Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 11:15 PM EDT

PDB ID	:	3HO8
Title	:	Crystal Structure of S. aureus Pyruvate Carboxylase in complex with Coenzyme A
Authors	:	Tong, L.; Yu, L.P.C.
Deposited on	:	2009-06-01
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

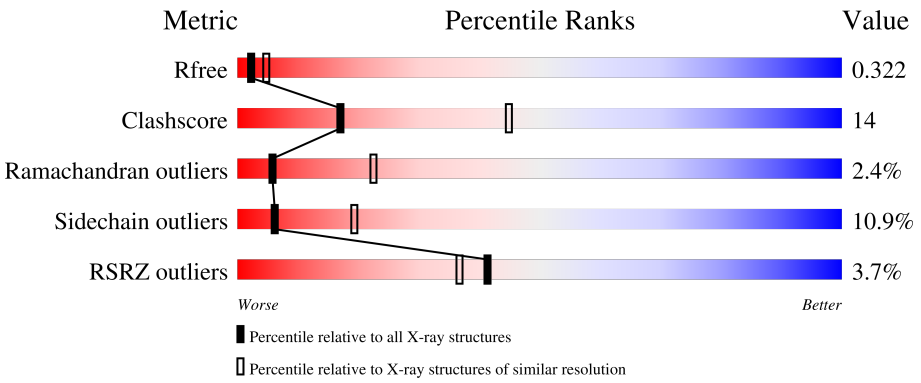
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	1150	4% 57% 26% • 14%
1	B	1150	% 52% 29% 5% 14%
1	C	1150	2% 56% 26% • 13%
1	D	1150	6% 54% 23% • 19%

2 Entry composition (i)

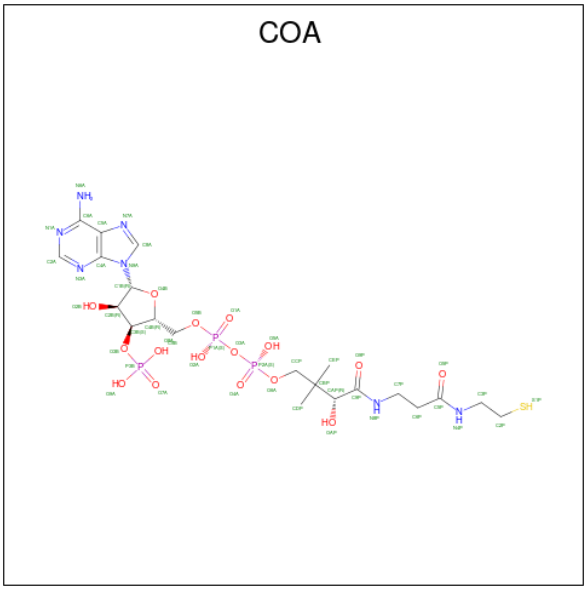
There are 4 unique types of molecules in this entry. The entry contains 31229 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	994	7880	5000	1329	1525	26	0	0	0
1	D	934	7396	4696	1250	1426	24	0	0	0
1	C	995	7889	5005	1330	1528	26	0	0	0
1	B	989	7838	4975	1321	1516	26	0	0	0

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	48	21	7	16	3	1	0	0
2	D	1	48	21	7	16	3	1	0	0

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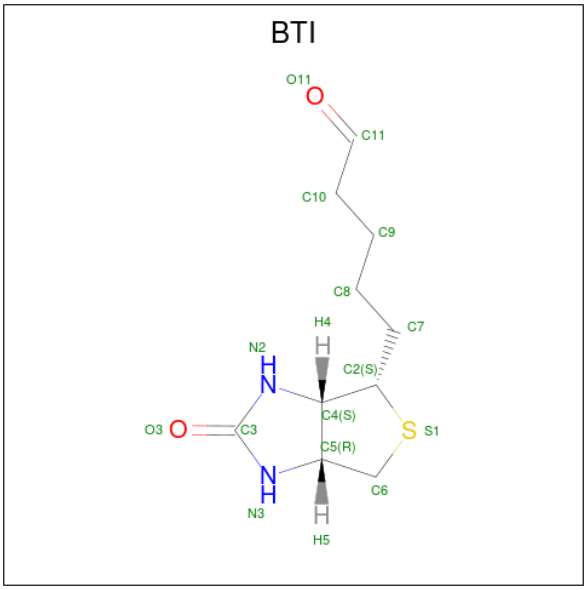
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	C	1	48	21	7	16	3	1	0	0
			Total	C	N	O	P	S		
2	B	1	48	21	7	16	3	1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	1	1	1	0	0
			Total	Mn		
3	D	1	1	1	0	0
			Total	Mn		
3	C	1	1	1	0	0
			Total	Mn		
3	B	1	1	1	0	0

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: $C_{10}H_{16}N_2O_2S$).



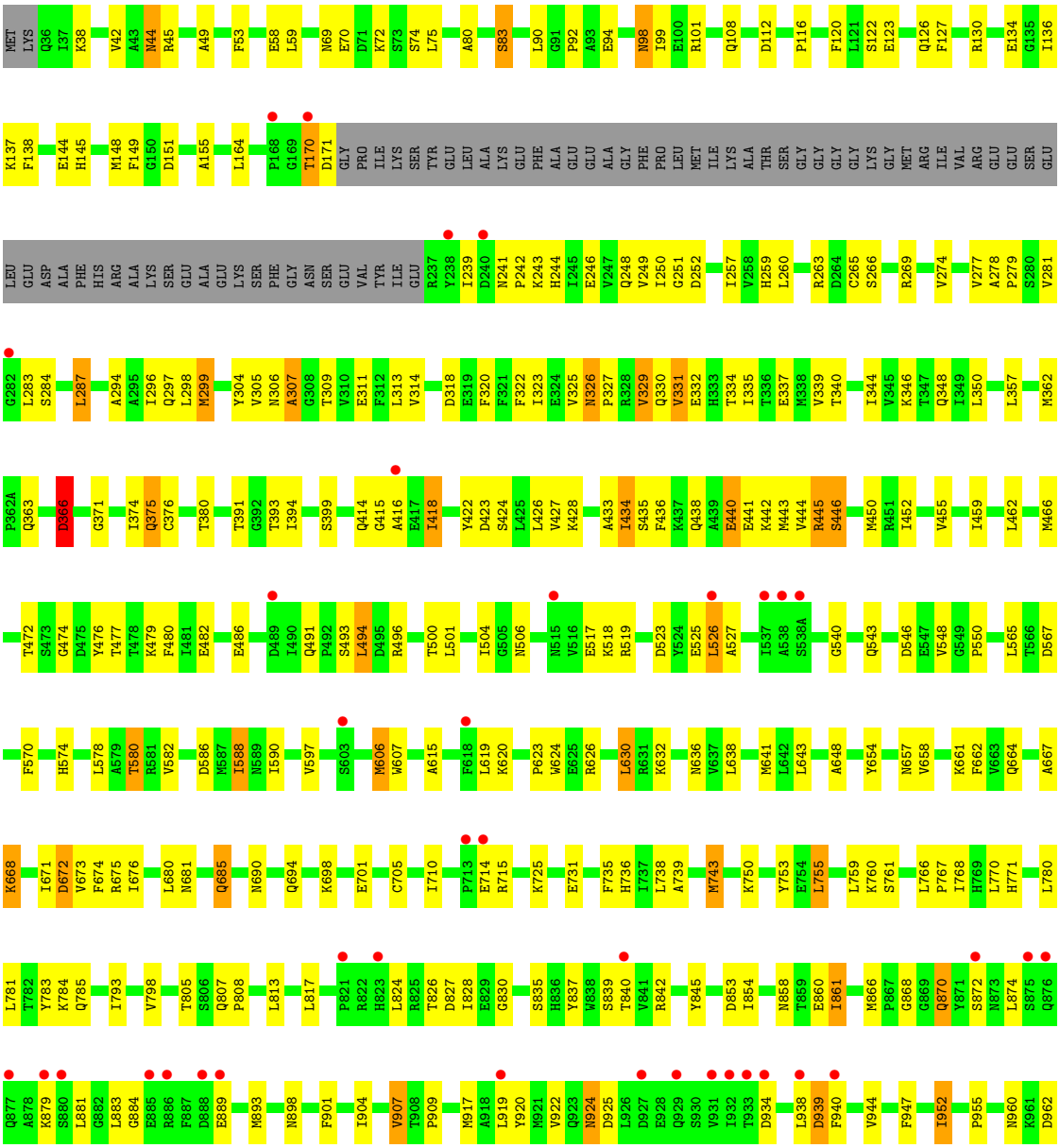
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	C	1	15	10	2	2	1	0	0
			Total	C	N	O	S		
4	B	1	15	10	2	2	1	0	0

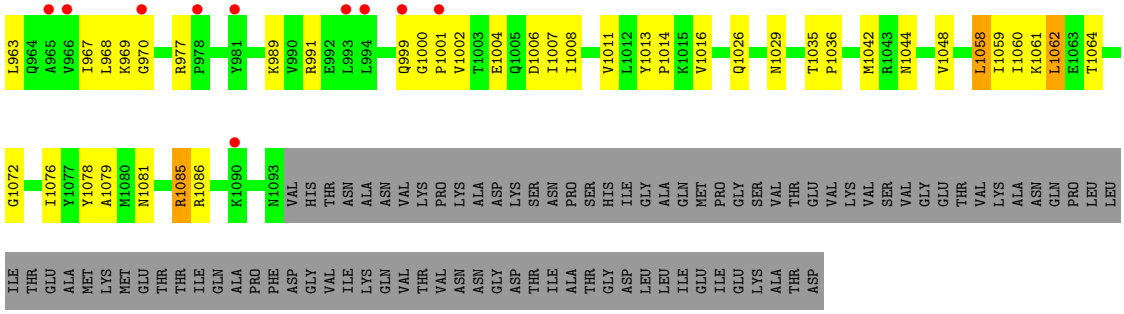
3 Residue-property plots (i)

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

- Molecule 1: Pyruvate carboxylase

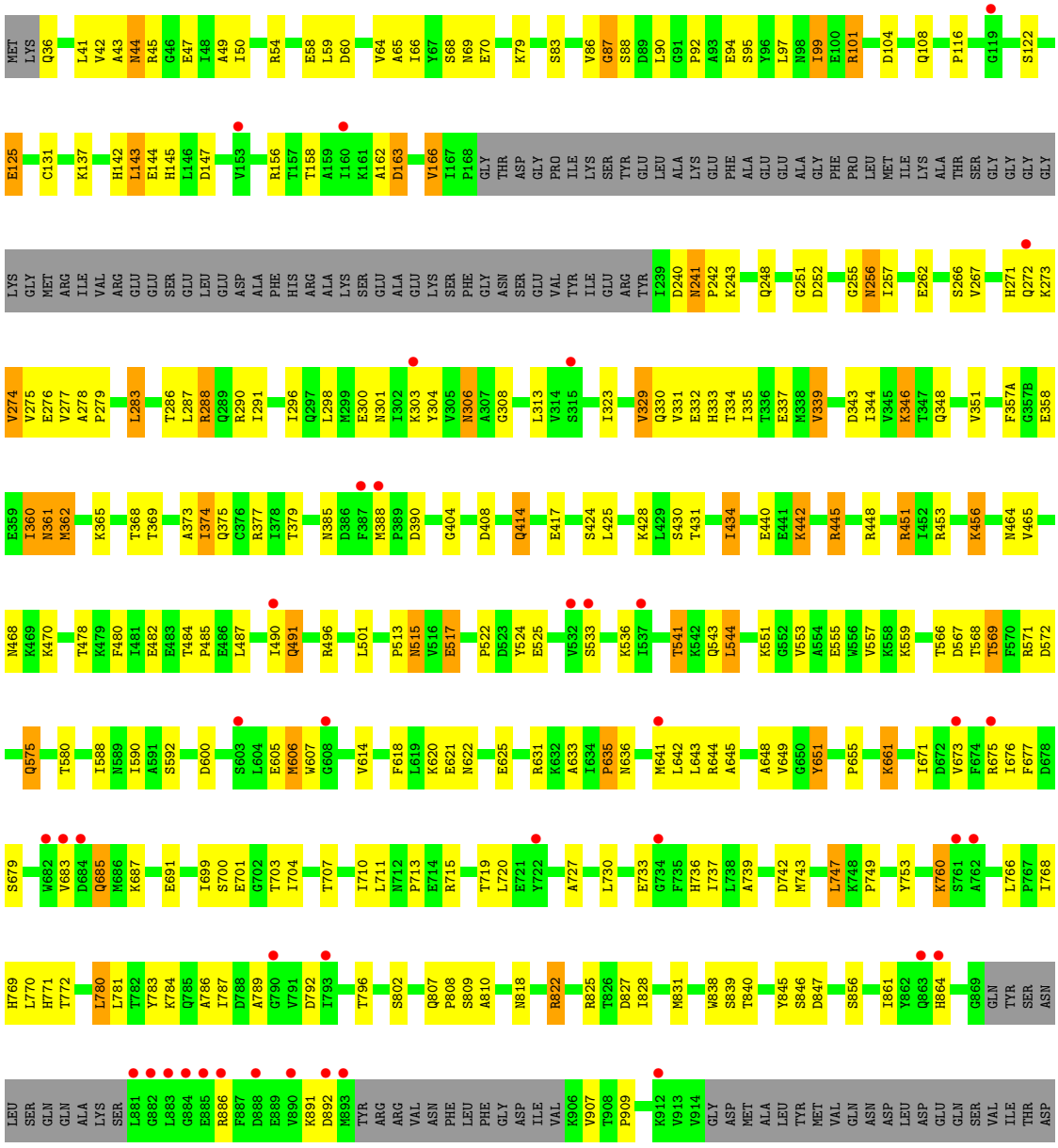
Chain A:

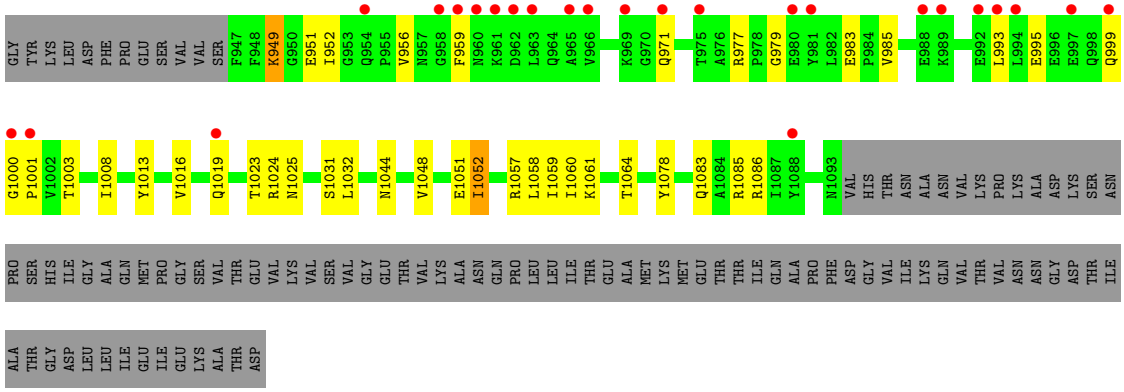




• Molecule 1: Pyruvate carboxylase

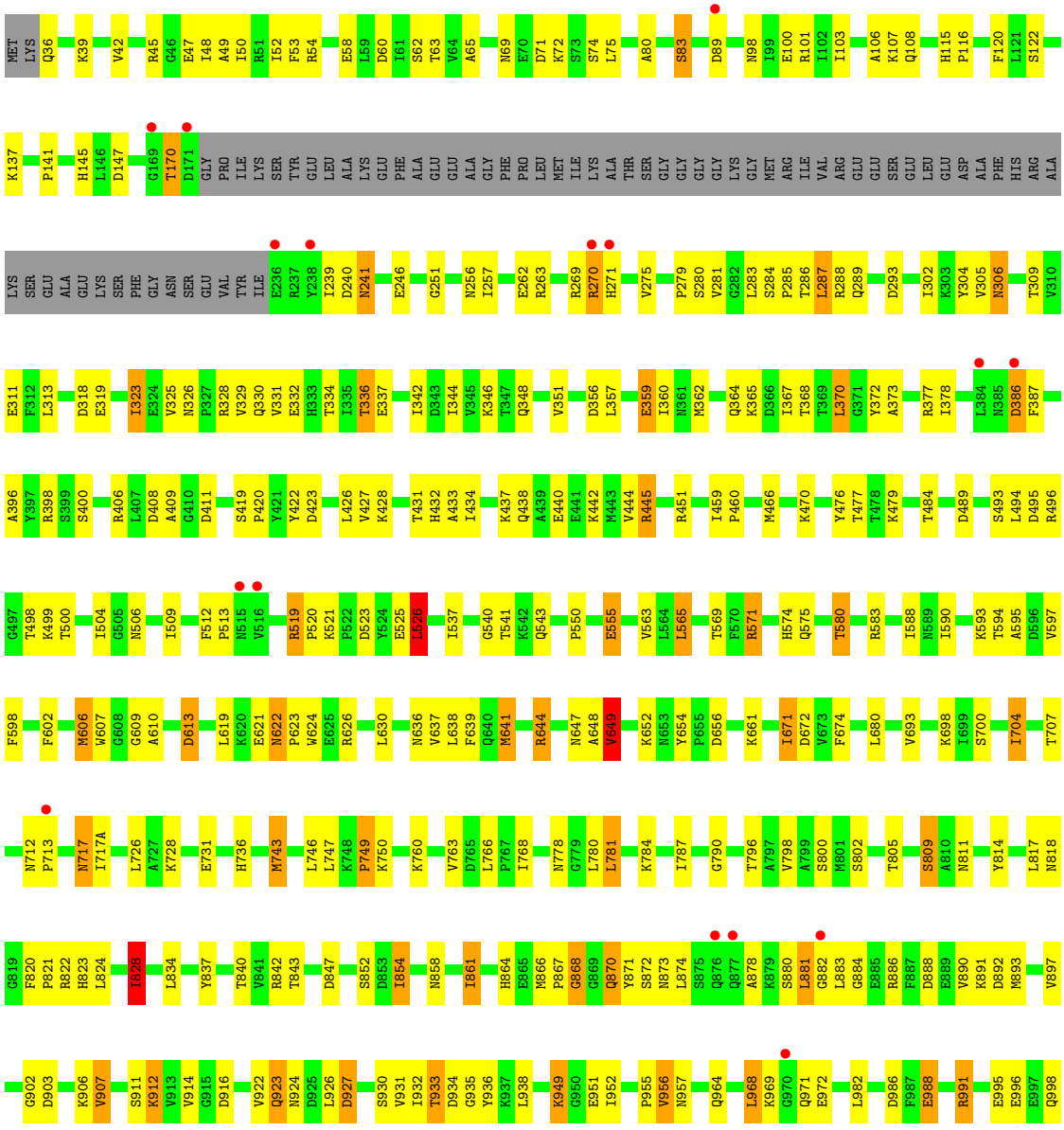
Chain D:

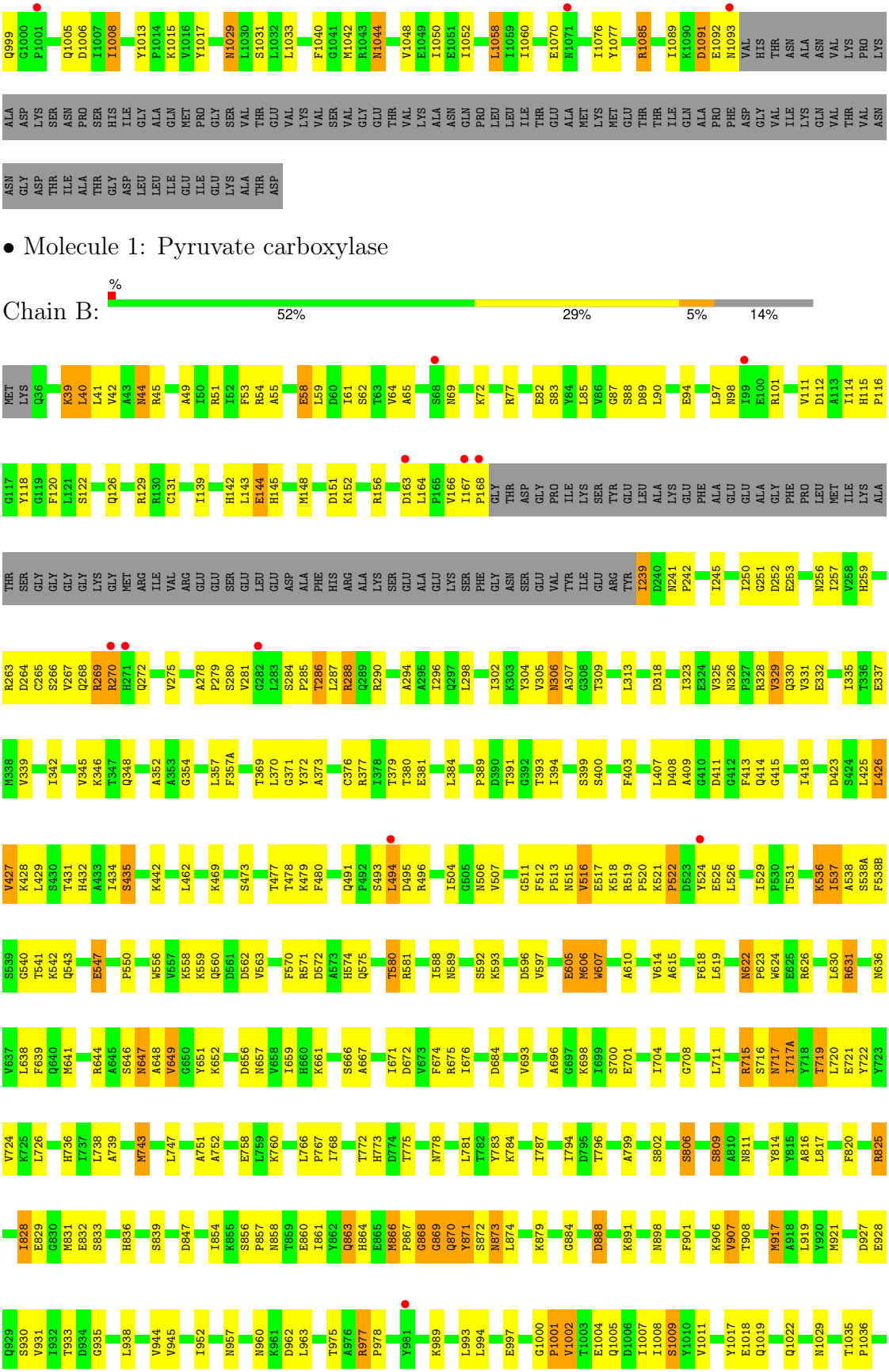




• Molecule 1: Pyruvate carboxylase

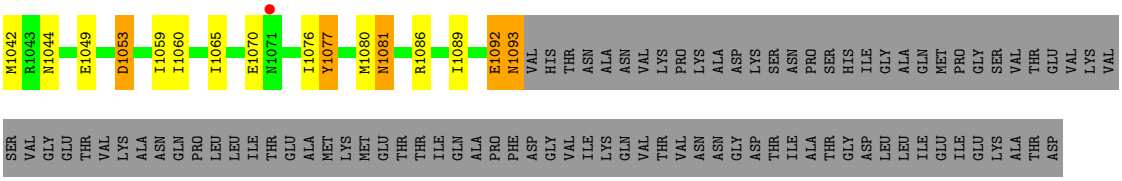
Chain C:





• Molecule 1: Pyruvate carboxylase

Chain B: % 52% 29% 5% 14%


M1042
R1043
N1044
E1049
D1053
I1059
I1060
I1065
E1070
N1071
I1076
Y1077
M1080
N1081
R1086
I1089
E1092
N1093
SER VAL GLY GLU THR VAL LYS ALA ASN GLN PRO LEU LEU ILE THR GLU ALA MET LYS MET GLU THR THR ILE GLN ALA PRO PHE ASP GLY VAL ILE LYS GLN VAL THR VAL ASN ASN GLY ASP THR ILE ALA THR GLY ASP LEU LEU ILE GLU ILE GLU LYS ALA THR ASP
VAL HIS THR ASN ALA ASN VAL LYS PRO LYS ALA ASP LYS SER ASN PRO SER HIS ILE GLY ALA GLN MET PRO GLY SER VAL THR GLU VAL LYS VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.59Å 164.47Å 373.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.90 29.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.97-2.90) 89.8 (29.98-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.264 , 0.328 0.266 , 0.322	Depositor DCC
R_{free} test set	5969 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	64.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	31229	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1935e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MN, BTI, COA

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	0.43	0/8033	0.60	1/10868 (0.0%)
1	B	0.49	0/7990	0.64	0/10810
1	C	0.50	0/8042	0.65	2/10880 (0.0%)
1	D	0.43	0/7537	0.60	0/10192
All	All	0.47	0/31602	0.62	3/42750 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	526	LEU	CA-CB-CG	5.56	128.09	115.30
1	C	828	ILE	CB-CA-C	-5.22	101.16	111.60
1	C	526	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	880	SER	Peptide

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	7880	0	7807	199	0
1	B	7838	0	7771	292	0
1	C	7889	0	7813	232	0
1	D	7396	0	7347	158	0
2	A	48	0	32	0	0
2	B	48	0	32	1	0
2	C	48	0	32	2	0
2	D	48	0	32	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	15	0	16	0	0
4	C	15	0	16	3	0
All	All	31229	0	30898	870	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 14.

