



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:15 AM UTC

PDB ID : 4PKH / pdb_00004pkh
Title : Complex of ADP-actin With the N-terminal Actin-Binding Domain of Tropomodulin
Authors : Rao, J.N.; Dominguez, R.
Deposited on : 2014-05-14
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

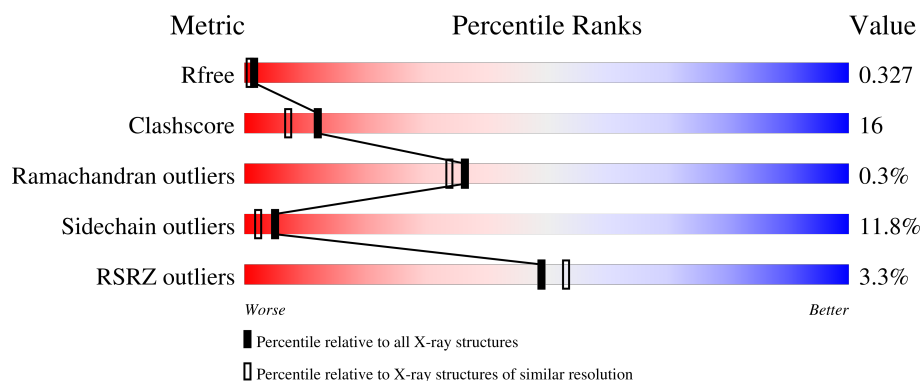
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	377	
1	D	377	
1	F	377	
1	I	377	
2	B	186	

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Mol	Chain	Length	Quality of chain
2	E	186	42%21%33%
2	G	186	6% 40%32%5%23%
2	J	186	7% 37%24%6%32%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31981 atoms, of which 15522 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	359	Total	C	H	N	O	S	0	2	0
			5592	1787	2775	469	541	20			
1	D	360	Total	C	H	N	O	S	0	1	0
			5609	1790	2786	473	541	19			
1	F	365	Total	C	H	N	O	S	0	0	0
			5678	1812	2821	481	544	20			
1	I	360	Total	C	H	N	O	S	0	1	0
			5609	1790	2786	473	540	20			

- Molecule 2 is a protein called Gelsolin,Tropomodulin-1 chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	165	Total	C	H	N	O	S	0	0	0
			2622	859	1291	225	246	1			
2	E	125	Total	C	H	N	O	S	0	0	0
			1944	642	952	165	184	1			
2	G	143	Total	C	H	N	O	S	0	0	0
			2245	738	1102	191	212	2			
2	J	126	Total	C	H	N	O	S	0	1	0
			1970	650	965	166	187	2			

There are 36 discrepancies between the modelled and reference sequences:

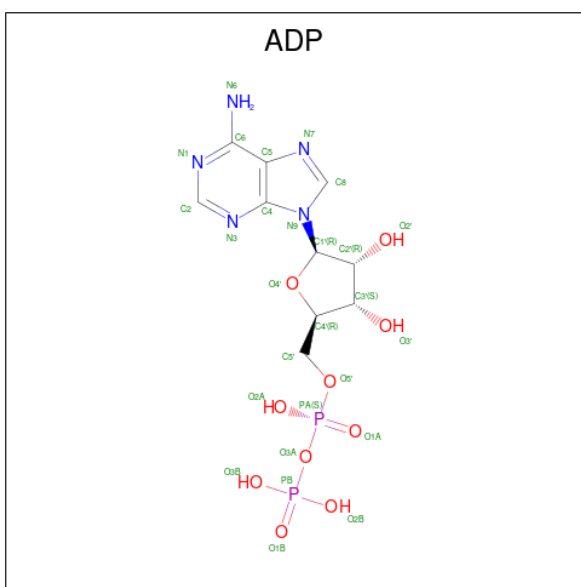
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	GLY	-	linker	UNP P06396
B	178	GLY	-	linker	UNP P06396
B	179	SER	-	linker	UNP P06396
B	180	GLY	-	linker	UNP P06396
B	181	GLY	-	linker	UNP P06396
B	182	SER	-	linker	UNP P06396
B	183	GLY	-	linker	UNP P06396
B	184	GLY	-	linker	UNP P06396

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Chain	Residue	Modelled	Actual	Comment	Reference
B	185	SER	-	linker	UNP P06396
E	177	GLY	-	linker	UNP P06396
E	178	GLY	-	linker	UNP P06396
E	179	SER	-	linker	UNP P06396
E	180	GLY	-	linker	UNP P06396
E	181	GLY	-	linker	UNP P06396
E	182	SER	-	linker	UNP P06396
E	183	GLY	-	linker	UNP P06396
E	184	GLY	-	linker	UNP P06396
E	185	SER	-	linker	UNP P06396
G	177	GLY	-	linker	UNP P06396
G	178	GLY	-	linker	UNP P06396
G	179	SER	-	linker	UNP P06396
G	180	GLY	-	linker	UNP P06396
G	181	GLY	-	linker	UNP P06396
G	182	SER	-	linker	UNP P06396
G	183	GLY	-	linker	UNP P06396
G	184	GLY	-	linker	UNP P06396
G	185	SER	-	linker	UNP P06396
J	177	GLY	-	linker	UNP P06396
J	178	GLY	-	linker	UNP P06396
J	179	SER	-	linker	UNP P06396
J	180	GLY	-	linker	UNP P06396
J	181	GLY	-	linker	UNP P06396
J	182	SER	-	linker	UNP P06396
J	183	GLY	-	linker	UNP P06396
J	184	GLY	-	linker	UNP P06396
J	185	SER	-	linker	UNP P06396

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	
			38	10	11	5	10	2	0
3	D	1	Total	C	H	N	O	P	
			38	10	11	5	10	2	0
3	F	1	Total	C	H	N	O	P	
			38	10	11	5	10	2	0
3	I	1	Total	C	H	N	O	P	
			38	10	11	5	10	2	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca		
			2	2	0	0
4	B	1	Total	Ca		
			1	1	0	0
4	D	2	Total	Ca		
			2	2	0	0
4	E	1	Total	Ca		
			1	1	0	0
4	F	2	Total	Ca		
			2	2	0	0
4	G	1	Total	Ca		
			1	1	0	0
4	I	2	Total	Ca		
			2	2	0	0
4	J	1	Total	Ca		
			1	1	0	0

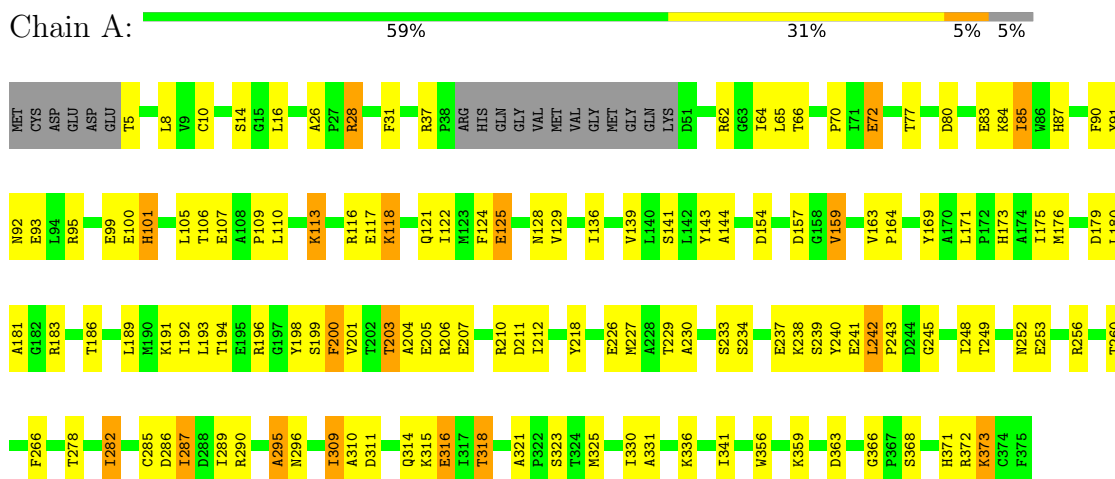
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total 88	O 88	0	0
5	B	82	Total 82	O 82	0	0
5	D	87	Total 87	O 87	0	0
5	E	77	Total 77	O 77	0	0
5	F	63	Total 63	O 63	0	0
5	G	49	Total 49	O 49	0	0
5	I	62	Total 62	O 62	0	0
5	J	40	Total 40	O 40	0	0

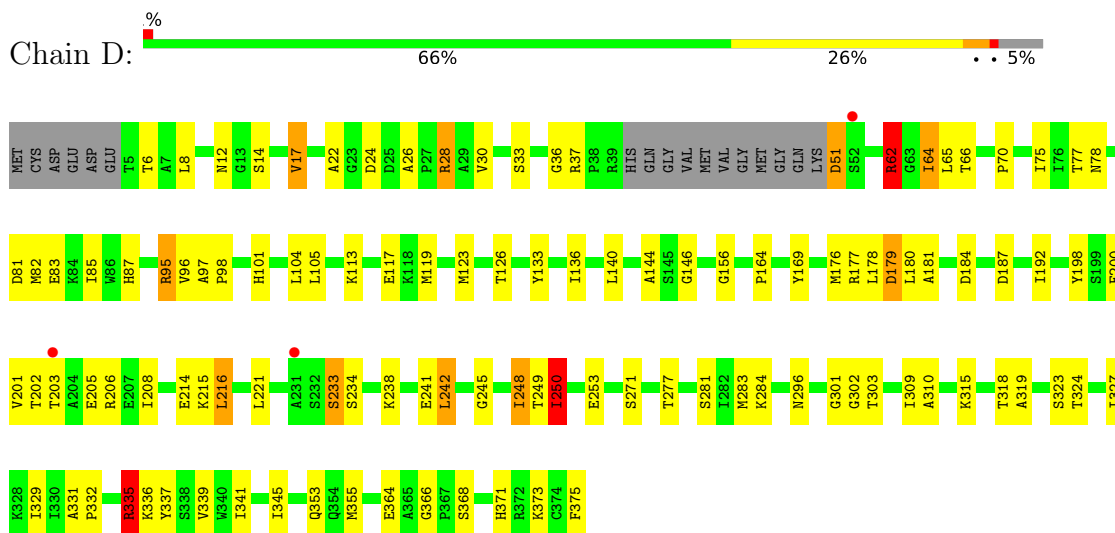
3 Residue-property plots

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: Actin, alpha skeletal muscle

