1:A:264:GLN:HB2	1:A:268:ILE:HD11	1.92	0.51
2:C:71:ALA:C	2:C:72:LEU:HD12	2.36	0.51
1:E:259:THR:HG22	1:E:260:MET:H	1.76	0.51
1:E:302:MET:HE3	1:E:549:LEU:HB3	1.93	0.51
1:E:691:LEU:CD2	1:E:724:LEU:HD12	2.41	0.51
1:A:267:ILE:CG2	1:A:268:ILE:N	2.72	0.50
1:A:267:ILE:HG22	1:A:268:ILE:N	2.24	0.50
1:E:291:LEU:CD2	1:E:311:LEU:HD22	2.39	0.50
1:E:728:HIS:O	1:E:729:TYR:C	2.54	0.50
1:E:223:VAL:O	1:E:679:ASN:HB2	2.12	0.50
1:A:467:PHE:HB2	1:A:473:TYR:CE1	2.47	0.50
1:A:584:ARG:HD2	1:A:589:GLU:OE1	2.12	0.50
2:D:151:PHE:CZ	2:D:157:ARG:HB3	2.47	0.50
2:D:47:GLU:HG2	2:D:192:ASN:HA	1.94	0.50
1:A:694:GLU:CB	1:B:697:ARG:HH21	2.21	0.50
2:D:111:THR:CG2	2:D:122:GLN:HG3	2.37	0.50
1:E:709:TRP:HA	1:E:732:LEU:HD21	1.94	0.50
1:B:327:THR:HG23	1:B:390:VAL:HG22	1.93	0.50
2:D:185:VAL:O	2:D:211:ARG:NH2	2.45	0.50
1:E:783:LYS:O	1:E:787:LYS:HB2	2.12	0.50
1:A:656:ARG:NH1	1:A:657:VAL:O	2.43	0.49
1:B:611:ILE:HD11	1:B:735:LEU:HB2	1.94	0.49
1:A:227:VAL:HG12	1:A:260:MET:HB2	1.95	0.49
1:E:133:LEU:HD23	1:E:148:LEU:HB3	1.94	0.49
2:F:113:ARG:HB2	2:F:120:ALA:HB2	1.95	0.49
1:A:327:THR:HG23	1:A:390:VAL:HG22	1.94	0.49
2:C:151:PHE:O	2:C:158:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:66:ASP:OD1	2:F:67:GLU:HG3	2.12	0.49
1:A:278:GLU:HA	1:A:281:GLN:O	2.13	0.49
3:A:1801:ANP:PG	1:B:670:PHE:HB3	2.53	0.49
1:B:300:THR:OG1	1:B:346:GLY:O	2.29	0.49
1:E:732:LEU:C	1:E:734:GLN:N	2.70	0.49
2:C:105:VAL:O	2:C:150:LEU:O	2.31	0.49
1:B:467:PHE:HB2	1:B:473:TYR:CE1	2.47	0.49
1:A:673:GLU:HG2	1:A:674:MET:CE	2.43	0.49
2:C:65:LYS:HA	2:C:68:LEU:HD12	1.93	0.49
2:F:151:PHE:O	2:F:158:ARG:NH1	2.46	0.49
1:A:300:THR:OG1	1:A:346:GLY:O	2.30	0.49
1:E:415:PRO:HB2	1:E:424:VAL:HG22	1.95	0.49
1:E:433:LEU:HD12	1:E:520:ALA:HB1	1.95	0.49
1:E:617:MET:O	1:E:758:PHE:CE2	2.65	0.49
1:B:621:SER:OG	3:B:1801:ANP:O2B	2.31	0.48
1:A:267:ILE:CG2	1:A:652:ARG:HG2	2.43	0.48
1:B:267:ILE:HG21	1:B:314:PRO:HD2	1.95	0.48
1:B:502:ILE:HD12	1:B:506:LEU:HD22	1.95	0.48
1:E:155:PHE:O	1:E:258:ILE:HA	2.14	0.48
2:C:47:GLU:HG2	2:C:192:ASN:HA	1.94	0.48
1:E:179:LEU:HD22	1:E:199:ARG:HD3	1.95	0.48
1:A:209:ALA:CB	1:A:238:GLY:HA3	2.42	0.48
1:B:527:LEU:O	1:B:531:LEU:HD13	2.13	0.48
1:B:266:SER:O	1:B:316:ARG:CD	2.60	0.48
1:E:412:ILE:HG22	1:E:413:ASP:N	2.28	0.48
1:B:584:ARG:HD2	1:B:589:GLU:OE1	2.13	0.48
1:B:622:THR:N	3:B:1801:ANP:O1A	2.38	0.48
2:C:295:ASP:CG	2:C:296:PRO:HD2	2.39	0.48
1:E:362:PRO:HG3	1:E:419:VAL:HG22	1.96	0.48
1:A:617:MET:SD	1:B:671:MET:CE	3.01	0.48
1:A:780:GLY:O	1:B:682:HIS:HE1	1.96	0.48
1:B:564:THR:HG23	2:D:195:ILE:CD1	2.43	0.48
1:A:243:TYR:O	1:A:247:THR:N	2.47	0.48
1:A:603:LEU:HD11	1:A:724:LEU:HD21	1.94	0.47
1:A:615:PRO:HB3	1:A:771:TYR:CG	2.48	0.47
1:E:730:PHE:HA	1:E:767:ALA:CB	2.43	0.47
2:F:234:LEU:HD22	2:F:294:ILE:CG2	2.44	0.47
1:A:780:GLY:O	1:B:682:HIS:CE1	2.67	0.47
1:B:279:ILE:CG2	1:B:311:LEU:HD13	2.44	0.47
2:C:162:ARG:O	2:C:163:THR:C	2.57	0.47
2:D:67:GLU:HG2	2:D:89:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLU:OE2	1:A:283:LEU:N	2.37	0.47
1:A:527:LEU:O	1:A:531:LEU:HD13	2.14	0.47
1:B:540:GLU:O	1:B:544:GLN:HG2	2.14	0.47
1:B:596:PHE:CZ	3:B:1801:ANP:N6	2.82	0.47
1:E:200:PRO:HB2	1:E:202:TRP:NE1	2.29	0.47
1:E:342:LEU:O	1:E:343:ARG:C	2.57	0.47
2:F:82:SER:O	2:F:86:LEU:HB3	2.15	0.47
1:E:732:LEU:C	1:E:734:GLN:H	2.22	0.47
1:E:755:THR:HG21	2:F:135:LYS:HB2	1.96	0.47
2:F:47:GLU:HG2	2:F:192:ASN:HA	1.95	0.47
2:F:71:ALA:C	2:F:72:LEU:HD12	2.40	0.47
1:B:267:ILE:CG1	1:B:314:PRO:O	2.63	0.47
1:E:624:MET:SD	1:E:726:ALA:HB2	2.54	0.47
1:B:603:LEU:HD11	1:B:724:LEU:HD21	1.95	0.47
1:E:400:PHE:HZ	1:E:541:ALA:HB1	1.80	0.47
1:A:279:ILE:CG2	1:A:311:LEU:HD13	2.45	0.47
1:B:251:THR:O	1:B:252:LEU:HD23	2.15	0.47
2:F:64:LYS:HG3	2:F:114:THR:HG21	1.97	0.47
1:E:393:LEU:HD22	1:E:548:ALA:HA	1.97	0.47
1:E:623:TYR:HB2	1:E:747:LEU:HD21	1.97	0.47
1:B:243:TYR:CE2	1:B:247:THR:HG21	2.50	0.47
1:E:137:TRP:HD1	1:E:181:ALA:CB	2.28	0.47
1:E:311:LEU:O	1:E:632:LEU:HD11	2.15	0.47
1:E:388:ALA:HB3	1:E:389:PRO:HD3	1.96	0.47
1:A:657:VAL:O	1:A:658:GLY:C	2.58	0.46
1:B:615:PRO:HB3	1:B:771:TYR:CG	2.50	0.46
2:C:234:LEU:HD22	2:C:294:ILE:CG2	2.44	0.46
2:D:234:LEU:HD22	2:D:294:ILE:CG2	2.44	0.46
2:D:247:THR:HB	2:D:248:PRO:HD2	1.96	0.46
1:E:412:ILE:HG22	1:E:413:ASP:H	1.80	0.46
1:E:242:GLN:HA	1:E:245:LYS:HD3	1.97	0.46
1:E:694:GLU:HG2	1:E:727:THR:HA	1.97	0.46
1:B:735:LEU:N	1:B:736:PRO:CD	2.79	0.46
1:E:174:ASN:O	1:E:174:ASN:CG	2.56	0.46
1:E:619:GLY:O	1:E:747:LEU:HG	2.15	0.46
1:B:267:ILE:CG2	1:B:268:ILE:N	2.78	0.46
2:C:113:ARG:HB2	2:C:120:ALA:HB2	1.96	0.46
1:A:640:VAL:HG13	1:A:641:PRO:HD2	1.98	0.46