All (870) 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:504:ILE:HG21	1:C:1042:MET:HE2	1.18	1.12
1:C:704:ILE:HG12	1:C:726:LEU:HD23	1.22	1.12
1:A:304:TYR:HE2	1:A:307:ALA:O	1.35	1.10
1:A:1085:ARG:HG2	1:A:1085:ARG:HH11	1.12	1.06
1:C:743:MET:HG3	1:C:907:VAL:HG13	1.38	1.04
1:B:825:ARG:HH11	1:B:825:ARG:HG2	1.20	1.02
1:D:451:ARG:HH22	2:D:2001:COA:H62	1.27	0.99
1:D:496:ARG:HE	1:D:1052:ILE:HG21	1.26	0.99
1:B:516:VAL:HG12	1:B:517:GLU:H	1.22	0.97
1:C:364:GLN:HA	1:C:367:ILE:HD12	1.46	0.96
1:A:44:ASN:HD22	1:A:45:ARG:H	1.13	0.96
1:A:304:TYR:CE2	1:A:307:ALA:O	2.17	0.95
1:B:288:ARG:HG3	1:B:288:ARG:HH11	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:MET:HE2	1:C:639:PHE:HB3	1.49	0.94
1:B:700:SER:H	1:B:736:HIS:HD2	1.17	0.91
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.34	0.91
1:D:43:ALA:HA	1:D:66:ILE:HD11	1.49	0.90
1:C:864:HIS:HD2	1:C:866:MET:H	1.19	0.90
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.36	0.89
1:B:644:ARG:HH11	1:B:647:ASN:HD21	1.15	0.89
1:D:277:VAL:HG22	1:D:374:ILE:HG22	1.54	0.88
1:C:506:ASN:OD1	4:C:2000:BTI:H92	1.73	0.88
1:C:870:GLN:HE22	1:C:911:SER:HB2	1.38	0.87
1:B:898:ASN:ND2	1:B:906:LYS:HE3	1.88	0.87
1:B:570:PHE:O	1:B:574:HIS:HE1	1.58	0.86
1:B:719:THR:HG22	1:B:721:GLU:H	1.40	0.86
1:C:574:HIS:HD2	1:C:580:THR:HA	1.41	0.85
1:B:1092:GLU:O	1:B:1093:ASN:HB2	1.77	0.85
1:B:917:MET:HG2	1:B:944:VAL:HG21	1.58	0.84
1:C:866:MET:CE	1:C:871:TYR:HA	2.07	0.83
1:A:442:LYS:O	1:A:446:SER:HB2	1.78	0.83
1:C:1044:ASN:HD22	1:C:1044:ASN:N	1.77	0.83
1:B:864:HIS:HD2	1:B:866:MET:H	1.28	0.81
1:B:516:VAL:HG12	1:B:517:GLU:N	1.95	0.81
1:C:743:MET:CG	1:C:907:VAL:HG13	2.10	0.80
1:A:418:ILE:HD12	1:A:418:ILE:H	1.47	0.80
1:C:704:ILE:CG1	1:C:726:LEU:HD23	2.09	0.80
1:D:162:ALA:O	1:D:163:ASP:HB2	1.82	0.80
1:A:1085:ARG:HG2	1:A:1085:ARG:NH1	1.88	0.79
1:C:626:ARG:O	1:C:630:LEU:HB2	1.82	0.79
1:B:866:MET:HG2	1:B:870:GLN:HB3	1.65	0.79
1:C:866:MET:HE2	1:C:871:TYR:HA	1.65	0.79
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.48	0.79
1:A:1058:LEU:HD12	1:A:1060:ILE:HD11	1.66	0.78
1:B:329:VAL:HG22	1:B:348:GLN:HE22	1.49	0.77
1:C:512:PHE:CZ	4:C:2000:BTI:H5	2.20	0.76
1:D:288:ARG:HA	1:D:291:ILE:HD12	1.64	0.76
1:A:313:LEU:HB2	1:A:323:ILE:HD11	1.67	0.76
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.51	0.76
1:B:306:ASN:HD21	1:B:348:GLN:HG3	1.49	0.75
1:B:409:ALA:HA	1:B:427:VAL:HG12	1.68	0.75
1:A:306:ASN:OD1	1:A:348:GLN:HG2	1.86	0.75
1:C:606:MET:CE	1:C:639:PHE:HB3	2.15	0.75
1:B:516:VAL:CG1	1:B:517:GLU:H	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ARG:HH11	1:C:1052:ILE:HD12	1.52	0.74
1:C:858:ASN:O	1:C:861:ILE:HG12	1.87	0.74
1:B:54:ARG:O	1:B:58:GLU:HG2	1.87	0.74
1:C:743:MET:HG3	1:C:907:VAL:CG1	2.16	0.74
1:B:873:ASN:H	1:B:873:ASN:ND2	1.86	0.74
1:A:44:ASN:HD22	1:A:45:ARG:N	1.84	0.73
1:C:717(A):ILE:HG12	1:C:957:ASN:HD21	1.53	0.73
1:B:901:PHE:CZ	1:B:917:MET:HG3	2.21	0.73
1:B:825:ARG:HG2	1:B:825:ARG:NH1	1.92	0.73
1:A:570:PHE:HB2	1:A:606:MET:HB3	1.71	0.73
1:D:677:PHE:HB3	1:D:703:THR:HB	1.69	0.73
1:C:357:LEU:O	1:C:362:MET:HB3	1.88	0.73
1:C:1044:ASN:HD22	1:C:1044:ASN:H	1.33	0.73
1:B:700:SER:H	1:B:736:HIS:CD2	2.06	0.72
1:D:277:VAL:HG22	1:D:374:ILE:CG2	2.19	0.72
1:A:658:VAL:HG11	1:A:1011:VAL:HG11	1.71	0.72
1:C:571:ARG:HD2	1:C:571:ARG:C	2.10	0.72
1:C:870:GLN:NE2	1:C:911:SER:HB2	2.05	0.72
1:C:555:GLU:HA	1:C:555:GLU:OE1	1.90	0.71
1:B:379:THR:HG22	1:B:425:LEU:HA	1.72	0.71
1:D:279:PRO:HD3	1:D:339:VAL:HG11	1.72	0.71
1:D:622:ASN:HB3	1:D:625:GLU:HB2	1.71	0.71
1:A:731:GLU:HG3	1:A:766:LEU:HD21	1.73	0.71
1:C:145:HIS:HE1	1:C:302:ILE:O	1.73	0.71
1:A:259:HIS:HB3	1:A:296:ILE:HD11	1.70	0.71
1:B:286:THR:O	1:B:290:ARG:HG3	1.91	0.70
1:C:563:VAL:HG21	1:C:787:ILE:HG12	1.74	0.70
1:C:924:ASN:HB2	1:C:926:LEU:CD2	2.20	0.70
1:D:283:LEU:HD23	1:D:288:ARG:HB2	1.73	0.70
1:D:337:GLU:HG2	1:D:344:ILE:HD12	1.74	0.70
1:C:396:ALA:HB2	1:C:1085:ARG:HD2	1.73	0.70
1:C:500:THR:O	1:C:504:ILE:HD12	1.91	0.70
1:B:717:ASN:H	1:B:717:ASN:HD22	1.40	0.70
1:C:504:ILE:HG21	1:C:1042:MET:CE	2.10	0.69
1:C:823:HIS:HD2	1:C:824:LEU:N	1.90	0.69
1:C:334:THR:HG23	1:C:406:ARG:CZ	2.22	0.69
1:B:644:ARG:HH11	1:B:647:ASN:ND2	1.89	0.69
1:B:869:GLY:O	1:B:871:TYR:N	2.26	0.69
1:A:335:ILE:HD11	1:A:374:ILE:HA	1.74	0.68
1:B:540:GLY:H	1:B:543:GLN:HE21	1.40	0.68
1:B:864:HIS:CD2	1:B:866:MET:H	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:LEU:HD23	1:C:496:ARG:HE	1.58	0.68
1:B:775:THR:HG23	1:B:861:ILE:HD13	1.75	0.68
1:B:719:THR:HG22	1:B:721:GLU:N	2.07	0.68
1:D:156:ARG:HG2	1:D:166:VAL:HG11	1.76	0.68
1:C:53:PHE:CD2	1:C:63:THR:HB	2.29	0.68
1:D:453:ARG:NE	2:D:2001:COA:O8A	2.27	0.67
1:C:823:HIS:HD2	1:C:824:LEU:H	1.42	0.67
1:C:311:GLU:HB2	1:C:323:ILE:HG22	1.75	0.67
1:B:1049:GLU:HG2	1:B:1059:ILE:HG13	1.76	0.67
1:D:252:ASP:HA	1:D:351:VAL:HG13	1.77	0.67
1:C:309:THR:HG21	1:C:330:GLN:NE2	2.09	0.67
1:D:408:ASP:HB2	1:D:428:LYS:HB3	1.77	0.67
1:D:335:ILE:O	1:D:339:VAL:HG23	1.95	0.67
1:B:917:MET:HG2	1:B:944:VAL:CG2	2.25	0.66
1:A:44:ASN:ND2	1:A:45:ARG:H	1.90	0.66
1:C:569:THR:OG1	1:C:798:VAL:HG23	1.95	0.66
1:B:960:ASN:HD22	1:B:963:LEU:H	1.43	0.66
1:B:873:ASN:H	1:B:873:ASN:HD22	1.43	0.66
1:A:309:THR:HB	1:A:326:ASN:ND2	2.09	0.66
1:D:1032:LEU:HD13	1:D:1052:ILE:HA	1.78	0.66
1:C:731:GLU:OE1	1:C:763:VAL:HB	1.95	0.66
1:A:250:ILE:HD11	1:A:344:ILE:HG23	1.78	0.66
1:D:44:ASN:HD22	1:D:45:ARG:H	1.42	0.66
1:B:719:THR:CG2	1:B:721:GLU:H	2.08	0.66
1:B:284:SER:HB2	1:B:285:PRO:HD2	1.78	0.65
1:B:644:ARG:HD2	1:B:647:ASN:HD21	1.61	0.65
1:A:525:GLU:HB3	1:A:840:THR:HG23	1.79	0.65
1:D:116:PRO:HB2	1:D:122:SER:HA	1.78	0.65
1:C:864:HIS:CD2	1:C:866:MET:H	2.08	0.65
1:A:249:VAL:HG11	1:A:299:MET:HG2	1.76	0.65
1:C:241:ASN:HB2	1:C:477:THR:OG1	1.95	0.65
1:C:866:MET:HE1	1:C:871:TYR:HA	1.77	0.65
1:C:1044:ASN:H	1:C:1044:ASN:ND2	1.92	0.65
1:D:651:TYR:H	1:D:651:TYR:HD2	1.43	0.65
1:D:949:LYS:HB3	1:D:951:GLU:HG2	1.78	0.64
1:B:641:MET:HE2	1:B:671:ILE:HG13	1.77	0.64
1:A:898:ASN:HD21	1:A:904:ILE:H	1.43	0.64
2:D:2001:COA:O2A	2:D:2001:COA:H10	1.97	0.64
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.62	0.64
1:A:783:TYR:CE1	1:A:808:PRO:HG2	2.33	0.64
1:B:575:GLN:HG3	1:B:580:THR:OG1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLU:OE1	1:D:346:LYS:NZ	2.30	0.64
1:B:142:HIS:H	1:B:145:HIS:HD2	1.45	0.64
1:B:543:GLN:HE22	1:B:636:ASN:CA	2.08	0.64
1:A:69:ASN:HD22	1:A:72:LYS:HE2	1.63	0.63
1:A:363:GLN:O	1:A:366:ASP:HB2	1.98	0.63
1:B:570:PHE:O	1:B:574:HIS:CE1	2.47	0.63
1:A:1044:ASN:HA	1:A:1062:LEU:CD2	2.27	0.63
1:A:1044:ASN:HA	1:A:1062:LEU:HD23	1.81	0.63
1:B:802:SER:OG	1:B:809:SER:HB2	1.98	0.63
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.81	0.63
1:C:309:THR:HG21	1:C:330:GLN:HE22	1.63	0.63
1:D:451:ARG:NH2	2:D:2001:COA:H62	2.08	0.63
1:C:263:ARG:HH11	1:C:336:THR:HB	1.61	0.63
1:C:680:LEU:HD11	1:C:952:ILE:HG22	1.81	0.63
1:D:334:THR:HG21	1:D:430:SER:OG	1.98	0.63
1:B:493:SER:O	1:B:495:ASP:N	2.31	0.63
1:B:720:LEU:HD11	1:B:758:GLU:HG3	1.80	0.63
1:A:251:GLY:HA3	1:A:257:ILE:HG13	1.81	0.63
1:A:879:LYS:HG2	1:A:884:GLY:HA3	1.79	0.63
1:C:881:LEU:HD12	1:C:882:GLY:H	1.63	0.63
1:B:306:ASN:HD22	1:B:307:ALA:N	1.97	0.63
1:D:567:ASP:OD2	1:D:569:THR:OG1	2.16	0.63
1:D:42:VAL:HG11	1:D:49:ALA:HA	1.79	0.62
1:B:288:ARG:HG3	1:B:288:ARG:NH1	2.09	0.62
1:C:927:ASP:H	1:C:930:SER:HB3	1.63	0.62
1:C:575:GLN:HG3	1:C:580:THR:OG1	1.99	0.62
1:A:130:ARG:HH12	1:A:134:GLU:HG2	1.63	0.62
1:A:309:THR:HB	1:A:326:ASN:HD21	1.64	0.62
1:B:306:ASN:HD22	1:B:307:ALA:H	1.46	0.62
1:B:814:TYR:CE2	1:B:828:ILE:HG12	2.35	0.62
1:B:377:ARG:HG3	1:B:377:ARG:HH11	1.64	0.62
1:D:513:PRO:O	1:D:515:ASN:HB2	1.98	0.62
1:B:543:GLN:NE2	1:B:636:ASN:HA	2.11	0.62
1:A:615:ALA:HA	1:A:619:LEU:HD12	1.82	0.61
1:B:263:ARG:HG2	1:B:278:ALA:HB2	1.81	0.61
1:B:269:ARG:HB2	1:B:269:ARG:NH1	2.14	0.61
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.12	0.61
1:D:730:LEU:HA	1:D:733:GLU:HB2	1.83	0.61
1:C:811:ASN:HD22	1:C:811:ASN:H	1.46	0.61
1:C:924:ASN:HB2	1:C:926:LEU:HD21	1.81	0.61
1:A:164:LEU:HD11	1:A:298:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:701:GLU:HG3	1:D:737:ILE:HB	1.81	0.61
1:B:536:LYS:O	1:B:538(A):SER:OG	2.16	0.61
1:A:394:ILE:O	1:A:415:GLY:HA2	2.00	0.61
1:C:63:THR:OG1	1:C:80:ALA:HA	2.00	0.61
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.36	0.61
1:C:593:LYS:O	1:C:597:VAL:HG23	2.00	0.61
1:B:376:CYS:HB3	1:B:462:LEU:HD13	1.82	0.61
1:C:509:ILE:HG21	1:C:1091:ASP:HB2	1.83	0.61
1:C:823:HIS:CD2	1:C:824:LEU:N	2.68	0.60
1:B:143:LEU:HD12	1:B:143:LEU:H	1.66	0.60
1:B:403:PHE:O	1:B:442:LYS:HE3	2.01	0.60
1:A:331:VAL:HG12	1:A:428:LYS:HD2	1.83	0.60
1:B:644:ARG:NH1	1:B:647:ASN:HD21	1.95	0.60
1:B:828:ILE:O	1:B:832:GLU:HG2	2.01	0.60
1:D:335:ILE:HG23	1:D:373:ALA:HB3	1.84	0.60
1:B:537:ILE:HA	1:B:538(B):PHE:CD1	2.37	0.60
1:C:805:THR:HG23	1:C:854:ILE:HD13	1.83	0.60
1:A:662:PHE:HA	1:A:1008:ILE:HD13	1.84	0.60
1:C:438:GLN:O	1:C:442:LYS:HG3	2.02	0.60
1:C:870:GLN:O	1:C:871:TYR:C	2.40	0.60
1:B:306:ASN:ND2	1:B:348:GLN:HG3	2.17	0.60
1:A:917:MET:HG2	1:A:944:VAL:HG21	1.84	0.60
1:A:960:ASN:HB3	1:A:963:LEU:HB3	1.83	0.60
1:C:378:ILE:HG22	1:C:426:LEU:HD12	1.82	0.60
1:D:517:GLU:HB2	1:D:847:ASP:OD1	2.02	0.59
1:C:823:HIS:CD2	1:C:824:LEU:H	2.19	0.59
1:D:404:GLY:O	1:D:431:THR:HA	2.02	0.59
1:D:86:VAL:O	1:D:87:GLY:O	2.21	0.59
1:D:700:SER:H	1:D:736:HIS:HD2	1.50	0.59
1:B:69:ASN:O	1:B:72:LYS:HG2	2.03	0.59
1:B:606:MET:HE1	1:B:671:ILE:CD1	2.31	0.59
1:B:1092:GLU:O	1:B:1093:ASN:CB	2.49	0.59
1:A:335:ILE:HD11	1:A:374:ILE:CA	2.33	0.59
1:B:772:THR:HG22	1:B:783:TYR:CE2	2.38	0.59
1:B:537:ILE:C	1:B:538(A):SER:H	2.05	0.59
1:A:99:ILE:HG12	1:A:127:PHE:HB2	1.85	0.59
1:A:626:ARG:O	1:A:630:LEU:HB2	2.03	0.58
1:B:952:ILE:HG22	1:B:952:ILE:O	2.03	0.58
1:B:512:PHE:CD2	1:B:513:PRO:HD2	2.38	0.58
1:C:337:GLU:HG2	1:C:342:ILE:O	2.03	0.58
1:B:251:GLY:O	1:B:306:ASN:N	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ASN:HB3	1:B:357(A):PHE:HE1	1.69	0.58
1:A:116:PRO:HB2	1:A:122:SER:HA	1.85	0.58
1:D:600:ASP:HB3	1:D:825:ARG:HD3	1.85	0.58
1:B:917:MET:SD	1:B:921:MET:CE	2.92	0.58
1:A:527:ALA:HB2	1:A:840:THR:HB	1.84	0.58
1:D:104:ASP:O	1:D:108:GLN:HG2	2.03	0.58
1:D:385:ASN:O	1:D:388:MET:HG2	2.03	0.58
1:B:606:MET:HE1	1:B:671:ILE:HD11	1.86	0.58
1:A:494:LEU:HD12	1:A:494:LEU:H	1.68	0.58
1:B:743:MET:HG3	1:B:907:VAL:HG13	1.86	0.58
1:B:856:SER:HB2	1:B:857:PRO:HD2	1.86	0.58
1:B:1000:GLY:N	1:B:1001:PRO:HD3	2.19	0.58
1:A:517:GLU:HB3	1:A:519:ARG:HH21	1.69	0.57
1:C:116:PRO:HB2	1:C:122:SER:HA	1.85	0.57
1:B:51:ARG:HH12	1:B:55:ALA:HB2	1.68	0.57
1:D:278:ALA:HB3	1:D:335:ILE:HG22	1.85	0.57
1:C:626:ARG:HG2	1:C:630:LEU:HD12	1.86	0.57
1:B:825:ARG:HH11	1:B:825:ARG:CG	2.05	0.57
1:D:710:ILE:HD13	1:D:720:LEU:HD13	1.85	0.57
1:B:537:ILE:O	1:B:538(A):SER:N	2.37	0.57
1:C:852:SER:OG	1:C:854:ILE:HG12	2.04	0.57
1:C:932:ILE:O	1:C:936:TYR:CE2	2.57	0.57
1:C:495:ASP:O	1:C:499:LYS:HD2	2.03	0.57
1:B:622:ASN:HD22	1:B:623:PRO:CD	2.17	0.57
1:B:773:HIS:C	1:B:775:THR:H	2.07	0.57
1:A:244:HIS:HD2	1:A:265:CYS:HB2	1.69	0.57
1:B:701:GLU:HG2	1:B:739:ALA:HB2	1.86	0.57
1:A:543:GLN:HA	1:A:546:ASP:HB2	1.87	0.57
1:B:164:LEU:HD21	1:B:294:ALA:HB1	1.85	0.57
1:A:920:TYR:O	1:A:924:ASN:ND2	2.37	0.57
1:C:991:ARG:O	1:C:995:GLU:HG2	2.05	0.57
1:B:960:ASN:ND2	1:B:963:LEU:H	2.02	0.57
1:A:445:ARG:HH21	1:C:54:ARG:HB3	1.70	0.56
1:A:438:GLN:O	1:A:442:LYS:HG3	2.05	0.56
1:C:513:PRO:HD3	4:C:2000:BTI:H11	1.86	0.56
1:B:331:VAL:HG23	1:B:332:GLU:OE1	2.05	0.56
1:B:1005:GLN:O	1:B:1009:SER:HB2	2.05	0.56
1:B:64:VAL:HG22	1:B:82:GLU:HB2	1.86	0.56
1:A:578:LEU:HD11	1:A:842:ARG:HG3	1.88	0.56
1:C:241:ASN:HB3	1:C:479:LYS:HD3	1.87	0.56
1:B:269:ARG:HB2	1:B:269:ARG:HH11	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:820:PHE:HB3	1:C:821:PRO:HD2	1.87	0.56
1:B:41:LEU:HB2	1:B:111:VAL:HG11	1.86	0.56
1:C:700:SER:H	1:C:736:HIS:HD2	1.52	0.56
1:A:685:GLN:HA	1:A:977:ARG:HD2	1.87	0.56
1:D:448:ARG:HB2	2:D:2001:COA:H21	1.88	0.56
1:C:496:ARG:HH11	1:C:1052:ILE:CD1	2.17	0.56
1:B:288:ARG:HH11	1:B:288:ARG:CG	2.12	0.56
1:C:881:LEU:HB2	1:C:884:GLY:H	1.71	0.55
1:D:783:TYR:CE1	1:D:808:PRO:HG2	2.41	0.55
1:B:811:ASN:H	1:B:811:ASN:HD22	1.52	0.55
1:B:917:MET:SD	1:B:921:MET:HE1	2.46	0.55
1:D:783:TYR:O	1:D:786:ALA:N	2.35	0.55
1:A:144:GLU:CD	1:A:144:GLU:H	2.09	0.55
1:B:879:LYS:HG3	1:B:884:GLY:HA2	1.89	0.55
1:A:391:THR:HG23	1:A:418:ILE:O	2.06	0.55
1:B:638:LEU:HD22	1:B:672:ASP:HB3	1.87	0.55
1:B:661:LYS:NZ	1:B:1004:GLU:OE2	2.32	0.55
1:C:311:GLU:OE1	1:C:326:ASN:ND2	2.30	0.55
1:C:357:LEU:HA	1:C:360:ILE:HD12	1.89	0.55
1:C:780:LEU:HD13	1:B:778:ASN:ND2	2.22	0.55
1:B:672:ASP:HA	1:B:698:LYS:HD2	1.87	0.55
1:A:968:LEU:C	1:A:970:GLY:H	2.08	0.55
1:D:240:ASP:C	1:D:242:PRO:HD3	2.26	0.55
1:D:496:ARG:NE	1:D:1052:ILE:HG21	2.09	0.55
1:C:39:LYS:HG3	1:C:62:SER:HB3	1.87	0.55
1:D:533:SER:HB3	1:D:536:LYS:HB2	1.89	0.55
1:A:440:GLU:O	1:A:444:VAL:HG13	2.07	0.54
1:A:525:GLU:HB3	1:A:840:THR:CG2	2.37	0.54
1:C:284:SER:HB2	1:C:285:PRO:HD2	1.89	0.54
1:C:760:LYS:CD	1:C:768:ILE:HD12	2.37	0.54
1:D:468:ASN:OD1	1:D:470:LYS:HG2	2.07	0.54
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.90	0.54
1:B:556:TRP:HA	1:B:559:LYS:HD3	1.88	0.54
1:C:519:ARG:HB2	1:C:520:PRO:HD2	1.88	0.54
1:C:370:LEU:O	1:C:432:HIS:HE1	1.91	0.54
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.71	0.54
1:A:252:ASP:O	1:A:305:VAL:HG22	2.07	0.54
1:A:145:HIS:CE1	1:A:304:TYR:HA	2.42	0.54
1:D:679:SER:HB3	1:D:909:PRO:HD2	1.90	0.54
1:B:720:LEU:O	1:B:724:VAL:HG23	2.07	0.54
1:B:1081:ASN:N	1:B:1081:ASN:HD22	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:GLN:O	1:D:333:HIS:ND1	2.32	0.54
1:C:359:GLU:H	1:C:359:GLU:CD	2.10	0.54
1:C:924:ASN:HB2	1:C:926:LEU:HD22	1.90	0.54
1:B:522:PRO:HA	1:B:524:TYR:HE1	1.72	0.54
1:B:563:VAL:HG21	1:B:787:ILE:HG12	1.89	0.54
1:B:644:ARG:HD2	1:B:647:ASN:ND2	2.22	0.54
1:A:938:LEU:O	1:A:939:ASP:O	2.25	0.54
1:A:574:HIS:HD2	1:A:580:THR:HA	1.73	0.53
1:A:586:ASP:OD1	1:A:1035:THR:OG1	2.25	0.53
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.74	0.53
1:C:931:VAL:O	1:C:935:GLY:HA3	2.08	0.53
1:B:45:ARG:NH2	1:B:411:ASP:OD2	2.40	0.53
1:D:541:THR:HA	1:D:544:LEU:HB2	1.89	0.53
1:B:239:ILE:HG21	1:B:313:LEU:HD23	1.89	0.53
1:B:675:ARG:HA	1:B:701:GLU:HB3	1.89	0.53
1:B:960:ASN:HD21	1:B:962:ASP:HB2	1.73	0.53
1:B:898:ASN:HD22	1:B:906:LYS:HE3	1.67	0.53
1:D:572:ASP:OD1	1:D:807:GLN:NE2	2.41	0.53
1:D:496:ARG:HE	1:D:1052:ILE:CG2	2.12	0.53
1:D:704:ILE:HD11	1:D:727:ALA:HB2	1.91	0.53
1:B:575:GLN:NE2	1:B:610:ALA:H	2.07	0.53
1:D:44:ASN:HD22	1:D:45:ARG:N	2.04	0.53
1:D:243:LYS:O	1:D:313:LEU:HA	2.09	0.53
1:D:414:GLN:O	1:D:414:GLN:HG3	2.09	0.53
1:C:48:ILE:O	1:C:52:ILE:HD12	2.08	0.53
1:C:52:ILE:HG12	1:C:115:HIS:CG	2.44	0.53
1:B:328:ARG:HD3	1:B:329:VAL:O	2.09	0.53
1:A:246:GLU:HG2	1:A:311:GLU:HG2	1.90	0.53
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.06	0.53
1:D:810:ALA:HB3	1:D:831:MET:HE3	1.90	0.53
1:B:504:ILE:HD13	1:B:1042:MET:HE2	1.91	0.53
1:C:280:SER:OG	1:C:283:LEU:HG	2.08	0.52
1:B:866:MET:SD	1:B:874:LEU:HD22	2.49	0.52
1:A:444:VAL:HG12	1:A:466:MET:HB3	1.91	0.52
1:D:445:ARG:NH1	1:B:54:ARG:HB3	2.25	0.52
1:C:263:ARG:HH21	1:C:330:GLN:HE21	1.56	0.52
1:D:641:MET:HE2	1:D:671:ILE:HG13	1.91	0.52
1:C:598:PHE:O	1:C:637:VAL:HG21	2.09	0.52
1:C:746:LEU:HD23	1:C:861:ILE:HG22	1.90	0.52
1:C:1006:ASP:HB3	1:C:1017:TYR:OH	2.10	0.52
1:B:263:ARG:HH21	1:B:330:GLN:HE22	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG22	1:A:374:ILE:HG23	1.91	0.52
1:D:94:GLU:HA	1:D:97:LEU:HB2	1.91	0.52
1:C:897:VAL:HG23	1:C:914:VAL:HG13	1.92	0.52
1:A:418:ILE:HD12	1:A:418:ILE:N	2.21	0.52
1:C:48:ILE:O	1:C:52:ILE:CD1	2.57	0.52
1:C:949:LYS:HB3	1:C:951:GLU:HG3	1.91	0.52
1:B:263:ARG:NH2	1:B:330:GLN:NE2	2.58	0.52
1:B:281:VAL:HG22	1:B:372:TYR:CE2	2.45	0.52
1:D:661:LYS:HB3	1:D:1008:ILE:HD13	1.92	0.52
1:D:339:VAL:O	1:D:369:THR:HA	2.09	0.52
1:D:360:ILE:O	1:D:361:ASN:C	2.47	0.52
1:B:118:TYR:CE2	1:B:331:VAL:HG12	2.45	0.52
1:B:930:SER:HA	1:B:933:THR:HB	1.91	0.52
1:C:239:ILE:HD12	1:C:313:LEU:HD23	1.91	0.52
1:C:328:ARG:HD2	1:C:329:VAL:O	2.10	0.52
1:C:802:SER:OG	1:C:809:SER:HB2	2.10	0.52
1:C:935:GLY:HA2	1:C:938:LEU:HD12	1.92	0.52
1:C:986:ASP:OD1	1:C:988:GLU:HG2	2.10	0.52
1:D:484:THR:HB	1:D:487:LEU:HD22	1.92	0.52
1:C:638:LEU:HD22	1:C:672:ASP:HB3	1.93	0.51
1:C:864:HIS:CD2	1:C:866:MET:HB2	2.45	0.51
1:B:541:THR:HB	1:B:638:LEU:HG	1.92	0.51
1:A:90:LEU:HD21	1:A:101:ARG:HD2	1.92	0.51
1:D:1052:ILE:HD11	1:D:1058:LEU:HD13	1.92	0.51
2:D:2001:COA:H2A	1:B:77:ARG:NH2	2.26	0.51
1:B:1060:ILE:HG12	1:B:1080:MET:HG3	1.93	0.51
1:A:690:ASN:HB2	1:A:735:PHE:CZ	2.46	0.51
1:A:1004:GLU:HA	1:A:1007:ILE:HD12	1.93	0.51
1:D:162:ALA:O	1:D:163:ASP:CB	2.55	0.51
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.92	0.51
1:C:661:LYS:HG2	1:C:1008:ILE:HG23	1.92	0.51
1:C:781:LEU:HD13	1:B:816:ALA:HB1	1.93	0.51
1:B:377:ARG:HD2	1:B:425:LEU:HD11	1.93	0.51
1:B:507:VAL:O	1:B:511:GLY:HA2	2.11	0.51
1:A:357:LEU:HD22	1:A:362:MET:HG3	1.92	0.51
1:C:624:TRP:CD2	1:C:1005:GLN:HG2	2.46	0.51
1:B:519:ARG:NH2	1:B:847:ASP:OD2	2.44	0.51
1:A:654:TYR:HB3	1:A:658:VAL:CG2	2.41	0.51
1:A:858:ASN:OD1	1:A:860:GLU:HG2	2.11	0.51
1:B:263:ARG:NH2	1:B:330:GLN:HE22	2.09	0.51
1:B:1059:ILE:H	1:B:1081:ASN:HD21	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ASP:OD2	1:A:872:SER:HB2	2.12	0.51
1:A:1062:LEU:HD12	1:A:1076:ILE:HG23	1.93	0.51
1:D:568:THR:HG22	1:D:605:GLU:HB3	1.92	0.51
1:C:661:LYS:HG2	1:C:1008:ILE:CG2	2.41	0.51
1:B:252:ASP:HB3	1:B:357:LEU:HD13	1.92	0.51
1:B:267:VAL:HG11	1:B:275:VAL:HB	1.93	0.51
1:C:65:ALA:HB3	1:C:83:SER:HB3	1.92	0.50
1:C:263:ARG:HH21	1:C:330:GLN:NE2	2.09	0.50
1:B:994:LEU:HD21	1:B:1017:TYR:HE2	1.75	0.50
1:A:42:VAL:HG11	1:A:49:ALA:HA	1.93	0.50
1:D:621:GLU:HB2	1:D:1031:SER:HB2	1.93	0.50
1:C:504:ILE:CG2	1:C:1042:MET:HE2	2.13	0.50
1:B:408:ASP:HB2	1:B:428:LYS:HG3	1.92	0.50
1:B:562:ASP:OD2	1:B:825:ARG:HD3	2.10	0.50
1:D:445:ARG:HD3	1:B:54:ARG:HA	1.92	0.50
1:D:999:GLN:HG2	1:D:1001:PRO:HD2	1.93	0.50
1:C:269:ARG:HG3	1:C:270:ARG:HG2	1.93	0.50
1:C:574:HIS:CD2	1:C:580:THR:HA	2.32	0.50
1:C:641:MET:HG2	1:C:671:ILE:HD12	1.94	0.50
1:A:898:ASN:ND2	1:A:904:ILE:H	2.09	0.50
1:D:1013:TYR:HB3	1:D:1016:VAL:HB	1.94	0.50
1:C:42:VAL:HG11	1:C:49:ALA:HA	1.92	0.50
1:C:541:THR:HG21	1:C:602:PHE:HA	1.92	0.50
1:B:266:SER:O	1:B:478:THR:HA	2.11	0.50
1:B:418:ILE:N	1:B:418:ILE:HD12	2.27	0.50
1:B:512:PHE:CG	1:B:513:PRO:HD2	2.46	0.50
1:A:441:GLU:OE2	1:C:58:GLU:HB3	2.12	0.50
1:A:641:MET:HB3	1:A:671:ILE:HD12	1.94	0.50
1:C:873:ASN:H	1:C:873:ASN:HD22	1.59	0.50
1:B:269:ARG:HG3	1:B:270:ARG:N	2.27	0.50
1:A:90:LEU:HD11	1:A:101:ARG:HD3	1.92	0.50
1:C:867:PRO:HD2	1:C:870:GLN:HE21	1.76	0.50
1:B:337:GLU:HG2	1:B:342:ILE:O	2.11	0.50
1:D:442:LYS:HE3	1:B:58:GLU:OE2	2.12	0.50
1:C:717:ASN:HD22	1:C:717:ASN:H	1.59	0.50
1:C:1033:LEU:HD22	1:C:1050:ILE:HG12	1.94	0.50
1:B:381:GLU:HA	1:B:389:PRO:HA	1.94	0.50
1:A:70:GLU:HG3	1:A:92:PRO:HB3	1.93	0.50
1:D:50:ILE:O	1:D:54:ARG:HG3	2.11	0.50
1:B:1065:ILE:HG12	1:B:1076:ILE:HG12	1.95	0.49
1:C:373:ALA:HA	1:C:431:THR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1052:ILE:HD13	1:C:1058:LEU:HD21	1.93	0.49
1:B:506:ASN:HD22	1:B:1089:ILE:HG23	1.77	0.49
1:A:130:ARG:NH1	1:A:134:GLU:HG2	2.27	0.49
1:A:314:VAL:HG22	1:A:320:PHE:HB2	1.94	0.49
1:B:743:MET:CG	1:B:907:VAL:HG13	2.41	0.49
1:A:53:PHE:CZ	1:A:80:ALA:HB2	2.47	0.49
1:A:540:GLY:H	1:A:543:GLN:HE21	1.58	0.49
1:D:501:LEU:HB3	1:D:1078:TYR:CE1	2.47	0.49
1:C:652:LYS:O	1:C:654:TYR:CE1	2.66	0.49
1:C:1076:ILE:HD11	1:C:1089:ILE:HG13	1.95	0.49
