



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:56 PM UTC

PDB ID : 3HO8 / pdb_00003ho8
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

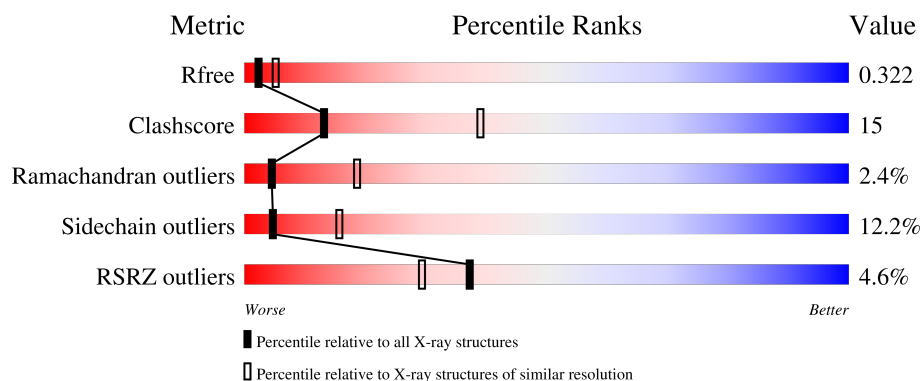
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	1150	5% 55% 27% • 14%
1	B	1150	• 50% 29% 6% 14%
1	C	1150	2% 55% 26% 5% 13%
1	D	1150	7% 53% 25% • 19%

2 Entry composition ⓘ

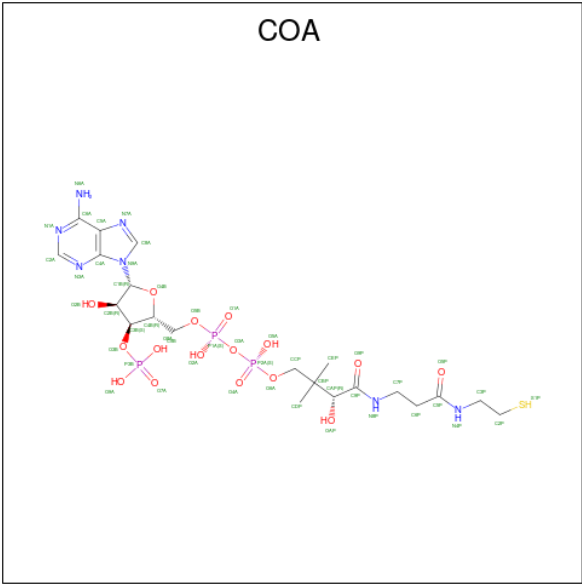
There are 4 unique types of molecules in this entry. The entry contains 31229 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

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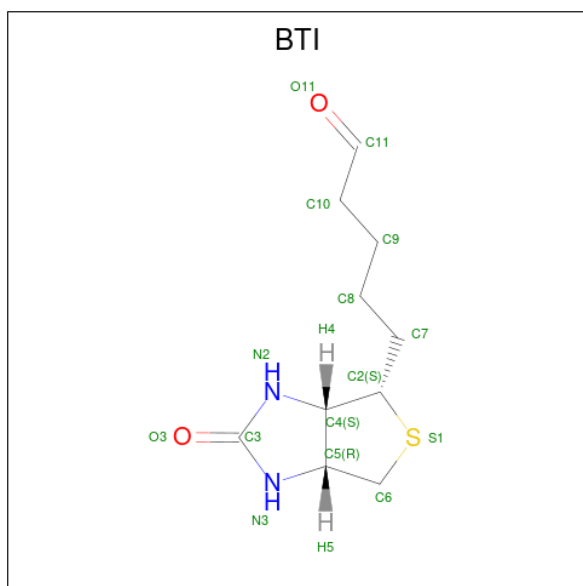
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	0
2	B	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	0

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).