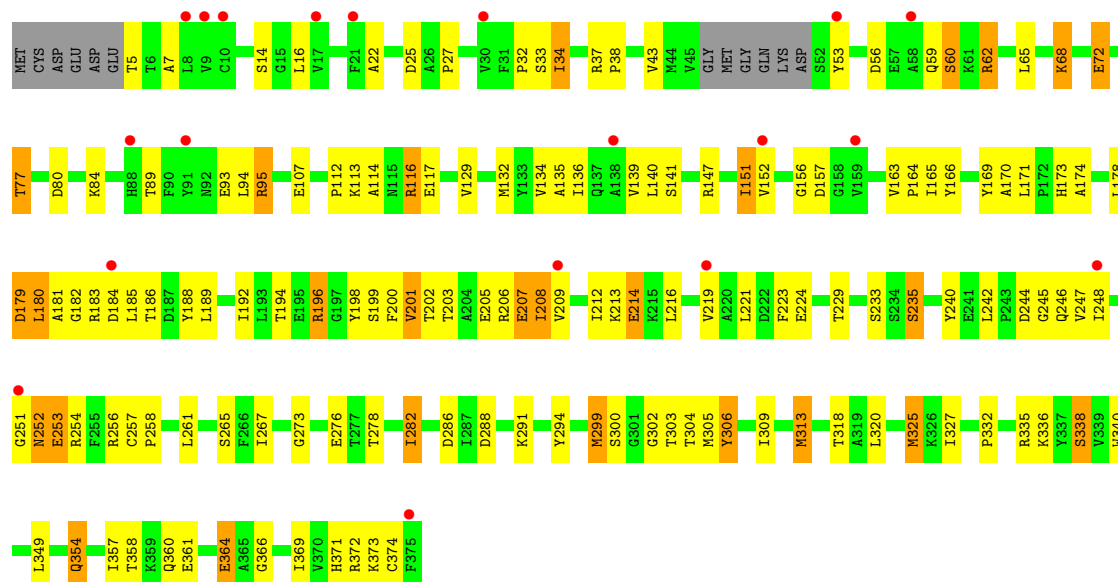


• Molecule 1: Actin, alpha skeletal muscle

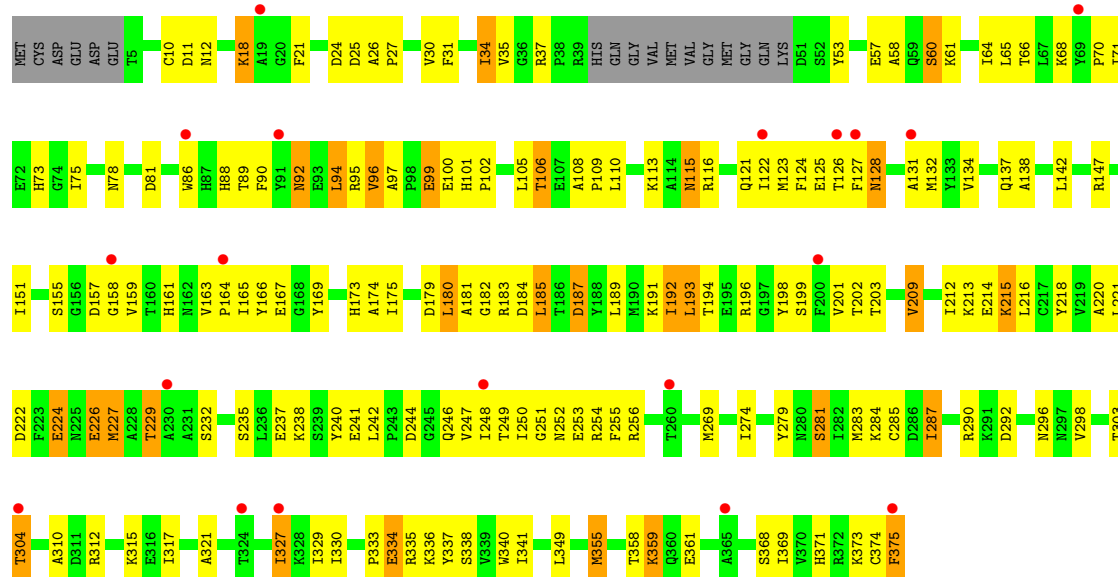


• Molecule 1: Actin, alpha skeletal muscle

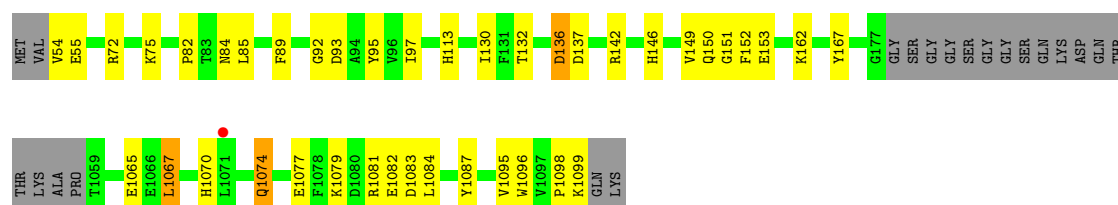




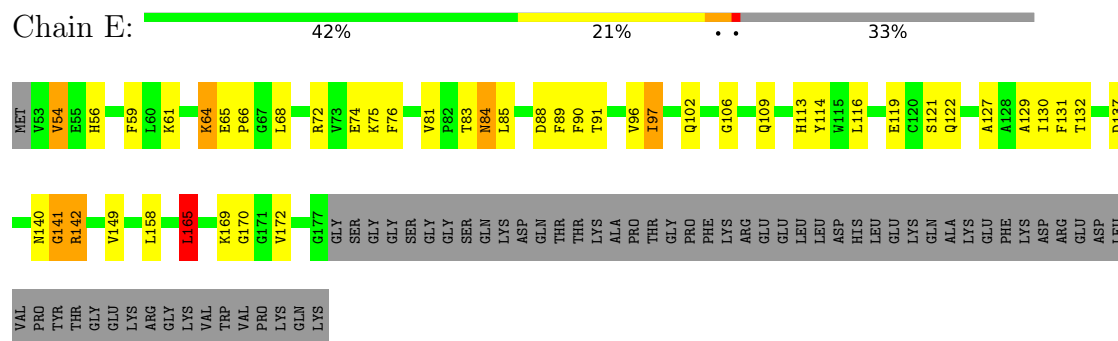
• Molecule 1: Actin, alpha skeletal muscle



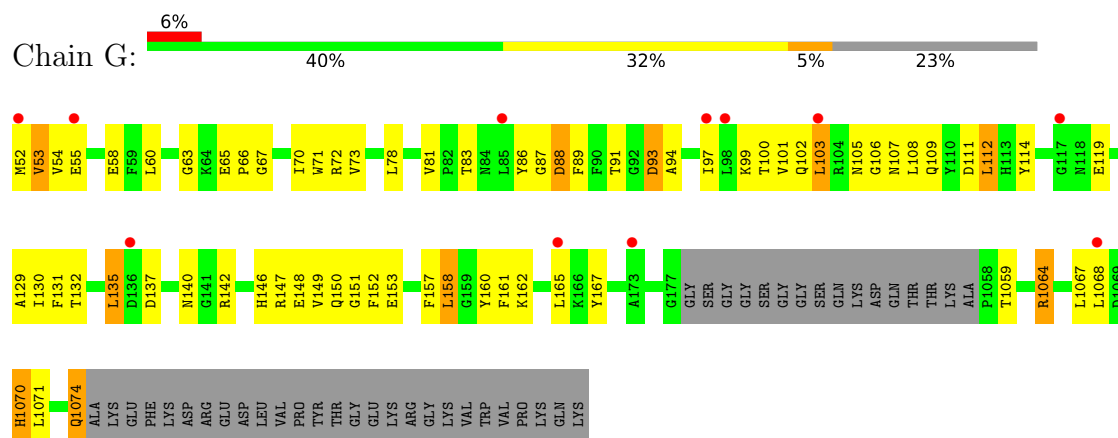
• Molecule 2: Gelsolin,Tropomodulin-1 chimera



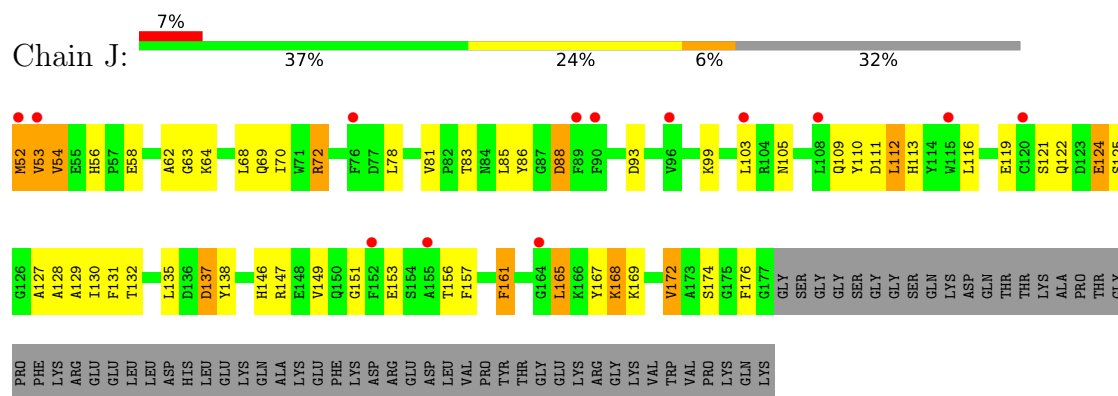
- Molecule 2: Gelsolin,Tropomodulin-1 chimera



- Molecule 2: Gelsolin,Tropomodulin-1 chimera



- Molecule 2: Gelsolin,Tropomodulin-1 chimera



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.22Å 135.14Å 140.55Å 90.00° 94.41° 90.00°	Depositor
Resolution (Å)	44.90 – 2.15 44.90 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.4 (44.90-2.15) 72.7 (44.90-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.274 , 0.326 0.282 , 0.327	Depositor DCC
R_{free} test set	2019 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	31981	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7803e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ADP, CA

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	1.22	10/2884 (0.3%)	1.29	19/3909 (0.5%)
1	D	1.27	9/2887 (0.3%)	1.34	25/3912 (0.6%)
1	F	0.79	0/2919	1.06	7/3955 (0.2%)
1	I	0.77	0/2887	1.06	7/3912 (0.2%)
2	B	1.29	7/1365 (0.5%)	1.16	2/1840 (0.1%)
2	E	1.59	9/1018 (0.9%)	1.30	8/1377 (0.6%)
2	G	0.88	0/1172	1.07	1/1581 (0.1%)
2	J	0.86	0/1035	1.02	2/1399 (0.1%)
All	All	1.08	35/16167 (0.2%)	1.18	71/21885 (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	1
1	D	0	2
1	I	0	2
All	All	0	5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	VAL	CA-CB	9.07	1.66	1.54
1	D	341	ILE	CA-CB	7.88	1.65	1.54
1	D	345	ILE	CA-C	7.67	1.62	1.52
2	E	114	TYR	CA-C	7.61	1.61	1.52
1	D	136	ILE	CA-C	7.45	1.60	1.52
2	E	142	ARG	CA-C	6.85	1.62	1.52
2	E	97	ILE	CA-C	6.85	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	113	HIS	N-CA	6.65	1.54	1.46
1	D	17	VAL	CA-CB	-6.27	1.46	1.54
2	B	132	THR	CA-C	6.27	1.60	1.52
2	E	129	ALA	CA-CB	-5.96	1.43	1.53
1	A	144	ALA	C-O	-5.85	1.16	1.24
1	A	106	THR	CA-C	-5.85	1.45	1.52
1	D	140	LEU	CA-C	5.77	1.60	1.52
1	A	341	ILE	CA-CB	5.76	1.61	1.54
2	B	142	ARG	CA-C	5.72	1.60	1.52
1	D	133	TYR	CA-C	-5.62	1.45	1.52
1	D	87	HIS	CA-C	-5.58	1.45	1.52
2	B	152	PHE	CA-C	5.56	1.60	1.52
2	B	97	ILE	CA-C	5.55	1.59	1.52
1	D	22	ALA	C-O	-5.54	1.17	1.23
2	E	149	VAL	N-CA	5.46	1.53	1.46
1	A	90	PHE	CA-C	5.44	1.59	1.52
2	E	97	ILE	CA-CB	-5.38	1.47	1.54
1	A	309	ILE	CA-CB	-5.34	1.47	1.54
1	A	282	ILE	CA-CB	-5.26	1.48	1.54
2	B	136	ASP	C-O	5.24	1.30	1.24
2	E	127	ALA	CA-CB	-5.20	1.45	1.53
1	A	122	ILE	CA-CB	-5.16	1.48	1.54
1	A	136	ILE	N-CA	-5.14	1.40	1.46
1	A	141	SER	CA-C	-5.13	1.46	1.52
1	D	12	ASN	CA-C	-5.06	1.46	1.52
2	E	131	PHE	CA-C	5.05	1.59	1.52
2	B	149	VAL	CA-CB	-5.04	1.48	1.54
2	B	92	GLY	C-O	5.03	1.29	1.24

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	366	GLY	CA-C-N	11.94	132.94	119.32
1	D	366	GLY	C-N-CA	11.94	132.94	119.32
1	D	339	VAL	N-CA-C	-8.99	102.08	110.53
1	D	335	ARG	N-CA-C	8.89	123.23	112.38
2	E	141	GLY	N-CA-C	-8.39	104.52	115.59
1	A	366	GLY	CA-C-N	8.16	127.80	119.56
1	A	366	GLY	C-N-CA	8.16	127.80	119.56
2	E	81	VAL	N-CA-C	7.77	115.31	108.63
1	D	77	THR	N-CA-C	7.73	123.77	113.72
2	E	132	THR	N-CA-C	-7.71	102.82	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	301	GLY	CA-C-O	-7.68	116.93	122.23
1	D	319	ALA	N-CA-C	-7.30	102.93	111.03
2	B	153	GLU	N-CA-C	7.15	119.53	110.24
1	D	26	ALA	N-CA-C	6.94	114.37	108.13
1	A	321	ALA	CA-C-N	6.81	126.84	119.90
1	A	321	ALA	C-N-CA	6.81	126.84	119.90
1	A	331	ALA	CA-C-N	-6.76	113.42	120.38
1	A	331	ALA	C-N-CA	-6.76	113.42	120.38
1	D	233	SER	N-CA-C	6.69	119.03	108.79
1	A	295	ALA	CA-C-N	-6.68	113.33	122.95
1	A	295	ALA	C-N-CA	-6.68	113.33	122.95
1	D	133	TYR	CA-C-N	-6.61	113.20	122.71
1	D	133	TYR	C-N-CA	-6.61	113.20	122.71
2	E	130	ILE	N-CA-C	-6.59	104.06	110.72
1	D	62	ARG	N-CA-C	6.48	119.17	111.33
1	A	26	ALA	N-CA-C	6.37	115.64	108.25
2	J	128	ALA	N-CA-C	-6.34	104.29	111.07
1	D	331	ALA	CA-C-N	-6.28	113.91	120.38
1	D	331	ALA	C-N-CA	-6.28	113.91	120.38
1	F	306	TYR	CA-C-N	5.91	127.23	119.84
1	F	306	TYR	C-N-CA	5.91	127.23	119.84
1	D	201	VAL	N-CA-C	5.88	119.29	111.17
1	F	141	SER	N-CA-C	-5.83	105.01	111.36
1	F	332	PRO	CA-C-N	5.76	125.62	119.28
1	F	332	PRO	C-N-CA	5.76	125.62	119.28
1	D	373	LYS	N-CA-C	5.64	118.37	111.82
1	A	91	TYR	N-CA-C	5.51	118.47	111.69
1	I	31	PHE	CA-C-N	5.45	125.46	119.90
1	I	31	PHE	C-N-CA	5.45	125.46	119.90
1	A	311	ASP	N-CA-C	-5.44	105.43	111.36
1	D	146	GLY	O-C-N	5.44	128.29	122.41
1	D	242	LEU	CA-C-N	5.44	124.96	119.19
1	D	242	LEU	C-N-CA	5.44	124.96	119.19
1	F	366	GLY	CA-C-N	5.38	125.09	119.82
1	F	366	GLY	C-N-CA	5.38	125.09	119.82
2	J	124	GLU	N-CA-C	-5.38	105.49	111.36
1	D	250	ILE	N-CA-C	5.32	116.14	108.48
1	A	101	HIS	N-CA-C	5.32	118.84	108.85
1	A	16	LEU	N-CA-C	5.30	117.07	108.26
1	A	125	GLU	N-CA-C	5.30	117.86	111.40
1	A	289	ILE	N-CA-C	5.29	118.06	112.83
2	G	93	ASP	N-CA-C	5.27	117.43	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	61	LYS	N-CA-C	-5.25	106.87	113.28
1	D	302	GLY	N-CA-C	5.23	120.09	113.24
1	A	159	VAL	N-CA-C	5.23	115.17	107.75
1	D	216	LEU	N-CA-C	5.22	119.81	113.38
1	D	215	LYS	N-CA-C	5.20	117.75	111.40
2	E	56	HIS	CA-C-N	-5.20	114.26	119.56
2	E	56	HIS	C-N-CA	-5.20	114.26	119.56
1	D	75	ILE	N-CA-C	5.12	115.96	108.53
1	A	129	VAL	CA-C-N	5.12	124.73	119.56
1	A	129	VAL	C-N-CA	5.12	124.73	119.56
1	I	159	VAL	N-CA-C	5.12	115.10	108.35
2	E	165	LEU	CA-CB-CG	5.08	134.08	116.30
1	I	287	ILE	N-CA-C	5.07	116.40	110.62
1	D	82	MET	N-CA-C	-5.04	105.78	111.28
1	A	368	SER	N-CA-C	-5.04	106.96	113.01
1	I	97	ALA	CA-C-N	5.02	125.30	119.47
1	I	97	ALA	C-N-CA	5.02	125.30	119.47
1	I	142	LEU	N-CA-C	-5.01	105.90	111.36
2	B	132	THR	N-CA-C	-5.01	105.71	111.07

