



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:00 AM UTC

PDB ID : 7CQT / pdb_00007cqt
Title : Crystal structure of Brassica juncea HMG-CoA synthase 1 mutant - S359A in complex with acetyl-CoA
Authors : Liao, P.; Hu, M.; Kong, G.K.W.; Hao, Q.; Chye, M.L.
Deposited on : 2020-08-11
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

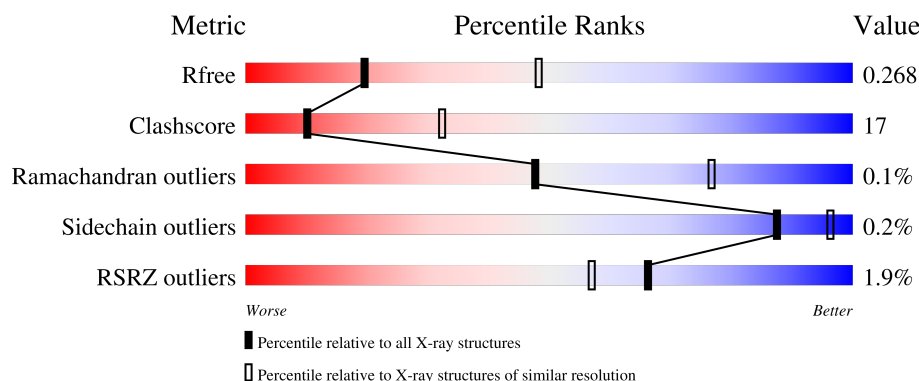
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	461	74% 23% ..
1	B	461	69% 27% ..
1	C	461	4% 59% 36% ..
1	D	461	66% 31% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14148 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.

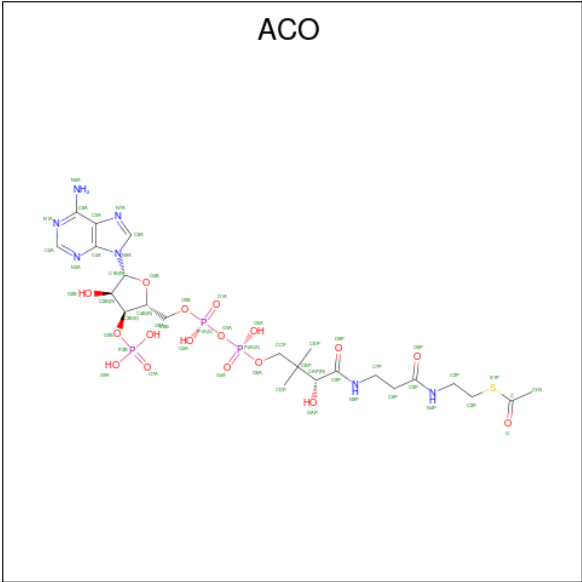
- Molecule 1 is a protein called 3-hydroxy-3-methylglutaryl coenzyme A synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3509	2237	575	674	23			
1	B	449	Total	C	N	O	S	0	0	0
			3500	2231	573	673	23			
1	C	447	Total	C	N	O	S	0	0	0
			3493	2227	572	671	23			
1	D	451	Total	C	N	O	S	0	0	0
			3517	2242	576	675	24			

There are 4 discrepancies between the modelled and reference sequences:

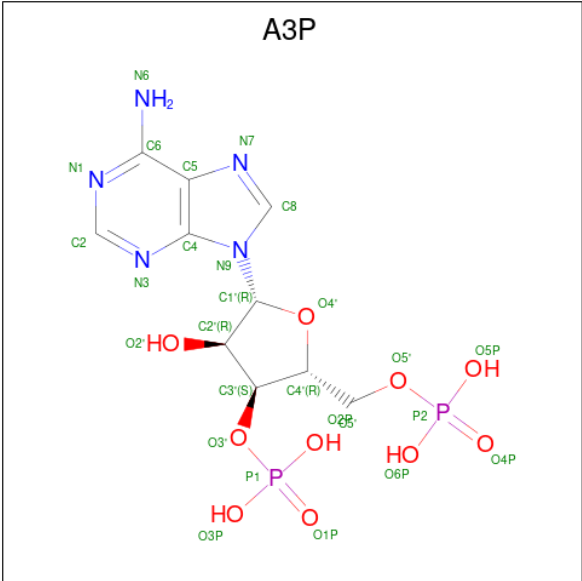
Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ALA	SER	engineered mutation	UNP Q9M6U3
B	359	ALA	SER	engineered mutation	UNP Q9M6U3
C	359	ALA	SER	engineered mutation	UNP Q9M6U3
D	359	ALA	SER	engineered mutation	UNP Q9M6U3

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



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-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

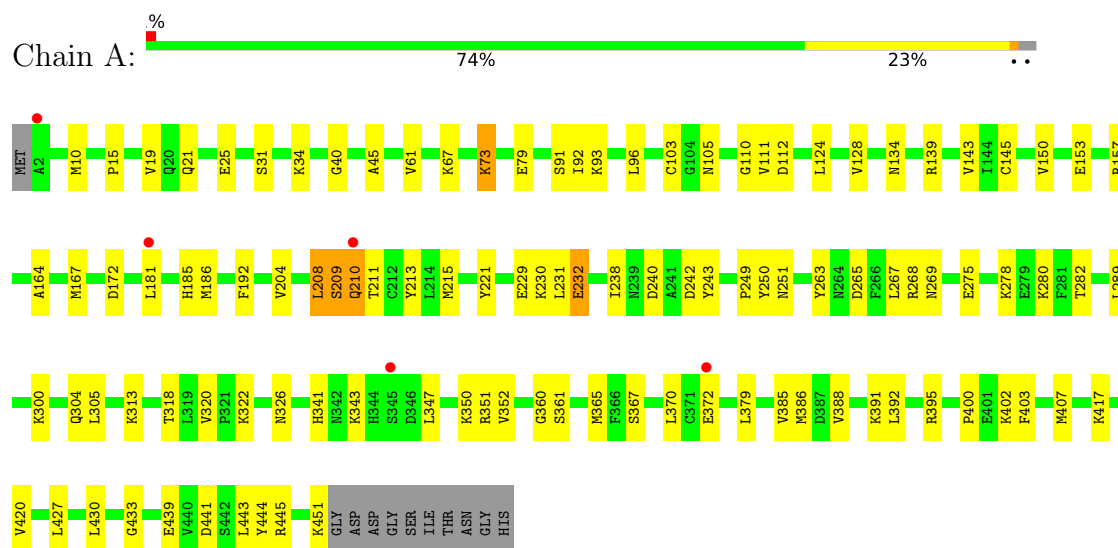


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

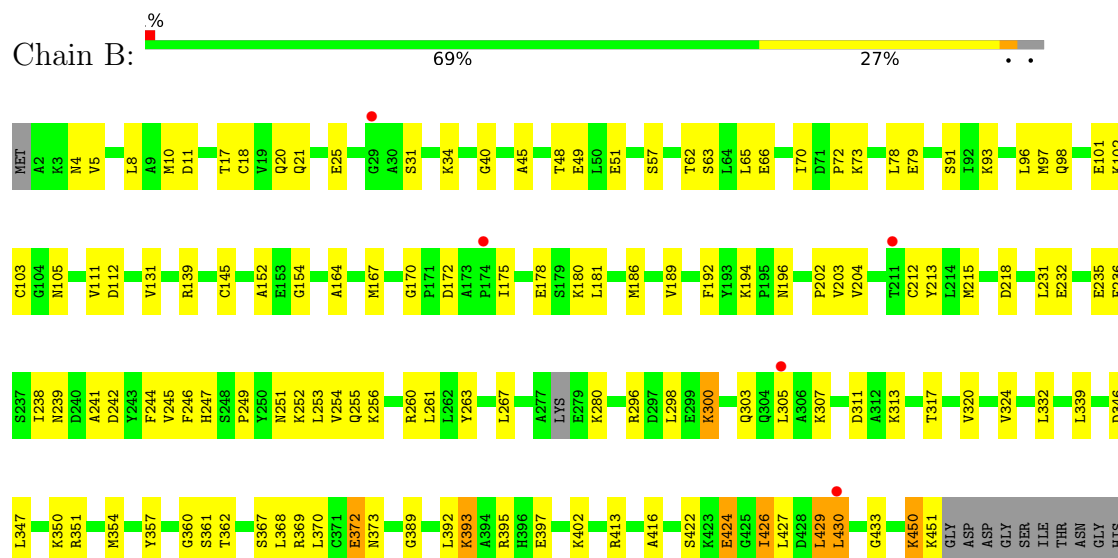
3 Residue-property plots [i](#)

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: 3-hydroxy-3-methylglutaryl coenzyme A synthase

