



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 10:53 AM EDT

PDB ID : 2ZPA
Title : Crystal Structure of tRNA(Met) Cytidine Acetyltransferase
Authors : Chimnaronk, S.; Manita, T.; Yao, M.; Tanaka, I.
Deposited on : 2008-07-08
Resolution : 2.35 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

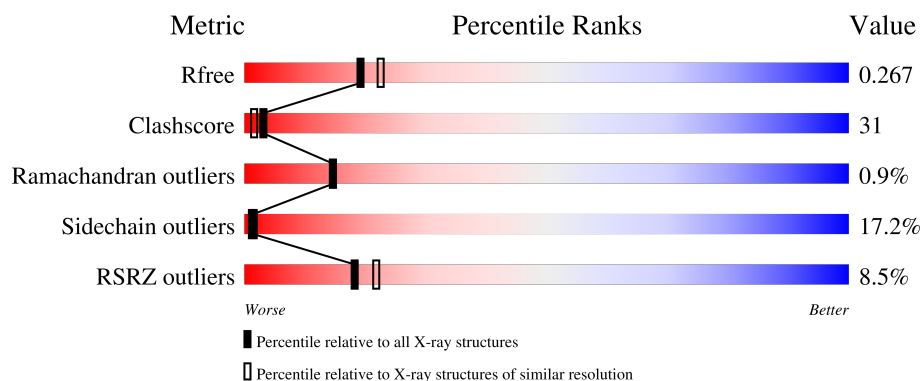
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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	671	<div> <div>3%</div> <div>61%</div> <div>29%</div> <div>8%</div> <div>.</div> </div>
1	B	671	<div> <div>13%</div> <div>48%</div> <div>38%</div> <div>11%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACO	A	700	X	-	-	-
2	ACO	B	701	X	-	-	-

2 Entry composition [i](#)

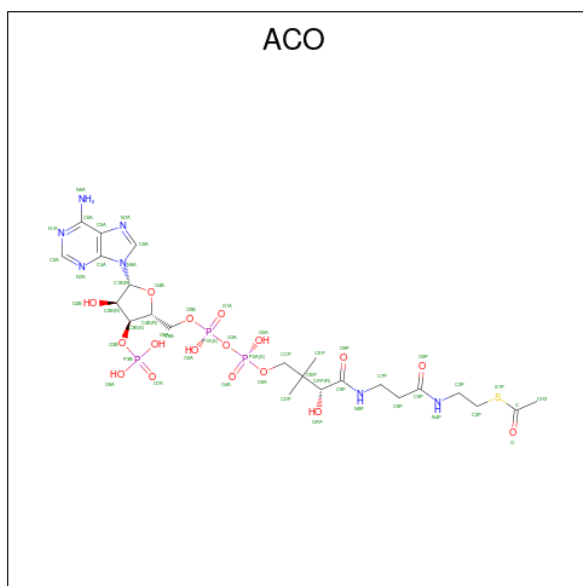
There are 5 unique types of molecules in this entry. The entry contains 10891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein ypfl.

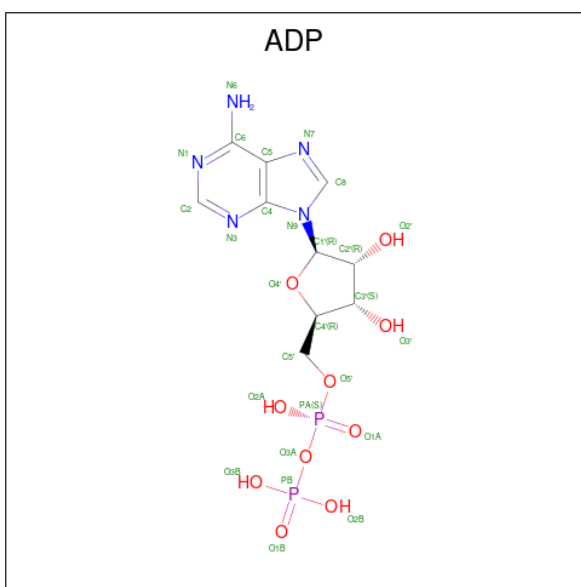
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	658	Total	C	N	O	S	Se	0	0	0
			5189	3291	951	929	8	10			
1	B	662	Total	C	N	O	S	Se	0	0	0
			5218	3309	955	935	8	11			

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



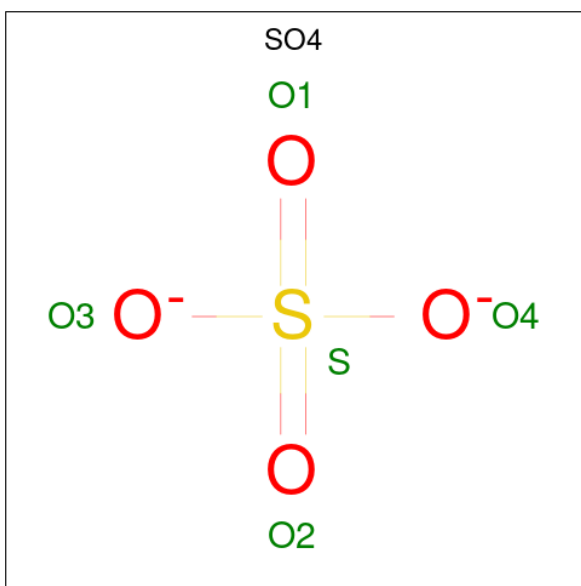
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

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



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

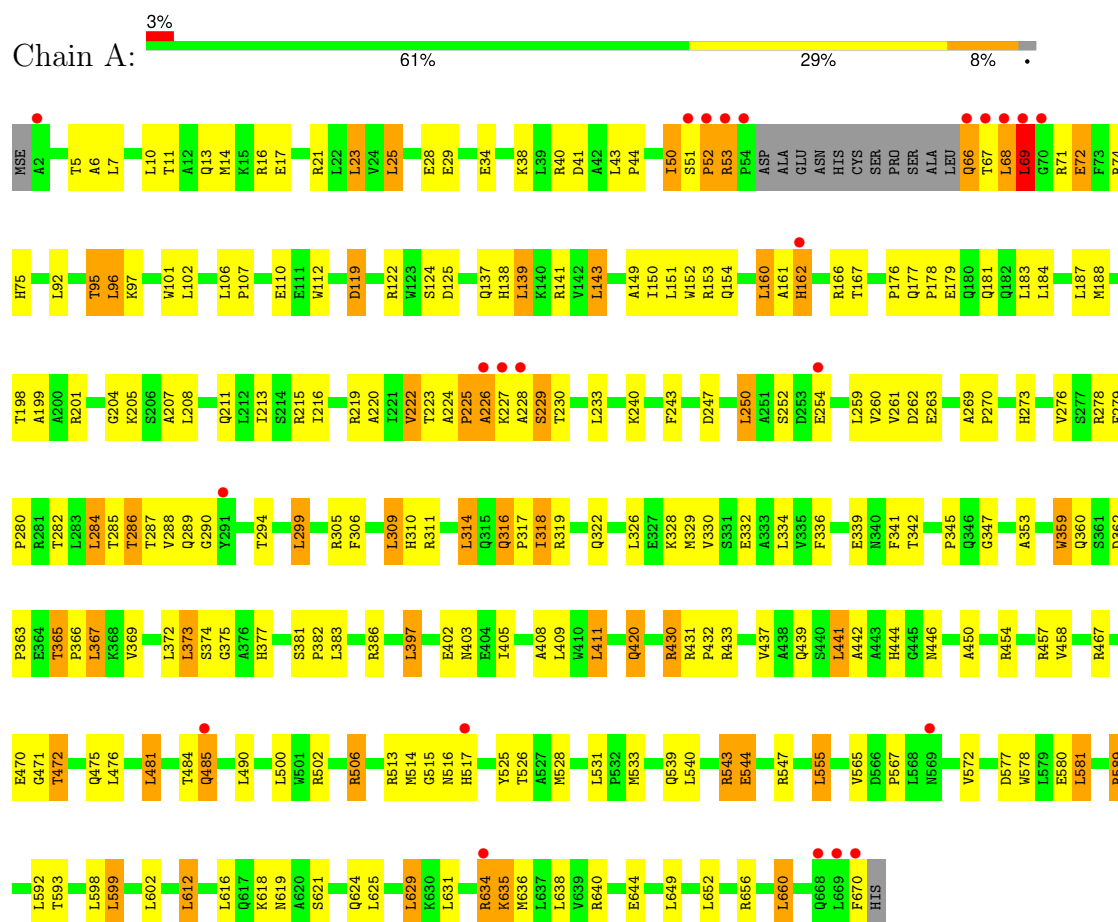
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	224	Total 224	O 224	0	0
5	B	126	Total 126	O 126	0	0

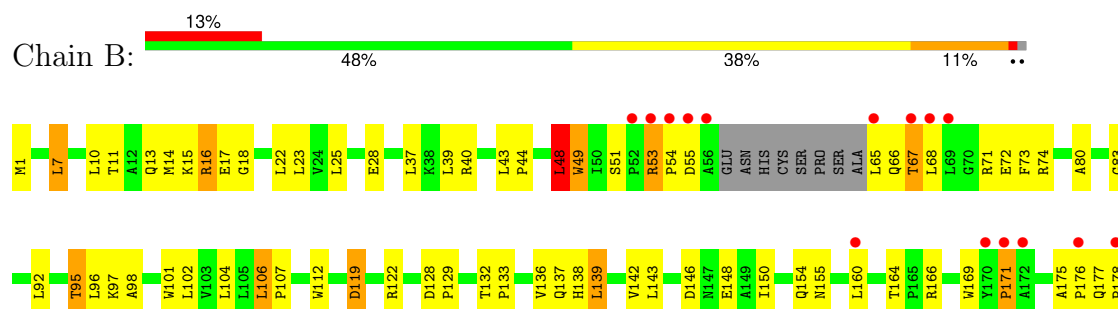
3 Residue-property plots [i](#)

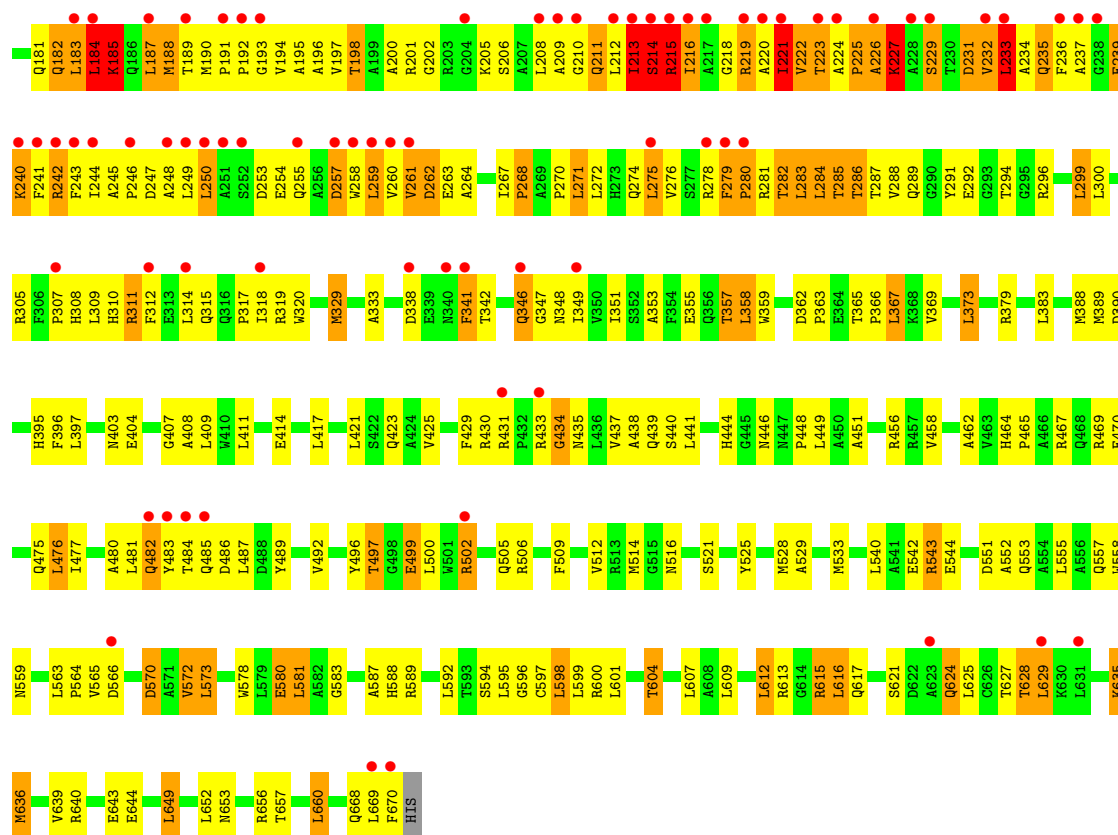
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Uncharacterized protein ypfI



