



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:08 PM UTC

PDB ID : 1MR9 / pdb_00001mr9
Title : Crystal structure of Streptogramin A Acetyltransferase with acetyl-CoA bound
Authors : Kehoe, L.E.; Snidwongse, J.; Courvalin, P.; Rafferty, J.B.; Murray, I.A.
Deposited on : 2002-09-18
Resolution : 3.00 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:

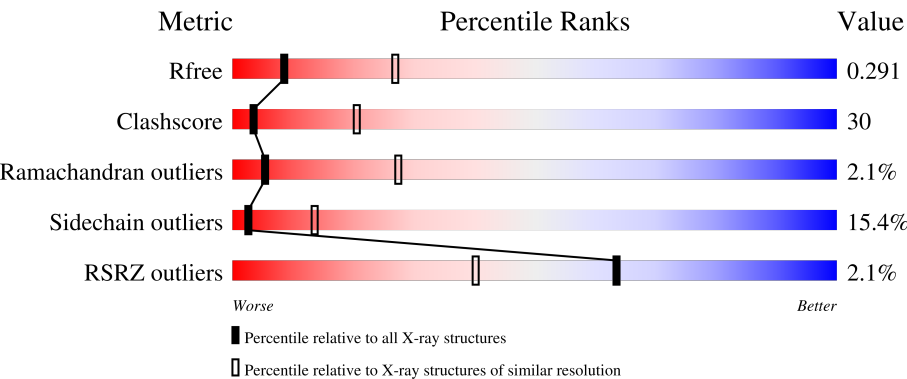
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	209	2% 51%39%7%
1	B	209	2% 49%40%7%
1	C	209	47%40%9%
1	X	209	2% 50%40%7%
1	Y	209	2% 42%43%10%

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Mol	Chain	Length	Quality of chain
1	Z	209	3% 40% 44% 11% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9672 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 Streptogramin A Acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	Se	0	0	0
			1576	1017	257	293	1	8			
1	B	203	Total	C	N	O	S	Se	0	0	0
			1570	1014	259	288	1	8			
1	C	202	Total	C	N	O	S	Se	0	0	0
			1557	1005	252	292	1	7			
1	X	203	Total	C	N	O	S	Se	0	0	0
			1569	1013	257	291	1	7			
1	Y	200	Total	C	N	O	S	Se	0	0	0
			1547	997	252	290	1	7			
1	Z	199	Total	C	N	O	S	Se	0	0	0
			1551	1004	252	287	1	7			

There are 48 discrepancies between the modelled and reference sequences:

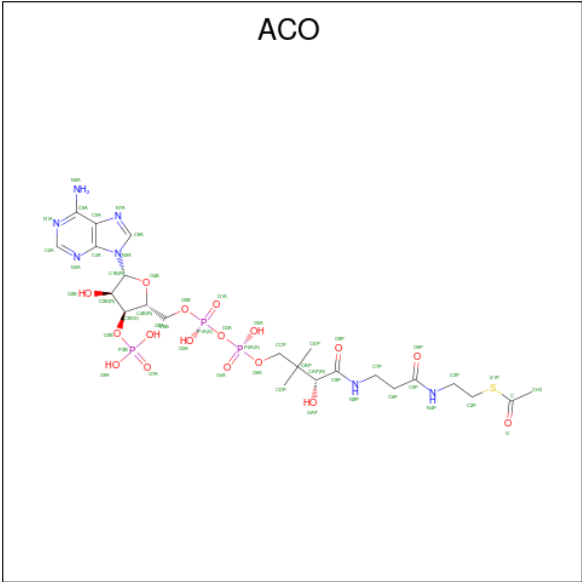
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P50870
A	6	MSE	MET	modified residue	UNP P50870
A	8	MSE	MET	modified residue	UNP P50870
A	77	MSE	MET	modified residue	UNP P50870
A	84	MSE	MET	modified residue	UNP P50870
A	102	MSE	MET	modified residue	UNP P50870
A	129	MSE	MET	modified residue	UNP P50870
A	154	MSE	MET	modified residue	UNP P50870
B	1	MSE	MET	modified residue	UNP P50870
B	6	MSE	MET	modified residue	UNP P50870
B	8	MSE	MET	modified residue	UNP P50870
B	77	MSE	MET	modified residue	UNP P50870
B	84	MSE	MET	modified residue	UNP P50870
B	102	MSE	MET	modified residue	UNP P50870
B	129	MSE	MET	modified residue	UNP P50870
B	154	MSE	MET	modified residue	UNP P50870
C	1	MSE	MET	modified residue	UNP P50870

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	MSE	MET	modified residue	UNP P50870
C	8	MSE	MET	modified residue	UNP P50870
C	77	MSE	MET	modified residue	UNP P50870
C	84	MSE	MET	modified residue	UNP P50870
C	102	MSE	MET	modified residue	UNP P50870
C	129	MSE	MET	modified residue	UNP P50870
C	154	MSE	MET	modified residue	UNP P50870
X	1	MSE	MET	modified residue	UNP P50870
X	6	MSE	MET	modified residue	UNP P50870
X	8	MSE	MET	modified residue	UNP P50870
X	77	MSE	MET	modified residue	UNP P50870
X	84	MSE	MET	modified residue	UNP P50870
X	102	MSE	MET	modified residue	UNP P50870
X	129	MSE	MET	modified residue	UNP P50870
X	154	MSE	MET	modified residue	UNP P50870
Y	1	MSE	MET	modified residue	UNP P50870
Y	6	MSE	MET	modified residue	UNP P50870
Y	8	MSE	MET	modified residue	UNP P50870
Y	77	MSE	MET	modified residue	UNP P50870
Y	84	MSE	MET	modified residue	UNP P50870
Y	102	MSE	MET	modified residue	UNP P50870
Y	129	MSE	MET	modified residue	UNP P50870
Y	154	MSE	MET	modified residue	UNP P50870
Z	1	MSE	MET	modified residue	UNP P50870
Z	6	MSE	MET	modified residue	UNP P50870
Z	8	MSE	MET	modified residue	UNP P50870
Z	77	MSE	MET	modified residue	UNP P50870
Z	84	MSE	MET	modified residue	UNP P50870
Z	102	MSE	MET	modified residue	UNP P50870
Z	129	MSE	MET	modified residue	UNP P50870
Z	154	MSE	MET	modified residue	UNP P50870

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

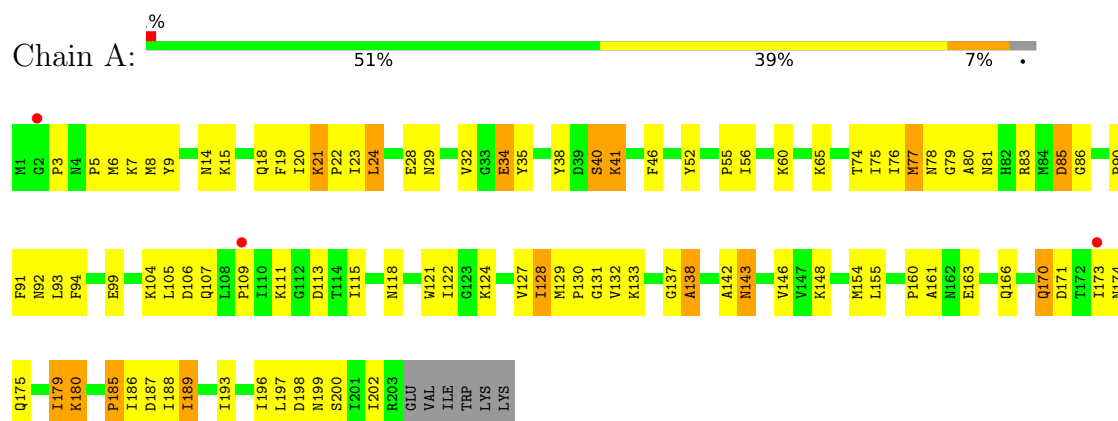


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	X	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	Y	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	Z	1	Total	C	N	O	P	S	0	0
			47	21	7	16	3			

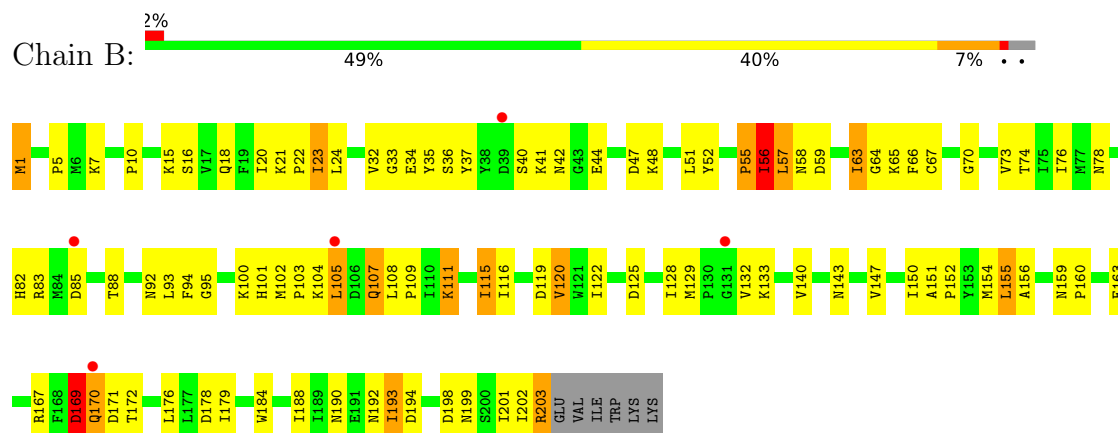
3 Residue-property plots

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.

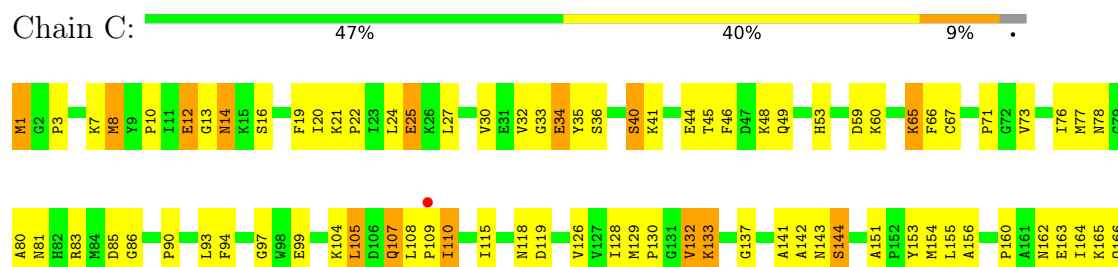
• Molecule 1: Streptogramin A Acetyltransferase



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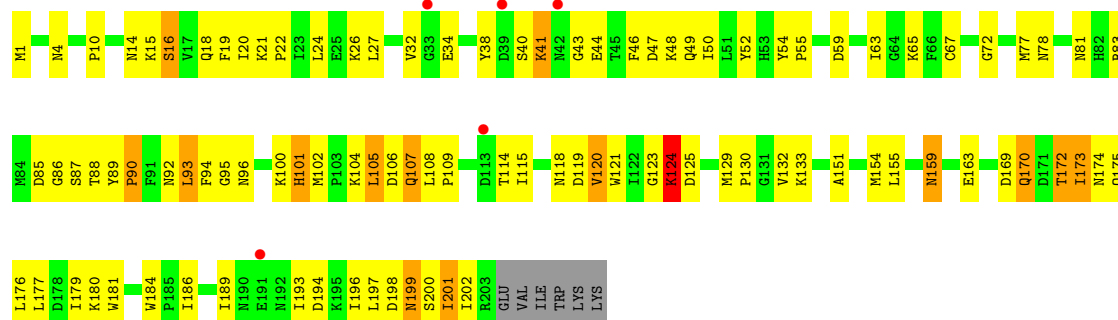


• Molecule 1: Streptogramin A Acetyltransferase

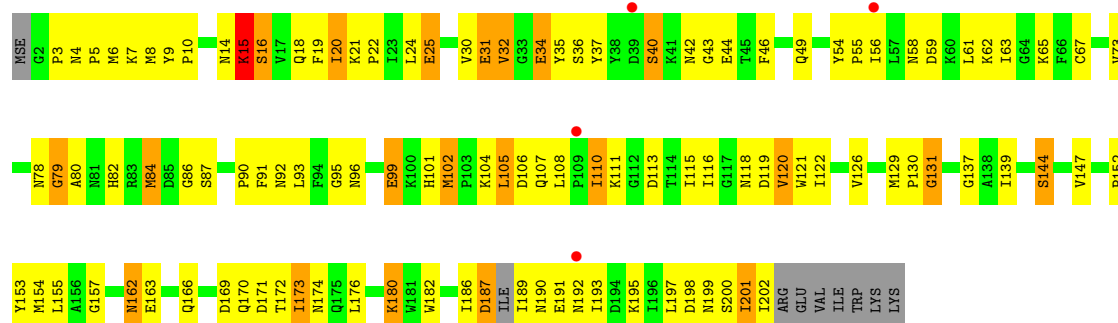




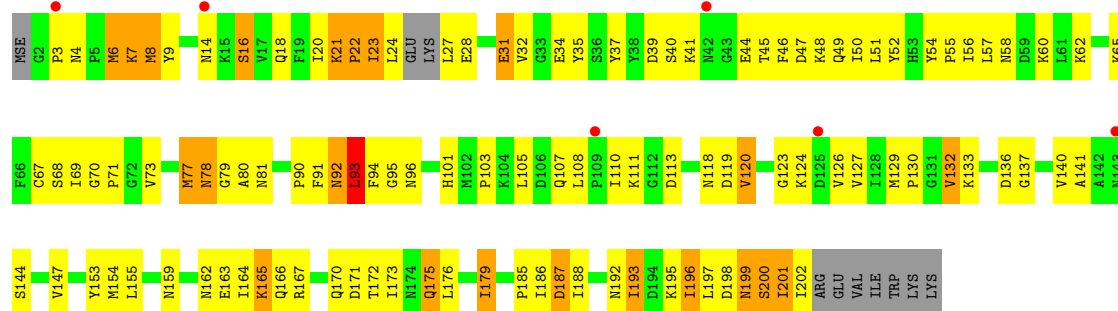
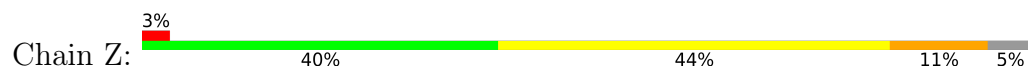
• Molecule 1: Streptogramin A Acetyltransferase



• Molecule 1: Streptogramin A Acetyltransferase



• Molecule 1: Streptogramin A Acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	181.52Å 184.53Å 186.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.7 (20.00-3.00) 89.3 (20.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.243 , 0.295 0.242 , 0.291	Depositor DCC
R_{free} test set	1425 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 85.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,l,k 0.024 for l,-k,h 0.028 for -k,-h,-l 0.012 for -k,-l,h 0.012 for l,-h,-k	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9672	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% 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: ACO

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	0.59	0/1608	0.70	0/2177
1	B	0.61	0/1602	0.73	0/2169
1	C	0.54	0/1589	0.72	0/2155
1	X	0.68	1/1601 (0.1%)	0.72	0/2169
1	Y	0.54	0/1578	0.72	0/2138
1	Z	0.60	0/1582	0.70	0/2139
All	All	0.60	1/9560 (0.0%)	0.71	0/12947

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	77	MSE	SE-CE	-5.88	1.77	1.95

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	MSE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1576	0	1541	86	0
1	B	1570	0	1538	93	0
1	C	1557	0	1504	93	0
1	X	1569	0	1530	97	0
1	Y	1547	0	1493	113	0
1	Z	1551	0	1525	109	0
2	A	51	0	34	3	0
2	B	102	0	68	8	0
2	X	51	0	34	5	0
2	Y	51	0	34	2	0
2	Z	47	0	29	1	0
All	All	9672	0	9330	567	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 30.