1:B:695:ILE:HD11	1:B:725:PHE:CE2	2.51	0.46
2:F:83:LEU:O	2:F:84:ASP:C	2.59	0.46
2:F:105:VAL:O	2:F:150:LEU:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:162:ARG:O	2:F:163:THR:C	2.58	0.46
1:A:656:ARG:CZ	1:A:673:GLU:HA	2.41	0.46
1:B:243:TYR:O	1:B:247:THR:N	2.49	0.46
1:E:410:ALA:O	1:E:425:ILE:HA	2.15	0.46
1:A:276:ASN:HB2	1:A:657:VAL:HG21	1.96	0.46
1:A:509:TYR:O	1:A:512:LYS:HG2	2.16	0.46
1:E:624:MET:HE1	1:E:692:MET:O	2.16	0.46
1:A:695:ILE:HD11	1:A:725:PHE:CE2	2.51	0.46
2:D:295:ASP:CG	2:D:296:PRO:HD2	2.41	0.46
1:E:278:GLU:O	1:E:290:THR:HB	2.16	0.46
1:E:611:ILE:HD11	1:E:735:LEU:HD12	1.98	0.46
1:E:300:THR:OG1	1:E:553:ASP:OD2	2.29	0.45
1:E:656:ARG:NH2	1:E:673:GLU:HG3	2.31	0.45
2:C:102:ILE:CG2	2:C:150:LEU:HD21	2.46	0.45
1:B:671:MET:HA	1:B:671:MET:HE2	1.97	0.45
1:B:776:ALA:O	1:B:781:VAL:HG23	2.16	0.45
1:E:166:MET:HE3	1:E:166:MET:HA	1.98	0.45
1:A:710:ALA:O	1:A:711:VAL:C	2.58	0.45
1:E:362:PRO:HG3	1:E:419:VAL:CG2	2.47	0.45
1:E:693:ASP:HA	1:E:726:ALA:HB3	1.98	0.45
2:F:80:ILE:CG2	2:F:90:ILE:HD13	2.46	0.45
1:A:624:MET:CE	1:A:724:LEU:HB2	2.43	0.45
1:E:301:PRO:HG2	1:E:347:ASP:HB2	1.99	0.45
2:C:162:ARG:O	2:C:163:THR:O	2.35	0.45
1:A:674:MET:HA	1:A:674:MET:HE2	1.98	0.45
1:A:627:THR:HA	1:A:630:ILE:HD12	1.99	0.45
1:B:624:MET:SD	1:B:726:ALA:HB2	2.57	0.45
1:E:264:GLN:O	1:E:265:ASP:C	2.60	0.45
1:B:471:HIS:HB3	1:B:492:ARG:HD3	1.97	0.45
1:B:614:GLY:N	1:B:767:ALA:HB2	2.31	0.45
1:E:654:PHE:CB	1:E:680:ILE:HG23	2.47	0.45
1:A:244:ALA:HA	1:A:247:THR:OG1	2.17	0.45
1:A:776:ALA:O	1:A:781:VAL:HG23	2.17	0.45
1:B:209:ALA:CB	1:B:238:GLY:HA3	2.46	0.45
2:C:51:ALA:C	2:C:149:ASP:OD1	2.57	0.45
2:C:247:THR:HB	2:C:248:PRO:HD2	1.98	0.45
1:E:277:LEU:HD12	1:E:279:ILE:HD11	1.99	0.45
1:A:735:LEU:N	1:A:736:PRO:CD	2.80	0.44
1:B:227:VAL:HG12	1:B:260:MET:HB2	1.98	0.44
1:E:137:TRP:CZ3	1:E:139:ASP:HB3	2.47	0.44
2:F:162:ARG:O	2:F:163:THR:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ARG:HG3	1:A:397:MET:HE3	1.98	0.44
1:A:728:HIS:ND1	1:B:698:GLY:O	2.51	0.44
1:B:705:LEU:O	1:B:706:SER:C	2.60	0.44
1:E:670:PHE:CZ	1:E:674:MET:HE3	2.53	0.44
1:A:705:LEU:O	1:A:706:SER:C	2.60	0.44
2:D:139:HIS:CG	2:D:140:PRO:HD2	2.53	0.44
1:B:244:ALA:HA	1:B:247:THR:OG1	2.18	0.44
1:B:267:ILE:HD11	1:B:313:MET:C	2.43	0.44
2:C:30:LEU:HD22	2:C:145:LEU:HD22	1.99	0.44
1:A:202:TRP:CD1	2:D:158:ARG:CZ	3.01	0.44
1:B:509:TYR:O	1:B:512:LYS:HG2	2.18	0.44
2:C:164:GLU:CG	2:C:165:LYS:H	2.30	0.44
1:A:268:ILE:C	1:A:269:MET:HG3	2.42	0.44
1:E:134:ALA:HB3	1:E:178:LEU:HD23	2.00	0.44
1:E:248:GLN:HG3	1:E:252:LEU:CD2	2.44	0.44
1:A:580:ILE:HD13	1:A:630:ILE:HD13	1.99	0.44
1:E:400:PHE:CZ	1:E:541:ALA:HB1	2.53	0.44
1:E:585:HIS:CG	1:E:586:PRO:HD2	2.53	0.44
1:B:493:GLN:HB3	1:B:500:ARG:HB2	2.00	0.43
1:E:693:ASP:O	1:E:694:GLU:C	2.61	0.43
1:A:347:ASP:OD2	1:A:350:ARG:CZ	2.67	0.43
1:B:640:VAL:HG13	1:B:641:PRO:HD2	2.00	0.43
1:E:269:MET:HG2	1:E:653:ILE:CG2	2.48	0.43
1:E:436:TRP:CZ2	1:E:519:LYS:HD3	2.53	0.43
1:B:437:ARG:O	1:B:441:ASP:HB2	2.18	0.43
1:B:695:ILE:HD11	1:B:725:PHE:HZ	1.80	0.43
2:C:251:ALA:HB1	2:C:285:GLN:HB2	1.99	0.43
2:D:160:PHE:N	2:D:160:PHE:CD1	2.84	0.43
1:A:243:TYR:CE2	1:A:247:THR:HG21	2.54	0.43
2:D:297:HIS:ND1	2:D:315:SER:N	2.66	0.43
1:E:182:GLU:HB2	1:E:198:ARG:NH2	2.33	0.43
1:E:578:ILE:HG12	1:E:650:ILE:HD11	2.00	0.43
1:E:746:HIS:HE1	1:E:765:GLY:HA3	1.84	0.43
1:B:297:SER:OG	1:B:561:ARG:HD3	2.18	0.43
1:B:564:THR:HG23	2:D:195:ILE:HD12	2.01	0.43
1:B:657:VAL:O	1:B:658:GLY:C	2.61	0.43
1:E:238:GLY:O	1:E:242:GLN:NE2	2.48	0.43
1:E:411:ILE:HG22	1:E:412:ILE:N	2.33	0.43
2:F:30:LEU:HD22	2:F:145:LEU:HD22	2.00	0.43
2:F:251:ALA:HB1	2:F:285:GLN:HB2	1.99	0.43
1:B:438:ALA:HA	1:B:441:ASP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:GLN:CD	1:E:252:LEU:HD21	2.44	0.43
1:E:652:ARG:O	1:E:653:ILE:HG13	2.19	0.43
2:F:108:LEU:HD12	2:F:147:VAL:HG22	2.00	0.43
1:E:705:LEU:O	1:E:706:SER:C	2.62	0.43
1:B:379:ARG:HG3	1:B:397:MET:HE3	1.99	0.43
2:D:30:LEU:HD22	2:D:145:LEU:HD22	2.01	0.43
1:B:267:ILE:HD13	1:B:313:MET:HA	2.00	0.43
1:B:652:ARG:HB3	1:B:654:PHE:CE2	2.54	0.43
1:E:436:TRP:HB3	1:E:517:LYS:N	2.34	0.43
2:F:51:ALA:C	2:F:149:ASP:OD1	2.57	0.43
2:F:112:SER:HB2	2:F:143:THR:HG23	2.01	0.43
1:B:266:SER:C	1:B:267:ILE:CG1	2.92	0.42
1:B:674:MET:HE2	1:B:674:MET:HA	2.00	0.42
2:D:80:ILE:CG2	2:D:83:LEU:HD21	2.49	0.42
2:D:251:ALA:HB1	2:D:285:GLN:HB2	2.01	0.42
1:E:132:LEU:HD12	1:E:173:THR:O	2.19	0.42
1:E:629:LEU:O	1:E:630:ILE:C	2.62	0.42
2:F:83:LEU:HD12	2:F:84:ASP:N	2.34	0.42
2:D:112:SER:HB2	2:D:143:THR:HG23	2.01	0.42
1:E:157:LEU:CD1	1:E:237:ALA:HB2	2.42	0.42