1:A:1013:TYR:HB3	1:A:1016:VAL:HB	1.95	0.49
1:D:651:TYR:CD2	1:D:651:TYR:N	2.79	0.49
1:D:343:ASP:CG	1:D:346:LYS:HB2	2.33	0.49
1:D:701:GLU:HG2	1:D:739:ALA:HB2	1.94	0.49
1:C:717(A):ILE:HG21	1:C:956:VAL:HG11	1.95	0.49
1:B:434:ILE:HD12	1:B:435:SER:H	1.78	0.49
1:A:394:ILE:HG13	1:A:418:ILE:HD11	1.94	0.49
1:B:542:LYS:HG3	1:B:631:ARG:HH12	1.77	0.49
1:B:622:ASN:HD22	1:B:623:PRO:N	2.10	0.49
1:B:888:ASP:HA	1:B:891:LYS:HE3	1.93	0.49
1:A:278:ALA:CB	1:A:335:ILE:HG23	2.42	0.48
1:A:332:GLU:HA	1:A:375:GLN:NE2	2.27	0.48
1:A:664:GLN:O	1:A:668:LYS:HB2	2.13	0.48
1:B:259:HIS:HB3	1:B:296:ILE:HD11	1.94	0.48
1:A:90:LEU:HD21	1:A:101:ARG:CD	2.42	0.48
1:D:251:GLY:HA2	1:D:256:ASN:O	2.14	0.48
1:C:289:GLN:OE1	1:C:293:ASP:OD2	2.31	0.48
1:B:370:LEU:O	1:B:432:HIS:CE1	2.66	0.48
1:B:434:ILE:HD12	1:B:435:SER:N	2.28	0.48
1:D:379:THR:HG22	1:D:425:LEU:HA	1.95	0.48
1:C:893:MET:O	1:C:897:VAL:HG22	2.12	0.48
1:B:641:MET:HE2	1:B:671:ILE:CG1	2.43	0.48
1:B:1018:GLU:O	1:B:1022:GLN:HG2	2.14	0.48
1:D:1051:GLU:HB3	1:D:1057:ARG:HG2	1.96	0.48
1:B:646:SER:O	1:B:659:ILE:HD11	2.13	0.48
1:A:624:TRP:CZ2	1:A:1008:ILE:HD11	2.48	0.48
1:A:755:LEU:HD12	1:A:759:LEU:HD11	1.95	0.48
1:C:337:GLU:HG3	1:C:344:ILE:HG12	1.96	0.48
1:C:537:ILE:HD12	1:C:595:ALA:HB3	1.96	0.48
1:B:144:GLU:H	1:B:144:GLU:CD	2.17	0.48
1:B:85:LEU:HD21	1:B:88:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:SER:HB2	1:A:476:TYR:HD2	1.77	0.48
1:A:371:GLY:HA3	1:A:434:ILE:HA	1.96	0.48
1:D:313:LEU:HD13	1:D:323:ILE:HG13	1.95	0.48
1:B:145:HIS:CE1	1:B:304:TYR:HA	2.49	0.48
1:B:606:MET:CE	1:B:607:TRP:HB2	2.44	0.48
1:D:143:LEU:H	1:D:143:LEU:HD23	1.79	0.48
1:D:606:MET:SD	1:D:606:MET:C	2.92	0.48
1:C:621:GLU:HB2	1:C:1031:SER:HB3	1.95	0.48
1:B:864:HIS:CD2	1:B:866:MET:HB2	2.49	0.48
1:A:83:SER:HB2	2:C:2001:COA:H61A	1.79	0.47
1:A:501:LEU:HB3	1:A:1078:TYR:CE1	2.49	0.47
1:C:287:LEU:C	1:C:289:GLN:H	2.18	0.47
1:B:614:VAL:HG13	1:B:618:PHE:HD1	1.79	0.47
1:A:883:LEU:HD13	1:A:922:VAL:HG12	1.95	0.47
1:B:40:LEU:HB2	1:B:61:ILE:HG21	1.96	0.47
1:B:817:LEU:O	1:B:820:PHE:HB2	2.14	0.47
1:A:394:ILE:O	1:A:414:GLN:O	2.32	0.47
1:C:360:ILE:C	1:C:362:MET:H	2.18	0.47
1:C:526:LEU:HD13	1:C:526:LEU:O	2.14	0.47
1:B:993:LEU:O	1:B:997:GLU:HG3	2.14	0.47
1:A:817:LEU:HD12	1:A:824:LEU:HB2	1.95	0.47
1:C:814:TYR:CE2	1:C:828:ILE:HG23	2.49	0.47
1:D:571:ARG:HH11	1:D:575:GLN:HE22	1.59	0.47
1:B:72:LYS:O	1:B:77:ARG:HD3	2.15	0.47
1:A:376:CYS:HB3	1:A:462:LEU:HD13	1.97	0.47
1:A:999:GLN:HG2	1:A:1001:PRO:HD2	1.97	0.47
1:C:927:ASP:OD1	1:C:927:ASP:N	2.48	0.47
1:C:47:GLU:OE1	1:C:428:LYS:NZ	2.47	0.47
1:C:760:LYS:HD2	1:C:768:ILE:HD12	1.96	0.47
1:C:890:VAL:HG22	1:C:922:VAL:HG21	1.96	0.47
1:B:747:LEU:HG	1:B:752:ALA:HB2	1.94	0.47
1:B:864:HIS:HD2	1:B:866:MET:N	2.06	0.47
1:A:435:SER:OG	1:A:438:GLN:HG2	2.15	0.47
1:C:543:GLN:OE1	1:C:636:ASN:HA	2.15	0.47
1:B:65:ALA:O	1:B:83:SER:HA	2.14	0.47
1:B:116:PRO:HB3	1:B:122:SER:HA	1.96	0.47
1:B:245:ILE:HD13	1:B:264:ASP:HA	1.97	0.47
1:C:47:GLU:HA	1:C:50:ILE:HD12	1.96	0.47
1:C:704:ILE:HD11	1:C:726:LEU:HB3	1.96	0.47
1:C:811:ASN:H	1:C:811:ASN:ND2	2.12	0.47
1:B:394:ILE:HD11	1:B:426:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLN:O	1:A:874:LEU:HB3	2.14	0.47
1:C:50:ILE:CD1	1:C:409:ALA:O	2.63	0.47
1:C:279:PRO:HD2	1:C:372:TYR:CD2	2.49	0.47
1:A:136:ILE:CG2	1:A:137:LYS:N	2.79	0.46
1:D:390:ASP:OD1	1:D:456:LYS:HD2	2.15	0.46
1:C:571:ARG:HH11	1:C:575:GLN:NE2	2.12	0.46
1:B:256:ASN:HB3	1:B:357(A):PHE:CE1	2.48	0.46
1:B:400:SER:O	1:B:407:LEU:HD11	2.15	0.46
1:A:940:PHE:CE2	1:A:967:ILE:HA	2.50	0.46
1:D:88:SER:C	1:D:90:LEU:H	2.18	0.46
1:D:142:HIS:HB2	1:D:145:HIS:CD2	2.51	0.46
1:C:398:ARG:NH2	1:C:451:ARG:NH1	2.63	0.46
1:C:622:ASN:HD21	1:C:624:TRP:HD1	1.63	0.46
1:D:70:GLU:HG3	1:D:92:PRO:HB3	1.96	0.46
1:B:345:VAL:O	1:B:348:GLN:HB3	2.14	0.46
1:C:870:GLN:O	1:C:873:ASN:N	2.48	0.46
1:B:373:ALA:HA	1:B:431:THR:O	2.14	0.46
1:B:571:ARG:HE	1:B:605:GLU:CD	2.18	0.46
1:A:680:LEU:HD22	1:A:955:PRO:HB3	1.98	0.46
1:A:690:ASN:O	1:A:694:GLN:HG2	2.15	0.46
1:D:566:THR:OG1	1:D:769:HIS:CE1	2.69	0.46
1:C:53:PHE:HD2	1:C:63:THR:HB	1.79	0.46
1:A:250:ILE:HD12	1:A:260:LEU:HD11	1.97	0.46
1:A:673:VAL:HG12	1:A:673:VAL:O	2.15	0.46
1:A:504:ILE:HG21	1:A:1042:MET:CE	2.45	0.46
1:D:1078:TYR:HB2	1:D:1085:ARG:HB3	1.98	0.46
1:C:141:PRO:HB3	1:C:305:VAL:O	2.14	0.46
1:B:370:LEU:O	1:B:432:HIS:HE1	1.99	0.46
1:A:149:PHE:HA	1:A:155:ALA:HB2	1.98	0.46
1:A:281:VAL:HB	1:A:474:GLY:HA3	1.98	0.46
1:A:597:VAL:HG13	1:A:827:ASP:HB3	1.97	0.46
1:C:881:LEU:C	1:C:883:LEU:H	2.18	0.46
1:A:738:LEU:HD21	1:A:759:LEU:HD13	1.97	0.46
1:D:266:SER:O	1:D:478:THR:HA	2.16	0.46
1:D:1024:ARG:HH21	1:D:1025:ASN:HD21	1.64	0.46
1:C:613:ASP:HB2	1:C:1013:TYR:CE2	2.51	0.46
1:B:647:ASN:HD22	1:B:647:ASN:H	1.64	0.46
1:C:700:SER:N	1:C:736:HIS:HD2	2.14	0.46
1:C:955:PRO:O	1:C:956:VAL:C	2.53	0.46
1:B:55:ALA:HA	1:B:58:GLU:HG3	1.97	0.46
1:A:329:VAL:HG22	1:A:348:GLN:HE22	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:LEU:CD1	1:A:759:LEU:HD11	2.46	0.45
1:C:69:ASN:HD22	1:C:72:LYS:HE3	1.81	0.45
1:C:269:ARG:O	1:C:270:ARG:C	2.55	0.45
1:C:1058:LEU:HB2	1:C:1060:ILE:HD11	1.97	0.45
1:B:717:ASN:HD22	1:B:717:ASN:N	2.10	0.45
1:A:98:ASN:HD22	1:A:101:ARG:H	1.63	0.45
1:A:170:THR:HG22	1:A:171:ASP:H	1.81	0.45
1:B:279:PRO:HD3	1:B:369:THR:HG21	1.99	0.45
1:B:593:LYS:O	1:B:597:VAL:HG23	2.16	0.45
1:D:753:TYR:CD1	1:D:789:ALA:HB2	2.51	0.45
1:D:861:ILE:H	1:D:861:ILE:HG13	1.61	0.45
1:D:951:GLU:HB2	1:D:952:ILE:HD12	1.97	0.45
1:C:287:LEU:C	1:C:289:GLN:N	2.70	0.45
1:C:408:ASP:HB2	1:C:428:LYS:HB2	1.98	0.45
1:C:912:LYS:HD3	1:C:916:ASP:OD2	2.15	0.45
1:D:567:ASP:O	1:D:605:GLU:N	2.44	0.45
1:D:590:ILE:HD11	1:D:838:TRP:CZ2	2.51	0.45
1:B:54:ARG:O	1:B:58:GLU:CG	2.61	0.45
1:B:371:GLY:HA2	1:B:434:ILE:O	2.16	0.45
1:A:322:PHE:CE2	1:A:325:VAL:HG23	2.50	0.45
1:D:643:LEU:O	1:D:676:ILE:HA	2.16	0.45
1:B:241:ASN:HB3	1:B:477:THR:HG21	1.98	0.45
1:B:251:GLY:HA3	1:B:257:ILE:HG12	1.98	0.45
1:B:529:ILE:HG21	1:B:589:ASN:O	2.17	0.45
1:B:676:ILE:HD11	1:B:693:VAL:HG21	1.98	0.45
1:A:479:LYS:HA	1:A:482:GLU:OE1	2.17	0.45
1:D:677:PHE:CB	1:D:703:THR:HB	2.41	0.45
1:D:802:SER:OG	1:D:809:SER:HB2	2.17	0.45
1:B:537:ILE:C	1:B:538(A):SER:N	2.70	0.45
1:B:794:ILE:HD12	1:B:796:THR:HG23	1.98	0.45
1:A:58:GLU:HG3	1:C:445:ARG:HG3	1.99	0.45
1:A:643:LEU:HD22	1:A:676:ILE:HG12	1.99	0.45
1:A:1061:LYS:HB3	1:A:1079:ALA:HB3	1.97	0.45
1:B:615:ALA:HA	1:B:619:LEU:HB2	1.99	0.45
1:A:283:LEU:HD22	1:A:287:LEU:HG	1.99	0.45
1:D:952:ILE:HG22	1:D:952:ILE:O	2.17	0.45
1:C:306:ASN:HA	1:C:351:VAL:HG11	1.98	0.45
1:B:39:LYS:CD	1:B:62:SER:HB2	2.47	0.45
1:A:322:PHE:HE2	1:A:325:VAL:HG23	1.82	0.45
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.52	0.45
1:A:638:LEU:HD22	1:A:672:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ILE:CG2	1:D:373:ALA:HB3	2.47	0.45
1:D:555:GLU:O	1:D:559:LYS:HG3	2.17	0.45
1:B:543:GLN:O	1:B:547:GLU:HG2	2.17	0.45
1:B:1035:THR:HB	1:B:1036:PRO:HD3	1.99	0.45
1:A:116:PRO:HG3	1:A:138:PHE:CZ	2.52	0.45
1:A:309:THR:HG21	1:A:330:GLN:HE22	1.81	0.45
1:A:346:LYS:HZ2	1:C:438:GLN:HE21	1.64	0.45
1:D:50:ILE:HG12	1:D:79:LYS:HG3	2.00	0.45
1:D:125:GLU:O	1:D:125:GLU:HG2	2.17	0.45
1:D:335:ILE:HG23	1:D:373:ALA:CB	2.46	0.45
1:C:778:ASN:ND2	1:B:816:ALA:HB2	2.33	0.45
1:B:265:CYS:O	1:B:268:GLN:NE2	2.49	0.45
1:A:504:ILE:HD13	1:A:1042:MET:CE	2.47	0.44
1:C:693:VAL:CG1	1:C:700:SER:OG	2.65	0.44
1:C:866:MET:HE2	1:C:871:TYR:CA	2.40	0.44
1:C:1070:GLU:H	1:C:1070:GLU:HG3	1.59	0.44
1:B:773:HIS:O	1:B:775:THR:N	2.50	0.44
1:D:993:LEU:C	1:D:995:GLU:H	2.20	0.44
1:C:700:SER:H	1:C:736:HIS:CD2	2.33	0.44
1:B:606:MET:SD	1:B:639:PHE:CD2	3.10	0.44
1:A:59:LEU:HD21	1:A:350:LEU:HD11	1.99	0.44
1:A:435:SER:OG	1:A:438:GLN:CG	2.66	0.44
1:A:753:TYR:HB2	1:A:785:GLN:HB3	1.99	0.44
1:D:568:THR:OG1	1:D:807:GLN:HG3	2.18	0.44
1:C:108:GLN:HG3	1:C:108:GLN:O	2.16	0.44
1:C:251:GLY:HA2	1:C:256:ASN:O	2.17	0.44
1:C:828:ILE:H	1:C:828:ILE:HG13	1.59	0.44
1:B:494:LEU:HB2	1:B:496:ARG:NH2	2.32	0.44
1:B:641:MET:CE	1:B:666:SER:HB3	2.48	0.44
1:B:1007:ILE:O	1:B:1011:VAL:HG23	2.18	0.44
1:D:501:LEU:HD22	1:D:1078:TYR:CD2	2.52	0.44
1:C:575:GLN:NE2	1:C:610:ALA:H	2.14	0.44
1:C:638:LEU:HD22	1:C:672:ASP:CB	2.47	0.44
1:C:927:ASP:O	1:C:931:VAL:HG23	2.16	0.44
1:B:626:ARG:HG2	1:B:630:LEU:HD12	1.98	0.44
1:B:935:GLY:HA2	1:B:938:LEU:HD12	1.99	0.44
1:A:243:LYS:HG3	1:A:266:SER:OG	2.17	0.44
1:A:248:GLN:HB2	1:A:263:ARG:HH12	1.81	0.44
1:A:339:VAL:HG23	1:A:340:THR:HG23	1.98	0.44
1:D:68:SER:HB3	1:D:95:SER:CB	2.48	0.44
1:B:42:VAL:HG12	1:B:44:ASN:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:LYS:HE2	1:B:767:PRO:HD3	1.97	0.44
1:A:242:PRO:O	1:A:477:THR:HB	2.18	0.44
1:A:266:SER:HB2	1:A:476:TYR:CD2	2.52	0.44
1:A:550:PRO:HB2	1:A:736:HIS:CE1	2.53	0.44
1:A:901:PHE:HZ	1:A:917:MET:HG3	1.83	0.44
1:C:422:TYR:O	1:C:423:ASP:C	2.56	0.44
1:A:861:ILE:HD11	1:A:866:MET:O	2.18	0.44
1:A:968:LEU:C	1:A:970:GLY:N	2.71	0.44
1:D:464:ASN:OD1	1:D:491:GLN:NE2	2.51	0.44
1:C:71:ASP:HB3	1:C:74:SER:HB3	1.99	0.44
1:C:496:ARG:HD2	1:C:1052:ILE:HD12	1.99	0.44
1:C:878:ALA:O	1:C:881:LEU:HA	2.18	0.44
1:C:874:LEU:O	1:C:878:ALA:HB2	2.17	0.44
1:B:550:PRO:HB2	1:B:736:HIS:CE1	2.52	0.44
1:B:560:GLN:OE1	1:B:825:ARG:NH2	2.51	0.44
1:A:798:VAL:CG1	1:A:835:SER:HA	2.48	0.44
1:D:241:ASN:N	1:D:242:PRO:CD	2.81	0.44
1:C:597:VAL:HG21	1:C:834:LEU:HG	2.00	0.44
1:B:493:SER:O	1:B:493:SER:OG	2.29	0.44
1:B:708:GLY:HA2	1:B:715:ARG:NH1	2.33	0.44
1:D:47:GLU:HG2	1:D:425:LEU:HD21	2.00	0.43
1:C:263:ARG:NH1	1:C:336:THR:HB	2.29	0.43
1:C:583:ARG:HG2	1:C:619:LEU:HD13	2.00	0.43
1:B:1059:ILE:N	1:B:1081:ASN:HD21	2.16	0.43
1:D:241:ASN:N	1:D:242:PRO:HD3	2.32	0.43
1:D:655:PRO:HG2	1:D:985:VAL:HG23	2.00	0.43
1:D:977:ARG:HH21	1:D:979:GLY:HA3	1.83	0.43
1:B:760:LYS:HG2	1:B:768:ILE:HD12	1.99	0.43
1:D:248:GLN:NE2	1:D:308:GLY:O	2.51	0.43
1:C:470:LYS:O	1:C:476:TYR:HB3	2.18	0.43
1:B:94:GLU:HA	1:B:97:LEU:HD12	2.00	0.43
1:B:167:ILE:HG13	1:B:168:PRO:HD2	2.00	0.43
1:B:380:THR:HG23	1:B:426:LEU:HD21	2.00	0.43
1:A:90:LEU:HD22	1:A:94:GLU:CG	2.48	0.43
1:A:346:LYS:NZ	1:C:438:GLN:HE21	2.16	0.43
1:A:781:LEU:HD12	1:D:780:LEU:HD12	2.00	0.43
1:B:516:VAL:CG1	1:B:517:GLU:N	2.65	0.43
1:C:313:LEU:HB2	1:C:323:ILE:HD13	1.99	0.43
1:B:142:HIS:CE1	1:B:305:VAL:HG21	2.53	0.43
1:B:309:THR:HB	1:B:326:ASN:HB2	1.99	0.43
1:B:377:ARG:HG3	1:B:377:ARG:NH1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ILE:HG13	1:B:418:ILE:CD1	2.48	0.43
1:A:500:THR:HG22	1:A:504:ILE:HD11	2.01	0.43
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.99	0.43
1:C:540:GLY:H	1:C:543:GLN:HG2	1.83	0.43
1:C:743:MET:SD	1:C:907:VAL:HG13	2.58	0.43
1:B:927:ASP:O	1:B:931:VAL:HG23	2.18	0.43
1:D:673:VAL:HG22	1:D:699:ILE:HD12	2.00	0.43
1:B:513:PRO:O	1:B:515:ASN:HB2	2.19	0.43
1:B:977:ARG:HA	1:B:978:PRO:HD3	1.91	0.43
1:A:380:THR:HG22	1:A:426:LEU:HD11	2.01	0.43
1:A:710:ILE:HD13	1:A:755:LEU:HD23	2.01	0.43
1:A:771:HIS:C	1:A:771:HIS:CD2	2.91	0.43
1:D:90:LEU:HD21	1:D:101:ARG:NH2	2.34	0.43
1:B:118:TYR:CZ	1:B:331:VAL:HG12	2.54	0.43
1:B:413:PHE:O	1:B:415:GLY:N	2.52	0.43
1:B:624:TRP:HB3	1:B:1005:GLN:HE22	1.83	0.43
1:B:711:LEU:HG	1:B:751:ALA:HB2	2.01	0.43
1:A:294:ALA:HA	1:A:297:GLN:HB2	2.00	0.43
1:A:399:SER:HA	1:A:450:MET:SD	2.59	0.43
1:A:1076:ILE:O	1:A:1086:ARG:HA	2.18	0.43
1:C:800:SER:O	1:C:842:ARG:NH1	2.52	0.43
1:C:964:GLN:O	1:C:968:LEU:HG	2.19	0.43
1:B:115:HIS:HA	1:B:116:PRO:HD3	1.72	0.43
1:B:126:GLN:HA	1:B:129:ARG:HH11	1.84	0.43
1:B:606:MET:HE1	1:B:671:ILE:HD13	1.99	0.43
1:A:38:LYS:HB2	1:A:112:ASP:OD1	2.19	0.43
1:A:755:LEU:O	1:A:759:LEU:HG	2.18	0.43
1:A:1002:VAL:HG13	1:A:1006:ASP:HB2	2.01	0.43
1:C:609:GLY:HA2	1:C:644:ARG:NH1	2.34	0.43
1:C:902:GLY:O	1:C:903:ASP:HB3	2.19	0.43
1:B:309:THR:O	1:B:325:VAL:HA	2.19	0.43
1:A:239:ILE:HG21	1:A:313:LEU:HD21	2.01	0.42
1:D:620:LYS:HD3	1:D:1023:THR:HG21	2.00	0.42
1:B:44:ASN:HD22	1:B:45:ARG:H	1.67	0.42
1:B:531:THR:HA	1:B:592:SER:OG	2.19	0.42
1:B:541:THR:CB	1:B:638:LEU:HG	2.49	0.42
1:B:860:GLU:HA	1:B:863:GLN:NE2	2.34	0.42
1:C:565:LEU:O	1:C:565:LEU:HD23	2.20	0.42
1:B:49:ALA:O	1:B:53:PHE:CD1	2.72	0.42
1:B:716:SER:OG	1:B:717(A):ILE:HD12	2.18	0.42
1:A:444:VAL:HG12	1:A:466:MET:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:VAL:HG12	1:D:274:VAL:HB	2.00	0.42
1:D:490:ILE:O	1:D:491:GLN:C	2.58	0.42
1:D:645:ALA:HB1	1:D:685:GLN:O	2.19	0.42
1:D:742:ASP:HB3	1:D:771:HIS:O	2.19	0.42
1:D:787:ILE:HA	1:D:822:ARG:HH21	1.84	0.42
1:A:287:LEU:HD22	1:A:318:ASP:OD1	2.18	0.42
1:A:570:PHE:HB2	1:A:606:MET:CB	2.45	0.42
1:A:889:GLU:O	1:A:893:MET:HB2	2.20	0.42
1:B:651:TYR:CZ	1:B:652:LYS:HD3	2.54	0.42
1:B:738:LEU:HD23	1:B:768:ILE:HG12	2.01	0.42
1:A:766:LEU:HA	1:A:767:PRO:HD2	1.87	0.42
1:D:276:GLU:OE2	1:D:332:GLU:HB3	2.19	0.42
1:D:783:TYR:O	1:D:784:LYS:C	2.57	0.42
1:C:647:ASN:O	1:C:649:VAL:N	2.47	0.42
1:B:45:ARG:HH22	1:B:411:ASP:CG	2.22	0.42
1:B:281:VAL:HG22	1:B:372:TYR:HE2	1.84	0.42
1:B:802:SER:HA	1:B:806:SER:HB3	2.02	0.42
1:A:326:ASN:HA	1:A:327:PRO:HD3	1.76	0.42
1:A:334:THR:HA	1:A:337:GLU:OE2	2.20	0.42
1:D:360:ILE:O	1:D:362:MET:N	2.53	0.42
1:D:522:PRO:HG2	1:D:524:TYR:CZ	2.55	0.42
1:C:750:LYS:HE2	1:B:820:PHE:CE2	2.54	0.42
1:B:571:ARG:NE	1:B:605:GLU:OE2	2.52	0.42
1:C:444:VAL:CG1	1:C:445:ARG:N	2.82	0.42
1:C:594:THR:HG23	1:C:598:PHE:HD1	1.83	0.42
1:C:883:LEU:HA	1:C:886:ARG:HB2	2.02	0.42
1:B:1000:GLY:N	1:B:1001:PRO:CD	2.76	0.42
1:A:615:ALA:HB3	1:A:623:PRO:HG3	2.00	0.42
1:C:671:ILE:HG22	1:C:674:PHE:CE2	2.54	0.42
1:C:867:PRO:O	1:C:868:GLY:O	2.37	0.42
1:B:379:THR:OG1	1:B:381:GLU:HG2	2.19	0.42
1:B:434:ILE:H	1:B:434:ILE:HG13	1.68	0.42
1:A:90:LEU:HD22	1:A:94:GLU:HG3	2.00	0.42
1:A:445:ARG:NH2	1:C:54:ARG:HB3	2.34	0.42
1:D:633:ALA:O	1:D:635:PRO:HD3	2.20	0.42
1:D:1058:LEU:HD23	1:D:1060:ILE:HD11	2.01	0.42
1:B:288:ARG:H	1:B:288:ARG:HG2	1.71	0.42
1:B:775:THR:CG2	1:B:861:ILE:HD13	2.47	0.42
1:A:597:VAL:HG22	1:A:830:GLY:HA3	2.02	0.42
1:C:494:LEU:HD23	1:C:496:ARG:NE	2.31	0.42
1:B:284:SER:CB	1:B:285:PRO:HD2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ASP:O	1:B:659:ILE:N	2.50	0.42
1:A:422:TYR:O	1:A:423:ASP:C	2.57	0.41
1:A:440:GLU:O	1:A:443:MET:HB3	2.20	0.41
1:A:588:ILE:HD13	1:A:588:ILE:O	2.20	0.41
1:D:273:LYS:O	1:D:377:ARG:NH2	2.53	0.41
1:C:53:PHE:CZ	1:C:65:ALA:HB2	2.55	0.41
1:B:118:TYR:CE2	1:B:331:VAL:CG1	3.03	0.41
1:B:145:HIS:HA	1:B:148:MET:HE2	2.02	0.41
1:B:572:ASP:HB2	1:B:605:GLU:OE1	2.20	0.41
1:B:667:ALA:HB1	1:B:698:LYS:HG3	2.02	0.41
1:A:701:GLU:OE1	1:A:739:ALA:HB2	2.20	0.41
1:A:731:GLU:HG3	1:A:766:LEU:CD2	2.46	0.41
1:D:251:GLY:O	1:D:306:ASN:N	2.51	0.41
1:D:772:THR:HG22	1:D:783:TYR:CZ	2.55	0.41
1:C:289:GLN:O	1:C:293:ASP:OD2	2.38	0.41
1:C:398:ARG:HH21	1:C:451:ARG:NH1	2.18	0.41
1:C:459:ILE:HB	1:C:460:PRO:HD3	2.02	0.41
1:B:264:ASP:HB2	1:B:280:SER:HB2	2.02	0.41
1:B:811:ASN:H	1:B:811:ASN:ND2	2.18	0.41
1:B:854:ILE:HD12	1:B:854:ILE:H	1.86	0.41
1:D:65:ALA:HB3	1:D:83:SER:HB3	2.02	0.41
1:D:242:PRO:HB2	1:D:313:LEU:HG	2.02	0.41
1:D:614:VAL:HG13	1:D:618:PHE:HB2	2.03	0.41
1:D:642:LEU:HD12	1:D:675:ARG:HB3	2.01	0.41
1:D:711:LEU:O	1:D:713:PRO:HD3	2.20	0.41
1:B:139:ILE:HG23	1:B:352:ALA:HB2	2.02	0.41
1:B:335:ILE:O	1:B:339:VAL:HG22	2.21	0.41
1:A:277:VAL:HG11	1:A:436:PHE:HE1	1.85	0.41
1:D:760:LYS:HG2	1:D:768:ILE:HD12	2.02	0.41
1:D:845:TYR:O	1:D:846:SER:C	2.58	0.41
1:C:329:VAL:HG13	1:C:348:GLN:NE2	2.35	0.41
1:C:433:ALA:HB3	1:C:438:GLN:HB3	2.03	0.41
1:C:923:GLN:HE21	1:C:923:GLN:HB2	1.66	0.41
1:B:339:VAL:HG12	1:B:432:HIS:CE1	2.55	0.41
1:B:828:ILE:HD12	1:B:829:GLU:H	1.86	0.41
1:A:1059:ILE:H	1:A:1081:ASN:ND2	2.18	0.41
1:C:440:GLU:OE2	1:C:466:MET:HB3	2.20	0.41
1:C:760:LYS:HE2	1:C:790:GLY:O	2.21	0.41
1:C:906:LYS:HD3	1:C:914:VAL:HG21	2.02	0.41
1:B:717(A):ILE:O	1:B:722:TYR:HB2	2.21	0.41
1:B:719:THR:CG2	1:B:720:LEU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:MET:SD	1:B:907:VAL:HG13	2.60	0.41
1:A:444:VAL:HG23	1:A:445:ARG:N	2.36	0.41
1:A:909:PRO:HD2	1:A:952:ILE:HD11	2.03	0.41
1:D:41:LEU:HD12	1:D:64:VAL:HG11	2.03	0.41
1:D:59:LEU:HG	1:D:346:LYS:HD2	2.02	0.41
1:D:145:HIS:CE1	1:D:304:TYR:HA	2.55	0.41
1:D:255:GLY:O	1:D:257:ILE:HG13	2.21	0.41
1:D:864:HIS:O	1:D:864:HIS:CD2	2.74	0.41
1:B:45:ARG:HG3	1:B:45:ARG:HH11	1.85	0.41
1:B:641:MET:HE3	1:B:674:PHE:CE1	2.55	0.41
1:B:647:ASN:O	1:B:649:VAL:N	2.52	0.41
1:B:994:LEU:HB3	1:B:1002:VAL:HG21	2.02	0.41
1:A:496:ARG:HH22	1:A:1029:ASN:HB2	1.86	0.41
1:D:641:MET:HE2	1:D:671:ILE:HG21	2.03	0.41
1:C:145:HIS:CE1	1:C:302:ILE:O	2.63	0.41
1:C:309:THR:O	1:C:325:VAL:HA	2.21	0.41
1:C:712:ASN:HA	1:C:713:PRO:HD2	1.90	0.41
1:C:890:VAL:O	1:C:891:LYS:C	2.59	0.41
1:B:622:ASN:HD21	1:B:624:TRP:HB2	1.85	0.41
1:B:701:GLU:CG	1:B:739:ALA:HB2	2.49	0.41
1:B:704:ILE:HG23	1:B:726:LEU:HD23	2.01	0.41
1:A:494:LEU:H	1:A:494:LEU:CD1	2.33	0.41
1:A:582:VAL:HA	1:A:845:TYR:CZ	2.55	0.41
1:A:881:LEU:HD12	1:A:919:LEU:HD12	2.03	0.41
1:D:286:THR:O	1:D:287:LEU:C	2.58	0.41
1:D:465:VAL:HG13	1:D:480:PHE:HE2	1.86	0.41
1:D:553:VAL:O	1:D:557:VAL:HG23	2.21	0.41
1:C:246:GLU:OE1	1:C:332:GLU:OE2	2.38	0.41
1:C:331:VAL:HG22	1:C:428:LYS:HD3	2.03	0.41
1:C:749:PRO:HG3	1:C:781:LEU:HB3	2.03	0.41
1:C:817:LEU:HD13	1:C:822:ARG:O	2.21	0.41
1:B:39:LYS:O	1:B:112:ASP:OD1	2.37	0.41
1:B:242:PRO:HB2	1:B:313:LEU:HG	2.02	0.41
1:B:867:PRO:O	1:B:868:GLY:C	2.59	0.41
2:B:2001:COA:C9P	2:B:2001:COA:H8A	2.51	0.41
1:C:419:SER:HA	1:C:420:PRO:HD3	1.94	0.41
1:C:717:ASN:HD22	1:C:717:ASN:N	2.18	0.41
1:C:840:THR:O	1:C:843:THR:HB	2.21	0.41
1:B:606:MET:HE3	1:B:607:TRP:HB2	2.01	0.41
1:B:811:ASN:ND2	1:B:831:MET:HG2	2.36	0.41
1:A:504:ILE:HG21	1:A:1042:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:LEU:O	1:C:289:GLN:N	2.54	0.40
1:C:622:ASN:HD22	1:C:623:PRO:CD	2.33	0.40
1:B:799:ALA:H	1:B:811:ASN:ND2	2.18	0.40
1:A:278:ALA:HA	1:A:279:PRO:HA	1.85	0.40
1:A:590:ILE:H	1:A:590:ILE:HG13	1.71	0.40
1:A:626:ARG:HG2	1:A:630:LEU:HD12	2.03	0.40
1:A:667:ALA:HB1	1:A:698:LYS:HG3	2.02	0.40
1:D:679:SER:HA	1:D:907:VAL:CG2	2.51	0.40
1:D:683:VAL:HG12	1:D:687:LYS:HE3	2.02	0.40
1:D:747:LEU:HD23	1:D:770:LEU:HD11	2.03	0.40
1:B:622:ASN:ND2	1:B:624:TRP:H	2.19	0.40
1:A:738:LEU:HD23	1:A:768:ILE:HG12	2.04	0.40
1:A:760:LYS:HG2	1:A:768:ILE:HD12	2.01	0.40
1:A:770:LEU:HD12	1:A:771:HIS:H	1.87	0.40
1:C:521:LYS:HD3	1:C:1040:PHE:HB2	2.04	0.40
1:B:870:GLN:O	1:B:874:LEU:HB2	2.21	0.40
1:A:74:SER:OG	1:A:75:LEU:N	2.54	0.40
1:A:452:ILE:HD12	1:A:459:ILE:HD11	2.04	0.40
1:A:681:ASN:HD21	1:A:705:CYS:N	2.20	0.40
1:A:1035:THR:HB	1:A:1036:PRO:HD3	2.03	0.40
1:D:796:THR:OG1	1:D:810:ALA:HB2	2.21	0.40
1:C:1029:ASN:ND2	1:C:1031:SER:OG	2.53	0.40
1:C:1077:TYR:CD1	1:C:1077:TYR:N	2.90	0.40
1:B:59:LEU:HD11	1:B:346:LYS:HG3	2.03	0.40
1:B:391:THR:OG1	1:B:418:ILE:O	2.37	0.40
1:B:624:TRP:HB3	1:B:1005:GLN:NE2	2.37	0.40
1:B:836:HIS:O	1:B:839:SER:HB3	2.21	0.40
1:B:1077:TYR:CD1	1:B:1077:TYR:N	2.89	0.40
1:A:736:HIS:O	1:A:766:LEU:HD12	2.21	0.40
1:A:947:PHE:HD2	1:A:952:ILE:HG21	1.87	0.40
1:C:141:PRO:HG3	1:C:304:TYR:OH	2.22	0.40
2:C:2001:COA:O2A	2:C:2001:COA:H10	2.20	0.40
1:B:114:ILE:HD12	1:B:131:CYS:SG	2.62	0.40
1:B:151:ASP:OD1	1:B:152:LYS:N	2.55	0.40
1:B:298:LEU:O	1:B:302:ILE:HG13	2.21	0.40
1:B:313:LEU:HB2	1:B:323:ILE:HD11	2.04	0.40
1:B:521:LYS:HA	1:B:522:PRO:HD3	1.88	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	990/1150 (86%)	862 (87%)	105 (11%)	23 (2%)	6	23
1	B	985/1150 (86%)	875 (89%)	89 (9%)	21 (2%)	7	26
1	C	991/1150 (86%)	887 (90%)	79 (8%)	25 (2%)	5	21
1	D	924/1150 (80%)	777 (84%)	123 (13%)	24 (3%)	5	20
All	All	3890/4600 (85%)	3401 (87%)	396 (10%)	93 (2%)	6	22