All (567) 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:B:1:MSE:H3	1:B:190:ASN:ND2	1.48	1.11
1:B:1:MSE:N	1:B:190:ASN:HD21	1.47	1.10
1:A:52:TYR:CD1	1:A:80:ALA:HB2	1.93	1.03
1:B:1:MSE:N	1:B:190:ASN:ND2	2.07	0.99
1:Z:65:LYS:H	1:Z:118:ASN:HD22	1.08	0.99
1:Z:154:MSE:HE2	1:Z:163:GLU:HB3	1.45	0.98
1:B:47:ASP:OD2	1:B:48:LYS:NZ	1.96	0.98
1:Y:104:LYS:H	1:Y:107:GLN:HE21	1.12	0.96
1:C:170:GLN:O	1:C:170:GLN:NE2	2.04	0.91
2:B:301:ACO:H4B	2:B:301:ACO:O7A	1.67	0.90
1:A:65:LYS:H	1:A:118:ASN:HD22	1.18	0.87
1:X:10:PRO:HG3	1:X:19:PHE:CD1	2.09	0.87
1:Z:176:LEU:HD11	1:Z:199:ASN:HD21	1.40	0.86
1:Y:104:LYS:H	1:Y:107:GLN:NE2	1.75	0.85
1:B:92:ASN:HD22	1:B:102:MSE:HA	1.40	0.85
1:X:176:LEU:HG	1:X:202:ILE:HD11	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:14:ASN:OD1	1:Z:16:SER:HB2	1.79	0.83
1:Z:18:GLN:HE22	1:Z:46:PHE:H	1.27	0.83
1:X:14:ASN:O	1:X:16:SER:N	2.12	0.82
1:Y:32:VAL:HG12	1:Y:63:ILE:HB	1.59	0.81
1:Z:118:ASN:N	1:Z:136:ASP:OD2	2.13	0.81
1:Z:92:ASN:O	1:Z:94:PHE:N	2.13	0.80
1:Y:170:GLN:NE2	1:Y:174:ASN:OD1	2.15	0.80
1:B:154:MSE:HE2	1:B:163:GLU:HB3	1.63	0.79
1:A:65:LYS:H	1:A:118:ASN:ND2	1.81	0.78
1:Y:67:CYS:SG	1:Y:120:VAL:HG13	2.24	0.78
1:Z:71:PRO:HG2	1:Z:124:LYS:HG3	1.65	0.78
1:B:1:MSE:HE3	1:B:190:ASN:CG	2.08	0.77
2:B:300:ACO:O7A	2:B:300:ACO:H4B	1.84	0.77
1:X:44:GLU:N	1:X:44:GLU:OE1	2.16	0.77
1:Y:9:TYR:CD2	1:Y:15:LYS:NZ	2.53	0.77
1:Y:65:LYS:H	1:Y:118:ASN:HD22	1.33	0.77
1:A:21:LYS:HG3	1:A:32:VAL:O	1.86	0.75
1:X:176:LEU:HD11	1:X:199:ASN:HD21	1.51	0.75
1:X:14:ASN:C	1:X:16:SER:H	1.94	0.74
1:Z:65:LYS:H	1:Z:118:ASN:ND2	1.84	0.74
1:Y:78:ASN:C	1:Y:80:ALA:H	1.96	0.74
1:Y:170:GLN:HE21	1:Y:174:ASN:CG	1.96	0.74
1:C:167:ARG:O	1:C:168:PHE:CD1	2.41	0.73
1:Z:137:GLY:O	1:Z:167:ARG:HD3	1.88	0.73
1:Y:110:ILE:O	1:Y:110:ILE:HG23	1.89	0.73
1:C:24:LEU:HB3	1:C:30:VAL:HG11	1.71	0.72
1:B:1:MSE:H3	1:B:190:ASN:HD21	0.76	0.72
1:Y:154:MSE:SE	1:Y:166:GLN:HG3	2.39	0.72
1:C:44:GLU:OE1	1:C:44:GLU:N	2.23	0.71
1:Y:104:LYS:N	1:Y:107:GLN:HE21	1.86	0.70
1:C:12:GLU:CD	1:C:12:GLU:H	2.00	0.70
1:Y:166:GLN:NE2	1:Y:173:ILE:HD12	2.06	0.70
1:Y:166:GLN:HE21	1:Y:173:ILE:HD12	1.56	0.70
1:Z:192:ASN:O	1:Z:196:ILE:HG13	1.90	0.70
1:Z:14:ASN:OD1	1:Z:16:SER:CB	2.40	0.69
2:A:302:ACO:C2A	1:C:160:PRO:HG3	2.22	0.69
1:B:51:LEU:HB2	1:B:76:ILE:HD13	1.74	0.69
1:X:177:LEU:O	1:X:180:LYS:HE2	1.91	0.69
1:A:160:PRO:HG3	2:B:300:ACO:C2A	2.23	0.69
1:Y:9:TYR:CG	1:Y:15:LYS:NZ	2.61	0.68
1:X:123:GLY:O	1:X:124:LYS:C	2.36	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:HA	1:B:140:VAL:HG22	1.75	0.68
1:Z:200:SER:C	1:Z:202:ILE:H	2.01	0.68
1:C:81:ASN:HB2	1:C:109:PRO:HG2	1.74	0.68
1:A:24:LEU:N	1:A:24:LEU:HD23	2.07	0.68
1:Y:78:ASN:O	1:Y:80:ALA:N	2.27	0.68
1:X:169:ASP:O	1:X:173:ILE:HG13	1.94	0.67
1:C:65:LYS:HB2	1:C:118:ASN:HD22	1.59	0.67
1:C:119:ASP:O	1:C:137:GLY:HA2	1.94	0.67
1:Z:198:ASP:C	1:Z:198:ASP:OD1	2.36	0.67
1:Y:187:ASP:O	1:Y:189:ILE:N	2.27	0.67
1:X:159:ASN:C	1:X:159:ASN:HD22	2.02	0.67
1:C:110:ILE:O	1:C:110:ILE:HG23	1.93	0.67
1:A:128:ILE:HG22	1:A:132:VAL:CG2	2.25	0.66
1:B:184:TRP:CH2	1:B:201:ILE:HD11	2.31	0.66
1:X:10:PRO:HG3	1:X:19:PHE:CE1	2.30	0.66
1:X:104:LYS:H	1:X:107:GLN:HE21	1.42	0.66
1:X:194:ASP:CG	1:Z:101:HIS:HD1	2.03	0.66
1:Y:34:GLU:O	1:Y:35:TYR:HB2	1.93	0.66
1:Z:21:LYS:HB3	1:Z:22:PRO:HD3	1.77	0.65
1:B:159:ASN:C	1:B:159:ASN:HD22	2.04	0.65
1:C:151:ALA:HB3	1:C:154:MSE:HG3	1.78	0.65
1:C:141:ALA:O	1:C:144:SER:HB2	1.95	0.65
1:A:127:VAL:HG21	1:B:143:ASN:ND2	2.11	0.65
1:X:198:ASP:OD1	1:X:200:SER:OG	2.14	0.65
1:B:34:GLU:O	1:B:35:TYR:HB2	1.95	0.65
1:B:92:ASN:ND2	1:B:102:MSE:HA	2.12	0.65
1:C:170:GLN:HE22	1:C:174:ASN:CG	2.05	0.64
1:C:105:LEU:O	1:C:108:LEU:N	2.30	0.64
1:X:34:GLU:OE1	1:X:34:GLU:N	2.29	0.64
1:X:104:LYS:H	1:X:107:GLN:NE2	1.96	0.64
1:X:65:LYS:HB2	1:X:118:ASN:HD22	1.62	0.64
1:Z:18:GLN:OE1	1:Z:45:THR:HA	1.98	0.63
1:A:154:MSE:CE	1:A:163:GLU:HB3	2.28	0.63
1:X:20:ILE:HG13	1:X:32:VAL:HG11	1.81	0.63
1:Y:195:LYS:HA	1:Y:198:ASP:OD1	1.99	0.63
1:B:122:ILE:HA	1:B:140:VAL:CG2	2.29	0.63
1:Z:164:ILE:HG22	1:Z:165:LYS:HG2	1.80	0.63
1:C:137:GLY:O	1:C:153:TYR:HA	1.98	0.62
1:C:200:SER:O	1:C:202:ILE:N	2.31	0.62
1:X:121:TRP:CZ2	2:X:305:ACO:H61	2.34	0.62
1:A:52:TYR:CG	1:A:80:ALA:HB2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:ACO:O7A	2:B:301:ACO:C4B	2.43	0.62
1:X:118:ASN:O	1:X:120:VAL:HG12	2.00	0.62
1:Y:36:SER:OG	1:Y:67:CYS:HB2	1.98	0.62
1:Y:110:ILE:O	1:Y:110:ILE:CG2	2.46	0.62
1:B:24:LEU:HD12	1:B:32:VAL:HG21	1.81	0.62
1:B:55:PRO:O	1:B:57:LEU:N	2.33	0.62
1:C:66:PHE:O	1:C:119:ASP:HA	1.99	0.62
1:X:176:LEU:CG	1:X:202:ILE:HD11	2.29	0.62
1:B:203:ARG:HG3	1:B:203:ARG:HH11	1.64	0.62
1:Z:92:ASN:C	1:Z:94:PHE:H	2.08	0.61
1:A:34:GLU:O	1:A:35:TYR:HB2	2.00	0.61
1:Z:92:ASN:OD1	1:Z:92:ASN:N	2.32	0.61
1:Z:40:SER:OG	1:Z:44:GLU:O	2.18	0.61
1:Z:14:ASN:OD1	1:Z:16:SER:N	2.29	0.61
1:Z:77:MSE:O	1:Z:79:GLY:N	2.34	0.60
1:A:175:GLN:O	1:A:179:ILE:HG23	2.02	0.60
1:B:1:MSE:HE3	1:B:190:ASN:CB	2.32	0.60
1:C:34:GLU:CD	1:C:34:GLU:H	2.09	0.60
1:A:185:PRO:O	1:A:188:ILE:N	2.35	0.60
1:Y:34:GLU:HG2	1:Y:65:LYS:HZ3	1.66	0.60
1:Z:46:PHE:CE2	1:Z:50:ILE:HD11	2.36	0.60
1:B:1:MSE:H1	1:B:190:ASN:ND2	1.99	0.60
1:A:21:LYS:CG	1:A:32:VAL:O	2.50	0.59
1:A:23:ILE:HG22	1:A:24:LEU:HD23	1.82	0.59
1:B:21:LYS:N	1:B:22:PRO:HD2	2.18	0.59
1:C:104:LYS:O	1:C:105:LEU:C	2.45	0.59
1:Y:10:PRO:HG3	1:Y:19:PHE:CE1	2.38	0.59
1:Z:78:ASN:ND2	1:Z:130:PRO:HB3	2.18	0.59
1:A:121:TRP:CZ2	2:A:302:ACO:H62	2.39	0.58
1:X:59:ASP:CG	1:X:78:ASN:HD22	2.11	0.58
1:Z:129:MSE:HG3	1:Z:147:VAL:HG12	1.85	0.58
1:C:198:ASP:OD1	1:C:198:ASP:C	2.46	0.58
1:Y:4:ASN:O	1:Y:6:MSE:N	2.37	0.58
1:Y:189:ILE:O	1:Y:190:ASN:C	2.47	0.58
1:B:1:MSE:HE3	1:B:190:ASN:HB3	1.86	0.58
1:Z:21:LYS:CB	1:Z:22:PRO:HD3	2.33	0.58
1:Z:24:LEU:HD12	1:Z:32:VAL:HG21	1.85	0.58
1:Y:25:GLU:OE1	1:Y:25:GLU:HA	2.03	0.58
1:C:83:ARG:NH2	1:C:85:ASP:OD2	2.35	0.57
1:Y:200:SER:C	1:Y:202:ILE:H	2.12	0.57
1:Z:141:ALA:O	1:Z:144:SER:OG	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASP:N	1:B:47:ASP:OD1	2.36	0.57
1:X:121:TRP:HZ2	2:X:305:ACO:H61	1.68	0.57
1:A:76:ILE:O	1:A:130:PRO:HG3	2.04	0.57
1:B:108:LEU:HB3	1:B:109:PRO:CD	2.35	0.57
1:C:34:GLU:O	1:C:35:TYR:HB2	2.04	0.57
1:Y:87:SER:OG	1:Z:119:ASP:OD1	2.21	0.57
1:Z:185:PRO:HD2	1:Z:188:ILE:HD13	1.85	0.57
1:A:38:TYR:CE2	1:A:40:SER:HA	2.40	0.57
1:C:155:LEU:O	1:C:164:ILE:N	2.37	0.57
1:X:86:GLY:HA3	1:Y:197:LEU:O	2.04	0.57
1:X:159:ASN:C	1:X:159:ASN:ND2	2.60	0.57
1:Z:126:VAL:HG12	1:Z:127:VAL:N	2.20	0.57
1:X:100:LYS:O	1:X:102:MSE:N	2.33	0.57
1:Z:45:THR:OG1	1:Z:47:ASP:OD2	2.18	0.57
1:B:18:GLN:O	1:B:37:TYR:HA	2.05	0.57
1:X:172:THR:HG23	1:X:202:ILE:CD1	2.34	0.56
1:B:169:ASP:OD2	1:B:171:ASP:N	2.36	0.56
1:C:129:MSE:O	1:C:132:VAL:HG13	2.05	0.56
1:Z:103:PRO:HA	1:Z:107:GLN:NE2	2.21	0.56
1:B:33:GLY:HA3	1:B:64:GLY:O	2.06	0.56
1:C:175:GLN:OE1	1:C:202:ILE:HB	2.05	0.56
1:X:24:LEU:HD12	1:X:32:VAL:HG21	1.88	0.56
1:X:100:LYS:C	1:X:102:MSE:H	2.13	0.56
1:X:176:LEU:HD11	1:X:199:ASN:ND2	2.19	0.56
1:X:196:ILE:HG12	1:X:201:ILE:HD13	1.88	0.56
1:A:171:ASP:HA	1:A:174:ASN:ND2	2.20	0.56
1:X:198:ASP:OD1	1:X:198:ASP:C	2.48	0.56
1:A:197:LEU:O	1:C:86:GLY:HA3	2.06	0.56
1:A:128:ILE:HG22	1:A:132:VAL:HG21	1.88	0.55
1:X:21:LYS:HB3	1:X:22:PRO:HD3	1.89	0.55
1:Y:186:ILE:O	1:Y:190:ASN:OD1	2.24	0.55
1:A:65:LYS:N	1:A:118:ASN:HD22	1.96	0.55
1:C:25:GLU:O	1:C:25:GLU:HG3	2.05	0.55
1:Y:95:GLY:HA2	1:Y:99:GLU:HG3	1.88	0.55
1:A:171:ASP:HA	1:A:174:ASN:HD22	1.72	0.55
1:B:101:HIS:CE1	1:C:193:ILE:HB	2.41	0.55
1:Y:91:PHE:HD1	1:Z:197:LEU:HD21	1.71	0.55
1:Z:52:TYR:CD1	1:Z:80:ALA:HB2	2.41	0.55
1:Z:92:ASN:O	1:Z:93:LEU:C	2.50	0.55
1:A:143:ASN:N	1:A:143:ASN:ND2	2.54	0.55
1:C:193:ILE:O	1:C:197:LEU:HG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:151:ALA:HB3	1:X:154:MSE:HG3	1.88	0.55
1:Y:54:TYR:CD2	1:Y:79:GLY:HA3	2.42	0.55
1:X:194:ASP:OD2	1:Z:101:HIS:ND1	2.37	0.55
1:Y:19:PHE:O	1:Y:22:PRO:HD2	2.07	0.55
1:Y:34:GLU:HG2	1:Y:65:LYS:NZ	2.22	0.55
1:Y:40:SER:HB2	1:Y:43:GLY:H	1.72	0.55
1:B:55:PRO:O	1:B:56:ILE:C	2.50	0.54
1:Y:92:ASN:HD22	1:Y:102:MSE:HG2	1.71	0.54
1:Z:171:ASP:O	1:Z:172:THR:C	2.50	0.54
1:C:104:LYS:O	1:C:107:GLN:HG3	2.08	0.54
1:A:154:MSE:HE2	1:A:163:GLU:CG	2.38	0.54
1:B:184:TRP:CZ3	1:B:201:ILE:HD11	2.43	0.54
1:Y:55:PRO:O	1:Y:58:ASN:N	2.40	0.54
1:A:35:TYR:OH	1:A:186:ILE:HG12	2.07	0.54
1:B:20:ILE:HG23	1:B:24:LEU:HG	1.89	0.54
1:C:81:ASN:CB	1:C:109:PRO:HG2	2.38	0.54
1:X:115:ILE:HB	1:X:133:LYS:HG3	1.88	0.54
1:Y:154:MSE:HE2	1:Y:163:GLU:HB3	1.89	0.54
1:A:80:ALA:HA	2:B:300:ACO:S1P	2.48	0.54
1:Y:21:LYS:HB3	1:Y:22:PRO:HD3	1.89	0.54
1:Z:4:ASN:C	1:Z:6:MSE:H	2.16	0.54
1:X:10:PRO:CG	1:X:19:PHE:CD1	2.88	0.54
1:C:97:GLY:N	1:C:99:GLU:OE1	2.41	0.53
1:Z:8:MSE:HA	1:Z:22:PRO:HB2	1.89	0.53
1:B:169:ASP:OD1	1:B:172:THR:OG1	2.22	0.53
1:C:13:GLY:O	1:C:14:ASN:C	2.51	0.53
1:A:21:LYS:N	1:A:22:PRO:HD2	2.23	0.53
1:B:92:ASN:OD1	1:B:93:LEU:N	2.39	0.53
1:A:154:MSE:SE	1:A:166:GLN:HG2	2.58	0.53
1:Z:70:GLY:O	1:Z:73:VAL:HG23	2.09	0.53
1:Y:21:LYS:N	1:Y:22:PRO:CD	2.71	0.53
1:Y:67:CYS:SG	1:Y:120:VAL:CG1	2.96	0.53
1:Y:96:ASN:HD22	1:Z:3:PRO:HB3	1.73	0.53
1:X:10:PRO:CG	1:X:19:PHE:CE1	2.91	0.53
1:Y:78:ASN:C	1:Y:80:ALA:N	2.63	0.53
1:A:77:MSE:O	1:A:79:GLY:N	2.42	0.53
1:B:104:LYS:O	1:B:105:LEU:C	2.52	0.53
1:B:203:ARG:HH11	1:B:203:ARG:CG	2.22	0.53
1:C:104:LYS:HG2	1:C:107:GLN:NE2	2.24	0.53
1:B:56:ILE:HA	1:X:104:LYS:HG3	1.90	0.53
1:Z:21:LYS:CB	1:Z:22:PRO:CD	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:176:LEU:HD11	1:Y:199:ASN:ND2	2.25	0.52
1:Z:200:SER:C	1:Z:202:ILE:N	2.67	0.52
1:C:200:SER:C	1:C:202:ILE:N	2.68	0.52
1:Y:4:ASN:C	1:Y:6:MSE:H	2.17	0.52
1:Z:7:LYS:HD2	1:Z:8:MSE:N	2.24	0.52
1:B:129:MSE:HG3	1:B:147:VAL:HG12	1.91	0.52
1:C:53:HIS:CD2	1:C:77:MSE:HG3	2.44	0.52
1:Z:154:MSE:SE	1:Z:166:GLN:HG2	2.58	0.52
1:Y:21:LYS:O	1:Y:25:GLU:CD	2.53	0.52
1:B:128:ILE:HG23	1:B:132:VAL:HG21	1.92	0.52
1:Z:52:TYR:CG	1:Z:80:ALA:HB2	2.45	0.52
1:Z:195:LYS:O	1:Z:201:ILE:HG23	2.10	0.52
1:Z:126:VAL:CG1	1:Z:127:VAL:N	2.73	0.52
1:Z:129:MSE:HB3	1:Z:130:PRO:HD2	1.92	0.52
1:A:7:LYS:O	1:A:19:PHE:HB2	2.09	0.52
1:A:170:GLN:HE21	1:A:170:GLN:CA	2.21	0.52
1:C:110:ILE:O	1:C:110:ILE:CG2	2.57	0.52
1:Y:20:ILE:HD11	1:Y:32:VAL:CG1	2.39	0.52
1:Y:189:ILE:O	1:Y:192:ASN:N	2.39	0.52
1:A:29:ASN:OD1	1:A:60:LYS:NZ	2.23	0.52
1:C:193:ILE:O	1:C:197:LEU:N	2.36	0.52
1:C:40:SER:OG	1:C:44:GLU:O	2.27	0.52
1:Z:23:ILE:HG22	1:Z:24:LEU:HD23	1.91	0.51
1:B:66:PHE:O	1:B:119:ASP:HA	2.11	0.51
1:Y:21:LYS:NZ	1:Y:25:GLU:OE2	2.35	0.51
1:Y:176:LEU:HD11	1:Y:199:ASN:HD21	1.75	0.51
1:X:90:PRO:HB2	1:X:93:LEU:HD23	1.93	0.51
1:Y:21:LYS:O	1:Y:25:GLU:OE1	2.28	0.51
1:Z:4:ASN:OD1	1:Z:6:MSE:HB2	2.11	0.51
1:Z:195:LYS:CB	1:Z:201:ILE:HG23	2.41	0.51
1:A:38:TYR:HE2	1:A:40:SER:HA	1.75	0.51
1:C:156:ALA:HA	1:C:162:ASN:O	2.11	0.51
1:X:155:LEU:HD11	2:X:305:ACO:H142	1.93	0.51
1:A:185:PRO:O	1:A:187:ASP:N	2.44	0.51
1:B:104:LYS:H	1:B:107:GLN:HE21	1.58	0.51
1:X:24:LEU:HD22	1:X:27:LEU:HD12	1.93	0.51
1:X:83:ARG:O	1:X:88:THR:HA	2.10	0.51
1:C:73:VAL:HG22	1:C:126:VAL:HB	1.93	0.51
1:X:4:ASN:OD1	1:X:4:ASN:C	2.53	0.50
1:Y:90:PRO:CB	1:Y:93:LEU:HD12	2.42	0.50
1:Z:21:LYS:C	1:Z:23:ILE:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:HD12	1:B:156:ALA:N	2.26	0.50
1:C:187:ASP:OD2	1:C:187:ASP:C	2.53	0.50
1:C:201:ILE:HD12	1:C:201:ILE:N	2.27	0.50
1:X:14:ASN:ND2	1:X:16:SER:OG	2.44	0.50
1:X:83:ARG:NH2	1:X:85:ASP:OD2	2.39	0.50
1:X:92:ASN:OD1	1:X:92:ASN:N	2.43	0.50
1:Y:18:GLN:O	1:Y:37:TYR:HA	2.11	0.50
1:B:20:ILE:CG2	1:B:32:VAL:HG11	2.41	0.50
1:B:70:GLY:O	1:B:73:VAL:HG23	2.12	0.50
1:X:90:PRO:O	1:X:93:LEU:HB2	2.12	0.50
1:Y:104:LYS:CB	1:Y:107:GLN:HE21	2.25	0.50
1:Y:129:MSE:HE3	1:Y:130:PRO:CD	2.41	0.50
1:A:86:GLY:O	1:B:167:ARG:NH2	2.38	0.50
1:A:14:ASN:OD1	1:A:14:ASN:C	2.54	0.49
1:A:83:ARG:NE	1:A:85:ASP:OD2	2.44	0.49
1:B:172:THR:O	1:B:176:LEU:N	2.29	0.49
2:B:301:ACO:O9P	1:C:141:ALA:HA	2.12	0.49
1:X:198:ASP:OD1	1:X:200:SER:CB	2.60	0.49
1:C:10:PRO:HG3	1:C:19:PHE:CD1	2.47	0.49
1:X:38:TYR:CE2	1:X:40:SER:HA	2.46	0.49
1:X:72:GLY:HA3	1:X:125:ASP:OD1	2.11	0.49
1:Y:169:ASP:OD1	1:Y:172:THR:N	2.40	0.49
1:Z:200:SER:O	1:Z:202:ILE:N	2.43	0.49
1:X:81:ASN:HB3	1:X:109:PRO:HG2	1.94	0.49
1:A:20:ILE:HD13	1:A:46:PHE:CD2	2.48	0.49
