



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:17 PM UTC

PDB ID : 1COW / pdb_00001cow
Title : BOVINE MITOCHONDRIAL F1-ATPASE COMPLEXED WITH AU-ROVERTIN B
Authors : van Raaij, M.J.; Abrahams, J.P.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 1996-05-08
Resolution : 3.10 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

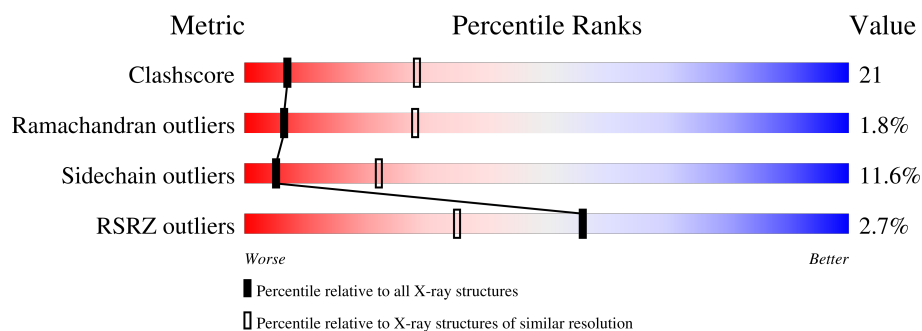
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	272	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23462 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 BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	conflict	UNP P19483
B	481	GLY	SER	conflict	UNP P19483
C	481	GLY	SER	conflict	UNP P19483

- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

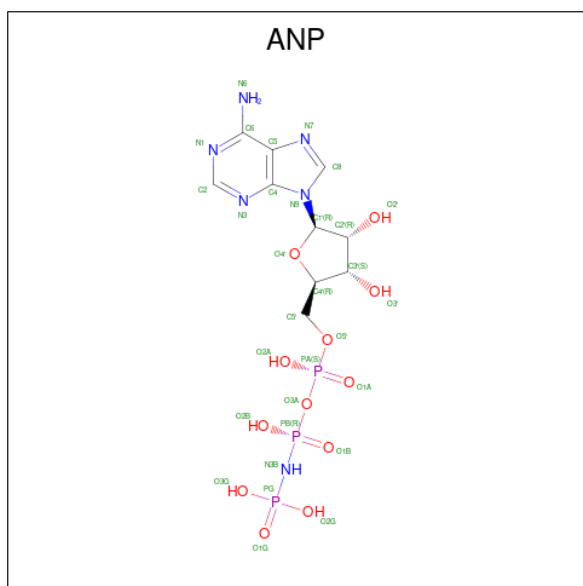
- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	122	Total	C	N	O	S	0	0	0
			945	591	171	176	7			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

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



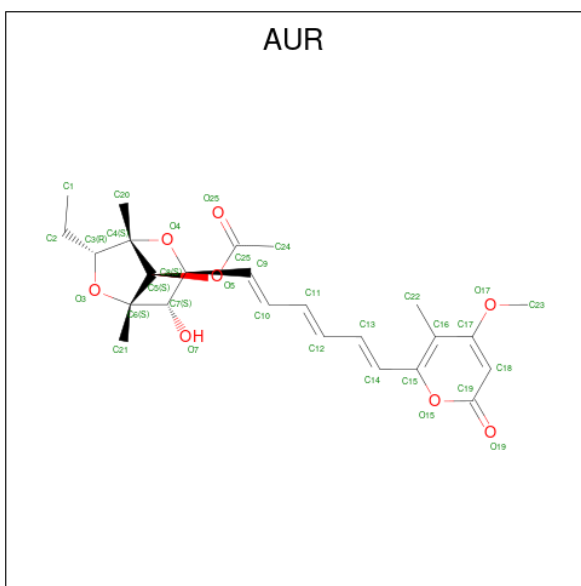
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 10 6 12 3	0	0
5	B	1	Total C N O P 31 10 6 12 3	0	0
5	C	1	Total C N O P 31 10 6 12 3	0	0
5	F	1	Total C N O P 31 10 6 12 3	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is AUROVERTIN B (CCD ID: AUR) (formula: $\text{C}_{25}\text{H}_{32}\text{O}_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total C O 33 25 8	0	0
7	F	1	Total C O 33 25 8	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	80	Total 80	O 80	0	0
8	B	84	Total 84	O 84	0	0
8	C	98	Total 98	O 98	0	0
8	D	94	Total 94	O 94	0	0
8	E	47	Total 47	O 47	0	0
8	F	92	Total 92	O 92	0	0
8	G	23	Total 23	O 23	0	0

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.

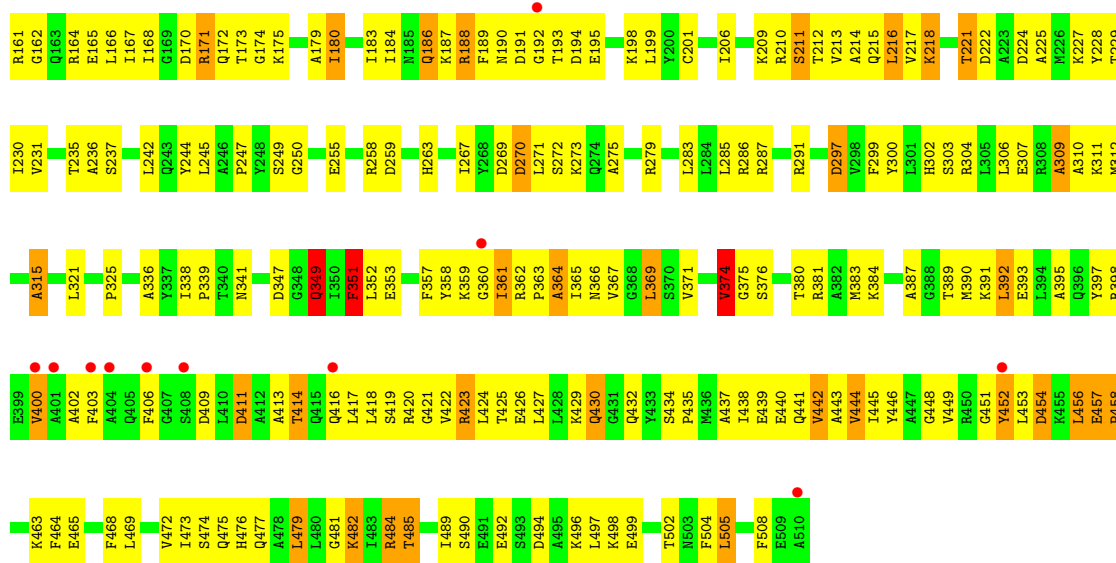
Chain A:

Amino Acid	Count
F464	1
F468	1
H471	1
V472	1
I473	1
S474	1
K475	1
H476	1
L473	1
L480	1
G481	1
K482	1
I483	1
R484	1
T485	1
D486	1
K487	1
K488	1
I489	1
S493	1
D494	1
A495	1
K496	1
L497	1
K498	1
F499	1
I500	1
V501	1
F508	1
E509	1
A510	1
K395	1
Q396	1
Y397	1
R398	1
E399	1
V400	1
A401	1
A402	1
F403	1
Q404	1
Q405	1
F406	1
Q407	1
S408	1
D409	1
L410	1
D411	1
A412	1
A413	1
T414	1
Q415	1
Q416	1
L417	1
L418	1
S419	1
R420	1
R423	1
L427	1
L428	1
K429	1
Q430	1
Q431	1
Q432	1
M436	1
A437	1
L438	1
E439	1
E440	1
Q441	1
V442	1
A443	1
V444	1
I445	1
V449	1
K450	1
Y452	1
L453	1
L454	1
K455	1
L456	1
E457	1
K460	1
I461	1
K312	1
N313	1
F316	1
G317	1
G318	1
G319	1
L324	1
P325	1
V326	1
D333	1
V334	1
Y337	1
T340	1
N341	1
V342	1
I343	1
S344	1
I345	1
L346	1
D347	1
G348	1
Q349	1
L352	1
E353	1
G360	1
I361	1
R362	1
P363	1
A364	1
L365	1
N366	1
V367	1
V371	1
S372	1
R373	1
S376	1
A377	1
Q378	1
A379	1
T380	1
M383	1
K384	1
Q385	1
V386	1
G451	1
Y452	1
L453	1
L454	1
K455	1
L456	1
E457	1
K460	1
I461	1
K218	1
R219	1
D222	1
V142	1
R143	1
D224	1
P144	1
A225	1
M226	1
L230	1
S233	1
A240	1
P241	1
Y244	1
L245	1
A246	1
P247	1
Q248	1
S249	1
M253	1
Y256	1
F257	1
R258	1
T267	1
Y268	1
D269	1
D270	1
K273	1
Q274	1
L283	1
L284	1
N185	1
L285	1
R286	1
R287	1
P288	1
T289	1
G290	1
R291	1
E292	1
A293	1
R294	1
D297	1
V298	1
K299	1
V304	1
M383	1
K384	1
Q385	1
V386	1
G451	1
Y452	1
L453	1
L454	1
K455	1
L456	1
E457	1
K460	1
I461	1
K139	1
I140	1
V142	1
R143	1
D224	1
P144	1
A225	1
M226	1
L230	1
S233	1
A240	1
P241	1
Y244	1
L245	1
A246	1
P247	1
Q248	1
S249	1
M253	1
Y256	1
F257	1
R258	1
T267	1
Y268	

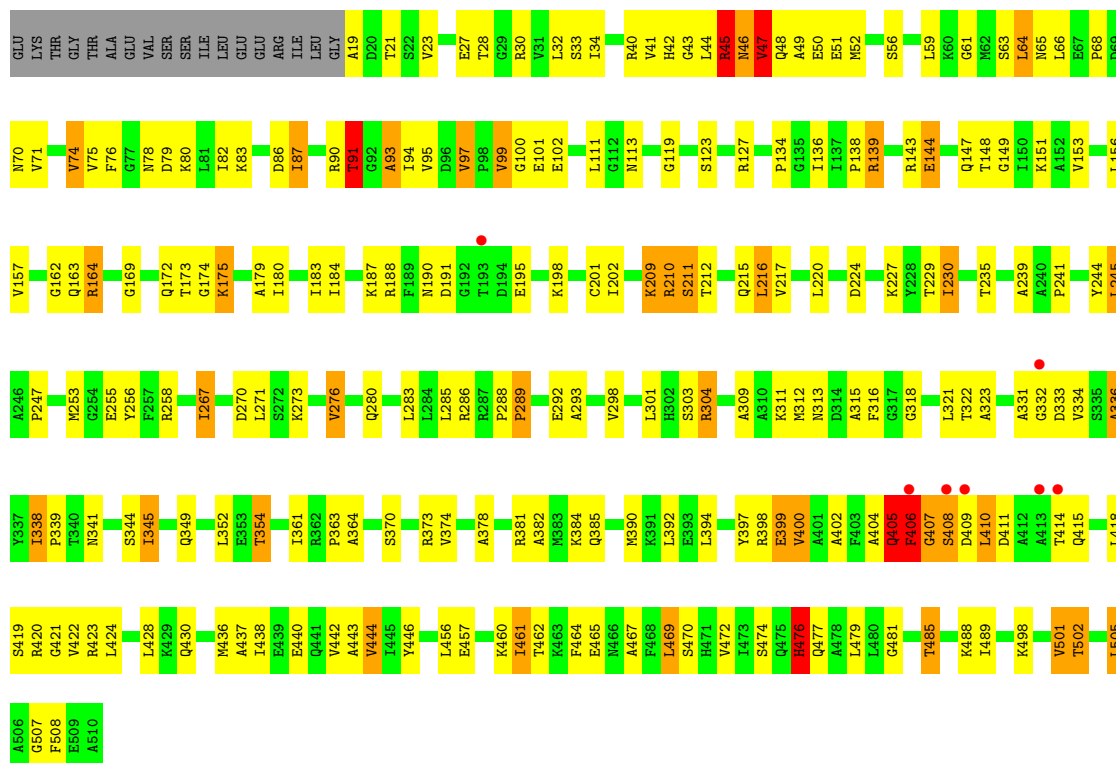
Chain B:

2% 43% 43% 9% 5%

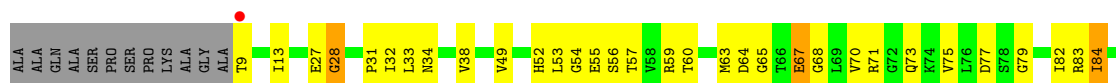
V73 F76 G77 N78 D79 K80 L81 D86 I87 R90 T91 I94 V95 D96 V97 P98 V99 E102 L103 V107 I115 D116 G117 K118 G119 G122 S123 R127 R128 P134 G135 I136 I137 P138 R139 E140 I140 S141 V142 R143 E144 P145 M146 Q147 K151 L156 V157 P158

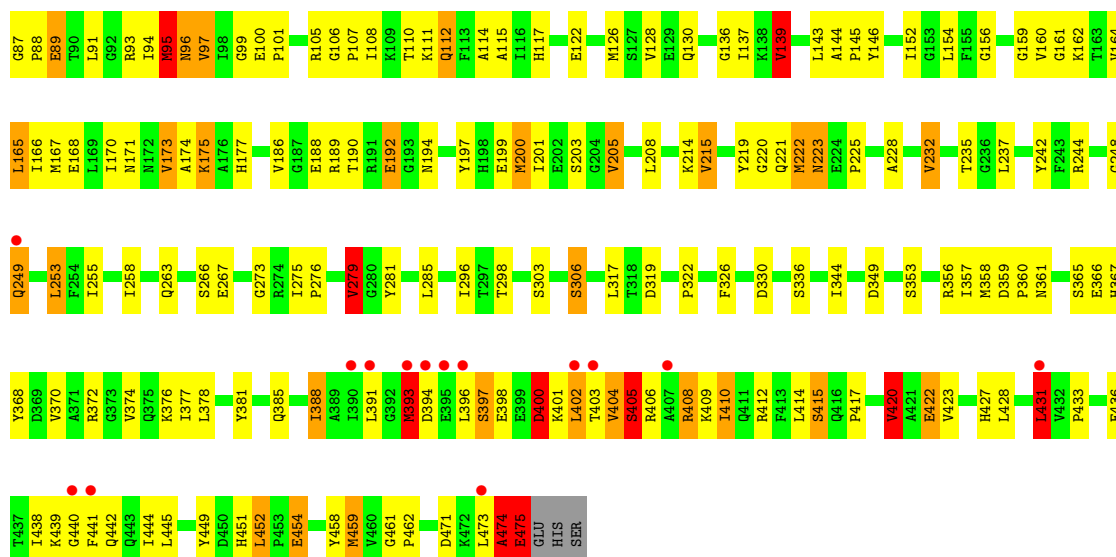


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

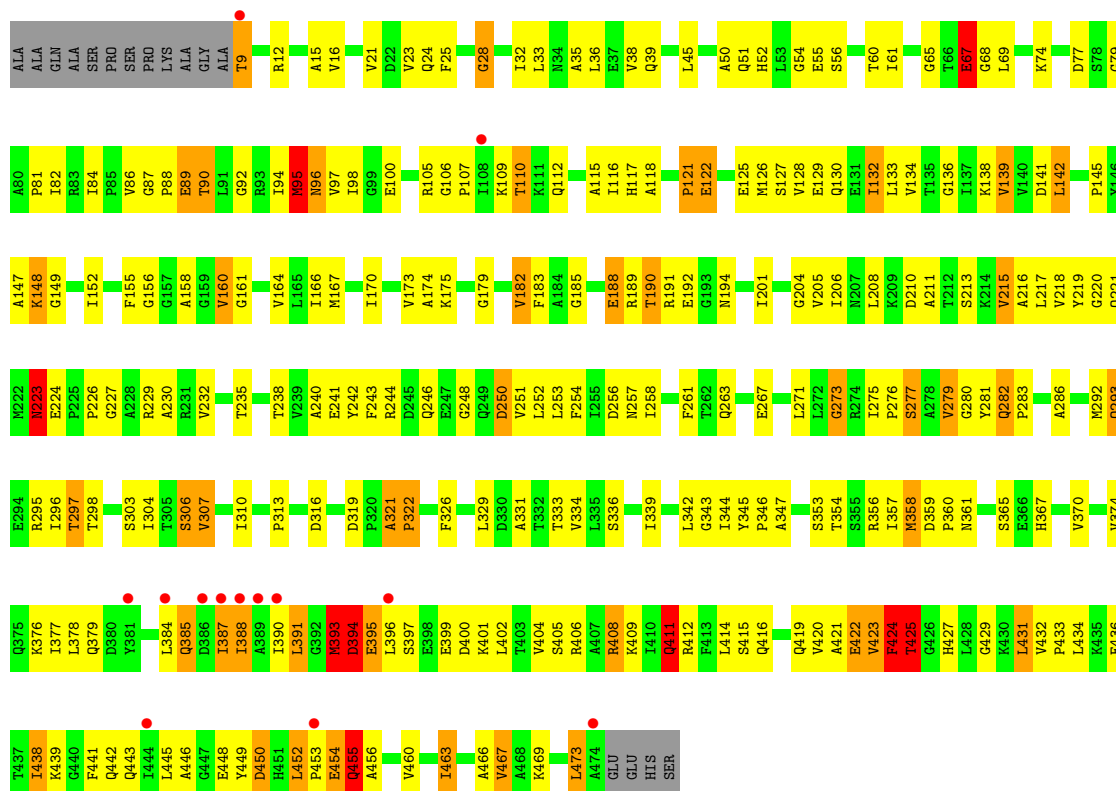


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

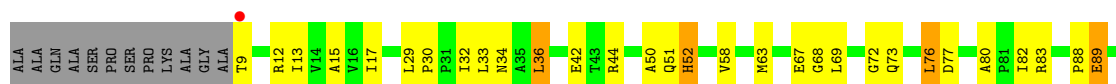




• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	283.40Å 107.60Å 140.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.10) 99.0 (20.00-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.44 (at 3.09Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , 0.280 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23462	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: AUR, ADP, MG, 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	1.18	5/3766 (0.1%)	1.66	50/5080 (1.0%)
1	B	1.22	6/3766 (0.2%)	1.68	57/5080 (1.1%)
1	C	1.22	2/3799 (0.1%)	1.67	56/5126 (1.1%)
2	D	1.20	2/3596 (0.1%)	1.62	50/4879 (1.0%)
2	E	1.18	4/3587 (0.1%)	1.64	38/4867 (0.8%)
2	F	1.23	1/3587 (0.0%)	1.66	52/4867 (1.1%)
3	G	1.21	3/949 (0.3%)	1.61	17/1266 (1.3%)
All	All	1.21	23/23050 (0.1%)	1.65	320/31165 (1.0%)

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	B	0	2
1	C	0	2
2	D	0	1
2	E	0	2
3	G	1	3
All	All	1	11

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	367	HIS	CD2-NE2	-8.50	1.28	1.37
1	B	214	ALA	CA-C	-7.96	1.42	1.52
1	A	211	SER	CA-C	-6.75	1.44	1.52
2	D	417	PRO	CA-C	-6.49	1.46	1.52
3	G	22	SER	CA-CB	-6.46	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	353	SER	CA-C	-6.44	1.45	1.52
1	B	156	LEU	CA-C	-6.15	1.44	1.52
3	G	250	PHE	N-CA	-6.13	1.38	1.46
1	B	315	ALA	CA-C	-5.99	1.44	1.52
1	C	41	VAL	CA-CB	-5.88	1.47	1.54
3	G	40	PRO	N-CD	5.80	1.55	1.47
1	B	484	ARG	CD-NE	-5.68	1.38	1.46
1	A	47	VAL	CA-CB	-5.67	1.48	1.54
1	A	471	HIS	CE1-NE2	-5.54	1.27	1.32
2	F	344	ILE	CA-CB	-5.48	1.47	1.54
1	C	409	ASP	N-CA	5.41	1.53	1.46
1	A	212	THR	C-N	-5.33	1.27	1.33
2	E	174	ALA	CA-CB	-5.30	1.45	1.53
2	E	50	ALA	CA-C	-5.27	1.45	1.52
1	B	218	LYS	C-N	-5.22	1.27	1.33
1	A	304	ARG	CD-NE	-5.07	1.39	1.46
2	E	321	ALA	C-O	-5.03	1.20	1.24
1	B	409	ASP	CG-OD2	5.02	1.34	1.25