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	868	GLY
1	A	939	ASP
1	D	87	GLY
1	D	163	ASP
1	D	272	GLN
1	D	361	ASN
1	C	170	THR
1	C	386	ASP
1	C	387	PHE
1	C	828	ILE
1	C	870	GLN
1	B	414	GLN
1	B	423	ASP
1	B	494	LEU
1	B	520	PRO
1	B	522	PRO
1	B	868	GLY
1	B	870	GLN
1	B	1001	PRO
1	A	148	MET
1	A	434	ILE
1	A	674	PHE

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Mol	Chain	Res	Type
1	A	925	ASP
1	A	1026	GLN
1	D	99	ILE
1	D	274	VAL
1	D	424	SER
1	D	515	ASN
1	D	959	PHE
1	C	89	ASP
1	C	747	LEU
1	C	854	ILE
1	C	868	GLY
1	C	881	LEU
1	B	538	ALA
1	B	1053	ASP
1	B	1070	GLU
1	A	366	ASP
1	A	416	ALA
1	A	648	ALA
1	A	761	SER
1	A	854	ILE
1	D	60	ASP
1	D	256	ASN
1	D	414	GLN
1	C	270	ARG
1	B	120	PHE
1	B	648	ALA
1	B	696	ALA
1	A	120	PHE
1	A	307	ALA
1	A	424	SER
1	A	480	PHE
1	D	241	ASN
1	D	271	HIS
1	D	648	ALA
1	C	106	ALA
1	C	288	ARG
1	C	648	ALA
1	C	649	VAL
1	C	933	THR
1	B	1002	VAL
1	A	433	ALA
1	A	494	LEU

