



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 06:10 PM JST

PDB ID : 8ZD3 / pdb_00008zd3
Title : Crystal structure of ALPK1-N+K in complex with CDP-heptose
Authors : She, Y.; Ding, J.J.; Shao, F.
Deposited on : 2024-05-01
Resolution : 2.30 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

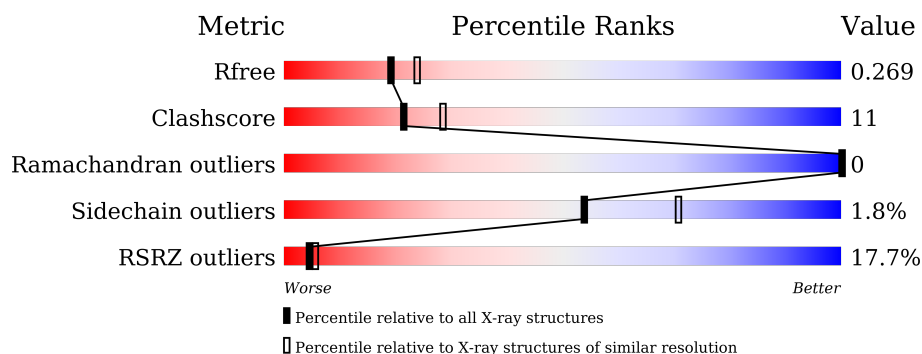
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	456	<div> <div>16%</div> <div>79%</div> <div>16%</div> <div>• •</div> </div>
1	C	456	<div> <div>16%</div> <div>79%</div> <div>16%</div> <div>5%</div> </div>
2	B	286	<div> <div>14%</div> <div>72%</div> <div>19%</div> <div>8%</div> </div>
2	D	286	<div> <div>20%</div> <div>71%</div> <div>13%</div> <div>• 15%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11342 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.

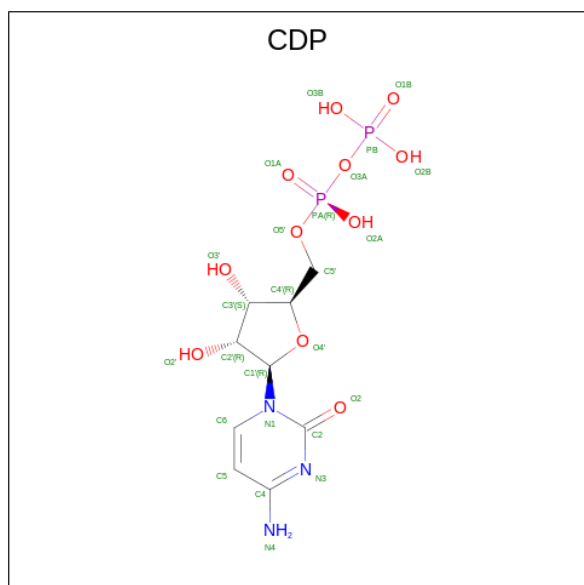
- Molecule 1 is a protein called Alpha-protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3417	2175	588	639	15			
1	C	435	Total	C	N	O	S	0	0	0
			3404	2166	585	638	15			

- Molecule 2 is a protein called Alpha-protein kinase 1.

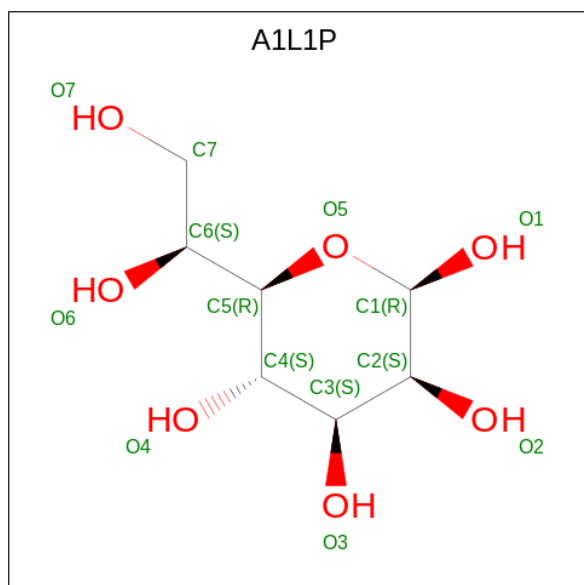
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	0	0
			2180	1409	370	395	6			
2	D	244	Total	C	N	O	S	0	0	0
			2028	1313	347	362	6			

- Molecule 3 is CYTIDINE-5'-DIPHOSPHATE (CCD ID: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	3	11	2		

- Molecule 4 is (2R,3S,4S,5S,6R)-6-[(1S)-1,2-bis(oxidanyl)ethyl]oxane-2,3,4,5-tetrol (CCD ID: A1L1P) (formula: C₇H₁₄O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	7	6		
4	C	1	Total	C	O	0	0
			13	7	6		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		

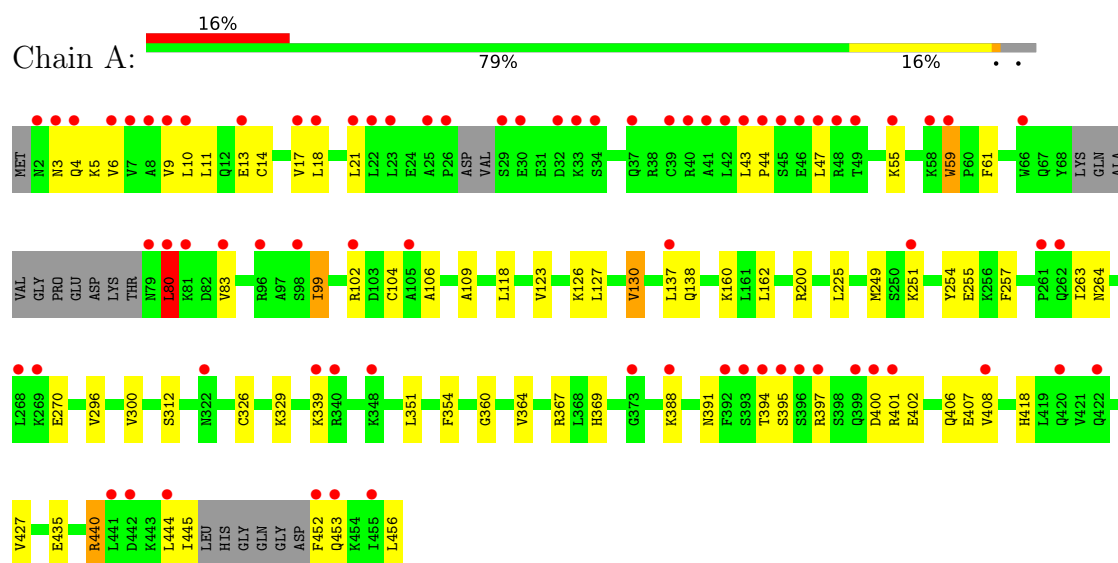
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total 79	O 79	0	0
6	B	48	Total 48	O 48	0	0
6	C	75	Total 75	O 75	0	0
6	D	33	Total 33	O 33	0	0