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	408	ARG	CD-NE-CZ	11.21	140.09	124.40
1	C	405	GLN	CA-C-N	10.81	136.46	121.33
1	C	405	GLN	C-N-CA	10.81	136.46	121.33
2	E	425	THR	N-CA-C	-10.30	100.33	113.72
2	F	139	VAL	CB-CA-C	-9.42	99.83	111.88
1	B	351	PHE	CA-CB-CG	8.83	122.63	113.80
2	F	282	GLN	CB-CG-CD	8.65	127.31	112.60
1	A	270	ASP	CA-CB-CG	8.64	121.24	112.60
1	A	78	ASN	CA-CB-CG	8.55	121.15	112.60
1	A	123	SER	N-CA-C	8.44	121.30	109.15
2	E	307	VAL	N-CA-CB	8.42	121.94	111.41
1	B	96	ASP	CA-CB-CG	8.39	120.99	112.60
1	B	270	ASP	CB-CA-C	-8.32	94.29	110.10
1	B	71	VAL	CA-C-N	-8.27	113.69	121.62
1	B	71	VAL	C-N-CA	-8.27	113.69	121.62
1	C	42	HIS	N-CA-C	8.24	123.70	112.90
2	F	221	GLN	N-CA-C	8.18	121.64	110.35
3	G	2	THR	N-CA-CB	8.15	124.26	110.49
2	D	408	ARG	NE-CZ-NH2	-8.08	111.93	119.20
1	B	210	ARG	N-CA-CB	8.02	121.64	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	209	LEU	CA-C-N	8.01	133.52	120.63
3	G	209	LEU	C-N-CA	8.01	133.52	120.63
1	B	375	GLY	N-CA-C	7.92	123.38	114.67
2	F	96	ASN	CB-CA-C	-7.89	94.07	110.40
2	D	475	GLU	N-CA-CB	7.82	123.79	110.50
1	B	475	GLN	N-CA-C	7.77	119.53	111.14
2	D	474	ALA	CA-C-N	7.74	135.63	121.70
2	D	474	ALA	C-N-CA	7.74	135.63	121.70
2	D	400	ASP	CA-CB-CG	7.71	120.31	112.60
1	B	192	GLY	O-C-N	7.63	130.13	122.88
2	D	221	GLN	N-CA-C	7.59	120.13	110.33
1	C	501	VAL	N-CA-CB	7.56	118.86	110.62
2	D	459	MET	CG-SD-CE	-7.50	84.41	100.90
2	F	225	PRO	O-C-N	7.46	124.66	121.15
1	A	170	ASP	CA-CB-CG	7.33	119.93	112.60
1	B	245	LEU	N-CA-C	7.32	119.25	111.28
1	B	270	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	508	PHE	N-CA-C	7.29	119.86	111.11
2	F	427	HIS	CA-CB-CG	7.26	121.06	113.80
2	F	97	VAL	CB-CA-C	-7.25	102.35	112.14
1	A	432	GLN	N-CA-CB	-7.25	100.08	110.44
1	B	24	ASP	CA-C-N	7.22	135.33	121.54
1	B	24	ASP	C-N-CA	7.22	135.33	121.54
2	D	393	MET	N-CA-C	7.18	122.34	113.50
1	A	245	LEU	N-CA-C	7.10	119.02	111.28
1	B	309	ALA	N-CA-C	-7.08	100.51	110.50
2	D	97	VAL	CB-CA-C	-6.99	102.58	112.22
3	G	22	SER	CA-CB-OG	6.96	125.01	111.10
3	G	211	ASN	CA-C-O	6.95	127.81	119.61
2	D	143	LEU	N-CA-C	6.92	121.86	113.41
1	A	149	GLY	N-CA-C	-6.92	105.51	115.27
2	F	96	ASN	N-CA-CB	-6.91	100.56	110.44
1	A	224	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	53	VAL	N-CA-CB	-6.89	102.87	112.52
2	E	219	TYR	N-CA-C	6.82	120.02	108.90
1	A	245	LEU	CB-CA-C	-6.80	99.50	110.79
2	E	250	ASP	CA-CB-CG	-6.78	105.82	112.60
1	A	74	VAL	N-CA-CB	-6.77	103.95	111.66
1	A	157	VAL	CA-CB-CG2	6.75	121.88	110.40
2	E	408	ARG	CD-NE-CZ	6.73	133.83	124.40
2	F	110	THR	CA-CB-CG2	6.73	121.94	110.50
1	B	409	ASP	CA-CB-CG	6.72	119.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	129	GLU	N-CA-C	6.72	119.65	109.23
1	C	476	HIS	N-CA-C	6.72	125.12	110.80
2	F	312	VAL	CA-C-N	6.72	127.08	119.83
2	F	312	VAL	C-N-CA	6.72	127.08	119.83
2	E	96	ASN	CA-CB-CG	6.71	119.31	112.60
1	B	403	PHE	N-CA-C	-6.71	104.04	111.36
1	C	345	ILE	N-CA-C	-6.70	106.49	112.12
1	A	24	ASP	CA-CB-CG	6.70	119.30	112.60
2	F	80	ALA	N-CA-CB	-6.64	98.56	110.37
1	A	476	HIS	N-CA-C	6.63	121.27	112.25
2	D	139	VAL	CB-CA-C	-6.62	103.22	111.70
1	C	164	ARG	CD-NE-CZ	-6.62	115.13	124.40
2	F	143	LEU	N-CA-C	6.62	121.57	112.90
1	A	270	ASP	CB-CA-C	-6.58	97.60	110.10
2	F	385	GLN	N-CA-C	6.58	120.17	111.75
1	C	476	HIS	CA-CB-CG	-6.53	107.27	113.80
3	G	266	ILE	CB-CG1-CD1	-6.51	100.12	113.80
2	D	408	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	A	269	ASP	CA-C-N	6.49	133.38	121.70
1	A	269	ASP	C-N-CA	6.49	133.38	121.70
3	G	15	ASN	CA-CB-CG	-6.46	106.14	112.60
2	F	275	ILE	N-CA-C	-6.45	103.02	109.02
1	A	95	VAL	N-CA-C	6.42	117.60	108.93
1	A	392	LEU	N-CA-C	6.42	118.36	111.36
2	D	454	GLU	CB-CA-C	-6.42	100.71	110.92
1	C	65	ASN	CA-C-N	-6.34	114.04	122.85
1	C	65	ASN	C-N-CA	-6.34	114.04	122.85
1	C	74	VAL	N-CA-CB	-6.29	103.67	110.53
2	D	402	LEU	N-CA-C	-6.28	105.75	113.41
1	C	304	ARG	N-CA-CB	-6.27	99.90	110.49
1	C	93	ALA	N-CA-C	6.26	119.14	109.07
2	F	256	ASP	CA-CB-CG	6.26	118.86	112.60
1	C	235	THR	N-CA-C	6.25	118.60	110.53
1	C	42	HIS	CA-C-N	-6.24	114.59	123.95
1	C	42	HIS	C-N-CA	-6.24	114.59	123.95
1	A	230	ILE	CB-CA-C	-6.23	101.41	110.63
1	C	149	GLY	N-CA-C	-6.22	106.04	115.00
2	E	306	SER	N-CA-C	6.22	119.09	109.07
2	D	349	ASP	CA-C-N	6.22	125.91	119.56
2	D	349	ASP	C-N-CA	6.22	125.91	119.56
1	A	143	ARG	NE-CZ-NH2	-6.21	113.61	119.20
2	E	394	ASP	N-CA-C	6.21	123.40	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	406	PHE	CA-CB-CG	6.21	120.01	113.80
1	A	25	LEU	N-CA-C	6.21	124.02	110.80
2	F	201	ILE	CA-C-N	6.19	128.90	120.54
2	F	201	ILE	C-N-CA	6.19	128.90	120.54
2	E	336	SER	N-CA-C	6.18	118.48	108.41
1	B	402	ALA	N-CA-C	6.17	118.00	110.41
2	F	461	GLY	CA-C-N	6.17	126.52	119.92
2	F	461	GLY	C-N-CA	6.17	126.52	119.92
1	C	276	VAL	N-CA-CB	6.13	118.88	110.54
1	B	158	PRO	N-CD-CG	6.12	112.38	103.20
2	D	175	LYS	N-CA-C	6.12	118.74	111.33
1	A	91	THR	N-CA-C	-6.11	105.99	113.50
2	F	259	PHE	N-CA-C	-6.09	104.72	111.36
1	A	75	VAL	N-CA-C	6.09	116.88	108.84
1	C	46	ASN	CA-CB-CG	6.08	118.68	112.60
1	B	259	ASP	CA-CB-CG	-6.08	106.52	112.60
1	C	230	ILE	CB-CA-C	-6.05	101.61	110.62
2	D	84	ILE	N-CA-C	6.04	114.55	107.84
2	E	106	GLY	CA-C-N	6.04	125.98	119.76
2	E	106	GLY	C-N-CA	6.04	125.98	119.76
2	D	95	MET	CA-C-N	6.03	133.43	122.02
2	D	95	MET	C-N-CA	6.03	133.43	122.02
1	B	299	PHE	N-CA-C	-6.02	104.80	111.36
1	B	374	VAL	N-CA-C	5.95	119.47	113.47
1	B	94	ILE	CA-C-O	-5.94	114.82	121.36
3	G	209	LEU	N-CA-CB	5.94	120.60	110.50
2	E	321	ALA	N-CA-CB	5.94	118.66	110.11
1	B	195	GLU	CA-C-O	5.93	126.79	119.97
2	E	431	LEU	CB-CA-C	5.93	120.79	111.72
1	C	75	VAL	N-CA-C	5.92	116.38	107.80
1	A	371	VAL	CB-CA-C	-5.89	100.34	110.30
2	F	417	PRO	CB-CA-C	-5.88	104.23	111.11
2	F	387	ILE	CB-CA-C	-5.87	104.33	112.02
2	F	394	ASP	CA-CB-CG	-5.86	106.74	112.60
1	C	191	ASP	CA-CB-CG	-5.86	106.75	112.60
1	B	362	ARG	CA-C-O	-5.85	114.24	119.86
1	C	472	VAL	N-CA-C	5.85	117.29	110.62
1	A	162	GLY	N-CA-C	-5.84	107.01	114.37
1	B	25	LEU	N-CA-C	5.84	123.24	110.80
1	C	113	ASN	CA-CB-CG	-5.83	106.77	112.60
2	D	404	VAL	N-CA-C	-5.83	104.83	110.72
2	E	110	THR	CA-CB-CG2	5.81	120.38	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	ILE	N-CA-CB	5.81	118.00	111.21
1	B	137	ILE	N-CA-C	5.80	119.92	112.67
1	B	349	GLN	N-CA-CB	5.79	121.33	111.66
1	A	452	TYR	N-CA-C	5.79	118.33	111.33
2	F	225	PRO	N-CA-CB	5.77	106.22	103.22
2	F	381	TYR	N-CA-C	-5.75	104.21	111.11
1	C	149	GLY	CA-C-O	5.73	125.33	118.97
2	D	420	VAL	N-CA-CB	-5.72	104.87	112.26
2	D	249	GLN	N-CA-C	5.70	118.22	110.35
1	A	285	LEU	CA-C-O	5.69	126.16	119.28
1	B	164	ARG	N-CA-C	-5.67	99.16	108.41
1	B	374	VAL	CB-CA-C	-5.66	104.51	110.62
2	E	94	ILE	N-CA-CB	5.65	118.94	111.25
3	G	32	ALA	N-CA-C	-5.64	104.77	111.03
2	E	96	ASN	N-CA-CB	-5.61	101.01	110.49
2	E	277	SER	N-CA-CB	5.61	119.03	109.10
2	F	330	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	479	LEU	N-CA-C	-5.58	105.11	111.14
1	B	119	GLY	CA-C-N	5.58	126.82	119.84
1	B	119	GLY	C-N-CA	5.58	126.82	119.84
1	C	45	ARG	N-CA-C	5.57	118.12	111.71
2	E	273	GLY	CA-C-N	-5.57	114.35	122.65
2	E	273	GLY	C-N-CA	-5.57	114.35	122.65
1	B	353	GLU	CB-CA-C	-5.56	100.11	109.72
1	C	47	VAL	CB-CA-C	-5.55	105.23	111.45
1	C	309	ALA	N-CA-C	-5.55	101.63	109.96
2	F	342	LEU	N-CA-C	-5.55	106.47	113.18
2	F	389	ALA	N-CA-C	5.54	118.25	111.82
1	B	297	ASP	N-CA-C	5.54	119.74	112.92
1	B	351	PHE	N-CA-CB	5.54	119.46	110.42
2	D	200	MET	CA-CB-CG	5.54	125.19	114.10
1	C	100	GLY	N-CA-C	5.54	117.69	112.04
2	F	279	VAL	CA-CB-CG2	5.54	119.81	110.40
2	D	215	VAL	CA-CB-CG1	-5.53	101.00	110.40
2	F	388	ILE	CB-CA-C	-5.53	103.98	112.05
2	F	52	HIS	ND1-CE1-NE2	5.52	113.92	108.40
1	C	43	GLY	O-C-N	5.51	124.94	121.85
1	A	47	VAL	N-CA-C	5.50	118.47	109.78
1	B	210	ARG	O-C-N	5.50	127.74	122.07
1	C	410	LEU	N-CA-C	5.50	118.51	109.76
3	G	40	PRO	CA-N-CD	-5.50	104.31	112.00
1	A	509	GLU	CA-C-N	5.49	131.58	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	GLU	C-N-CA	5.49	131.58	121.70
2	F	144	ALA	CA-C-N	5.48	125.49	119.90
2	F	144	ALA	C-N-CA	5.48	125.49	119.90
1	C	230	ILE	CA-C-N	-5.48	115.81	123.10
1	C	230	ILE	C-N-CA	-5.48	115.81	123.10
1	C	157	VAL	CA-C-N	5.48	125.49	119.90
1	C	157	VAL	C-N-CA	5.48	125.49	119.90
1	B	116	ASP	N-CA-C	-5.47	106.37	113.16
2	D	139	VAL	N-CA-CB	5.47	116.36	110.62
2	D	276	PRO	CB-CA-C	-5.46	103.82	110.98
1	B	151	LYS	N-CA-C	5.45	117.65	111.11
2	E	107	PRO	N-CA-C	5.45	119.64	111.14
2	E	95	MET	N-CA-C	5.44	117.66	109.23
1	A	299	PHE	N-CA-C	-5.43	105.26	111.07
2	D	160	VAL	N-CA-CB	5.42	118.17	112.21
3	G	250	PHE	CA-CB-CG	-5.42	108.38	113.80
2	E	395	GLU	CA-C-N	5.41	128.79	121.05
2	E	395	GLU	C-N-CA	5.41	128.79	121.05
1	B	297	ASP	CA-CB-CG	-5.41	107.19	112.60
2	D	139	VAL	N-CA-C	5.40	115.85	110.23
2	D	96	ASN	CA-CB-CG	-5.40	107.20	112.60
1	B	194	ASP	N-CA-C	5.40	119.03	109.96
2	E	422	GLU	N-CA-C	-5.40	107.24	113.88
1	C	138	PRO	N-CA-CB	5.38	108.57	103.19
1	C	370	SER	O-C-N	-5.37	117.04	123.06
1	C	354	THR	OG1-CB-CG2	-5.37	98.56	109.30
3	G	237	LYS	CB-CA-C	5.37	120.98	110.67
1	C	28	THR	CA-CB-CG2	5.37	119.62	110.50
1	A	34	ILE	CB-CG1-CD1	5.36	125.06	113.80
1	A	400	VAL	N-CA-C	5.36	119.91	112.35
1	C	119	GLY	CA-C-N	5.36	125.33	120.03
1	C	119	GLY	C-N-CA	5.36	125.33	120.03
2	D	96	ASN	CB-CA-C	-5.35	100.00	111.78
2	E	87	GLY	CA-C-N	5.34	124.98	119.05
2	E	87	GLY	C-N-CA	5.34	124.98	119.05
2	D	394	ASP	N-CA-C	5.34	117.52	111.11
2	E	424	PHE	N-CA-CB	5.33	119.50	110.49
2	D	222	MET	CB-CA-C	-5.33	98.55	110.21
2	F	370	VAL	N-CA-C	-5.32	105.35	110.72
1	A	431	GLY	N-CA-C	-5.32	104.29	112.85
2	F	353	SER	O-C-N	-5.31	117.00	123.16
1	C	289	PRO	CB-CA-C	-5.31	104.03	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	THR	CA-CB-CG2	5.30	119.52	110.50
1	A	92	GLY	N-CA-C	-5.30	108.69	115.42
2	D	215	VAL	CB-CA-C	-5.29	102.62	111.29
3	G	258	ILE	CB-CA-C	-5.27	105.02	112.14
1	B	103	LEU	N-CA-C	-5.27	107.02	113.50
1	C	210	ARG	N-CA-C	5.27	117.71	111.33
2	D	253	LEU	CA-C-N	-5.26	115.57	122.99
2	D	253	LEU	C-N-CA	-5.26	115.57	122.99
2	F	113	PHE	CA-CB-CG	-5.25	108.55	113.80
2	F	282	GLN	CA-CB-CG	-5.24	103.62	114.10
1	C	336	ALA	N-CA-C	5.24	117.68	110.35
2	E	354	THR	CA-CB-CG2	5.23	119.39	110.50
2	E	223	ASN	CB-CA-C	-5.23	99.07	109.99
1	A	475	GLN	CG-CD-NE2	-5.22	108.56	116.40
2	D	84	ILE	N-CA-CB	-5.22	108.23	111.83
3	G	221	THR	N-CA-CB	5.21	118.07	110.47
1	B	194	ASP	N-CA-CB	-5.20	101.81	110.23
2	D	431	LEU	CD1-CG-CD2	-5.20	99.37	110.80
3	G	12	SER	N-CA-C	5.20	117.02	111.36
1	C	415	GLN	N-CA-C	-5.19	105.69	112.23
2	E	51	GLN	CB-CG-CD	5.18	121.41	112.60
2	E	160	VAL	N-CA-C	-5.17	102.06	108.89
2	D	192	GLU	N-CA-C	5.17	116.92	111.28
3	G	211	ASN	N-CA-CB	-5.17	100.87	110.18
1	A	371	VAL	CA-CB-CG2	5.17	119.19	110.40
2	D	431	LEU	CB-CA-C	5.17	118.66	109.72
2	F	204	GLY	CA-C-N	-5.17	112.17	120.64
2	F	204	GLY	C-N-CA	-5.17	112.17	120.64
1	B	349	GLN	CA-CB-CG	5.16	124.43	114.10
1	C	245	LEU	CB-CA-C	-5.16	102.22	110.79
2	E	90	THR	N-CA-C	-5.15	107.12	113.41
2	F	354	THR	CA-CB-CG2	5.15	119.26	110.50
1	A	367	VAL	N-CA-C	5.14	115.86	110.62
2	E	156	GLY	N-CA-C	-5.14	106.20	112.68
1	A	94	ILE	CB-CA-C	5.14	118.57	111.38
2	D	101	PRO	N-CA-CB	5.14	108.12	103.34
1	A	233	SER	N-CA-C	5.13	116.76	108.34
2	D	173	VAL	CB-CA-C	-5.13	102.88	111.29
1	C	507	GLY	N-CA-C	-5.12	106.58	112.83
1	B	306	LEU	N-CA-C	5.12	119.02	112.87
1	C	94	ILE	N-CA-C	-5.12	102.98	109.58
2	F	77	ASP	CA-CB-CG	5.11	117.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ILE	CA-C-O	-5.11	115.82	121.29
1	A	222	ASP	CA-C-N	-5.11	114.11	122.54
1	A	222	ASP	C-N-CA	-5.11	114.11	122.54
2	D	377	ILE	N-CA-C	5.11	115.83	110.62
2	F	76	LEU	N-CA-C	5.10	117.22	108.90
2	F	225	PRO	CA-C-N	5.10	126.22	119.84
2	F	225	PRO	C-N-CA	5.10	126.22	119.84
1	B	477	GLN	CA-C-N	5.10	127.12	120.28
1	B	477	GLN	C-N-CA	5.10	127.12	120.28
2	E	298	THR	CB-CA-C	-5.10	102.74	111.31
1	B	287	ARG	CB-CA-C	5.09	116.75	109.26
2	E	367	HIS	CG-CD2-NE2	5.09	112.29	107.20
2	D	144	ALA	CA-C-N	5.09	125.09	119.90
2	D	144	ALA	C-N-CA	5.09	125.09	119.90
1	B	299	PHE	CA-C-O	5.09	125.81	120.42
1	A	324	LEU	CA-C-O	5.08	124.41	119.99
2	F	95	MET	CA-C-N	5.08	132.32	121.45
2	F	95	MET	C-N-CA	5.08	132.32	121.45
1	B	192	GLY	CA-C-N	5.08	131.23	121.54
1	B	192	GLY	C-N-CA	5.08	131.23	121.54
2	D	219	TYR	N-CA-C	5.08	117.69	109.06
1	C	91	THR	N-CA-C	-5.07	108.13	114.56
1	A	167	ILE	CA-C-N	-5.06	115.42	122.71
1	A	167	ILE	C-N-CA	-5.06	115.42	122.71
2	F	344	ILE	CB-CG1-CD1	-5.06	103.17	113.80
1	C	288	PRO	N-CA-CB	5.06	107.98	103.08
1	B	361	ILE	N-CA-CB	5.05	117.73	111.41
2	D	422	GLU	N-CA-C	-5.05	105.96	111.82
1	B	79	ASP	CA-CB-CG	5.04	117.64	112.60
3	G	210	ALA	CA-C-O	5.04	125.56	119.61
1	B	457	GLU	N-CA-C	5.04	116.25	109.24
1	C	209	LYS	N-CA-CB	-5.04	102.66	110.57
1	C	285	LEU	CA-C-O	5.04	125.45	119.56
2	D	96	ASN	N-CA-CB	-5.03	102.79	110.49
1	C	323	ALA	N-CA-C	5.03	117.60	109.40
1	B	180	ILE	N-CA-C	5.03	115.18	110.30
2	E	322	PRO	N-CD-CG	5.03	110.74	103.20
2	F	206	ILE	CB-CG1-CD1	5.03	124.36	113.80
2	F	348	VAL	N-CA-C	5.03	115.58	109.30
2	F	261	PHE	CA-C-O	5.02	126.09	120.82
2	F	381	TYR	CD1-CG-CD2	-5.01	110.58	118.10
2	E	218	VAL	N-CA-CB	5.01	117.78	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	PHE	CA-CB-CG	-5.01	108.79	113.80
2	D	165	LEU	N-CA-CB	5.01	117.48	110.12
1	C	230	ILE	O-C-N	-5.00	117.78	123.18
1	A	230	ILE	CA-C-N	-5.00	116.30	123.11
1	A	230	ILE	C-N-CA	-5.00	116.30	123.11
1	C	444	VAL	N-CA-CB	5.00	117.34	110.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	209	LEU	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	PHE	Mainchain
1	B	369	LEU	Mainchain
1	B	432	GLN	Mainchain
1	C	363	PRO	Mainchain
1	C	405	GLN	Mainchain
2	D	431	LEU	Mainchain
2	E	346	PRO	Mainchain
2	E	411	GLN	Sidechain
3	G	17	GLN	Mainchain,Sidechain
3	G	250	PHE	Mainchain