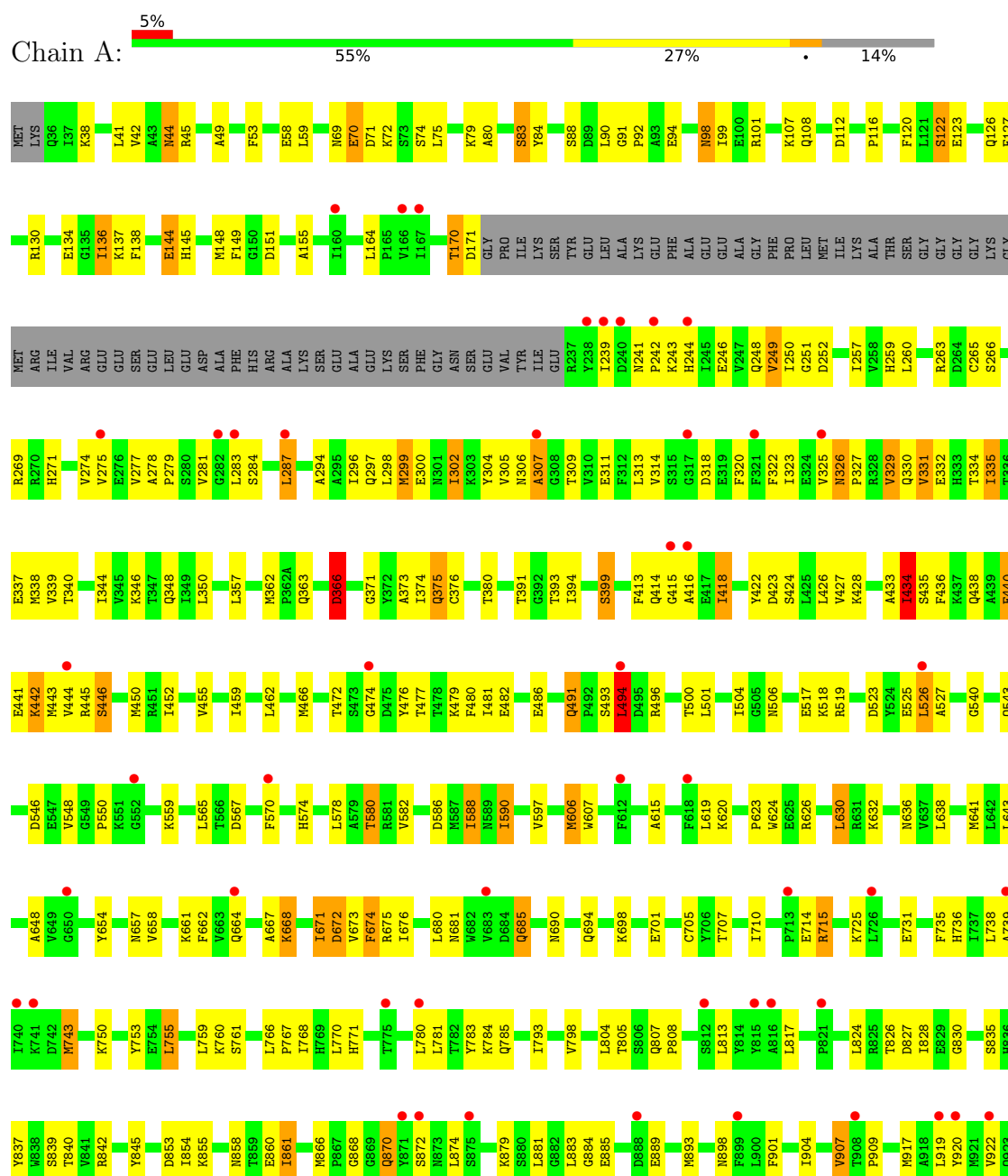


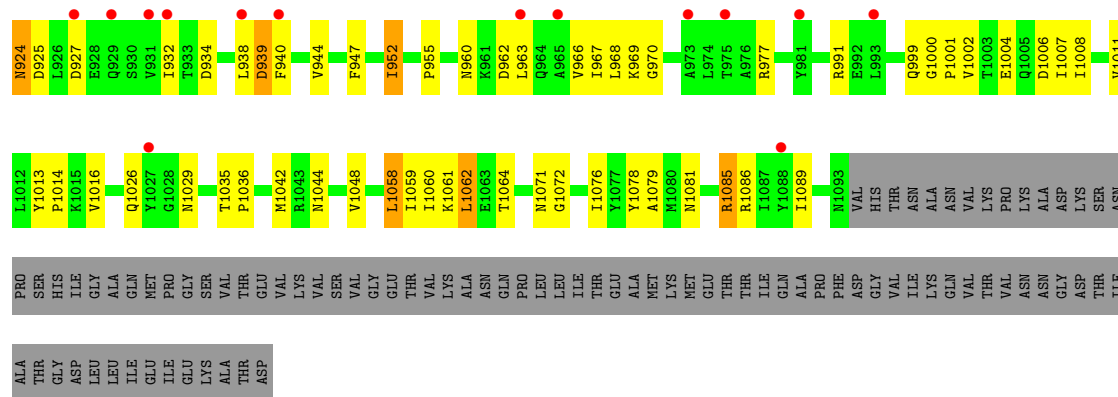
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S		
			15	10	2	2	1	0	0