• Molecule 1: Uncharacterized protein ypfI





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.30Å 100.99Å 263.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-2.35) 96.1 (20.00-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.49 (at 2.37Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.274 0.227 , 0.267	Depositor DCC
R_{free} test set	5079 reflections (7.68%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10891	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ACO, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/5306	0.77	7/7197 (0.1%)
1	B	0.49	2/5335 (0.0%)	0.82	16/7236 (0.2%)
All	All	0.48	2/10641 (0.0%)	0.79	23/14433 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	GLN	C-N	5.74	1.47	1.34
1	B	617	GLN	N-CA	5.51	1.57	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	CD-NE-CZ	14.20	143.47	123.60
1	A	66	GLN	C-N-CA	-10.02	96.65	121.70
1	B	49	TRP	N-CA-CB	9.03	126.86	110.60
1	B	187	LEU	N-CA-C	-8.68	87.57	111.00
1	A	226	ALA	N-CA-C	-8.12	89.08	111.00
1	B	213	ILE	C-N-CA	-7.18	103.76	121.70
1	A	52	PRO	CA-N-CD	-6.68	102.15	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	LEU	C-N-CA	6.47	137.88	121.70
1	B	226	ALA	N-CA-C	-6.12	94.48	111.00
1	B	213	ILE	CA-C-N	6.10	130.62	117.20
1	B	270	PRO	CA-N-CD	-5.87	103.29	111.50
1	A	52	PRO	N-CA-C	5.80	127.17	112.10
1	B	434	GLY	N-CA-C	-5.79	98.62	113.10
1	A	397	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	66	GLN	CA-C-N	5.53	129.37	117.20
1	B	185	LYS	C-N-CA	-5.43	108.12	121.70
1	B	227	LYS	N-CA-C	5.40	125.57	111.00
1	B	54	PRO	N-CA-C	-5.28	98.36	112.10
1	B	214	SER	CA-C-N	5.28	128.82	117.20
1	B	171	PRO	CA-N-CD	-5.26	104.14	111.50
1	B	617	GLN	N-CA-CB	-5.24	101.16	110.60
1	B	270	PRO	CA-C-N	-5.23	105.69	117.20
1	B	669	LEU	CB-CA-C	-5.08	100.55	110.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	TRP	Mainchain
1	B	48	LEU	Peptide
1	B	656	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	5189	0	5151	230	0
1	B	5218	0	5183	413	0
2	A	51	0	30	3	0
2	B	51	0	33	7	0
3	A	27	0	12	2	0
4	B	5	0	0	1	0
5	A	224	0	0	13	0
5	B	126	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10891	0	10409	643	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 31.