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	ASN	Mainchain
1	D	179	ASP	Peptide
1	D	296	ASN	Mainchain
1	I	235	SER	Peptide
1	I	57	GLU	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	2817	2775	2785	93	1
1	D	2823	2786	2794	58	0
1	F	2857	2821	2830	101	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2823	2786	2794	122	1
2	B	1331	1291	1295	21	0
2	E	992	952	955	31	0
2	G	1143	1102	1106	53	0
2	J	1005	965	966	46	1
3	A	27	11	12	0	0
3	D	27	11	12	2	0
3	F	27	11	12	5	0
3	I	27	11	12	3	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
4	I	2	0	0	0	0
4	J	1	0	0	0	0
5	A	88	0	0	10	0
5	B	82	0	0	2	0
5	D	87	0	0	1	0
5	E	77	0	0	7	0
5	F	63	0	0	7	0
5	G	49	0	0	4	0
5	I	62	0	0	13	0
5	J	40	0	0	5	0
All	All	16459	15522	15573	491	2

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 16.

All (491) 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:J:72:ARG:NH1	2:J:93:ASP:OD2	1.76	1.17
1:I:95:ARG:NH1	5:I:501:HOH:O	1.89	1.04
2:J:52:MET:SD	2:J:52:MET:N	2.33	1.01
2:J:88:ASP:OD2	2:J:168:LYS:NZ	1.96	0.98
1:I:226:GLU:OE2	5:I:526:HOH:O	1.86	0.92
1:A:83:GLU:OE2	2:B:1087:TYR:OH	1.88	0.91
1:I:173:HIS:NE2	1:I:284:LYS:O	2.03	0.91
3:I:401:ADP:O1A	5:I:514:HOH:O	1.89	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:LEU:HD21	1:D:277:THR:HG21	1.54	0.88
1:I:227:MET:SD	1:I:252:ASN:ND2	2.47	0.87
1:I:88:HIS:ND1	1:I:92:ASN:OD1	2.08	0.86
1:F:358:THR:N	1:F:361:GLU:OE2	2.08	0.86
1:D:24:ASP:OD2	1:D:28:ARG:NH1	2.10	0.85
1:A:169:TYR:OH	2:B:137:ASP:OD2	1.96	0.83
1:F:364:GLU:O	5:F:521:HOH:O	1.95	0.83
1:D:117:GLU:OE2	1:D:371:HIS:NE2	2.09	0.81
1:D:62:ARG:NH1	1:D:203:THR:OG1	2.14	0.81
2:G:91:THR:OG1	2:G:119:GLU:OE2	2.00	0.79
1:D:221:LEU:O	1:D:315:LYS:NZ	2.15	0.79
1:A:154:ASP:OD2	5:A:588:HOH:O	2.01	0.79
1:D:253:GLU:OE2	1:D:253:GLU:N	2.16	0.79
1:A:356:TRP:O	1:A:373:LYS:NZ	2.15	0.78
1:D:187:ASP:OD1	1:D:206:ARG:NH2	2.16	0.78
1:D:327:ILE:O	5:D:550:HOH:O	2.01	0.78
1:F:199:SER:O	2:G:1064:ARG:NH2	2.18	0.76
1:I:169:TYR:OH	2:J:137:ASP:OD1	2.04	0.75
2:J:116:LEU:HD12	2:J:147:ARG:NH1	2.03	0.74
1:A:295:ALA:O	5:A:551:HOH:O	2.06	0.74
2:G:148:GLU:OE1	5:G:1329:HOH:O	2.04	0.74
2:B:136:ASP:OD2	5:B:1374:HOH:O	2.06	0.73
2:G:67:GLY:N	2:G:100:THR:OG1	2.22	0.72
1:F:273:GLY:N	1:F:276:GLU:OE1	2.22	0.72
3:F:401:ADP:N1	5:F:531:HOH:O	2.21	0.71
1:I:174:ALA:O	1:I:281:SER:OG	2.07	0.71
1:I:252:ASN:HA	1:I:255:PHE:CE1	2.26	0.69
2:G:88:ASP:O	5:G:1311:HOH:O	2.09	0.69
2:G:1070:HIS:O	2:G:1074:GLN:N	2.24	0.69
1:F:117:GLU:OE2	5:F:562:HOH:O	2.08	0.69
1:F:156:GLY:O	1:F:303:THR:OG1	2.09	0.69
1:I:115:ASN:OD1	1:I:115:ASN:N	2.26	0.68
1:A:198:TYR:CZ	1:A:248:ILE:HG23	2.29	0.67
2:G:151:GLY:N	2:G:167:TYR:OH	2.28	0.66
2:G:137:ASP:OD2	5:G:1323:HOH:O	2.13	0.65
1:D:214:GLU:HG2	3:D:401:ADP:C5	2.32	0.65
1:I:212:ILE:HG23	1:I:216:LEU:HD12	1.78	0.65
2:B:162:LYS:NZ	5:B:1380:HOH:O	2.30	0.65
1:I:214:GLU:OE1	5:I:517:HOH:O	2.15	0.65
2:J:58:GLU:OE1	5:J:1317:HOH:O	2.15	0.65
1:A:95:ARG:O	5:A:530:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:GLU:OE1	1:F:77:THR:OG1	2.16	0.64
1:A:229:THR:O	1:A:233:SER:OG	2.04	0.64
1:A:186:THR:HG21	1:A:206:ARG:HE	1.63	0.64
2:E:74:GLU:OE1	5:E:1355:HOH:O	2.14	0.64
1:A:117:GLU:OE2	1:A:371:HIS:HE1	1.81	0.64
1:F:147:ARG:NH1	2:G:147:ARG:HH12	1.96	0.64
2:E:137:ASP:HA	5:E:1303:HOH:O	1.96	0.64
1:A:128:ASN:OD1	1:A:359:LYS:NZ	2.31	0.64
2:G:72:ARG:HD2	2:G:93:ASP:OD2	1.98	0.63
1:I:218:TYR:OH	1:I:226:GLU:OE1	2.15	0.63
1:A:100:GLU:HG2	1:A:101:HIS:CD2	2.33	0.63
1:D:169:TYR:OH	2:E:137:ASP:OD2	2.16	0.62
2:G:72:ARG:NH1	2:G:93:ASP:OD2	2.31	0.62
1:I:116:ARG:NH2	1:I:374:CYS:O	2.32	0.62
1:A:285:CYS:O	1:A:290:ARG:NH2	2.33	0.61
1:A:372:ARG:NH1	5:A:554:HOH:O	2.23	0.61
1:I:213:LYS:NZ	3:I:401:ADP:O2'	2.31	0.61
1:A:314:GLN:O	1:A:318:THR:OG1	2.14	0.61
1:D:178:LEU:CD2	1:D:277:THR:HG21	2.30	0.61
1:I:229:THR:O	1:I:232:SER:OG	2.09	0.61
1:F:240:TYR:C	1:F:247:VAL:HG13	2.26	0.60
1:F:114:ALA:HA	1:F:117:GLU:OE2	2.01	0.60
2:J:112:LEU:O	2:J:146:HIS:N	2.34	0.60
1:I:336:LYS:NZ	5:I:545:HOH:O	2.27	0.60
1:F:286:ASP:OD1	1:F:288:ASP:N	2.23	0.60
2:G:63:GLY:HA2	2:G:100:THR:HG21	1.83	0.60
2:E:72:ARG:NH1	2:E:172:VAL:HG23	2.17	0.59
1:I:355:MET:SD	5:I:543:HOH:O	2.57	0.59
1:A:194:THR:HG22	1:A:199:SER:HA	1.84	0.59
2:G:1068:LEU:O	2:G:1071:LEU:N	2.35	0.59
1:A:80:ASP:OD1	5:A:584:HOH:O	2.16	0.59
1:F:244:ASP:HB3	2:G:1067:LEU:HD12	1.84	0.59
2:G:83:THR:HA	2:G:86:TYR:CE1	2.37	0.59
1:A:196:ARG:NH2	1:A:249:THR:OG1	2.35	0.59
2:E:68:LEU:HD11	2:E:97:ILE:HG23	1.84	0.59
1:F:372:ARG:NH1	2:J:153[A]:GLU:OE2	2.36	0.59
1:D:95:ARG:HH21	1:D:95:ARG:HG3	1.68	0.59
2:E:141:GLY:N	5:E:1303:HOH:O	2.34	0.59
1:F:214:GLU:OE2	3:F:401:ADP:C4	2.55	0.59
1:A:157:ASP:OD2	1:A:183:ARG:NE	2.36	0.59
1:A:241:GLU:OE2	1:A:245:GLY:HA2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:66:PRO:O	5:E:1349:HOH:O	2.17	0.58
1:I:220:ALA:O	1:I:312:ARG:NH2	2.35	0.58
2:J:78:LEU:HD13	2:J:131:PHE:CD2	2.38	0.58
1:I:96:VAL:HG11	1:I:101:HIS:CE1	2.38	0.58
1:I:253:GLU:HA	1:I:256:ARG:HB2	1.84	0.58
2:E:89:PHE:CD2	2:E:165:LEU:HD13	2.38	0.58
2:J:137:ASP:HB3	5:J:1301:HOH:O	2.03	0.58
2:G:140:ASN:O	2:J:119:GLU:OE1	2.22	0.58
2:E:102:GLN:HE22	2:E:106:GLY:C	2.11	0.58
2:E:91:THR:OG1	2:E:119:GLU:OE2	2.13	0.57
1:I:317:ILE:O	1:I:321:ALA:N	2.37	0.57
1:F:37:ARG:NH1	1:F:68:LYS:NZ	2.53	0.57
1:D:214:GLU:HG2	3:D:401:ADP:C4	2.40	0.57
1:I:165:ILE:HG23	1:I:169:TYR:C	2.30	0.56
1:D:318:THR:HA	1:D:327:ILE:CD1	2.34	0.56
1:F:179:ASP:OD1	1:F:179:ASP:N	2.37	0.56
1:A:117:GLU:OE2	1:A:371:HIS:CE1	2.58	0.56
1:D:113:LYS:HG3	1:D:371:HIS:CE1	2.40	0.56
1:F:135:ALA:HB3	1:F:140:LEU:HD11	1.88	0.56
1:A:128:ASN:OD1	1:A:359:LYS:CE	2.54	0.56
1:A:207:GLU:OE2	1:A:210:ARG:NH1	2.37	0.56
2:E:64:LYS:N	5:E:1369:HOH:O	2.38	0.56
1:D:105:LEU:HD11	1:D:123:MET:HG3	1.87	0.56
1:A:95:ARG:NH1	2:B:1083:ASP:OD2	2.27	0.56
1:F:180:LEU:HD12	1:F:181:ALA:N	2.20	0.56
1:F:214:GLU:OE2	3:F:401:ADP:C5	2.59	0.56
1:I:251:GLY:N	1:I:253:GLU:OE2	2.39	0.56
2:J:116:LEU:HD12	2:J:147:ARG:HH12	1.71	0.56
2:E:72:ARG:NH1	2:E:172:VAL:CG2	2.69	0.56
1:I:25:ASP:HA	2:J:176:PHE:CE1	2.41	0.56
1:I:121:GLN:CG	1:I:125:GLU:OE2	2.54	0.55
1:I:73:HIS:HB3	1:I:179:ASP:OD1	2.06	0.55
1:I:180:LEU:HD11	1:I:185:LEU:HD11	1.88	0.55
1:A:118:LYS:NZ	5:A:580:HOH:O	2.38	0.55
1:A:242:LEU:N	1:A:242:LEU:CD1	2.70	0.55
2:E:97:ILE:HD12	2:E:97:ILE:N	2.21	0.55
1:I:181:ALA:N	1:I:184:ASP:OD2	2.39	0.55
1:A:218:TYR:OH	1:A:226:GLU:OE2	2.20	0.55
2:J:85:LEU:O	2:J:88:ASP:HB2	2.07	0.55
1:D:117:GLU:CD	1:D:371:HIS:HE2	2.11	0.55
1:I:240:TYR:O	1:I:248:ILE:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:GLU:N	1:F:224:GLU:OE1	2.41	0.54
2:G:103:LEU:HD23	2:G:105:ASN:H	1.71	0.54
1:A:200:PHE:HB3	1:A:205:GLU:HB3	1.89	0.54
1:D:28:ARG:HH11	1:D:28:ARG:CG	2.20	0.54
1:F:7:ALA:HB3	1:F:22:ALA:HB3	1.90	0.54
1:F:38:PRO:HA	1:F:65:LEU:HD23	1.90	0.54
1:I:349:LEU:HD11	2:J:130:ILE:HG21	1.90	0.54
1:D:51:ASP:OD1	1:D:51:ASP:N	2.40	0.54
2:E:89:PHE:HD2	2:E:165:LEU:HD13	1.71	0.54
1:A:198:TYR:CE1	1:A:248:ILE:HG23	2.43	0.54
1:I:180:LEU:HD12	1:I:181:ALA:N	2.22	0.54
1:A:157:ASP:OD2	1:A:183:ARG:NH1	2.41	0.53
1:A:200:PHE:HB3	1:A:205:GLU:CB	2.38	0.53
1:A:28:ARG:NH1	5:A:577:HOH:O	2.40	0.53
1:A:70:PRO:HG3	1:A:85:ILE:HD12	1.89	0.53
1:D:216:LEU:HD12	1:D:250:ILE:HD12	1.91	0.53
2:E:54:VAL:HG11	2:E:59:PHE:CD2	2.43	0.53
1:I:21:PHE:HB2	1:I:24:ASP:OD2	2.08	0.53
1:I:147:ARG:NH2	1:I:296:ASN:OD1	2.41	0.53