1:E:159:GLU:CD	1:E:232:ARG:HB3	2.45	0.42
1:E:334:PHE:HB3	1:E:338:LEU:HD12	2.01	0.42
2:F:102:ILE:CG2	2:F:150:LEU:HD21	2.49	0.42
1:A:493:GLN:HB3	1:A:500:ARG:HB2	2.01	0.42
1:A:267:ILE:HG21	1:A:652:ARG:HG2	2.00	0.42
1:A:738:LYS:HA	1:E:717:ASN:ND2	2.35	0.42
1:B:656:ARG:NH2	1:B:673:GLU:HB3	2.35	0.42
2:C:121:TRP:HA	2:C:136:PRO:HA	2.01	0.42
1:E:532:PHE:O	1:E:536:LEU:HD13	2.20	0.42
1:E:654:PHE:HB3	1:E:680:ILE:HG23	2.02	0.42
2:F:139:HIS:NE2	2:F:144:THR:OG1	2.49	0.42
1:A:614:GLY:N	1:A:767:ALA:HB2	2.34	0.42
1:B:269:MET:HG2	1:B:653:ILE:HD13	2.02	0.42
1:B:621:SER:OG	1:B:693:ASP:OD2	2.31	0.42
1:E:556:VAL:O	1:E:559:ALA:HB3	2.20	0.42
1:A:321:LEU:HD13	1:A:572:PHE:CZ	2.55	0.42
1:A:603:LEU:HD21	1:A:610:LEU:HG	2.00	0.42
2:F:295:ASP:CG	2:F:296:PRO:HD2	2.44	0.42
1:A:611:ILE:CD1	1:A:735:LEU:HB2	2.50	0.42
1:B:267:ILE:HD11	1:B:314:PRO:N	2.35	0.42
2:D:71:ALA:C	2:D:72:LEU:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:ILE:HB	2:D:329:VAL:HG21	2.01	0.42
1:E:327:THR:CG2	1:E:555:LEU:HD13	2.42	0.42
1:E:411:ILE:HG21	1:E:415:PRO:HG3	2.02	0.42
2:F:207:GLN:HG2	2:F:210:ARG:HH12	1.84	0.42
1:A:682:HIS:NE2	1:B:782:PRO:HG3	2.35	0.42
1:E:730:PHE:HA	1:E:767:ALA:HB1	2.02	0.42
1:A:748:ASP:HB2	1:A:763:GLN:HG3	2.01	0.41
1:E:573:ILE:O	1:E:648:GLY:HA2	2.20	0.41
2:F:227:ILE:HB	2:F:329:VAL:HG21	2.02	0.41
1:A:652:ARG:HB3	1:A:654:PHE:CE2	2.55	0.41
1:A:728:HIS:ND1	1:B:699:THR:HA	2.34	0.41
1:B:710:ALA:O	1:B:711:VAL:C	2.63	0.41
1:E:153:GLY:HA2	1:E:255:ILE:HG12	2.02	0.41
1:E:599:ASN:ND2	1:E:761:SER:HA	2.35	0.41
1:E:659:ALA:HB2	1:E:697:ARG:HD3	2.01	0.41
2:C:56:ILE:O	2:C:144:THR:HA	2.20	0.41
2:C:80:ILE:CG2	2:C:83:LEU:HD21	2.50	0.41
1:A:299:VAL:HG21	1:A:342:LEU:HB2	2.03	0.41
2:D:56:ILE:O	2:D:144:THR:HA	2.21	0.41
1:E:267:ILE:HG22	1:E:268:ILE:CG1	2.50	0.41
1:E:327:THR:HG23	1:E:390:VAL:CG2	2.50	0.41
2:C:67:GLU:HG2	2:C:89:ILE:HG22	2.02	0.41
2:D:44:ILE:HG23	2:D:189:LEU:HA	2.03	0.41
1:E:155:PHE:HB3	1:E:257:SER:O	2.21	0.41
1:E:609:MET:HB3	1:E:742:VAL:HG22	2.01	0.41
1:E:730:PHE:CD2	1:E:767:ALA:CB	2.94	0.41
2:D:108:LEU:HD12	2:D:147:VAL:HG22	2.03	0.41
1:E:575:LYS:HE2	1:E:606:GLN:HE22	1.85	0.41
1:E:615:PRO:HA	1:E:771:TYR:HB2	2.03	0.41
1:E:623:TYR:CZ	1:E:762:VAL:HG21	2.55	0.41
2:F:44:ILE:HG23	2:F:189:LEU:HA	2.02	0.41
2:F:67:GLU:HG2	2:F:89:ILE:HG22	2.02	0.41
1:B:580:ILE:HD13	1:B:630:ILE:HD13	2.02	0.41
2:D:162:ARG:HB3	2:D:167:GLU:HG2	2.03	0.41
1:E:781:VAL:HG11	1:E:786:ILE:HG12	2.01	0.41
1:A:265:ASP:OD1	1:A:267:ILE:HG12	2.20	0.41
1:A:282:ASN:OD1	1:A:284:ALA:N	2.54	0.41
1:A:592:LEU:HD12	1:A:593:ASN:H	1.85	0.41
1:A:723:THR:HG22	1:A:724:LEU:N	2.35	0.41
1:A:699:THR:HA	1:B:728:HIS:CD2	2.54	0.41
1:B:278:GLU:HA	1:B:281:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:LEU:HD21	1:B:610:LEU:HG	2.01	0.41
1:B:617:MET:HA	3:B:1801:ANP:C5'	2.51	0.41
1:B:783:LYS:NZ	1:B:787:LYS:HE3	2.36	0.41
1:E:691:LEU:HD21	1:E:724:LEU:HD12	2.03	0.41
1:B:569:SER:HB3	1:B:639:TYR:CZ	2.56	0.41
1:E:264:GLN:O	1:E:267:ILE:CG1	2.68	0.41
1:A:656:ARG:HE	1:A:673:GLU:HG3	1.84	0.40
1:A:697:ARG:HD3	1:B:697:ARG:HD2	2.03	0.40
1:B:460:LEU:HD22	1:B:481:GLN:HB3	2.03	0.40
1:B:611:ILE:CD1	1:B:735:LEU:HB2	2.51	0.40
1:E:650:ILE:HD13	1:E:689:LEU:CD2	2.48	0.40
1:E:752:HIS:O	1:E:753:GLY:C	2.64	0.40
1:A:460:LEU:HD22	1:A:481:GLN:HB3	2.03	0.40
2:C:109:THR:HA	2:C:123:ALA:O	2.21	0.40
1:E:575:LYS:CE	1:E:606:GLN:HE22	2.34	0.40
1:E:592:LEU:C	1:E:594:GLU:H	2.28	0.40
1:A:773:LEU:HD13	1:A:790:ARG:HG2	2.03	0.40
1:B:388:ALA:N	1:B:389:PRO:CD	2.84	0.40
1:B:627:THR:HA	1:B:630:ILE:HD12	2.03	0.40
2:C:112:SER:HB2	2:C:143:THR:HG23	2.03	0.40
1:A:621:SER:OG	1:A:693:ASP:OD2	2.30	0.40
1:A:788:ARG:HA	1:A:788:ARG:HD2	1.89	0.40
1:B:207:ASP:OD2	2:C:48:ARG:NH2	2.48	0.40
1:A:670:PHE:CG	1:B:616:ASN:ND2	2.89	0.40
1:A:696:GLY:O	1:A:729:TYR:OH	2.29	0.40
1:A:730:PHE:CD1	1:A:730:PHE:C	3.00	0.40
1:B:615:PRO:HD2	1:B:747:LEU:O	2.21	0.40
1:B:622:THR:HG21	3:B:1801:ANP:N7	2.37	0.40
1:B:748:ASP:HB2	1:B:763:GLN:HG3	2.03	0.40
1:E:361:ARG:HB3	1:E:417:VAL:O	2.21	0.40
1:E:609:MET:HA	1:E:723:THR:O	2.22	0.40
2:F:56:ILE:O	2:F:144:THR:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:LEU:O	1:E:420:ARG:NH1[2_858]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	659/800 (82%)	623 (94%)	34 (5%)	2 (0%)	36	71
1	B	659/800 (82%)	623 (94%)	33 (5%)	3 (0%)	24	63
1	E	582/800 (73%)	522 (90%)	52 (9%)	8 (1%)	9	39
2	C	277/369 (75%)	252 (91%)	21 (8%)	4 (1%)	9	39
2	D	277/369 (75%)	252 (91%)	23 (8%)	2 (1%)	18	55
2	F	277/369 (75%)	249 (90%)	23 (8%)	5 (2%)	6	33
All	All	2731/3507 (78%)	2521 (92%)	186 (7%)	24 (1%)	14	49