All (643) 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:A:67:THR:CG2	1:A:71:ARG:HD3	1.36	1.51
1:B:185:LYS:HG3	1:B:215:ARG:NH2	1.51	1.25
1:B:274:GLN:HB3	1:B:278:ARG:NH2	1.62	1.14
1:B:221:ILE:HG23	1:B:259:LEU:HA	1.34	1.08
1:B:215:ARG:NH1	1:B:215:ARG:HG3	1.60	1.08
1:A:506:ARG:NH1	1:A:506:ARG:HG3	1.52	1.08
1:A:67:THR:CG2	1:A:71:ARG:CD	2.31	1.07
1:B:215:ARG:HG3	1:B:215:ARG:HH11	1.08	1.07
1:A:250:LEU:HD13	1:A:278:ARG:HH22	1.18	1.07
1:B:185:LYS:CG	1:B:215:ARG:HH21	1.66	1.06
1:B:11:THR:HA	1:B:14:MSE:HE3	1.10	1.05
1:B:184:LEU:HD11	1:B:211:GLN:HG2	1.38	1.04
1:A:506:ARG:HH11	1:A:506:ARG:CG	1.70	1.04
1:B:214:SER:HB2	1:B:240:LYS:HG3	1.38	1.04
1:A:67:THR:HG21	1:A:71:ARG:CD	1.89	1.03
1:B:185:LYS:HB2	1:B:215:ARG:HE	1.21	1.03
1:A:506:ARG:HG3	1:A:506:ARG:HH11	0.89	1.02
1:B:10:LEU:HG	1:B:14:MSE:HE2	1.41	1.00
1:A:11:THR:HA	1:A:14:MSE:HE2	1.03	1.00
1:A:514:MSE:HE2	1:A:525:TYR:HB3	1.43	1.00
1:B:192:PRO:HA	1:B:281:ARG:HG2	1.43	1.00
1:B:458:VAL:HB	1:B:492:VAL:HG22	1.43	0.98
1:A:67:THR:HG22	1:A:67:THR:O	1.63	0.98
1:B:484:THR:HG23	1:B:533:MSE:HE1	1.44	0.97
1:B:612:LEU:O	1:B:616:LEU:HD12	1.64	0.97
1:B:359:TRP:CZ3	1:B:367:LEU:HD13	2.00	0.96
1:A:67:THR:HG21	1:A:71:ARG:HD3	0.99	0.96
1:B:497:THR:HG22	1:B:500:LEU:H	1.27	0.96
1:B:11:THR:CA	1:B:14:MSE:HE3	1.95	0.96
1:B:213:ILE:CG2	1:B:237:ALA:HB1	1.96	0.95
1:B:185:LYS:CB	1:B:215:ARG:HE	1.81	0.94
1:A:11:THR:HA	1:A:14:MSE:CE	1.98	0.93
1:A:514:MSE:HE2	1:A:525:TYR:CB	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLN:HB3	1:B:278:ARG:HH22	1.29	0.92
1:B:264:ALA:CB	1:B:284:LEU:HD11	1.99	0.91
1:B:184:LEU:HD11	1:B:211:GLN:CG	2.01	0.91
1:B:274:GLN:CB	1:B:278:ARG:HH22	1.84	0.90
1:A:250:LEU:HD22	1:A:278:ARG:HH21	1.36	0.90
1:B:264:ALA:HB3	1:B:284:LEU:HD11	1.54	0.89
1:B:346:GLN:HE21	1:B:346:GLN:HA	1.38	0.88
1:B:500:LEU:HD21	2:B:701:ACO:H21	1.55	0.88
2:A:700:ACO:H8A	2:A:700:ACO:O5B	1.73	0.88
1:B:223:THR:HG23	1:B:246:PRO:HD3	1.56	0.87
1:B:359:TRP:HZ3	1:B:367:LEU:HD13	1.36	0.87
1:A:11:THR:CA	1:A:14:MSE:HE2	1.98	0.87
1:B:274:GLN:CB	1:B:278:ARG:NH2	2.38	0.87
1:B:185:LYS:HB2	1:B:215:ARG:NE	1.90	0.86
1:A:226:ALA:HA	5:A:821:HOH:O	1.74	0.86
1:A:67:THR:HG23	1:A:71:ARG:HD3	1.55	0.85
1:B:430:ARG:HH11	1:B:670:PHE:HE1	1.24	0.85
1:B:214:SER:CB	1:B:240:LYS:HG3	2.05	0.85
1:B:365:THR:HB	1:B:366:PRO:HD3	1.55	0.85
1:B:215:ARG:NH1	1:B:215:ARG:O	2.10	0.85
1:B:262:ASP:HA	1:B:285:THR:HG23	1.59	0.84
1:B:289:GLN:CG	1:B:296:ARG:HH11	1.91	0.84
1:B:185:LYS:HG3	1:B:215:ARG:HH21	0.74	0.84
1:B:573:LEU:HD22	1:B:604:THR:HG21	1.60	0.83
1:B:311:ARG:HH11	1:B:311:ARG:HG3	1.43	0.83
1:B:11:THR:HA	1:B:14:MSE:CE	2.03	0.83
1:A:250:LEU:HD22	1:A:278:ARG:NH2	1.94	0.83
1:A:634:ARG:NH1	1:A:638:LEU:HB2	1.93	0.82
1:B:178:PRO:O	1:B:182:GLN:HG3	1.80	0.82
1:A:621:SER:OG	1:A:624:GLN:HG3	1.80	0.80
1:A:289:GLN:HG3	1:A:290:GLY:H	1.45	0.80
1:A:198:THR:HG21	1:A:311:ARG:HH21	1.47	0.80
1:B:7:LEU:HD13	1:B:160:LEU:CD2	2.12	0.80
1:A:471:GLY:O	1:A:475:GLN:HG3	1.81	0.80
1:B:244:ILE:HD11	1:B:248:ALA:HB3	1.64	0.80
1:A:250:LEU:HA	1:A:278:ARG:NH2	1.97	0.79
1:B:68:LEU:HG	1:B:71:ARG:HH12	1.46	0.79
1:B:215:ARG:NH1	1:B:215:ARG:CG	2.40	0.79
1:B:497:THR:HG23	1:B:499:GLU:HG3	1.64	0.79
1:B:262:ASP:HA	1:B:285:THR:CG2	2.12	0.79
1:A:67:THR:HG22	1:A:71:ARG:HD3	1.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LEU:HB3	1:B:282:THR:HG23	1.65	0.79
1:B:215:ARG:HH11	1:B:215:ARG:C	1.87	0.79
1:A:441:LEU:HD13	1:A:528:MSE:HE1	1.63	0.78
1:B:214:SER:C	1:B:216:ILE:H	1.87	0.78
1:B:212:LEU:HD12	1:B:212:LEU:H	1.47	0.78
1:B:497:THR:HG22	1:B:500:LEU:N	1.99	0.78
1:B:183:LEU:O	1:B:183:LEU:HD22	1.83	0.77
1:A:359:TRP:HZ3	1:A:367:LEU:HD13	1.48	0.77
1:B:7:LEU:HD13	1:B:160:LEU:HD22	1.66	0.77
1:B:190:MSE:HE2	1:B:258:TRP:CH2	2.19	0.77
1:B:213:ILE:HB	1:B:237:ALA:CB	2.14	0.77
1:B:215:ARG:O	1:B:215:ARG:CG	2.32	0.77
1:B:329:MSE:HE2	1:B:333:ALA:HB2	1.67	0.77
1:B:185:LYS:CE	1:B:189:THR:HA	2.15	0.77
1:A:634:ARG:O	1:A:634:ARG:HD3	1.85	0.76
1:B:215:ARG:NH1	1:B:216:ILE:HA	2.00	0.76
1:B:213:ILE:CB	1:B:237:ALA:HB1	2.15	0.76
1:B:275:LEU:CD2	1:B:279:PHE:HE2	2.00	0.75
1:B:213:ILE:HB	1:B:237:ALA:HB1	1.66	0.75
1:B:184:LEU:HD11	1:B:211:GLN:HB3	1.68	0.74
1:A:250:LEU:HD13	1:A:278:ARG:NH2	2.00	0.74
1:A:160:LEU:HD22	1:A:161:ALA:O	1.87	0.74
1:A:634:ARG:HD2	5:A:913:HOH:O	1.88	0.74
1:B:318:ILE:HD11	5:B:1017:HOH:O	1.87	0.74
1:B:215:ARG:HG3	1:B:215:ARG:O	1.87	0.73
1:B:624:GLN:O	1:B:628:THR:HG22	1.88	0.73
1:A:228:ALA:O	1:A:229:SER:C	2.26	0.73
1:B:188:MSE:HE1	1:B:283:LEU:HG	1.71	0.73
1:B:250:LEU:HD21	1:B:271:LEU:HD21	1.69	0.73
1:B:289:GLN:CD	1:B:296:ARG:HH11	1.91	0.73
1:B:214:SER:HB2	1:B:240:LYS:HZ3	1.51	0.73
1:B:309:LEU:HD23	1:B:310:HIS:N	2.03	0.72
1:B:184:LEU:HD11	1:B:211:GLN:CB	2.19	0.72
1:B:221:ILE:CG2	1:B:259:LEU:HA	2.18	0.72
1:B:215:ARG:HH11	1:B:215:ARG:CG	1.88	0.72
1:B:213:ILE:O	1:B:216:ILE:HG22	1.90	0.72
1:B:209:ALA:CB	1:B:233:LEU:HD21	2.20	0.72
1:B:231:ASP:O	1:B:235:GLN:HB3	1.91	0.71
1:A:437:VAL:HG13	1:A:528:MSE:HE3	1.73	0.71
1:B:636:MSE:HG2	5:B:980:HOH:O	1.88	0.71
1:B:240:LYS:HD3	1:B:240:LYS:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LYS:HD3	1:A:230:THR:HG21	1.72	0.71
1:B:185:LYS:HG3	1:B:215:ARG:CZ	2.21	0.70
1:B:268:PRO:HD3	1:B:521:SER:O	1.90	0.70
1:A:386:ARG:NH1	5:A:957:HOH:O	2.23	0.70
1:A:28:GLU:HG3	1:A:154:GLN:OE1	1.91	0.70
1:B:138:HIS:HB2	1:B:389:MSE:HE1	1.74	0.70
1:B:581:LEU:HD13	1:B:597:CYS:SG	2.32	0.69
1:B:373:LEU:HD13	1:B:408:ALA:HB3	1.74	0.69
1:A:67:THR:CG2	1:A:67:THR:O	2.37	0.69
1:A:506:ARG:NH1	1:A:506:ARG:CG	2.35	0.69
1:B:435:ASN:O	1:B:439:GLN:HG2	1.92	0.69
1:B:497:THR:CG2	1:B:500:LEU:H	2.02	0.69
1:B:215:ARG:HH12	1:B:216:ILE:HA	1.57	0.69
1:B:185:LYS:HE3	1:B:189:THR:HA	1.73	0.68
1:B:275:LEU:CD2	1:B:279:PHE:CE2	2.76	0.68
1:B:188:MSE:HE3	1:B:258:TRP:HZ2	1.58	0.68
1:B:213:ILE:HG21	1:B:237:ALA:HB1	1.75	0.68
1:B:221:ILE:O	1:B:260:VAL:HG22	1.92	0.68
1:B:222:VAL:HG13	1:B:242:ARG:O	1.94	0.67
1:B:244:ILE:HD11	1:B:248:ALA:CB	2.24	0.67
1:A:207:ALA:O	1:A:211:GLN:HG3	1.95	0.67
1:A:347:GLY:O	1:A:467:ARG:NH1	2.22	0.67
1:B:221:ILE:HD13	1:B:259:LEU:HG	1.74	0.67
1:B:347:GLY:O	1:B:467:ARG:NH1	2.28	0.67
1:B:240:LYS:HD3	1:B:240:LYS:H	1.60	0.67
1:A:263:GLU:OE2	1:A:287:THR:HG23	1.95	0.67
1:B:279:PHE:N	1:B:279:PHE:CD2	2.63	0.67
1:A:402:GLU:C	1:A:403:ASN:HD22	1.99	0.66
1:B:469:ARG:NE	2:B:701:ACO:O2B	2.28	0.66
1:B:184:LEU:O	1:B:212:LEU:HD21	1.93	0.66
1:B:607:LEU:O	1:B:613:ARG:NH1	2.27	0.66
1:B:259:LEU:O	1:B:282:THR:HA	1.95	0.66
1:B:209:ALA:C	1:B:233:LEU:HD21	2.17	0.66
1:B:484:THR:CG2	1:B:533:MSE:HE1	2.21	0.66
1:B:209:ALA:HB3	1:B:233:LEU:CD2	2.25	0.66
1:B:184:LEU:CD1	1:B:211:GLN:HG2	2.21	0.65
1:A:204:GLY:HA2	3:A:800:ADP:O1A	1.96	0.65
1:B:185:LYS:HD3	1:B:189:THR:HA	1.77	0.65
1:B:373:LEU:CD1	1:B:408:ALA:HB3	2.27	0.65
1:A:286:THR:HG21	1:A:299:LEU:HD11	1.79	0.65
1:B:259:LEU:HD23	1:B:260:VAL:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HG3	1:A:430:ARG:HH11	1.62	0.65
1:B:349:ILE:HD12	1:B:349:ILE:O	1.97	0.65
1:B:213:ILE:HD12	1:B:220:ALA:HB3	1.78	0.64
1:B:235:GLN:O	1:B:235:GLN:HG2	1.96	0.64
1:B:14:MSE:HE1	1:B:101:TRP:CZ2	2.32	0.64
1:B:259:LEU:HD11	1:B:275:LEU:HD13	1.79	0.64
1:B:263:GLU:OE1	1:B:286:THR:HA	1.97	0.64
1:B:188:MSE:HE1	1:B:283:LEU:CD2	2.28	0.64
1:B:14:MSE:HE1	1:B:101:TRP:CE2	2.33	0.64
1:B:512:VAL:HG13	1:B:544:GLU:HB3	1.80	0.64
1:B:221:ILE:CD1	1:B:259:LEU:HG	2.29	0.63
1:B:104:LEU:HG	1:B:106:LEU:HD13	1.79	0.63
1:B:214:SER:HB2	1:B:240:LYS:CG	2.22	0.63
1:A:199:ALA:HB3	1:A:205:LYS:HD3	1.80	0.63
1:A:359:TRP:CZ2	1:A:366:PRO:HB2	2.34	0.63
1:A:472:THR:HG23	5:A:887:HOH:O	1.99	0.63
1:B:51:SER:O	1:B:53:ARG:N	2.32	0.63
1:A:10:LEU:HD22	1:A:160:LEU:HD21	1.81	0.63
1:B:128:ASP:HB3	1:B:129:PRO:HD2	1.78	0.62
1:A:17:GLU:HB3	1:A:166:ARG:HG3	1.80	0.62
1:A:72:GLU:HG2	1:A:319:ARG:HH12	1.65	0.62
1:B:28:GLU:HB3	5:B:1006:HOH:O	1.99	0.62
1:A:96:LEU:HD21	1:A:102:LEU:HD23	1.80	0.62
1:B:264:ALA:HB2	1:B:284:LEU:HD11	1.79	0.62
1:B:208:LEU:HD13	1:B:208:LEU:C	2.20	0.62
1:B:223:THR:HA	1:B:243:PHE:CE1	2.34	0.62
1:B:279:PHE:HB3	1:B:280:PRO:HD2	1.82	0.62
1:B:196:ALA:CB	1:B:309:LEU:HD21	2.30	0.62
1:A:437:VAL:O	1:A:441:LEU:HD22	2.00	0.61
1:B:67:THR:C	1:B:68:LEU:HD12	2.20	0.61
1:B:259:LEU:HB3	1:B:282:THR:CG2	2.30	0.61
1:B:44:PRO:HA	5:B:968:HOH:O	2.00	0.61
1:A:227:LYS:HD3	1:A:230:THR:CG2	2.29	0.61
1:B:275:LEU:HD23	1:B:279:PHE:HE2	1.65	0.61
1:B:250:LEU:HD21	1:B:271:LEU:CD2	2.31	0.61
1:B:311:ARG:HH11	1:B:311:ARG:CG	2.10	0.61
1:A:44:PRO:HA	5:A:1013:HOH:O	1.98	0.61
1:A:188:MSE:HE1	1:A:215:ARG:O	2.01	0.61
1:B:292:GLU:N	1:B:292:GLU:OE2	2.34	0.61
1:B:482:GLN:OE1	1:B:482:GLN:HA	1.99	0.61
1:A:635:LYS:CD	1:A:635:LYS:H	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:HIS:CB	1:B:389:MSE:HE1	2.31	0.60
1:B:351:ILE:HD12	1:B:476:LEU:HD13	1.81	0.60
1:A:280:PRO:HD3	5:A:1004:HOH:O	2.01	0.60
1:B:214:SER:C	1:B:216:ILE:N	2.49	0.60
1:B:403:ASN:O	1:B:404:GLU:HG2	2.01	0.60
1:A:437:VAL:HG13	1:A:528:MSE:CE	2.31	0.60
1:B:48:LEU:HG	1:B:49:TRP:N	2.08	0.60
1:B:296:ARG:NH2	1:B:341:PHE:CE2	2.68	0.60
1:B:497:THR:CG2	1:B:499:GLU:HG3	2.29	0.60
1:B:621:SER:O	1:B:625:LEU:HD22	2.01	0.60
1:A:250:LEU:HA	1:A:278:ARG:HH21	1.65	0.60
1:A:372:LEU:HD22	1:A:405:ILE:HG22	1.83	0.60
1:A:539:GLN:O	1:A:543:ARG:HB2	2.01	0.60
1:B:209:ALA:HB3	1:B:233:LEU:HD21	1.84	0.60
1:B:214:SER:HB2	1:B:240:LYS:NZ	2.16	0.60
1:B:215:ARG:HH12	1:B:216:ILE:CA	2.15	0.60
1:B:359:TRP:HZ3	1:B:367:LEU:CD1	2.11	0.60
1:B:506:ARG:HG3	1:B:506:ARG:HH11	1.67	0.60
1:B:649:LEU:HB3	1:B:657:THR:HG21	1.82	0.60