4	B	1	Total	C	N	O	S		
			15	10	2	2	1	0	0

3 Residue-property plots [i](#)

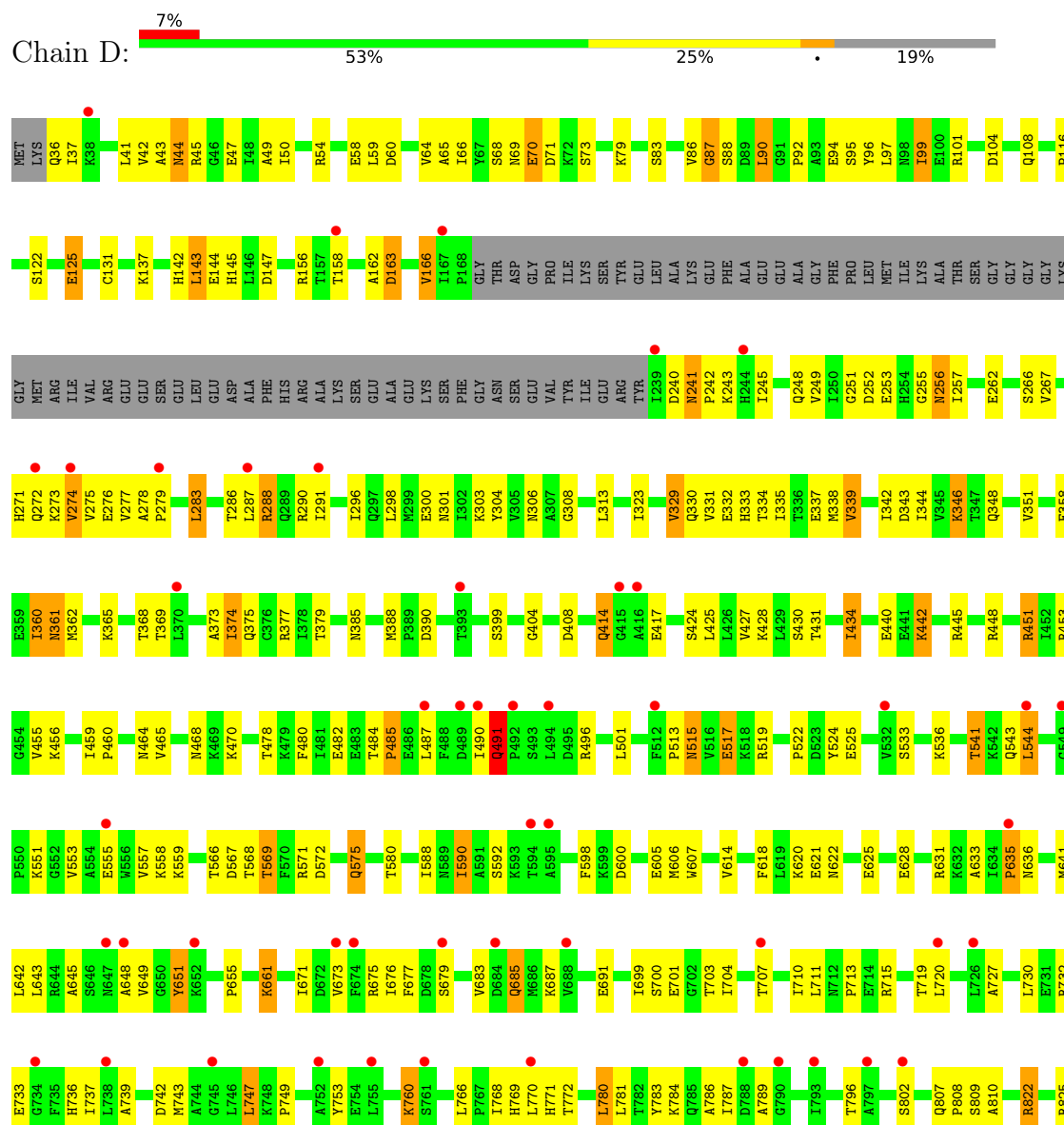
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