1:X:118:ASN:O	1:X:119:ASP:C	2.56	0.49
1:B:159:ASN:HD22	1:B:160:PRO:N	2.10	0.49
1:C:201:ILE:HD12	1:C:202:ILE:N	2.28	0.49
1:X:59:ASP:CB	1:X:78:ASN:HD22	2.25	0.49
1:B:20:ILE:HG22	1:B:32:VAL:HG11	1.94	0.49
1:C:151:ALA:HB3	1:C:154:MSE:CG	2.41	0.49
1:Y:90:PRO:CB	1:Y:93:LEU:HG	2.42	0.49
1:A:21:LYS:HG3	1:A:32:VAL:C	2.37	0.49
1:B:5:PRO:HG3	1:B:35:TYR:CZ	2.48	0.48
1:X:154:MSE:HE2	1:X:163:GLU:HG2	1.95	0.48
1:Z:198:ASP:OD1	1:Z:200:SER:OG	2.27	0.48
1:B:116:ILE:HG23	1:B:120:VAL:HG21	1.94	0.48
1:Z:34:GLU:O	1:Z:35:TYR:HB2	2.13	0.48
1:A:142:ALA:C	1:A:143:ASN:HD22	2.21	0.48
1:B:188:ILE:O	1:B:192:ASN:ND2	2.44	0.48
1:Y:101:HIS:CG	1:Z:193:ILE:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PRO:HB2	1:A:188:ILE:HG12	1.95	0.48
1:Z:20:ILE:CD1	1:Z:69:ILE:HD12	2.44	0.48
1:Z:78:ASN:HD21	1:Z:111:LYS:HB2	1.79	0.48
1:B:105:LEU:CD1	1:X:105:LEU:HD23	2.44	0.48
1:B:108:LEU:HB3	1:B:109:PRO:HD2	1.96	0.48
1:C:198:ASP:OD1	1:C:200:SER:CB	2.62	0.48
1:Y:30:VAL:HG13	1:Y:61:LEU:HD23	1.95	0.48
1:Y:129:MSE:HE3	1:Y:130:PRO:HD2	1.96	0.48
1:B:101:HIS:CG	1:C:193:ILE:HG21	2.49	0.48
1:C:10:PRO:CB	1:C:19:PHE:CE1	2.96	0.48
1:X:104:LYS:HB2	1:X:107:GLN:NE2	2.29	0.48
1:A:90:PRO:C	1:A:92:ASN:N	2.72	0.47
1:B:83:ARG:O	1:B:88:THR:HG22	2.14	0.47
1:B:111:LYS:HE3	2:B:301:ACO:O2A	2.14	0.47
1:C:65:LYS:H	1:C:118:ASN:ND2	2.11	0.47
1:X:44:GLU:HG3	1:X:49:GLN:OE1	2.14	0.47
1:B:85:ASP:O	1:C:199:ASN:HB2	2.14	0.47
1:Z:34:GLU:OE1	1:Z:65:LYS:HE2	2.15	0.47
1:A:83:ARG:HD2	1:A:107:GLN:HB3	1.96	0.47
1:A:198:ASP:C	1:A:200:SER:H	2.22	0.47
1:B:21:LYS:HB3	1:B:22:PRO:CD	2.43	0.47
1:Z:111:LYS:HZ2	1:Z:130:PRO:HG2	1.79	0.47
1:B:59:ASP:OD2	1:B:78:ASN:HB2	2.14	0.47
1:Y:86:GLY:HA3	1:Z:197:LEU:C	2.40	0.47
1:Y:191:GLU:O	1:Y:192:ASN:CG	2.58	0.47
1:Z:58:ASN:O	1:Z:58:ASN:CG	2.57	0.47
1:Z:95:GLY:O	1:Z:96:ASN:HB2	2.14	0.47
1:A:5:PRO:C	1:A:7:LYS:H	2.23	0.47
1:A:154:MSE:HE2	1:A:163:GLU:HB3	1.94	0.47
1:Z:159:ASN:C	1:Z:159:ASN:OD1	2.58	0.47
1:A:90:PRO:O	1:A:91:PHE:C	2.58	0.47
1:X:94:PHE:HB3	1:Y:3:PRO:HG3	1.96	0.47
1:X:170:GLN:NE2	1:X:170:GLN:CA	2.77	0.47
1:Y:49:GLN:HB3	1:Y:73:VAL:O	2.15	0.47
1:Y:90:PRO:HB2	1:Y:93:LEU:CG	2.44	0.47
1:Y:116:ILE:CG2	1:Y:120:VAL:HG11	2.45	0.47
1:Z:90:PRO:O	1:Z:91:PHE:C	2.57	0.47
1:A:146:VAL:HA	1:A:161:ALA:HB3	1.96	0.47
1:C:200:SER:C	1:C:202:ILE:H	2.23	0.47
1:Y:90:PRO:HB2	1:Y:93:LEU:HG	1.96	0.47
1:B:33:GLY:CA	1:B:64:GLY:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLU:O	1:B:44:GLU:HG2	2.14	0.47
1:X:59:ASP:OD1	1:X:59:ASP:N	2.43	0.47
1:X:83:ARG:NE	1:X:85:ASP:OD1	2.46	0.47
1:Y:20:ILE:CD1	1:Y:32:VAL:HG11	2.43	0.46
1:C:115:ILE:HB	1:C:133:LYS:HB3	1.98	0.46
1:X:101:HIS:CG	1:Y:193:ILE:HG21	2.50	0.46
1:A:81:ASN:HB3	1:A:109:PRO:HG2	1.96	0.46
1:A:91:PHE:CD2	1:B:193:ILE:HD13	2.51	0.46
1:Y:126:VAL:HG22	1:Y:144:SER:HB2	1.98	0.46
1:Y:169:ASP:OD1	1:Y:172:THR:CB	2.64	0.46
1:Z:35:TYR:CE1	1:Z:186:ILE:HD13	2.51	0.46
1:C:201:ILE:HD12	1:C:202:ILE:H	1.81	0.46
1:X:41:LYS:NZ	1:X:72:GLY:HA3	2.30	0.46
1:X:100:LYS:C	1:X:102:MSE:N	2.73	0.46
1:Y:65:LYS:H	1:Y:118:ASN:ND2	2.08	0.46
1:Z:92:ASN:C	1:Z:94:PHE:N	2.63	0.46
1:C:10:PRO:HB3	1:C:19:PHE:CE1	2.50	0.46
1:Y:171:ASP:O	1:Y:172:THR:C	2.58	0.46
1:Z:31:GLU:O	1:Z:62:LYS:HA	2.16	0.46
1:B:83:ARG:HG2	1:B:85:ASP:OD1	2.15	0.46
1:Y:20:ILE:HD11	1:Y:32:VAL:HG11	1.97	0.46
1:Y:199:ASN:C	1:Y:201:ILE:N	2.72	0.46
1:A:129:MSE:O	1:A:132:VAL:HG22	2.15	0.46
1:C:21:LYS:N	1:C:22:PRO:HD2	2.31	0.46
1:C:24:LEU:HB3	1:C:30:VAL:CG1	2.43	0.46
1:C:32:VAL:HG12	1:C:33:GLY:N	2.31	0.46
1:Y:34:GLU:CG	1:Y:65:LYS:NZ	2.79	0.46
1:C:59:ASP:HB3	1:C:78:ASN:HD22	1.81	0.46
1:A:155:LEU:CD1	2:A:302:ACO:H142	2.45	0.46
1:Z:51:LEU:HB3	1:Z:52:TYR:CD1	2.51	0.46
1:A:185:PRO:C	1:A:187:ASP:N	2.72	0.45
1:X:52:TYR:CZ	2:Y:303:ACO:S1P	3.10	0.45
1:Y:92:ASN:CB	1:Y:102:MSE:HA	2.46	0.45
1:Z:67:CYS:SG	1:Z:120:VAL:HG13	2.55	0.45
1:Z:176:LEU:HD11	1:Z:199:ASN:ND2	2.21	0.45
1:Z:187:ASP:OD2	1:Z:187:ASP:N	2.49	0.45
1:Z:21:LYS:HB3	1:Z:22:PRO:CD	2.44	0.45
1:B:36:SER:HA	1:B:67:CYS:O	2.17	0.45
1:B:92:ASN:O	1:B:95:GLY:N	2.49	0.45
1:X:181:TRP:O	1:X:184:TRP:HB2	2.16	0.45
1:Y:82:HIS:CE1	1:Y:90:PRO:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:14:ASN:O	1:Y:16:SER:N	2.49	0.45
1:A:127:VAL:HG21	1:B:143:ASN:HD21	1.81	0.45
1:A:170:GLN:HE21	1:A:170:GLN:C	2.24	0.45
1:B:115:ILE:O	1:B:115:ILE:HG22	2.17	0.45
1:X:18:GLN:HE22	1:X:46:PHE:N	2.15	0.45
1:Y:84:MSE:O	1:Z:167:ARG:NH2	2.50	0.45
1:Y:90:PRO:O	1:Y:91:PHE:C	2.58	0.45
1:C:77:MSE:HE3	1:C:77:MSE:HA	1.98	0.45
1:Z:90:PRO:HB2	1:Z:93:LEU:HD23	1.99	0.45
1:C:46:PHE:O	1:C:49:GLN:HB2	2.17	0.45
1:Y:31:GLU:O	1:Y:62:LYS:HA	2.18	0.45
1:Z:8:MSE:HB3	1:Z:9:TYR:CD1	2.52	0.45
1:Z:8:MSE:HE3	1:Z:23:ILE:CD1	2.47	0.45
1:A:111:LYS:HD2	1:A:130:PRO:HB2	1.99	0.44
1:B:133:LYS:O	1:B:150:ILE:N	2.49	0.44
1:X:170:GLN:NE2	1:X:170:GLN:HA	2.31	0.44
1:A:28:GLU:OE1	1:A:55:PRO:HB3	2.17	0.44
1:A:104:LYS:O	1:A:105:LEU:C	2.60	0.44
1:B:55:PRO:C	1:B:57:LEU:N	2.75	0.44
1:C:104:LYS:H	1:C:107:GLN:HE21	1.65	0.44
1:C:181:TRP:O	1:C:183:ASN:N	2.51	0.44
1:X:121:TRP:CZ2	2:X:305:ACO:C6P	3.00	0.44
1:Y:116:ILE:HG22	1:Y:120:VAL:HG11	1.99	0.44
1:Y:195:LYS:O	1:Y:199:ASN:N	2.49	0.44
1:Z:18:GLN:HE22	1:Z:46:PHE:N	2.04	0.44
1:Z:199:ASN:HD22	1:Z:199:ASN:HA	1.53	0.44
1:A:94:PHE:CD1	1:A:94:PHE:N	2.85	0.44
1:B:82:HIS:ND1	1:B:88:THR:O	2.42	0.44
1:X:21:LYS:N	1:X:22:PRO:CD	2.80	0.44
1:Y:129:MSE:HB3	1:Y:130:PRO:HD2	1.98	0.44
1:Z:77:MSE:C	1:Z:79:GLY:H	2.25	0.44
1:B:41:LYS:HE3	1:B:125:ASP:OD2	2.18	0.44
1:C:76:ILE:O	1:C:130:PRO:HG3	2.17	0.44
1:X:67:CYS:SG	1:X:120:VAL:HG13	2.57	0.44
1:X:175:GLN:OE1	1:X:202:ILE:HG23	2.18	0.44
1:Y:180:LYS:C	1:Y:182:TRP:H	2.26	0.44
1:Z:21:LYS:C	1:Z:23:ILE:N	2.74	0.44
1:C:104:LYS:HG3	1:C:107:GLN:CG	2.47	0.44
1:Z:129:MSE:O	1:Z:132:VAL:HG13	2.17	0.44
1:C:181:TRP:O	1:C:184:TRP:N	2.44	0.44
1:C:10:PRO:HG3	1:C:19:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:PRO:HG2	1:C:93:LEU:HD12	1.99	0.44
1:B:105:LEU:HD12	1:X:105:LEU:HD23	2.00	0.44
1:C:155:LEU:HD23	1:C:164:ILE:HB	1.99	0.44
1:C:181:TRP:C	1:C:183:ASN:N	2.74	0.44
1:Z:54:TYR:HB3	1:Z:56:ILE:HG22	1.99	0.44
1:B:1:MSE:CE	1:B:190:ASN:HB3	2.47	0.43
1:X:52:TYR:CE2	2:Y:303:ACO:S1P	3.11	0.43
1:Z:37:TYR:CE2	1:Z:68:SER:HA	2.53	0.43
1:A:115:ILE:O	1:A:133:LYS:HA	2.18	0.43
1:A:5:PRO:C	1:A:7:LYS:N	2.76	0.43
1:B:41:LYS:O	1:B:42:ASN:CG	2.61	0.43
1:C:21:LYS:O	1:C:25:GLU:N	2.51	0.43
1:X:95:GLY:O	1:X:96:ASN:C	2.61	0.43
1:X:151:ALA:HB3	1:X:154:MSE:CG	2.48	0.43
1:B:94:PHE:HB3	1:C:3:PRO:HG3	2.00	0.43
1:B:203:ARG:CG	1:B:203:ARG:NH1	2.81	0.43
1:C:198:ASP:OD1	1:C:200:SER:N	2.51	0.43
1:Z:7:LYS:HD2	1:Z:9:TYR:H	1.84	0.43
1:Z:78:ASN:ND2	1:Z:111:LYS:H	2.15	0.43
1:X:129:MSE:HB3	1:X:130:PRO:CD	2.47	0.43
1:Z:54:TYR:O	1:Z:55:PRO:C	2.62	0.43
1:Z:179:ILE:HD11	1:Z:201:ILE:HD12	2.00	0.43
1:A:52:TYR:CD1	1:A:80:ALA:CB	2.83	0.43
1:A:85:ASP:OD1	1:A:85:ASP:N	2.34	0.43
1:C:21:LYS:CB	1:C:22:PRO:CD	2.96	0.43
1:C:187:ASP:OD2	1:C:188:ILE:N	2.51	0.43
1:A:188:ILE:O	1:A:189:ILE:C	2.61	0.43
1:B:102:MSE:HG3	1:B:103:PRO:HD2	2.01	0.43
1:B:151:ALA:HB1	1:B:152:PRO:HD2	2.00	0.43
1:C:8:MSE:HE2	1:C:8:MSE:HB2	1.93	0.43
1:C:129:MSE:HE3	1:C:130:PRO:HD2	2.00	0.43
1:Z:81:ASN:HD21	1:Z:111:LYS:HZ2	1.66	0.43
1:Z:176:LEU:HA	1:Z:179:ILE:HG23	2.00	0.43
1:B:198:ASP:C	1:B:198:ASP:OD1	2.60	0.43
1:C:198:ASP:OD1	1:C:200:SER:HB2	2.18	0.43
1:X:40:SER:OG	1:X:44:GLU:OE1	2.37	0.43
1:A:142:ALA:O	1:A:143:ASN:C	2.62	0.43
1:B:52:TYR:HD1	1:B:76:ILE:HG23	1.83	0.43
1:C:78:ASN:O	1:C:80:ALA:N	2.52	0.43
1:X:173:ILE:O	1:X:174:ASN:C	2.61	0.43
1:Y:144:SER:OG	1:Y:157:GLY:HA2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:49:GLN:HB3	1:Z:73:VAL:O	2.19	0.43
1:B:83:ARG:O	1:B:88:THR:HA	2.19	0.43
1:X:193:ILE:O	1:X:197:LEU:HG	2.19	0.43
1:A:111:LYS:CD	1:A:130:PRO:HB2	2.49	0.42
1:X:47:ASP:N	1:X:47:ASP:OD1	2.50	0.42
1:X:105:LEU:HD22	1:X:105:LEU:HA	1.85	0.42
1:Y:59:ASP:OD1	1:Y:59:ASP:N	2.50	0.42
1:A:5:PRO:HA	1:A:19:PHE:CD1	2.54	0.42
1:Y:18:GLN:HE22	1:Y:46:PHE:H	1.68	0.42
1:Y:200:SER:C	1:Y:202:ILE:N	2.77	0.42
1:A:179:ILE:O	1:A:180:LYS:C	2.62	0.42
1:C:142:ALA:O	1:C:143:ASN:C	2.62	0.42
1:X:54:TYR:HA	1:X:55:PRO:HD3	1.91	0.42
1:X:193:ILE:HG21	1:Z:101:HIS:CD2	2.54	0.42
1:C:153:TYR:HB2	1:C:173:ILE:HG12	2.00	0.42
1:B:94:PHE:CE2	1:C:19:PHE:CE2	3.07	0.42
1:X:186:ILE:HA	1:X:189:ILE:HB	2.02	0.42
1:Y:18:GLN:HE22	1:Y:46:PHE:N	2.18	0.42
1:A:154:MSE:HE2	1:A:163:GLU:CD	2.44	0.42
1:Y:198:ASP:OD1	1:Y:198:ASP:C	2.62	0.42
1:A:3:PRO:HB3	1:C:94:PHE:HB3	2.00	0.42
1:A:143:ASN:N	1:A:143:ASN:HD22	2.18	0.42
1:B:159:ASN:HA	1:B:160:PRO:HA	1.89	0.42
1:X:26:LYS:HG3	1:X:27:LEU:HD23	2.00	0.42
1:X:105:LEU:O	1:X:106:ASP:C	2.63	0.42
1:X:196:ILE:CG1	1:X:201:ILE:HD13	2.49	0.42
1:Y:24:LEU:HD11	1:Y:46:PHE:HD2	1.84	0.42
1:Z:105:LEU:O	1:Z:108:LEU:N	2.51	0.42
1:Z:185:PRO:HB2	1:Z:188:ILE:HD12	2.01	0.42
1:B:7:LYS:HD3	1:B:10:PRO:HA	2.01	0.42
1:B:21:LYS:HB3	1:B:22:PRO:HD3	2.02	0.42
1:A:81:ASN:CG	1:A:111:LYS:HZ1	2.20	0.42
1:A:175:GLN:NE2	1:A:202:ILE:HB	2.33	0.42
1:C:20:ILE:HG12	1:C:36:SER:O	2.20	0.42
1:Y:25:GLU:OE1	1:Y:25:GLU:CA	2.67	0.42
1:Z:7:LYS:HD2	1:Z:7:LYS:C	2.45	0.42
1:Z:137:GLY:O	1:Z:153:TYR:HA	2.20	0.42
1:Y:162:ASN:O	1:Y:163:GLU:C	2.63	0.41
1:Z:175:GLN:O	1:Z:179:ILE:HG22	2.20	0.41
1:A:113:ASP:O	1:A:131:GLY:HA2	2.19	0.41
1:A:170:GLN:O	1:A:173:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:HG12	1:B:150:ILE:CD1	2.50	0.41
1:X:83:ARG:HG2	1:X:85:ASP:OD1	2.21	0.41
1:X:87:SER:HB3	1:Y:197:LEU:HD23	2.03	0.41
1:A:9:TYR:CE1	1:A:15:LYS:HD2	2.56	0.41
1:B:23:ILE:HG22	1:B:24:LEU:HD23	2.02	0.41
1:C:175:GLN:O	1:C:178:ASP:N	2.52	0.41
1:A:99:GLU:H	1:A:99:GLU:CD	2.27	0.41
1:Y:78:ASN:OD1	1:Y:111:LYS:CB	2.68	0.41
1:Z:77:MSE:C	1:Z:79:GLY:N	2.78	0.41
1:Z:164:ILE:HG21	2:Z:304:ACO:O4B	2.20	0.41
1:A:111:LYS:HZ3	2:B:300:ACO:CAP	2.33	0.41
1:Y:121:TRP:HB3	1:Y:139:ILE:HG12	2.02	0.41
1:C:12:GLU:CD	1:C:12:GLU:N	2.75	0.41
1:A:76:ILE:O	1:A:130:PRO:CG	2.68	0.41
1:Y:21:LYS:HA	1:Y:32:VAL:HG23	2.03	0.41
1:Y:34:GLU:CG	1:Y:65:LYS:HZ1	2.34	0.41
1:Y:104:LYS:O	1:Y:105:LEU:C	2.64	0.41
1:Z:8:MSE:HE3	1:Z:23:ILE:HG12	2.03	0.41
1:B:47:ASP:CG	1:B:48:LYS:NZ	2.76	0.41
1:B:51:LEU:HB2	1:B:76:ILE:CD1	2.45	0.41
1:B:63:ILE:HD13	1:B:116:ILE:HD12	2.03	0.41
1:B:193:ILE:O	1:B:194:ASP:C	2.64	0.41
1:B:199:ASN:O	1:B:202:ILE:HG12	2.20	0.41
1:C:78:ASN:C	1:C:80:ALA:H	2.27	0.41
1:C:181:TRP:O	1:C:182:TRP:C	2.63	0.41
1:Y:73:VAL:HG21	1:Y:122:ILE:HG22	2.03	0.41
1:Y:130:PRO:O	1:Y:131:GLY:C	2.63	0.41
1:Y:200:SER:O	1:Y:202:ILE:N	2.49	0.41
1:A:193:ILE:O	1:A:196:ILE:N	2.53	0.41
1:B:169:ASP:OD2	1:B:170:GLN:N	2.54	0.41
1:X:43:GLY:O	1:X:44:GLU:C	2.61	0.41
1:X:104:LYS:N	1:X:107:GLN:HE21	2.14	0.41
1:Y:105:LEU:C	1:Y:107:GLN:H	2.29	0.41
1:Z:172:THR:O	1:Z:173:ILE:C	2.63	0.41
1:A:128:ILE:CG2	1:A:132:VAL:HG21	2.51	0.40
1:A:137:GLY:O	1:A:138:ALA:O	2.39	0.40
1:X:115:ILE:O	1:X:133:LYS:HA	2.21	0.40
1:Y:54:TYR:CE2	1:Y:79:GLY:HA3	2.56	0.40
1:A:198:ASP:C	1:A:200:SER:N	2.79	0.40
1:Z:123:GLY:O	1:Z:126:VAL:HG23	2.21	0.40
1:A:8:MSE:O	1:A:18:GLN:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:41:LYS:N	1:X:44:GLU:OE2	2.51	0.40
1:Y:44:GLU:O	1:Y:44:GLU:HG2	2.21	0.40
1:Z:56:ILE:HG23	1:Z:57:LEU:CD2	2.50	0.40
2:X:305:ACO:S1P	1:Z:80:ALA:HA	2.62	0.40
1:Y:34:GLU:CD	1:Y:34:GLU:H	2.30	0.40
1:Y:40:SER:C	1:Y:42:ASN:N	2.78	0.40
1:Z:51:LEU:CB	1:Z:52:TYR:CD1	3.04	0.40
1:Z:58:ASN:O	1:Z:58:ASN:OD1	2.40	0.40
1:A:137:GLY:O	1:A:138:ALA:C	2.65	0.40
1:C:21:LYS:HA	1:C:32:VAL:HB	2.03	0.40
1:C:36:SER:OG	1:C:67:CYS:N	2.54	0.40
1:C:41:LYS:HB2	1:C:71:PRO:HB2	2.03	0.40
1:C:154:MSE:SE	1:C:166:GLN:HG2	2.71	0.40
1:X:89:TYR:HA	1:X:90:PRO:HD3	1.83	0.40
1:X:108:LEU:CD2	1:X:109:PRO:HD3	2.52	0.40
1:Y:119:ASP:O	1:Y:137:GLY:HA2	2.21	0.40
1:Y:129:MSE:HE3	1:Y:130:PRO:HD3	2.03	0.40
1:Y:152:PRO:O	1:Y:153:TYR:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	201/209 (96%)	180 (90%)	16 (8%)	5 (2%)	4	23
1	B	201/209 (96%)	174 (87%)	24 (12%)	3 (2%)	8	35
1	C	200/209 (96%)	173 (86%)	25 (12%)	2 (1%)	12	45
1	X	201/209 (96%)	178 (89%)	18 (9%)	5 (2%)	4	23
1	Y	196/209 (94%)	164 (84%)	26 (13%)	6 (3%)	3	19
1	Z	195/209 (93%)	171 (88%)	20 (10%)	4 (2%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1194/1254 (95%)	1040 (87%)	129 (11%)	25 (2%)	5	27