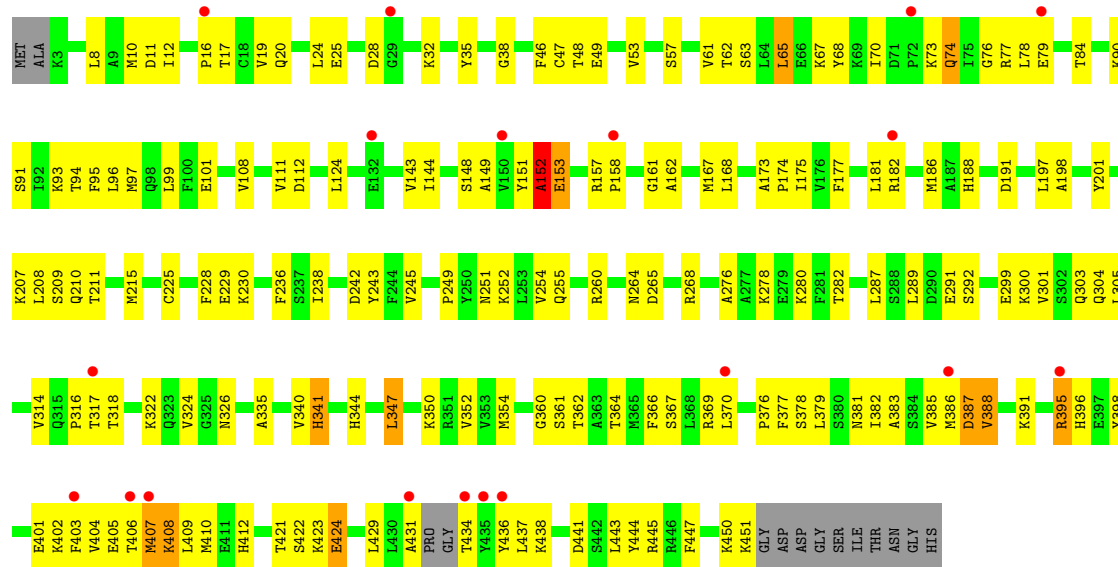


- Molecule 1: 3-hydroxy-3-methylglutaryl coenzyme A synthase

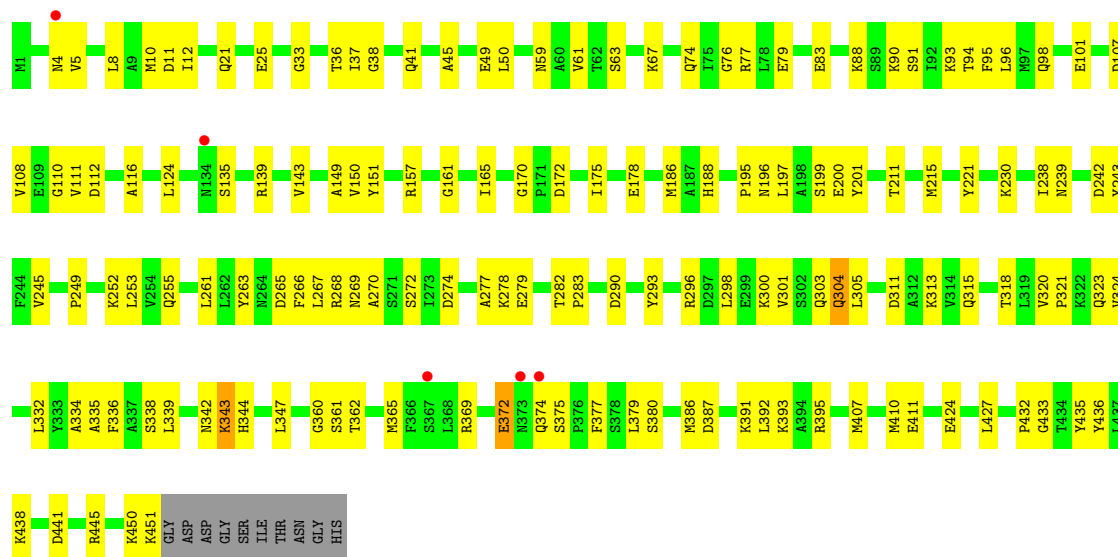


- Molecule 1: 3-hydroxy-3-methylglutaryl coenzyme A synthase





• Molecule 1: 3-hydroxy-3-methylglutaryl coenzyme A synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.61Å 121.61Å 118.61Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	34.62 – 2.80 34.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.7 (34.62-2.80) 84.4 (34.62-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.227 , 0.267 0.229 , 0.268	Depositor DCC
R_{free} test set	1989 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,-l,-k 0.001 for -h,l,k 0.031 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14148	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: ACO, A3P

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	1/3585 (0.0%)	0.71	9/4843 (0.2%)
1	B	0.40	2/3575 (0.1%)	0.79	16/4829 (0.3%)
1	C	0.48	0/3567	0.95	21/4816 (0.4%)
1	D	0.40	1/3593 (0.0%)	0.77	5/4853 (0.1%)
All	All	0.44	4/14320 (0.0%)	0.81	51/19341 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	VAL	CA-CB	-20.71	1.43	1.54
1	B	320	VAL	CA-CB	7.13	1.63	1.54
1	B	424	GLU	CG-CD	-5.73	1.37	1.52
1	D	343	LYS	CE-NZ	-5.33	1.33	1.49

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	407	MET	CA-CB-CG	-15.92	82.26	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	GLU	CA-CB-CG	10.43	134.96	114.10
1	B	300	LYS	CB-CG-CD	8.95	131.88	111.30
1	C	408	LYS	CB-CG-CD	-8.78	91.11	111.30
1	B	372	GLU	CA-CB-CG	-8.71	96.69	114.10
1	C	304	GLN	CA-CB-CG	-8.35	97.40	114.10
1	C	347	LEU	CB-CG-CD2	-8.12	86.33	110.70
1	C	424	GLU	CA-CB-CG	-7.51	99.08	114.10
1	C	73	LYS	CA-CB-CG	7.41	128.92	114.10
1	B	426	ILE	CA-CB-CG1	-7.01	98.48	110.40
1	B	393	LYS	CG-CD-CE	-6.83	95.59	111.30
1	C	398	TYR	CA-C-N	-6.79	110.84	120.49
1	C	398	TYR	C-N-CA	-6.79	110.84	120.49
1	D	304	GLN	CA-CB-CG	6.69	127.47	114.10
1	C	20	GLN	CB-CA-C	6.51	121.11	109.38
1	B	424	GLU	CB-CG-CD	-6.51	101.53	112.60
1	A	372	GLU	CA-CB-CG	6.51	127.12	114.10
1	D	342	ASN	CA-C-N	-6.48	110.74	122.54
1	D	342	ASN	C-N-CA	-6.48	110.74	122.54
1	A	73	LYS	CA-CB-CG	-6.41	101.29	114.10
1	D	372	GLU	CB-CG-CD	6.23	123.19	112.60
1	B	429	LEU	CA-C-N	-6.18	111.14	121.39
1	B	429	LEU	C-N-CA	-6.18	111.14	121.39
1	B	235	GLU	N-CA-CB	-5.69	101.64	110.29
1	B	430	LEU	CB-CG-CD1	5.65	127.64	110.70
1	C	74	GLN	CA-CB-CG	-5.58	102.93	114.10
1	A	372	GLU	CB-CG-CD	-5.53	103.20	112.60
1	A	172	ASP	N-CA-CB	-5.48	103.08	111.74
1	C	388	VAL	CG1-CB-CG2	5.46	122.81	110.80
1	A	210	GLN	CB-CG-CD	5.45	121.86	112.60
1	C	210	GLN	CA-CB-CG	5.38	124.87	114.10
1	B	424	GLU	CA-CB-CG	5.33	124.75	114.10
1	C	395	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	C	153	GLU	CA-CB-CG	5.32	124.73	114.10
1	C	153	GLU	CB-CA-C	5.28	118.42	109.50
1	C	341	HIS	CB-CA-C	-5.28	102.60	110.88
1	C	152	ALA	CA-C-N	-5.23	113.75	122.64
1	C	152	ALA	C-N-CA	-5.23	113.75	122.64
1	C	65	LEU	CB-CG-CD2	-5.20	95.10	110.70
1	B	416	ALA	CA-C-N	5.19	131.23	122.87
1	B	416	ALA	C-N-CA	5.19	131.23	122.87
1	A	400	PRO	CA-C-N	-5.17	112.55	121.66
1	A	400	PRO	C-N-CA	-5.17	112.55	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	408	LYS	CG-CD-CE	5.16	123.17	111.30
1	B	300	LYS	CG-CD-CE	-5.12	99.52	111.30
1	D	393	LYS	CB-CG-CD	-5.07	99.63	111.30
1	B	346	ASP	CB-CA-C	-5.06	100.84	109.65
1	B	424	GLU	CA-C-N	-5.04	111.52	121.41
1	B	424	GLU	C-N-CA	-5.04	111.52	121.41
1	A	232	GLU	CB-CG-CD	-5.02	104.06	112.60
1	A	210	GLN	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLU	Sidechain
1	B	450	LYS	Peptide
1	C	74	GLN	Peptide
1	D	438	LYS	Peptide
1	D	74	GLN	Sidechain

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	3509	0	3458	73	0
1	B	3500	0	3444	108	0
1	C	3493	0	3442	185	0
1	D	3517	0	3470	138	0
2	A	51	0	34	5	0
2	B	51	0	34	10	0
3	C	27	0	11	4	0
All	All	14148	0	13893	483	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 17.