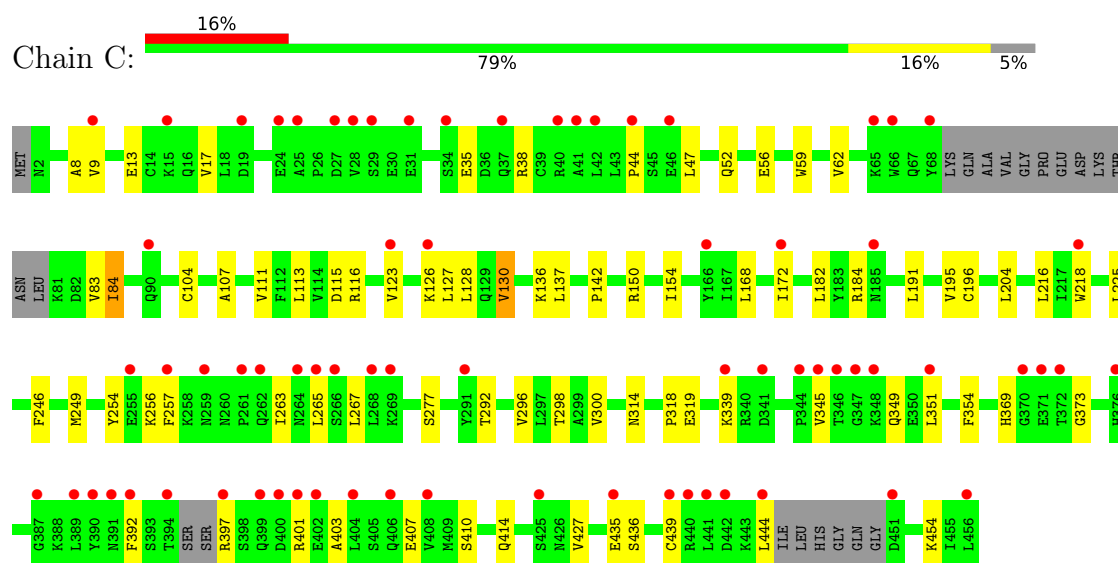
3 Residue-property plots

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

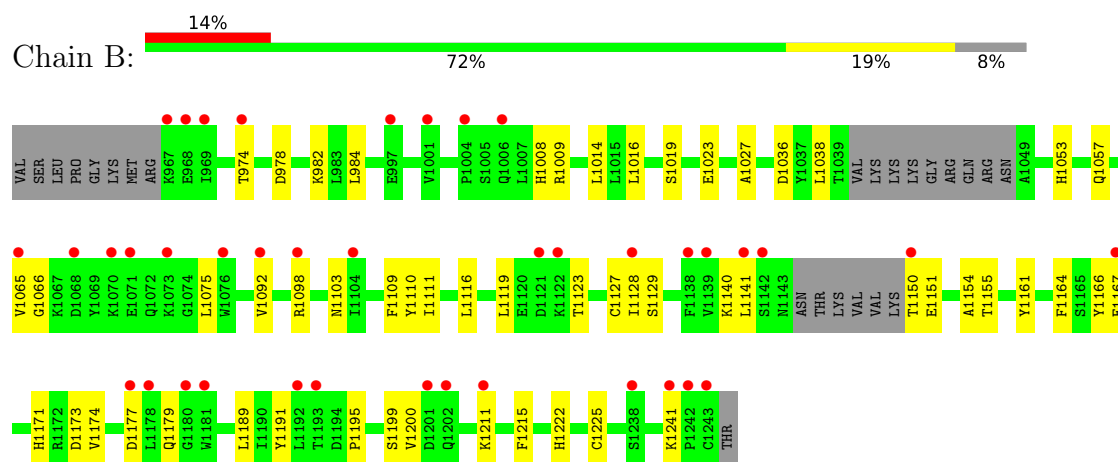
• Molecule 1: Alpha-protein kinase 1



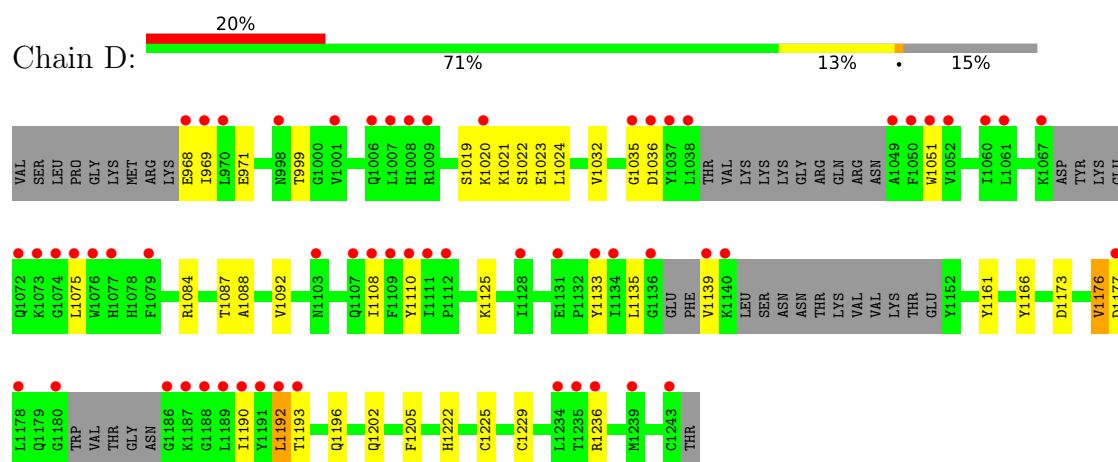
• Molecule 1: Alpha-protein kinase 1



• Molecule 2: Alpha-protein kinase 1



• Molecule 2: Alpha-protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.79Å 65.94Å 108.68Å 89.62° 107.77° 111.12°	Depositor
Resolution (Å)	30.55 – 2.30 30.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.55-2.30) 96.4 (30.55-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.240 , 0.269 0.239 , 0.269	Depositor DCC
R_{free} test set	66052 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11342	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: ZN, A1L1P, CDP

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	0.37	1/3473 (0.0%)	0.51	1/4693 (0.0%)
1	C	0.35	0/3460	0.49	2/4676 (0.0%)
2	B	0.36	0/2239	0.58	1/3029 (0.0%)
2	D	0.29	0/2080	0.48	1/2808 (0.0%)
All	All	0.35	1/11252 (0.0%)	0.51	5/15206 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	HIS	C-O	-5.88	1.16	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1035	GLY	CA-C-O	-6.74	115.54	122.28
1	C	369	HIS	N-CA-C	6.65	121.68	113.50
1	A	80	LEU	N-CA-C	-5.78	105.89	113.12
1	C	373	GLY	N-CA-C	-5.44	105.81	112.77
2	B	1009	ARG	N-CA-C	5.13	116.87	108.76

There are no chirality outliers.

There are no planarity outliers.

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	3417	0	3491	78	0
1	C	3404	0	3470	58	0
2	B	2180	0	2122	59	0
2	D	2028	0	1982	44	0
3	A	25	0	12	0	0
3	C	25	0	12	0	0
4	A	13	0	0	0	0
4	C	13	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	79	0	0	5	0
6	B	48	0	0	2	0
6	C	75	0	0	6	0
6	D	33	0	0	2	0
All	All	11342	0	11089	237	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 11.