1:B:249:LEU:HD13	1:B:249:LEU:C	2.21	0.60
1:B:430:ARG:NH1	1:B:670:PHE:HE1	1.95	0.60
1:B:185:LYS:CD	1:B:189:THR:HA	2.32	0.60
1:B:600:ARG:O	1:B:604:THR:HG22	2.01	0.60
1:A:373:LEU:CD1	1:A:408:ALA:HB3	2.32	0.59
1:B:200:ALA:HA	1:B:288:VAL:O	2.02	0.59
1:B:215:ARG:NH1	1:B:216:ILE:CA	2.65	0.59
1:B:276:VAL:HG12	1:B:276:VAL:O	2.01	0.59
1:B:341:PHE:CD1	1:B:342:THR:N	2.70	0.59
1:B:258:TRP:HA	1:B:281:ARG:O	2.02	0.59
1:B:264:ALA:HB3	1:B:284:LEU:CD1	2.30	0.59
1:A:359:TRP:CZ3	1:A:367:LEU:HD13	2.35	0.59
1:A:481:LEU:HD12	1:A:533:MSE:HE3	1.85	0.59
1:B:225:PRO:O	1:B:227:LYS:N	2.35	0.59
1:B:244:ILE:CG2	1:B:249:LEU:HD23	2.32	0.59
1:B:437:VAL:HG13	1:B:528:MSE:HE3	1.85	0.59
1:A:67:THR:HG22	1:A:71:ARG:HB2	1.85	0.59
1:B:80:ALA:HA	1:B:83:GLY:O	2.02	0.59
1:B:639:VAL:O	1:B:643:GLU:HG3	2.02	0.59
1:A:635:LYS:HD2	5:A:822:HOH:O	2.03	0.58
1:B:222:VAL:HB	1:B:260:VAL:CG2	2.31	0.58
1:B:188:MSE:HE1	1:B:283:LEU:CG	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PRO:HG3	1:B:267:ILE:HG13	1.86	0.58
1:A:514:MSE:HE2	1:A:525:TYR:HB2	1.83	0.58
1:B:184:LEU:HD23	1:B:212:LEU:HG	1.85	0.58
1:B:635:LYS:O	1:B:639:VAL:HG23	2.04	0.58
1:A:629:LEU:HB3	1:A:631:LEU:CD2	2.34	0.58
1:B:261:VAL:HG22	1:B:264:ALA:HB2	1.85	0.58
1:B:467:ARG:HD2	1:B:470:GLU:OE2	2.04	0.58
1:B:670:PHE:CD1	1:B:670:PHE:C	2.77	0.58
1:B:261:VAL:CG2	1:B:264:ALA:HB2	2.34	0.57
1:B:296:ARG:NH2	1:B:341:PHE:CZ	2.71	0.57
1:B:484:THR:O	1:B:485:GLN:HG3	2.03	0.57
1:A:68:LEU:HD12	1:A:68:LEU:H	1.69	0.57
1:B:214:SER:O	1:B:216:ILE:N	2.37	0.57
1:B:396:PHE:O	1:B:397:LEU:HD22	2.04	0.57
1:A:69:LEU:HD11	1:A:71:ARG:HD2	1.85	0.57
1:A:420:GLN:CD	1:A:420:GLN:H	2.07	0.57
1:B:195:ALA:HB1	1:B:312:PHE:HE2	1.68	0.57
1:B:222:VAL:HA	1:B:260:VAL:O	2.04	0.57
1:B:274:GLN:C	1:B:278:ARG:HH21	2.07	0.57
1:B:222:VAL:CG1	1:B:242:ARG:O	2.52	0.57
1:B:359:TRP:CH2	1:B:367:LEU:HD13	2.38	0.57
1:B:194:VAL:HG13	1:B:282:THR:OG1	2.05	0.56
1:B:244:ILE:HG23	1:B:249:LEU:HD23	1.86	0.56
1:A:14:MSE:HE1	1:A:101:TRP:NE1	2.20	0.56
1:A:50:ILE:HG21	1:A:92:LEU:HD22	1.86	0.56
1:A:176:PRO:HG2	1:A:181:GLN:NE2	2.20	0.56
1:B:189:THR:O	1:B:189:THR:OG1	2.22	0.56
1:B:259:LEU:HD23	1:B:260:VAL:H	1.68	0.56
1:B:594:SER:O	1:B:598:LEU:HB2	2.05	0.56
1:B:185:LYS:HA	1:B:188:MSE:HB3	1.86	0.56
1:A:345:PRO:HG2	1:A:467:ARG:HG3	1.88	0.56
1:A:619:ASN:HB3	5:A:990:HOH:O	2.05	0.56
1:A:67:THR:HG21	1:A:71:ARG:HH11	1.70	0.56
1:A:634:ARG:HH11	1:A:638:LEU:HB2	1.67	0.56
1:B:132:THR:HB	1:B:390:ASP:OD2	2.06	0.56
1:A:516:ASN:HD21	1:A:555:LEU:HD12	1.71	0.56
1:B:341:PHE:CE1	1:B:342:THR:HG23	2.41	0.56
1:B:190:MSE:C	1:B:191:PRO:O	2.41	0.55
1:B:13:GLN:O	1:B:17:GLU:HG3	2.05	0.55
1:B:245:ALA:HB1	1:B:246:PRO:HD2	1.89	0.55
1:B:363:PRO:O	1:B:367:LEU:HD22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLN:O	1:A:17:GLU:HG3	2.06	0.55
1:A:282:THR:HG22	1:A:284:LEU:HD13	1.89	0.55
1:A:213:ILE:HG23	1:A:220:ALA:HB3	1.88	0.55
1:B:246:PRO:O	1:B:249:LEU:HB3	2.06	0.55
1:A:25:LEU:HD12	1:A:152:TRP:HB3	1.87	0.55
1:A:309:LEU:HD13	1:A:310:HIS:N	2.21	0.55
1:A:318:ILE:HD12	1:A:318:ILE:O	2.07	0.55
1:A:430:ARG:HG3	1:A:430:ARG:NH1	2.21	0.55
1:B:257:ASP:O	1:B:280:PRO:HG2	2.07	0.55
1:B:68:LEU:HD12	1:B:68:LEU:N	2.22	0.55
1:B:551:ASP:OD2	1:B:596:GLY:HA3	2.06	0.54
1:A:382:PRO:O	1:A:386:ARG:HG2	2.06	0.54
1:B:469:ARG:HD3	2:B:701:ACO:C8A	2.37	0.54
1:B:190:MSE:SE	1:B:310:HIS:HD2	2.40	0.54
1:A:66:GLN:HB3	1:A:68:LEU:HD12	1.88	0.54
1:A:223:THR:HG22	1:A:261:VAL:HG22	1.89	0.54
1:A:369:VAL:HG12	1:A:373:LEU:HD22	1.90	0.54
1:A:629:LEU:HB3	1:A:631:LEU:HD21	1.89	0.54
1:B:92:LEU:O	1:B:95:THR:HG22	2.07	0.54
1:B:423:GLN:HE21	1:B:449:LEU:HD11	1.73	0.54
1:B:506:ARG:NE	1:B:506:ARG:HA	2.22	0.54
1:B:274:GLN:CA	1:B:278:ARG:NH2	2.70	0.54
1:B:500:LEU:CD2	2:B:701:ACO:H21	2.35	0.54
1:A:247:ASP:HB2	5:A:989:HOH:O	2.08	0.54
1:A:634:ARG:HD3	1:A:634:ARG:C	2.28	0.54
1:A:110:GLU:OE2	1:A:153:ARG:NH2	2.42	0.53
1:B:14:MSE:HE1	1:B:101:TRP:NE1	2.24	0.53
1:B:107:PRO:HB3	5:B:927:HOH:O	2.08	0.53
1:B:72:GLU:HB2	1:B:97:LYS:HG3	1.90	0.53
1:B:139:LEU:O	1:B:143:LEU:HG	2.08	0.53
1:B:467:ARG:NH2	1:B:470:GLU:OE1	2.41	0.53
1:A:373:LEU:HD13	1:A:408:ALA:HB3	1.89	0.53
1:B:506:ARG:HG3	1:B:506:ARG:NH1	2.24	0.53
1:B:213:ILE:HB	1:B:237:ALA:HB2	1.88	0.53
1:A:67:THR:HA	1:A:69:LEU:HD21	1.90	0.53
1:A:502:ARG:HH22	1:B:1:MSE:N	2.06	0.53
1:B:195:ALA:O	1:B:284:LEU:N	2.38	0.53
1:A:216:ILE:O	1:A:240:LYS:NZ	2.42	0.53
1:A:444:HIS:HD2	1:A:593:THR:OG1	1.91	0.53
1:B:259:LEU:CD2	1:B:260:VAL:N	2.72	0.53
1:B:299:LEU:HD13	1:B:299:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLU:HB2	1:B:97:LYS:CG	2.38	0.53
1:B:221:ILE:HG12	1:B:222:VAL:N	2.24	0.53
1:B:358:LEU:HD13	1:B:362:ASP:HB3	1.91	0.53
1:B:294:THR:HG21	1:B:299:LEU:HD23	1.89	0.53
1:A:198:THR:HG21	1:A:311:ARG:NH2	2.21	0.53
1:A:502:ARG:NH2	1:B:1:MSE:N	2.57	0.53
1:B:7:LEU:HD13	1:B:160:LEU:HD21	1.89	0.53
1:B:220:ALA:C	1:B:221:ILE:HG22	2.29	0.53
1:A:635:LYS:H	1:A:635:LYS:HD2	1.74	0.52
1:B:202:GLY:O	1:B:317:PRO:HA	2.10	0.52
1:A:250:LEU:CA	1:A:278:ARG:NH2	2.72	0.52
1:B:215:ARG:O	1:B:215:ARG:CD	2.58	0.52
1:B:649:LEU:HB3	1:B:657:THR:CG2	2.39	0.52
1:A:289:GLN:HG3	1:A:290:GLY:N	2.21	0.52
1:B:311:ARG:CG	1:B:311:ARG:NH1	2.72	0.52
1:A:162:HIS:ND1	1:A:162:HIS:N	2.56	0.52
1:B:198:THR:HB	1:B:286:THR:HG22	1.92	0.52
1:A:34:GLU:O	1:A:38:LYS:HG3	2.10	0.52
1:B:176:PRO:HB3	1:B:211:GLN:OE1	2.09	0.52
1:B:209:ALA:C	1:B:233:LEU:CD2	2.79	0.52
1:B:249:LEU:CD1	1:B:275:LEU:HG	2.40	0.52
1:A:68:LEU:HD13	1:A:68:LEU:O	2.09	0.51
1:A:139:LEU:O	1:A:143:LEU:HB2	2.10	0.51
1:A:402:GLU:C	1:A:403:ASN:ND2	2.63	0.51
1:A:514:MSE:HE3	1:A:526:THR:O	2.10	0.51
1:B:16:ARG:HG2	1:B:16:ARG:HH21	1.75	0.51
1:B:583:GLY:O	1:B:587:ALA:HB3	2.11	0.51
1:A:23:LEU:CD1	1:A:25:LEU:HD13	2.40	0.51
1:A:67:THR:HG21	1:A:71:ARG:NH1	2.26	0.51
1:A:177:GLN:HB3	1:A:178:PRO:HD2	1.93	0.51
1:B:395:HIS:NE2	1:B:456:ARG:NH2	2.58	0.51
1:A:289:GLN:CG	1:A:290:GLY:H	2.22	0.51
1:A:484:THR:HG22	1:A:485:GLN:N	2.25	0.51
1:B:175:ALA:HB1	1:B:176:PRO:HD2	1.93	0.51
1:B:512:VAL:HG13	1:B:544:GLU:CB	2.41	0.51
1:A:328:LYS:O	1:A:332:GLU:HG3	2.10	0.50
1:B:196:ALA:HB3	1:B:309:LEU:HD21	1.94	0.50
1:B:341:PHE:HD1	1:B:342:THR:H	1.60	0.50
1:B:489:TYR:HA	1:B:533:MSE:HG3	1.92	0.50
1:A:513:ARG:NH2	5:A:961:HOH:O	2.43	0.50
1:B:205:LYS:O	1:B:208:LEU:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:VAL:HG11	1:B:241:PHE:CD1	2.46	0.50
1:A:437:VAL:HG23	1:A:457:ARG:HD3	1.93	0.50
1:A:636:MSE:HG3	5:A:803:HOH:O	2.11	0.50
1:A:442:ALA:O	1:A:589:ARG:NH2	2.45	0.50
1:B:223:THR:HG23	1:B:224:ALA:N	2.26	0.50
1:B:621:SER:OG	1:B:624:GLN:HB2	2.11	0.50
1:A:23:LEU:HD22	1:A:150:ILE:HB	1.93	0.50
1:B:552:ALA:HA	1:B:563:LEU:HD22	1.93	0.50
1:B:250:LEU:O	1:B:250:LEU:CD1	2.60	0.49
1:B:262:ASP:OD1	1:B:285:THR:HG21	2.12	0.49
1:B:485:GLN:O	1:B:486:ASP:HB3	2.12	0.49
1:B:486:ASP:OD1	1:B:486:ASP:O	2.30	0.49
1:A:252:SER:HB2	1:A:254:GLU:OE2	2.12	0.49
1:A:467:ARG:HA	1:A:470:GLU:OE2	2.12	0.49
1:B:184:LEU:CD1	1:B:211:GLN:HB3	2.39	0.49
1:B:185:LYS:CG	1:B:215:ARG:HE	2.25	0.49
1:B:112:TRP:CD2	1:B:136:VAL:HG13	2.47	0.49
1:B:222:VAL:HG11	1:B:241:PHE:CE1	2.46	0.49
1:A:72:GLU:HG2	1:A:319:ARG:NH1	2.27	0.49
1:B:119:ASP:OD2	1:B:122:ARG:NH1	2.45	0.49
1:B:201:ARG:NH1	1:B:291:TYR:O	2.45	0.49
1:A:500:LEU:HD21	2:A:700:ACO:H22	1.94	0.49
1:B:205:LYS:HE3	1:B:287:THR:OG1	2.13	0.49
1:A:119:ASP:OD2	1:A:122:ARG:NH1	2.46	0.49
1:A:437:VAL:HG12	1:A:441:LEU:HD22	1.95	0.49
1:A:446:ASN:ND2	1:A:580:GLU:HG3	2.28	0.49
1:B:169:TRP:CZ3	1:B:171:PRO:HD3	2.47	0.49
1:B:525:TYR:CE2	1:B:559:ASN:HB3	2.48	0.49
1:A:397:LEU:HB2	1:A:409:LEU:HB3	1.95	0.48
1:B:346:GLN:HA	1:B:346:GLN:NE2	2.18	0.48
1:A:23:LEU:HD11	1:A:25:LEU:HD13	1.95	0.48
1:A:318:ILE:HG12	3:A:800:ADP:O4'	2.12	0.48
1:B:206:SER:O	1:B:233:LEU:HD22	2.13	0.48
1:A:69:LEU:N	1:A:69:LEU:HD23	2.28	0.48
1:A:345:PRO:HG2	1:A:467:ARG:CG	2.43	0.48
1:B:188:MSE:CE	1:B:258:TRP:HZ2	2.25	0.48
1:A:68:LEU:HD13	1:A:68:LEU:C	2.33	0.48
1:B:555:LEU:HD23	1:B:563:LEU:HD21	1.96	0.48
1:A:179:GLU:OE1	1:A:316:GLN:HB2	2.13	0.48
1:A:96:LEU:CD2	1:A:102:LEU:HD23	2.44	0.48
1:B:225:PRO:O	1:B:226:ALA:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:TRP:CZ3	1:B:367:LEU:CD1	2.84	0.48
1:B:502:ARG:HA	1:B:505:GLN:HB3	1.96	0.48
1:A:670:PHE:N	1:A:670:PHE:CD2	2.79	0.48
1:A:306:PHE:CB	1:A:309:LEU:HD23	2.44	0.47
1:A:353:ALA:HB2	1:A:397:LEU:HD13	1.95	0.47
1:B:132:THR:O	1:B:132:THR:OG1	2.30	0.47
1:A:502:ARG:NH2	1:B:1:MSE:H2	2.11	0.47
1:A:250:LEU:CD1	1:A:278:ARG:HH22	2.07	0.47
1:A:50:ILE:CG2	1:A:92:LEU:HD22	2.45	0.47
1:A:106:LEU:HB3	1:A:107:PRO:HD2	1.96	0.47
1:B:279:PHE:H	1:B:279:PHE:HD2	1.62	0.47
1:B:407:GLY:HA2	1:B:462:ALA:O	2.13	0.47
1:A:359:TRP:CE2	1:A:366:PRO:HB2	2.50	0.47
1:B:196:ALA:HB2	1:B:309:LEU:HD21	1.97	0.47
1:B:640:ARG:O	1:B:644:GLU:HG3	2.14	0.47
1:B:10:LEU:HD23	1:B:160:LEU:HD21	1.95	0.47
1:A:454:ARG:NH2	5:A:880:HOH:O	2.47	0.47
1:B:223:THR:CG2	1:B:224:ALA:N	2.78	0.47
1:B:18:GLY:HA2	1:B:98:ALA:HB1	1.96	0.47
1:B:233:LEU:C	1:B:233:LEU:HD13	2.35	0.47
1:B:581:LEU:CD1	1:B:597:CYS:SG	3.03	0.47
1:B:215:ARG:O	1:B:215:ARG:HD2	2.14	0.46
1:B:222:VAL:HG22	1:B:243:PHE:HD1	1.79	0.46
1:B:496:TYR:CD1	1:B:514:MSE:HE1	2.49	0.46
1:B:244:ILE:HG23	1:B:244:ILE:O	2.16	0.46
1:A:289:GLN:HG2	1:A:336:PHE:O	2.14	0.46
1:B:229:SER:HB3	1:B:231:ASP:OD1	2.15	0.46
1:B:184:LEU:HD21	1:B:211:GLN:HB3	1.97	0.46
1:B:506:ARG:NH2	2:B:701:ACO:O9A	2.48	0.46
1:A:68:LEU:HD12	1:A:68:LEU:N	2.31	0.46
1:A:506:ARG:NH1	2:A:700:ACO:P3B	2.89	0.46
1:B:10:LEU:C	1:B:14:MSE:HE2	2.36	0.46
1:B:310:HIS:HB3	1:B:312:PHE:CZ	2.51	0.46