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	3715	0	3815	169	0
1	B	3715	0	3814	174	0
1	C	3748	0	3845	146	0
2	D	3539	0	3593	153	0
2	E	3530	0	3587	192	0
2	F	3530	0	3587	146	0
3	G	945	0	1019	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	A	31	0	13	1	0
5	B	31	0	13	8	0
5	C	31	0	13	4	0
5	F	31	0	12	2	0
6	D	27	0	12	3	0
7	E	33	0	32	14	0
7	F	33	0	32	6	0
8	A	80	0	0	6	0
8	B	84	0	0	12	0
8	C	98	0	0	11	0
8	D	94	0	0	11	0
8	E	47	0	0	9	0
8	F	92	0	0	13	0
8	G	23	0	0	2	0
All	All	23462	0	23387	966	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (966) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.07	1.15
1:C:127:ARG:HH12	1:C:255:GLU:HB2	0.97	1.07
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.24	1.01
2:F:223:ASN:HD22	2:F:223:ASN:H	1.06	1.00
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.80	0.96
1:C:215:GLN:HG3	2:F:356:ARG:NH2	1.80	0.95
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.82	0.93
2:E:223:ASN:HD22	2:E:223:ASN:H	0.92	0.92
1:B:456:LEU:HD12	1:B:457:GLU:H	1.37	0.90
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.54	0.89
2:E:411:GLN:NE2	7:E:479:AUR:H5	1.86	0.89
1:B:172:GLN:HA	5:B:600:ANP:HNB1	1.37	0.88
2:D:223:ASN:H	2:D:223:ASN:HD22	1.21	0.85
2:E:223:ASN:HD22	2:E:223:ASN:N	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:93:ARG:HH11	2:F:93:ARG:HG2	1.40	0.84
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.61	0.82
2:E:223:ASN:H	2:E:223:ASN:ND2	1.70	0.81
2:F:89:GLU:HG3	2:F:109:LYS:O	1.81	0.81
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.64	0.80
2:E:96:ASN:HB3	2:E:100:GLU:H	1.47	0.80
1:A:26:GLU:HG2	1:A:46:ASN:ND2	1.97	0.79
2:F:225:PRO:HB2	8:F:632:HOH:O	1.81	0.79
1:B:211:SER:HB2	8:B:664:HOH:O	1.83	0.78
1:C:40:ARG:HH11	1:C:70:ASN:HD21	1.32	0.78
1:A:360:GLY:HA2	1:A:362:ARG:NH1	1.98	0.78
1:A:68:PRO:HD3	2:E:15:ALA:HB2	1.66	0.77
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.84	0.77
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.49	0.77
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.49	0.77
1:B:187:LYS:HE3	1:B:191:ASP:OD2	1.85	0.77
2:E:89:GLU:HG3	2:E:109:LYS:O	1.85	0.76
2:E:326:PHE:HB3	8:E:497:HOH:O	1.85	0.76
1:C:404:ALA:C	1:C:406:PHE:H	1.93	0.76
2:F:411:GLN:HG2	7:F:602:AUR:H7	1.67	0.76
2:F:324:THR:HA	8:F:608:HOH:O	1.86	0.76
1:B:63:SER:HA	1:B:73:VAL:HG12	1.68	0.76
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.68	0.76
2:D:93:ARG:HH12	2:D:105:ARG:HB2	1.52	0.75
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.00	0.75
2:D:93:ARG:HG2	2:D:93:ARG:HH11	1.51	0.74
1:C:99:VAL:HG22	1:C:253:MET:HA	1.70	0.74
2:D:223:ASN:HD22	2:D:223:ASN:N	1.80	0.74
1:A:25:LEU:H	1:A:25:LEU:HD23	1.51	0.74
1:C:52:MET:O	1:C:91:THR:HB	1.88	0.74
1:A:440:GLU:O	1:A:444:VAL:HG13	1.87	0.74
2:E:342:LEU:O	7:E:479:AUR:H14	1.88	0.73
1:A:297:ASP:HA	8:A:627:HOH:O	1.88	0.73
1:C:443:ALA:O	1:C:446:TYR:HB3	1.87	0.73
2:E:411:GLN:OE1	7:E:479:AUR:H9	1.87	0.73
1:B:141:SER:O	1:B:143:ARG:HD2	1.88	0.73
2:F:223:ASN:HD22	2:F:223:ASN:N	1.82	0.73
2:F:407:ALA:O	2:F:411:GLN:HB2	1.87	0.73
1:A:136:ILE:HG22	8:A:610:HOH:O	1.88	0.72
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.71	0.72
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:224:GLU:HG2	8:E:499:HOH:O	1.88	0.72
1:C:399:GLU:OE2	2:D:408:ARG:NH2	2.23	0.72
1:C:40:ARG:NH1	1:C:70:ASN:HD21	1.87	0.71
2:E:378:LEU:O	7:E:479:AUR:H241	1.89	0.71
1:C:398:ARG:HG2	8:C:625:HOH:O	1.90	0.71
2:E:408:ARG:NH2	2:E:412:ARG:NH2	2.38	0.71
2:F:95:MET:HE3	2:F:108:ILE:HD13	1.73	0.71
1:A:333:ASP:HB3	8:A:630:HOH:O	1.91	0.71
2:D:225:PRO:HB2	8:D:646:HOH:O	1.91	0.71
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.91	0.70
2:E:411:GLN:NE2	7:E:479:AUR:O25	2.24	0.70
1:A:44:LEU:O	1:A:47:VAL:HG22	1.92	0.70
1:C:40:ARG:HH11	1:C:70:ASN:ND2	1.88	0.70
2:E:441:PHE:O	2:E:445:LEU:HG	1.92	0.70
2:E:149:GLY:HA2	2:E:304:ILE:O	1.91	0.70
2:E:411:GLN:HE22	7:E:479:AUR:H5	1.55	0.70
3:G:2:THR:HG22	3:G:4:LYS:H	1.57	0.70
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.71	0.69
2:E:279:VAL:HG12	8:E:481:HOH:O	1.92	0.69
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.58	0.69
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.74	0.69
2:D:404:VAL:O	2:D:408:ARG:HG3	1.91	0.69
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.74	0.69
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.73	0.68
2:E:319:ASP:O	2:E:322:PRO:HD2	1.94	0.68
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.75	0.68
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.74	0.68
1:B:102:GLU:HG3	1:B:122:GLY:O	1.94	0.68
1:A:417:LEU:HD23	1:A:417:LEU:H	1.59	0.68
1:C:44:LEU:O	1:C:47:VAL:HG22	1.94	0.68
2:E:408:ARG:NH2	2:E:412:ARG:HH21	1.92	0.68
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.74	0.68
2:F:319:ASP:O	2:F:322:PRO:HD2	1.93	0.68
2:D:95:MET:HE3	2:D:99:GLY:HA2	1.74	0.67
1:B:393:GLU:OE1	1:B:424:LEU:HD11	1.94	0.67
2:F:159:GLY:HA2	5:F:600:ANP:HNB1	1.58	0.67
2:D:175:LYS:N	8:D:606:HOH:O	2.27	0.67
1:A:94:ILE:HG12	1:A:95:VAL:N	2.10	0.67
1:A:385:GLN:OE1	1:A:488:LYS:HB2	1.95	0.67
1:C:139:ARG:HB3	1:C:311:LYS:O	1.93	0.67
1:A:270:ASP:OD1	1:A:273:LYS:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:138:LYS:HG3	2:E:416:GLN:OE1	1.95	0.67
2:F:395:GLU:OE2	3:G:77:LEU:HA	1.95	0.67
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.78	0.66
2:E:267:GLU:O	2:E:271:LEU:HG	1.96	0.66
2:D:223:ASN:H	2:D:223:ASN:ND2	1.89	0.65
1:B:151:LYS:HG3	1:B:430:GLN:HE21	1.60	0.65
1:B:422:VAL:O	1:B:426:GLU:HG2	1.97	0.65
1:C:210:ARG:NH1	2:F:121:PRO:O	2.30	0.65
2:E:388:ILE:HG23	2:E:393:MET:HG3	1.78	0.65
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.96	0.65
1:A:175:LYS:HG3	1:A:352:LEU:HD12	1.78	0.65
1:A:341:ASN:O	1:A:345:ILE:HG13	1.97	0.65
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.60	0.65
1:A:147:GLN:OE1	1:A:438:ILE:HD13	1.97	0.65
3:G:254:ARG:NH2	8:G:273:HOH:O	2.28	0.65
2:E:455:GLN:O	2:E:469:LYS:HD3	1.97	0.64
1:B:381:ARG:O	1:B:384:LYS:HB2	1.96	0.64
2:D:473:LEU:C	2:D:475:GLU:H	2.04	0.64
2:F:93:ARG:NH2	2:F:106:GLY:O	2.31	0.64
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.63	0.63
2:F:372:ARG:NH2	8:F:683:HOH:O	2.28	0.63
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.81	0.63
1:C:488:LYS:HG2	1:C:489:ILE:H	1.63	0.63
2:D:162:LYS:N	6:D:600:ADP:O1B	2.30	0.63
1:B:175:LYS:NZ	8:B:649:HOH:O	2.30	0.63
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.64	0.62
1:B:151:LYS:NZ	1:B:429:LYS:O	2.32	0.62
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.28	0.62
2:E:425:THR:O	2:E:427:HIS:ND1	2.27	0.62
2:E:449:TYR:HB3	2:E:452:LEU:HB2	1.81	0.62
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.80	0.62
2:F:223:ASN:H	2:F:223:ASN:ND2	1.88	0.62
1:A:150:ILE:HA	1:A:430:GLN:HE22	1.63	0.62
1:A:485:THR:HG22	1:A:486:ASP:N	2.14	0.62
2:E:224:GLU:O	2:E:229:ARG:NH1	2.30	0.62
3:G:221:THR:HG22	8:G:295:HOH:O	1.99	0.62
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.81	0.62
2:D:473:LEU:O	2:D:475:GLU:N	2.33	0.62
1:A:82:ILE:HA	1:A:86:ASP:OD2	1.99	0.62
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.82	0.62
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.00	0.61
2:D:96:ASN:HB2	2:D:100:GLU:H	1.64	0.61
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.65	0.61
1:A:106:ARG:NH2	1:A:119:GLY:O	2.29	0.61
1:A:414:THR:O	1:A:418:LEU:HD22	2.00	0.61
1:C:211:SER:HB3	2:F:126:MET:HE2	1.82	0.61
2:E:275:ILE:HG23	3:G:266:ILE:HD13	1.82	0.61
2:E:412:ARG:NH1	7:E:479:AUR:O19	2.32	0.61
1:A:164:ARG:NH1	1:A:347:ASP:OD2	2.33	0.61
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.82	0.61
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.65	0.61
2:D:173:VAL:N	8:D:606:HOH:O	2.33	0.61
2:E:142:LEU:HD23	2:E:414:LEU:HD21	1.82	0.61
2:E:455:GLN:NE2	2:E:469:LYS:NZ	2.49	0.61
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.83	0.61
1:B:441:GLN:O	1:B:445:ILE:HG12	2.00	0.61
1:B:499:GLU:O	1:B:502:THR:HB	2.00	0.60
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.81	0.60
1:B:400:VAL:HB	1:B:418:LEU:HD13	1.83	0.60
1:C:172:GLN:HA	5:C:600:ANP:HNB1	1.65	0.60
2:D:53:LEU:HD11	2:D:59:ARG:HB2	1.83	0.60
2:D:406:ARG:O	2:D:410:ILE:HG13	2.00	0.60
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.63	0.60
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.84	0.60
2:F:151:LYS:HA	8:F:609:HOH:O	2.00	0.60
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.81	0.60
1:C:211:SER:O	1:C:215:GLN:HG2	2.00	0.60
2:F:93:ARG:HG2	2:F:93:ARG:NH1	2.09	0.60
1:A:151:LYS:H	1:A:430:GLN:NE2	1.99	0.60
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.81	0.60
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.83	0.60
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.01	0.60
1:B:151:LYS:CG	1:B:430:GLN:HE21	2.15	0.60
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.60
1:B:118:LYS:NZ	8:B:628:HOH:O	2.34	0.60
1:C:419:SER:O	1:C:423:ARG:HG2	2.02	0.60
2:E:39:GLN:HB2	2:E:74:LYS:HB2	1.84	0.60
2:E:242:TYR:C	2:E:244:ARG:H	2.10	0.59
2:D:93:ARG:NH2	2:D:106:GLY:O	2.34	0.59
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.67	0.59
1:A:211:SER:N	2:D:126:MET:HE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.84	0.59
1:B:151:LYS:NZ	1:B:427:LEU:O	2.31	0.59
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.18	0.59
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.36	0.59
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.84	0.59
3:G:23:MET:SD	3:G:232:MET:HE2	2.43	0.59
2:D:402:LEU:O	2:D:406:ARG:HG3	2.03	0.59
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.85	0.59
2:D:408:ARG:HD3	2:D:454:GLU:OE2	2.02	0.59
2:E:422:GLU:C	2:E:424:PHE:H	2.11	0.59
2:F:243:PHE:O	2:F:249:GLN:HB2	2.03	0.59
2:F:252:LEU:HD23	2:F:305:THR:HB	1.85	0.59
2:F:162:LYS:HE3	8:F:627:HOH:O	2.03	0.58
2:F:289:MET:HE2	8:F:636:HOH:O	2.03	0.58
2:E:421:ALA:O	2:E:425:THR:HB	2.03	0.58
1:A:48:GLN:HB3	2:E:68:GLY:O	2.03	0.58
1:B:349:GLN:NE2	8:B:615:HOH:O	2.35	0.58
2:D:156:GLY:HA2	8:D:651:HOH:O	2.02	0.58
1:C:344:SER:O	2:D:222:MET:HE1	2.03	0.58
2:E:316:ASP:OD2	3:G:254:ARG:NH1	2.36	0.58
2:F:234:LEU:O	2:F:237:LEU:HB3	2.02	0.58
1:A:130:GLY:HA2	1:A:308:ARG:NH1	2.19	0.58
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.69	0.58
1:B:391:LYS:O	1:B:395:ALA:N	2.36	0.58
2:E:438:ILE:O	2:E:442:GLN:HB2	2.03	0.58
1:A:145:PRO:O	1:A:161:ARG:HD2	2.03	0.58
1:A:313:ASN:O	1:A:316:PHE:N	2.29	0.58
2:E:246:GLN:HA	2:E:246:GLN:NE2	2.19	0.58
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.02	0.58
1:B:27:GLU:O	1:B:90:ARG:HG3	2.04	0.58
2:E:61:ILE:HG13	2:E:61:ILE:O	2.02	0.58
2:E:92:GLY:N	2:E:215:VAL:O	2.32	0.58
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.86	0.58
1:A:142:VAL:HG22	1:A:161:ARG:O	2.04	0.58
1:A:130:GLY:H	1:A:308:ARG:HH12	1.52	0.57
1:C:59:LEU:HD23	1:C:82:ILE:HD11	1.86	0.57
2:D:170:ILE:O	2:D:174:ALA:HB3	2.05	0.57
2:D:359:ASP:OD1	2:D:360:PRO:HD2	2.05	0.57
2:E:279:VAL:HG12	2:E:279:VAL:O	2.04	0.57
2:E:408:ARG:O	2:E:412:ARG:HG3	2.05	0.57
2:D:391:LEU:HD21	3:G:16:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.86	0.57
1:B:151:LYS:HG3	1:B:430:GLN:HG3	1.87	0.57
1:A:215:GLN:NE2	2:D:128:VAL:HB	2.20	0.57
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.70	0.57
2:F:374:VAL:O	2:F:377:ILE:HG22	2.04	0.57
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.85	0.57
3:G:38:LEU:HD11	3:G:42:ARG:NE	2.20	0.57
1:B:383:MET:O	1:B:387:ALA:N	2.34	0.57
2:D:83:ARG:HA	2:D:114:ALA:O	2.04	0.57
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.85	0.57
2:E:9:THR:HG21	2:E:28:GLY:O	2.05	0.57
1:A:121:ILE:HD13	1:A:121:ILE:H	1.70	0.56
1:B:171:ARG:HG3	1:B:171:ARG:NH1	2.19	0.56
1:C:175:LYS:HE3	5:C:600:ANP:O1B	2.05	0.56
2:E:400:ASP:O	2:E:404:VAL:HG23	2.04	0.56
1:A:134:PRO:O	1:A:139:ARG:NH2	2.29	0.56
1:A:164:ARG:NH2	1:A:345:ILE:O	2.39	0.56
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.87	0.56
1:C:143:ARG:N	8:C:646:HOH:O	2.27	0.56
1:C:345:ILE:HA	2:D:222:MET:HE1	1.88	0.56
2:D:93:ARG:HG2	2:D:93:ARG:NH1	2.19	0.56
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.71	0.56
2:E:25:PHE:O	2:E:56:SER:HB3	2.06	0.56
2:E:258:ILE:O	2:E:261:PHE:HB3	2.05	0.56
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.86	0.56
1:C:476:HIS:ND1	1:C:476:HIS:N	2.53	0.56
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.19	0.56
2:E:126:MET:HE1	2:E:297:THR:HG21	1.86	0.56
1:A:179:ALA:O	1:A:182:THR:HB	2.06	0.56
1:B:174:GLY:HA2	5:B:600:ANP:PA	2.46	0.56
1:C:91:THR:HG22	1:C:93:ALA:H	1.71	0.56
1:C:102:GLU:OE1	1:C:123:SER:HA	2.04	0.56
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.86	0.56
2:E:425:THR:C	2:E:427:HIS:H	2.14	0.56
2:F:314:ALA:O	2:F:315:ASP:HB2	2.05	0.56
1:B:221:THR:HG22	1:B:222:ASP:N	2.20	0.56
1:C:399:GLU:CD	2:D:408:ARG:HH22	2.13	0.56
1:B:165:GLU:O	1:B:325:PRO:HD2	2.06	0.56
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.87	0.56
2:E:167:MET:HE3	2:E:420:VAL:HG11	1.88	0.56
2:E:216:ALA:HB1	8:E:490:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:O	1:C:422:VAL:HG23	2.06	0.56
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.87	0.55
1:B:358:TYR:C	1:B:360:GLY:H	2.13	0.55
2:E:422:GLU:O	2:E:424:PHE:N	2.39	0.55
1:A:389:THR:O	1:A:393:GLU:HG2	2.06	0.55
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.88	0.55
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.87	0.55
8:A:634:HOH:O	2:D:376:LYS:HB2	2.07	0.55
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.89	0.55
3:G:20:THR:HG21	3:G:236:SER:N	2.21	0.55
2:D:38:VAL:HG22	2:D:75:VAL:HG22	1.88	0.55
1:C:45:ARG:NH2	1:C:68:PRO:O	2.40	0.55
2:D:397:SER:OG	2:D:400:ASP:HB2	2.07	0.55
2:F:93:ARG:NH1	2:F:105:ARG:HB2	2.21	0.55
1:B:175:LYS:HE3	5:B:600:ANP:O1B	2.07	0.55
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.05	0.55
2:E:409:LYS:HE2	2:E:452:LEU:O	2.07	0.55
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.89	0.55
2:D:263:GLN:NE2	8:D:618:HOH:O	2.29	0.55
2:D:263:GLN:O	2:D:267:GLU:HG3	2.07	0.55
2:E:394:ASP:C	2:E:396:LEU:H	2.14	0.55
2:F:409:LYS:NZ	2:F:452:LEU:O	2.26	0.55
1:C:436:MET:HE3	1:C:469:LEU:HD21	1.88	0.55
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.88	0.55
3:G:7:THR:O	3:G:11:LYS:HB2	2.07	0.55
1:C:174:GLY:HA2	5:C:600:ANP:PA	2.47	0.55
2:E:12:ARG:O	2:E:23:VAL:HG13	2.07	0.55
2:E:411:GLN:HG2	7:E:479:AUR:H7	1.88	0.55
2:F:95:MET:HG3	2:F:99:GLY:HA2	1.88	0.55
2:F:164:VAL:HG23	5:F:600:ANP:O1A	2.06	0.55
1:C:312:MET:O	1:C:318:GLY:HA2	2.07	0.54
1:C:467:ALA:O	1:C:470:SER:HB2	2.07	0.54
2:E:397:SER:O	2:E:401:LYS:HG3	2.06	0.54
2:F:251:VAL:HG12	2:F:252:LEU:N	2.22	0.54
1:A:26:GLU:HG2	1:A:46:ASN:HD21	1.73	0.54
1:A:438:ILE:O	1:A:442:VAL:HG13	2.07	0.54
1:A:213:VAL:O	1:A:216:LEU:HB3	2.08	0.54
1:B:32:LEU:HD11	1:B:42:HIS:HB2	1.89	0.54
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.72	0.54
2:E:148:LYS:HE3	2:E:250:ASP:OD2	2.07	0.54
2:E:221:GLN:N	2:E:224:GLU:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:PHE:O	1:C:408:SER:N	2.40	0.54
2:E:138:LYS:O	2:E:142:LEU:HB3	2.08	0.54
1:B:440:GLU:O	1:B:443:ALA:HB3	2.07	0.54
2:D:244:ARG:O	2:D:248:GLY:HA2	2.08	0.54
2:D:440:GLY:O	2:D:444:ILE:HG13	2.07	0.54
1:B:302:HIS:ND1	8:B:607:HOH:O	2.33	0.54
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.08	0.54
2:E:185:GLY:HA3	2:E:188:GLU:HG3	1.88	0.54