All (237) 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:8:ALA:HB1	1:C:126:LYS:NZ	1.48	1.27
1:A:55:LYS:HE2	1:A:106:ALA:CA	1.65	1.26
1:C:172:ILE:HD11	1:C:196:CYS:HB3	1.23	1.18
2:D:1092:VAL:HG21	2:D:1110:TYR:CD2	1.81	1.15
2:B:1098:ARG:NE	2:B:1164:PHE:HE1	1.48	1.12
1:A:137:LEU:HD23	1:A:138:GLN:HG3	1.30	1.08
1:A:55:LYS:CE	1:A:106:ALA:HA	1.86	1.06
1:A:444:LEU:HD23	1:A:445:ILE:HG13	1.38	1.02
2:D:1092:VAL:HG21	2:D:1110:TYR:CE2	1.96	1.00
2:B:1098:ARG:HD2	2:B:1164:PHE:CE1	1.98	0.98
2:B:1098:ARG:CD	2:B:1164:PHE:HE1	1.78	0.97
1:C:8:ALA:HB1	1:C:126:LYS:HZ3	1.27	0.96
1:A:55:LYS:NZ	1:A:106:ALA:HB2	1.81	0.94
2:D:1092:VAL:HG21	2:D:1110:TYR:HD2	1.33	0.94
1:A:55:LYS:HE2	1:A:106:ALA:HA	0.94	0.93
1:A:55:LYS:HZ3	1:A:106:ALA:HB2	1.30	0.93
1:A:339:LYS:HG2	1:A:354:PHE:HZ	1.31	0.92
1:C:8:ALA:HB1	1:C:126:LYS:HZ2	1.26	0.92
2:B:1098:ARG:NE	2:B:1164:PHE:CE1	2.38	0.91
1:A:104:CYS:SG	1:A:137:LEU:HD22	2.10	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1098:ARG:HE	2:B:1164:PHE:HE1	1.14	0.90
1:C:168:LEU:O	1:C:172:ILE:HD12	1.73	0.88
1:C:436:SER:HA	1:C:439:CYS:SG	2.15	0.87
2:B:1200:VAL:HG12	2:B:1211:LYS:HG3	1.57	0.87
1:A:264:ASN:OD1	1:A:445:ILE:HG23	1.72	0.87
1:A:339:LYS:HG2	1:A:354:PHE:CZ	2.09	0.86
1:A:55:LYS:NZ	1:A:106:ALA:CB	2.38	0.86
1:C:8:ALA:CB	1:C:126:LYS:NZ	2.39	0.85
1:A:137:LEU:CD2	1:A:138:GLN:HG3	2.07	0.84
1:A:55:LYS:HE2	1:A:106:ALA:CB	2.08	0.83
2:B:1098:ARG:CD	2:B:1164:PHE:CE1	2.57	0.82
1:C:172:ILE:HD11	1:C:196:CYS:CB	2.07	0.82
2:D:1020:LYS:CE	2:D:1087:THR:HG23	2.09	0.82
2:B:1092:VAL:HG21	2:B:1110:TYR:CD2	2.15	0.81
1:A:55:LYS:CE	1:A:106:ALA:CB	2.61	0.79
2:B:1116:LEU:HB2	2:B:1128:ILE:CG1	2.14	0.78
1:A:80:LEU:HD13	1:A:80:LEU:C	2.10	0.76
2:B:1092:VAL:HG21	2:B:1110:TYR:CE2	2.20	0.76
2:D:1092:VAL:CG2	2:D:1110:TYR:CD2	2.68	0.76
1:A:5:LYS:O	1:A:9:VAL:HG23	1.86	0.76
1:A:264:ASN:OD1	1:A:445:ILE:CG2	2.34	0.75
1:C:123:VAL:HG12	1:C:123:VAL:O	1.86	0.75
1:A:80:LEU:HD13	1:A:80:LEU:O	1.86	0.74
2:D:1092:VAL:CG2	2:D:1110:TYR:CE2	2.70	0.74
1:C:8:ALA:CB	1:C:126:LYS:HZ2	1.98	0.74
2:B:1200:VAL:HG11	2:B:1211:LYS:HE2	1.69	0.74
2:B:1116:LEU:HB2	2:B:1128:ILE:HG13	1.70	0.73
1:A:395:SER:OG	1:A:401:ARG:HG2	1.89	0.73
2:B:1200:VAL:HG11	2:B:1211:LYS:CE	2.19	0.73
1:C:218:TRP:CD1	1:C:263:ILE:HG23	2.24	0.73
2:B:1092:VAL:HG22	2:B:1161:TYR:CE1	2.24	0.72
1:C:172:ILE:CD1	1:C:196:CYS:HB3	2.13	0.72
1:A:14:CYS:O	1:A:18:LEU:HD13	1.90	0.72
1:A:339:LYS:CG	1:A:354:PHE:CZ	2.73	0.71
2:D:1222:HIS:O	2:D:1236:ARG:NH2	2.25	0.69
2:D:1108:ILE:HD13	2:D:1190:ILE:HB	1.76	0.68
2:B:1200:VAL:HG12	2:B:1211:LYS:CG	2.23	0.68
2:B:1222:HIS:CE1	2:B:1225:CYS:HA	2.29	0.67
2:D:1020:LYS:HE2	2:D:1087:THR:HG23	1.77	0.65
1:A:395:SER:HB2	1:A:400:ASP:OD2	1.96	0.65
2:D:1020:LYS:HD2	2:D:1087:THR:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:SER:OG	1:A:401:ARG:CG	2.44	0.65
2:D:1110:TYR:CZ	2:D:1192:LEU:HD12	2.32	0.64
2:B:1200:VAL:CG1	2:B:1211:LYS:CG	2.74	0.64
2:B:1092:VAL:CG2	2:B:1161:TYR:CE1	2.81	0.63
1:A:4:GLN:HG3	1:A:123:VAL:HG13	1.80	0.63
2:D:1125:LYS:HG2	2:D:1125:LYS:O	2.00	0.62
1:A:406:GLN:HG3	6:A:618:HOH:O	1.99	0.61
2:B:1092:VAL:CG2	2:B:1161:TYR:CZ	2.83	0.61
1:A:444:LEU:CD2	1:A:445:ILE:HG13	2.24	0.61
2:B:1215:PHE:CZ	2:B:1241:LYS:HG2	2.36	0.60
2:B:1200:VAL:CG1	2:B:1211:LYS:CE	2.79	0.60
2:D:968:GLU:HG3	2:D:971:GLU:OE1	2.00	0.60
1:A:391:ASN:O	1:A:394:THR:HG22	2.01	0.60
1:A:162:LEU:HD21	6:B:1401:HOH:O	2.01	0.60
2:B:1092:VAL:HG21	2:B:1110:TYR:HD2	1.64	0.59
1:A:126:LYS:O	1:A:130:VAL:HG13	2.03	0.59
2:D:999:THR:OG1	2:D:1075:LEU:HD12	2.02	0.59
1:C:8:ALA:HB1	1:C:126:LYS:CE	2.31	0.59
1:C:182:LEU:HD23	1:C:184:ARG:NH1	2.18	0.58
1:A:312:SER:OG	1:A:367:ARG:NH1	2.36	0.58
1:C:136:LYS:NZ	6:C:605:HOH:O	2.33	0.58
2:D:1177:ASP:HB3	2:D:1192:LEU:HD13	1.83	0.58
2:D:1110:TYR:OH	2:D:1192:LEU:HD12	2.04	0.58
1:A:137:LEU:HD23	1:A:138:GLN:CG	2.19	0.58
1:A:80:LEU:C	1:A:80:LEU:CD1	2.76	0.58
1:C:257:PHE:CE1	1:C:263:ILE:HD13	2.38	0.58
1:A:47:LEU:HD21	1:A:83:VAL:HG22	1.85	0.58
2:B:1200:VAL:CG1	2:B:1211:LYS:HE3	2.34	0.58
2:D:1020:LYS:NZ	2:D:1087:THR:HG23	2.18	0.58
1:C:427:VAL:HG13	1:C:435:GLU:OE2	2.04	0.57
1:A:13:GLU:O	1:A:17:VAL:HG23	2.04	0.57
1:C:254:TYR:HH	1:C:277:SER:HG	1.52	0.57
2:D:1139:VAL:N	6:D:1404:HOH:O	2.37	0.57
1:C:218:TRP:CD1	1:C:265:LEU:HG	2.40	0.56
1:C:298:THR:HG22	6:C:604:HOH:O	2.05	0.56
1:C:8:ALA:CB	1:C:126:LYS:HZ3	2.08	0.56
1:A:395:SER:CB	1:A:400:ASP:OD2	2.53	0.55
2:B:1151:GLU:HG3	1:C:314:ASN:O	2.06	0.55
2:B:1166:TYR:HA	2:B:1173:ASP:O	2.07	0.55
2:B:1092:VAL:HG23	2:B:1161:TYR:CZ	2.42	0.55
2:D:1092:VAL:CG2	2:D:1110:TYR:HE2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1116:LEU:CD1	2:B:1128:ILE:HD11	2.37	0.55
2:D:1084:ARG:HB2	2:D:1205:PHE:HB2	1.89	0.54
1:C:126:LYS:O	1:C:130:VAL:HG13	2.07	0.54
1:A:55:LYS:HZ1	1:A:106:ALA:CB	2.20	0.54
2:B:1177:ASP:HB3	2:B:1195:PRO:HA	1.89	0.54
1:C:128:LEU:HD12	1:C:154:ILE:HD13	1.90	0.54
2:D:1092:VAL:HG22	2:D:1161:TYR:CE1	2.43	0.54
1:C:218:TRP:HD1	1:C:265:LEU:HG	1.74	0.53
1:A:264:ASN:O	1:A:445:ILE:HG12	2.09	0.53
2:B:1103:ASN:HA	6:B:1401:HOH:O	2.07	0.53
1:A:4:GLN:HG3	1:A:123:VAL:CG1	2.38	0.53
1:A:397:ARG:NH2	6:A:605:HOH:O	2.41	0.52
2:B:1140:LYS:HG2	2:B:1179:GLN:HG2	1.92	0.52
1:C:115:ASP:OD2	1:C:150:ARG:NH2	2.34	0.52
1:C:44:PRO:HD2	1:C:47:LEU:HD12	1.90	0.52
1:C:142:PRO:HG2	6:C:633:HOH:O	2.09	0.52
1:C:403:ALA:O	1:C:407:GLU:HG3	2.09	0.52
1:A:44:PRO:HD2	1:A:47:LEU:HD12	1.91	0.51
1:A:225:LEU:HD11	1:A:444:LEU:HD22	1.91	0.51
1:C:397:ARG:N	6:C:611:HOH:O	2.43	0.51
1:A:251:LYS:O	1:A:255:GLU:HG2	2.11	0.51
1:A:55:LYS:HZ1	1:A:106:ALA:HB1	1.74	0.51
1:C:83:VAL:HG23	1:C:84:ILE:HD12	1.93	0.51
1:A:257:PHE:CE1	1:A:263:ILE:HD13	2.46	0.51
2:D:1225:CYS:HB3	2:D:1229:CYS:HB2	1.93	0.50
1:A:402:GLU:HG3	6:A:618:HOH:O	2.11	0.50
1:C:392:PHE:CE2	1:C:401:ARG:HB3	2.46	0.50
2:D:1192:LEU:C	2:D:1193:THR:HG23	2.37	0.50
2:B:1092:VAL:HG22	2:B:1161:TYR:CZ	2.46	0.50
1:C:339:LYS:HG2	1:C:354:PHE:HZ	1.77	0.50
2:B:1116:LEU:HB2	2:B:1128:ILE:CD1	2.41	0.49
1:C:35:GLU:OE2	1:C:38:ARG:NH2	2.42	0.49
2:D:1019:SER:OG	2:D:1022:SER:OG	2.29	0.49
2:B:1014:LEU:HG	2:B:1119:LEU:HD11	1.94	0.49
2:B:1092:VAL:HG21	2:B:1110:TYR:HE2	1.77	0.49
1:A:55:LYS:CE	1:A:106:ALA:HB2	2.34	0.48
2:D:1019:SER:O	2:D:1023:GLU:N	2.46	0.48
1:C:123:VAL:O	1:C:123:VAL:CG1	2.57	0.48
2:D:1166:TYR:HA	2:D:1173:ASP:O	2.13	0.48
2:B:1116:LEU:CB	2:B:1128:ILE:HD11	2.44	0.48
1:C:204:LEU:HD12	1:C:216:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1092:VAL:CG2	2:D:1110:TYR:HD2	2.14	0.48
1:A:391:ASN:HA	1:A:394:THR:HG22	1.96	0.48
2:B:1016:LEU:CD1	2:B:1027:ALA:HB2	2.44	0.48
2:D:1176:VAL:HA	6:D:1415:HOH:O	2.14	0.48
2:B:1008:HIS:NE2	2:B:1036:ASP:OD1	2.46	0.47
1:A:18:LEU:HD11	1:A:99:ILE:HD13	1.95	0.47
2:B:1116:LEU:HB2	2:B:1128:ILE:HD11	1.95	0.47
1:C:8:ALA:HB1	1:C:126:LYS:CD	2.43	0.47
2:D:1108:ILE:HG23	2:D:1192:LEU:HD21	1.96	0.47
2:B:1200:VAL:CG1	2:B:1211:LYS:HG2	2.44	0.47
2:D:1110:TYR:CE2	2:D:1192:LEU:HD12	2.49	0.47
2:B:1038:LEU:HD21	2:B:1065:VAL:HG21	1.97	0.47
1:A:360:GLY:O	1:A:364:VAL:HG23	2.15	0.47
2:D:1176:VAL:HG22	2:D:1196:GLN:HB2	1.97	0.47
1:A:18:LEU:HD12	1:A:99:ILE:HG21	1.98	0.46
1:C:13:GLU:O	1:C:17:VAL:HG23	2.15	0.46
1:A:21:LEU:HD22	1:A:102:ARG:HD3	1.97	0.46
1:C:436:SER:O	1:C:439:CYS:SG	2.72	0.46
2:D:1190:ILE:N	2:D:1190:ILE:HD12	2.30	0.46
2:D:1088:ALA:O	2:D:1092:VAL:HG23	2.16	0.46
1:A:14:CYS:O	1:A:18:LEU:CD1	2.61	0.46
1:A:296:VAL:O	1:A:300:VAL:HG22	2.16	0.46
1:A:3:ASN:OD1	1:A:6:VAL:HG23	2.15	0.46
2:B:1150:THR:HB	1:C:318:PRO:HG2	1.97	0.46
2:B:1109:PHE:CE1	2:B:1189:LEU:HD13	2.50	0.45
1:A:104:CYS:HG	1:A:137:LEU:HD22	1.80	0.45
1:A:10:LEU:HD12	1:A:10:LEU:O	2.16	0.45
1:A:351:LEU:HG	1:A:408:VAL:HG11	1.97	0.45
1:A:249:MET:CE	1:A:254:TYR:HA	2.47	0.45
1:C:349:GLN:HG2	6:C:604:HOH:O	2.16	0.45
1:C:225:LEU:CD2	1:C:444:LEU:HD22	2.47	0.45
1:C:345:VAL:HG11	1:C:351:LEU:HD12	2.00	0.44
2:B:1200:VAL:HG11	2:B:1211:LYS:HE3	1.96	0.44
1:C:267:LEU:C	1:C:267:LEU:HD12	2.43	0.44
1:A:452:PHE:CE2	1:A:456:LEU:HD11	2.52	0.44
2:B:1066:GLY:HA2	2:B:1129:SER:O	2.17	0.44
1:A:11:LEU:HD11	1:A:118:LEU:HD13	2.00	0.44
2:B:1016:LEU:HD13	2:B:1027:ALA:HB2	2.00	0.44
2:D:1192:LEU:O	2:D:1193:THR:HG23	2.18	0.44
2:D:969:ILE:HD12	2:D:969:ILE:H	1.82	0.44
1:A:200:ARG:NH2	6:A:610:HOH:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1075:LEU:HD23	2:B:1127:CYS:SG	2.58	0.44
2:B:1140:LYS:O	2:B:1141:LEU:HB2	2.16	0.43
1:A:270:GLU:OE2	1:A:440:ARG:NH2	2.48	0.43
1:A:59:TRP:HB2	1:A:61:PHE:O	2.19	0.43
2:B:1141:LEU:O	2:B:1155:THR:OG1	2.35	0.43
1:C:107:ALA:O	1:C:111:VAL:HG23	2.18	0.43
2:D:1020:LYS:CD	2:D:1087:THR:HG23	2.48	0.43
2:B:1200:VAL:HG12	2:B:1211:LYS:HE3	1.99	0.43
1:C:168:LEU:C	1:C:172:ILE:HD12	2.41	0.43
1:C:191:LEU:O	1:C:195:VAL:HG23	2.19	0.43
1:C:246:PHE:HA	1:C:249:MET:HE2	2.00	0.43
2:D:1125:LYS:O	2:D:1125:LYS:CG	2.67	0.43
1:A:55:LYS:CE	1:A:106:ALA:CA	2.56	0.43
1:A:160:LYS:NZ	6:A:608:HOH:O	2.43	0.43
1:A:395:SER:OG	1:A:401:ARG:HG3	2.18	0.42
1:A:444:LEU:HD23	1:A:444:LEU:C	2.44	0.42
1:A:9:VAL:O	1:A:13:GLU:HG2	2.19	0.42
1:A:127:LEU:O	1:A:130:VAL:HG22	2.20	0.42
2:D:1133:TYR:OH	2:D:1135:LEU:HD13	2.20	0.42
2:B:974:THR:HG22	2:B:1123:THR:OG1	2.18	0.42
2:B:978:ASP:OD2	2:B:982:LYS:HE2	2.19	0.42
2:B:1141:LEU:HG	2:B:1154:ALA:HB1	2.01	0.42
2:B:1167:GLU:OE1	2:B:1171:HIS:NE2	2.53	0.42
1:C:127:LEU:O	1:C:130:VAL:HG22	2.19	0.42
2:D:1192:LEU:O	2:D:1193:THR:CG2	2.68	0.42
1:A:18:LEU:HD11	1:A:99:ILE:CD1	2.50	0.42
2:D:1036:ASP:O	2:D:1051:TRP:CD1	2.73	0.42
1:C:115:ASP:CG	1:C:150:ARG:HE	2.28	0.42
1:A:326:CYS:O	1:A:329:LYS:HB3	2.20	0.42
1:A:427:VAL:HG23	1:A:435:GLU:OE2	2.20	0.41
2:D:1110:TYR:CE1	2:D:1192:LEU:HB2	2.54	0.41
1:A:55:LYS:HG3	1:A:109:ALA:CB	2.50	0.41
1:C:62:VAL:HG23	1:C:116:ARG:NH1	2.35	0.41
1:A:55:LYS:CG	1:A:109:ALA:HB2	2.49	0.41
1:A:388:LYS:HD3	1:A:407:GLU:HB3	2.01	0.41
1:C:115:ASP:HA	1:C:127:LEU:CD2	2.50	0.41
1:C:296:VAL:O	1:C:300:VAL:HG13	2.21	0.41
2:B:1019:SER:O	2:B:1023:GLU:N	2.54	0.41
1:C:249:MET:HE1	1:C:254:TYR:HD1	1.85	0.41
1:C:52:GLN:O	1:C:56:GLU:HG3	2.21	0.41
1:C:104:CYS:SG	1:C:137:LEU:HD23	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:SER:O	1:C:414:GLN:HG3	2.21	0.41
1:A:453:GLN:HA	1:A:456:LEU:HD12	2.03	0.41
1:A:257:PHE:CZ	1:A:263:ILE:HD13	2.56	0.41
2:B:1053:HIS:HA	2:B:1057:GLN:OE1	2.20	0.41
2:D:1133:TYR:HE1	2:D:1135:LEU:HB2	1.86	0.41
2:B:1092:VAL:CG2	2:B:1110:TYR:CE2	2.98	0.40
2:B:1111:ILE:HG13	2:B:1191:TYR:HB3	2.02	0.40
2:B:1173:ASP:OD1	2:B:1199:SER:OG	2.37	0.40
2:D:1092:VAL:HG21	2:D:1110:TYR:HE2	1.67	0.40
2:B:984:LEU:HD23	2:B:1027:ALA:O	2.21	0.40
1:C:319:GLU:HG3	6:C:623:HOH:O	2.21	0.40
2:D:1092:VAL:CG2	2:D:1161:TYR:CE1	3.04	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	429/456 (94%)	423 (99%)	6 (1%)	0	100	100
1	C	427/456 (94%)	419 (98%)	8 (2%)	0	100	100
2	B	256/286 (90%)	245 (96%)	11 (4%)	0	100	100
2	D	232/286 (81%)	227 (98%)	5 (2%)	0	100	100
All	All	1344/1484 (91%)	1314 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	376/391 (96%)	369 (98%)	7 (2%)	52	69
1	C	374/391 (96%)	366 (98%)	8 (2%)	48	66
2	B	237/259 (92%)	236 (100%)	1 (0%)	89	95
2	D	220/259 (85%)	214 (97%)	6 (3%)	40	57
All	All	1207/1300 (93%)	1185 (98%)	22 (2%)	54	71