1:A:184:LEU:HD13	1:A:208:LEU:HD12	1.97	0.46
1:B:154:GLN:O	1:B:155:ASN:HB2	2.15	0.46
1:A:369:VAL:HG13	1:A:408:ALA:HB1	1.98	0.46
1:B:222:VAL:HB	1:B:260:VAL:HG22	1.97	0.46
1:B:249:LEU:HD11	1:B:275:LEU:HG	1.98	0.46
1:A:6:ALA:HB1	1:A:160:LEU:HD12	1.98	0.46
1:B:319:ARG:HB2	1:B:320:TRP:CE3	2.51	0.46
1:A:259:LEU:HB2	1:A:279:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:O	1:B:257:ASP:OD1	2.34	0.46
1:B:435:ASN:HB3	1:B:438:ALA:HB3	1.96	0.46
1:B:214:SER:CB	1:B:240:LYS:HZ3	2.26	0.45
1:A:183:LEU:HD22	1:A:314:LEU:HD13	1.98	0.45
1:A:341:PHE:CZ	1:A:375:GLY:HA3	2.51	0.45
1:A:634:ARG:HH12	1:A:638:LEU:HD13	1.81	0.45
1:B:213:ILE:HG23	1:B:240:LYS:HB2	1.98	0.45
1:B:240:LYS:H	1:B:240:LYS:CD	2.17	0.45
1:B:279:PHE:HB3	1:B:280:PRO:CD	2.45	0.45
1:B:397:LEU:HB2	1:B:409:LEU:HB3	1.98	0.45
1:A:660:LEU:HD12	1:A:660:LEU:HA	1.67	0.45
1:B:469:ARG:HA	1:B:469:ARG:HD2	1.71	0.45
1:B:566:ASP:HB3	5:B:997:HOH:O	2.16	0.45
1:B:10:LEU:O	1:B:14:MSE:HG3	2.16	0.45
1:B:480:ALA:O	1:B:484:THR:CG2	2.64	0.45
1:A:149:ALA:O	1:A:151:LEU:HD22	2.16	0.45
1:A:437:VAL:HG12	1:A:441:LEU:CD2	2.47	0.45
1:B:208:LEU:C	1:B:208:LEU:CD1	2.85	0.45
1:B:193:GLY:O	1:B:281:ARG:HA	2.17	0.45
1:A:329:MSE:HE3	1:A:329:MSE:HB3	1.93	0.45
1:B:122:ARG:NH2	1:B:383:LEU:HD11	2.31	0.45
1:B:213:ILE:HG22	1:B:237:ALA:HB1	1.92	0.45
1:B:216:ILE:HD13	1:B:218:GLY:H	1.82	0.45
1:B:477:ILE:O	1:B:481:LEU:HD23	2.17	0.45
1:B:555:LEU:HD12	1:B:595:LEU:HD23	1.99	0.45
1:B:132:THR:HA	1:B:390:ASP:CG	2.37	0.44
1:A:69:LEU:CD1	1:A:71:ARG:HD2	2.47	0.44
1:A:306:PHE:HB2	1:A:309:LEU:HD23	1.99	0.44
1:B:263:GLU:H	1:B:285:THR:HG23	1.82	0.44
1:B:583:GLY:HA3	1:B:589:ARG:HD2	1.99	0.44
1:A:262:ASP:HB2	1:A:285:THR:OG1	2.18	0.44
1:A:432:PRO:HG2	1:A:439:GLN:OE1	2.17	0.44
1:B:17:GLU:HB3	1:B:166:ARG:HB2	1.99	0.44
1:B:259:LEU:HD13	1:B:282:THR:CG2	2.46	0.44
1:B:464:HIS:ND1	1:B:465:PRO:HD2	2.32	0.44
1:B:581:LEU:HG	1:B:601:LEU:HD22	1.99	0.44
2:B:701:ACO:N8P	2:B:701:ACO:H131	2.32	0.44
1:B:71:ARG:NH2	1:B:73:PHE:CZ	2.86	0.44
1:B:213:ILE:CD1	1:B:220:ALA:CB	2.95	0.44
1:B:250:LEU:O	1:B:250:LEU:HD12	2.17	0.44
1:B:578:TRP:HZ3	1:B:657:THR:CG2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ALA:O	1:A:230:THR:N	2.50	0.44
1:B:446:ASN:HA	1:B:580:GLU:OE2	2.18	0.44
1:B:215:ARG:HH12	1:B:216:ILE:CB	2.31	0.44
1:B:369:VAL:HG12	1:B:373:LEU:HD22	2.00	0.44
1:A:151:LEU:HD22	1:A:151:LEU:N	2.33	0.44
1:A:199:ALA:C	1:A:288:VAL:HG12	2.38	0.44
1:A:441:LEU:HD13	1:A:528:MSE:CE	2.41	0.44
1:B:188:MSE:HE1	1:B:283:LEU:HD23	1.99	0.44
1:B:239:GLU:C	1:B:241:PHE:N	2.71	0.44
1:B:542:GLU:HG3	1:B:543:ARG:N	2.33	0.44
1:A:92:LEU:HD23	1:A:102:LEU:HD21	1.99	0.44
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.80	0.44
1:A:289:GLN:NE2	1:A:374:SER:OG	2.49	0.43
1:B:209:ALA:HB3	1:B:233:LEU:HD23	1.97	0.43
1:B:213:ILE:CD1	1:B:220:ALA:HB3	2.45	0.43
1:B:216:ILE:HG23	1:B:218:GLY:O	2.17	0.43
1:B:264:ALA:CB	1:B:284:LEU:CD1	2.86	0.43
1:B:481:LEU:HA	1:B:484:THR:HG22	1.99	0.43
1:A:74:ARG:O	1:A:75:HIS:HB2	2.18	0.43
1:A:250:LEU:CD2	1:A:278:ARG:NH2	2.75	0.43
1:A:252:SER:OG	1:A:254:GLU:HG2	2.18	0.43
1:A:506:ARG:HA	1:A:506:ARG:HD2	1.11	0.43
1:B:649:LEU:C	1:B:657:THR:HG21	2.38	0.43
1:B:16:ARG:HH21	1:B:16:ARG:CG	2.32	0.43
1:B:138:HIS:HB2	1:B:389:MSE:CE	2.47	0.43
1:B:177:GLN:HB3	1:B:178:PRO:HD2	2.01	0.43
1:B:185:LYS:HD3	1:B:189:THR:CA	2.48	0.43
1:A:329:MSE:HE3	1:A:330:VAL:HG23	2.01	0.43
1:A:362:ASP:OD1	1:A:365:THR:CG2	2.66	0.43
1:B:212:LEU:HD12	1:B:212:LEU:N	2.23	0.43
1:B:249:LEU:HD11	1:B:275:LEU:CG	2.48	0.43
1:A:92:LEU:O	1:A:95:THR:HG22	2.19	0.43
1:B:192:PRO:HB3	1:B:280:PRO:HB2	2.00	0.43
1:B:355:GLU:HB2	1:B:357:THR:HG23	2.01	0.43
1:A:199:ALA:O	1:A:287:THR:HA	2.18	0.43
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.88	0.43
1:A:373:LEU:HD11	1:A:408:ALA:HB3	2.00	0.43
1:B:185:LYS:HG3	1:B:215:ARG:NE	2.34	0.43
1:B:346:GLN:HE21	1:B:346:GLN:CA	2.12	0.43
1:A:10:LEU:O	1:A:14:MSE:HG3	2.19	0.43
1:A:50:ILE:HD12	1:A:51:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:HH21	1:A:383:LEU:HD11	1.83	0.43
1:A:612:LEU:HD22	1:A:644:GLU:HB2	2.01	0.43
1:B:485:GLN:O	1:B:486:ASP:CB	2.66	0.43
1:A:273:HIS:NE2	1:A:305:ARG:HB3	2.33	0.43
1:A:326:LEU:HD12	1:A:329:MSE:CE	2.49	0.43
1:A:411:LEU:HD12	1:A:458:VAL:HA	2.01	0.43
1:B:181:GLN:HA	1:B:181:GLN:OE1	2.19	0.43
1:B:234:ALA:HB2	1:B:241:PHE:CD1	2.53	0.43
1:B:509:PHE:HB3	1:B:529:ALA:HB1	2.00	0.43
1:B:516:ASN:HB2	1:B:592:LEU:HD23	2.01	0.43
1:A:577:ASP:O	1:A:581:LEU:HD22	2.19	0.43
1:B:307:PRO:O	1:B:308:HIS:HB2	2.17	0.43
1:A:53:ARG:HE	1:A:53:ARG:HB3	1.45	0.42
1:A:184:LEU:HD13	1:A:208:LEU:CD1	2.49	0.42
1:A:262:ASP:HA	1:A:285:THR:OG1	2.19	0.42
1:B:284:LEU:HA	1:B:284:LEU:HD13	1.64	0.42
1:A:67:THR:CG2	1:A:71:ARG:HH11	2.32	0.42
1:B:210:GLY:N	1:B:233:LEU:HD22	2.34	0.42
1:B:245:ALA:O	1:B:249:LEU:CB	2.67	0.42
1:B:353:ALA:HB2	1:B:397:LEU:HD13	2.00	0.42
1:A:317:PRO:HD2	1:A:322:GLN:HB2	2.01	0.42
1:A:339:GLU:O	1:A:342:THR:HB	2.20	0.42
1:B:489:TYR:CD1	1:B:489:TYR:C	2.92	0.42
1:B:242:ARG:HD3	1:B:243:PHE:N	2.34	0.42
1:B:578:TRP:HZ3	1:B:657:THR:HG22	1.85	0.42
1:A:276:VAL:HG22	1:A:282:THR:HG21	2.01	0.42
1:B:355:GLU:OE1	1:B:395:HIS:ND1	2.46	0.42
1:A:92:LEU:CD2	1:A:102:LEU:HD21	2.49	0.42
1:B:496:TYR:OH	1:B:564:PRO:HG3	2.19	0.42
1:A:224:ALA:HB1	1:A:225:PRO:HD2	2.02	0.42
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.93	0.42
1:A:540:LEU:O	1:A:544:GLU:HB2	2.20	0.42
1:B:184:LEU:CD1	1:B:211:GLN:CG	2.87	0.42
1:B:184:LEU:CG	1:B:211:GLN:HB3	2.49	0.42
1:B:355:GLU:O	1:B:358:LEU:HB2	2.20	0.42
1:B:395:HIS:CD2	1:B:456:ARG:CZ	3.02	0.42
1:B:553:GLN:O	1:B:557:GLN:HG3	2.19	0.42
1:A:565:VAL:O	1:A:567:PRO:HD3	2.20	0.42
1:B:101:TRP:CH2	1:B:150:ILE:HG13	2.54	0.42
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.93	0.42
1:B:612:LEU:C	1:B:616:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:HD13	1:B:629:LEU:HA	1.88	0.42
1:B:232:VAL:HB	1:B:233:LEU:H	1.32	0.42
1:B:421:LEU:O	1:B:425:VAL:HG23	2.20	0.42
1:A:441:LEU:HB3	1:A:450:ALA:HB1	2.02	0.42
1:B:440:SER:OG	1:B:444:HIS:HD2	2.02	0.42
1:B:581:LEU:HD12	1:B:581:LEU:HA	1.84	0.42
1:A:13:GLN:HG3	1:A:16:ARG:HH21	1.84	0.41
1:A:40:ARG:HG3	1:A:41:ASP:N	2.35	0.41
1:B:11:THR:CA	1:B:14:MSE:CE	2.80	0.41
1:B:429:PHE:CD1	1:B:668:GLN:HA	2.54	0.41
1:B:609:LEU:HD22	1:B:644:GLU:HB3	2.02	0.41
1:A:227:LYS:O	1:A:228:ALA:C	2.58	0.41
1:B:51:SER:CB	5:B:1004:HOH:O	2.67	0.41
1:B:570:ASP:OD2	1:B:572:VAL:HG12	2.20	0.41
1:A:269:ALA:N	1:A:270:PRO:HD2	2.36	0.41
1:B:53:ARG:O	1:B:55:ASP:OD1	2.37	0.41
1:B:146:ASP:OD2	1:B:148:GLU:HB2	2.20	0.41
1:B:148:GLU:OE2	1:B:166:ARG:NH2	2.54	0.41
1:B:660:LEU:CD1	5:B:1020:HOH:O	2.69	0.41
1:A:106:LEU:HD13	1:A:112:TRP:CH2	2.54	0.41
1:B:244:ILE:O	1:B:249:LEU:HB2	2.20	0.41
1:B:317:PRO:HG2	1:B:320:TRP:O	2.20	0.41
1:B:429:PHE:CE2	1:B:588:HIS:HD2	2.38	0.41
1:A:7:LEU:HD12	1:A:7:LEU:HA	1.91	0.41
1:A:102:LEU:C	1:A:102:LEU:HD13	2.41	0.41
1:A:124:SER:O	1:A:125:ASP:HB2	2.20	0.41
1:A:233:LEU:HD23	1:A:233:LEU:O	2.21	0.41
1:B:65:LEU:O	1:B:66:GLN:HG2	2.21	0.41
1:B:221:ILE:CG1	1:B:222:VAL:N	2.84	0.41
1:A:69:LEU:HG	1:A:71:ARG:HG3	2.02	0.41
1:B:329:MSE:HE2	1:B:333:ALA:CB	2.45	0.41
1:B:434:GLY:O	1:B:439:GLN:NE2	2.51	0.41
1:B:499:GLU:O	1:B:500:LEU:C	2.55	0.41
1:A:294:THR:OG1	1:A:299:LEU:CD2	2.68	0.41
1:B:388:MSE:HG3	1:B:396:PHE:CE1	2.56	0.41
1:B:476:LEU:HD12	1:B:476:LEU:HA	1.90	0.41
1:A:362:ASP:O	1:A:366:PRO:HD2	2.20	0.41
1:A:578:TRP:CZ3	1:A:656:ARG:HG2	2.55	0.41
1:A:629:LEU:CB	1:A:631:LEU:CD2	2.99	0.41
1:B:133:PRO:O	1:B:137:GLN:HG3	2.20	0.41
1:B:195:ALA:HB3	1:B:283:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLY:N	4:B:801:SO4:O2	2.54	0.41
1:A:514:MSE:HE3	1:A:515:GLY:H	1.85	0.41
1:A:543:ARG:NH1	1:A:543:ARG:HG2	2.36	0.41
1:B:10:LEU:HG	1:B:14:MSE:CE	2.31	0.41
1:B:15:LYS:HE3	1:B:74:ARG:HH11	1.85	0.41
1:B:74:ARG:NH2	1:B:74:ARG:HB2	2.36	0.41
1:B:197:VAL:HG12	1:B:312:PHE:HB2	2.02	0.41
1:B:208:LEU:O	1:B:211:GLN:HB2	2.21	0.41
1:B:215:ARG:NH1	1:B:215:ARG:C	2.63	0.41
1:B:409:LEU:HG	1:B:411:LEU:HD22	2.02	0.41
1:B:414:GLU:HG2	1:B:435:ASN:HA	2.02	0.41
1:B:417:LEU:HD22	1:B:451:ALA:HB1	2.01	0.41
1:A:137:GLN:O	1:A:141:ARG:HG3	2.20	0.41
1:A:176:PRO:HG2	1:A:181:GLN:HE21	1.86	0.41
1:B:363:PRO:O	1:B:366:PRO:HD2	2.20	0.41
1:B:365:THR:HB	1:B:366:PRO:CD	2.39	0.41
1:A:138:HIS:HA	1:A:141:ARG:NH1	2.36	0.40
1:A:205:LYS:CE	1:A:287:THR:HG22	2.50	0.40
1:B:274:GLN:CG	1:B:278:ARG:HH22	2.31	0.40
1:B:274:GLN:HB3	1:B:278:ARG:HH21	1.70	0.40
1:B:653:ASN:O	1:B:657:THR:HG23	2.20	0.40
1:A:122:ARG:NH2	1:A:383:LEU:HD11	2.36	0.40
1:A:222:VAL:HA	1:A:260:VAL:O	2.21	0.40
1:B:7:LEU:CD1	1:B:160:LEU:HD22	2.44	0.40
1:B:249:LEU:HD11	1:B:275:LEU:HD21	2.02	0.40
1:A:184:LEU:HD12	1:A:184:LEU:HA	1.88	0.40
1:A:222:VAL:HG22	1:A:243:PHE:HD2	1.86	0.40
1:B:73:PHE:CD1	1:B:73:PHE:N	2.90	0.40
1:B:558:TRP:HH2	1:B:615:ARG:NH1	2.19	0.40
2:B:701:ACO:H131	2:B:701:ACO:HN8	1.87	0.40
1:A:363:PRO:O	1:A:367:LEU:HB2	2.21	0.40
1:A:484:THR:CG2	1:A:485:GLN:N	2.84	0.40
1:A:547:ARG:HD2	5:A:1012:HOH:O	2.22	0.40
1:A:599:LEU:HD11	1:A:616:LEU:HB3	2.03	0.40
1:B:274:GLN:C	1:B:278:ARG:NH2	2.74	0.40
1:B:446:ASN:O	1:B:448:PRO:HD3	2.21	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	654/671 (98%)	633 (97%)	18 (3%)	3 (0%)	25	28
1	B	658/671 (98%)	605 (92%)	44 (7%)	9 (1%)	9	7
All	All	1312/1342 (98%)	1238 (94%)	62 (5%)	12 (1%)	14	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	LEU
1	B	227	LYS
1	B	215	ARG
1	B	232	VAL
1	A	225	PRO
1	B	280	PRO
1	A	229	SER
1	B	213	ILE
1	B	225	PRO
1	B	221	ILE
1	B	233	LEU
1	A	69	LEU