1:A:260:THR:HG23	1:A:266:PHE:HB2	1.90	0.53
1:F:201:VAL:HG12	1:F:202:THR:H	1.74	0.53
1:F:216:LEU:N	1:F:216:LEU:HD22	2.23	0.53
1:F:372:ARG:CD	2:J:165:LEU:HD11	2.39	0.53
1:I:155:SER:OG	1:I:303:THR:HG23	2.09	0.53
1:I:218:TYR:HD1	1:I:254:ARG:NH1	2.05	0.53
1:I:355:MET:N	5:I:543:HOH:O	2.41	0.53
1:I:18:LYS:HG3	1:I:30:VAL:HG13	1.91	0.53
1:I:242:LEU:HD13	1:I:244:ASP:OD2	2.09	0.53
1:A:242:LEU:HB3	1:A:243:PRO:HD2	1.90	0.53
2:E:68:LEU:HD11	2:E:97:ILE:CG2	2.39	0.52
2:G:160:TYR:O	2:G:162:LYS:NZ	2.30	0.52
1:I:60:SER:O	1:I:60:SER:OG	2.25	0.52
1:I:99:GLU:OE2	1:I:100:GLU:HG3	2.10	0.52
1:F:357:ILE:HA	1:F:361:GLU:OE2	2.09	0.52
1:F:349:LEU:HD22	2:G:131:PHE:CE1	2.45	0.52
1:A:5:THR:HB	1:A:101:HIS:CE1	2.44	0.52
1:I:64:ILE:HG23	1:I:65:LEU:H	1.75	0.52
1:I:113:LYS:HG3	1:I:371:HIS:CE1	2.44	0.52
1:A:207:GLU:OE2	1:A:210:ARG:NE	2.42	0.52
1:F:372:ARG:NH1	2:J:153[B]:GLU:OE1	2.42	0.52
2:G:71:TRP:HB3	2:G:78:LEU:HG	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:251:GLY:CA	1:I:253:GLU:OE2	2.59	0.51
1:F:233:SER:OG	1:F:235:SER:N	2.38	0.51
1:D:233:SER:OG	1:D:234:SER:N	2.44	0.51
1:I:121:GLN:HG2	1:I:125:GLU:OE2	2.11	0.51
1:D:164:PRO:HG3	1:D:281:SER:OG	2.11	0.51
1:I:37:ARG:O	1:I:66:THR:OG1	2.26	0.51
1:I:26:ALA:HB3	5:I:540:HOH:O	2.11	0.51
1:I:182:GLY:CA	1:I:213:LYS:NZ	2.74	0.51
2:J:138:TYR:O	5:J:1325:HOH:O	2.19	0.51
1:F:252:ASN:OD1	1:F:252:ASN:N	2.37	0.51
1:I:252:ASN:CG	1:I:256:ARG:HE	2.19	0.51
1:A:325:MET:HA	1:A:325:MET:HE2	1.93	0.50
1:F:302:GLY:HA2	1:F:336:LYS:CG	2.41	0.50
2:G:150:GLN:O	2:G:152:PHE:HD1	1.94	0.50
2:J:72:ARG:NH1	2:J:172:VAL:HB	2.26	0.50
1:I:215:LYS:HD3	1:I:216:LEU:HD23	1.94	0.50
2:J:62:ALA:HA	2:J:69:GLN:HE22	1.75	0.50
1:F:216:LEU:HD22	1:F:216:LEU:H	1.76	0.50
1:D:70:PRO:HG3	1:D:85:ILE:CD1	2.42	0.50
1:F:291:LYS:HA	1:F:325:MET:HE1	1.94	0.50
1:I:78:ASN:CG	1:I:81:ASP:HB3	2.37	0.50
1:I:241:GLU:HA	1:I:247:VAL:HA	1.93	0.50
1:A:113:LYS:NZ	1:A:113:LYS:HB3	2.27	0.50
1:D:104:LEU:C	1:D:104:LEU:HD23	2.37	0.50
1:I:196:ARG:NH1	5:I:509:HOH:O	2.44	0.50
1:A:278:THR:O	1:A:282:ILE:HG13	2.11	0.49
1:A:363:ASP:C	2:B:1096:TRP:HD1	2.20	0.49
1:F:93:GLU:HA	5:F:555:HOH:O	2.11	0.49
1:F:357:ILE:HG23	1:F:369:ILE:HD12	1.94	0.49
2:G:106:GLY:HA3	1:I:334:GLU:HG3	1.94	0.49
1:I:184:ASP:O	1:I:187:ASP:N	2.45	0.49
1:I:253:GLU:H	1:I:253:GLU:CD	2.20	0.49
2:J:56:HIS:CE1	2:J:58:GLU:HB2	2.46	0.49
1:F:72:GLU:CD	1:F:77:THR:OG1	2.55	0.49
1:F:147:ARG:NH1	2:G:147:ARG:NH1	2.60	0.49
2:G:73:VAL:HB	2:G:94:ALA:HB3	1.93	0.49
1:D:216:LEU:HD12	1:D:250:ILE:CD1	2.42	0.49
1:A:31:PHE:CE1	1:A:93:GLU:HG3	2.48	0.49
1:F:209:VAL:O	1:F:213:LYS:N	2.44	0.49
1:D:198:TYR:CE1	1:D:248:ILE:HG13	2.48	0.49
1:A:207:GLU:O	1:A:211:ASP:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ILE:HG12	1:D:65:LEU:HG	1.94	0.49
1:I:222:ASP:OD1	1:I:222:ASP:C	2.55	0.49
1:A:62:ARG:NH1	1:A:204:ALA:HA	2.28	0.49
2:E:158:LEU:HD23	2:E:165:LEU:HD23	1.94	0.49
1:F:116:ARG:NH2	1:F:371:HIS:HA	2.28	0.49
2:G:94:ALA:HB2	5:G:1327:HOH:O	2.12	0.49
2:B:1081:ARG:NH2	2:B:1083:ASP:OD1	2.46	0.48
1:D:17:VAL:O	1:D:30:VAL:HA	2.13	0.48
2:G:89:PHE:CD2	2:G:165:LEU:HD11	2.48	0.48
1:I:251:GLY:C	1:I:253:GLU:OE2	2.56	0.48
1:A:113:LYS:HB3	1:A:113:LYS:HZ2	1.78	0.48
2:G:112:LEU:HD12	2:G:132:THR:HG23	1.94	0.48
1:I:189:LEU:HD23	1:I:209:VAL:HG13	1.94	0.48
1:A:363:ASP:O	2:B:1096:TRP:HD1	1.96	0.48
1:F:183:ARG:NE	5:F:539:HOH:O	2.37	0.48
1:I:285:CYS:O	1:I:290:ARG:NE	2.39	0.48
2:J:103:LEU:HD11	2:J:109:GLN:N	2.28	0.48
1:A:234:SER:OG	1:A:237:GLU:OE1	2.32	0.48
2:E:84:ASN:HD22	2:E:85:LEU:N	2.10	0.48
1:I:99:GLU:OE2	1:I:100:GLU:CG	2.62	0.48
1:I:287:ILE:HA	1:I:290:ARG:NE	2.28	0.48
1:F:32:PRO:HB2	1:F:34:ILE:HD12	1.96	0.48
2:J:157:PHE:CZ	2:J:161:PHE:HZ	2.31	0.48
2:G:129:ALA:O	2:G:132:THR:HB	2.14	0.48
1:A:62:ARG:NH1	1:A:203:THR:O	2.45	0.48
2:G:99:LYS:HB3	2:G:111:ASP:HB2	1.95	0.48
2:B:113:HIS:CE1	2:B:146:HIS:CD2	3.02	0.47
1:F:208:ILE:HG21	1:F:242:LEU:HD23	1.96	0.47
1:F:335:ARG:HA	1:F:338:SER:OG	2.13	0.47
2:J:72:ARG:HH12	2:J:172:VAL:HB	1.79	0.47
1:A:241:GLU:OE2	1:A:242:LEU:O	2.32	0.47
2:J:78:LEU:HD13	2:J:131:PHE:CG	2.48	0.47
1:D:303:THR:HG22	1:D:303:THR:O	2.13	0.47
1:A:189:LEU:HD21	1:A:212:ILE:HG22	1.97	0.47
1:D:6:THR:O	1:D:101:HIS:ND1	2.33	0.47
1:D:83:GLU:OE2	1:D:126:THR:HG21	2.14	0.47
1:I:166:TYR:CE2	1:I:167:GLU:OE2	2.67	0.47
1:F:185:LEU:HD11	1:F:261:LEU:HD21	1.96	0.47
1:F:299:MET:HG2	1:F:304:THR:HB	1.95	0.47
1:I:121:GLN:HG3	1:I:125:GLU:OE2	2.14	0.47
1:I:218:TYR:CD1	1:I:254:ARG:NH1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:252:ASN:HA	1:I:255:PHE:CZ	2.49	0.47
1:I:317:ILE:HG21	1:I:327:ILE:HG21	1.96	0.47
1:A:242:LEU:HD21	1:A:248:ILE:HD12	1.97	0.47
1:D:177:ARG:C	1:D:178:LEU:HD22	2.40	0.47
2:G:1070:HIS:CG	2:G:1071:LEU:N	2.79	0.47
1:A:252:ASN:ND2	1:A:256:ARG:HD2	2.30	0.47
1:D:70:PRO:HG3	1:D:85:ILE:HD12	1.95	0.47
2:J:174:SER:HA	5:J:1310:HOH:O	2.15	0.47
2:J:53:VAL:HG12	2:J:54:VAL:HG12	1.96	0.47
1:D:78:ASN:ND2	1:D:81:ASP:OD2	2.48	0.47
1:F:244:ASP:OD1	1:F:245:GLY:N	2.48	0.47
1:I:37:ARG:O	1:I:66:THR:N	2.42	0.47
1:I:108:ALA:HB1	1:I:109:PRO:HD2	1.96	0.47
1:I:157:ASP:O	1:I:181:ALA:HB3	2.15	0.47
1:I:187:ASP:OD1	1:I:191:LYS:HE3	2.14	0.47
1:D:318:THR:HA	1:D:327:ILE:HD12	1.97	0.46
1:I:287:ILE:HA	1:I:290:ARG:CD	2.45	0.46
2:J:147:ARG:HH12	2:J:149:VAL:HG22	1.79	0.46
1:F:258:PRO:HG3	1:F:306:TYR:CE1	2.50	0.46
1:F:282:ILE:HD12	1:F:294:TYR:CE1	2.50	0.46
1:A:64:ILE:C	1:A:65:LEU:HD12	2.41	0.46
1:F:113:LYS:HG3	1:F:114:ALA:N	2.30	0.46
1:D:28:ARG:NH1	1:D:28:ARG:CG	2.77	0.46
2:G:88:ASP:OD1	2:G:88:ASP:N	2.47	0.46
1:I:58:ALA:HB1	1:I:61:LYS:CG	2.45	0.46
1:A:10[A]:CYS:HB2	1:A:105:LEU:HD23	1.97	0.46
1:A:84:LYS:HG2	2:B:1087:TYR:CD2	2.50	0.46
2:J:70:ILE:HD12	2:J:86:TYR:CG	2.51	0.46
1:I:157:ASP:OD1	3:I:401:ADP:O3'	2.30	0.46
2:G:97:ILE:HG13	2:G:157:PHE:HE1	1.81	0.46
1:A:330:ILE:HD12	1:A:330:ILE:N	2.31	0.46
2:B:82:PRO:HG2	2:B:85:LEU:HD12	1.98	0.46
1:D:70:PRO:CG	1:D:85:ILE:CD1	2.94	0.46
1:F:166:TYR:N	1:F:169:TYR:O	2.45	0.46
1:A:87:HIS:CD2	2:B:1087:TYR:HB2	2.51	0.46
1:I:106:THR:HG21	1:I:137:GLN:HE21	1.80	0.46
1:I:180:LEU:HD11	1:I:185:LEU:CD1	2.46	0.46
1:I:349:LEU:CD1	2:J:130:ILE:HG21	2.45	0.46
1:I:237:GLU:HG2	1:I:251:GLY:HA2	1.97	0.45
1:I:310:ALA:HB1	5:I:535:HOH:O	2.17	0.45
2:B:1065:GLU:HA	2:B:1065:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ILE:CG1	1:D:65:LEU:N	2.80	0.45
1:F:37:ARG:NH1	1:F:68:LYS:HZ2	2.14	0.45
1:F:214:GLU:HA	3:F:401:ADP:C6	2.51	0.45
2:J:111:ASP:HB3	2:J:113:HIS:NE2	2.30	0.45
1:A:227:MET:O	1:A:230:ALA:HB3	2.17	0.45
1:F:147:ARG:CZ	2:G:147:ARG:NH1	2.79	0.45
1:I:304:THR:O	1:I:335:ARG:NH1	2.50	0.45
2:B:89:PHE:HD2	2:B:95:TYR:CD1	2.35	0.45
2:B:72:ARG:NH1	2:B:93:ASP:OD2	2.44	0.45
1:F:151:ILE:HB	1:F:164:PRO:HA	1.99	0.45
1:I:128:ASN:N	1:I:128:ASN:HD22	2.15	0.45
1:D:332:PRO:O	1:D:335:ARG:NE	2.42	0.45
1:F:151:ILE:HD12	1:F:164:PRO:HD3	1.99	0.45
2:G:97:ILE:HG13	2:G:157:PHE:CE1	2.52	0.45
2:E:54:VAL:HG11	2:E:59:PHE:CE2	2.52	0.45
1:F:113:LYS:CG	1:F:114:ALA:N	2.80	0.45
1:F:372:ARG:HD2	2:J:165:LEU:HD11	1.98	0.45
1:I:192:ILE:CD1	1:I:253:GLU:HB3	2.47	0.45
1:D:176:MET:HE3	1:D:284:LYS:HD2	1.99	0.45
1:I:216:LEU:HD22	1:I:238:LYS:HD3	1.98	0.45
2:G:70:ILE:HG23	2:G:97:ILE:CD1	2.47	0.44
2:G:108:LEU:HG	1:I:333:PRO:HB3	1.99	0.44
1:I:12:ASN:HD21	1:I:86:TRP:HE1	1.63	0.44
1:A:171:LEU:HB3	1:A:173:HIS:CE1	2.53	0.44
1:D:28:ARG:NH1	1:D:28:ARG:HG3	2.32	0.44