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	59	TRP
1	A	80	LEU
1	A	99	ILE
1	A	130	VAL
1	A	418	HIS
1	A	440	ARG
2	B	1174	VAL
1	C	9	VAL
1	C	59	TRP
1	C	84	ILE
1	C	113	LEU
1	C	130	VAL
1	C	256	LYS
1	C	292	THR
1	C	454	LYS
2	D	1021	LYS
2	D	1024	LEU
2	D	1032	VAL
2	D	1176	VAL
2	D	1192	LEU
2	D	1202	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN

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Mol	Chain	Res	Type
2	B	1090	HIS
2	B	1220	ASN
1	C	352	HIS
1	C	365	HIS
1	C	422	GLN
2	D	1006	GLN
2	D	1053	HIS
2	D	1103	ASN
2	D	1202	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CDP	A	501	4	24,26,26	3.82	12 (50%)	37,40,40	1.20	4 (10%)
3	CDP	C	501	4	24,26,26	3.80	12 (50%)	37,40,40	1.17	6 (16%)
4	A1L1P	C	502	3	13,13,14	1.73	2 (15%)	17,18,20	1.02	2 (11%)
4	A1L1P	A	502	3	13,13,14	1.76	2 (15%)	17,18,20	0.95	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
3	CDP	A	501	4	-	0/16/32/32	0/2/2/2
3	CDP	C	501	4	-	0/16/32/32	0/2/2/2
4	A1L1P	C	502	3	-	0/6/23/26	0/1/1/1
4	A1L1P	A	502	3	-	0/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	CDP	C2'-C3'	-9.68	1.26	1.53
3	C	501	CDP	C2'-C3'	-9.47	1.27	1.53
3	A	501	CDP	O4'-C4'	-7.81	1.27	1.45
3	C	501	CDP	O4'-C4'	-7.74	1.27	1.45
3	A	501	CDP	C4-N4	5.79	1.47	1.33
3	C	501	CDP	C1'-N1	-5.74	1.31	1.47
3	A	501	CDP	C1'-N1	-5.73	1.31	1.47
3	C	501	CDP	C3'-C4'	5.70	1.67	1.53
3	C	501	CDP	C4-N4	5.68	1.47	1.33
3	A	501	CDP	C3'-C4'	5.62	1.67	1.53
3	C	501	CDP	O4'-C1'	5.45	1.54	1.42
3	A	501	CDP	O4'-C1'	5.37	1.54	1.42
4	A	502	A1L1P	C2-C3	-4.51	1.45	1.52
4	C	502	A1L1P	C2-C3	-4.37	1.46	1.52
3	A	501	CDP	C2-N1	-3.55	1.32	1.40
3	C	501	CDP	C2-N1	-3.50	1.32	1.40
3	A	501	CDP	O2'-C2'	3.25	1.50	1.43
3	C	501	CDP	O2'-C2'	3.20	1.50	1.43
4	A	502	A1L1P	O5-C1	3.13	1.48	1.43
4	C	502	A1L1P	O5-C1	2.94	1.48	1.43
3	A	501	CDP	O2-C2	-2.91	1.18	1.23
3	C	501	CDP	O2-C2	-2.85	1.18	1.23
3	C	501	CDP	C6-N1	-2.70	1.31	1.38
3	A	501	CDP	C6-N1	-2.57	1.31	1.38
3	A	501	CDP	PB-O2B	2.50	1.64	1.54
3	C	501	CDP	PB-O2B	2.46	1.64	1.54
3	A	501	CDP	C2-N3	-2.24	1.31	1.36
3	C	501	CDP	C2-N3	-2.19	1.31	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	A1L1P	C7-C6-C5	-2.56	107.00	112.17
3	A	501	CDP	C2'-C3'-C4'	2.50	107.50	102.64
3	C	501	CDP	PA-O3A-PB	-2.40	124.58	132.83
3	A	501	CDP	C4'-O4'-C1'	-2.39	104.19	109.47
3	A	501	CDP	O2-C2-N3	-2.37	118.48	122.33
3	C	501	CDP	C4'-O4'-C1'	-2.37	104.25	109.47
3	A	501	CDP	PA-O3A-PB	-2.36	124.71	132.83
3	C	501	CDP	C2'-C3'-C4'	2.15	106.82	102.64
3	C	501	CDP	O2-C2-N3	-2.14	118.85	122.33
4	C	502	A1L1P	O7-C7-C6	-2.08	106.54	111.07
3	C	501	CDP	C5-C6-N1	-2.08	118.33	121.81
3	C	501	CDP	C5'-C4'-C3'	-2.07	107.44	115.18

There are no chirality outliers.