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	163	THR
2	D	117	GLN
1	E	265	ASP
1	E	420	ARG
1	E	753	GLY
1	E	755	THR
2	F	163	THR
2	F	266	ARG
1	B	594	GLU
1	B	658	GLY
1	A	283	LEU
1	A	658	GLY
1	E	593	ASN
1	E	769	LYS
2	F	267	LEU
1	B	268	ILE
1	E	778	LEU
2	C	296	PRO
2	C	117	GLN
2	D	93	GLY

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Mol	Chain	Res	Type
2	F	93	GLY
2	F	117	GLN
2	C	93	GLY
1	E	267	ILE

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	550/662 (83%)	538 (98%)	12 (2%)	45	64
1	B	550/662 (83%)	537 (98%)	13 (2%)	43	63
1	E	484/662 (73%)	455 (94%)	29 (6%)	17	39
2	C	235/308 (76%)	218 (93%)	17 (7%)	13	35
2	D	235/308 (76%)	218 (93%)	17 (7%)	13	35
2	F	235/308 (76%)	222 (94%)	13 (6%)	19	42
All	All	2289/2910 (79%)	2188 (96%)	101 (4%)	25	47

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	LEU
1	A	289	ASN
1	A	300	THR
1	A	319	ARG
1	A	333	ASP
1	A	349	GLU
1	A	461	ASP
1	A	493	GLN
1	A	536	LEU
1	A	671	MET
1	A	773	LEU
1	A	783	LYS
1	B	201	LEU
1	B	256	ARG

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Mol	Chain	Res	Type
1	B	300	THR
1	B	313	MET
1	B	349	GLU
1	B	461	ASP
1	B	488	ASN
1	B	493	GLN
1	B	536	LEU
1	B	671	MET
1	B	738	LYS
1	B	773	LEU
1	B	783	LYS
2	C	30	LEU
2	C	83	LEU
2	C	90	ILE
2	C	92	LEU
2	C	94	PHE
2	C	132	VAL
2	C	147	VAL
2	C	148	LEU
2	C	154	THR
2	C	159	LYS
2	C	171	ILE
2	C	227	ILE
2	C	252	GLU
2	C	263	MET
2	C	284	GLN
2	C	293	GLU
2	C	295	ASP
2	D	30	LEU
2	D	83	LEU
2	D	92	LEU
2	D	97	GLU
2	D	147	VAL
2	D	148	LEU
2	D	154	THR
2	D	159	LYS
2	D	171	ILE
2	D	188	ASN
2	D	204	GLU
2	D	227	ILE
2	D	252	GLU
2	D	263	MET

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Mol	Chain	Res	Type
2	D	264	ARG
2	D	266	ARG
2	D	298	GLN
1	E	128	ARG
1	E	152	SER
1	E	196	LEU
1	E	207	ASP
1	E	219	THR
1	E	229	ASN
1	E	242	GLN
1	E	261	GLU
1	E	263	GLU
1	E	269	MET
1	E	319	ARG
1	E	335	THR
1	E	386	ASP
1	E	395	GLU
1	E	405	ASP
1	E	439	LEU
1	E	517	LYS
1	E	536	LEU
1	E	579	ARG
1	E	627	THR
1	E	652	ARG
1	E	689	LEU
1	E	699	THR
1	E	706	SER
1	E	732	LEU
1	E	737	GLU
1	E	775	VAL
1	E	784	GLU
1	E	799	ILE
2	F	30	LEU
2	F	92	LEU
2	F	97	GLU
2	F	111	THR
2	F	147	VAL
2	F	154	THR
2	F	159	LYS
2	F	171	ILE
2	F	204	GLU
2	F	227	ILE

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Mol	Chain	Res	Type
2	F	234	LEU
2	F	252	GLU
2	F	266	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	276	ASN
1	A	325	GLN
1	A	471	HIS
1	A	538	HIS
1	A	626	GLN
1	A	679	ASN
1	A	717	ASN
1	B	212	GLN
1	B	229	ASN
1	B	276	ASN
1	B	325	GLN
1	B	471	HIS
1	B	488	ASN
1	B	538	HIS
1	B	602	ASN
1	B	643	GLN
1	B	679	ASN
1	B	744	ASN
2	C	198	GLN
2	C	231	HIS
2	D	117	GLN
2	D	118	GLN
2	D	122	GLN
2	D	188	ASN
1	E	381	GLN
1	E	526	GLN
1	E	599	ASN
1	E	606	GLN
1	E	683	ASN
1	E	714	ASN
1	E	744	ASN
1	E	746	HIS
2	F	33	ASN
2	F	118	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
3	ANP	E	1801	-	33,33,33	2.36	12 (36%)	45,52,52	2.18	15 (33%)
3	ANP	B	1801	-	33,33,33	2.00	10 (30%)	45,52,52	2.24	14 (31%)
3	ANP	A	1801	-	33,33,33	2.01	10 (30%)	45,52,52	2.42	13 (28%)