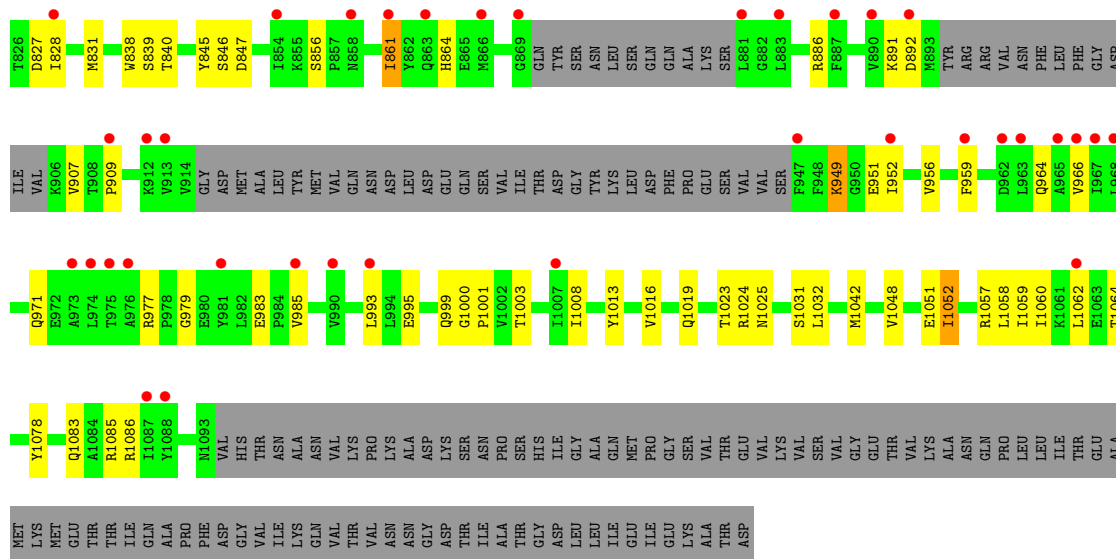
• Molecule 1: Pyruvate carboxylase



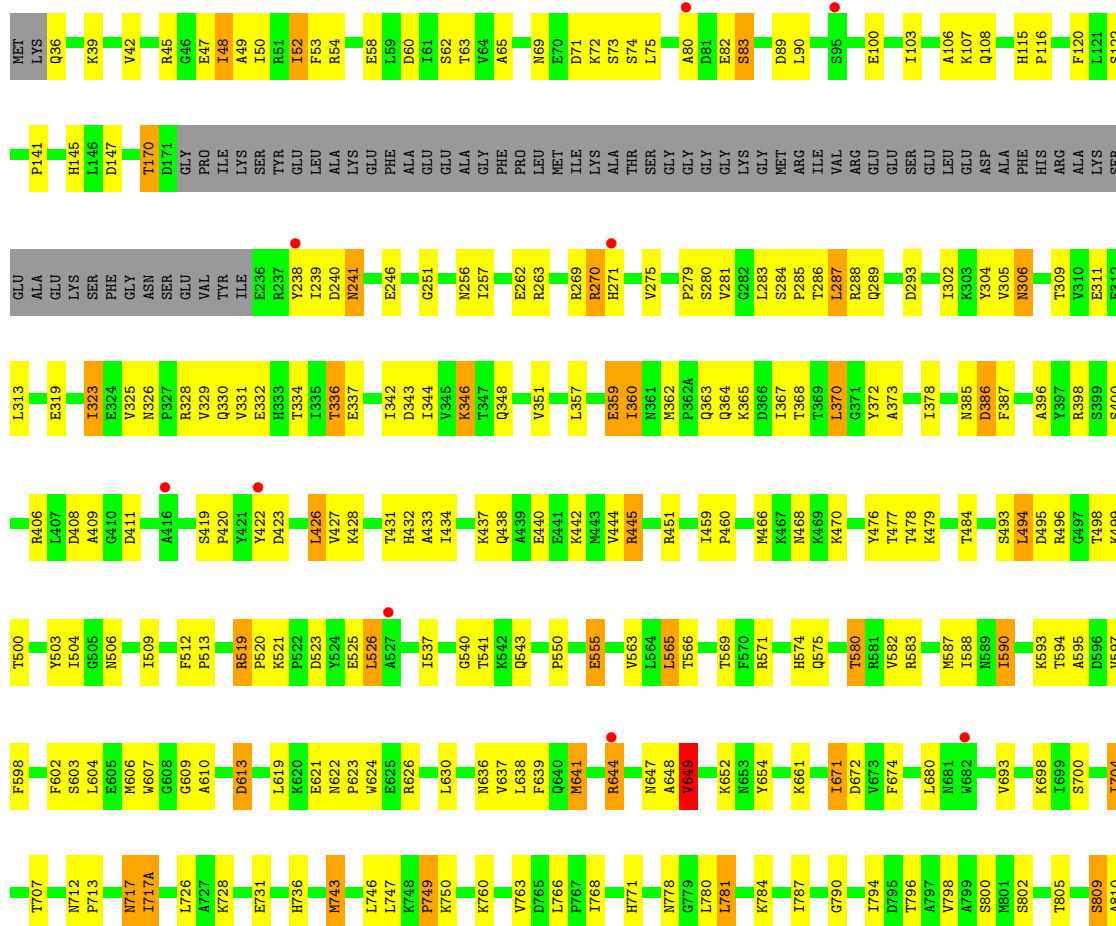


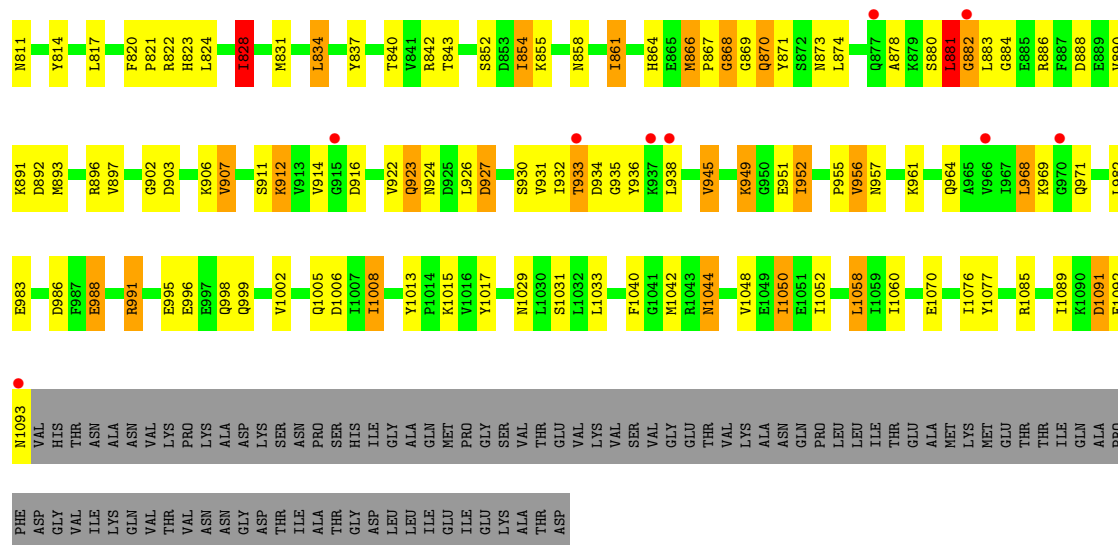
• Molecule 1: Pyruvate carboxylase



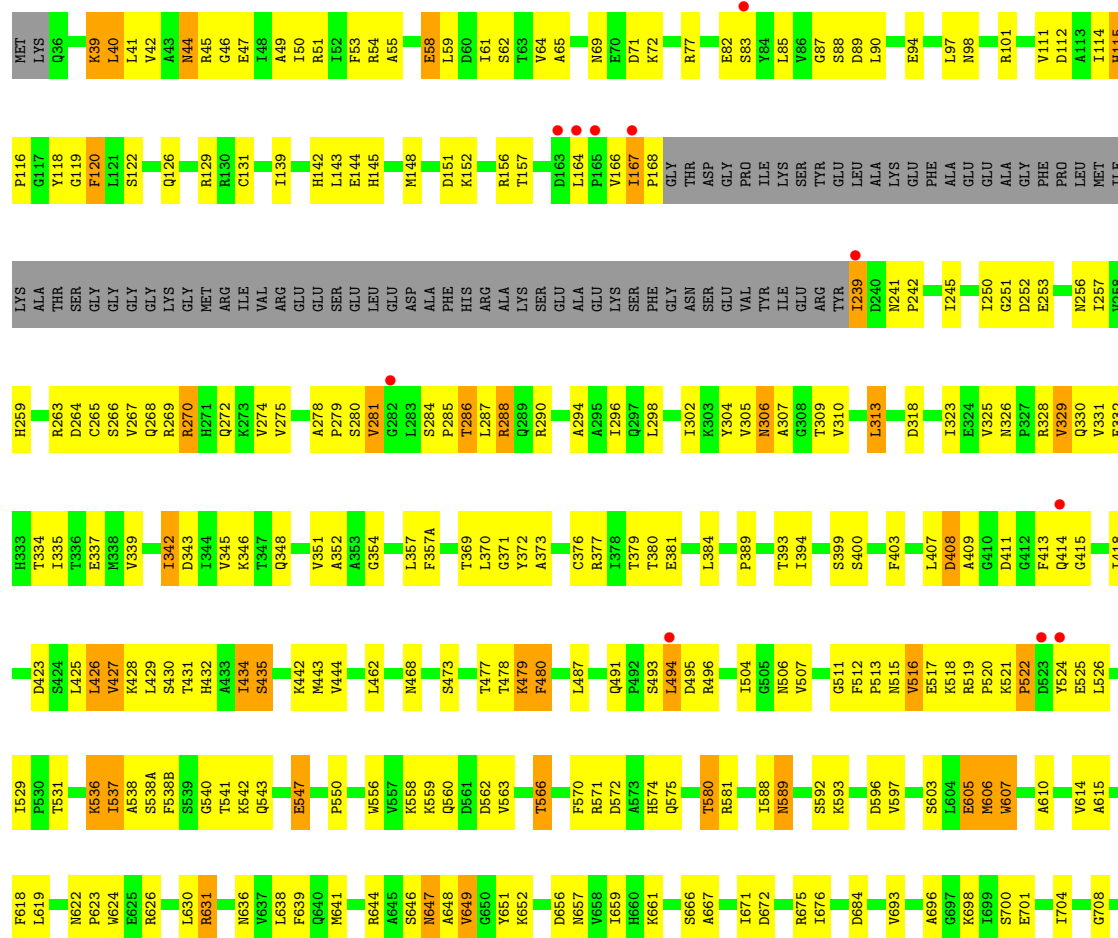


• Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase



GLY	ASP	HIS	S1009	N898	S806	L711
ASP	LEU	ILE	Y1010	F901	S809	R715
LEU	LEU	ALA	V1011	K906	A810	S716
ILE	ILE	GLN	Y1017	N811	N811	N717
GLU	GLU	MET	E1018	V907	I717A	I718
ILE	ILE	PRO	Q1019	T908	Y814	Y719