All (483) 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:182:ARG:NH2	1:D:135:SER:HB3	1.33	1.41
1:C:182:ARG:NH2	1:D:135:SER:CB	1.81	1.40
1:C:182:ARG:HH22	1:D:135:SER:CB	1.41	1.26
2:A:501:ACO:O4B	2:A:501:ACO:C1B	1.66	1.24
2:B:501:ACO:O4B	2:B:501:ACO:C1B	1.66	1.20
1:D:98:GLN:HA	1:D:101:GLU:HG3	1.28	1.15
1:C:318:THR:HB	1:C:322:LYS:HZ1	1.13	1.07
1:C:182:ARG:CZ	1:D:135:SER:HB3	1.84	1.06
1:C:341:HIS:CD2	1:C:388:VAL:HG13	1.91	1.05
1:D:4:ASN:OD1	1:D:172:ASP:HA	1.56	1.05
1:C:182:ARG:NH2	1:D:135:SER:CA	2.21	1.04
1:C:229:GLU:OE2	1:C:230:LYS:NZ	1.95	0.99
1:C:318:THR:HB	1:C:322:LYS:NZ	1.78	0.99
1:D:4:ASN:OD1	1:D:172:ASP:CA	2.11	0.98
1:A:265:ASP:OD1	1:A:268:ARG:NH2	1.99	0.96
1:D:344:HIS:CD2	1:D:380:SER:HA	2.01	0.95
1:D:344:HIS:HD2	1:D:380:SER:HA	1.31	0.95
1:D:59:ASN:HD21	1:D:435:TYR:H	1.09	0.95
1:C:386:MET:O	1:C:388:VAL:N	2.01	0.93
1:B:332:LEU:HD21	1:B:354:MET:HG2	1.47	0.93
1:B:372:GLU:HG3	1:B:373:ASN:N	1.80	0.93
1:C:182:ARG:HH21	1:D:135:SER:HA	1.33	0.92
1:C:324:VAL:HG22	1:C:395:ARG:HH22	1.35	0.92
1:A:186:MET:HB2	1:B:97:MET:HE2	1.51	0.91
1:B:181:LEU:HD22	1:B:367:SER:HB2	1.53	0.90
1:B:450:LYS:HG2	1:B:451:LYS:HB2	1.54	0.89
1:D:4:ASN:OD1	1:D:172:ASP:N	2.06	0.88
1:A:210:GLN:HG3	1:A:211:THR:H	1.37	0.88
1:A:210:GLN:HG3	1:A:211:THR:N	1.88	0.86
1:C:376:PRO:HA	1:C:381:ASN:HD22	1.40	0.85
1:D:201:TYR:OH	1:D:411:GLU:OE2	1.94	0.85
1:C:175:ILE:HA	1:C:370:LEU:HD22	1.57	0.84
1:B:280:LYS:HD2	1:B:305:LEU:HD11	1.59	0.83
1:C:182:ARG:NH2	1:D:135:SER:HA	1.88	0.83
1:C:347:LEU:HA	1:C:350:LYS:HE2	1.59	0.83
1:C:252:LYS:HA	1:C:255:GLN:HG3	1.61	0.83
1:D:269:ASN:HD21	1:D:278:LYS:HD3	1.43	0.82
1:C:12:ILE:HD11	1:C:386:MET:HE2	1.62	0.82
1:B:424:GLU:N	1:B:424:GLU:OE1	2.13	0.81
1:C:97:MET:HE2	1:D:186:MET:HB3	1.63	0.81
1:C:341:HIS:CD2	1:C:388:VAL:CG1	2.64	0.81
1:D:296:ARG:O	1:D:300:LYS:HG2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:MET:HB3	1:C:386:MET:HE3	1.63	0.80
1:C:65:LEU:HA	1:C:70:ILE:HD13	1.62	0.79
1:B:347:LEU:HB3	1:B:370:LEU:HD12	1.63	0.79
1:A:347:LEU:HB3	1:A:370:LEU:HD22	1.65	0.78
1:A:73:LYS:HD3	1:A:103:CYS:HB3	1.65	0.78
1:C:77:ARG:NH1	1:C:79:GLU:OE2	2.16	0.78
1:C:388:VAL:HA	1:C:391:LYS:HB2	1.65	0.77
1:A:150:VAL:HG12	1:A:407:MET:HE1	1.65	0.77
1:C:68:TYR:HB2	1:C:70:ILE:HD11	1.67	0.77
1:C:443:LEU:HD12	1:C:445:ARG:HH21	1.49	0.76
1:C:347:LEU:HD21	1:C:370:LEU:CB	2.15	0.76
1:C:402:LYS:O	1:C:406:THR:OG1	2.04	0.76
1:B:357:TYR:CD1	2:B:501:ACO:HH31	2.21	0.75
1:A:243:TYR:HB2	1:A:352:VAL:HG22	1.67	0.75
1:D:36:THR:HG22	1:D:37:ILE:HD12	1.69	0.74
1:C:245:VAL:HB	1:C:354:MET:HG2	1.69	0.74
1:A:280:LYS:HD3	1:A:305:LEU:HD21	1.67	0.74
1:D:300:LYS:O	1:D:304:GLN:NE2	2.20	0.74
1:B:49:GLU:OE1	1:B:413:ARG:NH1	2.20	0.74
1:B:34:LYS:NZ	2:B:501:ACO:O5A	2.20	0.73
1:D:374:GLN:HG2	1:D:375:SER:H	1.54	0.73
1:B:357:TYR:HD1	2:B:501:ACO:HH31	1.53	0.73
1:A:211:THR:O	1:A:215:MET:HG3	1.88	0.73
1:C:405:GLU:HG2	1:C:408:LYS:HE2	1.69	0.73
1:D:77:ARG:NH1	1:D:79:GLU:OE2	2.22	0.73
1:B:98:GLN:O	1:B:101:GLU:OE2	2.06	0.72
1:C:124:LEU:HD21	1:C:177:PHE:CZ	2.25	0.72
1:C:28:ASP:OD2	1:C:157:ARG:NH2	2.23	0.72
1:D:379:LEU:HD12	1:D:379:LEU:H	1.54	0.72
1:C:347:LEU:HD21	1:C:370:LEU:HB2	1.70	0.71
1:D:63:SER:OG	1:D:67:LYS:HD2	1.89	0.71
1:B:51:GLU:OE2	1:B:430:LEU:HD21	1.89	0.71
1:D:4:ASN:CG	1:D:172:ASP:HA	2.15	0.71
1:C:347:LEU:HD22	1:C:379:LEU:HD13	1.71	0.71
1:A:134:ASN:O	1:B:180:LYS:HE3	1.91	0.70
1:A:31:SER:HB2	2:A:501:ACO:H62A	1.57	0.69
1:B:252:LYS:O	1:B:256:LYS:HG3	1.92	0.69
1:B:192:PHE:HD1	1:B:204:VAL:HG22	1.56	0.69
1:C:182:ARG:HH21	1:D:135:SER:CA	1.93	0.69
1:B:186:MET:HG2	1:B:362:THR:HA	1.73	0.69
1:C:174:PRO:HG2	1:C:175:ILE:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:SER:O	1:C:61:VAL:HG22	1.92	0.69
1:C:369:ARG:C	1:C:370:LEU:HD23	2.17	0.69
1:D:320:VAL:HG23	1:D:321:PRO:HD3	1.75	0.69
1:C:181:LEU:HD23	1:C:367:SER:HB2	1.76	0.68
1:A:208:LEU:HD12	1:A:211:THR:HB	1.74	0.68
1:A:269:ASN:ND2	1:D:372:GLU:OE2	2.26	0.68
1:D:59:ASN:ND2	1:D:435:TYR:H	1.88	0.68
1:D:211:THR:O	1:D:215:MET:HG3	1.94	0.68
1:B:48:THR:HG22	1:B:49:GLU:H	1.59	0.67
1:D:151:TYR:HB2	1:D:157:ARG:HA	1.77	0.67
1:B:424:GLU:O	1:B:426:ILE:N	2.28	0.67
1:A:386:MET:O	1:A:391:LYS:HE2	1.94	0.66
1:C:78:LEU:HB3	1:C:93:LYS:HE3	1.77	0.66
1:D:269:ASN:ND2	1:D:278:LYS:HD3	2.10	0.66
1:A:181:LEU:HD22	1:A:367:SER:HB2	1.75	0.66
1:C:19:VAL:HG21	1:C:403:PHE:CG	2.31	0.66
1:C:211:THR:O	1:C:215:MET:HG3	1.94	0.66
1:C:347:LEU:C	1:C:347:LEU:HD23	2.20	0.66
1:A:443:LEU:HB2	1:A:445:ARG:HD3	1.78	0.66
1:B:426:ILE:HD13	1:B:429:LEU:HD21	1.78	0.66
1:C:24:LEU:HD23	1:C:35:TYR:HE1	1.61	0.66
1:D:98:GLN:HB3	1:D:101:GLU:OE1	1.95	0.66
1:C:382:ILE:HG22	1:C:386:MET:HG3	1.77	0.65
1:B:246:PHE:HB2	1:B:254:VAL:HG23	1.79	0.65
1:D:12:ILE:HD12	1:D:165:ILE:HG12	1.79	0.65
1:C:47:CYS:O	1:C:407:MET:HE1	1.97	0.64
1:C:376:PRO:HA	1:C:381:ASN:ND2	2.09	0.64
1:A:433:GLY:H	1:A:451:LYS:HB2	1.62	0.63
1:B:4:ASN:OD1	1:B:172:ASP:HA	1.99	0.63
1:C:347:LEU:CD2	1:C:370:LEU:HB2	2.27	0.63
1:C:383:ALA:HA	1:C:386:MET:HB2	1.80	0.63
1:B:5:VAL:HG21	1:B:131:VAL:HG11	1.81	0.63
1:C:67:LYS:HB3	1:C:385:VAL:HG13	1.82	0.62
1:C:186:MET:HE3	1:D:108:VAL:O	1.98	0.62
1:C:188:HIS:HB2	1:D:94:THR:O	2.00	0.62
1:D:238:ILE:O	1:D:313:LYS:NZ	2.32	0.62
1:C:422:SER:HB2	1:C:424:GLU:CD	2.23	0.62
1:C:409:LEU:HD12	1:C:412:HIS:HB3	1.82	0.62
1:A:210:GLN:CG	1:A:211:THR:N	2.61	0.61
1:C:24:LEU:HD23	1:C:35:TYR:CE1	2.35	0.61
1:D:83:GLU:OE1	1:D:116:ALA:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:GLN:HB3	1:D:395:ARG:HH12	1.66	0.61
1:A:289:LEU:HB2	1:D:374:GLN:NE2	2.16	0.60
1:C:67:LYS:HD2	1:C:385:VAL:HG13	1.83	0.60
1:B:263:TYR:CZ	1:B:267:LEU:HD21	2.36	0.60
1:B:332:LEU:HD21	1:B:354:MET:CG	2.26	0.60
1:A:238:ILE:HG12	1:A:265:ASP:OD2	2.01	0.60
1:A:300:LYS:NZ	1:A:304:GLN:HE21	2.00	0.60
1:C:124:LEU:HD21	1:C:177:PHE:HZ	1.67	0.59
1:D:344:HIS:HD2	1:D:380:SER:CA	2.11	0.59
1:C:347:LEU:HD23	1:C:347:LEU:O	2.02	0.59
1:D:301:VAL:O	1:D:305:LEU:HD12	2.02	0.59
1:D:12:ILE:O	1:D:391:LYS:NZ	2.35	0.59
1:B:181:LEU:HD22	1:B:367:SER:CB	2.28	0.59
1:C:8:LEU:HB2	1:C:168:LEU:HD12	1.85	0.59
1:D:186:MET:HG3	1:D:362:THR:HA	1.85	0.59
1:D:374:GLN:HG2	1:D:375:SER:N	2.16	0.59
1:C:401:GLU:OE2	1:C:401:GLU:N	2.35	0.59
1:D:242:ASP:O	1:D:243:TYR:HD1	1.85	0.59
1:B:392:LEU:HD22	1:B:395:ARG:HH21	1.67	0.58
1:C:421:THR:OG1	1:C:423:LYS:HE3	2.04	0.58
1:C:149:ALA:N	1:C:161:GLY:O	2.35	0.58
1:C:124:LEU:HA	1:C:143:VAL:HG21	1.86	0.58
1:C:407:MET:SD	1:C:410:MET:HG3	2.43	0.58
1:D:334:ALA:O	1:D:338:SER:HB2	2.03	0.58
1:C:10:MET:CG	1:C:167:MET:HG2	2.34	0.57
1:C:387:ASP:C	1:C:391:LYS:HD3	2.29	0.57
1:B:251:ASN:O	1:B:254:VAL:HG12	2.03	0.57
1:C:436:TYR:CE1	1:C:438:LYS:HG2	2.39	0.57
1:C:149:ALA:O	1:C:161:GLY:N	2.32	0.57
1:C:197:LEU:O	1:D:197:LEU:HD13	2.05	0.57
1:D:266:PHE:CD1	1:D:267:LEU:HD23	2.39	0.57
1:B:280:LYS:HZ3	1:B:305:LEU:HD21	1.70	0.57
1:C:10:MET:HE2	1:C:386:MET:HE1	1.86	0.57
1:B:21:GLN:O	1:B:25:GLU:HG3	2.05	0.57
1:C:317:THR:HG23	1:C:335:ALA:HB1	1.85	0.57
1:C:28:ASP:CG	1:C:157:ARG:HH21	2.13	0.57
1:D:252:LYS:HA	1:D:255:GLN:HG3	1.87	0.57
1:A:278:LYS:O	1:A:282:THR:HG23	2.05	0.57
1:C:8:LEU:HD23	1:C:173:ALA:HA	1.86	0.57