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.54
2:F:188:GLU:O	2:F:221:GLN:HB3	2.08	0.54
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.54
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.90	0.54
2:F:63:MET:HE1	2:F:231:ARG:HB2	1.90	0.54
1:C:30:ARG:NE	1:C:87:ILE:HD11	2.08	0.53
3:G:20:THR:HA	3:G:232:MET:HE3	1.89	0.53
3:G:43:VAL:HG12	3:G:43:VAL:O	2.08	0.53
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.23	0.53
1:B:300:TYR:O	1:B:304:ARG:HG2	2.08	0.53
1:C:392:LEU:HB3	2:D:458:TYR:OH	2.08	0.53
2:E:152:ILE:HA	2:E:331:ALA:O	2.09	0.53
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.90	0.53
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.42	0.53
2:E:116:ILE:HA	2:E:238:THR:OG1	2.08	0.53
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.90	0.53
2:D:366:GLU:O	2:D:370:VAL:HG23	2.09	0.53
1:B:352:LEU:HA	1:B:364:ALA:O	2.07	0.53
1:B:456:LEU:HD12	1:B:457:GLU:N	2.16	0.53
2:E:122:GLU:HB2	2:E:125:GLU:HG3	1.91	0.53
1:A:36:ASP:O	1:A:284:LEU:HD13	2.09	0.53
1:B:170:ASP:O	1:B:175:LYS:HE2	2.09	0.53
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.74	0.53
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.74	0.53
1:C:32:LEU:HB2	1:C:40:ARG:O	2.09	0.52
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.90	0.52
1:C:173:THR:HG22	1:C:354:THR:HG22	1.91	0.52
2:D:200:MET:HE3	2:D:215:VAL:HG21	1.91	0.52
1:B:137:ILE:HD13	2:F:103:ASP:HA	1.90	0.52
2:D:88:PRO:O	2:D:91:LEU:HD12	2.08	0.52
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.91	0.52
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.91	0.52
1:C:215:GLN:CG	2:F:356:ARG:HH22	2.00	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:439:LYS:O	2:E:442:GLN:HB3	2.09	0.52
2:F:151:LYS:HD3	2:F:328:HIS:O	2.09	0.52
1:A:184:ILE:HD12	1:A:223:ALA:HB3	1.91	0.52
1:C:390:MET:HE3	1:C:424:LEU:HD22	1.90	0.52
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.91	0.52
1:A:108:VAL:HA	1:A:113:ASN:O	2.09	0.52
1:A:224:ASP:HA	8:A:617:HOH:O	2.09	0.52
2:E:409:LYS:HZ2	2:E:450:ASP:HA	1.72	0.52
2:F:324:THR:O	2:F:324:THR:HG22	2.07	0.52
2:E:77:ASP:CG	2:E:79:GLY:H	2.18	0.52
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.91	0.51
2:F:151:LYS:HG2	8:F:609:HOH:O	2.09	0.51
1:A:268:TYR:HB2	1:A:325:PRO:HA	1.91	0.51
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.92	0.51
2:D:208:LEU:HA	8:D:609:HOH:O	2.10	0.51
1:A:48:GLN:HA	2:E:69:LEU:O	2.10	0.51
1:A:49:ALA:O	1:A:50:GLU:HB2	2.11	0.51
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.91	0.51
1:B:171:ARG:NH2	2:E:326:PHE:CD2	2.78	0.51
2:E:118:ALA:H	2:E:295:ARG:NH1	2.08	0.51
2:E:263:GLN:HB3	8:E:493:HOH:O	2.10	0.51
1:B:157:VAL:HG12	1:B:157:VAL:O	2.10	0.51
2:E:95:MET:HA	2:E:100:GLU:O	2.10	0.51
2:E:342:LEU:HB3	7:E:479:AUR:H12	1.92	0.51
2:F:408:ARG:NE	2:F:454:GLU:OE2	2.26	0.51
1:A:215:GLN:NE2	2:D:128:VAL:HG12	2.26	0.51
1:A:337:TYR:O	1:A:340:THR:HB	2.10	0.51
1:B:162:GLY:HA2	1:B:321:LEU:O	2.10	0.51
2:D:63:MET:HE3	2:D:228:ALA:HA	1.93	0.51
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.08	0.51
2:E:359:ASP:OD1	2:E:360:PRO:HD2	2.10	0.51
2:E:463:ILE:O	2:E:467:VAL:HG23	2.10	0.51
2:F:384:LEU:O	2:F:387:ILE:HD12	2.10	0.51
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.91	0.51
2:E:397:SER:H	2:E:400:ASP:HB2	1.75	0.51
2:F:266:SER:HB3	2:F:282:GLN:NE2	2.25	0.51
2:F:433:PRO:O	2:F:436:GLU:HB2	2.11	0.51
1:B:59:LEU:HD22	1:B:81:LEU:HD12	1.93	0.51
1:C:71:VAL:HG23	8:C:668:HOH:O	2.10	0.51
3:G:254:ARG:O	3:G:258:ILE:HG13	2.11	0.51
1:A:215:GLN:HE22	2:D:128:VAL:HB	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.92	0.51
1:C:30:ARG:HA	1:C:86:ASP:O	2.10	0.51
1:C:151:LYS:HE2	1:C:436:MET:SD	2.50	0.51
2:F:404:VAL:O	2:F:408:ARG:HG3	2.11	0.51
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.11	0.51
2:E:158:ALA:C	2:E:160:VAL:H	2.18	0.51
2:F:442:GLN:O	2:F:445:LEU:HB2	2.11	0.51
1:C:244:TYR:O	1:C:247:PRO:HD2	2.10	0.51
1:C:344:SER:HA	8:C:670:HOH:O	2.10	0.51
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.26	0.51
2:D:356:ARG:O	2:D:356:ARG:HG2	2.11	0.51
2:D:412:ARG:NH1	8:D:681:HOH:O	2.32	0.51
2:E:204:GLY:O	2:E:206:ILE:N	2.44	0.51
2:E:339:ILE:HD12	7:E:479:AUR:O7	2.11	0.51
2:E:385:GLN:HE22	7:E:479:AUR:H203	1.76	0.51
1:A:91:THR:C	1:A:93:ALA:H	2.20	0.50
1:A:151:LYS:HG2	1:A:430:GLN:HE21	1.74	0.50
1:A:460:LYS:N	1:A:460:LYS:HD2	2.26	0.50
1:B:279:ARG:NH1	8:B:624:HOH:O	2.32	0.50
1:A:56:SER:O	1:A:58:GLY:N	2.44	0.50
2:F:97:VAL:HG13	2:F:232:VAL:HA	1.93	0.50
1:A:258:ARG:O	1:A:319:GLY:HA3	2.11	0.50
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.94	0.50
1:B:297:ASP:HA	8:B:622:HOH:O	2.12	0.50
1:C:143:ARG:HB2	8:C:634:HOH:O	2.11	0.50
2:F:228:ALA:O	2:F:232:VAL:HG22	2.11	0.50
1:A:99:VAL:HG23	1:A:253:MET:HA	1.94	0.50
1:B:211:SER:O	1:B:215:GLN:HG3	2.12	0.50
1:B:420:ARG:O	1:B:423:ARG:N	2.45	0.50
2:D:54:GLY:O	2:D:55:GLU:HB2	2.12	0.50
2:D:168:GLU:HG3	2:D:168:GLU:O	2.10	0.50
1:B:69:ASP:O	1:B:70:ASN:HB3	2.12	0.50
2:E:96:ASN:OD1	2:E:97:VAL:N	2.44	0.50
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.93	0.50
2:E:296:ILE:HD13	2:E:306:SER:HB2	1.92	0.50
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.93	0.50
1:B:434:SER:N	1:B:435:PRO:HD3	2.26	0.50
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.94	0.50
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.94	0.50
2:F:455:GLN:H	2:F:455:GLN:CD	2.19	0.50
1:C:361:ILE:O	1:C:361:ILE:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:196:LEU:O	2:F:200:MET:HB2	2.12	0.49
2:F:304:ILE:HG22	2:F:304:ILE:O	2.12	0.49
2:F:467:VAL:O	2:F:470:ALA:HB3	2.12	0.49
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.93	0.49
1:B:445:ILE:O	1:B:449:VAL:HG23	2.12	0.49
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.94	0.49
2:D:367:HIS:HB2	8:D:641:HOH:O	2.11	0.49
2:E:419:GLN:HG3	2:E:429:GLY:HA3	1.94	0.49
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.26	0.49
2:E:469:LYS:O	2:E:473:LEU:HG	2.13	0.49
1:A:151:LYS:HE2	1:A:427:LEU:O	2.13	0.49
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.93	0.49
1:B:68:PRO:HD3	2:F:15:ALA:HB2	1.94	0.49
1:B:464:PHE:O	1:B:468:PHE:HB3	2.12	0.49
2:D:177:HIS:O	2:D:214:LYS:NZ	2.37	0.49
2:E:244:ARG:O	2:E:248:GLY:HA2	2.10	0.49
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.93	0.49
2:E:402:LEU:HD23	2:E:406:ARG:NH2	2.26	0.49
2:E:408:ARG:HH22	2:E:412:ARG:NH2	2.07	0.49
2:E:455:GLN:NE2	2:E:469:LYS:HZ1	2.10	0.49
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.95	0.49
3:G:30:LYS:HA	3:G:33:ARG:HE	1.77	0.49
1:C:49:ALA:O	1:C:50:GLU:HB2	2.13	0.49
2:D:122:GLU:OE1	2:D:122:GLU:HA	2.11	0.49
2:E:227:GLY:O	2:E:230:ALA:HB3	2.12	0.49
1:A:404:ALA:C	1:A:406:PHE:H	2.21	0.49
2:E:292:MET:SD	2:E:293:GLN:NE2	2.86	0.49
2:E:449:TYR:O	2:E:452:LEU:HB2	2.13	0.49
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.28	0.49
2:D:449:TYR:HD1	2:D:452:LEU:HD21	1.77	0.49
2:F:152:ILE:HG22	2:F:153:GLY:N	2.27	0.49
3:G:10:LEU:HG	3:G:246:LEU:HB3	1.94	0.49
1:B:303:SER:HB2	2:F:222:MET:HB3	1.95	0.49
2:D:105:ARG:HH11	2:D:208:LEU:HD22	1.77	0.49
2:D:422:GLU:HG2	2:D:427:HIS:O	2.12	0.49
2:F:138:LYS:HE2	2:F:416:GLN:HB2	1.94	0.49
2:F:342:LEU:HD13	7:F:602:AUR:H10	1.95	0.49
3:G:16:ILE:HA	3:G:19:ILE:HD12	1.95	0.49
1:C:209:LYS:HE2	1:C:212:THR:OG1	2.13	0.49
1:C:354:THR:HG23	8:C:649:HOH:O	2.12	0.49
2:D:145:PRO:HB2	2:D:357:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:414:LEU:HG	2:E:441:PHE:CE2	2.48	0.49
2:F:44:ARG:NH2	8:F:648:HOH:O	2.38	0.49
1:A:392:LEU:O	1:A:396:GLN:HG3	2.13	0.48
1:C:331:ALA:O	1:C:333:ASP:N	2.45	0.48
2:F:339:ILE:O	2:F:342:LEU:HB2	2.13	0.48
3:G:239:ALA:O	3:G:243:ILE:HG13	2.12	0.48
1:B:128:ARG:HD3	8:B:654:HOH:O	2.12	0.48
2:D:105:ARG:HH11	2:D:208:LEU:CD2	2.26	0.48
2:D:279:VAL:HG12	2:D:279:VAL:O	2.12	0.48
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.95	0.48
1:C:390:MET:HE1	1:C:428:LEU:HD21	1.95	0.48
2:D:473:LEU:C	2:D:475:GLU:N	2.72	0.48
1:A:241:PRO:O	1:A:244:TYR:HB3	2.14	0.48
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.77	0.48
1:C:381:ARG:O	1:C:385:GLN:HG3	2.13	0.48
2:E:405:SER:OG	2:E:406:ARG:N	2.46	0.48
1:B:136:ILE:HG23	2:F:194:ASN:HA	1.94	0.48
1:B:215:GLN:NE2	2:E:130:GLN:NE2	2.62	0.48
2:D:203:SER:OG	2:D:205:VAL:HG23	2.14	0.48
2:E:223:ASN:N	2:E:223:ASN:ND2	2.42	0.48
2:E:385:GLN:NE2	7:E:479:AUR:C20	2.77	0.48
1:A:441:GLN:O	1:A:445:ILE:HG12	2.13	0.48
2:D:471:ASP:O	2:D:474:ALA:N	2.47	0.48
2:D:84:ILE:N	2:D:114:ALA:O	2.41	0.48
2:E:394:ASP:C	2:E:396:LEU:N	2.71	0.48
1:A:415:GLN:HA	1:A:418:LEU:HD23	1.96	0.48
1:A:496:LYS:HG2	1:A:500:ILE:HD11	1.96	0.48
1:B:134:PRO:O	1:B:139:ARG:NH2	2.35	0.48
2:D:96:ASN:CB	2:D:100:GLU:H	2.26	0.48
2:E:67:GLU:H	2:E:67:GLU:HG3	1.51	0.48
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.48
1:C:148:THR:HG21	1:C:153:VAL:HG11	1.95	0.48
2:F:266:SER:HB3	2:F:282:GLN:HE21	1.79	0.48
1:A:151:LYS:HG2	1:A:430:GLN:NE2	2.29	0.48
1:A:215:GLN:NE2	2:D:128:VAL:CB	2.77	0.48
1:A:267:ILE:HA	1:A:324:LEU:O	2.14	0.48
1:A:291:ARG:HA	3:G:262:LEU:HD13	1.96	0.48
1:A:376:SER:C	1:A:378:ALA:N	2.72	0.48
1:B:389:THR:HG22	1:B:392:LEU:HD12	1.96	0.48
2:F:93:ARG:HH12	2:F:105:ARG:HB2	1.79	0.48
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:SER:C	1:A:378:ALA:H	2.21	0.47
1:B:212:THR:O	1:B:216:LEU:HB2	2.14	0.47
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.95	0.47
2:E:423:VAL:O	2:E:424:PHE:HB2	2.14	0.47
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.28	0.47
3:G:36:ARG:O	3:G:40:PRO:HD3	2.14	0.47
1:B:172:GLN:CA	5:B:600:ANP:HNB1	2.20	0.47
1:B:358:TYR:C	1:B:360:GLY:N	2.72	0.47
1:B:390:MET:HE3	1:B:424:LEU:HD22	1.95	0.47
1:C:352:LEU:HA	1:C:364:ALA:O	2.13	0.47
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.96	0.47
1:A:209:LYS:HZ1	2:D:330:ASP:CG	2.20	0.47
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.29	0.47
2:D:298:THR:HG23	2:D:303:SER:HA	1.97	0.47
2:E:16:VAL:HG22	2:E:21:VAL:HG13	1.95	0.47
2:E:166:ILE:O	2:E:170:ILE:HG13	2.14	0.47
2:E:282:GLN:H	2:E:282:GLN:NE2	2.12	0.47
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.96	0.47
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.13	0.47
1:A:468:PHE:O	1:A:472:VAL:HG13	2.14	0.47
1:B:183:ILE:O	1:B:186:GLN:HB2	2.14	0.47
1:C:304:ARG:NH1	8:C:629:HOH:O	2.47	0.47
1:C:373:ARG:HA	6:D:600:ADP:O3'	2.13	0.47
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.97	0.47
3:G:217:LEU:O	3:G:221:THR:HG23	2.14	0.47
1:A:218:LYS:HE2	1:A:222:ASP:OD2	2.15	0.47
1:B:363:PRO:C	1:B:365:ILE:H	2.22	0.47
1:B:479:LEU:HD22	1:B:482:LYS:HD2	1.95	0.47
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.96	0.47
2:E:415:SER:O	2:E:416:GLN:HB2	2.14	0.47
2:F:439:LYS:O	2:F:442:GLN:N	2.48	0.47
1:A:53:VAL:HG13	1:A:89:LYS:O	2.15	0.47
1:A:386:VAL:HG21	1:A:442:VAL:HB	1.97	0.47
1:A:415:GLN:O	1:A:415:GLN:HG2	2.14	0.47
1:A:445:ILE:O	1:A:449:VAL:HB	2.14	0.47
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.97	0.47
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.97	0.47
1:C:402:ALA:O	1:C:405:GLN:HG3	2.14	0.47
2:D:49:VAL:HA	2:D:60:THR:HG22	1.96	0.47
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.50	0.47
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ALA:O	1:A:406:PHE:N	2.48	0.47
8:B:627:HOH:O	2:F:189:ARG:HG2	2.14	0.47
1:C:336:ALA:HB3	1:C:339:PRO:HG2	1.95	0.47
2:D:130:GLN:HE22	2:D:356:ARG:CD	2.28	0.47
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.29	0.47
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.97	0.47
2:F:155:PHE:HB2	2:F:334:VAL:HA	1.97	0.47
2:F:205:VAL:O	2:F:213:SER:HA	2.14	0.47
1:B:33:SER:HB2	2:E:52:HIS:O	2.15	0.47
1:C:23:VAL:HG12	1:C:23:VAL:O	2.15	0.47
2:F:385:GLN:HE22	7:F:602:AUR:H202	1.80	0.47
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.28	0.46
1:C:280:GLN:OE1	2:F:287:THR:HG23	2.15	0.46
3:G:6:ILE:HG23	3:G:246:LEU:HD22	1.97	0.46
2:D:273:GLY:HA2	3:G:272:LEU:HD22	1.98	0.46
2:E:54:GLY:O	2:E:55:GLU:HB2	2.14	0.46
2:E:189:ARG:HB2	2:E:192:GLU:HG3	1.97	0.46
1:A:130:GLY:N	1:A:308:ARG:HH12	2.12	0.46
1:B:273:LYS:HB3	8:B:666:HOH:O	2.15	0.46
2:D:161:GLY:HA3	8:D:639:HOH:O	2.15	0.46
2:D:405:SER:O	2:D:409:LYS:HG3	2.14	0.46
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.98	0.46
2:E:454:GLU:C	2:E:456:ALA:H	2.23	0.46
2:F:409:LYS:HD3	2:F:457:PHE:CE1	2.51	0.46
1:B:285:LEU:O	1:B:286:ARG:HB2	2.16	0.46
1:B:366:ASN:ND2	1:B:369:LEU:HG	2.31	0.46
2:E:210:ASP:OD1	2:E:211:ALA:N	2.47	0.46
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.30	0.46
3:G:2:THR:HG22	3:G:4:LYS:N	2.29	0.46
1:B:440:GLU:O	1:B:444:VAL:HG13	2.15	0.46
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.96	0.46
2:E:358:MET:HE3	2:E:358:MET:HB3	1.83	0.46
2:F:175:LYS:NZ	8:F:692:HOH:O	2.48	0.46
2:F:251:VAL:HG12	2:F:252:LEU:H	1.80	0.46
2:F:381:TYR:CD1	2:F:385:GLN:NE2	2.79	0.46
1:B:145:PRO:O	1:B:161:ARG:HD2	2.15	0.46
1:B:201:CYS:O	1:B:229:THR:HA	2.16	0.46
1:C:267:ILE:N	1:C:267:ILE:HD12	2.30	0.46
1:C:400:VAL:HG13	8:C:671:HOH:O	2.15	0.46
2:D:357:ILE:O	2:D:359:ASP:N	2.48	0.46
1:B:499:GLU:HA	1:B:502:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.97	0.46
2:E:77:ASP:OD1	2:E:79:GLY:N	2.45	0.46
2:E:251:VAL:HG12	2:E:252:LEU:N	2.31	0.46
3:G:212:ILE:HD13	3:G:212:ILE:HA	1.85	0.46
1:A:52:MET:O	1:A:91:THR:HG23	2.16	0.46
1:B:357:PHE:HZ	5:B:600:ANP:O4'	1.98	0.46
1:C:292:GLU:O	1:C:293:ALA:HB3	2.15	0.46
2:F:13:ILE:HD13	2:F:69:LEU:HD13	1.98	0.46
2:D:9:THR:HG21	2:D:28:GLY:O	2.16	0.46
2:E:98:ILE:HB	8:E:489:HOH:O	2.15	0.46
2:F:170:ILE:O	2:F:174:ALA:HB3	2.15	0.46
1:A:164:ARG:HD3	1:A:347:ASP:OD2	2.15	0.46
1:A:286:ARG:NE	8:D:644:HOH:O	2.48	0.46
1:A:347:ASP:C	1:A:373:ARG:HH11	2.24	0.46
1:B:190:ASN:HA	1:B:198:LYS:HG2	1.98	0.46
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.51	0.46
1:B:452:TYR:O	1:B:453:LEU:HD23	2.15	0.46
2:D:154:LEU:HD22	2:D:165:LEU:HD23	1.98	0.46
2:F:421:ALA:O	2:F:425:THR:HG23	2.15	0.46
1:A:99:VAL:CG2	1:A:253:MET:HA	2.46	0.45
2:E:374:VAL:O	2:E:377:ILE:HG22	2.17	0.45
2:F:453:PRO:HG2	2:F:473:LEU:HD12	1.98	0.45
1:B:437:ALA:O	1:B:440:GLU:N	2.46	0.45
2:D:105:ARG:NH1	2:D:208:LEU:CD2	2.79	0.45
1:B:311:LYS:HD2	1:B:312:MET:O	2.17	0.45
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.98	0.45
2:D:438:ILE:O	2:D:442:GLN:HB2	2.16	0.45
2:E:423:VAL:O	2:E:423:VAL:HG12	2.16	0.45
1:A:34:ILE:HD12	1:A:79:ASP:HB3	1.97	0.45
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.99	0.45
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.31	0.45
2:F:32:ILE:O	2:F:33:LEU:HB2	2.17	0.45
3:G:23:MET:HE2	3:G:23:MET:HB3	1.75	0.45
1:A:53:VAL:HG12	1:A:54:GLU:N	2.32	0.45
1:A:105:GLY:HA2	1:A:226:MET:O	2.16	0.45
1:A:411:ASP:OD1	1:A:413:ALA:HB3	2.16	0.45
1:B:65:ASN:HD22	2:F:17:ILE:CG1	2.30	0.45
1:C:136:ILE:O	2:D:194:ASN:OD1	2.34	0.45
1:C:498:LYS:O	1:C:502:THR:OG1	2.30	0.45
2:D:77:ASP:CG	2:D:79:GLY:H	2.23	0.45
2:D:112:GLN:OE1	2:D:112:GLN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:411:GLN:CG	7:E:479:AUR:H7	2.46	0.45
1:B:96:ASP:HB2	1:B:127:ARG:O	2.17	0.45
1:B:413:ALA:O	1:B:417:LEU:HG	2.17	0.45
1:B:451:GLY:C	1:B:453:LEU:H	2.25	0.45
1:C:144:GLU:OE2	1:C:311:LYS:NZ	2.49	0.45
1:C:162:GLY:HA2	1:C:321:LEU:O	2.17	0.45
2:E:121:PRO:HD3	8:E:502:HOH:O	2.15	0.45
2:E:182:VAL:HG21	2:E:240:ALA:HB2	1.99	0.45
2:F:440:GLY:O	2:F:444:ILE:HG13	2.17	0.45