1:A:180:LEU:HD12	1:A:181:ALA:N	2.32	0.44
1:D:144:ALA:HB1	2:E:122:GLN:NE2	2.33	0.44
1:F:188:TYR:HB2	1:F:267:ILE:HD11	2.00	0.44
1:I:138:ALA:CB	1:I:163:VAL:HG11	2.48	0.44
1:I:151:ILE:HA	1:I:164:PRO:HA	2.00	0.44
2:E:96:VAL:C	2:E:97:ILE:HD12	2.42	0.44
1:F:278:THR:HG21	1:F:313:MET:HE1	1.99	0.44
1:D:156:GLY:O	1:D:181:ALA:HB1	2.17	0.44
2:J:129:ALA:O	2:J:132:THR:HB	2.18	0.44
1:A:100:GLU:CG	1:A:101:HIS:CD2	3.00	0.44
1:F:107:GLU:OE2	1:F:134:VAL:HG22	2.18	0.44
1:I:11:ASP:OD1	1:I:106:THR:HG21	2.17	0.44
1:A:92:ASN:N	1:A:92:ASN:HD22	2.14	0.44
1:D:180:LEU:HA	1:D:184:ASP:OD2	2.18	0.44
2:E:65:GLU:N	5:E:1369:HOH:O	2.46	0.44
1:F:372:ARG:HD3	2:J:165:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:354:GLN:HG3	2:G:54:VAL:HA	1.99	0.44
2:G:101:VAL:O	2:G:109:GLN:N	2.41	0.44
1:A:99:GLU:OE2	1:A:99:GLU:N	2.48	0.44
1:A:164:PRO:O	1:A:171:LEU:HD12	2.18	0.44
1:D:8:LEU:HD11	1:D:96:VAL:HG21	1.99	0.44
1:F:136:ILE:CG2	1:F:139:VAL:HG23	2.48	0.44
1:F:200:PHE:C	1:F:205:GLU:OE2	2.61	0.44
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.99	0.44
2:B:1074:GLN:NE2	2:B:1077:GLU:OE2	2.50	0.43
2:E:90:PHE:HB3	2:E:170:GLY:O	2.18	0.43
1:F:208:ILE:HG21	1:F:242:LEU:CD2	2.48	0.43
2:B:1067:LEU:C	2:B:1067:LEU:CD2	2.92	0.43
1:F:165:ILE:HA	1:F:170:ALA:HA	2.00	0.43
1:I:35:VAL:CG2	1:I:81:ASP:OD1	2.66	0.43
1:D:336:LYS:HE2	1:D:337:TYR:CE2	2.53	0.43
1:F:112:PRO:O	1:F:116:ARG:HG3	2.19	0.43
2:G:58:GLU:HB3	2:G:71:TRP:NE1	2.33	0.43
1:I:58:ALA:HB1	1:I:61:LYS:HG2	2.01	0.43
1:A:92:ASN:N	1:A:92:ASN:ND2	2.65	0.43
1:A:316:GLU:OE2	1:A:316:GLU:CA	2.66	0.43
2:B:1070:HIS:NE2	2:B:1074:GLN:OE1	2.52	0.43
1:F:84:LYS:HA	5:F:550:HOH:O	2.18	0.43
1:F:219:VAL:CG2	1:F:258:PRO:HB2	2.48	0.43
2:G:53:VAL:HG22	2:G:54:VAL:N	2.33	0.43
1:I:122:ILE:CG2	1:I:127:PHE:HE2	2.32	0.43
1:I:155:SER:O	1:I:303:THR:HG22	2.18	0.43
1:A:171:LEU:HD12	1:A:171:LEU:N	2.33	0.43
1:F:354:GLN:HE21	2:G:54:VAL:HG23	1.84	0.43
1:I:221:LEU:HD12	1:I:315:LYS:HD3	2.00	0.43
1:A:121:GLN:O	1:A:125:GLU:HG3	2.19	0.43
1:D:303:THR:O	1:D:303:THR:CG2	2.67	0.43
2:E:75:LYS:O	2:E:76:PHE:HB2	2.18	0.43
1:F:196:ARG:HA	1:F:196:ARG:NE	2.34	0.43
1:I:158:GLY:HA2	1:I:183:ARG:HH22	1.84	0.43
1:I:124:PHE:CE1	1:I:359:LYS:HA	2.53	0.43
1:I:196:ARG:NH1	1:I:251:GLY:HA3	2.33	0.43
1:A:248:ILE:CG2	1:A:249:THR:N	2.81	0.43
1:F:192:ILE:O	1:F:196:ARG:HG2	2.18	0.43
1:F:223:PHE:HZ	1:F:256:ARG:HG3	1.83	0.43
1:F:302:GLY:HA2	1:F:336:LYS:HD2	2.01	0.43
2:G:1068:LEU:HD12	2:G:1068:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:124:GLU:CD	5:J:1310:HOH:O	2.61	0.43
1:A:238:LYS:HG3	1:A:239:SER:H	1.84	0.43
1:D:178:LEU:HD21	1:D:277:THR:CG2	2.39	0.43
1:D:309:ILE:HG23	1:D:310:ALA:N	2.33	0.43
1:I:358:THR:HG23	1:I:361:GLU:OE2	2.19	0.43
2:J:165:LEU:C	2:J:165:LEU:HD22	2.44	0.43
1:F:372:ARG:HH12	2:J:151:GLY:HA2	1.84	0.42
1:A:196:ARG:NH2	5:A:567:HOH:O	2.51	0.42
1:D:192:ILE:HD12	1:D:253:GLU:HG3	2.01	0.42
1:D:200:PHE:HA	1:D:205:GLU:OE2	2.19	0.42
1:D:242:LEU:O	1:D:245:GLY:N	2.48	0.42
1:I:27:PRO:HD3	1:I:340:TRP:CE3	2.54	0.42
2:E:84:ASN:HD22	2:E:84:ASN:N	2.18	0.42
1:F:164:PRO:HG3	1:F:174:ALA:CB	2.49	0.42
1:F:305:MET:HE2	1:F:336:LYS:HD3	2.02	0.42
2:G:87:GLY:HA2	2:G:161:PHE:CE1	2.55	0.42
1:I:349:LEU:HD21	2:J:127:ALA:HB2	2.00	0.42
2:J:122:GLN:HA	2:J:125:SER:OG	2.19	0.42
1:D:37:ARG:NH2	1:D:81:ASP:OD1	2.46	0.42
1:I:371:HIS:O	1:I:375:PHE:HB3	2.18	0.42
2:B:151:GLY:N	2:B:167:TYR:OH	2.45	0.42
1:F:157:ASP:N	3:F:401:ADP:H5'1	2.33	0.42
1:F:349:LEU:HD11	2:G:130:ILE:HG21	2.01	0.42
1:I:21:PHE:CD1	1:I:21:PHE:N	2.88	0.42
1:I:329:ILE:N	1:I:329:ILE:HD12	2.33	0.42
2:J:151:GLY:N	2:J:167:TYR:OH	2.52	0.42
1:A:8:LEU:HG	1:A:101:HIS:HB3	2.02	0.42
1:A:109:PRO:HB3	1:A:175:ILE:HD13	2.02	0.42
1:A:169:TYR:CD1	2:E:169:LYS:HE3	2.55	0.42
1:A:192:ILE:HD12	1:A:253:GLU:CB	2.48	0.42
1:F:251:GLY:C	1:F:253:GLU:H	2.27	0.42
1:F:203:THR:O	1:F:203:THR:OG1	2.37	0.42
1:I:109:PRO:HB2	1:I:175:ILE:HD13	2.01	0.42
1:I:361:GLU:HB3	1:I:369:ILE:CD1	2.49	0.42
2:J:63:GLY:HA2	2:J:110:TYR:CE1	2.54	0.42
1:D:355:MET:HE3	2:E:54:VAL:HG23	2.01	0.42
2:G:112:LEU:HD21	2:G:135:LEU:HD13	2.01	0.42
2:J:147:ARG:HG3	2:J:147:ARG:HH11	1.84	0.42
1:A:107:GLU:OE1	1:A:116:ARG:HD2	2.20	0.42
2:E:54:VAL:O	2:E:54:VAL:HG12	2.20	0.42
2:E:84:ASN:HD22	2:E:85:LEU:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:ARG:NH1	5:F:525:HOH:O	2.38	0.42
1:F:212:ILE:HG23	1:F:216:LEU:HD23	2.02	0.42
2:G:149:VAL:O	2:G:150:GLN:C	2.62	0.42
1:I:193:LEU:HD23	1:I:198:TYR:CD2	2.55	0.42
1:F:171:LEU:HB3	1:F:173:HIS:CE1	2.55	0.42
2:G:53:VAL:HG22	2:G:54:VAL:H	1.85	0.42
1:I:240:TYR:HD2	1:I:248:ILE:HD11	1.85	0.42
1:I:341:ILE:HD11	5:I:532:HOH:O	2.18	0.42
1:A:163:VAL:HG13	1:A:175:ILE:HG12	2.01	0.41
1:I:252:ASN:CB	1:I:255:PHE:CZ	3.02	0.41
1:D:36:GLY:HA2	1:D:66:THR:O	2.20	0.41
1:A:143:TYR:CD2	2:B:130:ILE:HG12	2.56	0.41
1:A:191:LYS:HD2	1:A:191:LYS:HA	1.95	0.41
1:I:337:TYR:HA	5:I:525:HOH:O	2.20	0.41
2:E:140:ASN:C	2:E:142:ARG:N	2.79	0.41
1:F:165:ILE:HG23	1:F:169:TYR:C	2.46	0.41
1:F:223:PHE:CZ	1:F:256:ARG:HG3	2.55	0.41
1:F:372:ARG:HD3	2:J:165:LEU:CD1	2.50	0.41
1:D:202:THR:HB	1:D:205:GLU:HG3	2.03	0.41
1:F:182:GLY:HA2	1:F:185:LEU:HD12	2.01	0.41
1:I:102:PRO:HA	1:I:131:ALA:O	2.21	0.41
1:I:336:LYS:CE	5:I:545:HOH:O	2.67	0.41
1:A:212:ILE:HG13	1:A:240:TYR:CE2	2.56	0.41
1:A:286:ASP:OD1	1:A:287:ILE:N	2.54	0.41
2:B:1096:TRP:CH2	2:B:1098:PRO:HA	2.56	0.41
2:E:88:ASP:OD2	5:E:1354:HOH:O	2.22	0.41
1:F:202:THR:OG1	1:F:203:THR:N	2.51	0.41
1:A:233:SER:O	1:A:234:SER:CB	2.69	0.41
2:G:70:ILE:HG22	2:G:81:VAL:HG21	2.03	0.41
1:I:58:ALA:CB	1:I:61:LYS:HG3	2.51	0.41
1:A:10[B]:CYS:HB3	1:A:105:LEU:HD23	2.01	0.41
1:A:100:GLU:CG	1:A:101:HIS:NE2	2.84	0.41
1:A:124:PHE:O	1:A:128:ASN:HA	2.21	0.41
1:D:97:ALA:HA	1:D:98:PRO:HD3	1.94	0.41
1:F:207:GLU:C	1:F:207:GLU:CD	2.88	0.41
1:I:53:TYR:CD2	1:I:65:LEU:HD11	2.56	0.41
1:I:106:THR:HG23	1:I:137:GLN:CG	2.51	0.41
1:A:72:GLU:HG2	1:A:77:THR:HG21	2.03	0.41
1:A:193:LEU:O	1:A:198:TYR:N	2.44	0.41
1:A:336:LYS:HB2	5:A:503:HOH:O	2.21	0.41
1:F:56:ASP:HA	1:F:59:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:THR:O	1:F:94:LEU:HD13	2.21	0.41
1:F:94:LEU:C	1:F:95:ARG:HD3	2.46	0.41
2:G:87:GLY:CA	2:G:161:PHE:CE1	3.04	0.41
1:A:309:ILE:HG23	1:A:310:ALA:N	2.36	0.41
1:F:114:ALA:HA	1:F:117:GLU:CD	2.46	0.41
1:F:354:GLN:HG3	2:G:53:VAL:O	2.21	0.41
1:I:10[B]:CYS:HB3	1:I:105:LEU:CD2	2.50	0.41
1:I:70:PRO:HG2	1:I:71:ILE:HD12	2.03	0.41
1:I:90:PHE:HZ	1:I:123:MET:HE1	1.86	0.41
1:I:96:VAL:CG1	1:I:101:HIS:CE1	3.04	0.41
1:I:126:THR:O	1:I:128:ASN:ND2	2.54	0.41
1:D:310:ALA:HA	1:D:329:ILE:HG21	2.03	0.40
1:F:180:LEU:HA	1:F:184:ASP:OD2	2.22	0.40
2:G:1064:ARG:O	2:G:1068:LEU:HD12	2.21	0.40
1:I:194:THR:HA	1:I:198:TYR:O	2.21	0.40
1:I:304:THR:O	1:I:335:ARG:CZ	2.69	0.40
2:J:147:ARG:NH1	2:J:147:ARG:HG3	2.36	0.40
1:A:316:GLU:OE2	1:A:316:GLU:HA	2.22	0.40
1:F:27:PRO:HD3	1:F:340:TRP:CD2	2.56	0.40
1:F:60:SER:HA	1:F:62:ARG:CZ	2.51	0.40
1:A:110:LEU:N	1:A:110:LEU:HD23	2.36	0.40
1:A:314:GLN:O	1:A:318:THR:N	2.48	0.40
2:G:66:PRO:HA	2:G:100:THR:OG1	2.22	0.40
2:G:153:GLU:HB2	2:G:158:LEU:HD23	2.03	0.40
2:J:53:VAL:C	2:J:54:VAL:HG12	2.47	0.40
2:J:68:LEU:CD2	2:J:70:ILE:HG13	2.51	0.40
1:A:62:ARG:HG2	1:A:62:ARG:HH21	1.87	0.40
1:F:198:TYR:CD2	1:F:248:ILE:HD12	2.56	0.40
1:I:279:TYR:CE1	1:I:283:MET:SD	3.14	0.40
1:F:357:ILE:HD11	1:F:373:LYS:HB2	2.03	0.40
1:I:89:THR:O	1:I:94:LEU:HG	2.21	0.40