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	15	LYS
1	Z	93	LEU
1	Z	201	ILE
1	B	56	ILE
1	C	105	LEU
1	C	201	ILE
1	X	101	HIS
1	Y	15	LYS
1	Y	79	GLY
1	Y	201	ILE
1	A	41	LYS
1	A	199	ASN
1	B	169	ASP
1	X	124	LYS
1	Z	22	PRO
1	Z	78	ASN
1	A	138	ALA
1	X	173	ILE
1	A	78	ASN
1	B	55	PRO
1	X	90	PRO
1	Y	8	MSE
1	A	185	PRO
1	Y	5	PRO
1	Y	131	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/175 (97%)	147 (87%)	22 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	167/175 (95%)	143 (86%)	24 (14%)	3	15
1	C	165/175 (94%)	136 (82%)	29 (18%)	2	10
1	X	167/175 (95%)	148 (89%)	19 (11%)	5	24
1	Y	165/175 (94%)	138 (84%)	27 (16%)	2	12
1	Z	167/175 (95%)	134 (80%)	33 (20%)	1	8
All	All	1000/1050 (95%)	846 (85%)	154 (15%)	2	13

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MSE
1	A	21	LYS
1	A	24	LEU
1	A	34	GLU
1	A	40	SER
1	A	41	LYS
1	A	56	ILE
1	A	74	THR
1	A	75	ILE
1	A	77	MSE
1	A	85	ASP
1	A	93	LEU
1	A	106	ASP
1	A	122	ILE
1	A	124	LYS
1	A	128	ILE
1	A	143	ASN
1	A	148	LYS
1	A	170	GLN
1	A	179	ILE
1	A	180	LYS
1	A	189	ILE
1	B	1	MSE
1	B	15	LYS
1	B	16	SER
1	B	23	ILE
1	B	40	SER
1	B	56	ILE
1	B	57	LEU
1	B	58	ASN