1:C:441:ASP:OD2	1:C:445:ARG:N	2.37	0.57
1:D:242:ASP:O	1:D:313:LYS:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:VAL:HG23	1:B:170:GLY:C	2.30	0.56
1:C:378:SER:O	1:C:382:ILE:HD12	2.05	0.56
1:D:11:ASP:OD2	1:D:63:SER:OG	2.09	0.56
1:B:20:GLN:HG3	1:B:397:GLU:OE1	2.05	0.56
1:C:16:PRO:HA	1:C:395:ARG:HG3	1.86	0.56
1:C:249:PRO:HA	1:C:326:ASN:CG	2.30	0.56
1:D:45:ALA:HB3	1:D:324:VAL:HG13	1.86	0.56
1:B:296:ARG:O	1:B:300:LYS:HG3	2.06	0.56
1:C:68:TYR:HB2	1:C:70:ILE:CD1	2.35	0.56
1:D:5:VAL:HG23	1:D:170:GLY:C	2.30	0.56
1:D:407:MET:O	1:D:411:GLU:HG3	2.06	0.56
1:A:444:TYR:OH	1:B:196:ASN:ND2	2.39	0.56
1:D:238:ILE:HD12	1:D:265:ASP:OD2	2.06	0.56
1:B:40:GLY:HA3	1:B:251:ASN:HB3	1.88	0.56
1:C:124:LEU:HD12	1:C:167:MET:HE1	1.88	0.56
1:D:343:LYS:O	1:D:347:LEU:HG	2.05	0.55
1:A:21:GLN:O	1:A:25:GLU:HG3	2.05	0.55
1:B:10:MET:HG2	1:B:167:MET:HG2	1.87	0.55
1:C:405:GLU:HA	1:C:408:LYS:HE2	1.88	0.55
1:A:318:THR:OG1	1:A:322:LYS:NZ	2.38	0.55
1:C:124:LEU:HD23	1:C:124:LEU:C	2.32	0.55
1:D:277:ALA:CB	1:D:305:LEU:HD23	2.37	0.55
1:C:431:ALA:O	1:C:434:THR:N	2.40	0.55
1:B:280:LYS:NZ	1:B:305:LEU:HD21	2.21	0.55
1:D:149:ALA:N	1:D:161:GLY:O	2.36	0.55
1:D:277:ALA:HB1	1:D:305:LEU:HD23	1.89	0.55
1:A:300:LYS:HZ3	1:A:304:GLN:HE21	1.55	0.55
1:B:256:LYS:HG2	1:B:303:GLN:NE2	2.22	0.55
1:C:341:HIS:CG	1:C:388:VAL:CG1	2.90	0.55
1:A:263:TYR:CZ	1:A:267:LEU:HD11	2.42	0.54
1:C:387:ASP:HB3	1:C:391:LYS:HD2	1.89	0.54
1:B:101:GLU:CD	1:B:102:LYS:H	2.15	0.54
1:B:239:ASN:HA	1:B:313:LYS:HZ1	1.73	0.54
1:B:422:SER:HB2	1:B:424:GLU:CD	2.32	0.54
1:C:11:ASP:OD2	1:C:63:SER:OG	2.20	0.54
1:A:10:MET:HG2	1:A:167:MET:HG2	1.89	0.54
1:A:427:LEU:HD13	1:A:430:LEU:HD12	1.89	0.54
1:B:17:THR:HG22	1:B:429:LEU:HD11	1.89	0.54
1:B:192:PHE:CD1	1:B:204:VAL:HG22	2.41	0.54
1:C:198:ALA:HA	1:D:197:LEU:HD13	1.89	0.54
1:A:91:SER:HB2	1:A:112:ASP:CG	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LYS:NZ	2:B:501:ACO:O7A	2.39	0.54
1:C:243:TYR:HE1	1:C:350:LYS:HE3	1.73	0.54
1:B:91:SER:HB2	1:B:112:ASP:CG	2.33	0.54
1:C:157:ARG:HB3	1:C:158:PRO:HD3	1.88	0.54
1:D:243:TYR:CD2	1:D:339:LEU:HD11	2.43	0.54
1:C:32:LYS:HD3	1:C:32:LYS:C	2.32	0.53
1:D:424:GLU:OE1	1:D:424:GLU:N	2.34	0.53
1:C:230:LYS:N	1:C:230:LYS:HD2	2.24	0.53
1:C:347:LEU:HD21	1:C:370:LEU:HD12	1.88	0.53
1:C:347:LEU:HD11	1:C:370:LEU:HD12	1.90	0.53
1:C:94:THR:O	1:D:188:HIS:HB2	2.08	0.53
1:C:265:ASP:OD1	1:C:268:ARG:NH2	2.42	0.53
1:D:150:VAL:HG12	1:D:201:TYR:HE1	1.73	0.53
1:C:19:VAL:HG21	1:C:403:PHE:CD2	2.44	0.53
1:C:423:LYS:CE	1:C:438:LYS:HA	2.39	0.53
1:C:38:GLY:HA2	3:C:501:A3P:H5'2	1.90	0.52
1:C:68:TYR:CE2	1:C:385:VAL:HG11	2.43	0.52
1:D:300:LYS:O	1:D:304:GLN:CD	2.52	0.52
1:C:249:PRO:O	1:C:326:ASN:HB2	2.09	0.52
1:C:53:VAL:HG11	1:C:84:THR:OG1	2.10	0.52
1:B:239:ASN:HA	1:B:313:LYS:NZ	2.25	0.52
1:A:360:GLY:N	1:A:361:SER:HA	2.25	0.52
1:C:152:ALA:O	1:C:157:ARG:HD3	2.10	0.52
1:A:209:SER:O	1:A:213:TYR:N	2.24	0.52
1:B:31:SER:OG	2:B:501:ACO:N6A	2.34	0.52
1:B:213:TYR:HA	1:B:357:TYR:CE2	2.45	0.52
1:B:360:GLY:N	1:B:361:SER:HA	2.24	0.52
1:C:423:LYS:HE2	1:C:436:TYR:HE1	1.76	0.51
1:A:19:VAL:HG21	1:A:403:PHE:CG	2.45	0.51
1:B:245:VAL:CG1	1:B:354:MET:HG3	2.40	0.51
1:B:389:GLY:O	1:B:393:LYS:HE3	2.10	0.51
1:C:238:ILE:HG12	1:C:265:ASP:OD2	2.10	0.51
1:D:239:ASN:HA	1:D:313:LYS:NZ	2.25	0.51
1:D:150:VAL:HG22	1:D:407:MET:HE1	1.93	0.51
1:C:289:LEU:HA	1:C:292:SER:OG	2.09	0.51
1:D:243:TYR:HE2	1:D:347:LEU:HD21	1.75	0.51
1:C:191:ASP:HB2	1:C:209:SER:HA	1.92	0.51
1:C:396:HIS:CG	1:C:429:LEU:HD22	2.45	0.51
1:A:124:LEU:HD22	1:A:167:MET:HE1	1.93	0.51
1:D:178:GLU:CG	1:D:369:ARG:HG3	2.41	0.51
1:D:59:ASN:HD21	1:D:435:TYR:N	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ASP:O	1:D:139:ARG:NH1	2.45	0.50
1:C:252:LYS:HE3	3:C:501:A3P:O3P	2.11	0.50
1:A:420:VAL:HG22	1:A:439:GLU:HB3	1.94	0.50
1:B:79:GLU:HG3	1:B:111:VAL:O	2.12	0.50
1:B:178:GLU:OE2	1:B:369:ARG:NE	2.43	0.50
1:D:221:TYR:HA	1:D:365:MET:HE1	1.93	0.50
1:D:274:ASP:OD1	1:D:277:ALA:HB3	2.12	0.49
1:A:34:LYS:NZ	2:A:501:ACO:O5A	2.40	0.49
1:B:249:PRO:HB3	2:B:501:ACO:S1P	2.53	0.49
1:B:72:PRO:HB2	1:B:103:CYS:SG	2.53	0.49
1:C:278:LYS:O	1:C:282:THR:HG23	2.12	0.49
1:D:243:TYR:CE2	1:D:347:LEU:HD21	2.47	0.49
1:C:91:SER:HB2	1:C:112:ASP:CG	2.37	0.49
1:B:389:GLY:O	1:B:393:LYS:HB2	2.12	0.49
1:C:360:GLY:N	1:C:361:SER:HA	2.27	0.49
1:B:204:VAL:HG11	2:B:501:ACO:H71	1.94	0.49
1:C:198:ALA:HA	1:D:197:LEU:CD1	2.42	0.49
1:C:16:PRO:O	1:C:395:ARG:HG2	2.13	0.48
1:C:347:LEU:CD2	1:C:370:LEU:CB	2.87	0.48
1:C:300:LYS:HA	1:C:303:GLN:CG	2.43	0.48
1:D:36:THR:HA	1:D:41:GLN:O	2.12	0.48
1:A:79:GLU:HG3	1:A:111:VAL:O	2.13	0.48
1:C:450:LYS:HD2	1:C:451:LYS:HB3	1.96	0.48
1:D:441:ASP:OD2	1:D:445:ARG:NH1	2.46	0.48
1:B:427:LEU:HD13	1:B:427:LEU:O	2.13	0.48
1:C:78:LEU:HD11	1:C:96:LEU:HD12	1.93	0.48
1:D:305:LEU:HD12	1:D:305:LEU:H	1.79	0.48
1:B:242:ASP:OD1	1:B:350:LYS:HD2	2.14	0.48
1:A:347:LEU:HB2	1:A:379:LEU:HD13	1.96	0.48
1:A:124:LEU:HA	1:A:143:VAL:HG21	1.96	0.48
1:D:318:THR:C	1:D:321:PRO:HD2	2.39	0.48
1:A:240:ASP:O	1:A:351:ARG:NE	2.43	0.48
1:B:241:ALA:HB3	1:B:244:PHE:CE1	2.49	0.48
1:C:151:TYR:HA	1:C:201:TYR:HE1	1.78	0.48
1:D:8:LEU:HD11	1:D:170:GLY:O	2.14	0.48
1:A:300:LYS:O	1:A:300:LYS:HG2	2.08	0.47
1:C:10:MET:HG3	1:C:167:MET:HG2	1.95	0.47
1:C:381:ASN:O	1:C:385:VAL:HG23	2.13	0.47
1:D:239:ASN:HA	1:D:313:LYS:HZ1	1.78	0.47
1:B:332:LEU:HD23	1:B:332:LEU:O	2.15	0.47
1:C:243:TYR:HE2	1:C:316:PRO:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:VAL:O	1:C:317:THR:HB	2.14	0.47
1:D:21:GLN:O	1:D:25:GLU:HG3	2.14	0.47
1:B:51:GLU:CD	1:B:430:LEU:HD21	2.40	0.47
1:C:57:SER:HB3	1:C:96:LEU:HD21	1.95	0.47
1:B:175:ILE:CG2	1:B:368:LEU:HD13	2.45	0.47
1:B:189:VAL:HG21	1:B:212:CYS:SG	2.55	0.47
1:C:67:LYS:HD2	1:C:385:VAL:CG1	2.45	0.47
1:B:402:LYS:HA	1:B:402:LYS:HD3	1.74	0.47
1:C:76:GLY:O	1:C:108:VAL:HA	2.15	0.47
1:C:77:ARG:HD3	1:C:79:GLU:OE2	2.15	0.47
1:C:382:ILE:O	1:C:386:MET:HG3	2.15	0.47
1:D:265:ASP:OD1	1:D:268:ARG:NH1	2.46	0.47
1:D:433:GLY:H	1:D:451:LYS:C	2.22	0.47
1:A:280:LYS:HB2	1:A:305:LEU:HD11	1.97	0.47
1:C:260:ARG:O	1:C:264:ASN:ND2	2.47	0.47
1:C:276:ALA:O	1:C:280:LYS:HG3	2.15	0.47
1:C:364:THR:HG22	1:C:366:PHE:HD1	1.80	0.47
1:A:181:LEU:HD22	1:A:367:SER:CB	2.43	0.46
1:B:18:CYS:O	1:B:397:GLU:HA	2.15	0.46
1:C:124:LEU:HD12	1:C:167:MET:CE	2.45	0.46
1:C:197:LEU:HD23	1:D:88:LYS:HG3	1.96	0.46
1:C:444:TYR:CG	1:D:195:PRO:HB2	2.50	0.46
1:D:8:LEU:HD23	1:D:377:PHE:CE1	2.50	0.46
1:D:242:ASP:C	1:D:243:TYR:CD1	2.93	0.46
1:A:242:ASP:OD2	1:A:350:LYS:HD2	2.14	0.46
1:D:5:VAL:HG23	1:D:170:GLY:O	2.15	0.46
1:C:181:LEU:HD11	1:C:228:PHE:HB2	1.98	0.46
1:D:111:VAL:CG1	1:D:112:ASP:N	2.79	0.46
1:B:5:VAL:HG21	1:B:131:VAL:CG1	2.45	0.46
1:C:46:PHE:CD1	1:C:407:MET:HE2	2.50	0.46
1:D:49:GLU:HA	1:D:410:MET:SD	2.56	0.46
1:D:50:LEU:HB3	1:D:436:TYR:HB2	1.98	0.46
1:A:61:VAL:HG21	1:A:96:LEU:HD12	1.98	0.46
1:B:8:LEU:HD11	1:B:170:GLY:HA3	1.98	0.46
1:B:238:ILE:O	1:B:313:LYS:NZ	2.47	0.46
1:A:229:GLU:O	1:A:229:GLU:HG2	2.16	0.45
1:A:242:ASP:CG	1:A:350:LYS:HD2	2.40	0.45
1:B:152:ALA:C	1:B:154:GLY:H	2.23	0.45
1:D:91:SER:HB2	1:D:112:ASP:CG	2.41	0.45