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
3	ANP	E	1801	-	-	1/18/38/38	0/3/3/3
3	ANP	B	1801	-	-	7/18/38/38	0/3/3/3
3	ANP	A	1801	-	-	2/18/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1801	ANP	PG-N3B	5.54	1.77	1.63
3	E	1801	ANP	C5-C4	5.50	1.48	1.39
3	E	1801	ANP	PB-N3B	5.23	1.77	1.63
3	B	1801	ANP	C5-C4	4.92	1.47	1.39
3	A	1801	ANP	PB-N3B	4.72	1.75	1.63
3	A	1801	ANP	C5-C4	4.61	1.47	1.39
3	B	1801	ANP	PG-N3B	4.31	1.74	1.63
3	B	1801	ANP	PB-N3B	4.09	1.74	1.63
3	A	1801	ANP	PG-N3B	4.07	1.74	1.63
3	E	1801	ANP	PB-O3A	3.64	1.63	1.59
3	E	1801	ANP	PA-O3A	3.42	1.63	1.59
3	E	1801	ANP	PG-O1G	3.40	1.51	1.46
3	A	1801	ANP	C5-C6	3.19	1.49	1.41
3	B	1801	ANP	C5-C6	3.15	1.49	1.41
3	B	1801	ANP	PG-O2G	-3.09	1.48	1.56
3	E	1801	ANP	PB-O1B	2.98	1.50	1.46
3	E	1801	ANP	C5-C6	2.98	1.49	1.41
3	A	1801	ANP	PB-O1B	2.90	1.50	1.46
3	A	1801	ANP	PG-O1G	2.71	1.50	1.46
3	B	1801	ANP	PB-O2B	-2.71	1.49	1.56
3	A	1801	ANP	C5-N7	-2.61	1.34	1.39
3	B	1801	ANP	PB-O1B	2.51	1.50	1.46
3	B	1801	ANP	C8-N7	2.49	1.36	1.31
3	E	1801	ANP	C5-N7	-2.47	1.34	1.39
3	A	1801	ANP	PB-O3A	2.46	1.62	1.59
3	B	1801	ANP	PG-O3G	-2.44	1.50	1.56
3	A	1801	ANP	C8-N7	2.43	1.36	1.31
3	E	1801	ANP	PG-O2G	-2.38	1.50	1.56
3	B	1801	ANP	C5-N7	-2.35	1.34	1.39
3	A	1801	ANP	PG-O3G	-2.30	1.50	1.56
3	E	1801	ANP	PG-O3G	-2.28	1.50	1.56
3	E	1801	ANP	C8-N7	2.03	1.35	1.31

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	ANP	C5-C4-N3	-7.74	116.06	126.72
3	B	1801	ANP	C5-C4-N3	-6.51	117.75	126.72
3	E	1801	ANP	C5-C4-N3	-5.56	119.06	126.72
3	A	1801	ANP	N3-C4-N9	5.33	136.24	127.17
3	B	1801	ANP	N3-C4-N9	5.21	136.03	127.17
3	E	1801	ANP	N3-C4-N9	5.12	135.88	127.17
3	E	1801	ANP	O1G-PG-N3B	-4.67	104.90	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	ANP	O1G-PG-N3B	-4.56	105.05	111.77
3	B	1801	ANP	O1G-PG-N3B	-4.45	105.21	111.77
3	A	1801	ANP	C2-N3-C4	4.36	122.49	111.83
3	A	1801	ANP	C4-C5-N7	-4.30	105.67	110.58
3	B	1801	ANP	C2-N3-C4	4.27	122.25	111.83
3	E	1801	ANP	O1B-PB-N3B	-4.18	105.62	111.77
3	A	1801	ANP	O1B-PB-N3B	-4.13	105.69	111.77
3	A	1801	ANP	O2G-PG-O3G	3.89	118.06	107.59
3	B	1801	ANP	O2B-PB-O1B	3.88	118.20	109.87
3	E	1801	ANP	O2B-PB-O1B	3.71	117.83	109.87
3	B	1801	ANP	N3-C2-N1	-3.69	123.00	128.58
3	B	1801	ANP	C4-C5-N7	-3.66	106.40	110.58
3	E	1801	ANP	N3-C2-N1	-3.55	123.22	128.58
3	E	1801	ANP	C2-N3-C4	3.48	120.33	111.83
3	B	1801	ANP	O1B-PB-N3B	-3.44	106.70	111.77
3	A	1801	ANP	O2B-PB-O1B	3.16	116.65	109.87
3	B	1801	ANP	O5'-C5'-C4'	3.13	119.65	108.99
3	E	1801	ANP	C4-N9-C8	2.98	108.87	105.74
3	E	1801	ANP	C3'-C2'-C1'	2.95	107.05	101.46
3	A	1801	ANP	C5-N7-C8	2.93	108.06	103.45
3	A	1801	ANP	C3'-C2'-C1'	2.86	106.87	101.46
3	B	1801	ANP	C5-N7-C8	2.78	107.81	103.45
3	E	1801	ANP	C4-C5-N7	-2.77	107.42	110.58
3	B	1801	ANP	C4-N9-C8	2.75	108.63	105.74
3	A	1801	ANP	N3-C2-N1	-2.73	124.45	128.58
3	E	1801	ANP	C2-N1-C6	2.48	122.80	118.73
3	E	1801	ANP	C5-N7-C8	2.47	107.34	103.45
3	E	1801	ANP	O3A-PB-N3B	2.37	113.17	106.59
3	B	1801	ANP	C6-C5-N7	2.30	136.53	132.09
3	E	1801	ANP	O5'-C5'-C4'	2.23	116.58	108.99
3	E	1801	ANP	N6-C6-N1	2.22	123.31	118.38
3	A	1801	ANP	C1'-N9-C8	-2.20	122.21	127.09
3	B	1801	ANP	N9-C8-N7	-2.12	110.93	113.94
3	A	1801	ANP	O5'-C5'-C4'	2.09	116.12	108.99
3	B	1801	ANP	O2G-PG-O3G	2.03	113.03	107.59

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	ANP	PB-N3B-PG-O1G
3	A	1801	ANP	PA-O3A-PB-O2B