3:G:82:HIS:H	3:G:82:HIS:CD2	2.35	0.45
1:A:267:ILE:N	1:A:267:ILE:HD12	2.32	0.45
1:B:187:LYS:HD2	1:B:224:ASP:O	2.16	0.45
1:B:492:GLU:O	1:B:496:LYS:HB2	2.17	0.45
1:C:46:ASN:HB2	1:C:90:ARG:HH11	1.82	0.45
2:D:189:ARG:O	2:D:192:GLU:HB2	2.16	0.45
1:A:407:GLY:HA2	1:A:410:LEU:HD21	1.97	0.45
1:B:146:MET:HE3	1:B:146:MET:O	2.17	0.45
1:B:338:ILE:O	1:B:341:ASN:HB2	2.17	0.45
1:B:443:ALA:O	1:B:446:TYR:HB3	2.17	0.45
2:E:454:GLU:O	2:E:456:ALA:N	2.50	0.45
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.98	0.45
3:G:38:LEU:HD11	3:G:42:ARG:HE	1.81	0.45
1:B:309:ALA:O	1:B:310:ALA:HB2	2.17	0.45
1:B:481:GLY:O	1:B:485:THR:HB	2.16	0.45
2:E:256:ASP:HA	2:E:257:ASN:HA	1.61	0.45
2:F:327:ALA:HB3	8:F:682:HOH:O	2.16	0.45
1:A:157:VAL:N	1:A:158:PRO:CD	2.79	0.45
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.52	0.45
1:A:479:LEU:O	1:A:482:LYS:HB2	2.16	0.45
1:C:90:ARG:HE	1:C:90:ARG:HB3	1.58	0.45
1:C:179:ALA:O	1:C:183:ILE:HG13	2.16	0.45
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.99	0.45
2:E:422:GLU:C	2:E:424:PHE:N	2.74	0.45
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.99	0.45
3:G:35:GLU:O	3:G:39:LYS:HG2	2.16	0.45
1:A:240:ALA:N	1:A:241:PRO:HD2	2.32	0.44
1:B:138:PRO:HB2	1:B:312:MET:HE1	1.98	0.44
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.16	0.44
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.82	0.44
1:C:442:VAL:O	1:C:446:TYR:HB2	2.17	0.44
2:D:412:ARG:HH11	2:D:412:ARG:HG3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.52	0.44
2:E:387:ILE:HG22	2:E:388:ILE:N	2.32	0.44
2:F:327:ALA:HB2	8:F:681:HOH:O	2.16	0.44
2:F:386:ASP:O	2:F:389:ALA:HB3	2.17	0.44
2:D:32:ILE:O	2:D:33:LEU:HB2	2.17	0.44
2:E:397:SER:C	2:E:399:GLU:N	2.72	0.44
2:F:379:GLN:O	2:F:382:LYS:HB3	2.18	0.44
1:A:32:LEU:HD21	1:A:42:HIS:HB2	1.99	0.44
1:B:206:ILE:HD13	1:B:247:PRO:HG3	1.99	0.44
1:C:97:VAL:HG12	1:C:111:LEU:O	2.18	0.44
2:D:253:LEU:O	2:D:306:SER:HA	2.17	0.44
2:E:204:GLY:C	2:E:206:ILE:N	2.76	0.44
2:E:384:LEU:O	2:E:388:ILE:HG12	2.17	0.44
1:A:137:ILE:N	1:A:138:PRO:CD	2.80	0.44
1:B:389:THR:HA	1:B:392:LEU:HG	1.99	0.44
2:E:32:ILE:O	2:E:33:LEU:HB2	2.18	0.44
2:E:86:VAL:O	2:E:110:THR:HG21	2.16	0.44
2:E:189:ARG:O	2:E:192:GLU:N	2.51	0.44
2:F:431:LEU:HA	2:F:431:LEU:HD12	1.80	0.44
1:B:297:ASP:OD1	1:B:297:ASP:N	2.48	0.44
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.99	0.44
1:B:367:VAL:HG12	1:B:391:LYS:HE3	2.00	0.44
1:C:382:ALA:O	1:C:385:GLN:HB2	2.18	0.44
1:C:397:TYR:CD1	1:C:421:GLY:HA3	2.53	0.44
2:F:298:THR:HG22	2:F:299:THR:N	2.32	0.44
3:G:7:THR:O	3:G:11:LYS:HD2	2.16	0.44
3:G:213:ILE:HD13	3:G:213:ILE:HA	1.82	0.44
1:A:420:ARG:HA	1:A:420:ARG:HD3	1.60	0.44
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.99	0.44
1:B:49:ALA:O	1:B:50:GLU:HB2	2.17	0.44
1:B:423:ARG:HE	1:B:458:PRO:CD	2.29	0.44
1:C:139:ARG:HD3	8:C:688:HOH:O	2.17	0.44
1:C:172:GLN:HA	5:C:600:ANP:N3B	2.32	0.44
2:F:410:ILE:HG13	2:F:444:ILE:HG21	2.00	0.44
2:F:455:GLN:HA	7:F:602:AUR:O19	2.17	0.44
2:F:463:ILE:HG22	8:F:643:HOH:O	2.18	0.44
1:A:347:ASP:C	1:A:373:ARG:NH1	2.76	0.44
1:A:423:ARG:NH2	1:A:456:LEU:O	2.51	0.44
1:C:481:GLY:O	1:C:485:THR:HB	2.18	0.44
2:D:67:GLU:CD	2:D:67:GLU:H	2.26	0.44
2:D:220:GLY:HA3	2:D:232:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:271:LEU:C	2:E:273:GLY:H	2.24	0.44
2:F:9:THR:O	2:F:76:LEU:HA	2.17	0.44
1:C:286:ARG:NH1	8:C:632:HOH:O	2.49	0.44
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.81	0.44
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.53	0.44
2:D:461:GLY:HA3	2:D:462:PRO:HD3	1.81	0.44
1:A:215:GLN:HG3	2:D:356:ARG:HH11	1.73	0.44
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.82	0.44
1:B:465:GLU:O	1:B:469:LEU:HB2	2.18	0.44
2:D:344:ILE:HG23	2:D:415:SER:HB3	2.00	0.44
2:D:358:MET:HB3	2:D:358:MET:HE3	1.70	0.44
2:E:138:LYS:HE2	2:E:432:VAL:HG21	2.00	0.44
2:E:220:GLY:HA3	2:E:232:VAL:HG21	2.00	0.44
2:E:455:GLN:HE21	2:E:469:LYS:NZ	2.16	0.44
2:F:434:LEU:O	2:F:438:ILE:HG12	2.17	0.44
3:G:13:ILE:HG22	3:G:243:ILE:HG12	2.00	0.44
1:A:107:VAL:HG12	1:A:115:ILE:HD11	2.00	0.43
1:A:311:LYS:NZ	1:A:318:GLY:O	2.43	0.43
1:B:65:ASN:HD22	2:F:17:ILE:HG13	1.82	0.43
1:B:383:MET:O	1:B:387:ALA:HB3	2.18	0.43
2:D:201:ILE:C	2:D:203:SER:N	2.75	0.43
2:E:201:ILE:HD13	2:E:208:LEU:HD11	2.00	0.43
2:F:435:LYS:HG3	2:F:436:GLU:N	2.33	0.43
1:B:270:ASP:OD2	1:B:273:LYS:HG3	2.17	0.43
1:B:358:TYR:O	1:B:360:GLY:N	2.51	0.43
1:C:27:GLU:O	1:C:90:ARG:HG3	2.18	0.43
2:E:241:GLU:HA	2:E:304:ILE:HD11	2.00	0.43
2:F:296:ILE:HG21	2:F:296:ILE:HD13	1.76	0.43
1:A:34:ILE:HG22	2:D:52:HIS:HB2	1.99	0.43
2:D:201:ILE:C	2:D:203:SER:H	2.27	0.43
2:E:242:TYR:C	2:E:244:ARG:N	2.72	0.43
2:F:282:GLN:H	2:F:282:GLN:HG2	1.23	0.43
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.33	0.43
1:B:172:GLN:HA	5:B:600:ANP:N3B	2.19	0.43
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.53	0.43
2:D:388:ILE:HD12	2:D:393:MET:SD	2.58	0.43
2:E:376:LYS:O	2:E:379:GLN:HB2	2.18	0.43
2:F:12:ARG:HG2	2:F:72:GLY:O	2.19	0.43
2:F:445:LEU:HD23	2:F:445:LEU:HA	1.83	0.43
1:A:385:GLN:OE1	1:A:488:LYS:HE3	2.17	0.43
1:B:168:ILE:O	1:B:351:PHE:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:HB3	8:B:610:HOH:O	2.17	0.43
1:C:169:GLY:O	1:C:175:LYS:HE2	2.18	0.43
1:C:399:GLU:O	1:C:402:ALA:N	2.51	0.43
2:D:83:ARG:HA	2:D:115:ALA:HA	2.00	0.43
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.53	0.43
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.48	0.43
2:F:453:PRO:HB2	2:F:455:GLN:HG2	2.00	0.43
1:B:505:LEU:HD13	1:B:505:LEU:HA	1.87	0.43
2:D:164:VAL:O	2:D:167:MET:HB2	2.17	0.43
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.99	0.43
2:F:83:ARG:HA	2:F:115:ALA:HA	2.01	0.43
1:A:28:THR:CG2	1:A:29:GLY:N	2.81	0.43
1:A:268:TYR:O	1:A:326:VAL:HG23	2.19	0.43
1:A:383:MET:O	1:A:386:VAL:HG23	2.18	0.43
1:A:400:VAL:HG13	1:A:403:PHE:CD2	2.53	0.43
1:B:283:LEU:HD12	2:E:277:SER:HB3	2.00	0.43
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.43
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.53	0.43
2:E:139:VAL:HG13	2:E:414:LEU:HD22	2.00	0.43
2:E:155:PHE:N	2:E:155:PHE:CD1	2.87	0.43
2:F:409:LYS:HG2	2:F:454:GLU:HA	2.00	0.43
1:A:400:VAL:HG12	1:A:418:LEU:HD11	2.00	0.43
1:B:271:LEU:HB3	1:B:302:HIS:CE1	2.54	0.43
1:C:33:SER:HB2	2:F:52:HIS:O	2.19	0.43
2:D:171:ASN:O	8:D:606:HOH:O	2.21	0.43
2:E:88:PRO:C	2:E:90:THR:H	2.27	0.43
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.43
3:G:13:ILE:HD13	3:G:242:MET:SD	2.58	0.43
1:A:83:LYS:H	1:A:86:ASP:CG	2.27	0.43
1:B:151:LYS:H	1:B:430:GLN:NE2	2.16	0.43
1:B:174:GLY:HA2	5:B:600:ANP:O5'	2.19	0.43
1:C:201:CYS:O	1:C:229:THR:HA	2.19	0.43
2:D:459:MET:HB3	2:D:459:MET:HE3	1.38	0.43
2:E:452:LEU:HA	2:E:453:PRO:HD3	1.71	0.43
2:F:412:ARG:CD	2:F:454:GLU:HB3	2.48	0.43
1:A:403:PHE:CZ	3:G:22:SER:HB2	2.54	0.43
1:B:156:LEU:HD13	1:B:367:VAL:HG11	2.01	0.43
1:B:421:GLY:O	1:B:425:THR:OG1	2.30	0.43
1:C:144:GLU:H	1:C:144:GLU:HG3	1.60	0.43
1:C:384:LYS:HB2	1:C:384:LYS:HE3	1.91	0.43
2:E:434:LEU:O	2:E:438:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:42:ARG:C	3:G:44:TYR:H	2.27	0.43
1:B:147:GLN:OE1	1:B:438:ILE:HD13	2.18	0.42
1:B:209:LYS:NZ	2:E:356:ARG:NH1	2.67	0.42
1:B:479:LEU:HD11	1:B:497:LEU:HD13	2.00	0.42
1:B:489:ILE:HG22	1:B:494:ASP:HB2	2.00	0.42
2:D:445:LEU:HD23	2:D:445:LEU:HA	1.84	0.42
2:E:21:VAL:O	2:E:60:THR:OG1	2.35	0.42
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.35	0.42
1:B:423:ARG:O	1:B:426:GLU:N	2.49	0.42
1:C:374:VAL:HG11	1:C:378:ALA:HB2	2.00	0.42
2:D:70:VAL:HG12	2:D:71:ARG:N	2.33	0.42
2:D:96:ASN:HB2	2:D:100:GLU:N	2.34	0.42
1:A:288:PRO:HA	1:A:289:PRO:HD3	1.87	0.42
1:A:485:THR:C	1:A:487:GLY:N	2.77	0.42
1:B:272:SER:O	1:B:275:ALA:HB3	2.19	0.42
2:D:33:LEU:HD13	2:D:117:HIS:CG	2.55	0.42
1:A:172:GLN:HA	5:A:600:ANP:N3B	2.34	0.42
1:A:398:ARG:HH11	1:A:398:ARG:HD2	1.70	0.42
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.42
1:B:383:MET:SD	1:B:387:ALA:HB2	2.59	0.42
1:C:45:ARG:HA	1:C:45:ARG:HD3	1.40	0.42
1:C:51:GLU:HG2	1:C:52:MET:N	2.34	0.42
1:C:190:ASN:O	1:C:198:LYS:HE2	2.20	0.42
1:C:457:GLU:O	1:C:460:LYS:HB2	2.19	0.42
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.42
2:D:412:ARG:C	2:D:414:LEU:N	2.76	0.42
2:D:412:ARG:O	2:D:415:SER:OG	2.35	0.42
2:F:36:LEU:N	2:F:36:LEU:HD23	2.34	0.42
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.53	0.42
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.42
1:C:390:MET:HE2	1:C:428:LEU:HD11	2.01	0.42
2:D:93:ARG:HE	2:D:108:ILE:HG12	1.83	0.42
2:D:319:ASP:O	2:D:322:PRO:HD2	2.19	0.42
2:F:468:ALA:O	2:F:471:ASP:N	2.52	0.42
1:B:52:MET:HG2	1:B:95:VAL:HG22	2.02	0.42
1:B:235:THR:O	1:B:237:SER:N	2.52	0.42
1:C:338:ILE:O	1:C:341:ASN:N	2.52	0.42
2:D:159:GLY:N	6:D:600:ADP:O3B	2.49	0.42
2:E:343:GLY:O	2:E:345:TYR:HD1	2.02	0.42
2:E:443:GLN:HA	2:E:446:ALA:HB3	2.01	0.42
2:E:443:GLN:O	2:E:446:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:454:GLU:C	2:E:456:ALA:N	2.78	0.42
1:A:293:ALA:HB2	3:G:265:ILE:HD13	2.02	0.42
1:B:175:LYS:H	5:B:600:ANP:PB	2.42	0.42
2:D:188:GLU:O	2:D:222:MET:HG3	2.20	0.42
2:E:385:GLN:NE2	7:E:479:AUR:H203	2.35	0.42
1:A:91:THR:OG1	1:A:93:ALA:HB3	2.20	0.42
1:B:44:LEU:O	1:B:47:VAL:HG22	2.20	0.42
1:B:439:GLU:O	1:B:442:VAL:HG23	2.20	0.42
1:C:239:ALA:HB1	1:C:241:PRO:HD2	2.02	0.42
1:C:303:SER:HB2	2:D:222:MET:HB3	2.02	0.42
1:C:398:ARG:NH1	8:C:625:HOH:O	2.50	0.42
1:B:180:ILE:HD11	1:B:216:LEU:HD21	2.01	0.42
2:D:368:TYR:O	2:D:372:ARG:HG2	2.20	0.42
2:E:253:LEU:O	2:E:306:SER:HA	2.20	0.42
2:F:408:ARG:O	2:F:412:ARG:NH1	2.43	0.42
1:A:97:VAL:N	1:A:127:ARG:O	2.38	0.42
1:B:269:ASP:HA	1:B:270:ASP:HA	1.89	0.42
1:B:291:ARG:HD3	8:B:633:HOH:O	2.19	0.42
1:C:271:LEU:HD23	1:C:271:LEU:HA	1.85	0.42
2:D:64:ASP:CG	2:D:65:GLY:H	2.27	0.42
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.55	0.42
2:D:451:HIS:CD2	2:D:452:LEU:HD23	2.55	0.42
2:F:469:LYS:O	2:F:473:LEU:HG	2.20	0.42
1:C:74:VAL:HG13	1:C:241:PRO:HG3	2.01	0.41
2:E:105:ARG:NH1	8:E:516:HOH:O	2.49	0.41
2:F:96:ASN:HB2	2:F:100:GLU:H	1.85	0.41
2:F:432:VAL:HA	2:F:433:PRO:HD3	1.88	0.41
3:G:266:ILE:HD13	3:G:266:ILE:HG21	1.76	0.41
1:A:69:ASP:O	1:A:70:ASN:HB3	2.20	0.41
1:A:394:LEU:O	1:A:397:TYR:HB3	2.20	0.41
1:B:249:SER:O	1:B:250:GLY:C	2.62	0.41
1:B:438:ILE:HD12	1:B:438:ILE:HA	1.85	0.41
2:D:105:ARG:NH1	2:D:208:LEU:HD23	2.35	0.41
2:D:165:LEU:O	2:D:165:LEU:HG	2.20	0.41
2:E:456:ALA:HB1	2:E:466:ALA:O	2.20	0.41
2:F:89:GLU:CD	2:F:89:GLU:H	2.28	0.41
1:A:130:GLY:HA2	1:A:308:ARG:HH12	1.85	0.41
1:B:76:PHE:O	1:B:242:LEU:HD21	2.20	0.41
1:B:230:ILE:HG22	1:B:231:VAL:N	2.35	0.41
1:C:465:GLU:O	1:C:465:GLU:HG2	2.20	0.41
2:F:12:ARG:HA	2:F:73:GLN:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:188:GLU:H	2:F:221:GLN:NE2	2.18	0.41
3:G:9:ARG:NH2	3:G:242:MET:HE2	2.35	0.41
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.20	0.41
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.27	0.41
1:C:64:LEU:HD12	1:C:64:LEU:HA	1.90	0.41
1:C:76:PHE:CD1	1:C:241:PRO:HB2	2.56	0.41
1:C:505:LEU:O	1:C:508:PHE:HB3	2.21	0.41
2:D:154:LEU:HD13	2:D:165:LEU:HD23	2.02	0.41
1:C:164:ARG:HH11	1:C:164:ARG:HD2	1.49	0.41
2:D:374:VAL:O	2:D:378:LEU:HG	2.21	0.41
2:E:155:PHE:CE1	2:E:310:ILE:HD12	2.55	0.41
2:F:346:PRO:C	2:F:348:VAL:H	2.29	0.41
1:B:199:LEU:HA	1:B:263:HIS:O	2.21	0.41
1:B:255:GLU:HG2	1:B:258:ARG:CZ	2.51	0.41
1:B:336:ALA:HB3	1:B:339:PRO:HD2	2.02	0.41
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.20	0.41
1:C:134:PRO:CD	1:C:258:ARG:HH12	2.33	0.41
1:C:220:LEU:HD23	1:C:220:LEU:HA	1.69	0.41
1:C:469:LEU:HD12	1:C:469:LEU:HA	1.93	0.41
2:E:275:ILE:O	2:E:283:PRO:HG3	2.21	0.41
2:F:298:THR:CG2	2:F:299:THR:N	2.83	0.41
2:F:439:LYS:HE3	2:F:443:GLN:NE2	2.25	0.41
1:B:66:LEU:O	2:F:15:ALA:HA	2.21	0.41
1:C:51:GLU:OE2	1:C:90:ARG:HB3	2.20	0.41
2:E:136:GLY:HA2	2:E:432:VAL:O	2.20	0.41
2:F:342:LEU:HD13	7:F:602:AUR:C10	2.51	0.41
1:A:185:ASN:O	1:A:188:ARG:HG3	2.20	0.41
1:A:483:ILE:HA	8:A:680:HOH:O	2.20	0.41
1:A:485:THR:C	1:A:487:GLY:H	2.29	0.41
1:A:496:LYS:O	1:A:500:ILE:HG13	2.20	0.41
1:B:67:GLU:O	1:B:69:ASP:N	2.54	0.41
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.41
1:B:213:VAL:O	1:B:216:LEU:HB3	2.21	0.41
1:C:283:LEU:HD21	1:C:289:PRO:HB3	2.01	0.41
1:C:420:ARG:HG3	1:C:420:ARG:HH11	1.86	0.41
2:D:281:TYR:HB3	2:D:285:LEU:HD12	2.01	0.41
2:E:35:ALA:HB2	2:E:82:ILE:HG13	2.01	0.41
2:E:65:GLY:C	2:E:67:GLU:H	2.27	0.41
2:E:138:LYS:NZ	2:E:460:VAL:O	2.43	0.41
2:E:173:VAL:HG12	2:E:179:GLY:O	2.20	0.41
2:E:286:ALA:N	8:E:484:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:96:ASN:HD22	2:F:100:GLU:CG	2.34	0.41
1:A:151:LYS:H	1:A:151:LYS:HG2	1.72	0.41
1:B:166:LEU:HD23	1:B:349:GLN:HB3	2.03	0.41
1:C:19:ALA:O	1:C:21:THR:HG23	2.21	0.41
2:D:449:TYR:C	2:D:451:HIS:H	2.28	0.41
2:E:84:ILE:HD13	2:E:235:THR:HG23	2.02	0.41
2:E:96:ASN:HB3	2:E:100:GLU:N	2.26	0.41
2:E:138:LYS:HE3	2:E:416:GLN:HB2	2.02	0.41
1:A:79:ASP:OD1	1:A:79:ASP:N	2.54	0.40
1:A:307:GLU:OE1	2:E:190:THR:HB	2.21	0.40
1:B:48:GLN:HB3	2:F:68:GLY:HA2	2.02	0.40
1:B:363:PRO:C	1:B:365:ILE:N	2.79	0.40
1:B:468:PHE:HB2	1:B:504:PHE:CE2	2.56	0.40
2:D:94:ILE:HD11	2:D:197:TYR:CD1	2.56	0.40
2:D:200:MET:CE	2:D:215:VAL:HG21	2.50	0.40
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.40
2:E:77:ASP:C	2:E:79:GLY:H	2.29	0.40
2:E:281:TYR:CE1	2:E:321:ALA:HB2	2.56	0.40
2:F:89:GLU:CD	2:F:89:GLU:N	2.79	0.40
1:B:28:THR:CG2	1:B:29:GLY:N	2.83	0.40
1:B:244:TYR:O	1:B:247:PRO:HD2	2.21	0.40
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.94	0.40
1:C:52:MET:HE2	1:C:76:PHE:HE2	1.86	0.40
2:D:82:ILE:O	2:D:115:ALA:HA	2.21	0.40
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.50	0.40
2:E:147:ALA:HB2	2:E:357:ILE:HD13	2.04	0.40
2:F:126:MET:HE3	8:F:639:HOH:O	2.21	0.40
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.02	0.40
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.51	0.40
1:A:343:ILE:HG23	1:A:349:GLN:CD	2.46	0.40
1:A:411:ASP:OD1	1:A:413:ALA:N	2.54	0.40
1:A:439:GLU:HG2	1:A:484:ARG:HB2	2.04	0.40
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.40
1:B:157:VAL:N	1:B:158:PRO:CD	2.84	0.40
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.86	0.40
1:C:456:LEU:HD23	1:C:461:ILE:HG12	2.03	0.40
2:D:146:TYR:HB3	2:D:152:ILE:HD11	2.03	0.40
2:D:449:TYR:C	2:D:451:HIS:N	2.79	0.40
2:F:385:GLN:HE22	7:F:602:AUR:C20	2.34	0.40
3:G:261:GLU:O	3:G:264:GLU:N	2.54	0.40
1:B:423:ARG:NE	1:B:458:PRO:HD3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.55	0.40
1:C:163:GLN:O	1:C:322:THR:HG23	2.21	0.40
2:D:381:TYR:O	2:D:385:GLN:HG3	2.22	0.40
2:E:334:VAL:HG23	2:E:353:SER:HA	2.04	0.40
2:F:50:ALA:O	2:F:51:GLN:HB3	2.19	0.40
1:A:56:SER:C	1:A:58:GLY:N	2.79	0.40
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.87	0.40
1:B:454:ASP:C	1:B:456:LEU:H	2.29	0.40
2:F:63:MET:HE3	2:F:63:MET:HB3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/510 (95%)	430 (89%)	44 (9%)	11 (2%)	5	23
1	B	485/510 (95%)	430 (89%)	45 (9%)	10 (2%)	5	25
1	C	490/510 (96%)	438 (89%)	46 (9%)	6 (1%)	10	37
2	D	465/482 (96%)	415 (89%)	45 (10%)	5 (1%)	11	39
2	E	464/482 (96%)	401 (86%)	46 (10%)	17 (4%)	2	15
2	F	464/482 (96%)	422 (91%)	40 (9%)	2 (0%)	30	61
3	G	116/272 (43%)	98 (84%)	16 (14%)	2 (2%)	7	30
All	All	2969/3248 (91%)	2634 (89%)	282 (10%)	53 (2%)	6	28