All (2) 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:A:66:THR:OG1	1:I:224:GLU:OE2[2_557]	2.06	0.14
1:F:25:ASP:OD2	2:J:105:ASN:HD21[1_455]	1.57	0.03

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	357/377 (95%)	348 (98%)	9 (2%)	0	100	100
1	D	357/377 (95%)	349 (98%)	8 (2%)	0	100	100
1	F	361/377 (96%)	341 (94%)	19 (5%)	1 (0%)	36	34
1	I	357/377 (95%)	339 (95%)	17 (5%)	1 (0%)	36	34
2	B	161/186 (87%)	156 (97%)	5 (3%)	0	100	100
2	E	123/186 (66%)	118 (96%)	4 (3%)	1 (1%)	16	10
2	G	139/186 (75%)	135 (97%)	3 (2%)	1 (1%)	18	13
2	J	125/186 (67%)	122 (98%)	1 (1%)	2 (2%)	7	3
All	All	1980/2252 (88%)	1908 (96%)	66 (3%)	6 (0%)	36	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	201	VAL
2	G	53	VAL
2	E	54	VAL
1	I	34	ILE
2	J	54	VAL
2	J	53	VAL

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	307/320 (96%)	286 (93%)	21 (7%)	14	10
1	D	307/320 (96%)	283 (92%)	24 (8%)	11	7
1	F	310/320 (97%)	257 (83%)	53 (17%)	2	0
1	I	307/320 (96%)	258 (84%)	49 (16%)	2	1
2	B	138/153 (90%)	126 (91%)	12 (9%)	9	5
2	E	102/153 (67%)	95 (93%)	7 (7%)	14	9
2	G	119/153 (78%)	101 (85%)	18 (15%)	3	1
2	J	104/153 (68%)	87 (84%)	17 (16%)	2	1
All	All	1694/1892 (90%)	1493 (88%)	201 (12%)	5	2

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	28	ARG
1	A	37	ARG
1	A	72	GLU
1	A	85	ILE
1	A	113	LYS
1	A	118	LYS
1	A	159	VAL
1	A	176	MET
1	A	179[A]	ASP
1	A	179[B]	ASP
1	A	200	PHE
1	A	201	VAL
1	A	203	THR
1	A	242	LEU
1	A	287	ILE
1	A	315	LYS
1	A	316	GLU
1	A	318	THR
1	A	323	SER
1	A	373	LYS
2	B	54	VAL
2	B	55	GLU
2	B	75	LYS
2	B	84	ASN
2	B	150	GLN
2	B	1067	LEU

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Mol	Chain	Res	Type
2	B	1074	GLN
2	B	1079	LYS
2	B	1082	GLU
2	B	1084	LEU
2	B	1095	VAL
2	B	1099	LYS
1	D	14	SER
1	D	28	ARG
1	D	33	SER
1	D	51	ASP
1	D	62	ARG
1	D	64	ILE
1	D	95	ARG
1	D	119	MET
1	D	179	ASP
1	D	208	ILE
1	D	238	LYS
1	D	241	GLU
1	D	248	ILE
1	D	249	THR
1	D	250	ILE
1	D	271	SER
1	D	283	MET
1	D	323	SER
1	D	324	THR
1	D	335	ARG
1	D	353	GLN
1	D	364	GLU
1	D	368	SER
1	D	375	PHE
2	E	64	LYS
2	E	83	THR
2	E	84	ASN
2	E	109	GLN
2	E	116	LEU
2	E	121	SER
2	E	165	LEU
1	F	5	THR
1	F	14	SER
1	F	16	LEU
1	F	33	SER
1	F	34	ILE

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Mol	Chain	Res	Type
1	F	43	VAL
1	F	53	TYR
1	F	60	SER
1	F	62	ARG
1	F	68	LYS
1	F	72	GLU
1	F	77	THR
1	F	80	ASP
1	F	95	ARG
1	F	116	ARG
1	F	129	VAL
1	F	132	MET
1	F	151	ILE
1	F	152	VAL
1	F	163	VAL
1	F	178	LEU
1	F	179	ASP
1	F	180	LEU
1	F	186	THR
1	F	189	LEU
1	F	194	THR
1	F	196	ARG
1	F	206	ARG
1	F	207	GLU
1	F	208	ILE
1	F	214	GLU
1	F	221	LEU
1	F	229	THR
1	F	235	SER
1	F	246	GLN
1	F	252	ASN
1	F	253	GLU
1	F	254	ARG
1	F	265	SER
1	F	282	ILE
1	F	299	MET
1	F	300	SER
1	F	309	ILE
1	F	313	MET
1	F	318	THR
1	F	320	LEU
1	F	325	MET

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Mol	Chain	Res	Type
1	F	327	ILE
1	F	338	SER
1	F	354	GLN
1	F	360	GLN
1	F	364	GLU
1	F	374	CYS
2	G	52	MET
2	G	55	GLU
2	G	60	LEU
2	G	65	GLU
2	G	88	ASP
2	G	102	GLN
2	G	103	LEU
2	G	107	ASN
2	G	112	LEU
2	G	114	TYR
2	G	135	LEU
2	G	142	ARG
2	G	146	HIS
2	G	158	LEU
2	G	1059	THR
2	G	1064	ARG
2	G	1070	HIS
2	G	1074	GLN
1	I	18	LYS
1	I	34	ILE
1	I	60	SER
1	I	68	LYS
1	I	75	ILE
1	I	92	ASN
1	I	94	LEU
1	I	96	VAL
1	I	99	GLU
1	I	106	THR
1	I	110	LEU
1	I	115	ASN
1	I	128	ASN
1	I	132	MET
1	I	134	VAL
1	I	161	HIS
1	I	180	LEU
1	I	185	LEU

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Mol	Chain	Res	Type
1	I	187	ASP
1	I	192	ILE
1	I	193	LEU
1	I	199	SER
1	I	201	VAL
1	I	202	THR
1	I	203	THR
1	I	209	VAL
1	I	215	LYS
1	I	224	GLU
1	I	226	GLU
1	I	227	MET
1	I	229	THR
1	I	246	GLN
1	I	249	THR
1	I	250	ILE
1	I	269	MET
1	I	274	ILE
1	I	281	SER
1	I	292	ASP
1	I	298	VAL
1	I	304	THR
1	I	327	ILE
1	I	330	ILE
1	I	334	GLU
1	I	338	SER
1	I	355	MET
1	I	359	LYS
1	I	368	SER
1	I	373	LYS
1	I	375	PHE
2	J	52	MET
2	J	64	LYS
2	J	72	ARG
2	J	81	VAL
2	J	83	THR
2	J	88	ASP
2	J	99	LYS
2	J	112	LEU
2	J	121	SER
2	J	135	LEU
2	J	137	ASP

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Mol	Chain	Res	Type
2	J	156	THR
2	J	161	PHE
2	J	165	LEU
2	J	168	LYS
2	J	169	LYS
2	J	172	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	121	GLN
1	A	161	HIS
1	A	162	ASN
1	A	371	HIS
2	B	107	ASN
1	D	92	ASN
1	D	115	ASN
1	D	161	HIS
1	D	297	ASN
1	D	353	GLN
2	E	84	ASN
2	E	102	GLN
2	E	122	GLN
2	E	134	GLN
2	E	145	GLN
1	F	59	GLN
1	F	73	HIS
1	F	87	HIS
1	F	161	HIS
1	F	162	ASN
1	F	280	ASN
1	F	360	GLN
1	F	371	HIS
2	G	134	GLN
2	G	146	HIS
2	G	1070	HIS
1	I	12	ASN
1	I	59	GLN
1	I	111	ASN
1	I	128	ASN
1	I	137	GLN

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Mol	Chain	Res	Type
1	I	225	ASN
1	I	297	ASN
1	I	371	HIS
2	J	69	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](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	D	401	4	28,29,29	1.86	5 (17%)	43,45,45	2.05	15 (34%)
3	ADP	F	401	-	28,29,29	1.59	6 (21%)	43,45,45	2.02	14 (32%)
3	ADP	I	401	4	28,29,29	1.57	4 (14%)	43,45,45	2.21	19 (44%)
3	ADP	A	401	4	28,29,29	1.55	4 (14%)	43,45,45	2.38	16 (37%)