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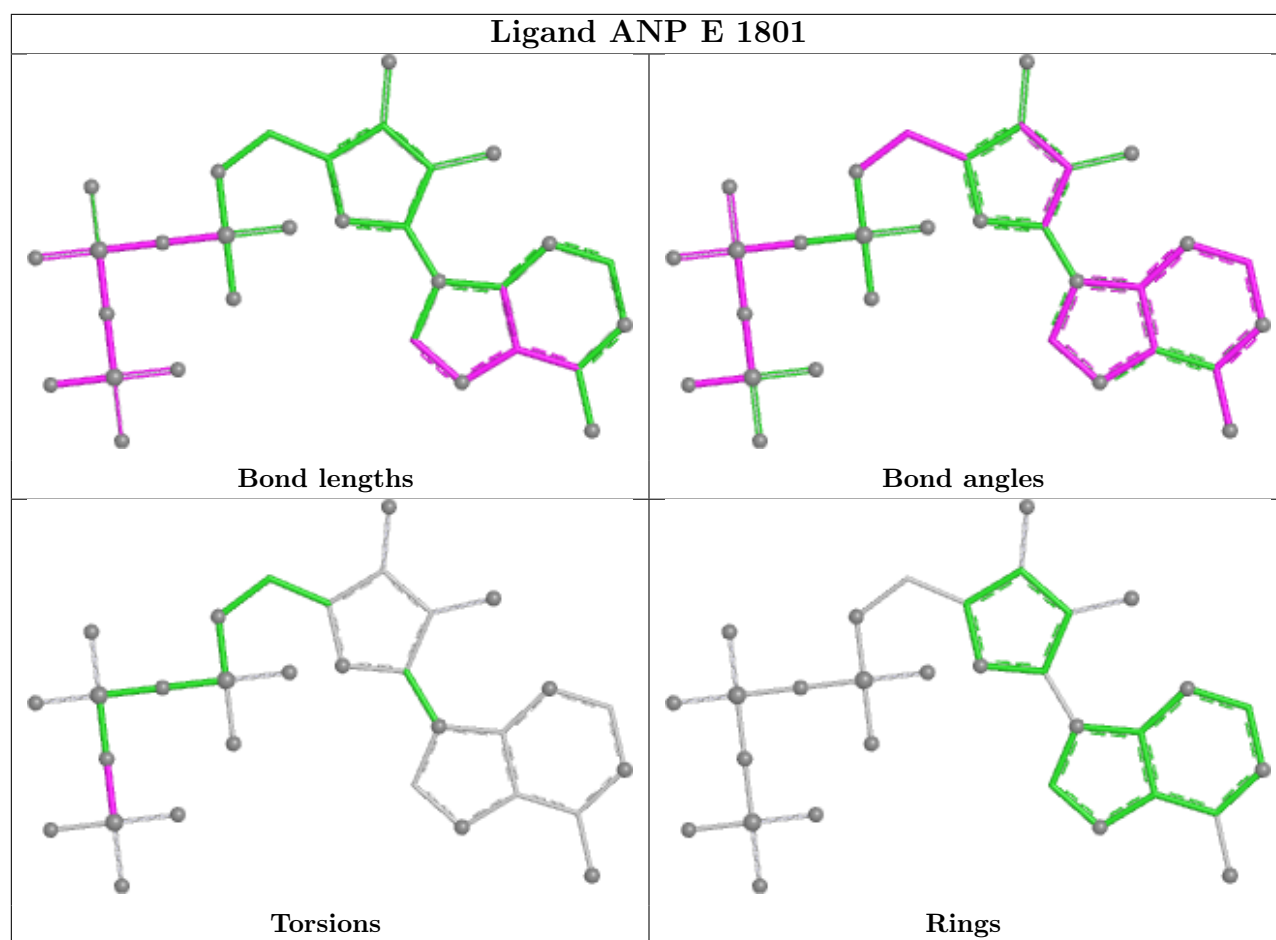
Mol	Chain	Res	Type	Atoms
3	B	1801	ANP	PB-N3B-PG-O1G
3	B	1801	ANP	PA-O3A-PB-O2B
3	B	1801	ANP	C5'-O5'-PA-O1A
3	B	1801	ANP	C5'-O5'-PA-O2A
3	E	1801	ANP	PB-N3B-PG-O1G
3	B	1801	ANP	O4'-C4'-C5'-O5'
3	B	1801	ANP	C5'-O5'-PA-O3A
3	B	1801	ANP	C3'-C4'-C5'-O5'

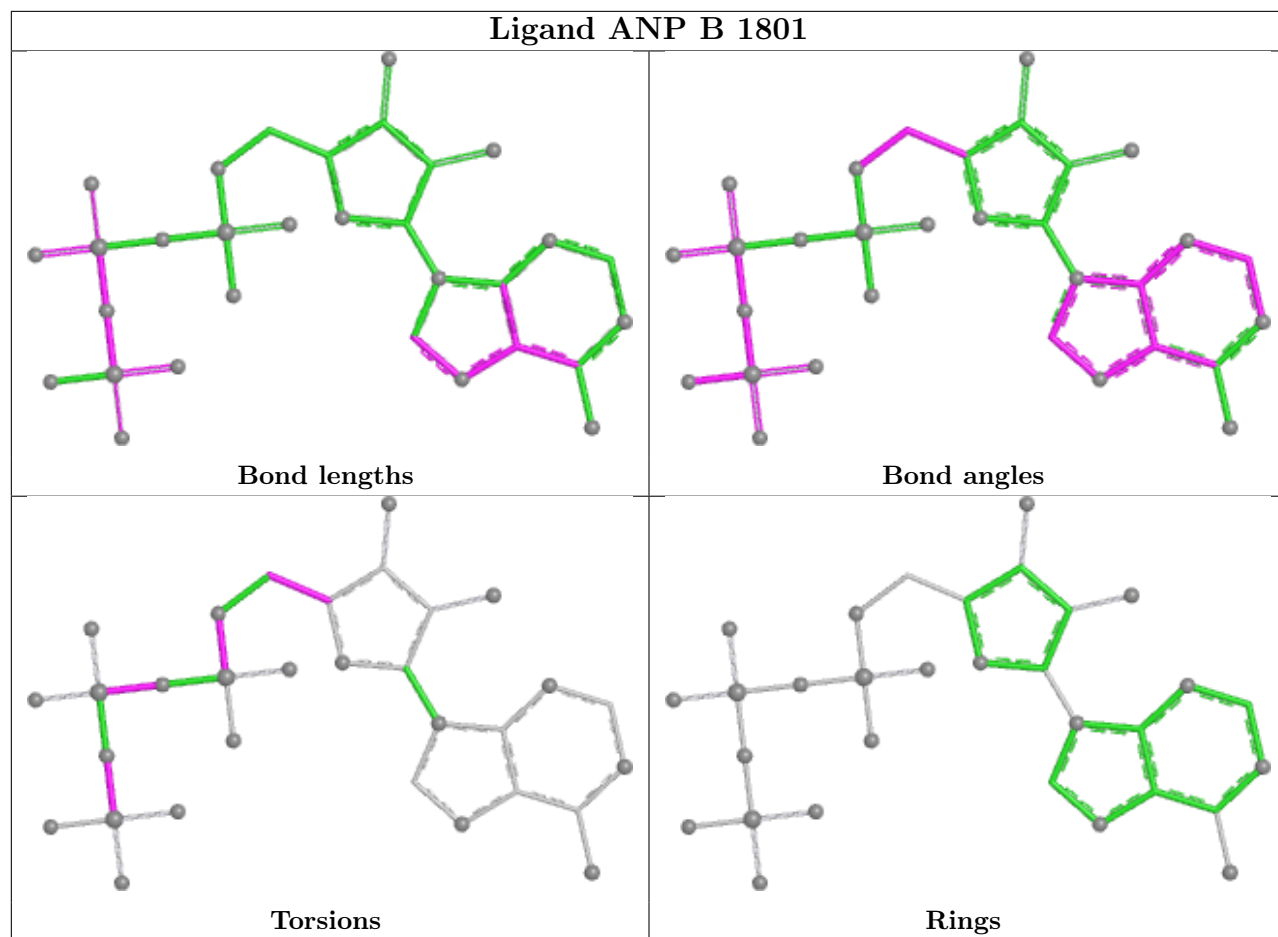
There are no ring outliers.