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	532/532 (100%)	460 (86%)	72 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	535/532 (101%)	424 (79%)	111 (21%)	1	0
All	All	1067/1064 (100%)	884 (83%)	183 (17%)	1	1

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	21	ARG
1	A	23	LEU
1	A	25	LEU
1	A	29	GLU
1	A	43	LEU
1	A	50	ILE
1	A	52	PRO
1	A	53	ARG
1	A	68	LEU
1	A	69	LEU
1	A	72	GLU
1	A	95	THR
1	A	96	LEU
1	A	97	LYS
1	A	119	ASP
1	A	139	LEU
1	A	143	LEU
1	A	160	LEU
1	A	162	HIS
1	A	167	THR
1	A	187	LEU
1	A	219	ARG
1	A	222	VAL
1	A	250	LEU
1	A	284	LEU
1	A	286	THR
1	A	299	LEU
1	A	309	LEU
1	A	314	LEU
1	A	316	GLN
1	A	318	ILE
1	A	334	LEU
1	A	360	GLN
1	A	365	THR
1	A	367	LEU

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Mol	Chain	Res	Type
1	A	373	LEU
1	A	377	HIS
1	A	381	SER
1	A	411	LEU
1	A	420	GLN
1	A	430	ARG
1	A	431	ARG
1	A	433	ARG
1	A	441	LEU
1	A	472	THR
1	A	476	LEU
1	A	481	LEU
1	A	485	GLN
1	A	506	ARG
1	A	517	HIS
1	A	531	LEU
1	A	543	ARG
1	A	544	GLU
1	A	555	LEU
1	A	572	VAL
1	A	581	LEU
1	A	589	ARG
1	A	592	LEU
1	A	598	LEU
1	A	599	LEU
1	A	602	LEU
1	A	612	LEU
1	A	618	LYS
1	A	625	LEU
1	A	629	LEU
1	A	634	ARG
1	A	635	LYS
1	A	640	ARG
1	A	649	LEU
1	A	652	LEU
1	A	660	LEU
1	B	7	LEU
1	B	16	ARG
1	B	22	LEU
1	B	23	LEU
1	B	25	LEU
1	B	37	LEU

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	40	ARG
1	B	43	LEU
1	B	48	LEU
1	B	53	ARG
1	B	67	THR
1	B	95	THR
1	B	96	LEU
1	B	102	LEU
1	B	106	LEU
1	B	119	ASP
1	B	139	LEU
1	B	142	VAL
1	B	164	THR
1	B	183	LEU
1	B	184	LEU
1	B	185	LYS
1	B	187	LEU
1	B	188	MSE
1	B	198	THR
1	B	211	GLN
1	B	213	ILE
1	B	214	SER
1	B	215	ARG
1	B	216	ILE
1	B	219	ARG
1	B	221	ILE
1	B	222	VAL
1	B	223	THR
1	B	229	SER
1	B	231	ASP
1	B	233	LEU
1	B	235	GLN
1	B	236	PHE
1	B	239	GLU
1	B	240	LYS
1	B	242	ARG
1	B	247	ASP
1	B	250	LEU
1	B	253	ASP
1	B	254	GLU
1	B	255	GLN

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Mol	Chain	Res	Type
1	B	257	ASP
1	B	259	LEU
1	B	261	VAL
1	B	262	ASP
1	B	268	PRO
1	B	271	LEU
1	B	272	LEU
1	B	275	LEU
1	B	279	PHE
1	B	282	THR
1	B	283	LEU
1	B	284	LEU
1	B	285	THR
1	B	286	THR
1	B	299	LEU
1	B	300	LEU
1	B	305	ARG
1	B	311	ARG
1	B	315	GLN
1	B	329	MSE
1	B	338	ASP
1	B	341	PHE
1	B	346	GLN
1	B	348	ASN
1	B	357	THR
1	B	358	LEU
1	B	367	LEU
1	B	373	LEU
1	B	379	ARG
1	B	431	ARG
1	B	433	ARG
1	B	441	LEU
1	B	475	GLN
1	B	476	LEU
1	B	482	GLN
1	B	483	TYR
1	B	487	LEU
1	B	497	THR
1	B	499	GLU
1	B	502	ARG
1	B	540	LEU
1	B	543	ARG

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Mol	Chain	Res	Type
1	B	565	VAL
1	B	570	ASP
1	B	572	VAL
1	B	573	LEU
1	B	580	GLU
1	B	581	LEU
1	B	598	LEU
1	B	599	LEU
1	B	604	THR
1	B	612	LEU
1	B	615	ARG
1	B	616	LEU
1	B	624	GLN
1	B	627	THR
1	B	628	THR
1	B	629	LEU
1	B	635	LYS
1	B	636	MSE
1	B	649	LEU
1	B	652	LEU
1	B	660	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	114	ASN
1	A	115	GLN
1	A	134	HIS
1	A	137	GLN
1	A	181	GLN
1	A	255	GLN
1	A	274	GLN
1	A	322	GLN
1	A	348	ASN
1	A	403	ASN
1	A	423	GLN
1	A	444	HIS
1	A	505	GLN
1	A	516	ASN
1	A	569	ASN
1	A	668	GLN