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Mol	Chain	Res	Type
1	A	620	LYS
1	A	826	THR
1	D	491	GLN
1	D	886	ARG
1	C	120	PHE
1	C	241	ASN
1	C	306	ASN
1	C	400	SER
1	C	934	ASP
1	B	480	PHE
1	A	1014	PRO
1	B	869	GLY
1	A	1072	GLY
1	D	635	PRO
1	C	956	VAL
1	B	87	GLY
1	B	166	VAL
1	B	354	GLY
1	D	649	VAL
1	D	749	PRO
1	D	1000	GLY
1	C	550	PRO
1	C	749	PRO
1	D	434	ILE
1	D	485	PRO
1	D	828	ILE
1	C	861	ILE
1	A	1000	GLY
1	B	516	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	860/987 (87%)	783 (91%)	77 (9%)	9 29
1	B	856/987 (87%)	762 (89%)	94 (11%)	6 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	861/987 (87%)	759 (88%)	102 (12%)	5 16
1	D	806/987 (82%)	711 (88%)	95 (12%)	5 16
All	All	3383/3948 (86%)	3015 (89%)	368 (11%)	6 19

All (368) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	83	SER
1	A	98	ASN
1	A	108	GLN
1	A	123	GLU
1	A	126	GLN
1	A	151	ASP
1	A	170	THR
1	A	241	ASN
1	A	269	ARG
1	A	274	VAL
1	A	284	SER
1	A	287	LEU
1	A	299	MET
1	A	326	ASN
1	A	329	VAL
1	A	331	VAL
1	A	366	ASP
1	A	375	GLN
1	A	393	THR
1	A	418	ILE
1	A	427	VAL
1	A	440	GLU
1	A	445	ARG
1	A	446	SER
1	A	455	VAL
1	A	472	THR
1	A	486	GLU
1	A	491	GLN
1	A	493	SER
1	A	506	ASN
1	A	518	LYS
1	A	523	ASP
1	A	526	LEU

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Mol	Chain	Res	Type
1	A	548	VAL
1	A	565	LEU
1	A	567	ASP
1	A	580	THR
1	A	588	ILE
1	A	606	MET
1	A	607	TRP
1	A	630	LEU
1	A	632	LYS
1	A	657	ASN
1	A	661	LYS
1	A	668	LYS
1	A	672	ASP
1	A	685	GLN
1	A	714	GLU
1	A	715	ARG
1	A	725	LYS
1	A	743	MET
1	A	750	LYS
1	A	755	LEU
1	A	780	LEU
1	A	784	LYS
1	A	793	ILE
1	A	805	THR
1	A	807	GLN
1	A	813	LEU
1	A	828	ILE
1	A	839	SER
1	A	861	ILE
1	A	870	GLN
1	A	907	VAL
1	A	924	ASN
1	A	934	ASP
1	A	952	ILE
1	A	962	ASP
1	A	969	LYS
1	A	989	LYS
1	A	991	ARG
1	A	1048	VAL
1	A	1058	LEU
1	A	1062	LEU
1	A	1064	THR

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Mol	Chain	Res	Type
1	A	1085	ARG
1	D	36	GLN
1	D	44	ASN
1	D	69	ASN
1	D	99	ILE
1	D	101	ARG
1	D	125	GLU
1	D	131	CYS
1	D	137	LYS
1	D	143	LEU
1	D	144	GLU
1	D	147	ASP
1	D	158	THR
1	D	166	VAL
1	D	262	GLU
1	D	283	LEU
1	D	288	ARG
1	D	290	ARG
1	D	296	ILE
1	D	298	LEU
1	D	300	GLU
1	D	301	ASN
1	D	303	LYS
1	D	306	ASN
1	D	329	VAL
1	D	331	VAL
1	D	339	VAL
1	D	346	LYS
1	D	357(A)	PHE
1	D	358	GLU
1	D	360	ILE
1	D	362	MET
1	D	365	LYS
1	D	368	THR
1	D	374	ILE
1	D	375	GLN
1	D	417	GLU
1	D	434	ILE
1	D	440	GLU
1	D	442	LYS
1	D	445	ARG
1	D	451	ARG

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Mol	Chain	Res	Type
1	D	456	LYS
1	D	482	GLU
1	D	517	GLU
1	D	525	GLU
1	D	541	THR
1	D	543	GLN
1	D	544	LEU
1	D	551	LYS
1	D	569	THR
1	D	575	GLN
1	D	580	THR
1	D	588	ILE
1	D	592	SER
1	D	606	MET
1	D	607	TRP
1	D	631	ARG
1	D	636	ASN
1	D	644	ARG
1	D	651	TYR
1	D	661	LYS
1	D	685	GLN
1	D	691	GLU
1	D	707	THR
1	D	715	ARG
1	D	719	THR
1	D	743	MET
1	D	747	LEU
1	D	760	LYS
1	D	766	LEU
1	D	780	LEU
1	D	781	LEU
1	D	792	ASP
1	D	818	ASN
1	D	822	ARG
1	D	827	ASP
1	D	839	SER
1	D	840	THR
1	D	856	SER
1	D	891	LYS
1	D	892	ASP
1	D	949	LYS
1	D	956	VAL

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Mol	Chain	Res	Type
1	D	971	GLN
1	D	983	GLU
1	D	1003	THR
1	D	1019	GLN
1	D	1044	ASN
1	D	1048	VAL
1	D	1052	ILE
1	D	1059	ILE
1	D	1061	LYS
1	D	1064	THR
1	D	1083	GLN
1	D	1086	ARG
1	C	36	GLN
1	C	45	ARG
1	C	60	ASP
1	C	75	LEU
1	C	83	SER
1	C	98	ASN
1	C	100	GLU
1	C	101	ARG
1	C	103	ILE
1	C	107	LYS
1	C	137	LYS
1	C	147	ASP
1	C	170	THR
1	C	240	ASP
1	C	257	ILE
1	C	262	GLU
1	C	271	HIS
1	C	275	VAL
1	C	281	VAL
1	C	286	THR
1	C	287	LEU
1	C	318	ASP
1	C	319	GLU
1	C	323	ILE
1	C	336	THR
1	C	346	LYS
1	C	356	ASP
1	C	359	GLU
1	C	365	LYS
1	C	368	THR

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Mol	Chain	Res	Type
1	C	370	LEU
1	C	377	ARG
1	C	386	ASP
1	C	411	ASP
1	C	427	VAL
1	C	434	ILE
1	C	437	LYS
1	C	445	ARG
1	C	484	THR
1	C	489	ASP
1	C	493	SER
1	C	498	THR
1	C	519	ARG
1	C	523	ASP
1	C	525	GLU
1	C	526	LEU
1	C	555	GLU
1	C	565	LEU
1	C	571	ARG
1	C	580	THR
1	C	588	ILE
1	C	606	MET
1	C	607	TRP
1	C	613	ASP
1	C	622	ASN
1	C	641	MET
1	C	644	ARG
1	C	649	VAL
1	C	656	ASP
1	C	671	ILE
1	C	704	ILE
1	C	707	THR
1	C	717	ASN
1	C	728	LYS
1	C	743	MET
1	C	766	LEU
1	C	781	LEU
1	C	784	LYS
1	C	796	THR
1	C	809	SER
1	C	818	ASN
1	C	828	ILE

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Mol	Chain	Res	Type
1	C	847	ASP
1	C	872	SER
1	C	888	ASP
1	C	892	ASP
1	C	907	VAL
1	C	912	LYS
1	C	923	GLN
1	C	927	ASP
1	C	933	THR
1	C	949	LYS
1	C	968	LEU
1	C	969	LYS
1	C	971	GLN
1	C	972	GLU
1	C	982	LEU
1	C	988	GLU
1	C	991	ARG
1	C	996	GLU
1	C	998	GLN
1	C	999	GLN
1	C	1008	ILE
1	C	1015	LYS
1	C	1029	ASN
1	C	1044	ASN
1	C	1048	VAL
1	C	1058	LEU
1	C	1085	ARG
1	C	1091	ASP
1	C	1092	GLU
1	C	1093	ASN
1	B	39	LYS
1	B	40	LEU
1	B	44	ASN
1	B	58	GLU
1	B	89	ASP
1	B	90	LEU
1	B	98	ASN
1	B	101	ARG
1	B	144	GLU
1	B	156	ARG
1	B	163	ASP
1	B	239	ILE

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Mol	Chain	Res	Type
1	B	250	ILE
1	B	253	GLU
1	B	269	ARG
1	B	270	ARG
1	B	272	GLN
1	B	286	THR
1	B	287	LEU
1	B	288	ARG
1	B	306	ASN
1	B	318	ASP
1	B	329	VAL
1	B	384	LEU
1	B	393	THR
1	B	399	SER
1	B	426	LEU
1	B	427	VAL
1	B	429	LEU
1	B	435	SER
1	B	469	LYS
1	B	473	SER
1	B	479	LYS
1	B	491	GLN
1	B	518	LYS
1	B	525	GLU
1	B	526	LEU
1	B	536	LYS
1	B	537	ILE
1	B	547	GLU
1	B	580	THR
1	B	581	ARG
1	B	588	ILE
1	B	596	ASP
1	B	605	GLU
1	B	606	MET
1	B	607	TRP
1	B	622	ASN
1	B	631	ARG
1	B	647	ASN
1	B	649	VAL
1	B	657	ASN
1	B	684	ASP
1	B	715	ARG

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Mol	Chain	Res	Type
1	B	717	ASN
1	B	717(A)	ILE
1	B	719	THR
1	B	743	MET
1	B	766	LEU
1	B	781	LEU
1	B	784	LYS
1	B	806	SER
1	B	809	SER
1	B	825	ARG
1	B	828	ILE
1	B	833	SER
1	B	858	ASN
1	B	863	GLN
1	B	866	MET
1	B	871	TYR
1	B	872	SER
1	B	873	ASN
1	B	888	ASP
1	B	907	VAL
1	B	908	THR
1	B	917	MET
1	B	919	LEU
1	B	928	GLU
1	B	945	VAL
1	B	957	ASN
1	B	975	THR
1	B	977	ARG
1	B	989	LYS
1	B	1008	ILE
1	B	1009	SER
1	B	1019	GLN
1	B	1029	ASN
1	B	1044	ASN
1	B	1053	ASP
1	B	1077	TYR
1	B	1081	ASN
1	B	1086	ARG
1	B	1092	GLU
1	B	1093	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	ASN
1	A	98	ASN
1	A	126	GLN
1	A	241	ASN
1	A	244	HIS
1	A	254	HIS
1	A	326	ASN
1	A	330	GLN
1	A	375	GLN
1	A	414	GLN
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	575	GLN
1	A	664	GLN
1	A	685	GLN
1	A	736	HIS
1	A	778	ASN
1	A	811	ASN
1	A	898	ASN
1	A	924	ASN
1	A	960	ASN
1	A	1025	ASN
1	A	1081	ASN
1	D	44	ASN
1	D	145	HIS
1	D	289	GLN
1	D	330	GLN
1	D	364	GLN
1	D	414	GLN
1	D	464	ASN
1	D	491	GLN
1	D	506	ASN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	653	ASN
1	D	694	GLN
1	D	736	HIS
1	D	778	ASN
1	D	811	ASN
1	D	818	ASN