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	57	SER

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Mol	Chain	Res	Type
1	A	405	GLN
1	B	25	LEU
1	B	364	ALA
1	C	407	GLY
2	E	393	MET
2	E	423	VAL
2	E	424	PHE
1	A	364	ALA
1	B	236	ALA
1	C	332	GLY
1	C	408	SER
1	C	411	ASP
1	C	476	HIS
2	D	28	GLY
2	D	474	ALA
2	E	28	GLY
2	E	161	GLY
2	E	205	VAL
2	E	243	PHE
2	E	455	GLN
3	G	81	ILE
1	A	404	ALA
1	A	409	ASP
1	B	359	LYS
1	B	452	TYR
2	E	347	ALA
2	F	347	ALA
1	A	337	TYR
1	A	484	ARG
1	B	458	PRO
2	E	122	GLU
2	F	327	ALA
1	A	401	ALA
1	A	464	PHE
1	B	315	ALA
1	B	411	ASP
2	E	67	GLU
2	E	175	LYS
2	E	190	THR
2	E	454	GLU
1	B	68	PRO
2	D	405	SER

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Mol	Chain	Res	Type
3	G	43	VAL
1	C	461	ILE
2	E	121	PRO
2	E	279	VAL
1	B	95	VAL
2	D	279	VAL
2	D	107	PRO
2	E	388	ILE
1	A	130	GLY

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	393/412 (95%)	333 (85%)	60 (15%)	3	12
1	B	393/412 (95%)	340 (86%)	53 (14%)	4	16
1	C	397/412 (96%)	355 (89%)	42 (11%)	6	26
2	D	377/386 (98%)	339 (90%)	38 (10%)	7	28
2	E	376/386 (97%)	334 (89%)	42 (11%)	6	24
2	F	376/386 (97%)	341 (91%)	35 (9%)	8	31
3	G	102/230 (44%)	92 (90%)	10 (10%)	7	29
All	All	2414/2624 (92%)	2134 (88%)	280 (12%)	5	22

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	25	LEU
1	A	34	ILE
1	A	38	ILE
1	A	40	ARG
1	A	45	ARG
1	A	48	GLN
1	A	50	GLU

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Mol	Chain	Res	Type
1	A	56	SER
1	A	79	ASP
1	A	80	LYS
1	A	88	VAL
1	A	89	LYS
1	A	94	ILE
1	A	99	VAL
1	A	101	GLU
1	A	102	GLU
1	A	103	LEU
1	A	121	ILE
1	A	123	SER
1	A	129	VAL
1	A	140	ILE
1	A	142	VAL
1	A	147	GLN
1	A	151	LYS
1	A	159	ILE
1	A	164	ARG
1	A	173	THR
1	A	175	LYS
1	A	188	ARG
1	A	193	THR
1	A	195	GLU
1	A	206	ILE
1	A	211	SER
1	A	219	ARG
1	A	270	ASP
1	A	334	VAL
1	A	344	SER
1	A	367	VAL
1	A	371	VAL
1	A	380	THR
1	A	386	VAL
1	A	393	GLU
1	A	409	ASP
1	A	417	LEU
1	A	418	LEU
1	A	420	ARG
1	A	436	MET
1	A	439	GLU
1	A	442	VAL

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Mol	Chain	Res	Type
1	A	444	VAL
1	A	449	VAL
1	A	453	LEU
1	A	455	LYS
1	A	457	GLU
1	A	472	VAL
1	A	473	ILE
1	A	479	LEU
1	A	485	THR
1	A	489	ILE
1	B	38	ILE
1	B	47	VAL
1	B	60	LYS
1	B	79	ASP
1	B	80	LYS
1	B	87	ILE
1	B	97	VAL
1	B	99	VAL
1	B	123	SER
1	B	137	ILE
1	B	141	SER
1	B	143	ARG
1	B	171	ARG
1	B	173	THR
1	B	186	GLN
1	B	188	ARG
1	B	189	PHE
1	B	193	THR
1	B	211	SER
1	B	216	LEU
1	B	217	VAL
1	B	218	LYS
1	B	221	THR
1	B	227	LYS
1	B	307	GLU
1	B	349	GLN
1	B	351	PHE
1	B	361	ILE
1	B	371	VAL
1	B	374	VAL
1	B	376	SER
1	B	380	THR

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Mol	Chain	Res	Type
1	B	392	LEU
1	B	398	ARG
1	B	400	VAL
1	B	414	THR
1	B	416	GLN
1	B	419	SER
1	B	423	ARG
1	B	430	GLN
1	B	442	VAL
1	B	444	VAL
1	B	454	ASP
1	B	456	LEU
1	B	472	VAL
1	B	474	SER
1	B	476	HIS
1	B	479	LEU
1	B	482	LYS
1	B	484	ARG
1	B	485	THR
1	B	490	SER
1	B	505	LEU
1	C	45	ARG
1	C	47	VAL
1	C	56	SER
1	C	63	SER
1	C	64	LEU
1	C	83	LYS
1	C	87	ILE
1	C	91	THR
1	C	97	VAL
1	C	99	VAL
1	C	101	GLU
1	C	139	ARG
1	C	144	GLU
1	C	175	LYS
1	C	195	GLU
1	C	211	SER
1	C	216	LEU
1	C	217	VAL
1	C	227	LYS
1	C	245	LEU
1	C	267	ILE

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Mol	Chain	Res	Type
1	C	276	VAL
1	C	298	VAL
1	C	301	LEU
1	C	334	VAL
1	C	338	ILE
1	C	349	GLN
1	C	399	GLU
1	C	400	VAL
1	C	406	PHE
1	C	414	THR
1	C	440	GLU
1	C	444	VAL
1	C	462	THR
1	C	469	LEU
1	C	474	SER
1	C	477	GLN
1	C	479	LEU
1	C	485	THR
1	C	501	VAL
1	C	502	THR
1	C	505	LEU
2	D	27	GLU
2	D	56	SER
2	D	67	GLU
2	D	89	GLU
2	D	95	MET
2	D	97	VAL
2	D	111	LYS
2	D	112	GLN
2	D	137	ILE
2	D	139	VAL
2	D	166	ILE
2	D	190	THR
2	D	199	GLU
2	D	205	VAL
2	D	223	ASN
2	D	232	VAL
2	D	249	GLN
2	D	266	SER
2	D	279	VAL
2	D	306	SER
2	D	336	SER

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Mol	Chain	Res	Type
2	D	361	ASN
2	D	365	SER
2	D	388	ILE
2	D	393	MET
2	D	397	SER
2	D	400	ASP
2	D	403	THR
2	D	405	SER
2	D	410	ILE
2	D	415	SER
2	D	420	VAL
2	D	423	VAL
2	D	428	LEU
2	D	431	LEU
2	D	439	LYS
2	D	452	LEU
2	D	475	GLU
2	E	9	THR
2	E	36	LEU
2	E	67	GLU
2	E	89	GLU
2	E	95	MET
2	E	127	SER
2	E	128	VAL
2	E	132	ILE
2	E	133	LEU
2	E	139	VAL
2	E	142	LEU
2	E	148	LYS
2	E	164	VAL
2	E	182	VAL
2	E	188	GLU
2	E	194	ASN
2	E	213	SER
2	E	215	VAL
2	E	223	ASN
2	E	282	GLN
2	E	293	GLN
2	E	297	THR
2	E	333	THR
2	E	344	ILE
2	E	358	MET

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Mol	Chain	Res	Type
2	E	365	SER
2	E	385	GLN
2	E	387	ILE
2	E	391	LEU
2	E	393	MET
2	E	394	ASP
2	E	395	GLU
2	E	411	GLN
2	E	425	THR
2	E	431	LEU
2	E	438	ILE
2	E	450	ASP
2	E	452	LEU
2	E	455	GLN
2	E	463	ILE
2	E	467	VAL
2	E	473	LEU
2	F	34	ASN
2	F	36	LEU
2	F	42	GLU
2	F	67	GLU
2	F	89	GLU
2	F	93	ARG
2	F	95	MET
2	F	97	VAL
2	F	112	GLN
2	F	127	SER
2	F	137	ILE
2	F	139	VAL
2	F	166	ILE
2	F	191	ARG
2	F	200	MET
2	F	201	ILE
2	F	205	VAL
2	F	208	LEU
2	F	223	ASN
2	F	232	VAL
2	F	258	ILE
2	F	268	VAL
2	F	279	VAL
2	F	292	MET
2	F	357	ILE

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Mol	Chain	Res	Type
2	F	386	ASP
2	F	387	ILE
2	F	393	MET
2	F	397	SER
2	F	405	SER
2	F	410	ILE
2	F	423	VAL
2	F	428	LEU
2	F	455	GLN
2	F	467	VAL
3	G	4	LYS
3	G	20	THR
3	G	22	SER
3	G	77	LEU
3	G	82	HIS
3	G	85	VAL
3	G	211	ASN
3	G	221	THR
3	G	254	ARG
3	G	258	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	208	GLN
1	A	215	GLN
1	A	396	GLN
1	A	430	GLN
1	A	476	HIS
1	B	65	ASN
1	B	215	GLN
1	B	430	GLN
1	B	466	ASN
1	B	503	ASN
1	C	70	ASN
1	C	260	ASN
1	C	416	GLN
2	D	171	ASN
2	D	221	GLN
2	D	223	ASN
2	D	442	GLN

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Mol	Chain	Res	Type
2	E	39	GLN
2	E	130	GLN
2	E	221	GLN
2	E	223	ASN
2	E	246	GLN
2	E	282	GLN
2	E	379	GLN
2	E	385	GLN
2	E	442	GLN
2	E	455	GLN
2	F	34	ASN
2	F	51	GLN
2	F	96	ASN
2	F	194	ASN
2	F	221	GLN
2	F	223	ASN
2	F	249	GLN
2	F	282	GLN
2	F	293	GLN
2	F	308	GLN
2	F	443	GLN
3	G	82	HIS
3	G	225	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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
5	ANP	A	600	4	33,33,33	1.68	7 (21%)	45,52,52	2.06	10 (22%)
5	ANP	C	600	4	33,33,33	1.73	8 (24%)	45,52,52	1.72	7 (15%)
5	ANP	F	600	4	33,33,33	1.59	8 (24%)	45,52,52	2.25	6 (13%)
6	ADP	D	600	4	28,29,29	1.25	2 (7%)	43,45,45	1.32	5 (11%)
7	AUR	E	479	-	33,35,35	1.74	6 (18%)	32,52,52	2.01	10 (31%)
5	ANP	B	600	4	33,33,33	1.37	7 (21%)	45,52,52	1.86	7 (15%)
7	AUR	F	602	-	33,35,35	1.37	4 (12%)	32,52,52	2.04	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	A	600	4	-	3/18/38/38	0/3/3/3
5	ANP	C	600	4	-	9/18/38/38	0/3/3/3
5	ANP	F	600	4	-	5/18/38/38	0/3/3/3
6	ADP	D	600	4	-	1/16/32/32	0/3/3/3
7	AUR	E	479	-	-	2/17/55/55	0/4/3/3
5	ANP	B	600	4	-	2/18/38/38	0/3/3/3
7	AUR	F	602	-	-	2/17/55/55	0/4/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	479	AUR	C7-C8	-5.35	1.47	1.53
5	A	600	ANP	PA-O3A	5.30	1.65	1.59
5	C	600	ANP	PB-O3A	5.12	1.65	1.59
5	F	600	ANP	PA-O3A	4.89	1.64	1.59
5	C	600	ANP	PA-O3A	4.76	1.64	1.59
5	A	600	ANP	PB-O3A	4.50	1.64	1.59
7	F	602	AUR	C7-C8	-4.06	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	479	AUR	O5-C5	-4.04	1.36	1.44
7	F	602	AUR	O5-C5	-3.91	1.36	1.44
6	D	600	ADP	PA-O3A	3.87	1.63	1.59
7	E	479	AUR	O15-C19	-3.33	1.32	1.39
7	F	602	AUR	O15-C19	-3.23	1.33	1.39
5	F	600	ANP	O3'-C3'	-3.13	1.35	1.43
5	C	600	ANP	PG-O3G	-3.10	1.48	1.56
7	E	479	AUR	O4-C8	3.09	1.48	1.44
7	E	479	AUR	O3-C6	3.03	1.51	1.45
5	B	600	ANP	PB-O2B	-2.95	1.49	1.56
5	B	600	ANP	PA-O3A	2.94	1.62	1.59
5	A	600	ANP	PG-O3G	-2.80	1.49	1.56
5	C	600	ANP	PG-O2G	-2.67	1.49	1.56
5	B	600	ANP	PG-O2G	-2.60	1.49	1.56
7	F	602	AUR	O3-C6	2.59	1.50	1.45
5	A	600	ANP	PB-O2B	-2.56	1.50	1.56
5	C	600	ANP	PG-O1G	2.50	1.50	1.46
5	F	600	ANP	PG-O3G	-2.46	1.50	1.56
5	F	600	ANP	PA-O5'	-2.42	1.49	1.59
5	C	600	ANP	PA-O5'	-2.39	1.50	1.59
5	A	600	ANP	C2-N1	-2.33	1.29	1.33
5	B	600	ANP	PA-O5'	-2.29	1.50	1.59
5	C	600	ANP	O5'-C5'	-2.28	1.36	1.44
5	B	600	ANP	PG-O1G	2.25	1.49	1.46
5	F	600	ANP	PB-O2B	-2.25	1.50	1.56
5	A	600	ANP	PG-O2G	-2.22	1.50	1.56
5	A	600	ANP	PA-O5'	-2.22	1.50	1.59
5	F	600	ANP	PB-O3A	2.18	1.61	1.59
5	F	600	ANP	PG-O2G	-2.18	1.51	1.56
5	B	600	ANP	PG-O3G	-2.16	1.51	1.56
5	B	600	ANP	PB-O3A	2.09	1.61	1.59
5	C	600	ANP	PB-O2B	-2.08	1.51	1.56
6	D	600	ADP	PA-O5'	-2.08	1.51	1.59
7	E	479	AUR	C21-C6	-2.00	1.47	1.52
5	F	600	ANP	PA-O2A	-2.00	1.46	1.55

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	600	ANP	O1G-PG-N3B	-9.57	97.68	111.77
5	F	600	ANP	O2G-PG-O3G	6.91	126.17	107.59
5	A	600	ANP	O2B-PB-O1B	6.40	123.61	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	ANP	O2G-PG-O3G	6.10	124.00	107.59
5	A	600	ANP	O2G-PG-O1G	5.89	128.21	113.45
5	C	600	ANP	O2B-PB-O1B	5.86	122.44	109.87
5	A	600	ANP	O1G-PG-N3B	-5.79	103.24	111.77
7	F	602	AUR	O4-C8-C7	5.36	115.78	110.28
5	F	600	ANP	O2B-PB-O1B	5.27	121.17	109.87
7	E	479	AUR	C17-C18-C19	-5.16	115.25	120.29
5	B	600	ANP	O2G-PG-O1G	-5.01	100.89	113.45
5	B	600	ANP	O1B-PB-N3B	4.99	119.11	111.77
7	E	479	AUR	O7-C7-C8	4.47	118.41	109.90
5	C	600	ANP	O1G-PG-N3B	-4.41	105.28	111.77
7	F	602	AUR	O5-C25-C24	4.31	118.77	111.09
7	F	602	AUR	C5-O5-C25	-4.14	111.37	117.65
7	F	602	AUR	C17-C18-C19	-4.08	116.30	120.29
7	F	602	AUR	O5-C25-O25	-3.99	115.28	122.99
5	B	600	ANP	O1G-PG-N3B	-3.96	105.93	111.77
6	D	600	ADP	O4'-C1'-N9	-3.89	100.62	108.09
7	E	479	AUR	C20-C4-C3	-3.87	106.91	113.54
5	C	600	ANP	O2G-PG-O3G	3.81	117.83	107.59
5	C	600	ANP	O3A-PA-O1A	-3.77	99.35	110.70
5	A	600	ANP	O3A-PA-O1A	3.57	121.45	110.70
5	F	600	ANP	O1B-PB-N3B	3.40	116.78	111.77
5	F	600	ANP	O2G-PG-O1G	-3.34	105.08	113.45
5	A	600	ANP	O1B-PB-N3B	-3.31	106.89	111.77
7	E	479	AUR	O25-C25-C24	-3.25	113.26	124.77
5	A	600	ANP	O2G-PG-O3G	-3.20	98.98	107.59
5	B	600	ANP	O2B-PB-O1B	3.03	116.37	109.87
5	B	600	ANP	O3A-PA-O1A	-2.98	101.73	110.70
5	C	600	ANP	O2G-PG-O1G	-2.95	106.05	113.45
6	D	600	ADP	O2A-PA-O3A	-2.83	99.62	107.27
7	E	479	AUR	O15-C19-C18	2.72	120.98	117.09
5	C	600	ANP	C4-N9-C1'	-2.71	120.29	126.63
7	F	602	AUR	C20-C4-C3	-2.70	108.91	113.54
7	E	479	AUR	C22-C16-C15	-2.51	120.29	122.97
7	E	479	AUR	C8-C9-C10	2.48	130.92	125.88
5	F	600	ANP	O3A-PB-N3B	-2.44	99.84	106.59
5	A	600	ANP	O2'-C2'-C3'	2.32	119.25	111.82
7	F	602	AUR	O25-C25-C24	-2.25	116.79	124.77
5	B	600	ANP	N3-C2-N1	2.22	131.95	128.58
6	D	600	ADP	N3-C2-N1	2.17	131.87	128.58
7	E	479	AUR	O7-C7-C6	2.17	114.58	109.87
5	A	600	ANP	C2'-C1'-N9	-2.14	107.99	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	602	AUR	C13-C12-C11	-2.12	119.82	124.72
5	C	600	ANP	C1'-N9-C8	2.11	131.78	127.09
7	E	479	AUR	C7-C8-C9	-2.10	110.07	112.75
5	A	600	ANP	O5'-C5'-C4'	2.10	116.13	108.99
6	D	600	ADP	C2-N3-C4	-2.09	106.74	111.83
6	D	600	ADP	O2B-PB-O1B	2.05	118.84	110.83
7	E	479	AUR	O5-C25-O25	-2.03	119.06	122.99
5	A	600	ANP	O2A-PA-O3A	-2.01	101.84	107.27

There are no chirality outliers.