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	ADP	D	401	4	-	0/16/32/32	0/3/3/3
3	ADP	F	401	-	-	5/16/32/32	0/3/3/3
3	ADP	I	401	4	-	0/16/32/32	0/3/3/3
3	ADP	A	401	4	-	1/16/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ADP	PA-O3A	5.88	1.65	1.59
3	I	401	ADP	C5-C4	4.57	1.47	1.39
3	D	401	ADP	C5-C4	4.50	1.47	1.39
3	F	401	ADP	C5-C4	4.49	1.47	1.39
3	A	401	ADP	C5-C4	4.18	1.46	1.39
3	A	401	ADP	C5-C6	4.08	1.52	1.41
3	I	401	ADP	C8-N7	3.59	1.38	1.31
3	F	401	ADP	PA-O3A	3.38	1.63	1.59
3	F	401	ADP	C4-N9	-3.30	1.30	1.37
3	D	401	ADP	C4-N9	-3.17	1.31	1.37
3	D	401	ADP	C5-C6	2.85	1.48	1.41
3	I	401	ADP	C4-N9	-2.55	1.32	1.37
3	A	401	ADP	PB-O3B	-2.46	1.45	1.54
3	F	401	ADP	C8-N7	2.45	1.36	1.31
3	F	401	ADP	C5-N7	-2.37	1.34	1.39
3	I	401	ADP	C5-N7	-2.34	1.34	1.39
3	F	401	ADP	C5-C6	2.28	1.47	1.41
3	A	401	ADP	C8-N9	-2.19	1.33	1.37
3	D	401	ADP	C1'-N9	2.10	1.52	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	C5-C4-N3	-7.14	116.89	126.72
3	I	401	ADP	C4-N9-C8	5.72	111.74	105.74
3	D	401	ADP	O4'-C1'-N9	5.59	118.83	108.09
3	A	401	ADP	C4-C5-N7	-5.34	104.47	110.58
3	A	401	ADP	N3-C4-N9	5.31	136.20	127.17
3	D	401	ADP	C5-C4-N3	-5.12	119.66	126.72
3	F	401	ADP	O4'-C1'-N9	5.07	117.83	108.09
3	F	401	ADP	C5-C4-N3	-5.03	119.79	126.72
3	A	401	ADP	C2-N3-C4	4.16	121.98	111.83
3	I	401	ADP	N9-C8-N7	-4.15	108.05	113.94
3	A	401	ADP	O3B-PB-O3A	-4.02	91.17	104.64
3	I	401	ADP	C5-C4-N3	-3.95	121.28	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	C5-N7-C8	3.84	109.48	103.45
3	F	401	ADP	N3-C4-N9	3.82	133.66	127.17
3	I	401	ADP	N3-C4-N9	3.74	133.53	127.17
3	D	401	ADP	N3-C4-N9	3.67	133.41	127.17
3	F	401	ADP	C4-C5-N7	-3.55	106.52	110.58
3	I	401	ADP	O3'-C3'-C2'	-3.52	100.54	111.82
3	F	401	ADP	C4-N9-C8	3.46	109.37	105.74
3	F	401	ADP	C2-N3-C4	3.27	119.83	111.83
3	I	401	ADP	C4-C5-N7	-3.25	106.86	110.58
3	I	401	ADP	N3-C2-N1	-3.18	123.77	128.58
3	D	401	ADP	C4-C5-N7	-3.14	107.00	110.58
3	A	401	ADP	C4-N9-C8	3.07	108.97	105.74
3	F	401	ADP	N3-C2-N1	-3.07	123.93	128.58
3	D	401	ADP	C2-N3-C4	3.00	119.17	111.83
3	I	401	ADP	C2-N1-C6	3.00	123.67	118.73
3	I	401	ADP	C5-N7-C8	3.00	108.17	103.45
3	I	401	ADP	C4-N9-C1'	-2.96	119.70	126.63
3	D	401	ADP	O3B-PB-O1B	2.82	121.84	110.83
3	A	401	ADP	O3B-PB-O1B	2.80	121.75	110.83
3	A	401	ADP	C6-C5-N7	2.75	137.40	132.09
3	A	401	ADP	N9-C8-N7	-2.65	110.17	113.94
3	I	401	ADP	C2-N3-C4	2.61	118.22	111.83
3	I	401	ADP	O3A-PB-O1B	-2.60	97.38	111.04
3	D	401	ADP	O3A-PA-O1A	2.59	118.48	110.70
3	D	401	ADP	O3'-C3'-C4'	-2.56	103.74	111.08
3	F	401	ADP	O2B-PB-O3A	2.55	113.18	104.64
3	I	401	ADP	O3B-PB-O2B	2.50	117.16	107.80
3	D	401	ADP	C5'-C4'-C3'	-2.50	106.23	115.21
3	D	401	ADP	C6-C5-N7	2.45	136.82	132.09
3	I	401	ADP	C6-C5-N7	2.44	136.80	132.09
3	A	401	ADP	O4'-C1'-N9	2.42	112.74	108.09
3	A	401	ADP	O2A-PA-O1A	2.34	123.35	112.44
3	I	401	ADP	O4'-C1'-C2'	2.33	111.61	106.62
3	F	401	ADP	N9-C8-N7	-2.30	110.67	113.94
3	A	401	ADP	C2'-C3'-C4'	2.30	107.06	102.61
3	I	401	ADP	O3B-PB-O1B	2.28	119.73	110.83
3	A	401	ADP	O3A-PB-O1B	-2.27	99.12	111.04
3	I	401	ADP	O4'-C4'-C3'	2.26	109.64	105.15
3	D	401	ADP	N3-C2-N1	-2.24	125.19	128.58
3	F	401	ADP	C2'-C1'-N9	-2.19	107.86	113.30
3	F	401	ADP	C6-C5-N7	2.18	136.29	132.09
3	F	401	ADP	C5-N7-C8	2.17	106.87	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	O3B-PB-O3A	-2.17	97.37	104.64
3	D	401	ADP	O4'-C4'-C3'	2.17	109.45	105.15
3	D	401	ADP	C4-N9-C8	2.16	108.01	105.74
3	F	401	ADP	O5'-C5'-C4'	2.12	116.20	108.99
3	I	401	ADP	C2'-C1'-N9	-2.08	108.12	113.30
3	A	401	ADP	O3B-PB-O2B	2.07	115.58	107.80
3	D	401	ADP	O2A-PA-O3A	-2.07	101.67	107.27
3	I	401	ADP	O2A-PA-O3A	2.07	112.87	107.27
3	F	401	ADP	O2A-PA-O1A	2.06	122.04	112.44
3	A	401	ADP	N3-C2-N1	-2.06	125.47	128.58

There are no chirality outliers.

All (6) torsion outliers are listed below:

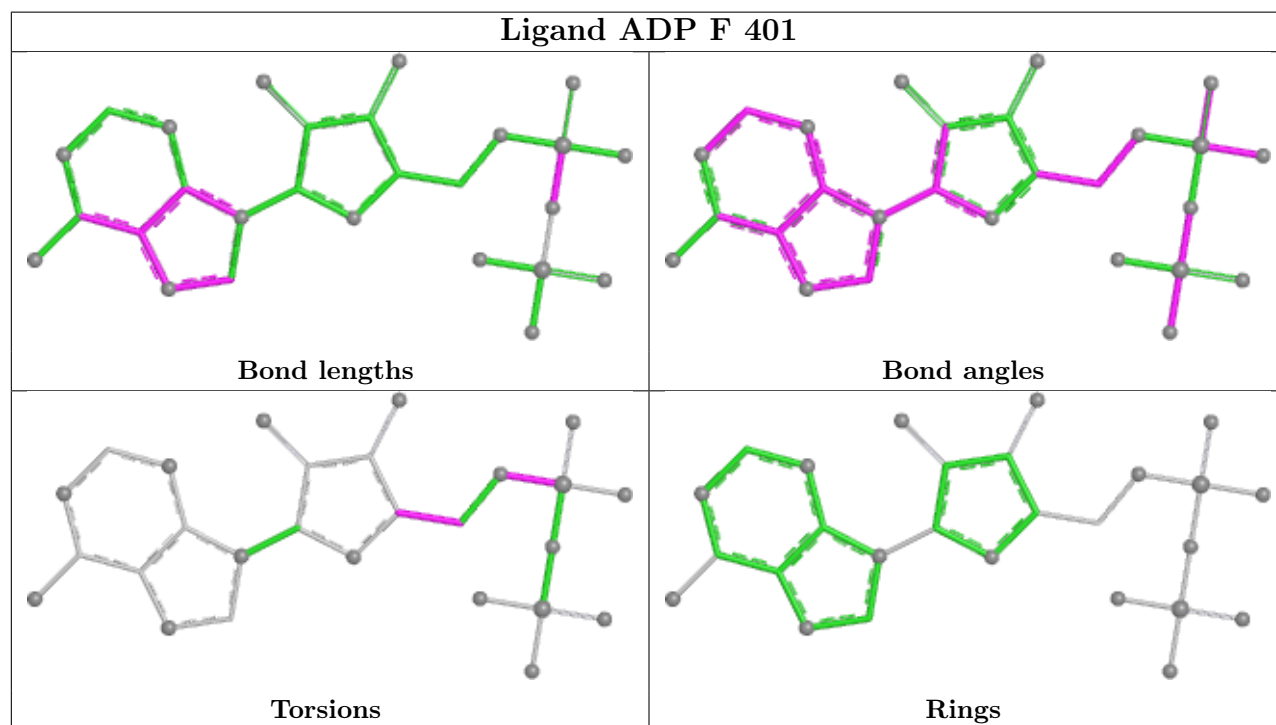
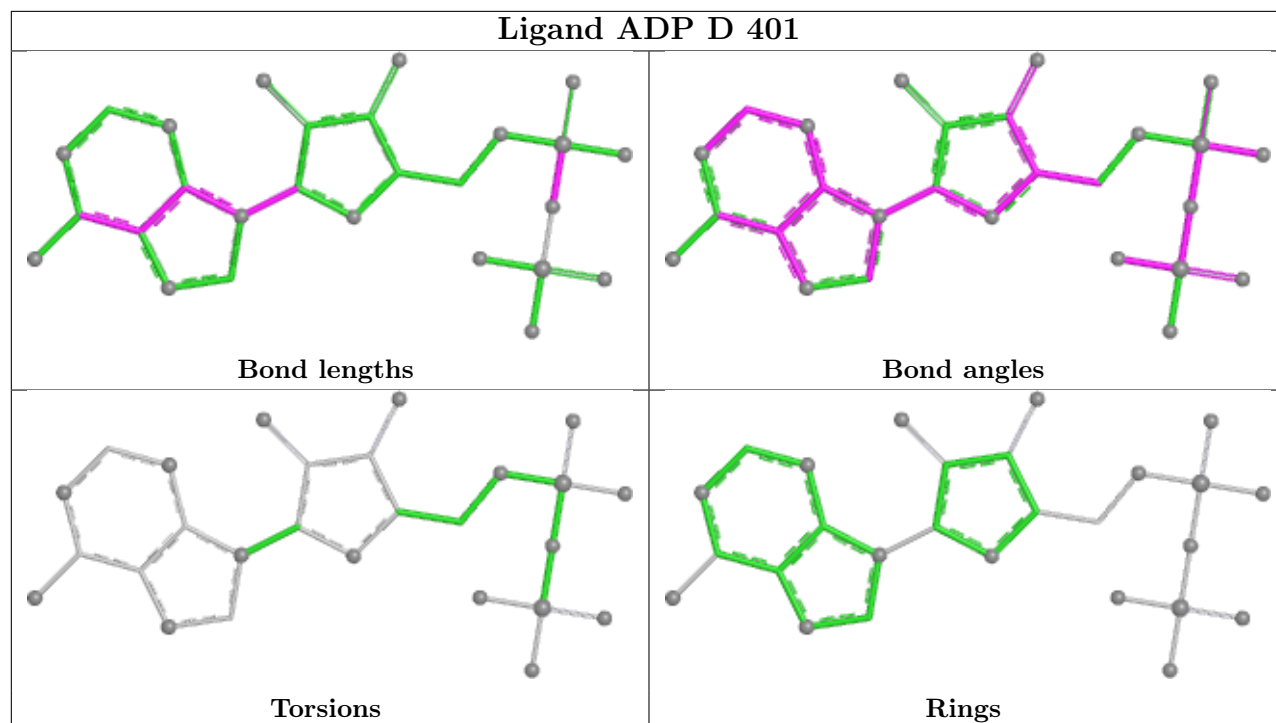
Mol	Chain	Res	Type	Atoms
3	F	401	ADP	C5'-O5'-PA-O2A
3	F	401	ADP	O4'-C4'-C5'-O5'
3	F	401	ADP	C3'-C4'-C5'-O5'
3	A	401	ADP	PA-O3A-PB-O3B
3	F	401	ADP	C5'-O5'-PA-O1A
3	F	401	ADP	C5'-O5'-PA-O3A