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Mol	Chain	Res	Type
1	D	864	HIS
1	D	1005	GLN
1	D	1025	ASN
1	D	1026	GLN
1	D	1029	ASN
1	D	1044	ASN
1	C	44	ASN
1	C	69	ASN
1	C	98	ASN
1	C	126	GLN
1	C	145	HIS
1	C	271	HIS
1	C	297	GLN
1	C	326	ASN
1	C	330	GLN
1	C	432	HIS
1	C	438	GLN
1	C	464	ASN
1	C	574	HIS
1	C	575	GLN
1	C	622	ASN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	811	ASN
1	C	818	ASN
1	C	823	HIS
1	C	864	HIS
1	C	870	GLN
1	C	873	ASN
1	C	876	GLN
1	C	898	ASN
1	C	923	GLN
1	C	957	ASN
1	C	1005	GLN
1	C	1025	ASN
1	C	1029	ASN
1	C	1044	ASN
1	C	1083	GLN
1	B	44	ASN
1	B	142	HIS
1	B	145	HIS

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Mol	Chain	Res	Type
1	B	241	ASN
1	B	297	GLN
1	B	306	ASN
1	B	326	ASN
1	B	330	GLN
1	B	333	HIS
1	B	348	GLN
1	B	414	GLN
1	B	438	GLN
1	B	491	GLN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN
1	B	589	ASN
1	B	617	ASN
1	B	622	ASN
1	B	647	ASN
1	B	657	ASN
1	B	717	ASN
1	B	736	HIS
1	B	771	HIS
1	B	778	ASN
1	B	811	ASN
1	B	858	ASN
1	B	864	HIS
1	B	873	ASN
1	B	877	GLN
1	B	898	ASN
1	B	923	GLN
1	B	960	ASN
1	B	999	GLN
1	B	1005	GLN
1	B	1019	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1044	ASN
1	B	1081	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
2	COA	C	2001	-	43,50,50	1.08	1 (2%)	56,75,75	1.57	6 (10%)
4	BTI	B	2000	-	15,16,16	1.62	2 (13%)	20,21,21	1.95	3 (15%)
2	COA	A	2001	-	43,50,50	1.39	3 (6%)	56,75,75	1.67	7 (12%)
2	COA	B	2001	-	43,50,50	1.26	4 (9%)	56,75,75	1.72	8 (14%)
4	BTI	C	2000	-	15,16,16	1.70	2 (13%)	20,21,21	2.23	3 (15%)
2	COA	D	2001	-	43,50,50	1.07	1 (2%)	56,75,75	1.64	5 (8%)

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	COA	C	2001	-	-	14/44/64/64	0/3/3/3
4	BTI	B	2000	-	-	3/6/27/27	0/2/2/2
2	COA	A	2001	-	-	16/44/64/64	0/3/3/3
2	COA	B	2001	-	-	17/44/64/64	0/3/3/3
4	BTI	C	2000	-	-	5/6/27/27	0/2/2/2
2	COA	D	2001	-	-	4/44/64/64	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	COA	P2A-O3A	5.00	1.64	1.59
4	C	2000	BTI	O3-C3	4.72	1.33	1.23
4	B	2000	BTI	O3-C3	4.41	1.32	1.23
2	A	2001	COA	P1A-O3A	4.10	1.63	1.59
4	C	2000	BTI	C2-S1	-3.68	1.76	1.82
2	B	2001	COA	P3B-O7A	3.59	1.61	1.50
4	B	2000	BTI	C2-S1	-3.42	1.77	1.82
2	C	2001	COA	P3B-O7A	3.40	1.61	1.50
2	A	2001	COA	P3B-O7A	3.29	1.60	1.50
2	D	2001	COA	P3B-O7A	3.04	1.59	1.50
2	B	2001	COA	P1A-O3A	2.94	1.62	1.59
2	B	2001	COA	P3B-O3B	2.83	1.64	1.59
2	B	2001	COA	P3B-O9A	-2.04	1.47	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2001	COA	O4B-C1B-N9A	-7.91	98.26	108.75
4	B	2000	BTI	C6-C5-N3	-6.36	104.99	113.18
4	C	2000	BTI	C2-C4-N2	-6.31	106.66	113.34
4	C	2000	BTI	C6-C5-N3	-6.26	105.12	113.18
2	A	2001	COA	O4B-C1B-N9A	-6.19	100.54	108.75
2	C	2001	COA	C4B-O4B-C1B	-5.93	104.50	109.92
2	B	2001	COA	O4B-C1B-N9A	-5.64	101.27	108.75
2	B	2001	COA	C4B-O4B-C1B	-5.62	104.78	109.92
2	D	2001	COA	N3A-C2A-N1A	-5.39	121.36	128.67
2	A	2001	COA	N3A-C2A-N1A	-5.25	121.55	128.67
2	C	2001	COA	N3A-C2A-N1A	-4.98	121.91	128.67
2	C	2001	COA	O4B-C1B-N9A	-4.84	102.32	108.75
2	A	2001	COA	C4B-O4B-C1B	-4.82	105.51	109.92
2	B	2001	COA	N3A-C2A-N1A	-4.61	122.42	128.67
4	B	2000	BTI	C2-C4-N2	-4.45	108.63	113.34
2	B	2001	COA	O4B-C4B-C5B	-3.70	97.48	109.33
2	A	2001	COA	C7P-N8P-C9P	3.47	128.77	122.55
2	B	2001	COA	CDP-CBP-CAP	3.45	114.65	108.77
2	D	2001	COA	C4B-O4B-C1B	-3.42	106.80	109.92
2	A	2001	COA	O8A-P3B-O7A	-2.65	100.52	110.83
2	C	2001	COA	C4A-C5A-N7A	-2.53	106.67	109.34
4	C	2000	BTI	N2-C3-N3	2.50	111.74	108.85
4	B	2000	BTI	N2-C3-N3	2.38	111.59	108.85
2	B	2001	COA	CEP-CBP-CCP	2.27	111.97	108.22
2	B	2001	COA	O8A-P3B-O7A	-2.21	102.23	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	COA	O9A-P3B-O7A	2.18	119.33	110.83
2	C	2001	COA	O8A-P3B-O7A	-2.09	102.68	110.83
2	C	2001	COA	CDP-CBP-CAP	2.09	112.32	108.77
2	D	2001	COA	O8A-P3B-O7A	-2.03	102.92	110.83
2	D	2001	COA	CDP-CBP-CAP	2.03	112.23	108.77
2	A	2001	COA	C6P-C7P-N8P	2.03	116.31	112.00
2	A	2001	COA	C3B-C2B-C1B	2.02	104.34	99.89

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	COA	CCP-O6A-P2A-O3A
2	A	2001	COA	CCP-O6A-P2A-O4A
2	A	2001	COA	CCP-O6A-P2A-O5A
2	A	2001	COA	C9P-CAP-CBP-CCP
2	D	2001	COA	S1P-C2P-C3P-N4P
2	C	2001	COA	CCP-O6A-P2A-O3A
2	C	2001	COA	CCP-O6A-P2A-O4A
2	C	2001	COA	CCP-O6A-P2A-O5A
2	C	2001	COA	C9P-CAP-CBP-CCP
2	C	2001	COA	C9P-CAP-CBP-CDP
2	C	2001	COA	OAP-CAP-CBP-CEP
2	C	2001	COA	C9P-CAP-CBP-CEP
2	B	2001	COA	C5B-O5B-P1A-O1A
2	B	2001	COA	CDP-CBP-CCP-O6A
2	B	2001	COA	OAP-CAP-CBP-CCP
2	B	2001	COA	C9P-CAP-CBP-CCP
2	B	2001	COA	OAP-CAP-CBP-CDP
2	B	2001	COA	C9P-CAP-CBP-CDP
2	B	2001	COA	OAP-CAP-CBP-CEP
2	B	2001	COA	C9P-CAP-CBP-CEP
2	B	2001	COA	O9P-C9P-CAP-CBP
2	B	2001	COA	N8P-C9P-CAP-CBP
2	B	2001	COA	O9P-C9P-CAP-OAP
2	B	2001	COA	N8P-C9P-CAP-OAP
2	B	2001	COA	S1P-C2P-C3P-N4P
4	C	2000	BTI	S1-C2-C7-C8
4	C	2000	BTI	C4-C2-C7-C8
4	B	2000	BTI	S1-C2-C7-C8
4	B	2000	BTI	C4-C2-C7-C8
2	A	2001	COA	C6P-C7P-N8P-C9P

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Mol	Chain	Res	Type	Atoms
2	D	2001	COA	C2B-C3B-O3B-P3B
2	A	2001	COA	C2B-C3B-O3B-P3B
2	B	2001	COA	C2B-C3B-O3B-P3B
4	C	2000	BTI	C2-C7-C8-C9
2	B	2001	COA	C6P-C7P-N8P-C9P
2	A	2001	COA	C4B-C3B-O3B-P3B
2	B	2001	COA	C4B-C3B-O3B-P3B
4	C	2000	BTI	C7-C8-C9-C10
2	C	2001	COA	C6P-C7P-N8P-C9P
2	C	2001	COA	OAP-CAP-CBP-CDP
4	B	2000	BTI	C7-C8-C9-C10
2	A	2001	COA	N8P-C9P-CAP-OAP
2	A	2001	COA	C9P-CAP-CBP-CDP
4	C	2000	BTI	C11-C10-C9-C8
2	B	2001	COA	CEP-CBP-CCP-O6A
2	C	2001	COA	OAP-CAP-CBP-CCP
2	C	2001	COA	C4B-C3B-O3B-P3B
2	A	2001	COA	C3B-O3B-P3B-O9A
2	C	2001	COA	C3B-O3B-P3B-O9A
2	C	2001	COA	C2B-C3B-O3B-P3B
2	A	2001	COA	O5P-C5P-C6P-C7P
2	D	2001	COA	C4B-C3B-O3B-P3B
2	A	2001	COA	N4P-C5P-C6P-C7P
2	A	2001	COA	C9P-CAP-CBP-CEP
2	A	2001	COA	OAP-CAP-CBP-CEP
2	A	2001	COA	P2A-O3A-P1A-O1A
2	A	2001	COA	P2A-O3A-P1A-O2A
2	D	2001	COA	C3B-O3B-P3B-O9A
2	C	2001	COA	S1P-C2P-C3P-N4P

There are no ring outliers.

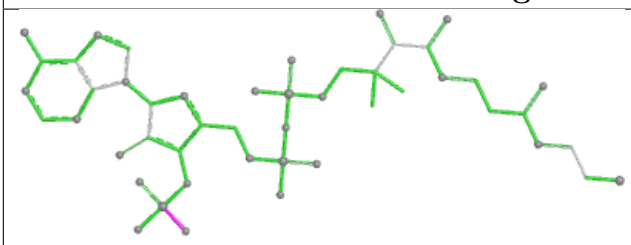
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	COA	2	0
2	B	2001	COA	1	0
4	C	2000	BTI	3	0
2	D	2001	COA	6	0

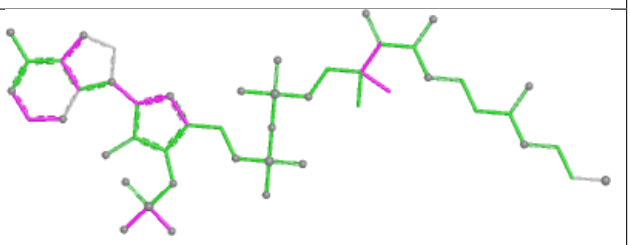
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