1:B:186:MET:HE3	1:B:186:MET:HB2	1.39	0.45
1:C:423:LYS:HE3	1:C:438:LYS:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:TYR:HE1	2:A:501:ACO:H31	1.80	0.45
1:C:10:MET:HG2	1:C:167:MET:HG2	1.98	0.45
1:B:145:CYS:O	1:B:164:ALA:HA	2.15	0.45
1:C:370:LEU:HD23	1:C:370:LEU:N	2.30	0.45
1:D:200:GLU:H	1:D:200:GLU:CD	2.22	0.45
1:B:231:LEU:HB3	1:B:232:GLU:OE1	2.16	0.45
1:D:93:LYS:HD3	1:D:93:LYS:C	2.41	0.45
1:B:175:ILE:HG22	1:B:368:LEU:HD13	1.99	0.45
1:D:150:VAL:HG12	1:D:201:TYR:CE1	2.50	0.45
1:D:175:ILE:HD13	1:D:336:PHE:CE2	2.52	0.45
1:B:57:SER:HB3	1:B:96:LEU:HD21	1.99	0.45
1:C:382:ILE:O	1:C:386:MET:N	2.31	0.45
1:A:145:CYS:O	1:A:164:ALA:HA	2.17	0.45
1:D:282:THR:HG22	1:D:283:PRO:HD3	1.97	0.45
1:B:251:ASN:O	1:B:255:GLN:HG3	2.17	0.45
1:B:307:LYS:HD3	1:B:311:ASP:OD1	2.17	0.45
1:C:347:LEU:HD21	1:C:370:LEU:CD1	2.47	0.45
1:C:437:LEU:HD12	1:C:447:PHE:O	2.17	0.45
1:B:105:ASN:OD1	1:B:139:ARG:NH2	2.50	0.44
1:B:245:VAL:HG13	1:B:354:MET:HG3	1.99	0.44
1:C:347:LEU:CD1	1:C:370:LEU:HD12	2.47	0.44
1:C:90:LYS:HE3	1:C:95:PHE:CE2	2.52	0.44
1:C:188:HIS:CD2	1:D:98:GLN:OE1	2.70	0.44
1:D:255:GLN:OE1	1:D:303:GLN:NE2	2.50	0.44
1:B:236:PHE:HE2	1:B:351:ARG:NH1	2.16	0.44
1:D:230:LYS:HE2	1:D:230:LYS:HB3	1.72	0.44
1:B:73:LYS:HD3	1:B:103:CYS:O	2.17	0.44
1:B:263:TYR:CE2	1:B:298:LEU:HD11	2.52	0.44
1:D:221:TYR:HD1	1:D:365:MET:HE1	1.82	0.44
1:D:386:MET:O	1:D:391:LYS:HE3	2.17	0.44
1:D:343:LYS:HZ2	1:D:343:LYS:HG2	1.75	0.44
1:B:73:LYS:HG3	1:B:103:CYS:SG	2.57	0.44
1:D:221:TYR:HA	1:D:365:MET:CE	2.48	0.44
1:D:249:PRO:HG2	1:D:253:LEU:HD23	2.00	0.44
1:D:392:LEU:O	1:D:395:ARG:HG3	2.18	0.44
1:A:402:LYS:HA	1:A:402:LYS:HD3	1.75	0.44
1:B:263:TYR:CD2	1:B:298:LEU:HD11	2.52	0.44
1:C:188:HIS:ND1	1:D:95:PHE:HA	2.33	0.44
1:B:256:LYS:HG2	1:B:303:GLN:HE22	1.82	0.44
1:B:62:THR:O	1:B:66:GLU:HG3	2.17	0.43
1:C:225:CYS:SG	1:C:236:PHE:HB3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:PRO:HA	1:D:451:LYS:HG2	2.00	0.43
1:A:31:SER:CB	2:A:501:ACO:H62A	2.25	0.43
1:D:290:ASP:OD1	1:D:290:ASP:N	2.51	0.43
1:D:374:GLN:CG	1:D:375:SER:N	2.80	0.43
1:B:78:LEU:HB3	1:B:93:LYS:HE3	2.00	0.43
1:C:53:VAL:O	1:C:57:SER:OG	2.31	0.43
1:C:61:VAL:HG23	1:C:62:THR:H	1.83	0.43
1:C:301:VAL:O	1:C:305:LEU:HG	2.18	0.43
1:A:67:LYS:HB3	1:A:385:VAL:HG13	2.01	0.43
1:A:343:LYS:O	1:A:347:LEU:HG	2.18	0.43
1:B:45:ALA:HB3	1:B:324:VAL:HG13	2.00	0.43
1:B:245:VAL:HG23	1:B:317:THR:HB	2.00	0.43
1:D:215:MET:HG2	1:D:293:TYR:CZ	2.54	0.43
1:C:186:MET:HE1	1:D:110:GLY:O	2.18	0.43
1:A:231:LEU:HB3	1:A:232:GLU:OE1	2.19	0.43
1:D:33:GLY:O	1:D:38:GLY:N	2.45	0.43
1:C:111:VAL:HG22	1:C:112:ASP:H	1.82	0.43
1:C:208:LEU:HD23	1:C:208:LEU:HA	1.81	0.43
1:D:178:GLU:HG2	1:D:369:ARG:HG3	2.01	0.43
1:D:433:GLY:O	1:D:450:LYS:HG3	2.19	0.43
1:C:25:GLU:HG2	1:C:35:TYR:CD1	2.54	0.43
1:C:70:ILE:N	1:C:70:ILE:HD12	2.33	0.43
1:C:151:TYR:O	1:C:153:GLU:N	2.52	0.43
1:C:340:VAL:O	1:C:344:HIS:HB3	2.19	0.43
1:C:422:SER:HB2	1:C:424:GLU:OE2	2.19	0.43
1:D:111:VAL:HG12	1:D:112:ASP:N	2.34	0.43
1:B:11:ASP:OD2	1:B:63:SER:HB3	2.19	0.43
1:B:422:SER:HB2	1:B:424:GLU:OE1	2.18	0.42
1:D:196:ASN:ND2	1:D:199:SER:HB3	2.34	0.42
1:D:270:ALA:C	1:D:272:SER:H	2.26	0.42
1:D:335:ALA:O	1:D:338:SER:HB3	2.19	0.42
1:A:93:LYS:NZ	1:A:110:GLY:O	2.38	0.42
1:A:105:ASN:OD1	1:A:139:ARG:NH2	2.53	0.42
1:A:185:HIS:C	1:A:186:MET:HG2	2.43	0.42
1:C:175:ILE:HG23	1:C:370:LEU:CD2	2.49	0.42
1:A:40:GLY:HA3	1:A:251:ASN:HB3	2.00	0.42
1:B:247:HIS:CD2	2:B:501:ACO:HH32	2.54	0.42
1:C:46:PHE:HD1	1:C:407:MET:HE2	1.84	0.42
1:C:61:VAL:HG23	1:C:62:THR:N	2.34	0.42
1:C:207:LYS:O	1:C:207:LYS:HG3	2.19	0.42
1:C:387:ASP:O	1:C:387:ASP:CG	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:MET:HE2	1:D:10:MET:HB3	1.91	0.42
1:D:61:VAL:HG21	1:D:96:LEU:HD12	2.00	0.42
1:D:124:LEU:HA	1:D:143:VAL:HG21	2.01	0.42
1:A:124:LEU:O	1:A:128:VAL:HG23	2.19	0.42
1:A:229:GLU:OE2	1:A:230:LYS:NZ	2.52	0.42
1:B:422:SER:C	1:B:424:GLU:OE1	2.62	0.42
1:B:433:GLY:H	1:B:451:LYS:HA	1.83	0.42
1:C:49:GLU:HA	1:C:410:MET:SD	2.60	0.42
1:C:61:VAL:HG21	1:C:99:LEU:CD2	2.49	0.42
1:A:153:GLU:HA	1:A:157:ARG:HE	1.85	0.42
1:A:221:TYR:HB2	1:A:365:MET:HE1	2.02	0.42
1:A:341:HIS:ND1	1:A:388:VAL:HG22	2.34	0.42
1:C:186:MET:SD	1:C:362:THR:HG22	2.60	0.42
1:C:280:LYS:HD2	1:C:305:LEU:CD2	2.50	0.42
1:C:407:MET:SD	1:C:410:MET:CG	3.06	0.42
1:B:98:GLN:C	1:B:101:GLU:OE2	2.62	0.42
2:B:501:ACO:O4B	2:B:501:ACO:N9A	2.43	0.42
1:C:17:THR:HG21	1:C:48:THR:HG21	2.02	0.41
1:D:245:VAL:HG12	1:D:332:LEU:CD1	2.50	0.41
1:C:91:SER:HB2	1:C:112:ASP:OD2	2.20	0.41
1:C:242:ASP:CG	1:C:350:LYS:HB2	2.44	0.41
1:C:243:TYR:HB2	1:C:352:VAL:HG12	2.02	0.41
1:C:287:LEU:HD22	1:C:291:GLU:HB3	2.02	0.41
1:A:242:ASP:O	1:A:313:LYS:HG2	2.19	0.41
1:D:360:GLY:N	1:D:361:SER:HA	2.34	0.41
1:A:417:LYS:HE2	1:A:444:TYR:CZ	2.54	0.41
1:B:317:THR:HG22	1:B:339:LEU:HB2	2.01	0.41
1:C:404:VAL:O	1:C:408:LYS:HG3	2.20	0.41
1:B:424:GLU:C	1:B:426:ILE:H	2.27	0.41
1:C:49:GLU:HG2	1:C:421:THR:HB	2.02	0.41
1:D:90:LYS:HE3	1:D:95:PHE:CE2	2.55	0.41
1:D:178:GLU:CD	1:D:369:ARG:HG3	2.46	0.41
1:A:392:LEU:HD22	1:A:395:ARG:NH1	2.35	0.41
1:C:38:GLY:CA	3:C:501:A3P:H5'2	2.50	0.41
1:C:143:VAL:O	1:C:144:ILE:HD13	2.20	0.41
1:D:263:TYR:CD1	1:D:298:LEU:HD11	2.55	0.41
1:D:311:ASP:HA	1:D:315:GLN:HB2	2.03	0.41
1:A:249:PRO:O	1:A:326:ASN:HB2	2.21	0.41
1:B:213:TYR:CZ	1:B:253:LEU:HD21	2.55	0.41
1:C:148:SER:HA	1:C:162:ALA:HA	2.03	0.41
1:C:186:MET:HG2	1:C:362:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:HD1	1:A:204:VAL:HG22	1.86	0.41
1:A:441:ASP:OD2	1:A:445:ARG:NE	2.54	0.41
1:B:261:LEU:HD23	1:B:261:LEU:HA	1.89	0.41
1:C:424:GLU:H	1:C:424:GLU:HG2	1.19	0.41
1:D:266:PHE:HD1	1:D:267:LEU:HD23	1.84	0.41
1:B:215:MET:HE2	1:B:215:MET:HB3	1.91	0.41
1:B:242:ASP:OD2	1:B:242:ASP:N	2.51	0.41
1:C:229:GLU:HG2	1:C:230:LYS:HD2	2.03	0.41
1:C:299:GLU:O	1:C:303:GLN:HG2	2.21	0.41
1:D:76:GLY:HA3	1:D:139:ARG:HD3	2.02	0.41
1:D:261:LEU:HD23	1:D:261:LEU:HA	1.88	0.41
1:D:347:LEU:HA	1:D:347:LEU:HD23	1.49	0.41
1:B:263:TYR:CE2	1:B:267:LEU:HD21	2.55	0.41
1:C:8:LEU:HD22	1:C:377:PHE:CD2	2.56	0.41
1:D:334:ALA:O	1:D:338:SER:N	2.54	0.41
1:A:92:ILE:O	1:A:96:LEU:HD23	2.21	0.40
1:C:251:ASN:O	1:C:254:VAL:HB	2.21	0.40
1:C:376:PRO:CA	1:C:381:ASN:HD22	2.22	0.40
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.90	0.40
1:B:354:MET:HE1	1:B:368:LEU:HD12	2.03	0.40
1:C:405:GLU:HG2	1:C:408:LYS:CE	2.44	0.40
1:D:387:ASP:O	1:D:391:LYS:HG2	2.20	0.40
1:B:194:LYS:HG2	1:B:202:PRO:HB3	2.03	0.40
1:D:427:LEU:HD23	1:D:427:LEU:O	2.20	0.40
1:A:15:PRO:HG2	1:A:45:ALA:HB1	2.03	0.40
1:A:427:LEU:CD1	1:A:430:LEU:HD12	2.49	0.40
1:B:65:LEU:HA	1:B:70:ILE:HB	2.04	0.40
1:C:387:ASP:HB3	1:C:391:LYS:CD	2.50	0.40
3:C:501:A3P:H2'	3:C:501:A3P:H8	1.65	0.40
1:D:279:GLU:O	1:D:282:THR:HG22	2.22	0.40
1:B:218:ASP:OD2	1:B:260:ARG:NH2	2.52	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	448/461 (97%)	427 (95%)	21 (5%)	0	100	100
1	B	445/461 (96%)	421 (95%)	24 (5%)	0	100	100
1	C	443/461 (96%)	416 (94%)	25 (6%)	2 (0%)	24	55
1	D	449/461 (97%)	420 (94%)	29 (6%)	0	100	100
All	All	1785/1844 (97%)	1684 (94%)	99 (6%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	152	ALA
1	C	387	ASP