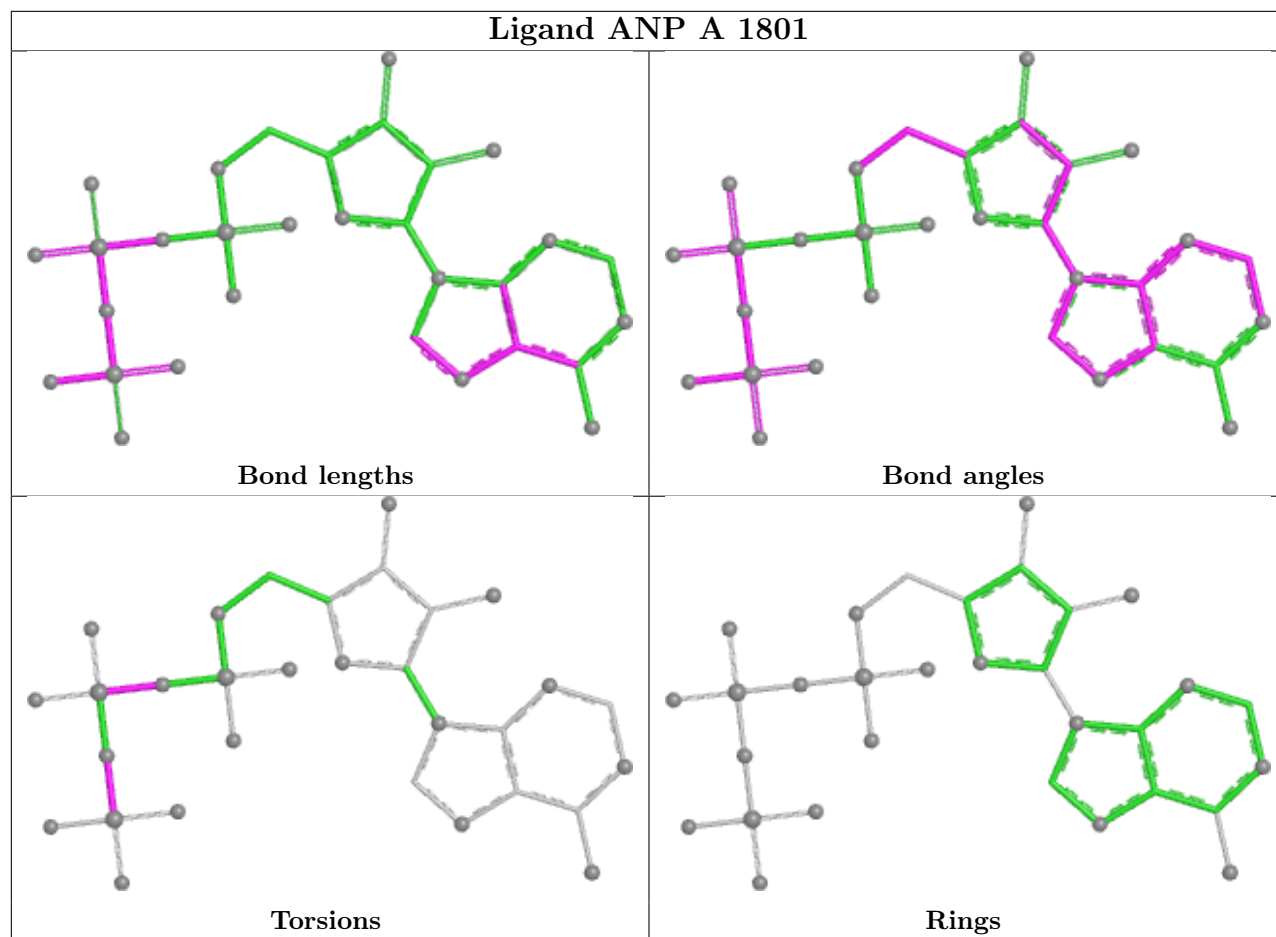
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1801	ANP	7	0
3	A	1801	ANP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	663/800 (82%)	0.49	30 (4%)	38	35	139, 203, 285, 347	0
1	B	663/800 (82%)	0.47	26 (3%)	43	38	162, 230, 292, 329	0
1	E	588/800 (73%)	0.87	57 (9%)	13	17	176, 236, 298, 405	0
2	C	285/369 (77%)	0.60	21 (7%)	20	23	150, 186, 253, 315	0
2	D	285/369 (77%)	0.93	36 (12%)	8	13	202, 277, 357, 420	0
2	F	285/369 (77%)	0.78	27 (9%)	14	18	200, 280, 355, 460	0
All	All	2769/3507 (78%)	0.65	197 (7%)	22	24	139, 230, 316, 460	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	330	ALA	5.9
1	E	329	GLY	5.2
2	F	70	LEU	5.2
2	F	82	SER	5.0
1	A	276	ASN	4.8
1	E	614	GLY	4.6
2	D	115	ALA	4.6
2	D	317	LEU	4.4
2	F	69	ALA	4.4
1	E	732	LEU	4.3
1	E	331	LEU	4.3
1	B	774	ALA	4.3
2	D	69	ALA	4.3
2	C	83	LEU	4.2
1	E	147	THR	4.2
2	D	146	GLU	4.1
2	C	270	HIS	4.1
1	B	587	VAL	4.1
2	D	318	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	585	HIS	4.0
2	D	319	HIS	3.9
2	D	82	SER	3.9
1	E	586	PRO	3.7
1	B	566	ASN	3.7
1	E	785	VAL	3.7
1	E	693	ASP	3.6
1	E	145	TYR	3.6
1	E	315	VAL	3.6
1	E	658	GLY	3.6
2	C	84	ASP	3.5
2	F	140	PRO	3.5
1	E	134	ALA	3.5
1	B	743	ALA	3.5
1	A	201	LEU	3.4
1	E	612	ILE	3.4
2	F	139	HIS	3.4
2	F	138	ALA	3.4
1	A	701	THR	3.4
1	A	635	TYR	3.4
2	D	54	ILE	3.4
2	C	243	PRO	3.3
1	E	136	ILE	3.3
1	E	397	MET	3.3
2	C	315	SER	3.3
2	D	198	GLN	3.3
2	C	323	TYR	3.3
1	B	511	ASP	3.2
1	B	390	VAL	3.2
2	D	138	ALA	3.2
1	B	633	MET	3.1
2	D	134	VAL	3.1
2	F	104	SER	3.1
1	E	133	LEU	3.1
1	E	782	PRO	3.0
1	B	307	LEU	3.0
2	D	80	ILE	3.0
2	D	31	VAL	3.0
1	B	638	SER	3.0
1	E	372	PHE	2.9
1	E	635	TYR	2.8
1	B	636	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	427	SER	2.8
1	B	659	ALA	2.8
1	E	417	VAL	2.8
1	A	469	ALA	2.8
2	D	73	ALA	2.8
2	C	67	GLU	2.7
2	D	124	TYR	2.7
1	E	772	GLY	2.7
2	C	82	SER	2.7
2	C	275	ALA	2.7
2	D	276	TYR	2.7
1	A	470	VAL	2.7
1	B	628	ALA	2.7
1	E	729	TYR	2.7
1	A	672	VAL	2.7
1	E	521	LEU	2.7
1	E	589	GLU	2.7
1	A	242	GLN	2.6
1	B	423	GLY	2.6
2	C	327	LEU	2.6
2	F	141	VAL	2.6
1	A	148	LEU	2.6
1	E	170	LEU	2.6
2	C	132	VAL	2.6
2	D	68	LEU	2.6
1	A	368	MET	2.6
1	E	613	THR	2.6
2	F	72	LEU	2.5
2	F	108	LEU	2.5
1	B	436	TRP	2.5
2	D	178	ILE	2.5
2	F	103	SER	2.5
1	E	399	GLU	2.5
2	C	256	PHE	2.5
1	E	697	ARG	2.5
2	F	84	ASP	2.5
1	E	178	LEU	2.5
2	D	239	TRP	2.5
1	A	203	GLU	2.5
2	F	137	ALA	2.5
2	D	218	THR	2.5
2	F	73	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	555	LEU	2.4
2	D	22	ARG	2.4
2	C	125	ALA	2.4
1	E	735	LEU	2.4
1	A	304	SER	2.4
2	D	188	ASN	2.4
1	E	633	MET	2.4
2	C	101	SER	2.4
1	E	779	ALA	2.4
1	A	370	HIS	2.4
2	F	67	GLU	2.4
2	D	106	SER	2.4
2	C	317	LEU	2.4
1	E	336	ALA	2.4
1	E	786	ILE	2.4
1	A	432	GLU	2.4
2	D	110	LEU	2.4
1	B	294	VAL	2.4
2	C	276	TYR	2.4
1	E	332	GLN	2.4
1	A	244	ALA	2.4
2	F	34	SER	2.4
2	F	219	ALA	2.4
2	D	236	LEU	2.4
1	A	721	ALA	2.3
1	E	699	THR	2.3
2	D	23	PRO	2.3
1	B	336	ALA	2.3
1	B	345	VAL	2.3
2	D	320	ASP	2.3
1	A	480	GLY	2.3
1	E	784	GLU	2.3
1	B	155	PHE	2.3
1	B	315	VAL	2.3
1	E	432	GLU	2.3
1	E	780	GLY	2.3
1	A	659	ALA	2.3
2	C	279	LYS	2.3
1	E	788	ARG	2.3
1	E	676	GLU	2.2
1	A	633	MET	2.2
1	E	623	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	256	PHE	2.2
1	A	577	GLY	2.2
1	E	148	LEU	2.2
1	B	239	ALA	2.2
2	C	258	VAL	2.2
1	E	401	ALA	2.2
1	E	624	MET	2.2
2	F	198	GLN	2.2
1	B	693	ASP	2.2
2	D	214	ALA	2.2
1	B	729	TYR	2.2
1	E	707	LEU	2.2
2	F	71	ALA	2.2
2	D	292	LEU	2.2
2	F	208	LYS	2.2
1	A	693	ASP	2.2
1	B	439	LEU	2.1
1	A	699	THR	2.1
1	A	257	SER	2.1
1	B	368	MET	2.1
1	E	177	GLU	2.1
2	D	81	ALA	2.1
1	A	576	PRO	2.1
1	E	701	THR	2.1
2	F	150	LEU	2.1
2	D	133	THR	2.1
2	C	49	GLY	2.1
2	F	29	GLU	2.1
1	A	372	PHE	2.1
1	A	150	ILE	2.1
1	E	638	SER	2.1
1	E	706	SER	2.1
1	A	241	LEU	2.1
1	E	722	LEU	2.1
1	E	673	GLU	2.1
2	D	87	GLU	2.1
2	F	134	VAL	2.1
2	D	149	ASP	2.1
2	D	125	ALA	2.1
2	F	100	ALA	2.1
2	C	296	PRO	2.1
2	F	97	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	72	LEU	2.0
1	A	243	TYR	2.0
1	E	328	ILE	2.0
1	B	465	VAL	2.0
1	A	687	TYR	2.0
2	F	89	ILE	2.0
1	E	777	ALA	2.0
2	C	320	ASP	2.0
1	E	629	LEU	2.0
2	F	148	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