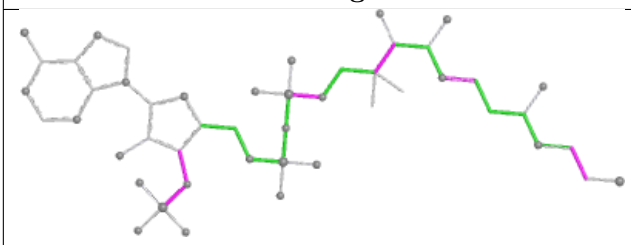
Ligand COA C 2001



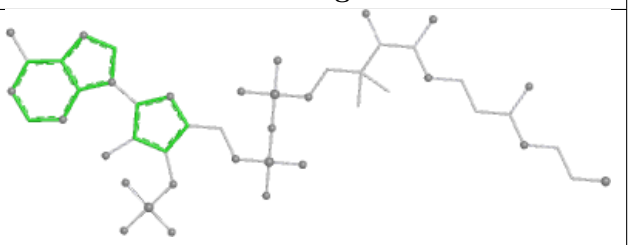
Bond lengths



Bond angles

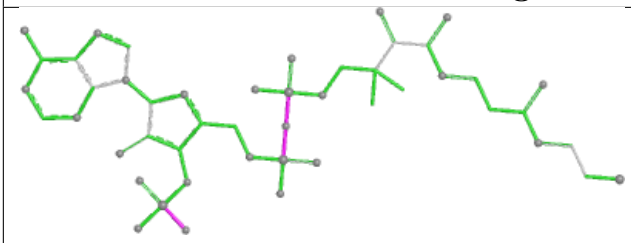


Torsions

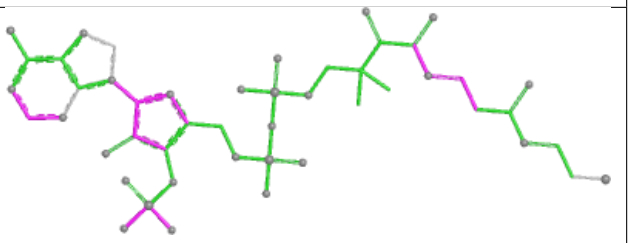


Rings

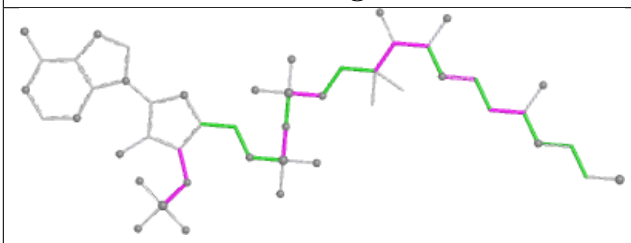
Ligand COA A 2001



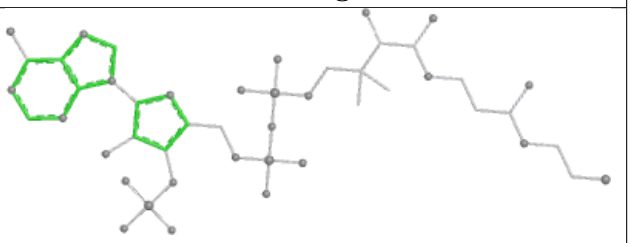
Bond lengths



Bond angles

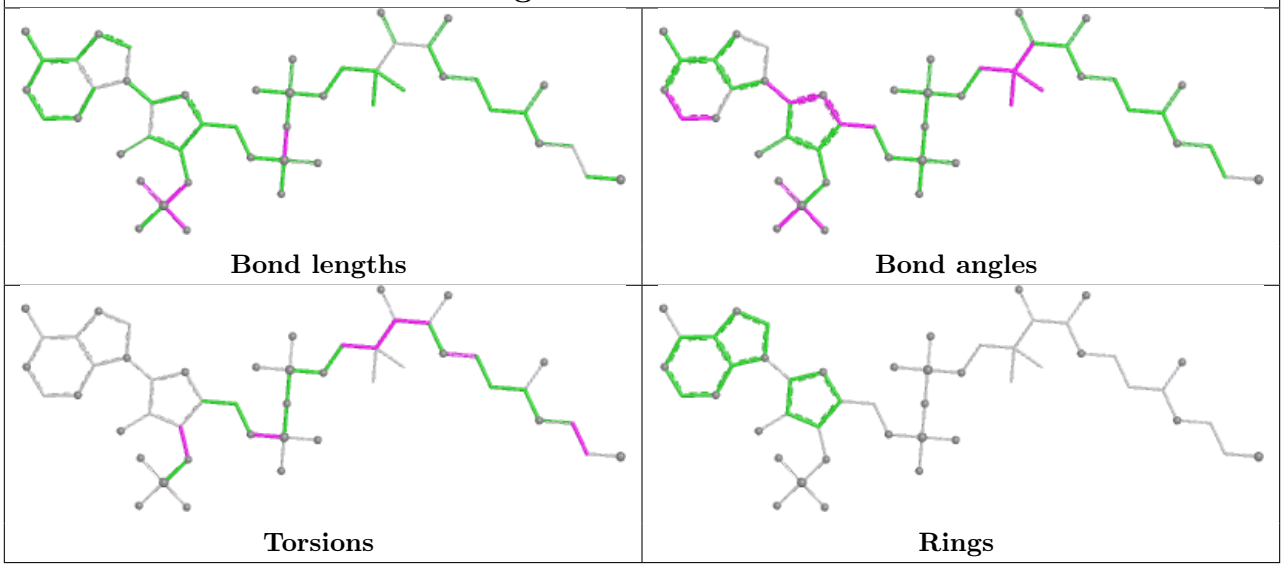


Torsions

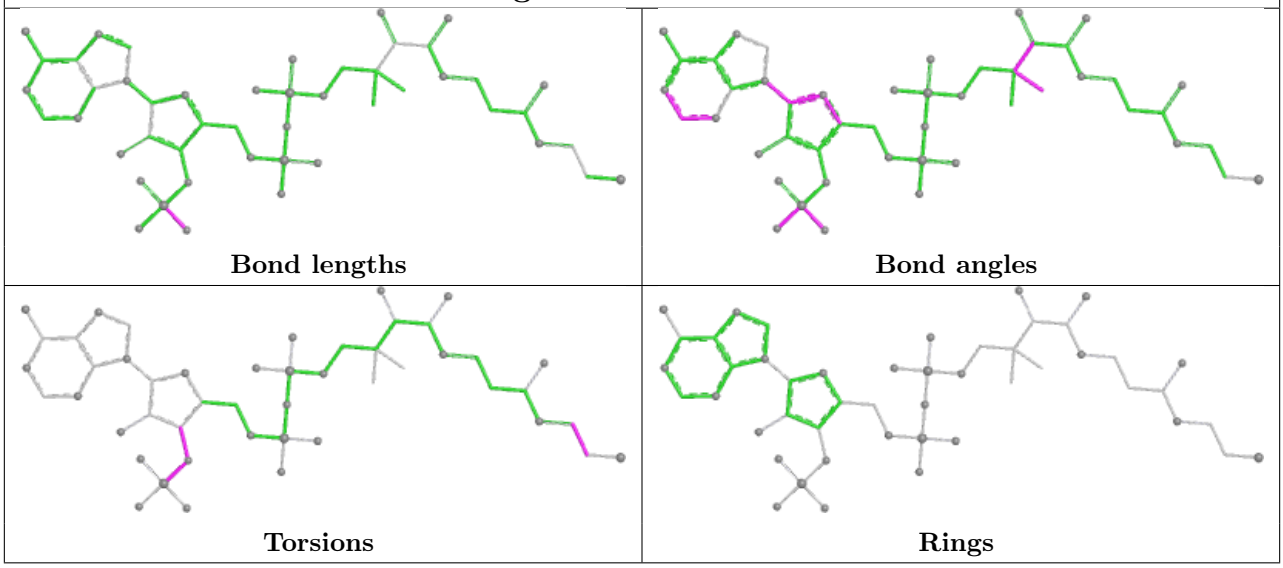


Rings

Ligand COA B 2001



Ligand COA D 2001



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	994/1150 (86%)	0.21	48 (4%)	30	27	39, 76, 117, 151	0
1	B	989/1150 (86%)	-0.20	12 (1%)	79	79	26, 52, 83, 102	0
1	C	995/1150 (86%)	-0.17	19 (1%)	66	65	29, 52, 83, 107	0
1	D	934/1150 (81%)	0.41	64 (6%)	16	13	41, 83, 128, 173	0
All	All	3912/4600 (85%)	0.06	143 (3%)	41	37	26, 64, 111, 173	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	962	ASP	9.6
1	D	965	ALA	6.8
1	D	981	TYR	6.4
1	D	975	THR	5.7
1	D	966	VAL	5.0
1	D	153	VAL	4.9
1	D	959	PHE	4.9
1	A	713	PRO	4.8
1	D	885	GLU	4.4
1	D	892	ASP	4.3
1	D	272	GLN	4.3
1	D	883	LEU	4.2
1	C	970	GLY	4.1
1	D	961	LYS	4.1
1	A	993	LEU	4.1
1	A	929	GLN	4.0
1	D	684	ASP	3.9
1	D	999	GLN	3.9
1	A	282	GLY	3.9
1	D	958	GLY	3.9
1	A	970	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	933	THR	3.8
1	C	236	GLU	3.7
1	A	876	GLN	3.7
1	A	999	GLN	3.6
1	A	538(A)	SER	3.6
1	A	932	ILE	3.6
1	C	238	TYR	3.5
1	D	994	LEU	3.5
1	A	489	ASP	3.5
1	D	537	ILE	3.5
1	D	886	ARG	3.4
1	A	714	GLU	3.4
1	D	533	SER	3.3
1	D	490	ILE	3.3
1	D	790	GLY	3.2
1	D	971	GLN	3.2
1	D	890	VAL	3.2
1	A	965	ALA	3.2
1	D	893	MET	3.1
1	D	988	GLU	3.1
1	A	888	ASP	3.1
1	A	875	SER	3.1
1	C	877	GLN	3.1
1	D	1000	GLY	3.1
1	B	282	GLY	3.1
1	A	940	PHE	3.1
1	D	641	MET	3.1
1	A	238	TYR	3.1
1	D	1001	PRO	3.0
1	C	882	GLY	2.9
1	A	1001	PRO	2.9
1	A	877	GLN	2.9
1	D	683	VAL	2.9
1	A	603	SER	2.8
1	D	882	GLY	2.8
1	D	989	LYS	2.8
1	A	885	GLU	2.8
1	C	89	ASP	2.8
1	B	494	LEU	2.8
1	C	515	ASN	2.8
1	B	163	ASP	2.8
1	A	931	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	879	LYS	2.7
1	A	170	THR	2.7
1	A	927	ASP	2.7
1	D	963	LEU	2.7
1	B	271	HIS	2.7
1	D	888	ASP	2.6
1	D	603	SER	2.6
1	C	876	GLN	2.6
1	A	618	PHE	2.6
1	C	1093	ASN	2.6
1	A	821	PRO	2.6
1	C	384	LEU	2.6
1	D	960	ASN	2.6
1	D	734	GLY	2.5
1	A	168	PRO	2.5
1	A	240	ASP	2.5
1	D	863	GLN	2.5
1	D	969	LYS	2.5
1	D	388	MET	2.5
1	D	864	HIS	2.5
1	C	171	ASP	2.5
1	C	169	GLY	2.5
1	A	537	ILE	2.5
1	A	872	SER	2.4
1	A	919	LEU	2.4
1	D	682	TRP	2.4
1	B	270	ARG	2.4
1	D	1019	GLN	2.4
1	D	992	GLU	2.4
1	C	270	ARG	2.4
1	A	934	ASP	2.4
1	A	880	SER	2.4
1	A	994	LEU	2.4
1	B	168	PRO	2.3
1	C	271	HIS	2.3
1	A	938	LEU	2.3
1	A	886	ARG	2.3
1	A	526	LEU	2.3
1	C	1071	ASN	2.3
1	C	1001	PRO	2.3
1	D	608	GLY	2.3
1	A	538	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	884	GLY	2.3
1	B	524	TYR	2.3
1	A	515	ASN	2.2
1	B	1071	ASN	2.2
1	D	387	PHE	2.2
1	B	99	ILE	2.2
1	B	981	TYR	2.2
1	A	1090	LYS	2.2
1	D	761	SER	2.2
1	D	673	VAL	2.2
1	D	954	GLN	2.2
1	D	119	GLY	2.2
1	D	881	LEU	2.2
1	D	160	ILE	2.2
1	D	762	ALA	2.2
1	C	713	PRO	2.1
1	C	386	ASP	2.1
1	D	980	GLU	2.1
1	C	516	VAL	2.1
1	D	793	ILE	2.1
1	D	675	ARG	2.1
1	A	889	GLU	2.1
1	D	997	GLU	2.1
1	B	68	SER	2.1
1	A	981	TYR	2.1
1	D	1088	TYR	2.1
1	D	912	LYS	2.1
1	D	993	LEU	2.0
1	D	315	SER	2.0
1	A	966	VAL	2.0
1	A	416	ALA	2.0
1	B	167	ILE	2.0
1	D	532	VAL	2.0
1	A	823	HIS	2.0
1	A	978	PRO	2.0
1	D	722	TYR	2.0
1	A	840	THR	2.0
1	D	303	LYS	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)

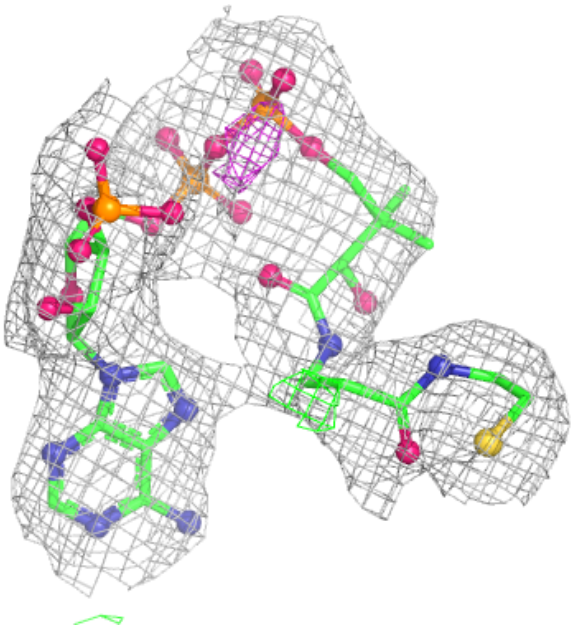
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

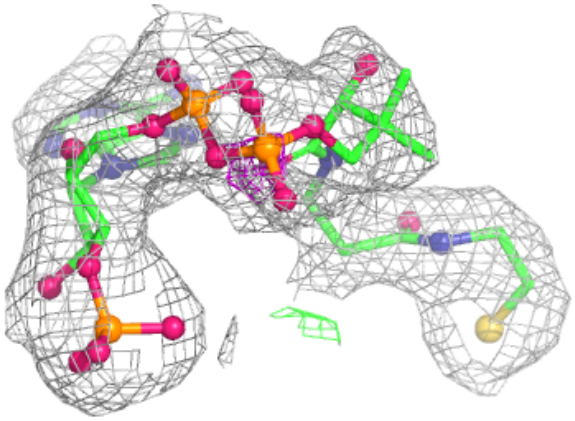
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	A	2002	1/1	0.91	0.08	86,86,86,86	0
2	COA	D	2001	48/48	0.94	0.15	45,51,55,56	0
3	MN	B	2002	1/1	0.94	0.08	60,60,60,60	0
4	BTI	B	2000	15/15	0.94	0.13	47,53,54,55	0
4	BTI	C	2000	15/15	0.95	0.12	36,40,42,43	0
3	MN	C	2002	1/1	0.96	0.07	65,65,65,65	0
2	COA	B	2001	48/48	0.96	0.14	37,40,43,45	0
2	COA	C	2001	48/48	0.97	0.12	32,36,48,51	0
3	MN	D	2002	1/1	0.97	0.10	65,65,65,65	0
2	COA	A	2001	48/48	0.97	0.13	44,48,57,59	0

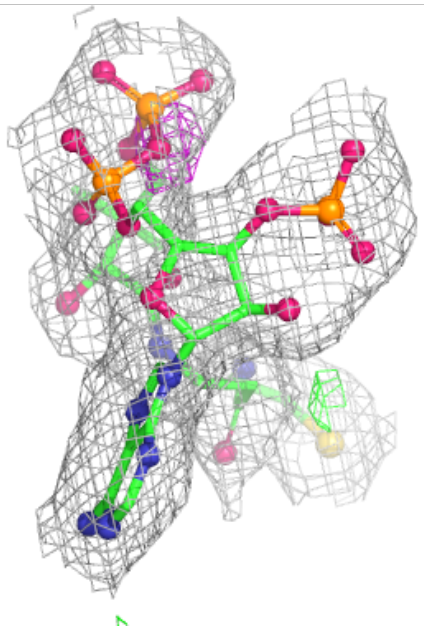
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA D 2001:

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

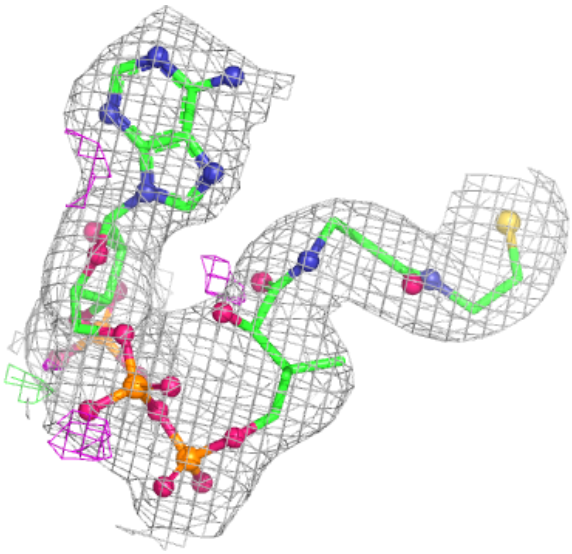


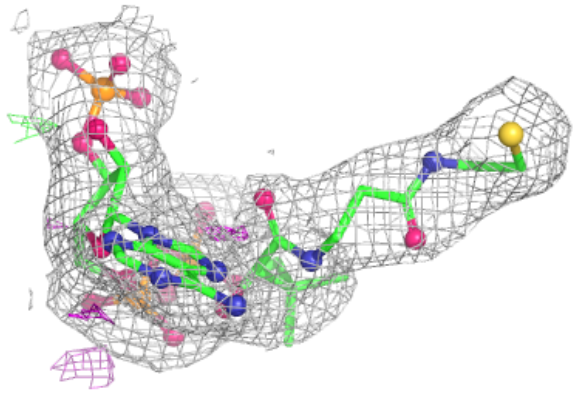


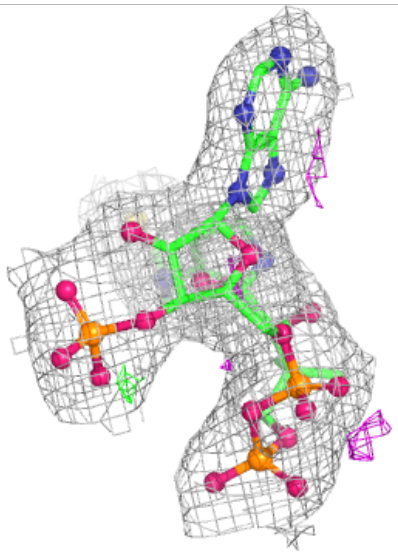


Electron density around COA B 2001:

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

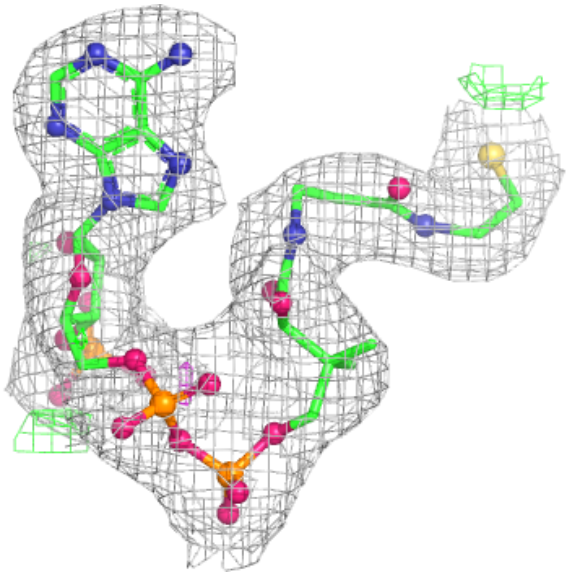


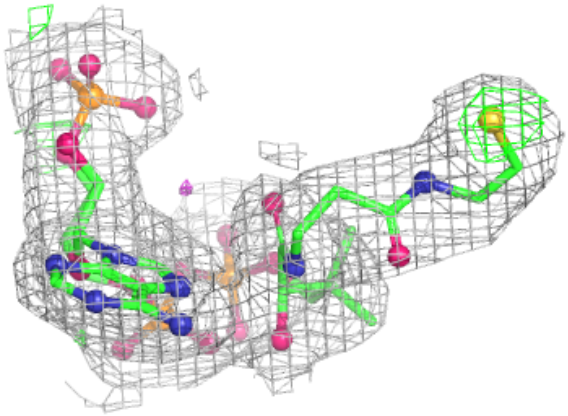


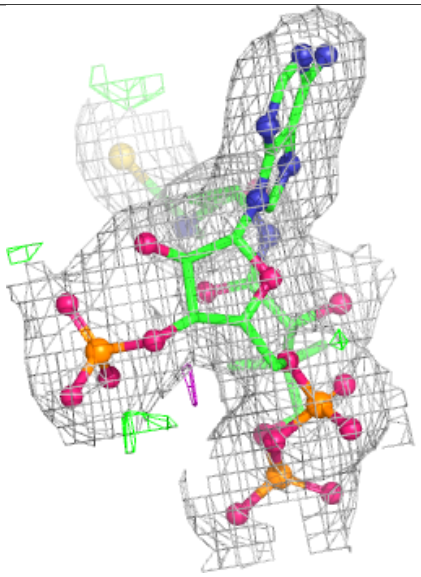


Electron density around COA C 2001:

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

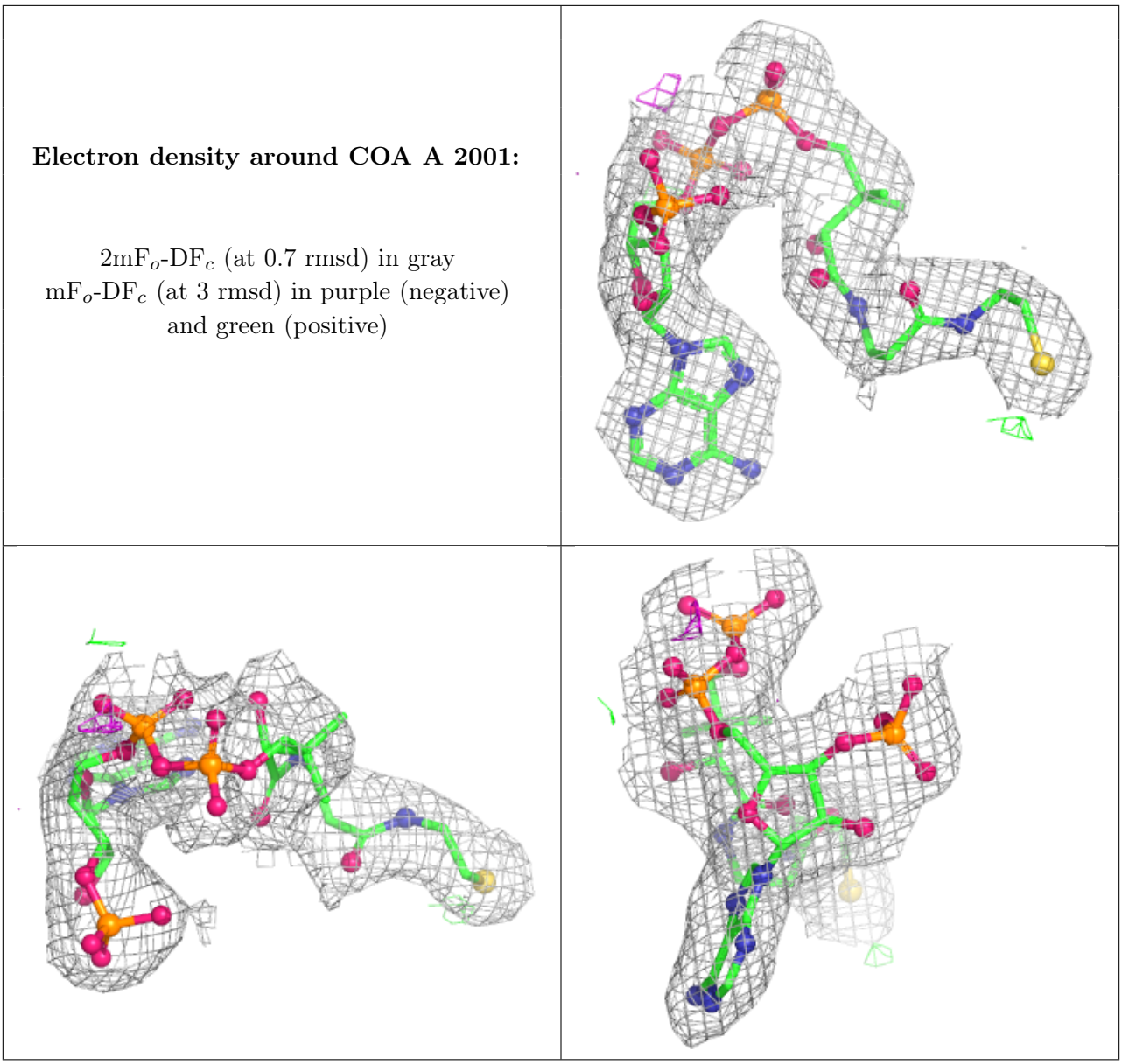






Electron density around COA A 2001:

$2mF_o$-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.