5.3.2 Protein sidechains [i](#)

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	380/388 (98%)	378 (100%)	2 (0%)	81	93
1	B	379/388 (98%)	378 (100%)	1 (0%)	86	95
1	C	379/388 (98%)	379 (100%)	0	100	100
1	D	381/388 (98%)	381 (100%)	0	100	100
All	All	1519/1552 (98%)	1516 (100%)	3 (0%)	87	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LEU
1	A	209	SER
1	B	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	294	GLN
1	A	304	GLN
1	A	344	HIS
1	B	20	GLN
1	B	41	GLN
1	B	196	ASN
1	B	239	ASN
1	B	255	GLN
1	B	269	ASN
1	B	381	ASN
1	C	342	ASN
1	C	373	ASN
1	D	59	ASN
1	D	134	ASN
1	D	239	ASN
1	D	255	GLN
1	D	269	ASN
1	D	303	GLN
1	D	344	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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A3P	C	501	-	29,29,29	3.43	11 (37%)	44,45,45	2.85	15 (34%)
2	ACO	A	501	-	51,53,53	3.30	19 (37%)	73,79,79	1.88	16 (21%)
2	ACO	B	501	-	51,53,53	3.41	19 (37%)	73,79,79	1.95	15 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A3P	C	501	-	-	10/15/31/31	0/3/3/3
2	ACO	A	501	-	-	19/51/67/67	0/3/3/3
2	ACO	B	501	-	-	17/51/67/67	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ACO	P2A-O3A	12.49	1.73	1.59
2	A	501	ACO	P2A-O3A	11.21	1.71	1.59
2	A	501	ACO	O4B-C1B	10.69	1.66	1.42
2	B	501	ACO	O4B-C1B	10.67	1.66	1.42
3	C	501	A3P	C3'-C4'	-8.81	1.30	1.52
3	C	501	A3P	C2'-C1'	-8.35	1.27	1.53
2	B	501	ACO	C5P-N4P	7.10	1.50	1.33
2	A	501	ACO	C5P-N4P	6.92	1.49	1.33
3	C	501	A3P	C2'-C3'	6.62	1.67	1.53
2	A	501	ACO	O4B-C4B	-6.52	1.30	1.45
3	C	501	A3P	O4'-C1'	6.48	1.57	1.42
2	B	501	ACO	O4B-C4B	-6.36	1.30	1.45
2	B	501	ACO	C2B-C1B	-6.18	1.34	1.53
2	A	501	ACO	C2B-C1B	-6.07	1.34	1.53
2	A	501	ACO	C9P-N8P	5.64	1.46	1.33
2	B	501	ACO	P1A-O3A	5.54	1.65	1.59
2	B	501	ACO	C9P-N8P	5.47	1.46	1.33
3	C	501	A3P	O4'-C4'	4.85	1.55	1.45
2	A	501	ACO	C6A-N6A	4.80	1.46	1.34
2	B	501	ACO	C6A-N6A	4.78	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ACO	P1A-O3A	4.39	1.64	1.59
3	C	501	A3P	P1-O3'	3.87	1.66	1.59
3	C	501	A3P	C6-N6	3.74	1.43	1.34
2	B	501	ACO	O3B-C3B	-3.59	1.31	1.44
2	A	501	ACO	O3B-C3B	-3.49	1.32	1.44
2	A	501	ACO	C6P-C5P	3.33	1.58	1.51
2	A	501	ACO	P3B-O3B	2.96	1.64	1.59
2	B	501	ACO	O5P-C5P	-2.92	1.17	1.23
2	A	501	ACO	C3B-C4B	2.88	1.60	1.52
2	B	501	ACO	P2A-O6A	2.87	1.70	1.59
2	B	501	ACO	C3B-C4B	2.86	1.60	1.52
2	A	501	ACO	O5P-C5P	-2.84	1.17	1.23
2	B	501	ACO	C6P-C5P	2.83	1.57	1.51
2	A	501	ACO	P2A-O6A	2.81	1.70	1.59
3	C	501	A3P	P2-O5'	2.64	1.68	1.60
3	C	501	A3P	C5-N7	-2.61	1.34	1.39
3	C	501	A3P	C5-C4	-2.55	1.34	1.39
2	B	501	ACO	P3B-O3B	2.49	1.63	1.59
2	B	501	ACO	C5A-C4A	-2.46	1.34	1.39
2	A	501	ACO	C5A-C4A	-2.43	1.34	1.39
2	A	501	ACO	P1A-O5B	2.33	1.68	1.59
3	C	501	A3P	C5'-C4'	2.31	1.58	1.51
2	B	501	ACO	P1A-O5B	2.21	1.68	1.59
2	B	501	ACO	C5A-N7A	-2.14	1.35	1.39
2	B	501	ACO	OAP-CAP	-2.11	1.38	1.42
2	B	501	ACO	C2A-N1A	2.08	1.37	1.33
2	A	501	ACO	OAP-CAP	-2.06	1.38	1.42
2	A	501	ACO	C2A-N1A	2.06	1.37	1.33
2	A	501	ACO	C5A-N7A	-2.01	1.35	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	A3P	C1'-N9-C8	-8.55	108.11	127.09
3	C	501	A3P	C4-N9-C1'	7.00	143.01	126.63
2	A	501	ACO	N6A-C6A-N1A	-6.54	103.81	118.38
3	C	501	A3P	N6-C6-N1	-6.43	104.05	118.38
2	A	501	ACO	N3A-C2A-N1A	-6.06	119.41	128.58
2	B	501	ACO	N6A-C6A-N1A	-5.95	105.13	118.38
2	B	501	ACO	N3A-C2A-N1A	-5.90	119.65	128.58
3	C	501	A3P	N3-C2-N1	-5.44	120.34	128.58
3	C	501	A3P	C5-C6-N6	5.24	136.27	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ACO	C7P-C6P-C5P	-5.11	103.88	112.39
2	A	501	ACO	C5A-C6A-N6A	5.00	135.66	123.29
2	B	501	ACO	C5A-C4A-N3A	-4.75	120.18	126.72
2	A	501	ACO	C5A-C4A-N3A	-4.45	120.58	126.72
2	B	501	ACO	N9A-C8A-N7A	-4.45	107.62	113.94
3	C	501	A3P	C5-C4-N3	-4.45	120.59	126.72
2	B	501	ACO	C5A-C6A-N6A	4.45	134.29	123.29
2	A	501	ACO	N9A-C8A-N7A	-4.40	107.69	113.94
3	C	501	A3P	N9-C8-N7	-4.30	107.84	113.94
3	C	501	A3P	C4'-O4'-C1'	-3.72	101.26	109.47
2	A	501	ACO	C2P-C3P-N4P	-3.61	104.87	112.41
2	A	501	ACO	C2A-N3A-C4A	3.51	120.39	111.83
2	B	501	ACO	C2A-N3A-C4A	3.47	120.30	111.83
3	C	501	A3P	N3-C4-N9	3.29	132.76	127.17
2	B	501	ACO	O9P-C9P-N8P	-3.18	116.26	122.98
3	C	501	A3P	C2-N3-C4	2.98	119.11	111.83
3	C	501	A3P	C4-N9-C8	2.96	108.85	105.74
2	B	501	ACO	N3A-C4A-N9A	2.94	132.17	127.17
2	A	501	ACO	C5A-N7A-C8A	2.92	108.04	103.45
3	C	501	A3P	O4'-C1'-N9	2.92	113.70	108.09
2	B	501	ACO	C5A-N7A-C8A	2.89	107.99	103.45
3	C	501	A3P	C5-N7-C8	2.78	107.82	103.45
2	A	501	ACO	O9P-C9P-N8P	-2.61	117.47	122.98
2	B	501	ACO	CAP-C9P-N8P	2.57	121.36	116.48
2	B	501	ACO	C4A-N9A-C8A	2.53	108.40	105.74
2	B	501	ACO	C3P-N4P-C5P	-2.45	118.27	122.82
2	A	501	ACO	C4A-C5A-N7A	-2.39	107.85	110.58
2	A	501	ACO	C7P-C6P-C5P	-2.38	108.43	112.39
2	A	501	ACO	C5A-C4A-N9A	2.32	108.34	105.81
2	B	501	ACO	C6P-C5P-N4P	2.31	120.55	116.34
2	A	501	ACO	N3A-C4A-N9A	2.30	131.08	127.17
3	C	501	A3P	O4'-C1'-C2'	-2.23	101.85	106.62
2	A	501	ACO	C4A-N9A-C8A	2.22	108.07	105.74
2	A	501	ACO	C6P-C7P-N8P	-2.21	107.29	112.00
2	B	501	ACO	O4B-C1B-N9A	-2.19	103.89	108.09
3	C	501	A3P	C6-C5-C4	2.05	119.97	117.18
2	A	501	ACO	C2P-S1P-C	2.03	111.17	101.42