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Mol	Chain	Res	Type
1	B	35	HIS
1	B	82	HIS
1	B	115	GLN
1	B	134	HIS
1	B	155	ASN
1	B	177	GLN
1	B	182	GLN
1	B	273	HIS
1	B	310	HIS
1	B	315	GLN
1	B	346	GLN
1	B	371	GLN
1	B	419	GLN
1	B	423	GLN
1	B	444	HIS
1	B	446	ASN
1	B	588	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACO	B	701	-	47,53,53	2.95	18 (38%)	60,79,79	4.65	31 (51%)
2	ACO	A	700	-	47,53,53	3.81	17 (36%)	60,79,79	5.40	31 (51%)
3	ADP	A	800	-	24,29,29	1.36	2 (8%)	29,45,45	1.79	5 (17%)
4	SO4	B	801	-	4,4,4	0.35	0	6,6,6	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	B	701	-	1/1/12/14	12/47/67/67	0/3/3/3
2	ACO	A	700	-	1/1/12/14	17/47/67/67	0/3/3/3
3	ADP	A	800	-	-	6/12/32/32	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	ACO	O5P-C5P	17.50	1.58	1.23
2	B	701	ACO	O5P-C5P	8.20	1.39	1.23
2	A	700	ACO	O9P-C9P	7.31	1.37	1.23
2	B	701	ACO	P1A-O3A	-6.97	1.52	1.59
2	A	700	ACO	P1A-O3A	-6.38	1.52	1.59
2	A	700	ACO	CH3-C	-6.06	1.25	1.50
2	A	700	ACO	C5P-N4P	5.87	1.47	1.33
2	A	700	ACO	C2A-N1A	5.33	1.43	1.33
2	B	701	ACO	C5P-N4P	5.17	1.45	1.33
2	A	700	ACO	C2A-N3A	5.17	1.40	1.32
2	B	701	ACO	C2A-N1A	5.14	1.43	1.33
2	B	701	ACO	O9P-C9P	5.05	1.33	1.23
2	B	701	ACO	CH3-C	-4.95	1.30	1.50
2	A	700	ACO	O4B-C1B	4.78	1.47	1.40
2	B	701	ACO	P3B-O3B	4.57	1.67	1.59
2	A	700	ACO	P3B-O3B	4.52	1.67	1.59
2	B	701	ACO	C6P-C5P	4.45	1.60	1.51
2	B	701	ACO	O4B-C4B	4.36	1.54	1.45
2	B	701	ACO	P3B-O7A	3.99	1.62	1.50
2	B	701	ACO	O4B-C1B	3.98	1.46	1.40
2	A	700	ACO	P2A-O3A	3.89	1.63	1.59
3	A	800	ADP	O4'-C1'	3.81	1.45	1.40
2	B	701	ACO	CCP-CBP	-3.62	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ACO	C2A-N3A	3.58	1.37	1.32
2	A	700	ACO	C1B-N9A	3.48	1.58	1.49
2	A	700	ACO	C6A-C5A	3.19	1.55	1.43
2	B	701	ACO	OAP-CAP	-2.83	1.37	1.42
2	B	701	ACO	C6A-C5A	2.82	1.53	1.43
3	A	800	ADP	C8-N7	-2.81	1.29	1.34
2	A	700	ACO	OAP-CAP	2.74	1.47	1.42
2	A	700	ACO	O4B-C4B	2.71	1.51	1.45
2	A	700	ACO	P3B-O7A	2.70	1.58	1.50
2	B	701	ACO	P2A-O3A	2.59	1.62	1.59
2	B	701	ACO	C4A-N3A	2.28	1.38	1.35
2	A	700	ACO	CDP-CBP	2.22	1.58	1.53
2	B	701	ACO	C5B-C4B	2.06	1.57	1.51
2	A	700	ACO	C6P-C5P	2.00	1.55	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ACO	C2P-C3P-N4P	16.47	146.81	112.41
2	A	700	ACO	CEP-CBP-CAP	15.46	135.13	108.77
2	A	700	ACO	O5P-C5P-C6P	-15.37	94.17	122.02
2	B	701	ACO	O5P-C5P-C6P	-15.24	94.41	122.02
2	B	701	ACO	C2P-C3P-N4P	14.14	141.94	112.41
2	B	701	ACO	O5P-C5P-N4P	-13.49	96.56	123.03
2	A	700	ACO	CEP-CBP-CDP	-12.41	84.46	109.20
2	A	700	ACO	CAP-C9P-N8P	-11.39	94.86	116.48
2	A	700	ACO	O5P-C5P-N4P	-10.65	102.14	123.03
2	A	700	ACO	O6A-CCP-CBP	10.15	126.86	110.55
2	B	701	ACO	O6A-CCP-CBP	8.28	123.85	110.55
2	B	701	ACO	C1B-N9A-C4A	-8.12	112.38	126.64
2	B	701	ACO	CAP-C9P-N8P	-7.81	101.67	116.48
2	A	700	ACO	C3P-N4P-C5P	-7.78	108.34	122.82
2	B	701	ACO	CEP-CBP-CAP	7.65	121.80	108.77
2	A	700	ACO	O9P-C9P-CAP	7.49	141.80	120.89
2	A	700	ACO	C2P-S1P-C	7.30	136.55	101.42
2	B	701	ACO	C2P-S1P-C	7.28	136.45	101.42
2	B	701	ACO	C6P-C5P-N4P	6.44	128.08	116.34
2	A	700	ACO	CDP-CBP-CAP	-6.33	97.97	108.77
2	A	700	ACO	CDP-CBP-CCP	5.42	117.17	108.22
2	B	701	ACO	O9P-C9P-CAP	5.36	135.87	120.89
2	B	701	ACO	CDP-CBP-CAP	-5.36	99.64	108.77
2	A	700	ACO	C6P-C7P-N8P	-5.34	100.64	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ACO	CEP-CBP-CCP	-5.32	99.44	108.22
2	B	701	ACO	C7P-N8P-C9P	5.23	131.95	122.55
3	A	800	ADP	N3-C2-N1	-5.20	121.62	128.67
2	A	700	ACO	OAP-CAP-CBP	4.98	121.72	110.18
2	B	701	ACO	O4B-C1B-N9A	-4.96	102.17	108.75
2	A	700	ACO	C7P-N8P-C9P	4.92	131.38	122.55
2	B	701	ACO	O3B-C3B-C2B	4.80	128.89	111.68
3	A	800	ADP	O2A-PA-O3A	4.39	119.14	107.27
2	A	700	ACO	C7P-C6P-C5P	-4.35	105.15	112.39
2	B	701	ACO	C4B-O4B-C1B	-4.31	105.97	109.92
2	B	701	ACO	C3P-N4P-C5P	4.21	130.66	122.82
2	A	700	ACO	O-C-S1P	-3.79	107.33	122.65
2	B	701	ACO	O-C-S1P	-3.75	107.47	122.65
2	A	700	ACO	P1A-O5B-C5B	-3.75	99.85	121.35
2	A	700	ACO	O4B-C4B-C5B	-3.68	97.56	109.33
2	B	701	ACO	C7P-C6P-C5P	-3.58	106.44	112.39
2	B	701	ACO	O4B-C4B-C5B	3.47	120.47	109.33
2	A	700	ACO	OAP-CAP-C9P	3.34	123.32	109.38
2	A	700	ACO	C1B-N9A-C4A	3.22	132.31	126.64
2	B	701	ACO	P3B-O3B-C3B	3.11	131.75	123.43
2	B	701	ACO	O2A-P1A-O3A	-3.09	98.93	107.27
2	A	700	ACO	CEP-CBP-CCP	-2.95	103.35	108.22
2	A	700	ACO	C6P-C5P-N4P	2.86	121.56	116.34
3	A	800	ADP	O4'-C1'-N9	-2.78	105.06	108.75
2	A	700	ACO	O2A-P1A-O5B	2.74	119.98	107.57
3	A	800	ADP	O2A-PA-O1A	-2.65	100.11	112.44
3	A	800	ADP	O3A-PA-O1A	-2.62	102.81	110.70
2	A	700	ACO	O5B-C5B-C4B	2.62	117.92	108.99
2	B	701	ACO	CDP-CBP-CCP	2.60	112.52	108.22
2	A	700	ACO	C5B-C4B-C3B	-2.50	106.04	114.38
2	A	700	ACO	O4B-C1B-N9A	-2.44	105.51	108.75
2	B	701	ACO	C4A-C5A-N7A	2.42	111.90	109.34
2	A	700	ACO	C4A-C5A-N7A	2.37	111.84	109.34
2	B	701	ACO	C3B-C2B-C1B	2.37	105.09	99.89
2	A	700	ACO	P2A-O6A-CCP	2.29	133.62	121.12
2	A	700	ACO	C3B-C2B-C1B	2.28	104.90	99.89
2	B	701	ACO	O3A-P2A-O4A	2.25	117.47	110.70
2	B	701	ACO	P2A-O6A-CCP	2.16	132.86	121.12
2	B	701	ACO	N3A-C2A-N1A	-2.07	125.86	128.67
2	B	701	ACO	O3A-P1A-O1A	2.03	116.81	110.70
2	B	701	ACO	OAP-CAP-C9P	2.03	117.85	109.38
2	B	701	ACO	OAP-CAP-CBP	2.02	114.85	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ACO	C5A-C6A-N1A	-2.01	115.44	120.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	700	ACO	C2B
2	B	701	ACO	C2B

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	ACO	O4B-C4B-C5B-O5B
2	A	700	ACO	C5B-O5B-P1A-O3A
2	A	700	ACO	CEP-CBP-CCP-O6A
2	A	700	ACO	C9P-CAP-CBP-CCP
2	A	700	ACO	C9P-CAP-CBP-CDP
2	A	700	ACO	C9P-CAP-CBP-CEP
2	A	700	ACO	N8P-C9P-CAP-OAP
2	A	700	ACO	S1P-C2P-C3P-N4P
2	B	701	ACO	O4B-C4B-C5B-O5B
2	B	701	ACO	C5B-O5B-P1A-O1A
2	B	701	ACO	C5B-O5B-P1A-O3A
2	B	701	ACO	N8P-C9P-CAP-OAP
2	B	701	ACO	O5P-C5P-N4P-C3P
2	B	701	ACO	C3P-C2P-S1P-C
2	B	701	ACO	CH3-C-S1P-C2P
3	A	800	ADP	C5'-O5'-PA-O1A
3	A	800	ADP	C5'-O5'-PA-O3A
3	A	800	ADP	O4'-C4'-C5'-O5'
2	A	700	ACO	O5P-C5P-N4P-C3P
3	A	800	ADP	C3'-C4'-C5'-O5'
2	A	700	ACO	C6P-C7P-N8P-C9P
2	A	700	ACO	C3B-C4B-C5B-O5B
2	B	701	ACO	C3B-C4B-C5B-O5B
2	A	700	ACO	CH3-C-S1P-C2P
2	A	700	ACO	O9P-C9P-CAP-OAP
2	B	701	ACO	O9P-C9P-CAP-OAP
2	B	701	ACO	C6P-C7P-N8P-C9P
2	B	701	ACO	C9P-CAP-CBP-CEP
3	A	800	ADP	PB-O3A-PA-O2A
2	B	701	ACO	C9P-CAP-CBP-CCP
2	A	700	ACO	C3P-C2P-S1P-C

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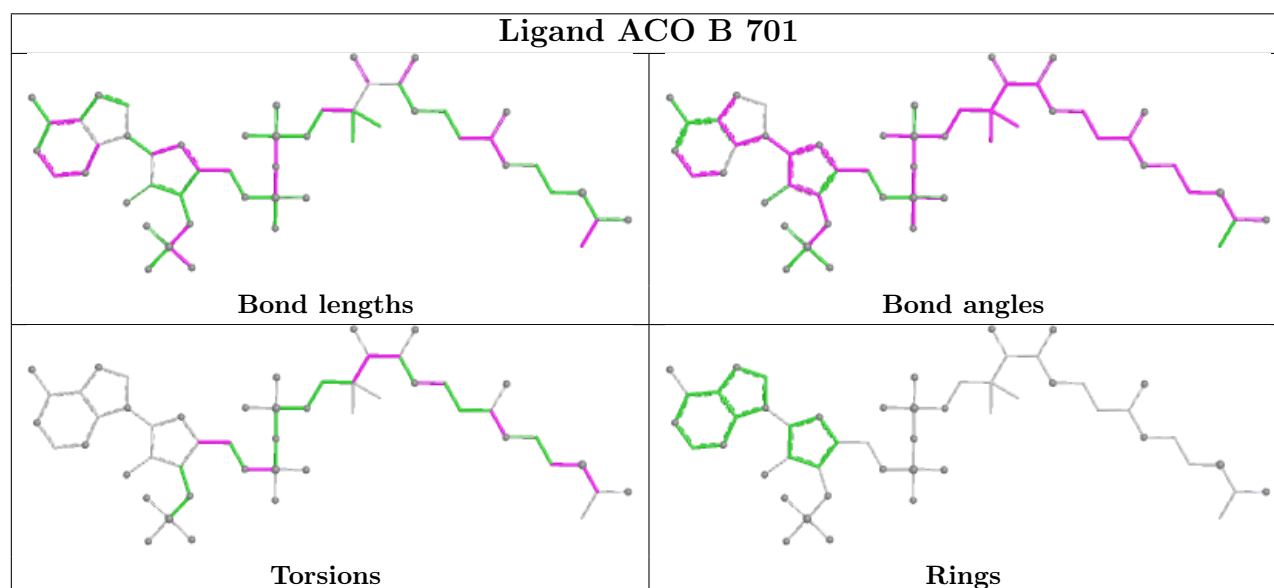
Mol	Chain	Res	Type	Atoms
2	A	700	ACO	C5B-O5B-P1A-O1A
2	A	700	ACO	C3B-O3B-P3B-O8A
2	A	700	ACO	C6P-C5P-N4P-C3P
3	A	800	ADP	PB-O3A-PA-O1A