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Mol	Chain	Res	Type
1	B	63	ILE
1	B	65	LYS
1	B	74	THR
1	B	100	LYS
1	B	105	LEU
1	B	107	GLN
1	B	111	LYS
1	B	115	ILE
1	B	120	VAL
1	B	155	LEU
1	B	169	ASP
1	B	170	GLN
1	B	178	ASP
1	B	179	ILE
1	B	193	ILE
1	B	203	ARG
1	C	1	MSE
1	C	7	LYS
1	C	8	MSE
1	C	12	GLU
1	C	14	ASN
1	C	16	SER
1	C	25	GLU
1	C	27	LEU
1	C	34	GLU
1	C	40	SER
1	C	45	THR
1	C	48	LYS
1	C	60	LYS
1	C	65	LYS
1	C	107	GLN
1	C	110	ILE
1	C	128	ILE
1	C	132	VAL
1	C	133	LYS
1	C	144	SER
1	C	163	GLU
1	C	165	LYS
1	C	169	ASP
1	C	170	GLN
1	C	179	ILE
1	C	187	ASP

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Mol	Chain	Res	Type
1	C	193	ILE
1	C	198	ASP
1	C	201	ILE
1	X	1	MSE
1	X	16	SER
1	X	41	LYS
1	X	48	LYS
1	X	50	ILE
1	X	63	ILE
1	X	93	LEU
1	X	105	LEU
1	X	107	GLN
1	X	114	THR
1	X	120	VAL
1	X	124	LYS
1	X	132	VAL
1	X	159	ASN
1	X	170	GLN
1	X	172	THR
1	X	179	ILE
1	X	199	ASN
1	X	201	ILE
1	Y	7	LYS
1	Y	15	LYS
1	Y	16	SER
1	Y	20	ILE
1	Y	25	GLU
1	Y	31	GLU
1	Y	32	VAL
1	Y	34	GLU
1	Y	40	SER
1	Y	56	ILE
1	Y	84	MSE
1	Y	99	GLU
1	Y	102	MSE
1	Y	105	LEU
1	Y	106	ASP
1	Y	108	LEU
1	Y	110	ILE
1	Y	113	ASP
1	Y	115	ILE
1	Y	120	VAL