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ACO	CDP-CBP-CCP-O6A
2	A	501	ACO	CEP-CBP-CCP-O6A
2	A	501	ACO	CAP-CBP-CCP-O6A
2	A	501	ACO	O9P-C9P-CAP-OAP
2	A	501	ACO	N8P-C9P-CAP-OAP
2	A	501	ACO	CAP-C9P-N8P-C7P
2	A	501	ACO	S1P-C2P-C3P-N4P
2	A	501	ACO	O-C-S1P-C2P
2	A	501	ACO	CH3-C-S1P-C2P
2	B	501	ACO	CCP-O6A-P2A-O3A
2	B	501	ACO	CCP-O6A-P2A-O4A
2	B	501	ACO	CDP-CBP-CCP-O6A
2	B	501	ACO	CEP-CBP-CCP-O6A
2	B	501	ACO	CAP-CBP-CCP-O6A
2	B	501	ACO	N8P-C9P-CAP-OAP
2	B	501	ACO	CAP-C9P-N8P-C7P
2	B	501	ACO	C5P-C6P-C7P-N8P
2	B	501	ACO	O-C-S1P-C2P
2	B	501	ACO	CH3-C-S1P-C2P
3	C	501	A3P	C5'-O5'-P2-O4P
3	C	501	A3P	C5'-O5'-P2-O5P
3	C	501	A3P	C5'-O5'-P2-O6P
2	A	501	ACO	O9P-C9P-N8P-C7P
2	B	501	ACO	O9P-C9P-N8P-C7P
3	C	501	A3P	C4'-C3'-O3'-P1
3	C	501	A3P	C2'-C3'-O3'-P1
3	C	501	A3P	C3'-C4'-C5'-O5'
3	C	501	A3P	O4'-C4'-C5'-O5'
2	B	501	ACO	O9P-C9P-CAP-OAP
2	A	501	ACO	O9P-C9P-CAP-CBP
2	B	501	ACO	O9P-C9P-CAP-CBP
2	A	501	ACO	N8P-C9P-CAP-CBP
2	B	501	ACO	N8P-C9P-CAP-CBP
2	A	501	ACO	P2A-O3A-P1A-O1A
2	B	501	ACO	C3P-C2P-S1P-C
3	C	501	A3P	C3'-O3'-P1-O1P
2	A	501	ACO	O5P-C5P-C6P-C7P
2	A	501	ACO	N4P-C5P-C6P-C7P
3	C	501	A3P	C3'-O3'-P1-O2P
3	C	501	A3P	C3'-O3'-P1-O3P
2	A	501	ACO	CBP-CCP-O6A-P2A
2	B	501	ACO	CBP-CCP-O6A-P2A
2	A	501	ACO	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
2	A	501	ACO	C5P-C6P-C7P-N8P
2	A	501	ACO	P2A-O3A-P1A-O2A
2	B	501	ACO	P1A-O3A-P2A-O5A

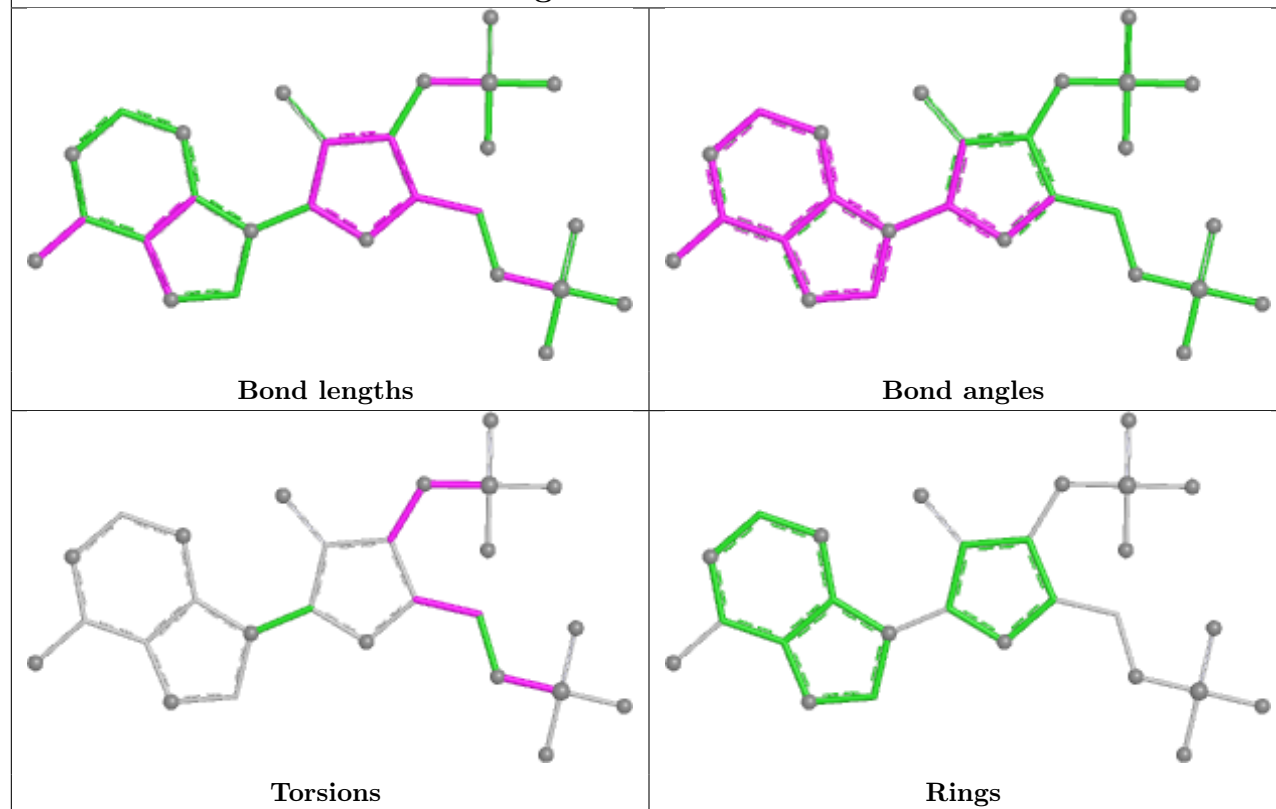
There are no ring outliers.