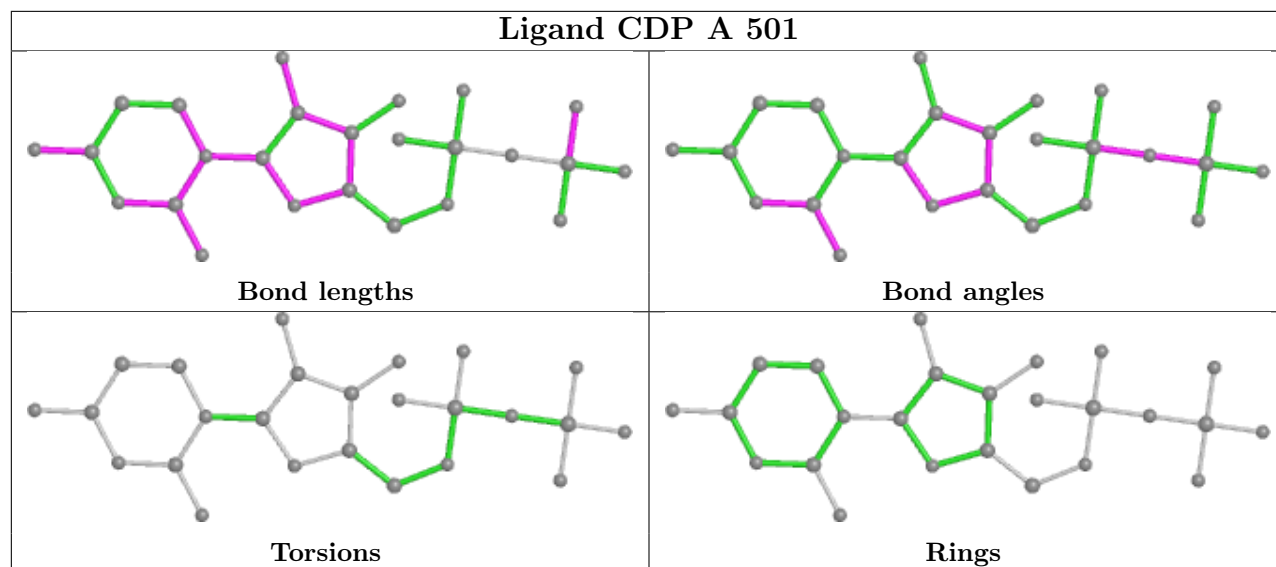
There are no torsion outliers.

There are no ring outliers.

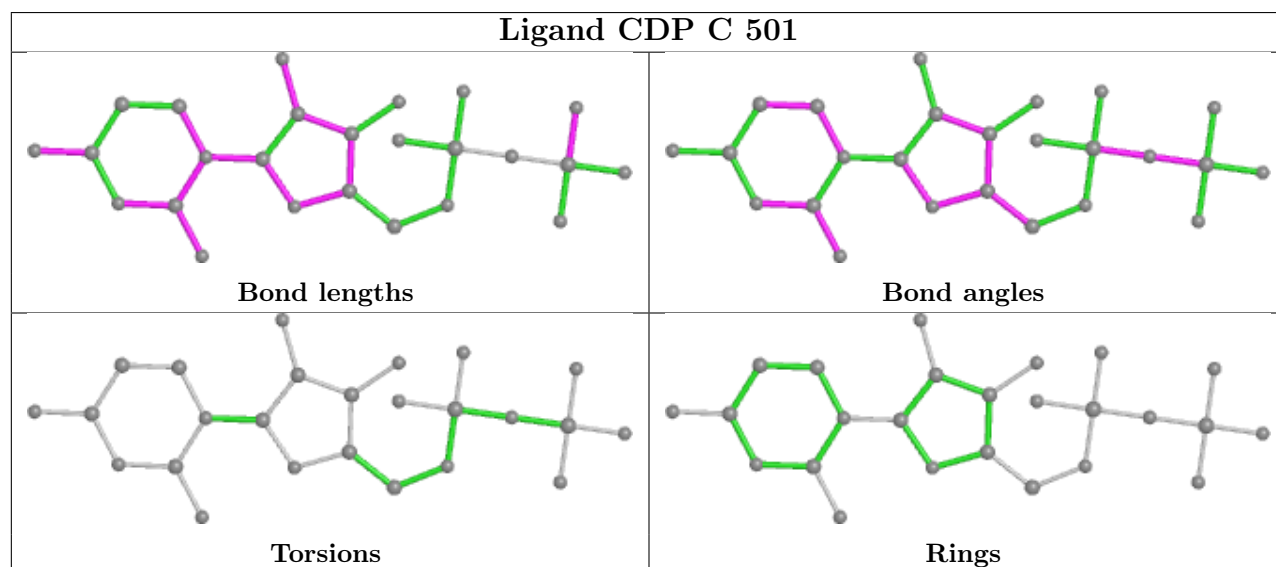
No monomer is involved in short contacts.

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.