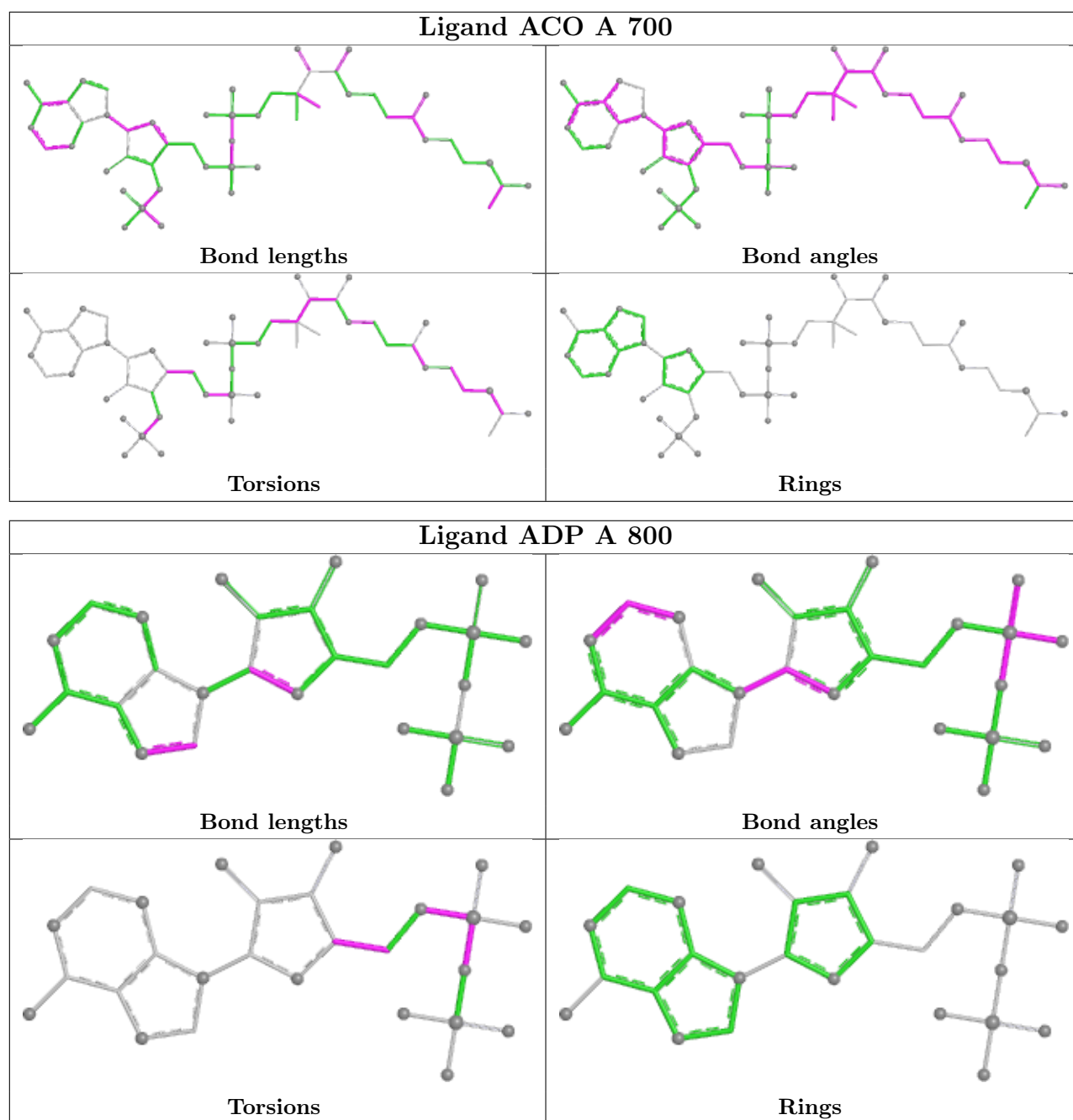
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ACO	7	0
2	A	700	ACO	3	0
3	A	800	ADP	2	0
4	B	801	SO4	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	648/671 (96%)	-0.03	23 (3%)	47	53	18, 35, 62, 90	0
1	B	651/671 (97%)	0.74	88 (13%)	8	10	22, 49, 99, 100	0
All	All	1299/1342 (96%)	0.36	111 (8%)	18	22	18, 42, 95, 100	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	PRO	6.3
1	B	258	TRP	5.7
1	A	54	PRO	5.4
1	B	65	LEU	5.2
1	B	217	ALA	4.7
1	B	184	LEU	4.7
1	B	484	THR	4.7
1	B	187	LEU	4.5
1	A	228	ALA	4.4
1	B	221	ILE	4.4
1	B	56	ALA	4.4
1	B	216	ILE	4.3
1	A	2	ALA	4.3
1	B	212	LEU	4.2
1	B	226	ALA	4.2
1	B	482	GLN	4.2
1	B	232	VAL	4.1
1	B	251	ALA	4.0
1	B	483	TYR	4.0
1	B	241	PHE	4.0
1	A	52	PRO	3.9
1	B	55	ASP	3.9
1	B	244	ILE	3.9
1	B	209	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	226	ALA	3.8
1	B	275	LEU	3.8
1	B	53	ARG	3.7
1	B	341	PHE	3.5
1	B	189	THR	3.5
1	A	66	GLN	3.5
1	B	318	ILE	3.5
1	B	191	PRO	3.4
1	B	312	PHE	3.4
1	A	670	PHE	3.4
1	B	69	LEU	3.4
1	A	70	GLY	3.4
1	B	502	ARG	3.3
1	B	237	ALA	3.3
1	B	243	PHE	3.2
1	B	183	LEU	3.1
1	A	668	GLN	3.1
1	B	670	PHE	3.1
1	A	67	THR	3.1
1	B	215	ARG	3.1
1	B	229	SER	3.1
1	B	208	LEU	3.0
1	B	238	GLY	3.0
1	B	340	ASN	3.0
1	B	220	ALA	3.0
1	A	634	ARG	3.0
1	B	192	PRO	3.0
1	A	517	HIS	2.9
1	B	349	ILE	2.9
1	B	52	PRO	2.9
1	A	291	TYR	2.9
1	B	236	PHE	2.9
1	B	214	SER	2.9
1	B	279	PHE	2.8
1	B	246	PRO	2.8
1	B	219	ARG	2.8
1	B	249	LEU	2.8
1	B	250	LEU	2.8
1	B	623	ALA	2.8
1	B	170	TYR	2.7
1	B	233	LEU	2.7
1	B	314	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	669	LEU	2.7
1	B	255	GLN	2.7
1	B	228	ALA	2.7
1	B	252	SER	2.6
1	B	223	THR	2.6
1	B	257	ASP	2.6
1	A	254	GLU	2.5
1	B	431	ARG	2.5
1	B	566	ASP	2.5
1	B	307	PRO	2.5
1	A	68	LEU	2.4
1	B	68	LEU	2.4
1	B	171	PRO	2.4
1	B	160	LEU	2.4
1	A	162	HIS	2.4
1	B	248	ALA	2.4
1	A	51	SER	2.3
1	B	278	ARG	2.3
1	A	485	GLN	2.3
1	B	259	LEU	2.3
1	B	224	ALA	2.3
1	B	178	PRO	2.3
1	B	338	ASP	2.3
1	B	346	GLN	2.2
1	B	485	GLN	2.2
1	B	261	VAL	2.2
1	A	69	LEU	2.2
1	A	569	ASN	2.2
1	B	242	ARG	2.1
1	B	172	ALA	2.1
1	B	193	GLY	2.1
1	B	210	GLY	2.1
1	B	629	LEU	2.1
1	B	631	LEU	2.1
1	A	227	LYS	2.1
1	B	67	THR	2.1
1	A	53	ARG	2.1
1	B	433	ARG	2.1
1	B	176	PRO	2.1
1	A	669	LEU	2.1
1	B	204	GLY	2.0
1	B	280	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	260	VAL	2.0
1	B	240	LYS	2.0
1	B	213	ILE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

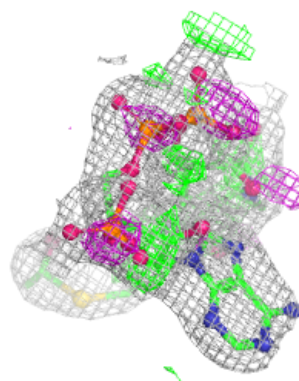
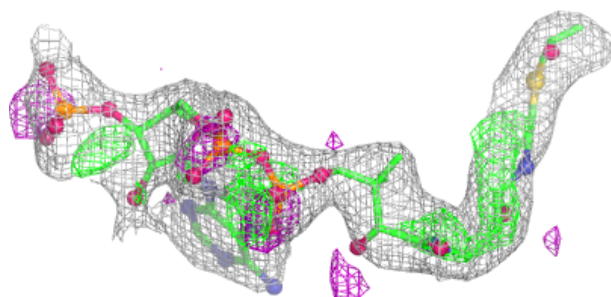
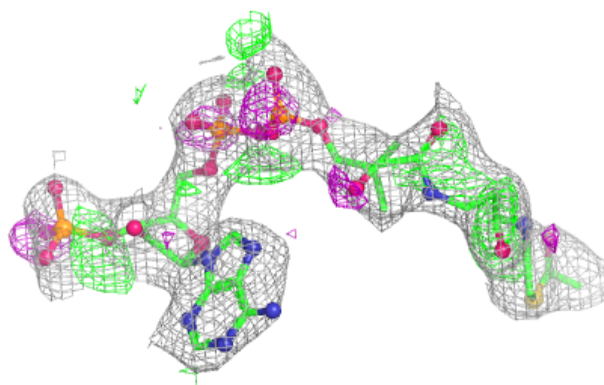
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	801	5/5	0.76	0.12	77,78,78,79	0
2	ACO	B	701	51/51	0.87	0.18	24,50,93,95	0
2	ACO	A	700	51/51	0.88	0.19	18,66,88,89	0
3	ADP	A	800	27/27	0.94	0.09	29,38,39,43	0

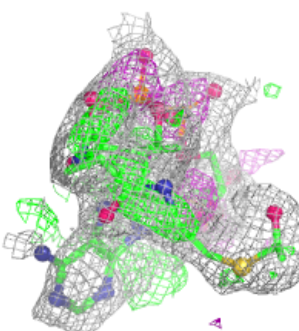
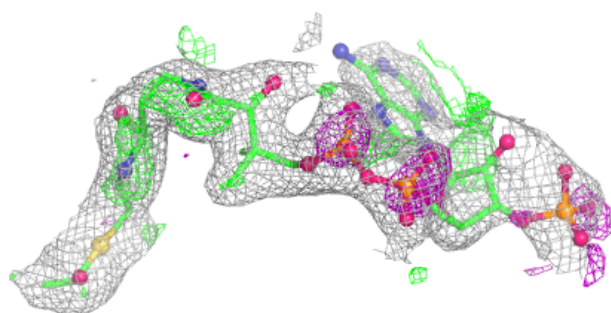
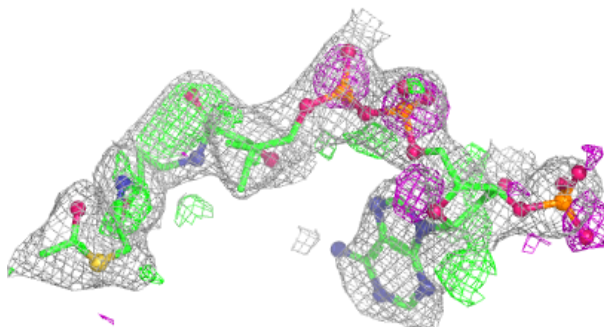
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

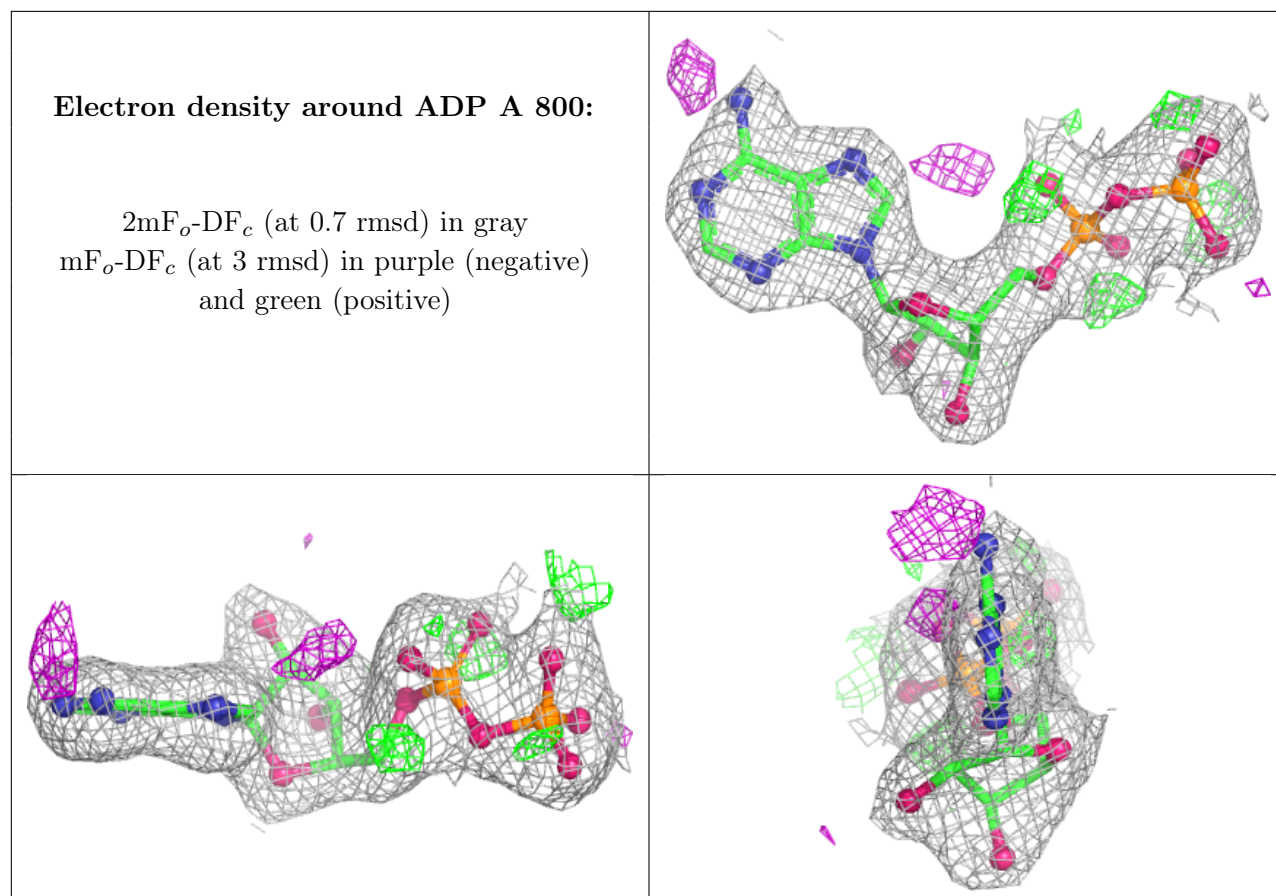
Electron density around ACO B 701:

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

**Electron density around ACO A 700:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.