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Mol	Chain	Res	Type
1	Y	144	SER
1	Y	147	VAL
1	Y	155	LEU
1	Y	162	ASN
1	Y	173	ILE
1	Y	180	LYS
1	Y	187	ASP
1	Z	6	MSE
1	Z	7	LYS
1	Z	8	MSE
1	Z	16	SER
1	Z	21	LYS
1	Z	23	ILE
1	Z	27	LEU
1	Z	28	GLU
1	Z	31	GLU
1	Z	39	ASP
1	Z	41	LYS
1	Z	48	LYS
1	Z	60	LYS
1	Z	77	MSE
1	Z	92	ASN
1	Z	93	LEU
1	Z	110	ILE
1	Z	113	ASP
1	Z	120	VAL
1	Z	132	VAL
1	Z	133	LYS
1	Z	140	VAL
1	Z	155	LEU
1	Z	162	ASN
1	Z	165	LYS
1	Z	170	GLN
1	Z	175	GLN
1	Z	179	ILE
1	Z	187	ASP
1	Z	193	ILE
1	Z	196	ILE
1	Z	199	ASN
1	Z	200	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	118	ASN
1	A	143	ASN
1	A	162	ASN
1	A	166	GLN
1	A	170	GLN
1	A	174	ASN
1	A	175	GLN
1	B	58	ASN
1	B	81	ASN
1	B	107	GLN
1	B	118	ASN
1	B	143	ASN
1	B	159	ASN
1	B	162	ASN
1	B	166	GLN
1	B	170	GLN
1	B	190	ASN
1	C	18	GLN
1	C	49	GLN
1	C	53	HIS
1	C	78	ASN
1	C	107	GLN
1	C	118	ASN
1	C	162	ASN
1	C	166	GLN
1	C	170	GLN
1	X	14	ASN
1	X	18	GLN
1	X	78	ASN
1	X	107	GLN
1	X	118	ASN
1	X	159	ASN
1	X	199	ASN
1	Y	18	GLN
1	Y	96	ASN
1	Y	107	GLN
1	Y	118	ASN
1	Y	159	ASN
1	Y	162	ASN
1	Y	166	GLN
1	Y	170	GLN
1	Y	183	ASN

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Mol	Chain	Res	Type
1	Y	192	ASN
1	Y	199	ASN
1	Z	18	GLN
1	Z	78	ASN
1	Z	81	ASN
1	Z	107	GLN
1	Z	118	ASN
1	Z	170	GLN
1	Z	199	ASN

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](#)

6 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	301	-	51,53,53	1.84	10 (19%)	73,79,79	2.30	17 (23%)
2	ACO	Y	303	-	51,53,53	1.73	11 (21%)	73,79,79	2.11	14 (19%)
2	ACO	A	302	-	51,53,53	1.78	10 (19%)	73,79,79	2.08	17 (23%)
2	ACO	X	305	-	51,53,53	1.93	9 (17%)	73,79,79	2.24	17 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACO	B	300	-	51,53,53	1.89	10 (19%)	73,79,79	2.06	16 (21%)
2	ACO	Z	304	-	47,49,53	1.98	9 (19%)	69,74,79	2.07	14 (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
2	ACO	B	301	-	-	12/51/67/67	0/3/3/3
2	ACO	Y	303	-	-	13/51/67/67	0/3/3/3
2	ACO	A	302	-	-	23/51/67/67	0/3/3/3
2	ACO	X	305	-	-	11/51/67/67	0/3/3/3
2	ACO	B	300	-	-	14/51/67/67	0/3/3/3
2	ACO	Z	304	-	-	12/47/63/67	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	304	ACO	P1A-O3A	-7.22	1.51	1.59
2	Z	304	ACO	P2A-O3A	-7.20	1.51	1.59
2	X	305	ACO	P2A-O3A	-6.97	1.52	1.59
2	B	301	ACO	P2A-O3A	-6.95	1.52	1.59
2	B	300	ACO	P2A-O3A	-6.94	1.52	1.59
2	X	305	ACO	P1A-O3A	-6.90	1.52	1.59
2	B	300	ACO	P1A-O3A	-6.39	1.52	1.59
2	B	301	ACO	P1A-O3A	-6.32	1.52	1.59
2	A	302	ACO	P2A-O3A	-6.13	1.52	1.59
2	Y	303	ACO	P1A-O3A	-5.82	1.53	1.59
2	A	302	ACO	P1A-O3A	-5.50	1.53	1.59
2	Y	303	ACO	P3B-O3B	-5.16	1.50	1.59
2	B	300	ACO	P3B-O3B	-4.90	1.50	1.59
2	Y	303	ACO	P2A-O3A	-4.89	1.54	1.59
2	A	302	ACO	P3B-O3B	-4.85	1.51	1.59
2	X	305	ACO	P3B-O3B	-4.56	1.51	1.59
2	Z	304	ACO	P3B-O3B	-4.55	1.51	1.59
2	B	301	ACO	P3B-O3B	-4.37	1.51	1.59
2	X	305	ACO	C5A-N7A	-4.10	1.31	1.39
2	B	300	ACO	C5A-N7A	-3.51	1.32	1.39
2	A	302	ACO	C5A-N7A	-3.41	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	304	ACO	C5A-N7A	-3.33	1.33	1.39
2	B	301	ACO	C5A-N7A	-3.31	1.33	1.39
2	Y	303	ACO	C5A-N7A	-3.23	1.33	1.39
2	A	302	ACO	C4A-N9A	-2.80	1.31	1.37
2	A	302	ACO	C-S1P	-2.70	1.60	1.75
2	X	305	ACO	C-S1P	-2.59	1.61	1.75
2	B	301	ACO	C5A-C4A	2.51	1.43	1.39
2	Y	303	ACO	C4A-N9A	-2.51	1.32	1.37
2	B	301	ACO	C-S1P	-2.46	1.61	1.75
2	B	300	ACO	C-S1P	-2.45	1.61	1.75
2	Z	304	ACO	C8A-N7A	2.44	1.36	1.31
2	Y	303	ACO	C5A-C4A	2.44	1.43	1.39
2	Y	303	ACO	C2B-C3B	-2.43	1.47	1.53
2	Z	304	ACO	C4A-N9A	-2.40	1.32	1.37
2	Z	304	ACO	C5A-C4A	2.39	1.43	1.39
2	Y	303	ACO	C-S1P	-2.38	1.62	1.75
2	A	302	ACO	C5A-C4A	2.34	1.43	1.39
2	B	300	ACO	C4A-N9A	-2.33	1.32	1.37
2	B	301	ACO	C4A-N9A	-2.33	1.32	1.37
2	X	305	ACO	C5A-C4A	2.30	1.43	1.39
2	X	305	ACO	C2B-C3B	-2.29	1.48	1.53
2	Z	304	ACO	P1A-O5B	-2.25	1.50	1.59
2	B	301	ACO	C5A-C6A	2.25	1.47	1.41
2	Y	303	ACO	C5A-C6A	2.25	1.47	1.41
2	X	305	ACO	C4A-N9A	-2.24	1.33	1.37
2	A	302	ACO	C2B-C3B	-2.23	1.48	1.53
2	A	302	ACO	C8A-N7A	2.18	1.35	1.31
2	Y	303	ACO	C8A-N7A	2.18	1.35	1.31
2	B	300	ACO	P1A-O5B	-2.17	1.50	1.59
2	Z	304	ACO	P2A-O6A	-2.16	1.50	1.59
2	B	300	ACO	C8A-N7A	2.15	1.35	1.31
2	B	301	ACO	C8A-N7A	2.12	1.35	1.31
2	B	300	ACO	C5A-C4A	2.11	1.42	1.39
2	Y	303	ACO	P1A-O5B	-2.05	1.51	1.59
2	X	305	ACO	P2A-O6A	-2.03	1.51	1.59
2	B	301	ACO	P1A-O5B	-2.03	1.51	1.59
2	A	302	ACO	P1A-O5B	-2.02	1.51	1.59
2	B	300	ACO	C5A-C6A	2.00	1.46	1.41

All (95) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	ACO	O9A-P3B-O3B	8.69	139.70	105.85
2	B	300	ACO	O9A-P3B-O3B	8.68	139.68	105.85
2	X	305	ACO	O9A-P3B-O3B	8.61	139.40	105.85
2	B	301	ACO	O9A-P3B-O3B	8.55	139.16	105.85
2	Z	304	ACO	O9A-P3B-O3B	8.51	139.01	105.85
2	Y	303	ACO	O9A-P3B-O3B	8.46	138.81	105.85
2	X	305	ACO	O3A-P1A-O1A	-7.39	88.47	110.70
2	B	301	ACO	O3A-P2A-O4A	-7.23	88.95	110.70
2	B	301	ACO	O3A-P1A-O1A	-6.15	92.19	110.70
2	X	305	ACO	C5A-C4A-N3A	-6.04	118.40	126.72
2	B	301	ACO	C5A-C4A-N3A	-6.02	118.43	126.72
2	B	300	ACO	C5A-C4A-N3A	-5.90	118.59	126.72
2	Z	304	ACO	C5A-C4A-N3A	-5.88	118.62	126.72
2	Z	304	ACO	O3A-P1A-O1A	-5.78	93.31	110.70
2	Y	303	ACO	O2A-P1A-O3A	-5.73	91.78	107.27
2	Y	303	ACO	C5A-C4A-N3A	-5.73	118.83	126.72
2	A	302	ACO	C5A-C4A-N3A	-5.63	118.96	126.72
2	B	300	ACO	O3A-P1A-O1A	-5.62	93.79	110.70
2	A	302	ACO	O3A-P2A-O4A	-5.55	94.01	110.70
2	X	305	ACO	N3A-C4A-N9A	5.47	136.47	127.17
2	B	301	ACO	N3A-C4A-N9A	5.33	136.24	127.17
2	B	300	ACO	N3A-C4A-N9A	5.15	135.92	127.17
2	Y	303	ACO	N3A-C4A-N9A	5.05	135.75	127.17
2	Z	304	ACO	N3A-C4A-N9A	5.02	135.70	127.17
2	B	301	ACO	O5B-P1A-O1A	-4.93	89.40	108.94
2	A	302	ACO	N3A-C4A-N9A	4.88	135.46	127.17
2	X	305	ACO	O5B-P1A-O1A	-4.87	89.65	108.94
2	Y	303	ACO	O2A-P1A-O5B	4.65	128.63	107.57
2	B	300	ACO	O5B-P1A-O1A	-4.23	92.16	108.94
2	Z	304	ACO	O5B-P1A-O1A	-4.22	92.21	108.94
2	B	301	ACO	O6A-P2A-O4A	-4.15	92.49	108.94
2	X	305	ACO	O5A-P2A-O3A	-4.11	96.15	107.27
2	Z	304	ACO	N3A-C2A-N1A	-3.79	122.84	128.58
2	X	305	ACO	C7P-N8P-C9P	-3.74	115.83	122.55
2	B	300	ACO	N3A-C2A-N1A	-3.74	122.92	128.58
2	X	305	ACO	N3A-C2A-N1A	-3.73	122.94	128.58
2	B	300	ACO	O5A-P2A-O3A	-3.69	97.30	107.27
2	Y	303	ACO	N3A-C2A-N1A	-3.67	123.02	128.58
2	A	302	ACO	N3A-C2A-N1A	-3.65	123.05	128.58
2	Y	303	ACO	O3A-P2A-O4A	-3.62	99.81	110.70
2	B	301	ACO	N3A-C2A-N1A	-3.61	123.12	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	304	ACO	C2A-N3A-C4A	3.54	120.47	111.83
2	B	301	ACO	C2A-N3A-C4A	3.53	120.46	111.83
2	Y	303	ACO	C2A-N3A-C4A	3.51	120.39	111.83
2	B	300	ACO	C2A-N3A-C4A	3.50	120.37	111.83
2	A	302	ACO	O6A-P2A-O4A	-3.46	95.21	108.94
2	Y	303	ACO	O9A-P3B-O7A	-3.45	97.39	110.83
2	X	305	ACO	C2A-N3A-C4A	3.44	120.23	111.83
2	A	302	ACO	C2A-N3A-C4A	3.41	120.16	111.83
2	Y	303	ACO	O3B-P3B-O7A	-3.28	97.63	109.33
2	A	302	ACO	O2A-P1A-O5B	3.26	122.33	107.57
2	Z	304	ACO	O3A-P2A-O4A	-3.25	100.94	110.70
2	A	302	ACO	O3A-P1A-O1A	-3.12	101.33	110.70
2	Y	303	ACO	C4A-N9A-C8A	3.02	108.91	105.74
2	A	302	ACO	O5B-P1A-O1A	3.01	120.86	108.94
2	A	302	ACO	O9A-P3B-O7A	-3.01	99.12	110.83
2	X	305	ACO	O9A-P3B-O7A	-2.95	99.35	110.83
2	B	300	ACO	C4A-N9A-C8A	2.95	108.83	105.74
2	B	301	ACO	C4A-N9A-C8A	2.90	108.78	105.74
2	B	300	ACO	N9A-C8A-N7A	-2.89	109.83	113.94
2	A	302	ACO	C4A-N9A-C8A	2.86	108.74	105.74
2	B	301	ACO	O9A-P3B-O8A	-2.74	97.53	107.80
2	A	302	ACO	N9A-C8A-N7A	-2.73	110.06	113.94
2	Y	303	ACO	N9A-C8A-N7A	-2.72	110.07	113.94
2	Z	304	ACO	O9A-P3B-O7A	-2.67	100.45	110.83
2	Z	304	ACO	N9A-C8A-N7A	-2.64	110.19	113.94
2	B	301	ACO	N9A-C8A-N7A	-2.64	110.19	113.94
2	B	300	ACO	O9A-P3B-O7A	-2.56	100.85	110.83
2	Z	304	ACO	C4A-N9A-C8A	2.55	108.42	105.74
2	Z	304	ACO	O5A-P2A-O3A	-2.52	100.47	107.27
2	X	305	ACO	C4A-N9A-C8A	2.47	108.33	105.74
2	X	305	ACO	C6A-C5A-C4A	2.46	120.54	117.18
2	X	305	ACO	N9A-C8A-N7A	-2.42	110.50	113.94
2	A	302	ACO	O3B-P3B-O7A	-2.41	100.74	109.33
2	Y	303	ACO	O6A-P2A-O4A	-2.41	99.39	108.94
2	B	301	ACO	O9A-P3B-O7A	-2.40	101.48	110.83
2	B	300	ACO	O9A-P3B-O8A	-2.36	98.96	107.80
2	X	305	ACO	O3A-P2A-O4A	-2.25	103.92	110.70
2	B	300	ACO	O3A-P2A-O4A	-2.25	103.94	110.70
2	X	305	ACO	O3B-P3B-O7A	-2.23	101.39	109.33
2	X	305	ACO	C2P-S1P-C	-2.21	90.80	101.42
2	Z	304	ACO	O9A-P3B-O8A	-2.19	99.61	107.80
2	B	301	ACO	C6A-C5A-C4A	2.18	120.15	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	ACO	C6A-C5A-C4A	2.18	120.15	117.18
2	B	301	ACO	C2P-S1P-C	-2.15	91.06	101.42
2	X	305	ACO	O5A-P2A-O6A	-2.14	97.86	107.57
2	A	302	ACO	C6A-C5A-C4A	2.11	120.06	117.18
2	Z	304	ACO	O3B-P3B-O7A	-2.11	101.81	109.33
2	B	301	ACO	C3B-C2B-C1B	2.09	104.49	99.89
2	A	302	ACO	O9A-P3B-O8A	-2.06	100.08	107.80
2	B	300	ACO	O3B-P3B-O7A	-2.05	102.03	109.33
2	A	302	ACO	O2A-P1A-O3A	-2.04	101.76	107.27
2	Y	303	ACO	C2P-S1P-C	-2.02	91.69	101.42
2	B	300	ACO	C2B-C3B-C4B	2.01	106.76	103.24
2	B	301	ACO	C7P-N8P-C9P	-2.00	118.95	122.55