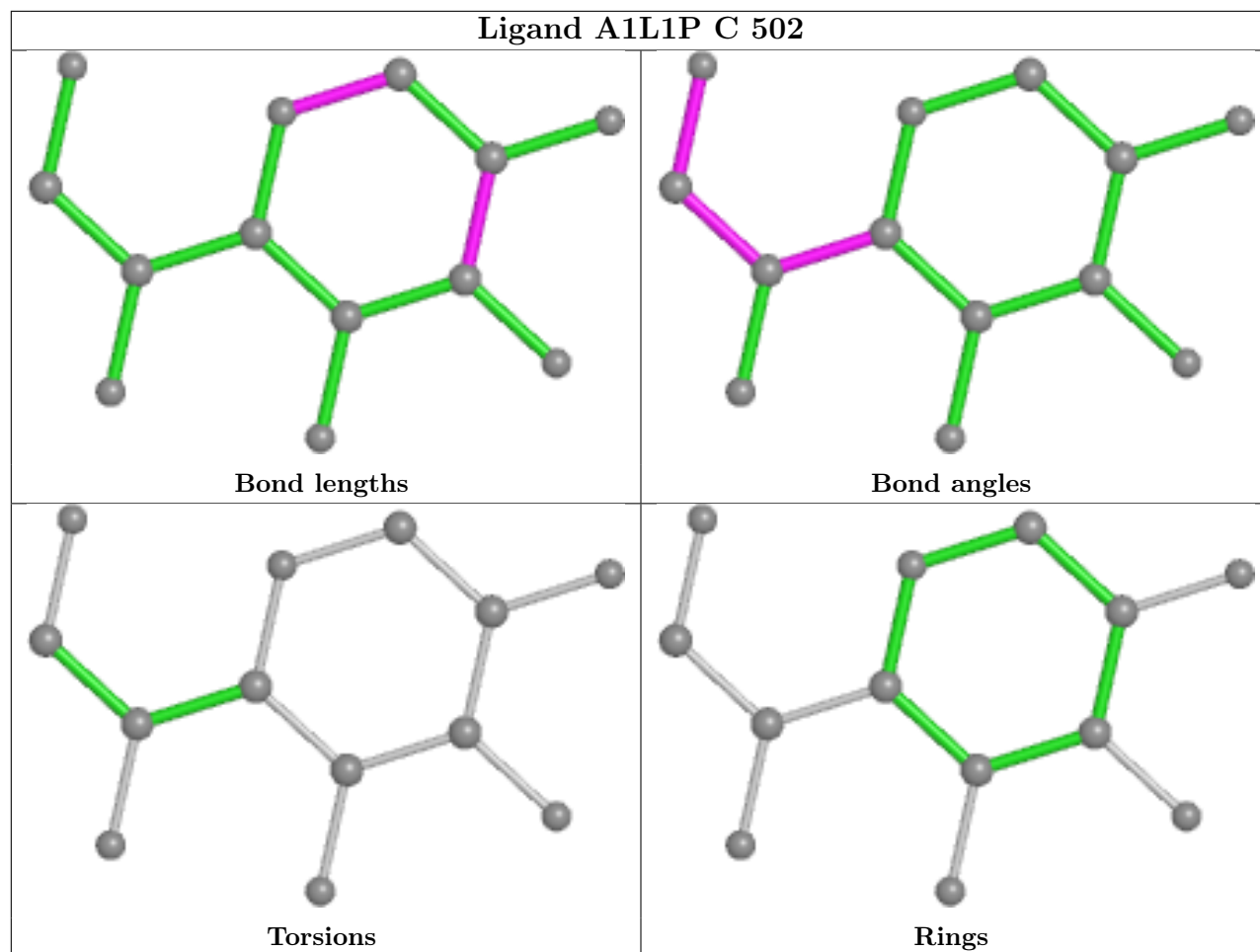
Ligand CDP A 501

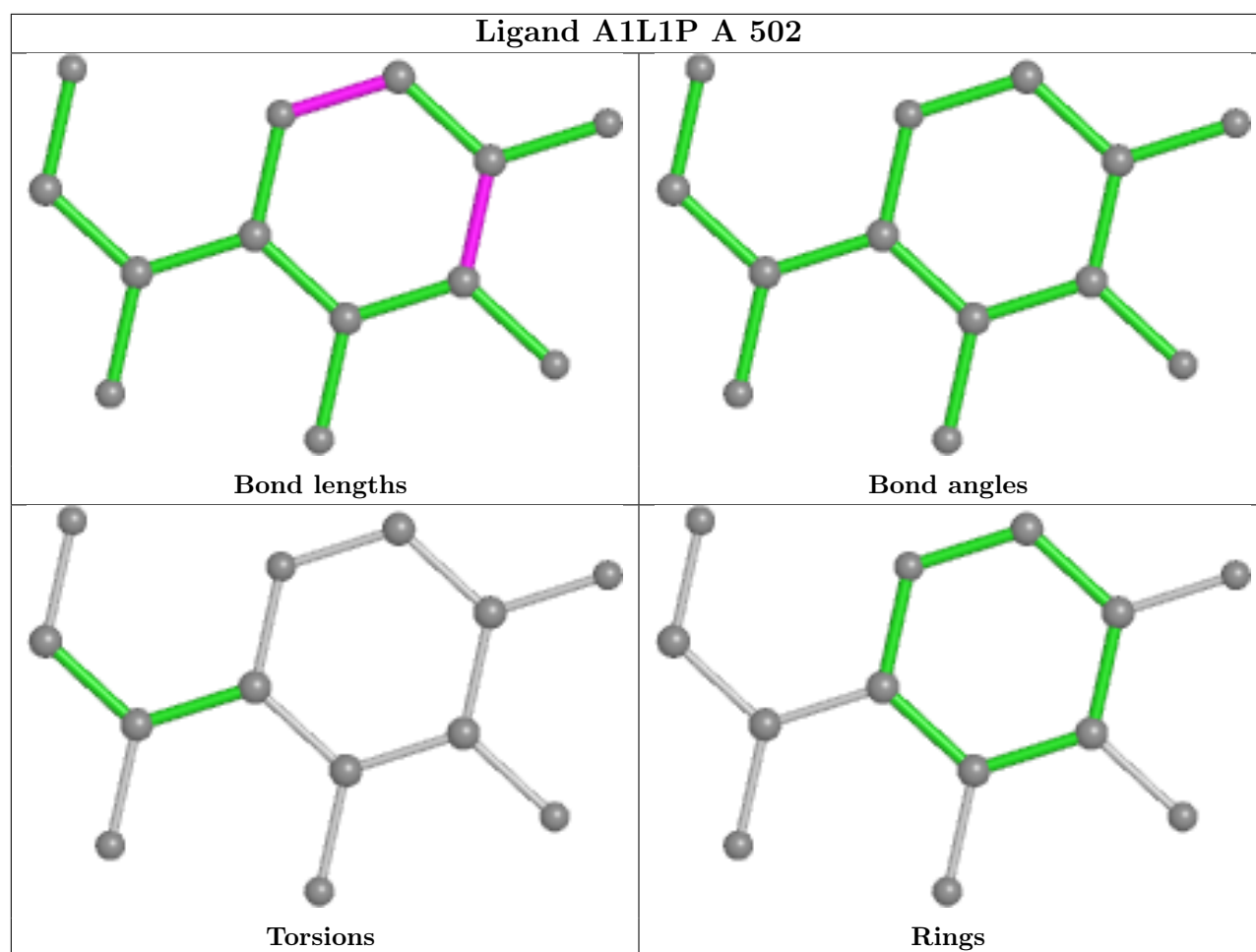


Ligand CDP C 501



Ligand A1L1P C 502





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	437/456 (95%)	1.06	75 (17%) 5 6	29, 47, 87, 107	0
1	C	435/456 (95%)	0.99	72 (16%) 5 6	29, 46, 84, 151	0
2	B	262/286 (91%)	1.02	39 (14%) 7 8	28, 46, 77, 95	0
2	D	244/286 (85%)	1.37	58 (23%) 2 3	30, 57, 84, 105	0
All	All	1378/1484 (92%)	1.08	244 (17%) 4 5	28, 48, 85, 151	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1121	ASP	7.0
2	D	1049	ALA	5.7
1	A	400	ASP	5.3
2	B	1243	CYS	5.3
1	A	26	PRO	5.1
1	A	66	TRP	4.9
2	B	1150	THR	4.8
1	A	42	LEU	4.8
2	D	1108	ILE	4.7
1	C	268	LEU	4.4
1	C	390	TYR	4.3
2	D	1076	TRP	4.3
1	C	31	GLU	4.3
2	D	1186	GLY	4.2
1	A	10	LEU	4.2
2	B	1177	ASP	4.1
1	A	58	LYS	4.1
1	A	444	LEU	4.1
2	B	1178	LEU	4.1
1	A	394	THR	4.1
1	A	79	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	1128	ILE	3.9
2	B	1211	LYS	3.9
1	A	80	LEU	3.9
1	A	43	LEU	3.8
2	D	1139	VAL	3.8
1	A	22	LEU	3.8
1	A	261	PRO	3.7
2	D	1111	ILE	3.7
1	C	394	THR	3.7
2	D	1243	CYS	3.7
2	D	968	GLU	3.6
1	C	404	LEU	3.6
1	A	13	GLU	3.6
2	D	1073	LYS	3.5
1	A	6	VAL	3.5
2	D	1007	LEU	3.5
1	A	41	ALA	3.5
1	C	392	PHE	3.5
1	A	3	ASN	3.5
1	A	32	ASP	3.5
1	C	27	ASP	3.5
1	C	371	GLU	3.5
1	A	441	LEU	3.4
1	C	400	ASP	3.4
1	C	291	TYR	3.4
1	A	39	CYS	3.4
2	D	1006	GLN	3.4
1	C	123	VAL	3.4
2	D	1136	GLY	3.4
2	B	1068	ASP	3.4
1	A	59	TRP	3.4
2	D	1110	TYR	3.3
2	D	1061	LEU	3.3
1	A	33	LYS	3.3
2	D	1235	THR	3.3
2	B	1076	TRP	3.3
1	A	4	GLN	3.3
1	C	425	SER	3.3
1	A	2	ASN	3.3
1	A	269	LYS	3.2
2	B	967	LYS	3.2
1	C	66	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	1074	GLY	3.2
2	D	1107	GLN	3.2
1	C	456	LEU	3.2
2	B	1238	SER	3.2
1	A	401	ARG	3.2
1	C	41	ALA	3.2
1	A	137	LEU	3.1
2	D	1038	LEU	3.1
1	A	44	PRO	3.1
1	A	40	ARG	3.1
2	D	1239	MET	3.1
1	C	68	TYR	3.1
1	C	172	ILE	3.0
2	D	1072	GLN	3.0
1	C	28	VAL	3.0
1	A	8	ALA	3.0
1	A	397	ARG	3.0
1	A	47	LEU	3.0
2	D	1109	PHE	3.0
1	A	392	PHE	3.0
1	C	269	LYS	3.0
2	D	1050	PHE	3.0
1	A	25	ALA	3.0
2	B	1141	LEU	2.9
2	B	1092	VAL	2.9
2	D	1177	ASP	2.9
1	A	48	ARG	2.9
1	C	401	ARG	2.9
1	C	441	LEU	2.9
1	C	442	ASP	2.8
1	A	9	VAL	2.8
1	C	44	PRO	2.8
1	C	65	LYS	2.8
2	D	1067	LYS	2.8
1	A	21	LEU	2.8
2	D	1008	HIS	2.8
2	D	1051	TRP	2.8
2	D	970	LEU	2.8
2	D	969	ILE	2.8
1	A	96	ARG	2.8
1	C	372	THR	2.8
1	C	265	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	998	ASN	2.8
1	A	455	ILE	2.7
1	A	396	SER	2.7
2	B	1098	ARG	2.7
2	D	1036	ASP	2.7
1	C	37	GLN	2.7
2	D	1075	LEU	2.7
1	C	339	LYS	2.7
2	B	1241	LYS	2.7
2	D	1037	TYR	2.7
1	C	185	ASN	2.7
1	C	259	ASN	2.7
2	B	1065	VAL	2.7
2	D	1191	TYR	2.7
1	C	391	ASN	2.7
2	B	969	ILE	2.7
1	C	451	ASP	2.7
1	A	37	GLN	2.7
2	D	1020	LYS	2.7
1	A	373	GLY	2.6
1	C	440	ARG	2.6
2	B	1192	LEU	2.6
1	C	387	GLY	2.6
2	D	1009	ARG	2.6
2	D	1192	LEU	2.6
2	D	1190	ILE	2.6
1	C	266	SER	2.6
1	C	257	PHE	2.6
1	C	370	GLY	2.6
1	C	46	GLU	2.6
1	A	34	SER	2.6
2	D	1188	GLY	2.6
2	D	1133	TYR	2.6
1	A	29	SER	2.6
1	A	399	GLN	2.6
2	D	1077	HIS	2.6
1	C	345	VAL	2.5
2	D	1234	LEU	2.5
1	A	395	SER	2.5
1	C	42	LEU	2.5
1	C	376	HIS	2.5
1	C	406	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	1180	GLY	2.5
2	D	1001	VAL	2.5
1	C	444	LEU	2.5
2	D	1134	ILE	2.5
2	B	1142	SER	2.5
2	B	1181	TRP	2.5
2	B	1180	GLY	2.5
1	A	55	LYS	2.5
2	B	1193	THR	2.5
1	A	46	GLU	2.4
1	C	347	GLY	2.4
1	A	83	VAL	2.4
2	B	1201	ASP	2.4
1	A	102	ARG	2.4
1	A	422	GLN	2.4
1	C	397	ARG	2.4
2	D	1178	LEU	2.4
1	C	19	ASP	2.4
2	B	1122	LYS	2.4
1	A	105	ALA	2.4
1	A	452	PHE	2.4
2	D	1079	PHE	2.4
1	A	45	SER	2.4
1	A	23	LEU	2.4
1	A	7	VAL	2.3
1	A	17	VAL	2.3
2	B	1139	VAL	2.3
2	B	974	THR	2.3
2	B	968	GLU	2.3
2	B	1070	LYS	2.3
2	D	1128	ILE	2.3
2	D	1236	ARG	2.3
1	A	262	GLN	2.3
2	D	1035	GLY	2.3
1	C	408	VAL	2.3
2	D	1187	LYS	2.3
1	A	442	ASP	2.3
1	C	34	SER	2.3
1	C	40	ARG	2.3
1	C	264	ASN	2.3
1	C	348	LYS	2.3
1	C	218	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	262	GLN	2.3
1	A	348	LYS	2.3
2	D	1140	LYS	2.3
1	C	344	PRO	2.3
1	A	393	SER	2.3
2	D	1189	LEU	2.2
2	D	1193	THR	2.2
1	C	90	GLN	2.2
1	C	24	GLU	2.2
1	C	389	LEU	2.2
1	C	346	THR	2.2
2	B	1104	ILE	2.2
1	A	18	LEU	2.2
2	B	1004	PRO	2.2
1	C	9	VAL	2.2
1	A	420	GLN	2.2
1	A	268	LEU	2.2
1	A	81	LYS	2.2
2	B	1073	LYS	2.2
1	C	29	SER	2.1
1	C	351	LEU	2.1
1	A	251	LYS	2.1
1	C	15	LYS	2.1
1	A	408	VAL	2.1
2	D	1052	VAL	2.1
1	C	255	GLU	2.1
1	C	261	PRO	2.1
2	B	1242	PRO	2.1
1	A	453	GLN	2.1
1	C	399	GLN	2.1
1	C	25	ALA	2.1
1	C	166	TYR	2.1
2	B	1071	GLU	2.1
2	B	1138	PHE	2.1
1	A	322	ASN	2.1
1	A	388	LYS	2.1
2	B	1006	GLN	2.1
1	C	402	GLU	2.1
1	A	339	LYS	2.1
1	C	439	CYS	2.1
2	B	1202	GLN	2.1
1	A	30	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	435	GLU	2.0
2	B	997	GLU	2.0
2	B	1167	GLU	2.0
2	D	1131	GLU	2.0
1	A	340	ARG	2.0
1	A	98	SER	2.0
2	D	1060	ILE	2.0
1	A	49	THR	2.0
2	B	1001	VAL	2.0
1	C	341	ASP	2.0
1	C	126	LYS	2.0
2	D	1103	ASN	2.0
2	D	1112	PRO	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](#)