GLU	GLU	GLY	Q1022	M917	T615	L720
LYS	LYS	SER	A918	A918	A816	E721
ALA	ALA	VAL	N1029	L919	L817	Y722
THR	THR	THR	GLU	Y920	F820	Y723
GLU	GLU	GLU	M821	M821	Y724	Y724
VAL	VAL	VAL	T1035	D927	K825	K725
LYS	LYS	LYS	P1036	E928	T825	L726
VAL	VAL	SER	M1042	D827	D827	L726
SER	SER	SER	GLY	Q929	H736	H736
GLY	GLY	GLY	V1048	S930	E829	I737
GLU	GLU	GLU	E1049	V931	Q830	L738
THR	THR	THR	D1053	I932	H831	A739
VAL	VAL	VAL	LYS	T932	E832	
LYS	LYS	LYS	D934	D934	S833	M743
ALA	ALA	ALA	I1059	G935		
ASN	ASN	ASN	I1060	H836	L747	L747
GLN	GLN	GLN	L838	S839	A751	A751
PRO	PRO	PRO	E1063	V944	A752	A752
LEU	LEU	LEU	T1064	V945	D847	
LEU	LEU	LEU	I1065		E758	E758
ILE	ILE	ILE	E1070	I952	I854	L759
THR	THR	THR	N1071	N857	K855	K760
GLU	GLU	GLU	G1072		S856	
ALA	ALA	ALA		N960	P857	
MET	MET	MET	I1076	D962	E860	L766
LYS	LYS	LYS	Y1077	L963	I861	P767
GLU	GLU	GLU	M1080	N1081	Q862	L768
THR	THR	THR		T975	H863	H771
ILE	ILE	ILE	I1089	A976	H864	T772
GLN	GLN	GLN		R977	E865	T773
ALA	ALA	ALA	E1092	P978	N866	D774
PRO	PRO	PRO	N1093	K869	P867	T775
PHE	PHE	PHE	VAL	V990	Q868	N778
ASP	ASP	ASP	HIS	L993	Q869	
GLY	GLY	GLY	THR	L994	Q870	L781
VAL	VAL	VAL	ILE	N873	X871	I782
ILE	ILE	ILE	ASN	L874	S872	Y783
LYS	LYS	LYS	ALA	E987	N874	K784
LYS	LYS	LYS	ASN			
GLN	GLN	GLN	VAL			I787
VAL	VAL	VAL	LYS		K879	
THR	THR	THR	PRO	G1000	S880	I794
VAL	VAL	VAL	LYS	P1001	L881	D795
ASN	ASN	ASN	ALA	V1002		T796
ASN	ASN	ASN	GLY	T1003	Q884	A797
GLY	GLY	GLY	ASP	E1004		V798
ASP	ASP	ASP	LYS	Q1005	D888	A799
THR	THR	THR	SER	D1006		
ILE	ILE	ILE	ASN	I1007	K891	S802
ALA	ALA	ALA	PRO	I1008		
THR	THR	THR	SER			