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	ACO	C5B-O5B-P1A-O1A
2	A	302	ACO	CCP-O6A-P2A-O4A
2	A	302	ACO	CCP-O6A-P2A-O5A
2	A	302	ACO	CDP-CBP-CCP-O6A
2	A	302	ACO	CEP-CBP-CCP-O6A
2	A	302	ACO	CAP-CBP-CCP-O6A
2	A	302	ACO	OAP-CAP-CBP-CCP
2	A	302	ACO	C9P-CAP-CBP-CCP
2	A	302	ACO	OAP-CAP-CBP-CEP
2	A	302	ACO	C9P-CAP-CBP-CEP
2	B	300	ACO	C5B-O5B-P1A-O3A
2	B	300	ACO	CCP-O6A-P2A-O3A
2	B	300	ACO	CCP-O6A-P2A-O5A
2	B	300	ACO	CDP-CBP-CCP-O6A
2	B	300	ACO	CEP-CBP-CCP-O6A
2	B	300	ACO	CAP-CBP-CCP-O6A
2	B	301	ACO	CCP-O6A-P2A-O5A
2	B	301	ACO	CAP-C9P-N8P-C7P
2	B	301	ACO	C3P-C2P-S1P-C
2	B	301	ACO	O-C-S1P-C2P
2	B	301	ACO	CH3-C-S1P-C2P
2	X	305	ACO	CAP-C9P-N8P-C7P
2	Y	303	ACO	C5B-O5B-P1A-O3A
2	Y	303	ACO	S1P-C2P-C3P-N4P
2	Z	304	ACO	C5B-O5B-P1A-O1A

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Mol	Chain	Res	Type	Atoms
2	Z	304	ACO	CCP-O6A-P2A-O3A
2	Z	304	ACO	CCP-O6A-P2A-O4A
2	Z	304	ACO	CCP-O6A-P2A-O5A
2	Z	304	ACO	CDP-CBP-CCP-O6A
2	Z	304	ACO	CEP-CBP-CCP-O6A
2	Z	304	ACO	CAP-CBP-CCP-O6A
2	Y	303	ACO	O4B-C4B-C5B-O5B
2	B	300	ACO	C4B-C3B-O3B-P3B
2	B	301	ACO	C4B-C3B-O3B-P3B
2	X	305	ACO	C4B-C3B-O3B-P3B
2	X	305	ACO	O9P-C9P-N8P-C7P
2	A	302	ACO	C4B-C3B-O3B-P3B
2	Y	303	ACO	C4B-C3B-O3B-P3B
2	Y	303	ACO	C6P-C5P-N4P-C3P
2	Y	303	ACO	C3B-C4B-C5B-O5B
2	B	300	ACO	C2B-C3B-O3B-P3B
2	A	302	ACO	O-C-S1P-C2P
2	A	302	ACO	CH3-C-S1P-C2P
2	Y	303	ACO	O5P-C5P-N4P-C3P
2	A	302	ACO	C6P-C5P-N4P-C3P
2	A	302	ACO	O5P-C5P-N4P-C3P
2	A	302	ACO	OAP-CAP-CBP-CDP
2	X	305	ACO	P1A-O3A-P2A-O4A
2	B	301	ACO	S1P-C2P-C3P-N4P
2	B	300	ACO	P1A-O3A-P2A-O6A
2	X	305	ACO	P1A-O3A-P2A-O6A
2	Z	304	ACO	P1A-O3A-P2A-O6A
2	B	300	ACO	P2A-O3A-P1A-O1A
2	B	301	ACO	P2A-O3A-P1A-O2A
2	Y	303	ACO	C3P-C2P-S1P-C
2	X	305	ACO	C2B-C3B-O3B-P3B
2	X	305	ACO	O-C-S1P-C2P
2	B	301	ACO	O9P-C9P-N8P-C7P
2	A	302	ACO	CCP-O6A-P2A-O3A
2	B	300	ACO	CCP-O6A-P2A-O4A
2	B	301	ACO	C5B-O5B-P1A-O1A
2	B	301	ACO	C5B-O5B-P1A-O3A
2	X	305	ACO	C5B-O5B-P1A-O3A
2	Y	303	ACO	C5B-O5B-P1A-O1A
2	Z	304	ACO	C5B-O5B-P1A-O3A
2	A	302	ACO	C2B-C3B-O3B-P3B
2	Y	303	ACO	C2B-C3B-O3B-P3B

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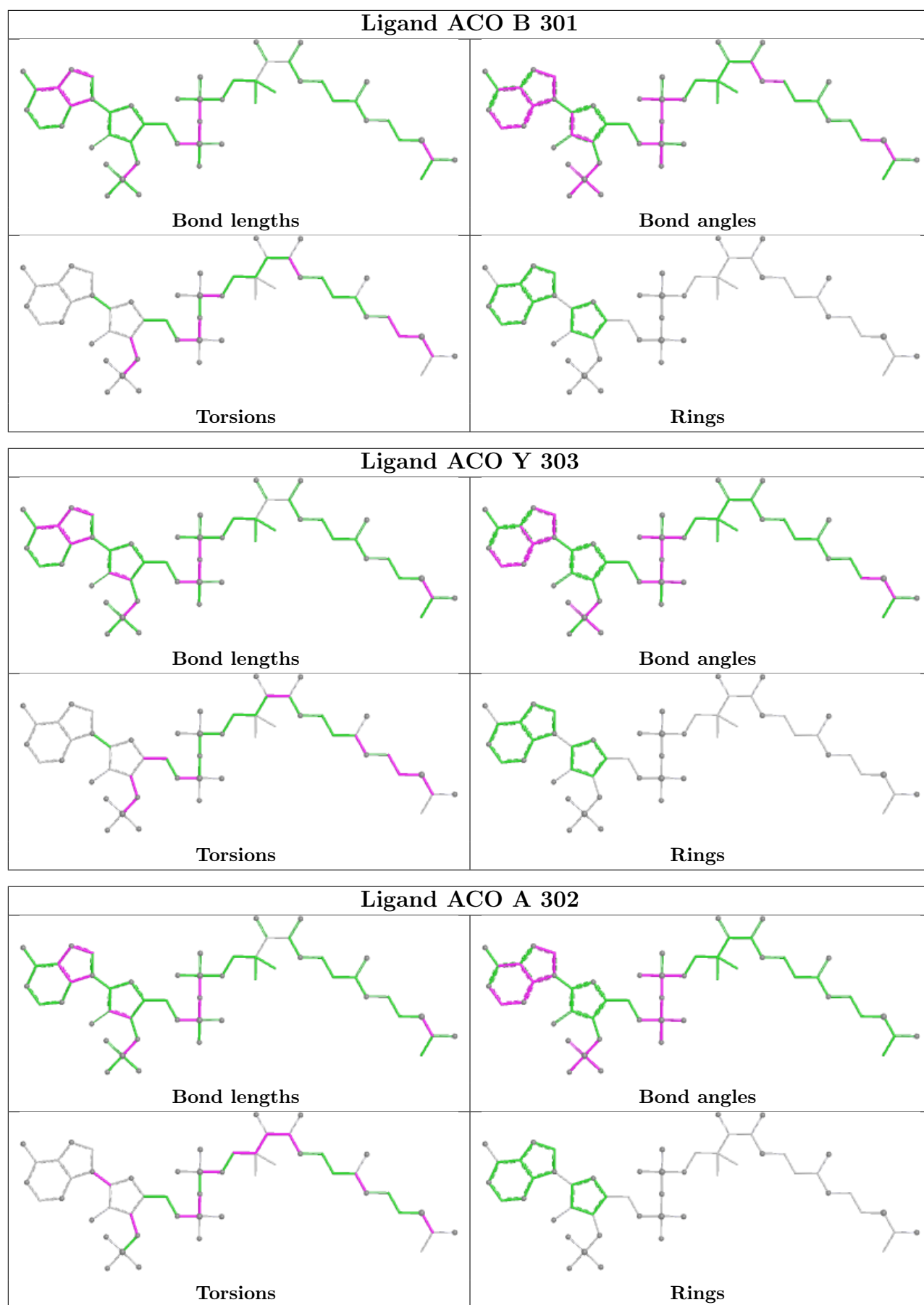
Mol	Chain	Res	Type	Atoms
2	Z	304	ACO	C5P-C6P-C7P-N8P
2	Z	304	ACO	P1A-O3A-P2A-O4A
2	B	301	ACO	C3B-O3B-P3B-O8A
2	Y	303	ACO	O-C-S1P-C2P
2	B	300	ACO	C2P-C3P-N4P-C5P
2	B	300	ACO	O9P-C9P-CAP-OAP
2	A	302	ACO	CAP-C9P-N8P-C7P
2	Y	303	ACO	C3B-O3B-P3B-O7A
2	X	305	ACO	CH3-C-S1P-C2P
2	A	302	ACO	C9P-CAP-CBP-CDP
2	A	302	ACO	P2A-O3A-P1A-O2A
2	A	302	ACO	C2B-C1B-N9A-C8A
2	X	305	ACO	C3B-O3B-P3B-O7A
2	A	302	ACO	N8P-C9P-CAP-OAP
2	B	300	ACO	N8P-C9P-CAP-OAP
2	X	305	ACO	N8P-C9P-CAP-OAP
2	Y	303	ACO	N8P-C9P-CAP-OAP
2	Z	304	ACO	N8P-C9P-CAP-OAP

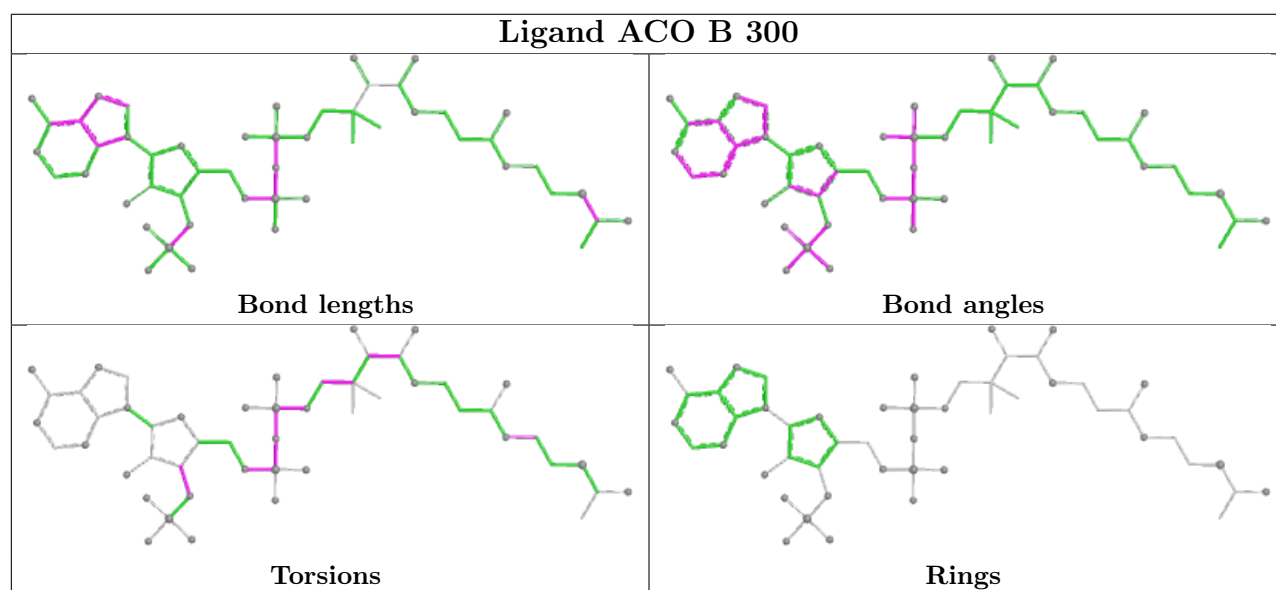
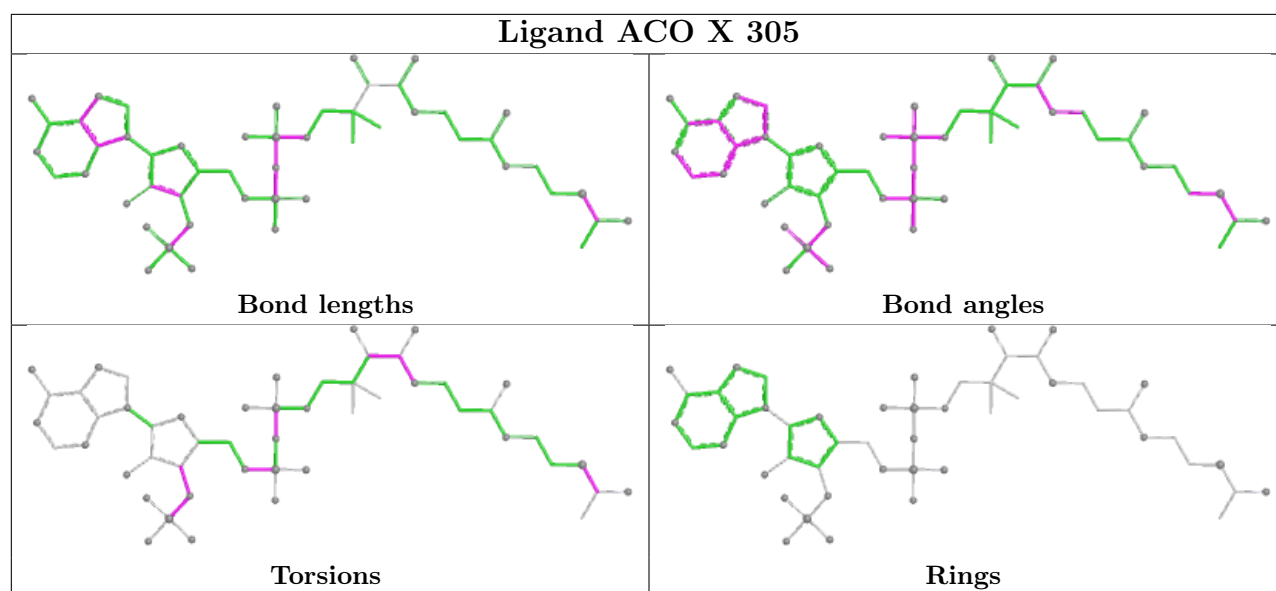
There are no ring outliers.