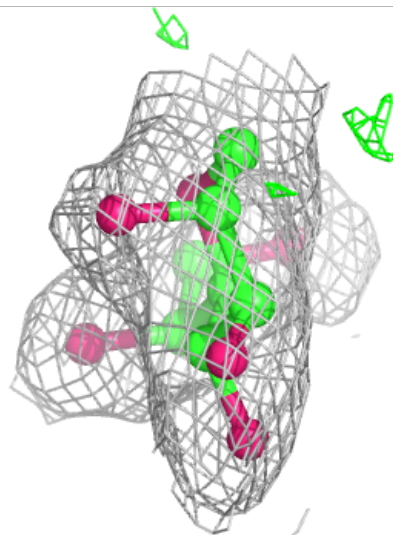
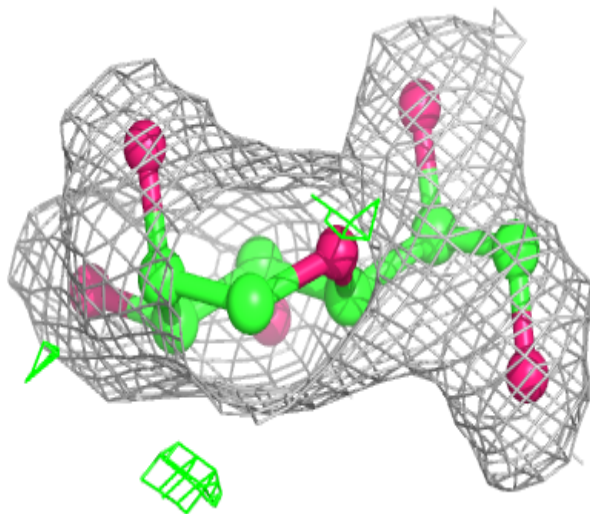
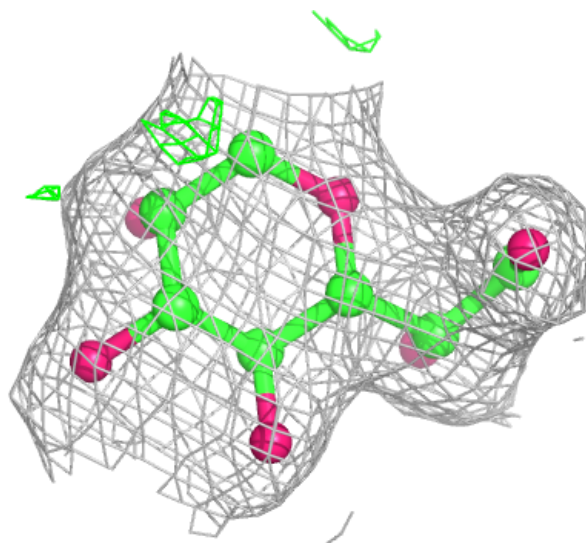
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1L1P	A	502	13/14	0.91	0.10	30,30,30,30	0
4	A1L1P	C	502	13/14	0.92	0.09	30,30,30,30	0
3	CDP	A	501	25/25	0.94	0.09	30,30,30,30	0
3	CDP	C	501	25/25	0.95	0.08	30,30,30,30	0
5	ZN	D	1301	1/1	0.98	0.05	54,54,54,54	0
5	ZN	B	1301	1/1	0.99	0.09	30,30,30,30	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.

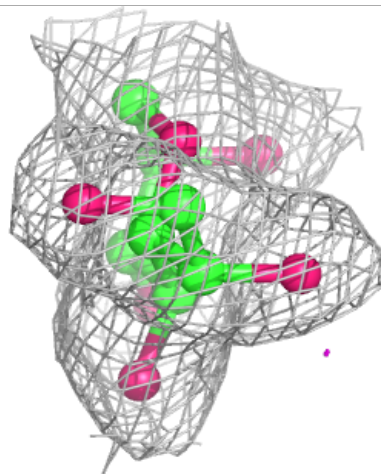
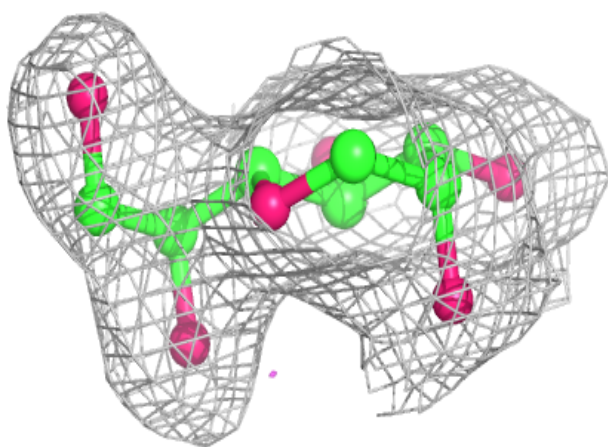
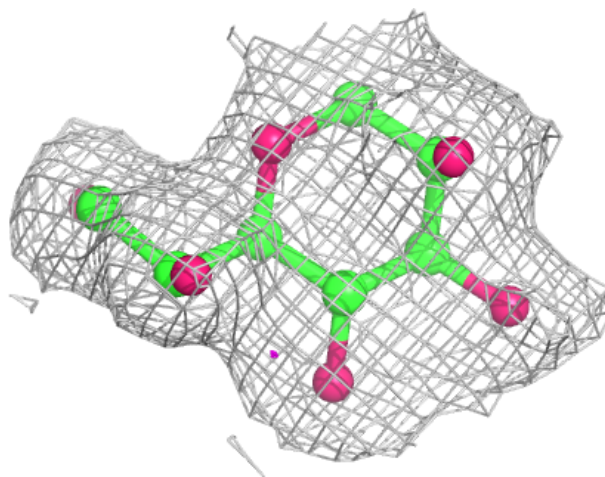
Electron density around A1L1P A 502:

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



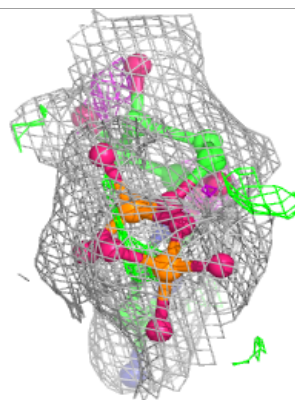
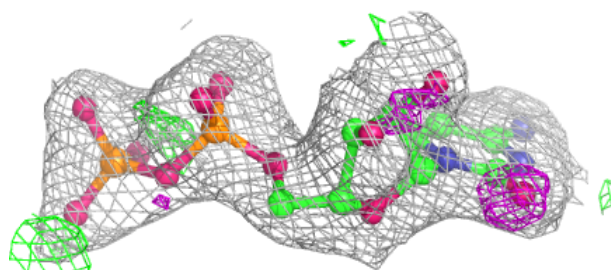
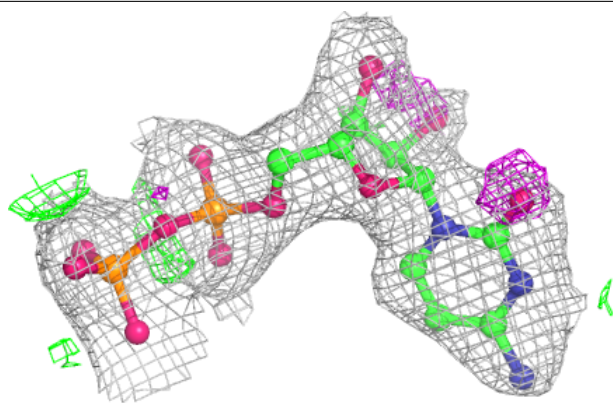
Electron density around A1L1P C 502:

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



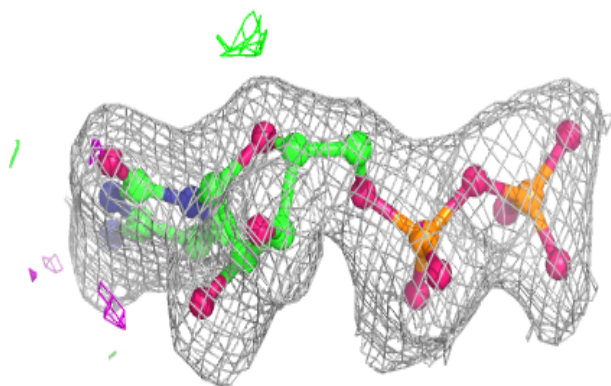
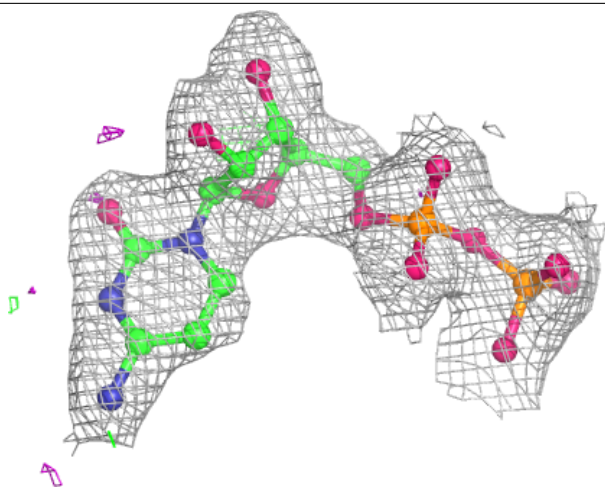
Electron density around CDP A 501:

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



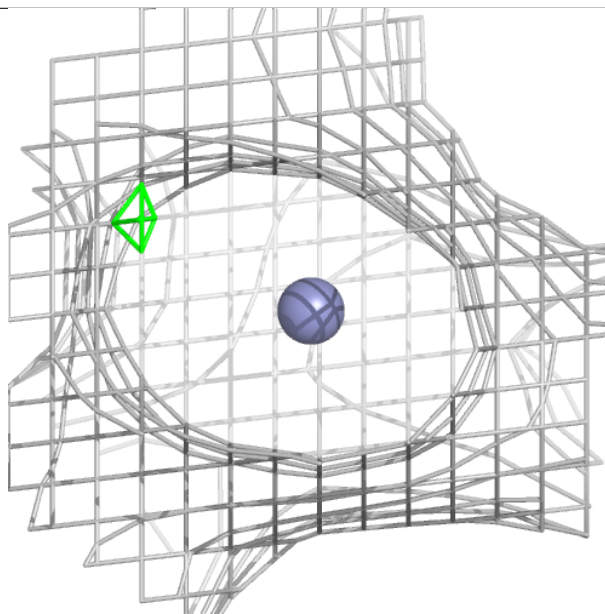
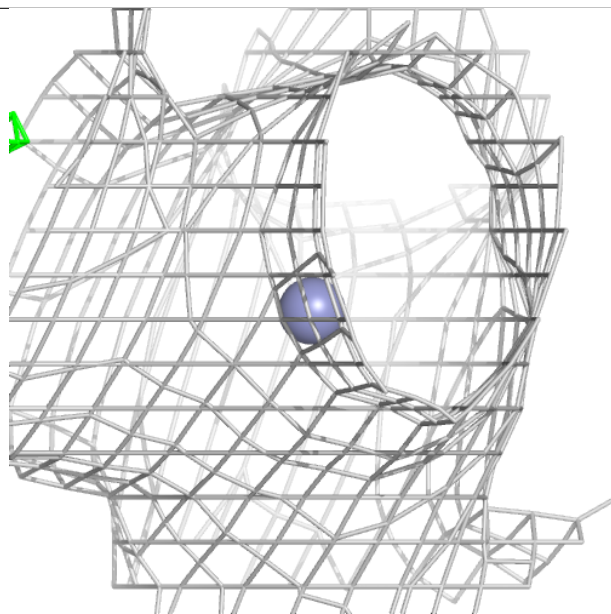
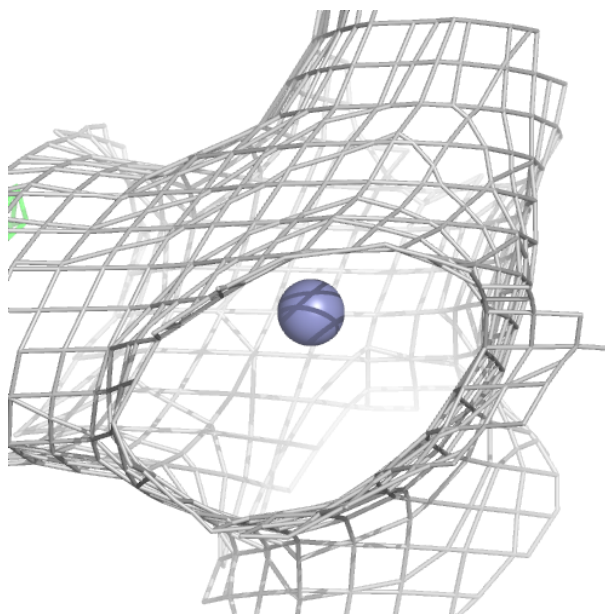
Electron density around CDP C 501:

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



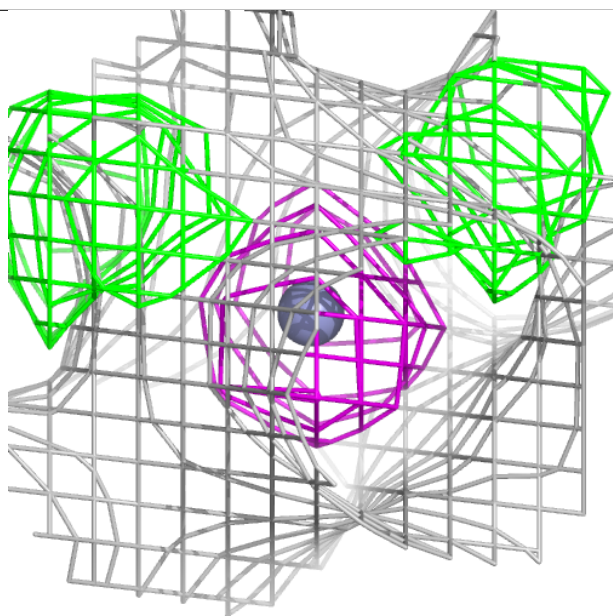
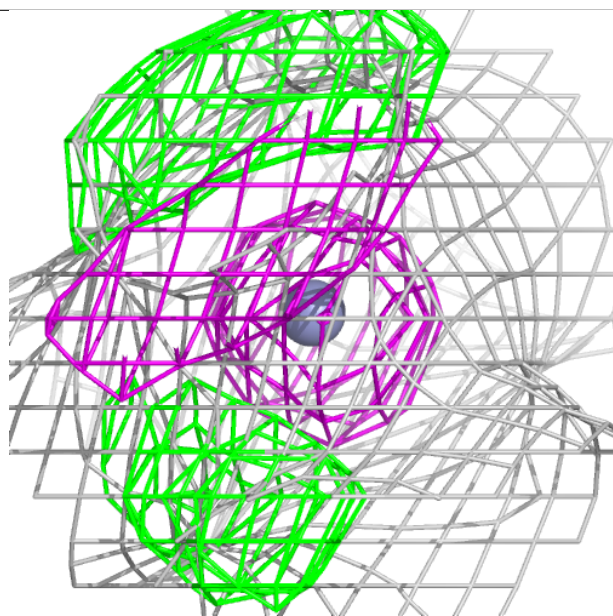
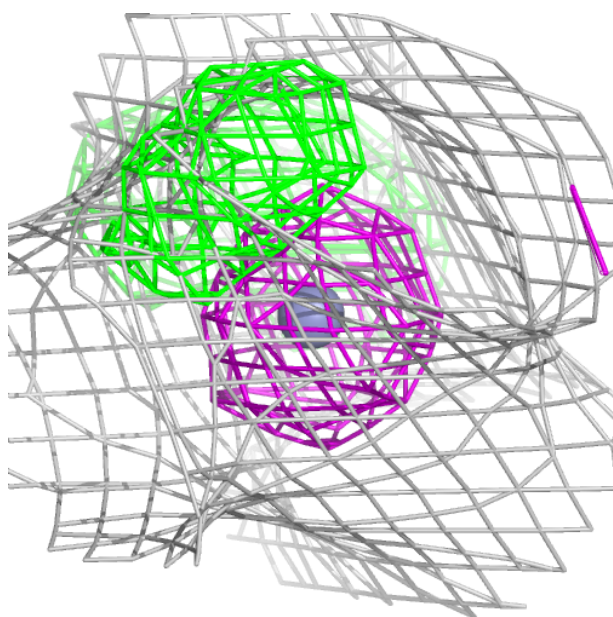
Electron density around ZN D 1301:

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



Electron density around ZN B 1301:

$2mF_o-DF_c$ (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.