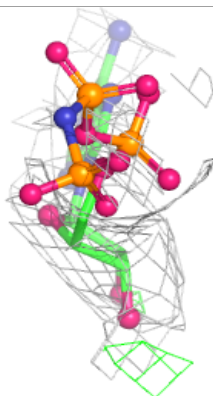
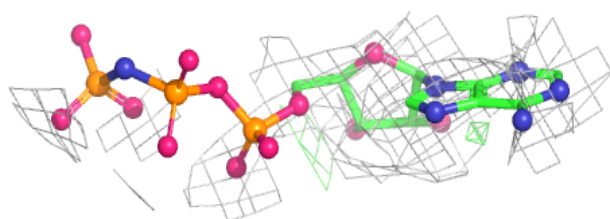
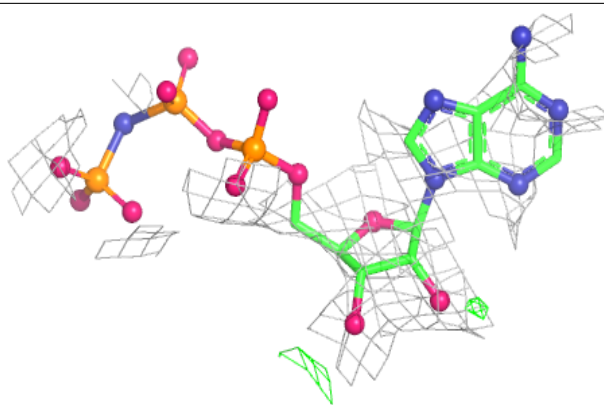
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	E	1801	31/31	0.84	0.12	232,262,291,292	0
3	ANP	A	1801	31/31	0.93	0.09	160,165,174,175	0
3	ANP	B	1801	31/31	0.94	0.08	185,196,210,211	0

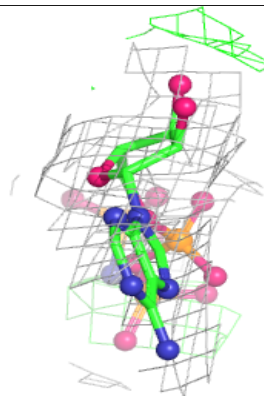
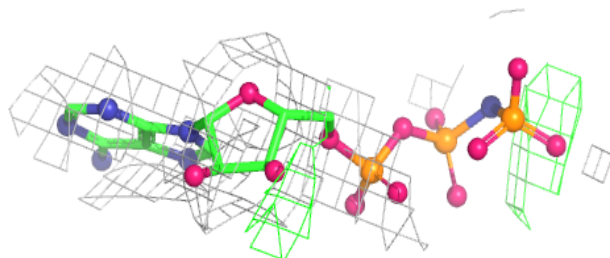
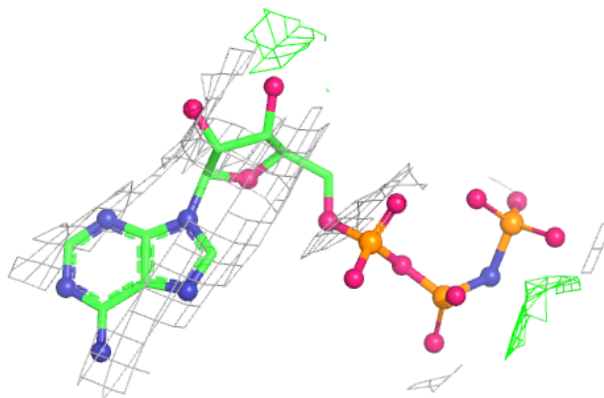
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP E 1801:

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

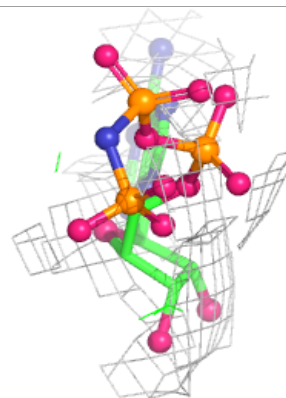
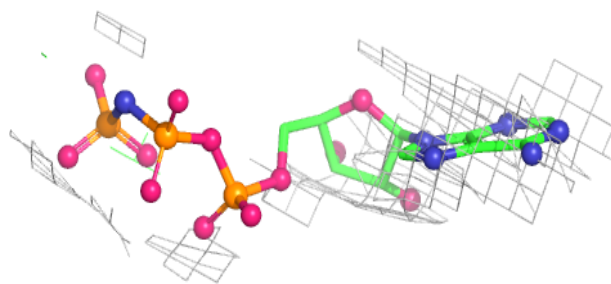
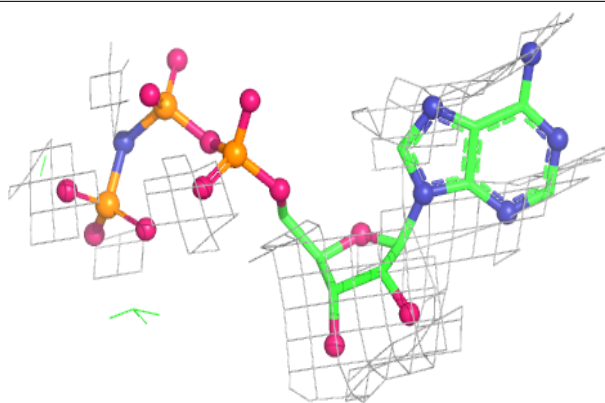
**Electron density around ANP A 1801:**

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



Electron density around ANP B 1801:

$2mF_o-DF_c$ (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.