All (24) torsion outliers are listed below:

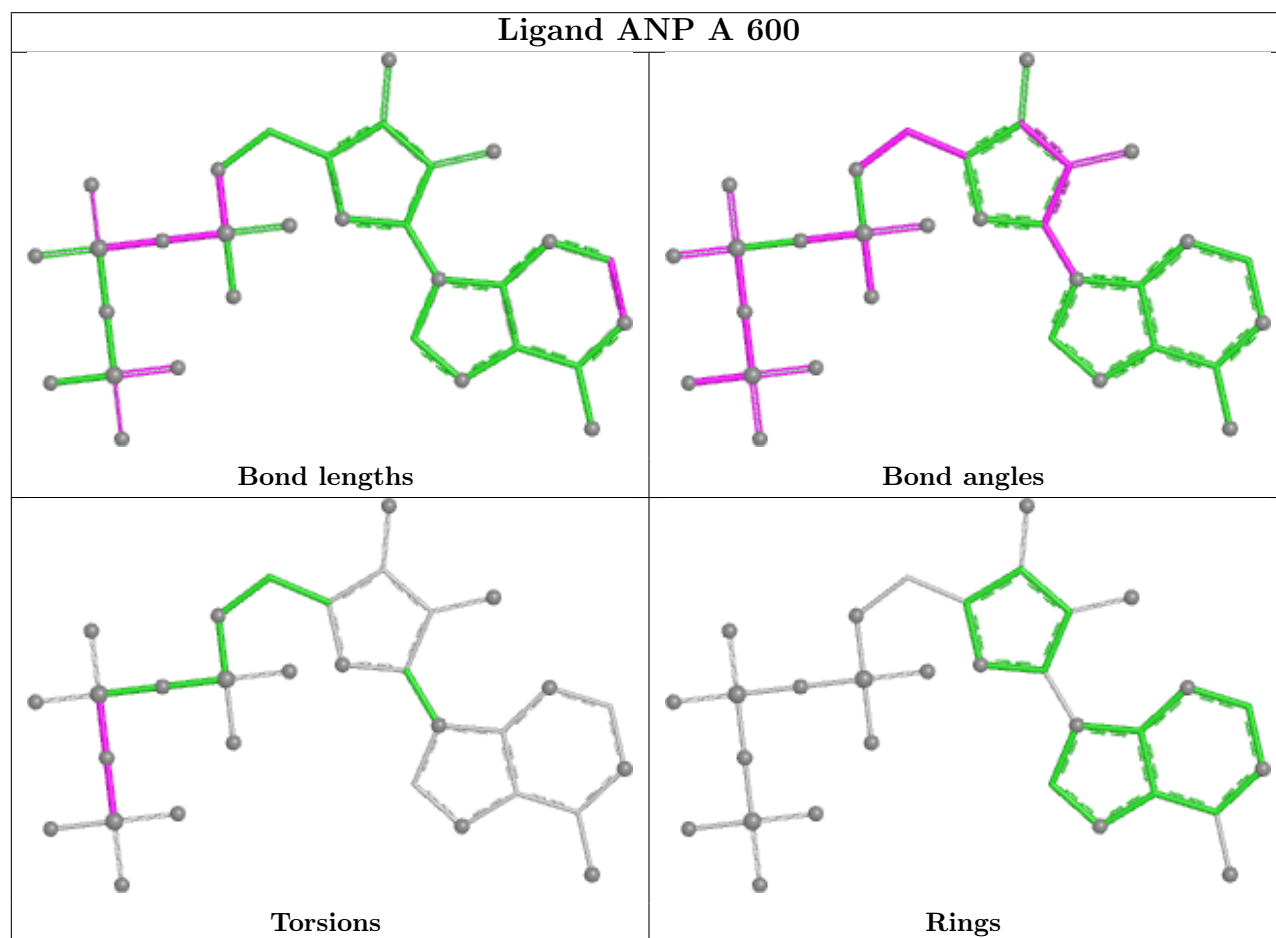
Mol	Chain	Res	Type	Atoms
5	A	600	ANP	PB-N3B-PG-O1G
5	A	600	ANP	PG-N3B-PB-O1B
5	A	600	ANP	PG-N3B-PB-O3A
5	B	600	ANP	PB-N3B-PG-O1G
5	B	600	ANP	PG-N3B-PB-O1B
5	C	600	ANP	PB-N3B-PG-O1G
5	C	600	ANP	PG-N3B-PB-O1B
5	C	600	ANP	PA-O3A-PB-O2B
5	C	600	ANP	C5'-O5'-PA-O1A
5	C	600	ANP	C5'-O5'-PA-O2A
5	F	600	ANP	PB-N3B-PG-O1G
5	F	600	ANP	PG-N3B-PB-O1B
5	F	600	ANP	PG-N3B-PB-O3A
5	F	600	ANP	PA-O3A-PB-O2B
7	F	602	AUR	C1-C2-C3-O3
7	E	479	AUR	C24-C25-O5-C5
5	C	600	ANP	C5'-O5'-PA-O3A
5	C	600	ANP	O4'-C4'-C5'-O5'
6	D	600	ADP	PA-O3A-PB-O3B
5	F	600	ANP	PA-O3A-PB-O1B
5	C	600	ANP	C3'-C4'-C5'-O5'
7	E	479	AUR	C1-C2-C3-O3
5	C	600	ANP	PG-N3B-PB-O3A
7	F	602	AUR	C18-C17-O17-C23

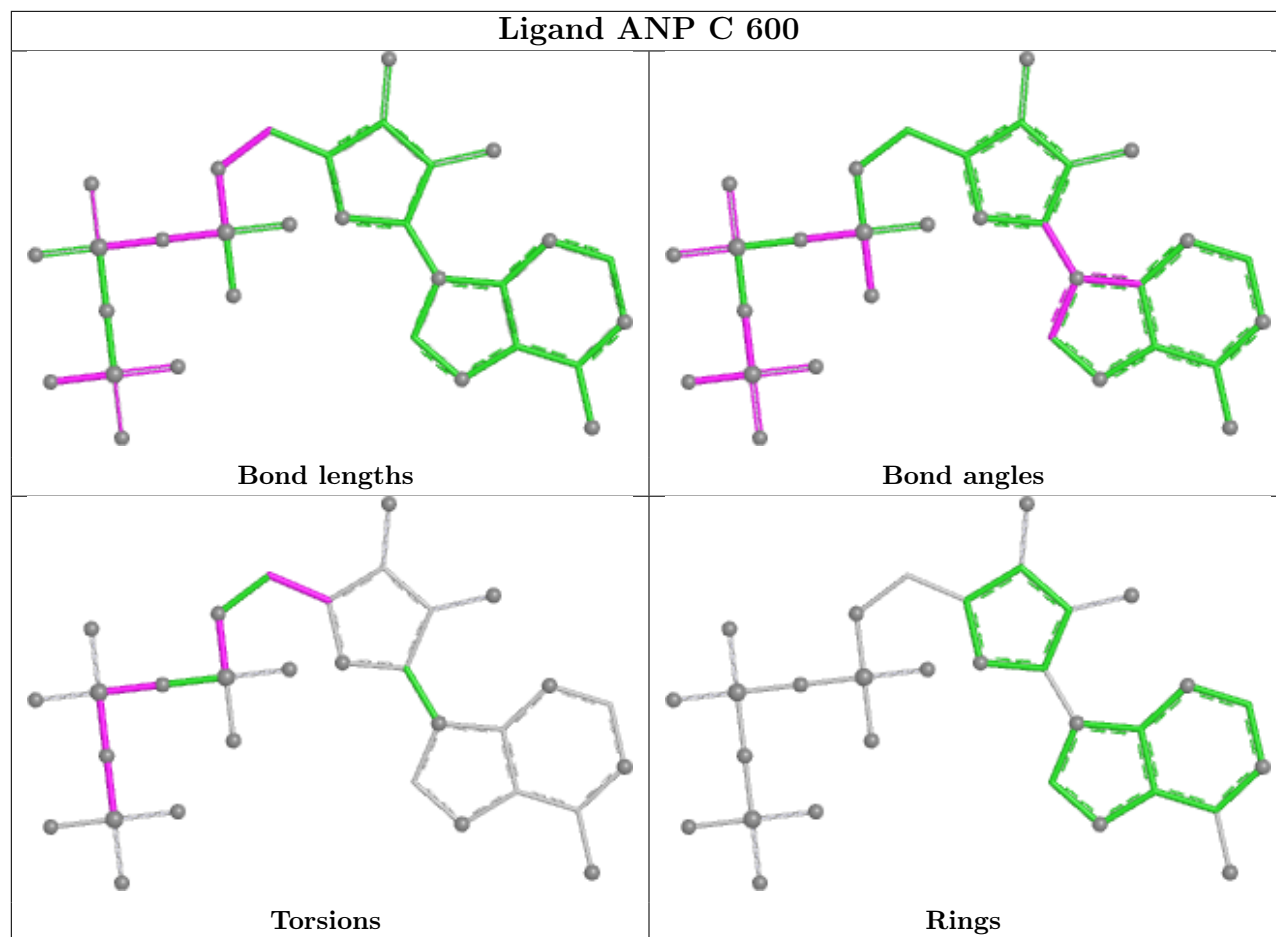
There are no ring outliers.

7 monomers are involved in 38 short contacts:

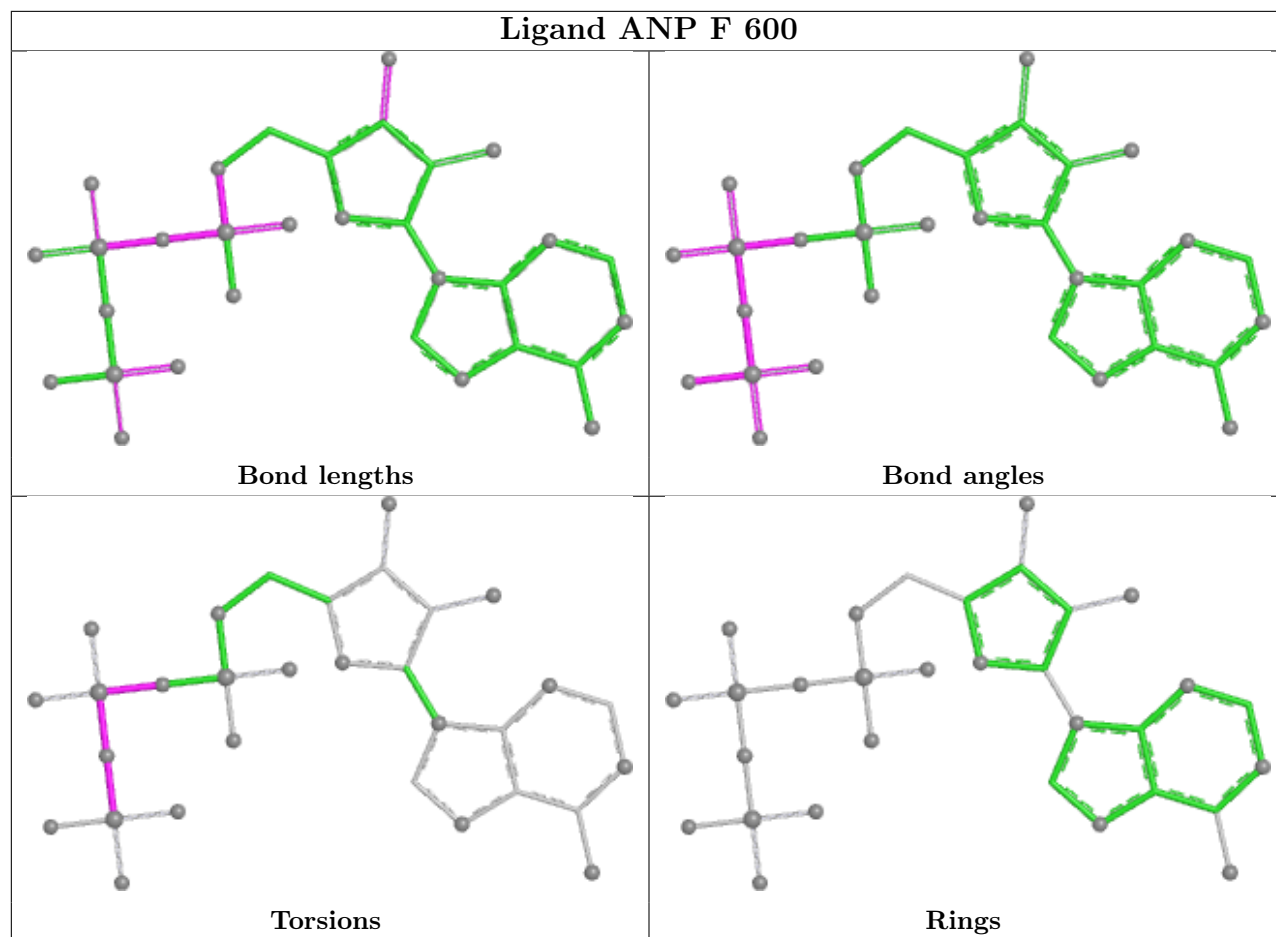
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ANP	1	0
5	C	600	ANP	4	0
5	F	600	ANP	2	0
6	D	600	ADP	3	0
7	E	479	AUR	14	0
5	B	600	ANP	8	0
7	F	602	AUR	6	0

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.

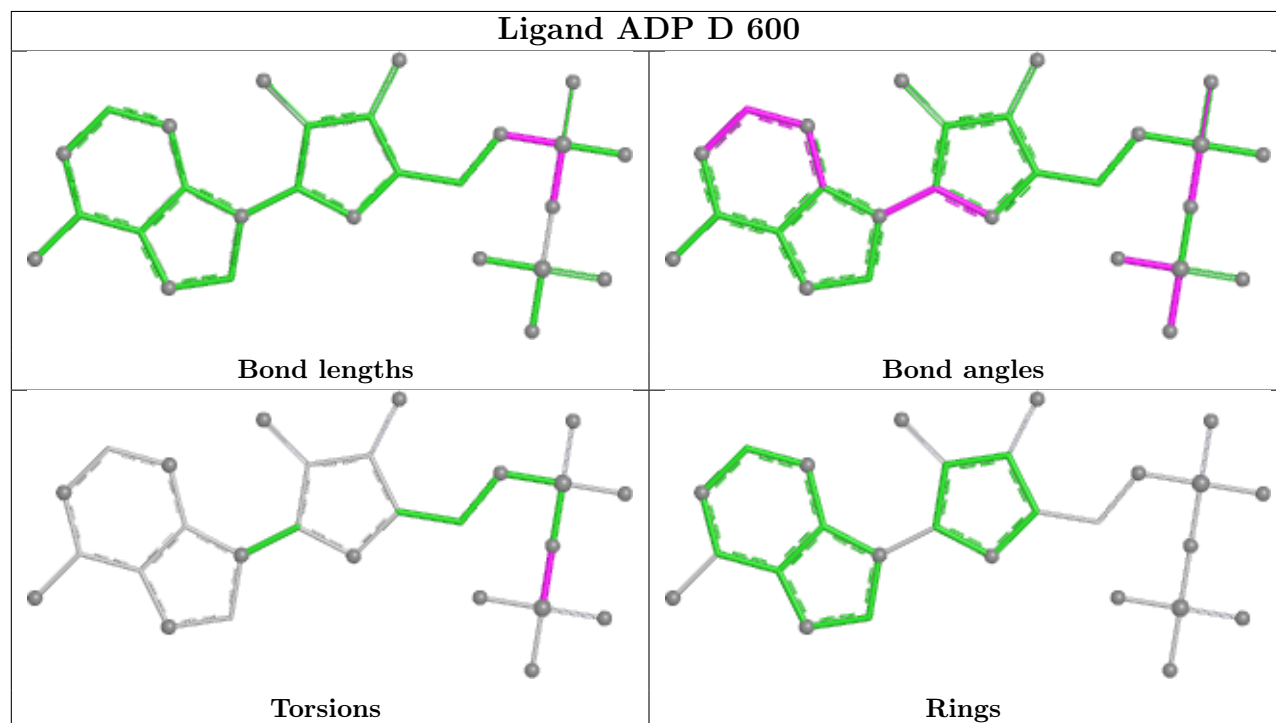


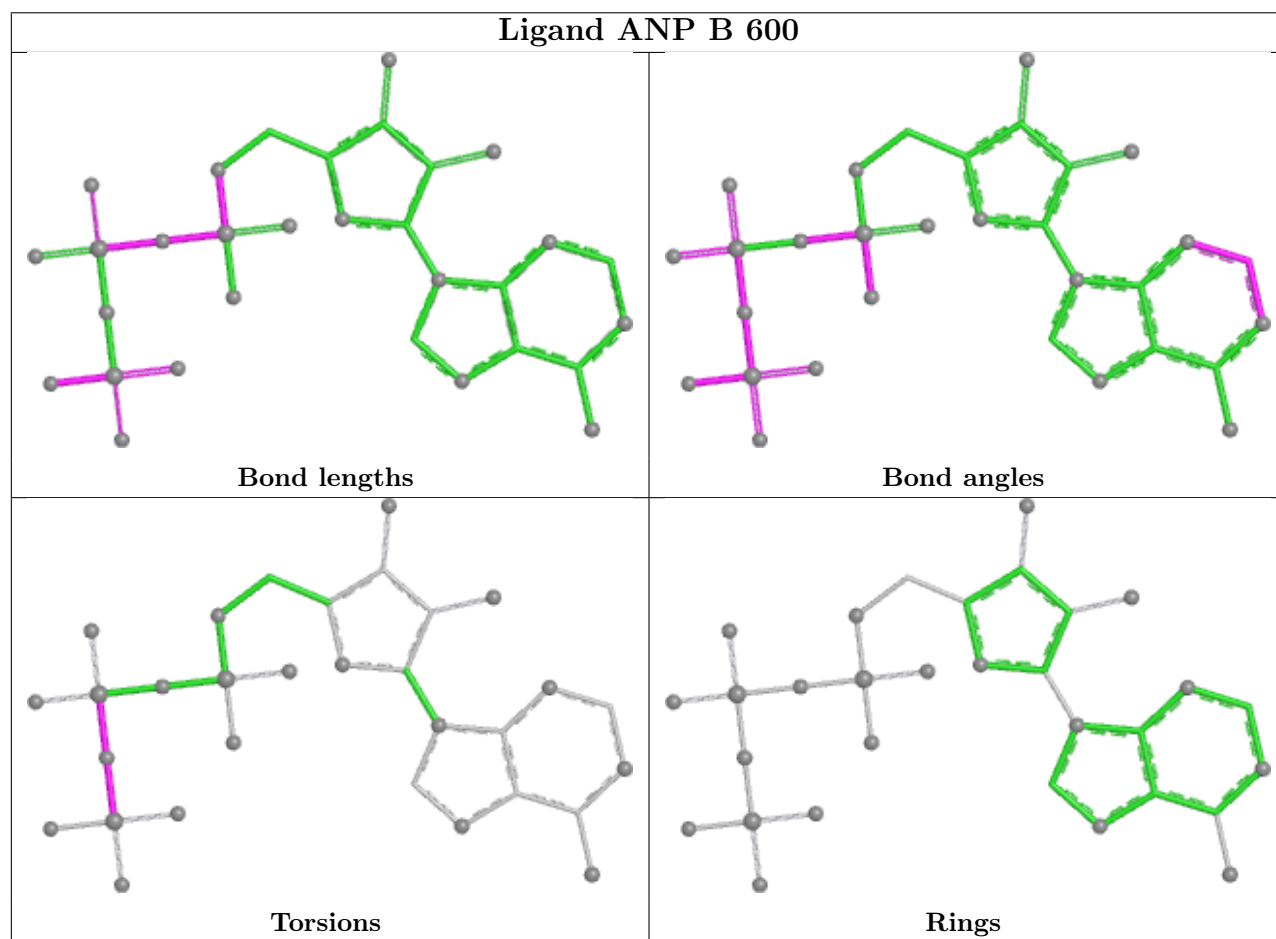
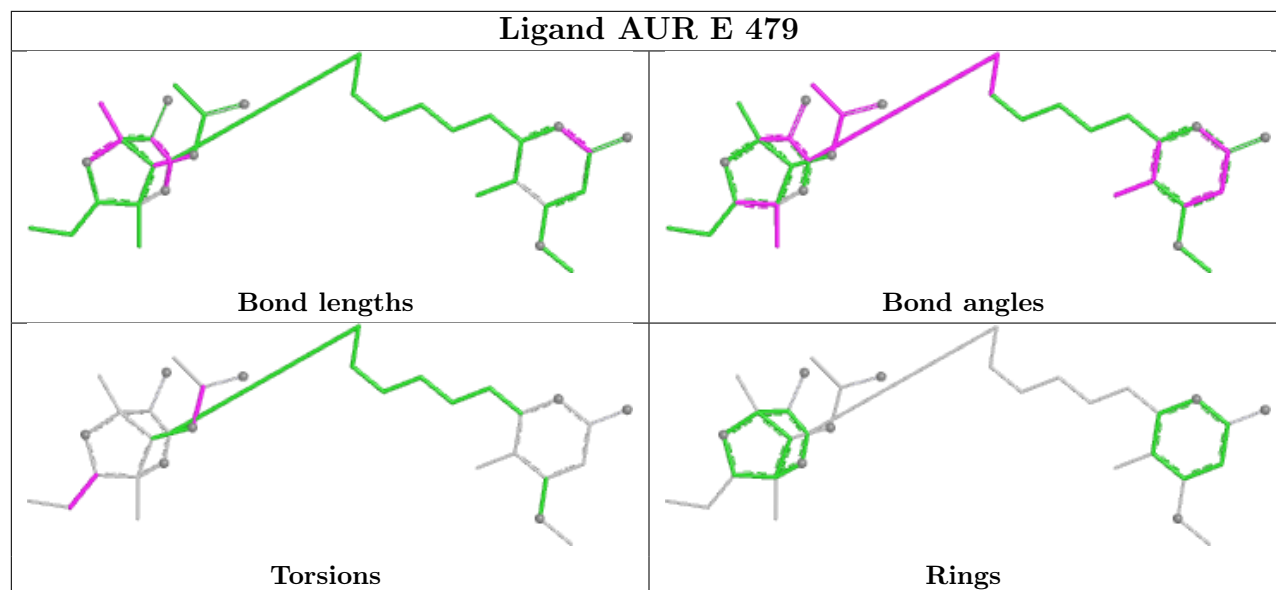