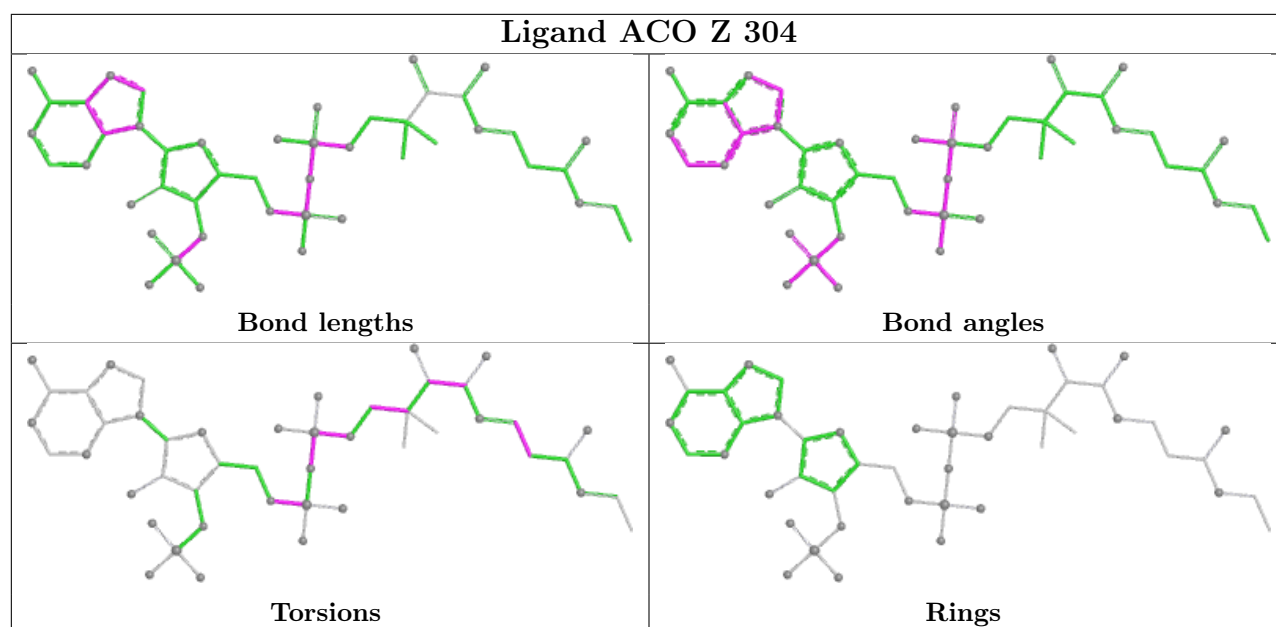
6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	ACO	4	0
2	Y	303	ACO	2	0
2	A	302	ACO	3	0
2	X	305	ACO	5	0
2	B	300	ACO	4	0
2	Z	304	ACO	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	195/209 (93%)	0.23	3 (1%)	72 49	66, 66, 66, 66	0
1	B	195/209 (93%)	0.46	5 (2%)	57 34	66, 66, 66, 66	0
1	C	194/209 (92%)	0.39	1 (0%)	87 72	66, 66, 66, 66	0
1	X	195/209 (93%)	0.24	5 (2%)	57 34	66, 66, 66, 66	0
1	Y	193/209 (92%)	0.54	4 (2%)	63 40	66, 66, 66, 66	0
1	Z	192/209 (91%)	0.48	6 (3%)	51 30	66, 66, 66, 66	0
All	All	1164/1254 (92%)	0.39	24 (2%)	63 40	66, 66, 66, 66	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	14	ASN	3.2
1	Y	39	ASP	3.1
1	X	39	ASP	3.0
1	B	85	ASP	2.8
1	B	170	GLN	2.8
1	X	42	ASN	2.8
1	Y	109	PRO	2.8
1	Y	192	ASN	2.6
1	Y	56	ILE	2.6
1	Z	109	PRO	2.4
1	A	109	PRO	2.2
1	B	105	LEU	2.2
1	X	113	ASP	2.2
1	A	173	ILE	2.1
1	X	33	GLY	2.1
1	Z	42	ASN	2.1
1	B	39	ASP	2.1
1	C	109	PRO	2.1
1	A	2	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	Z	3	PRO	2.0
1	X	191	GLU	2.0
1	Z	143	ASN	2.0
1	Z	125	ASP	2.0
1	B	131	GLY	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](#)

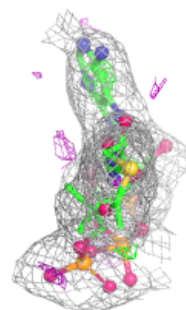
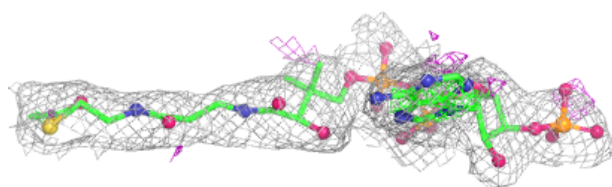
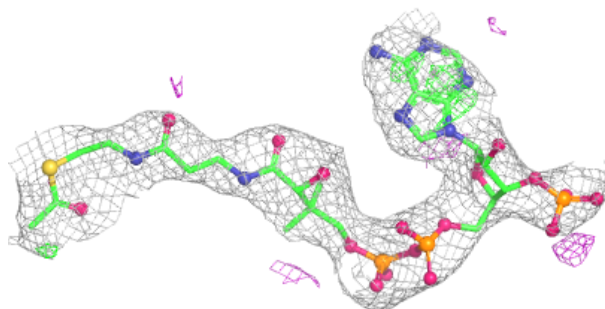
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	ACO	Y	303	51/51	0.81	0.16	65,65,65,65	0
2	ACO	B	301	51/51	0.83	0.14	65,65,65,65	0
2	ACO	X	305	51/51	0.83	0.14	65,65,65,65	0
2	ACO	A	302	51/51	0.83	0.13	65,65,65,65	0
2	ACO	B	300	51/51	0.86	0.12	65,65,65,65	0
2	ACO	Z	304	47/51	0.87	0.14	65,65,65,65	0

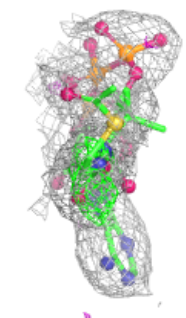
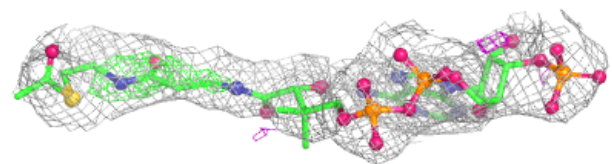
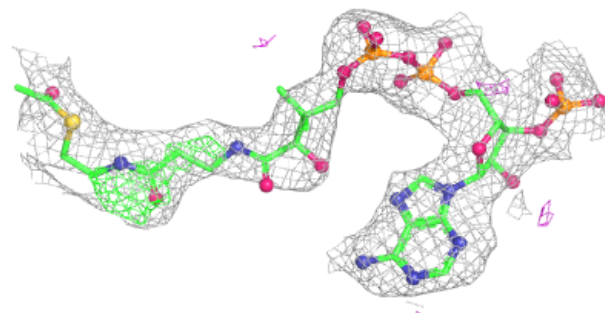
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO Y 303:

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

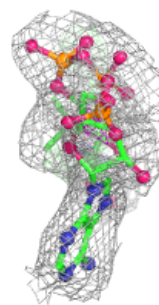
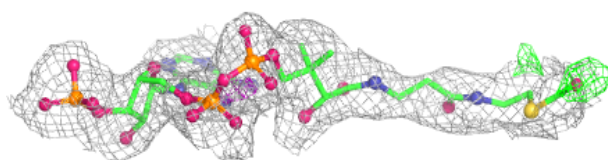
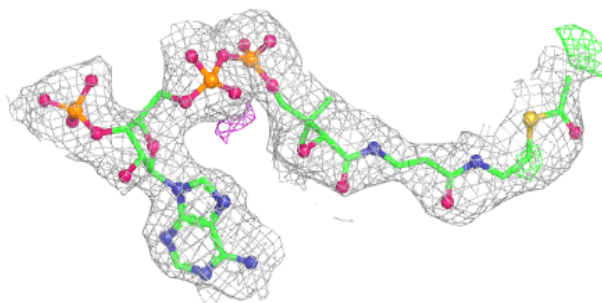
**Electron density around ACO B 301:**

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

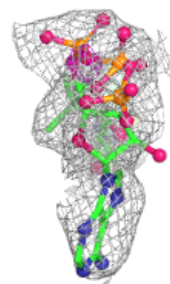
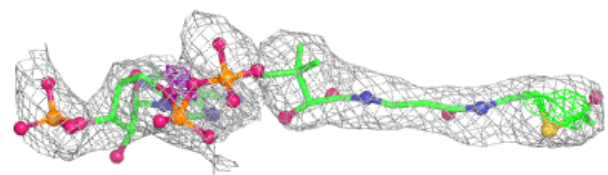
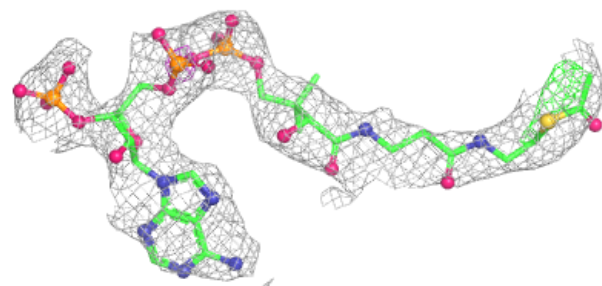


Electron density around ACO X 305:

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

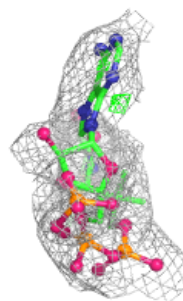
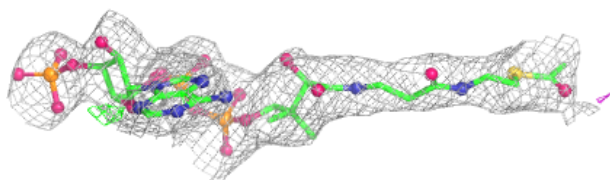
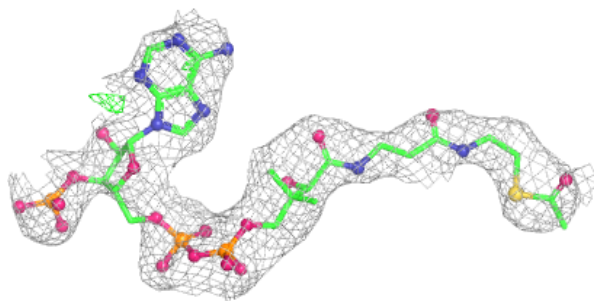
**Electron density around ACO A 302:**

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

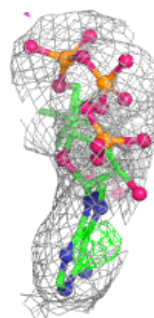
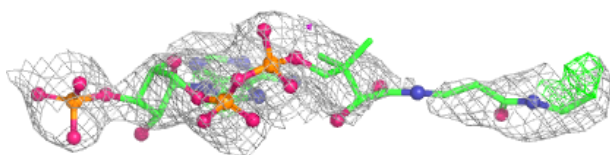
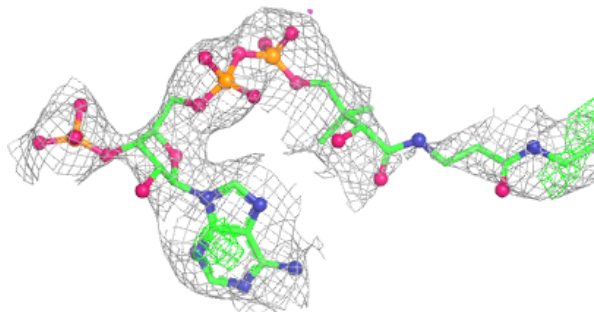


Electron density around ACO B 300:

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

**Electron density around ACO Z 304:**

$2mF_o-DF_c$ (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.