3 monomers are involved in 19 short contacts:

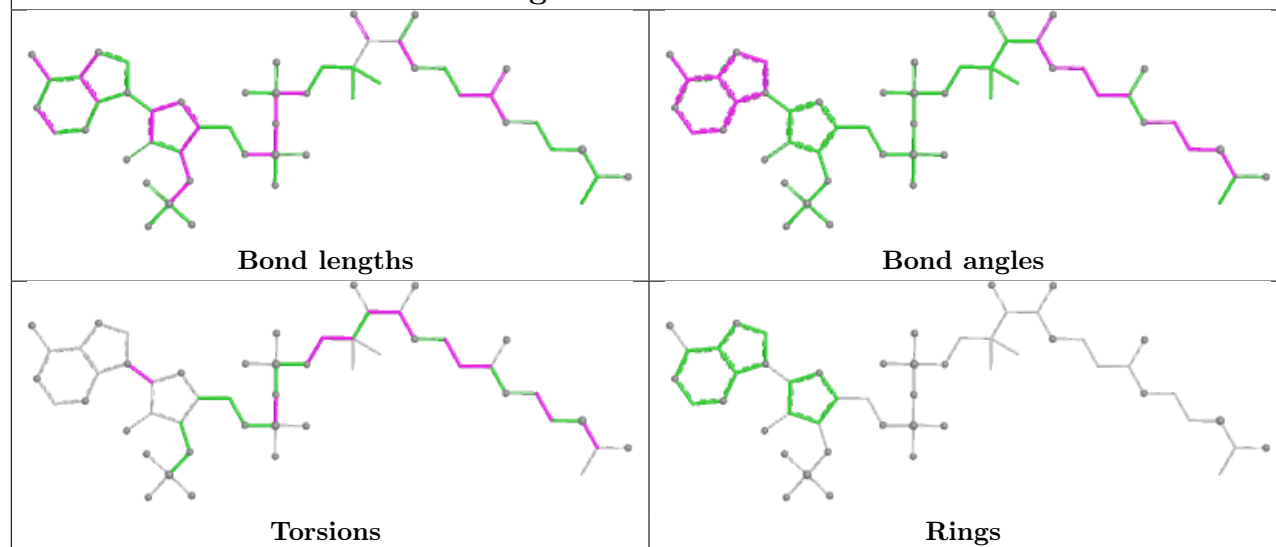
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	A3P	4	0
2	A	501	ACO	5	0
2	B	501	ACO	10	0

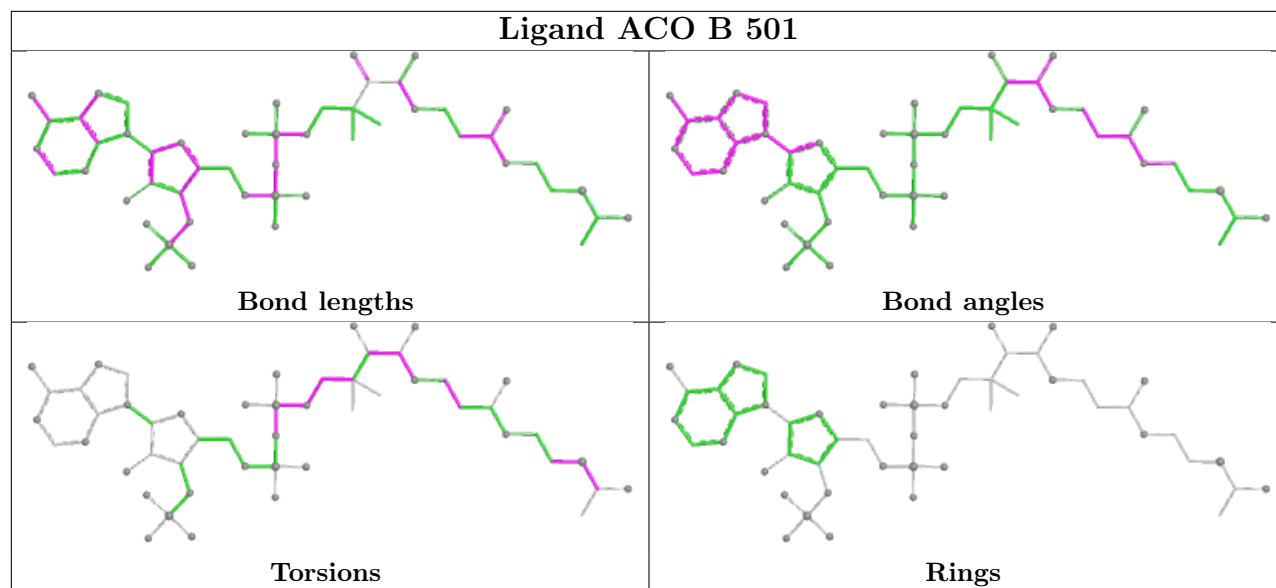
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A3P C 501



Ligand ACO A 501





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	450/461 (97%)	0.12	5 (1%) 78 70	41, 63, 89, 114	0
1	B	449/461 (97%)	0.23	5 (1%) 78 70	43, 68, 110, 135	0
1	C	447/461 (96%)	0.53	19 (4%) 40 31	49, 82, 112, 129	0
1	D	451/461 (97%)	0.36	5 (1%) 78 70	47, 74, 104, 128	0
All	All	1797/1844 (97%)	0.31	34 (1%) 66 57	41, 71, 108, 135	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	407	MET	4.2
1	A	372	GLU	3.3
1	B	305	LEU	3.3
1	B	211	THR	3.2
1	D	134	ASN	3.1
1	A	210	GLN	3.0
1	B	29	GLY	2.9
1	C	431	ALA	2.8
1	D	4	ASN	2.7
1	B	430	LEU	2.7
1	C	79	GLU	2.7
1	A	2	ALA	2.7
1	C	395	ARG	2.7
1	C	182	ARG	2.6
1	D	373	ASN	2.6
1	A	181	LEU	2.4
1	C	403	PHE	2.4
1	C	436	TYR	2.4
1	A	345	SER	2.3
1	C	317	THR	2.3
1	C	158	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	72	PRO	2.3
1	C	132	GLU	2.2
1	B	174	PRO	2.2
1	D	374	GLN	2.2
1	C	29	GLY	2.2
1	C	16	PRO	2.2
1	C	370	LEU	2.2
1	C	406	THR	2.1
1	D	367	SER	2.1
1	C	435	TYR	2.1
1	C	150	VAL	2.0
1	C	434	THR	2.0
1	C	386	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

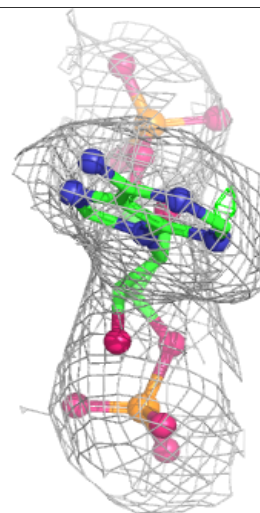
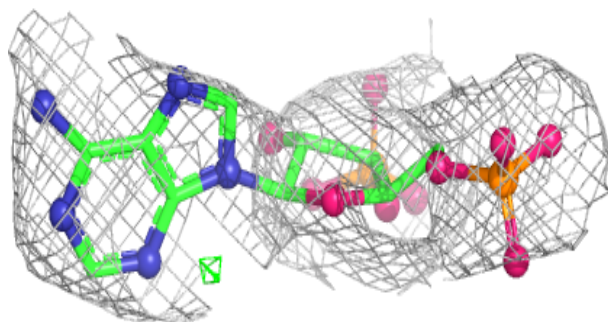
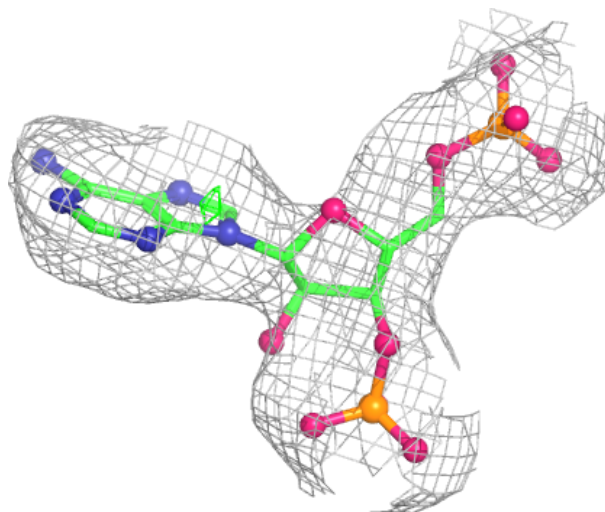
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A3P	C	501	27/27	0.81	0.11	83,99,107,121	0
2	ACO	A	501	51/51	0.89	0.10	49,65,78,92	0
2	ACO	B	501	51/51	0.90	0.11	44,67,85,115	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.

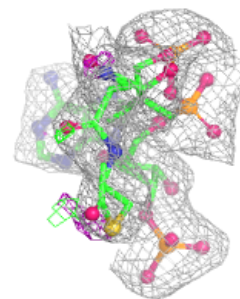
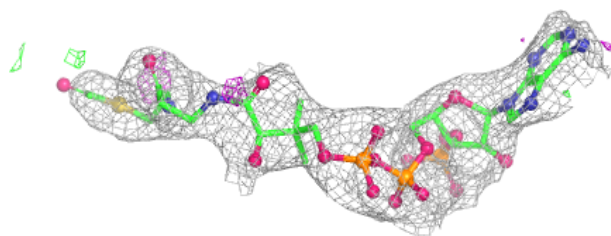
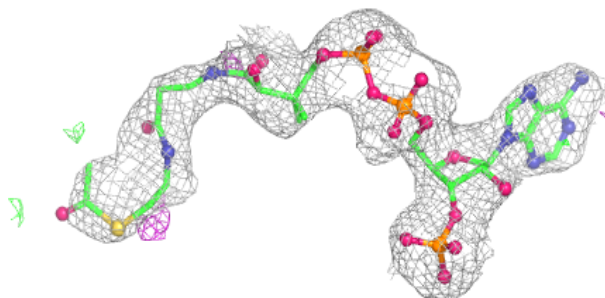
Electron density around A3P C 501:

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

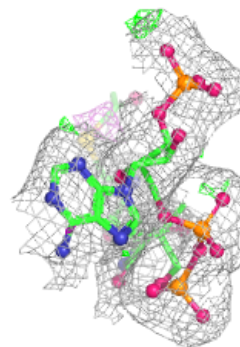
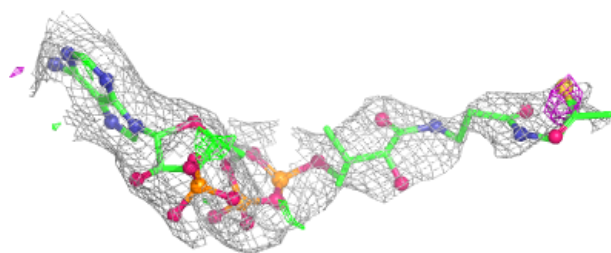
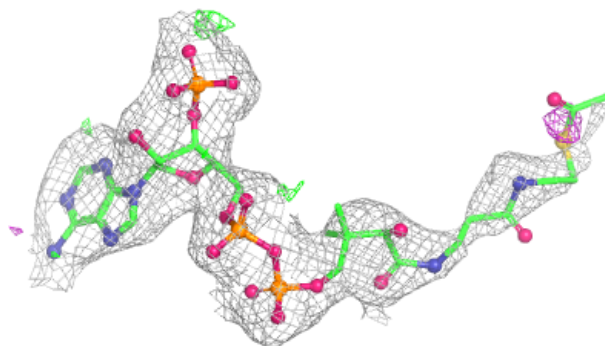


Electron density around ACO A 501:

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

**Electron density around ACO B 501:**

$2mF_o-DF_c$ (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.