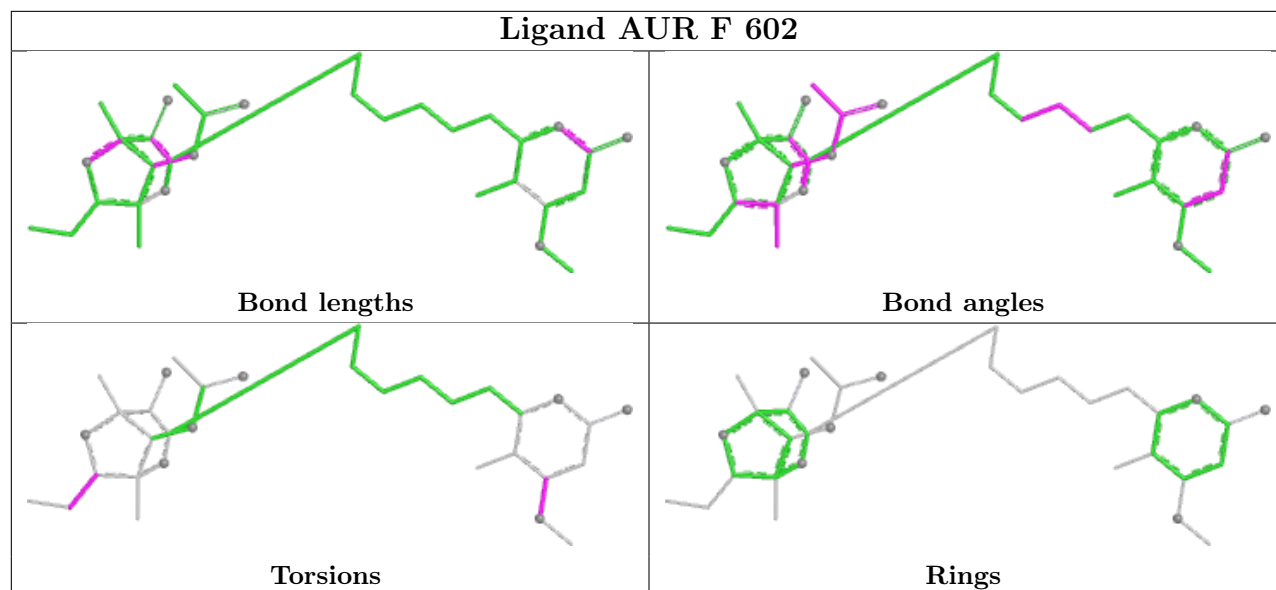
Ligand ANP F 600



Ligand ADP D 600







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	487/510 (95%)	0.00	10 (2%) 63 42	4, 40, 81, 100	0
1	B	487/510 (95%)	0.01	11 (2%) 61 39	1, 35, 93, 100	0
1	C	492/510 (96%)	-0.15	7 (1%) 73 53	7, 30, 71, 100	0
2	D	467/482 (96%)	0.10	15 (3%) 50 30	8, 37, 87, 100	0
2	E	466/482 (96%)	0.33	13 (2%) 55 34	3, 53, 100, 100	0
2	F	466/482 (96%)	-0.14	3 (0%) 85 70	3, 30, 76, 91	0
3	G	122/272 (44%)	1.00	23 (18%) 3 1	7, 79, 100, 100	0
All	All	2987/3248 (91%)	0.06	82 (2%) 56 35	1, 38, 92, 100	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	510	ALA	4.3
3	G	86	ALA	4.1
3	G	26	VAL	4.0
3	G	25	MET	3.8
2	D	396	LEU	3.7
1	C	408	SER	3.7
1	A	93	ALA	3.5
2	E	390	ILE	3.4
3	G	209	LEU	3.3
3	G	29	ALA	3.3
2	D	9	THR	3.3
2	E	389	ALA	3.2
2	E	388	ILE	3.2
1	A	94	ILE	3.2
2	D	390	ILE	3.2
2	D	473	LEU	3.1
1	B	403	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	414	THR	3.0
1	A	406	PHE	3.0
2	E	387	ILE	3.0
3	G	218	LYS	2.9
1	C	332	GLY	2.9
1	A	405	GLN	2.9
3	G	41	ALA	2.9
2	D	395	GLU	2.9
3	G	85	VAL	2.8
3	G	43	VAL	2.8
2	F	9	THR	2.8
1	B	510	ALA	2.7
1	B	408	SER	2.7
3	G	216	SER	2.7
3	G	24	LYS	2.6
3	G	213	ILE	2.6
1	B	406	PHE	2.6
2	D	391	LEU	2.6
3	G	12	SER	2.6
1	C	409	ASP	2.5
3	G	40	PRO	2.5
1	C	406	PHE	2.5
3	G	214	TYR	2.5
2	F	249	GLN	2.5
1	B	404	ALA	2.5
2	D	393	MET	2.5
1	A	408	SER	2.5
1	B	400	VAL	2.4
2	E	386	ASP	2.4
1	C	414	THR	2.3
2	D	403	THR	2.3
2	E	474	ALA	2.3
3	G	210	ALA	2.3
2	F	393	MET	2.3
2	E	444	ILE	2.3
2	E	384	LEU	2.3
2	D	394	ASP	2.3
1	B	401	ALA	2.2
1	C	413	ALA	2.2
3	G	27	ALA	2.2
2	D	441	PHE	2.2
3	G	211	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	453	PRO	2.2
1	B	452	TYR	2.2
2	D	402	LEU	2.2
2	D	440	GLY	2.2
3	G	7	THR	2.2
2	E	108	ILE	2.2
1	B	360	GLY	2.2
3	G	90	LYS	2.2
2	E	9	THR	2.1
3	G	44	TYR	2.1
1	A	402	ALA	2.1
1	A	489	ILE	2.1
2	D	431	LEU	2.1
1	B	192	GLY	2.1
2	D	407	ALA	2.1
2	D	249	GLN	2.1
1	A	140	ILE	2.0
2	E	396	LEU	2.0
3	G	89	MET	2.0
1	C	193	THR	2.0
2	E	381	TYR	2.0
3	G	221	THR	2.0
1	B	416	GLN	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](#)

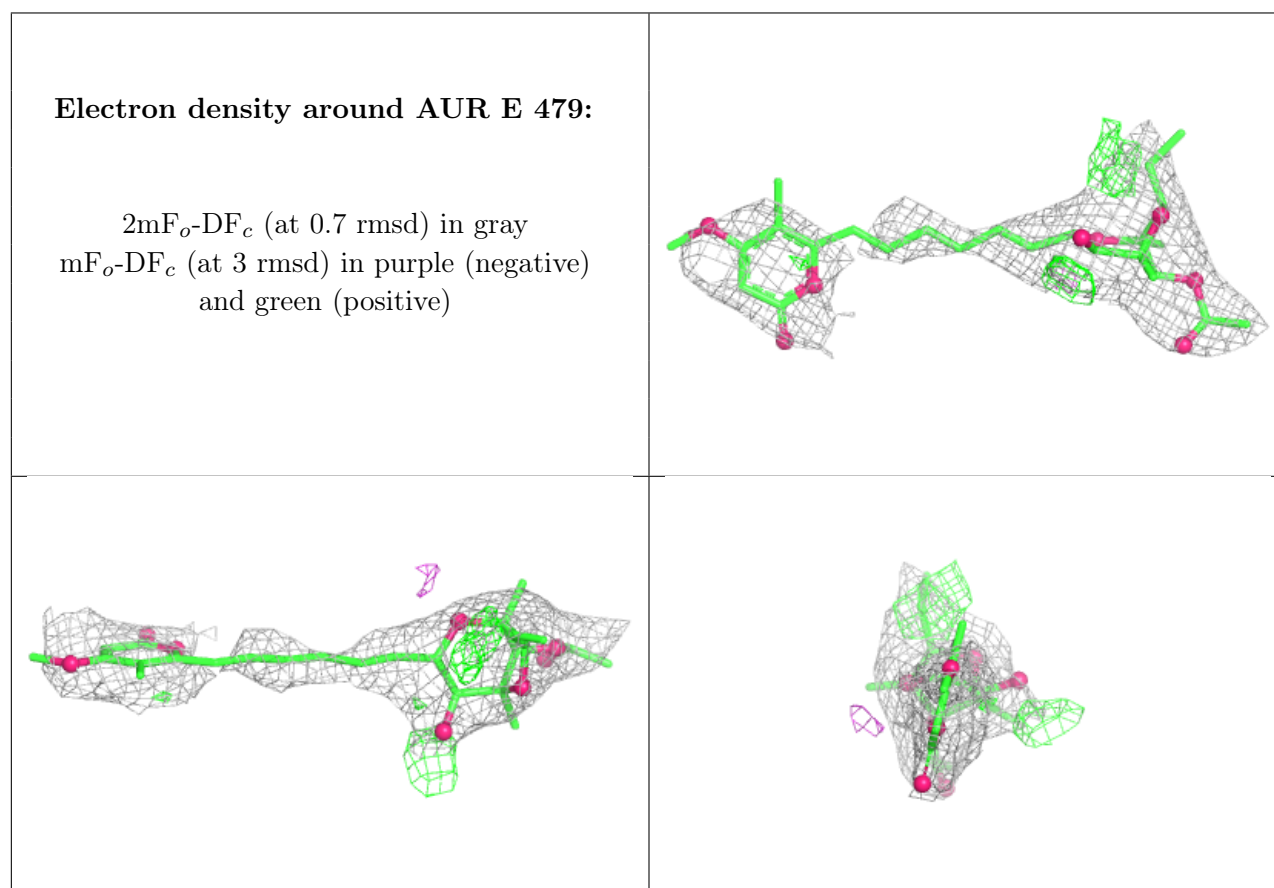
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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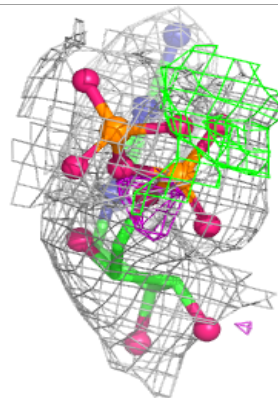
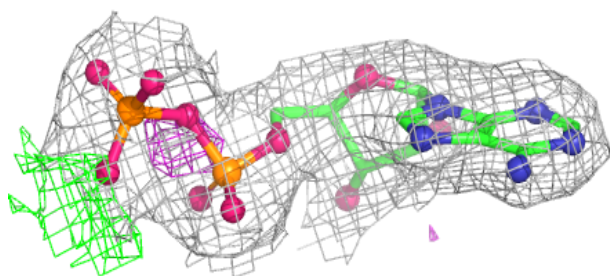
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	AUR	E	479	33/33	0.81	0.26	61,64,87,87	33
4	MG	B	601	1/1	0.83	0.13	35,35,35,35	0
4	MG	F	601	1/1	0.92	0.15	19,19,19,19	0
6	ADP	D	600	27/27	0.94	0.09	16,30,34,36	0
4	MG	C	601	1/1	0.94	0.07	19,19,19,19	0
4	MG	A	601	1/1	0.95	0.10	14,14,14,14	0
7	AUR	F	602	33/33	0.95	0.11	16,22,53,56	33
5	ANP	F	600	31/31	0.96	0.08	21,25,34,36	0
4	MG	D	601	1/1	0.96	0.23	16,16,16,16	0
5	ANP	B	600	31/31	0.96	0.08	18,37,44,47	0
5	ANP	C	600	31/31	0.96	0.08	7,20,25,27	0
5	ANP	A	600	31/31	0.97	0.08	17,31,44,45	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.

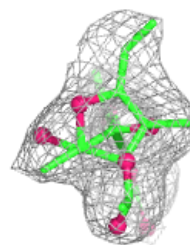
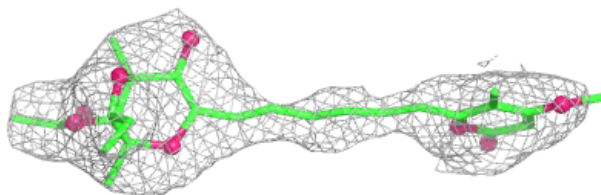
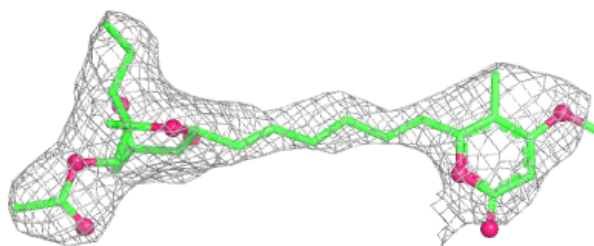


Electron density around ADP D 600:

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

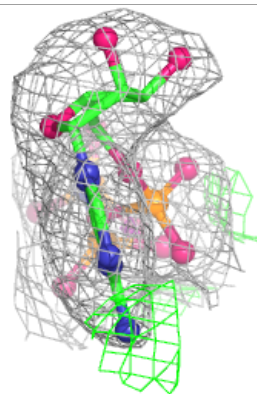
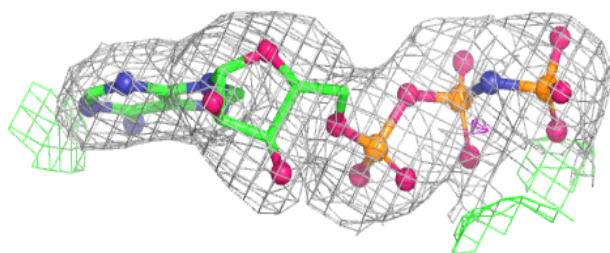
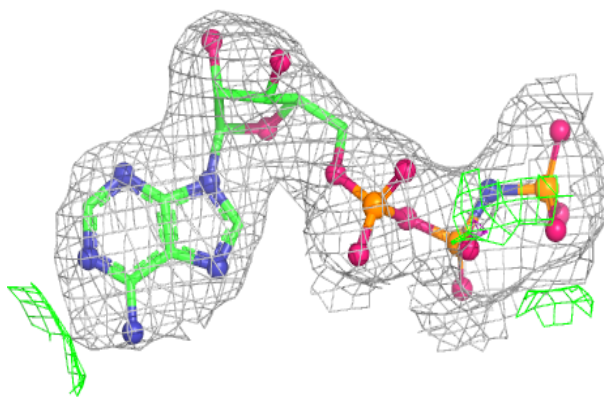
**Electron density around AUR F 602:**

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

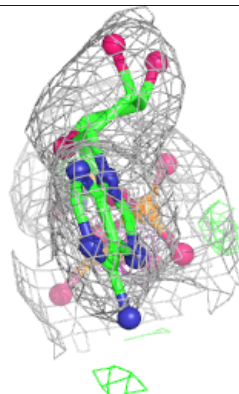
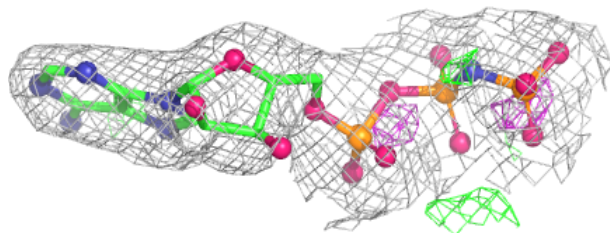
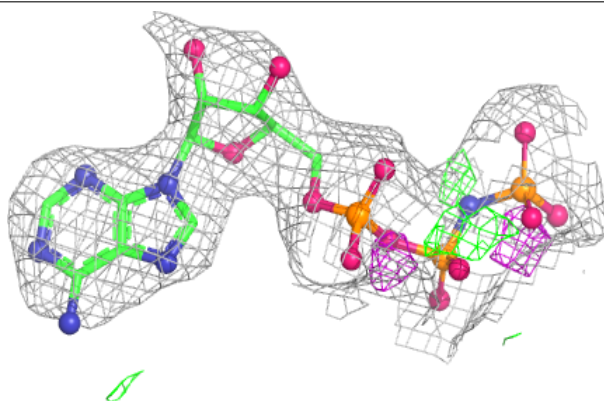


Electron density around ANP F 600:

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

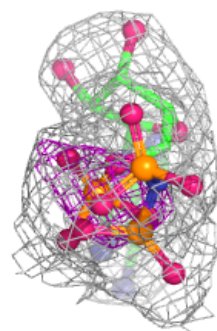
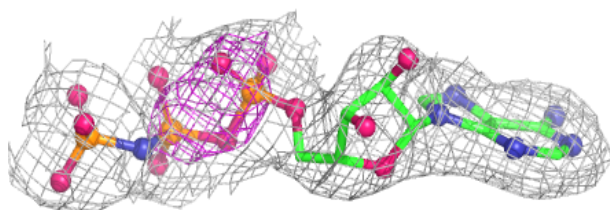
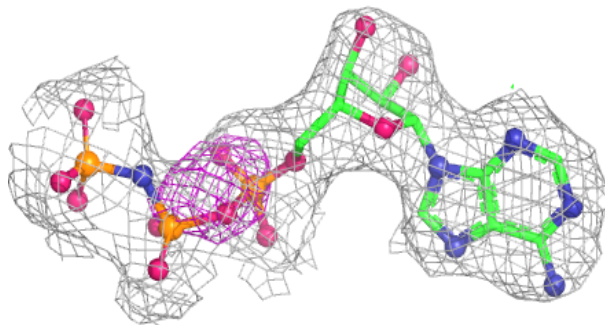
**Electron density around ANP B 600:**

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

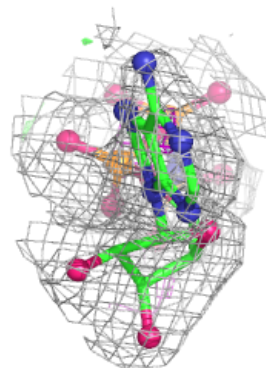
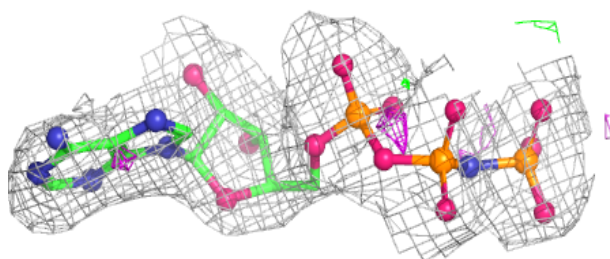
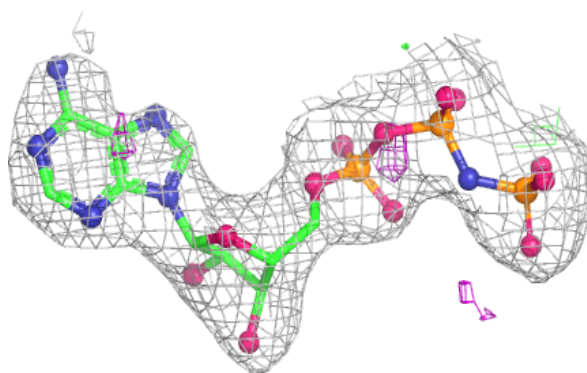


Electron density around ANP C 600:

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

**Electron density around ANP A 600:**

$2mF_o-DF_c$ (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.