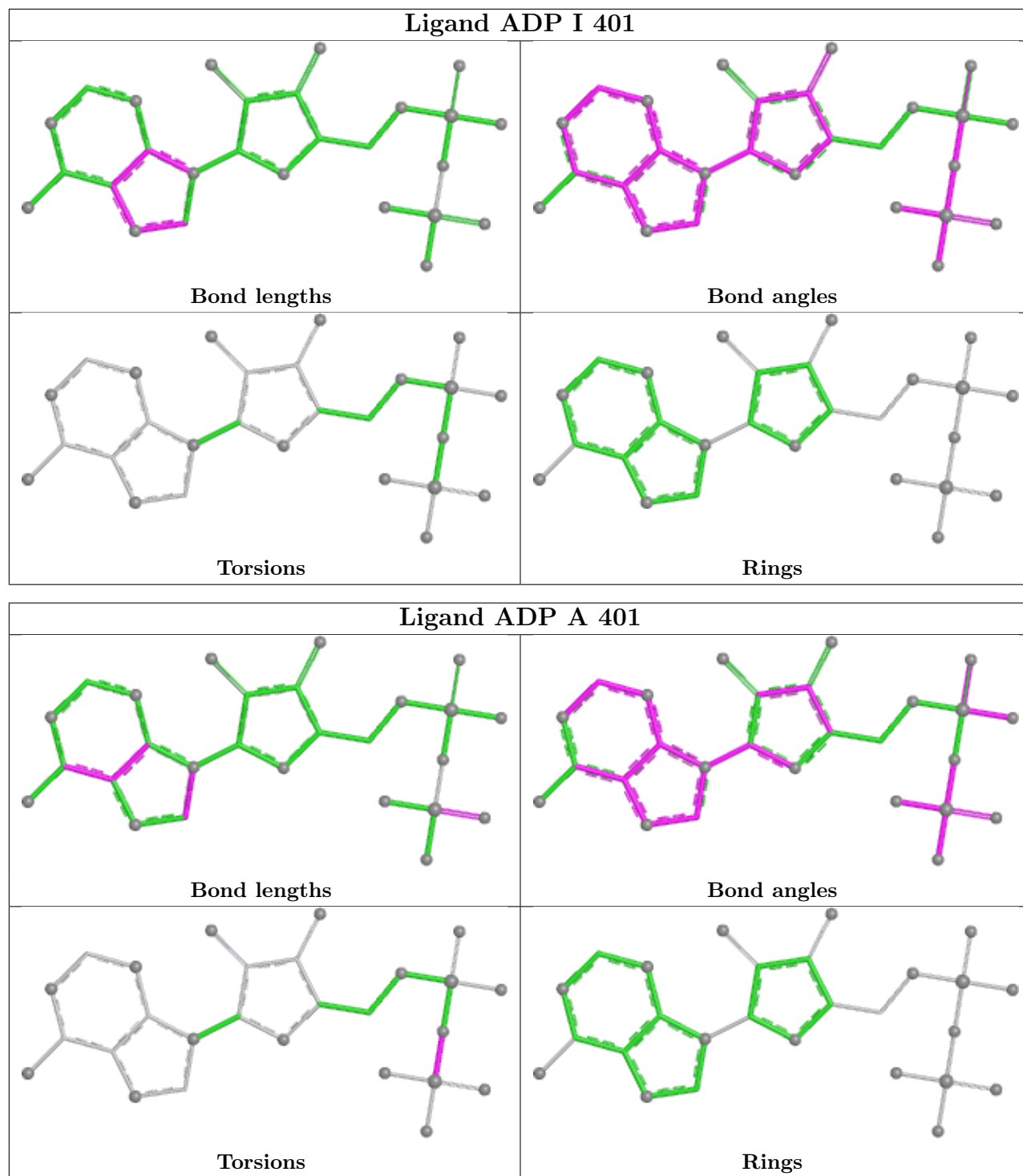
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	ADP	2	0
3	F	401	ADP	5	0
3	I	401	ADP	3	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	359/377 (95%)	-0.47	0 100 100	17, 50, 88, 129	3 (0%)
1	D	360/377 (95%)	-0.64	3 (0%) 82 84	11, 42, 89, 123	1 (0%)
1	F	365/377 (96%)	0.57	19 (5%) 33 36	60, 87, 138, 199	0
1	I	360/377 (95%)	0.75	19 (5%) 32 36	44, 90, 139, 180	1 (0%)
2	B	165/186 (88%)	-0.54	1 (0%) 85 87	19, 41, 111, 147	0
2	E	125/186 (67%)	-0.85	0 100 100	16, 32, 59, 106	0
2	G	143/186 (76%)	0.78	11 (7%) 19 22	62, 84, 121, 180	0
2	J	126/186 (67%)	0.96	13 (10%) 12 13	52, 87, 119, 159	1 (0%)
All	All	2003/2252 (88%)	0.06	66 (3%) 49 53	11, 74, 121, 199	6 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	365	ALA	4.3
2	J	108	LEU	3.7
1	I	375	PHE	3.6
1	I	327	ILE	3.4
1	I	230	ALA	3.3
1	I	131	ALA	3.3
1	I	164	PRO	3.3
1	F	30	VAL	3.2
2	G	117	GLY	3.2
2	G	97	ILE	3.1
2	J	53	VAL	3.1
1	F	375	PHE	3.1
2	J	96	VAL	3.1
1	F	8	LEU	3.0
2	J	152	PHE	3.0
1	I	91	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	86	TRP	2.9
1	I	158	GLY	2.9
1	I	126	THR	2.8
2	G	85	LEU	2.8
1	I	69	TYR	2.8
1	F	58	ALA	2.8
1	F	152	VAL	2.8
2	G	103	LEU	2.7
2	J	90	PHE	2.7
2	B	1071	LEU	2.7
1	I	127	PHE	2.7
2	J	89	PHE	2.7
1	F	159	VAL	2.6
1	D	203	THR	2.6
2	J	115	TRP	2.6
1	F	17	VAL	2.5
1	F	209	VAL	2.5
1	I	304	THR	2.5
2	G	173	ALA	2.5
1	F	9	VAL	2.4
1	F	248	ILE	2.4
1	I	248	ILE	2.4
2	G	55	GLU	2.4
1	I	19	ALA	2.4
2	J	120	CYS	2.3
2	J	103	LEU	2.3
1	F	219	VAL	2.3
1	F	88	HIS	2.2
1	I	122	ILE	2.2
2	G	136	ASP	2.2
2	J	76	PHE	2.2
1	F	251	GLY	2.2
2	G	98	LEU	2.2
1	I	260	THR	2.2
1	F	138	ALA	2.2
1	F	10	CYS	2.2
2	J	52	MET	2.2
2	G	165	LEU	2.1
1	F	184	ASP	2.1
2	J	164	GLY	2.1
1	D	52	SER	2.1
1	I	324	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	21	PHE	2.1
1	D	231	ALA	2.1
1	I	200	PHE	2.1
2	J	155	ALA	2.1
2	G	52	MET	2.0
2	G	1068	LEU	2.0
1	F	53	TYR	2.0
1	F	91	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	I	401	27/27	0.98	0.06	35,48,59,62	0
4	CA	D	402	1/1	0.98	0.06	64,64,64,64	0
4	CA	F	402	1/1	0.98	0.10	91,91,91,91	0
4	CA	I	402	1/1	0.98	0.07	81,81,81,81	0
4	CA	I	403	1/1	0.98	0.11	67,67,67,67	0
4	CA	A	403	1/1	0.99	0.05	40,40,40,40	0
4	CA	B	1201	1/1	0.99	0.03	26,26,26,26	0
3	ADP	D	401	27/27	0.99	0.04	16,30,40,42	0
4	CA	D	403	1/1	0.99	0.04	63,63,63,63	0
4	CA	E	1201	1/1	0.99	0.05	24,24,24,24	0
3	ADP	F	401	27/27	0.99	0.06	38,57,69,74	0
4	CA	F	403	1/1	0.99	0.12	55,55,55,55	0
4	CA	G	1201	1/1	0.99	0.10	56,56,56,56	0
3	ADP	A	401	27/27	0.99	0.04	18,41,55,57	0
4	CA	A	402	1/1	0.99	0.05	63,63,63,63	0

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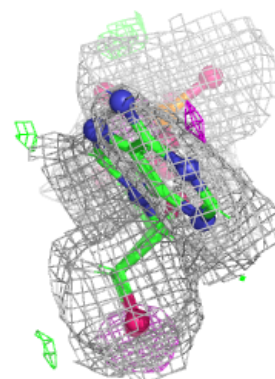
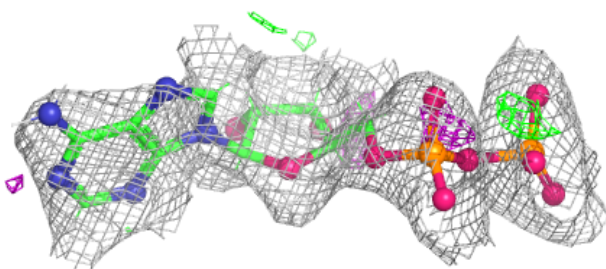
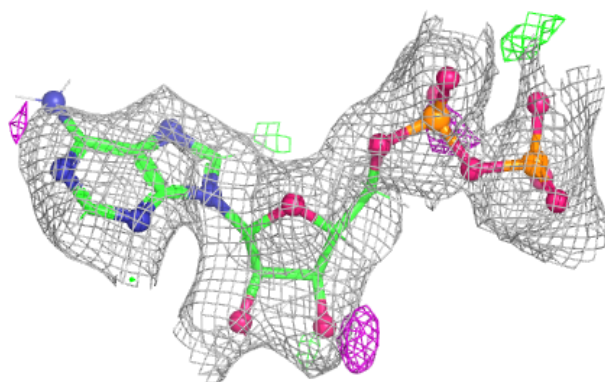
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	J	1201	1/1	0.99	0.07	60,60,60,60	0

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

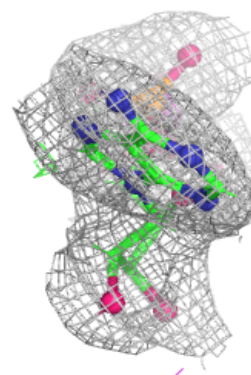
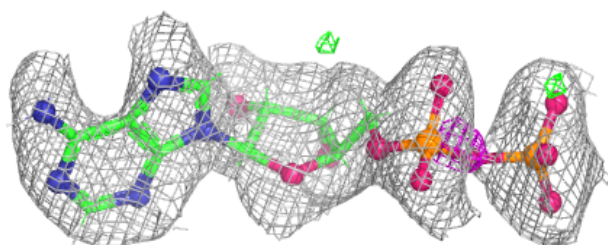
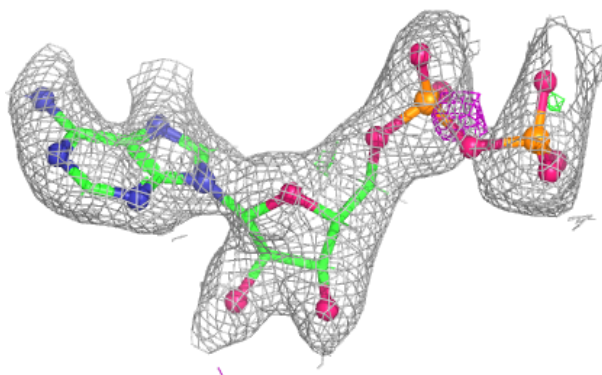
Electron density around ADP I 401:

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

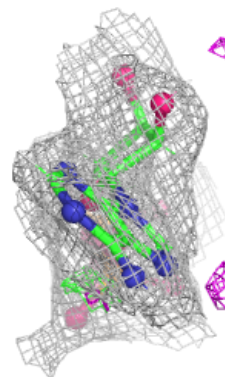
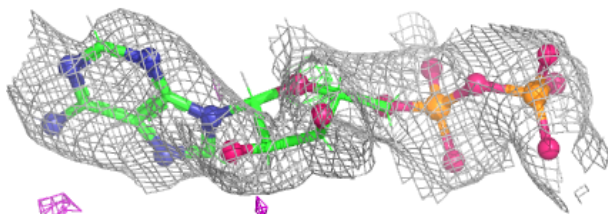
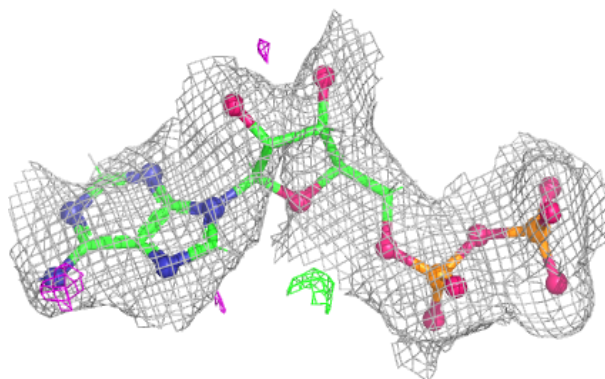


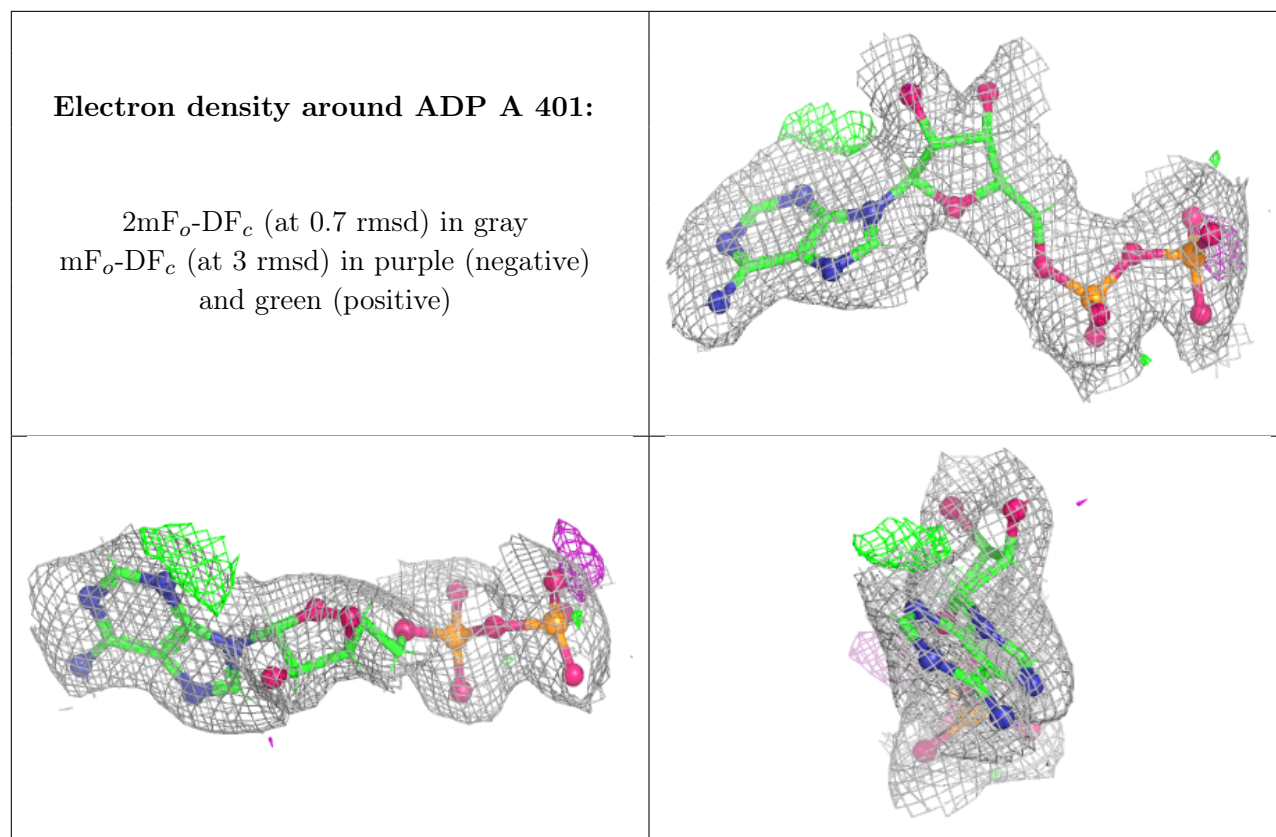
Electron density around ADP D 401:

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

**Electron density around ADP F 401:**

$2mF_o-DF_c$ (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.