4 Data and refinement statistics

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 29.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.97-2.90) 89.7 (29.97-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.264 , 0.328 0.267 , 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)	0.29 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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: 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	0.56	0/8033	0.91	12/10868 (0.1%)
1	B	0.62	1/7990 (0.0%)	0.95	10/10810 (0.1%)
1	C	0.62	1/8042 (0.0%)	0.93	5/10880 (0.0%)
1	D	0.55	0/7537	0.91	4/10192 (0.0%)
All	All	0.59	2/31602 (0.0%)	0.92	31/42750 (0.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	945	VAL	CA-CB	6.92	1.62	1.54
1	C	945	VAL	CA-CB	5.74	1.61	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	938	LEU	N-CA-C	7.32	119.33	111.36
1	A	91	GLY	CA-C-N	7.31	128.97	119.84
1	A	91	GLY	C-N-CA	7.31	128.97	119.84
1	C	882	GLY	N-CA-C	-7.18	105.92	115.40
1	B	115	HIS	CA-C-N	6.81	126.28	118.85
1	B	115	HIS	C-N-CA	6.81	126.28	118.85
1	A	79	LYS	N-CA-C	-6.65	105.19	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	828	ILE	CB-CA-C	-6.18	101.16	111.29
1	B	828	ILE	CB-CA-C	-6.14	103.86	112.14
1	B	820	PHE	CA-C-N	6.00	125.48	119.24
1	B	820	PHE	C-N-CA	6.00	125.48	119.24
1	C	1002	VAL	N-CA-C	5.93	116.55	107.77
1	D	491	GLN	CA-C-N	5.59	125.25	119.05
1	D	491	GLN	C-N-CA	5.59	125.25	119.05
1	B	1072	GLY	N-CA-C	-5.56	107.09	115.32
1	D	399	SER	N-CA-C	5.51	117.01	109.18
1	B	935	GLY	N-CA-C	5.39	119.17	112.64
1	C	238	TYR	N-CA-C	5.38	118.32	109.76
1	A	526	LEU	N-CA-C	5.37	117.57	111.02
1	D	37	ILE	N-CA-C	5.29	120.35	109.34
1	A	271	HIS	N-CA-C	-5.28	104.43	111.87
1	B	906	LYS	N-CA-C	5.24	115.93	108.54
1	B	468	ASN	N-CA-C	5.18	117.73	109.96
1	A	927	ASP	N-CA-C	5.15	115.04	108.24
1	A	671	ILE	N-CA-C	5.14	117.04	109.63
1	A	715	ARG	N-CA-C	-5.13	105.59	111.14
1	A	491	GLN	CB-CA-C	5.11	116.32	109.42
1	C	468	ASN	N-CA-C	5.05	117.75	110.28
1	A	84	TYR	N-CA-C	5.04	117.28	108.76
1	A	491	GLN	CA-C-N	5.04	125.03	119.89
1	A	491	GLN	C-N-CA	5.04	125.03	119.89

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 ⓘ

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	212	0
1	B	7838	0	7771	303	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7889	0	7813	251	0
1	D	7396	0	7347	168	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	923	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 15.

All (923) 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:606:MET:HE2	1:C:639:PHE:HB3	1.20	1.15
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:C:866:MET:HE2	1:C:871:TYR:HA	1.39	1.02
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:504:ILE:HG21	1:C:1042:MET:HE3	1.60	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:C:504:ILE:HG21	1:C:1042:MET:CE	2.10	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: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:C:571:ARG:HD2	1:C:571:ARG:C	2.10	0.77
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:B:516:VAL:CG1	1:B:517:GLU:H	1.98	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:870:GLN:NE2	1:C:911:SER:HB2	2.05	0.72
1:A:504:ILE:HG21	1:A:1042:MET:HE3	1.71	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:823:HIS:HD2	1:C:824:LEU:N	1.90	0.69
1:C:866:MET:HE2	1:C:871:TYR:CA	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:870:GLN:O	1:C:871:TYR:C	2.40	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:641:MET:HE2	1:B:671:ILE:HG13	1.79	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
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:537:ILE:C	1:B:538(A):SER:H	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:893:MET:HE3	1:C:896:ARG:HB2	1.81	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:B:504:ILE:HG21	1:B:1042:MET:HE3	1.81	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:C:1042:MET:HE1	1:C:1060:ILE:HG22	1.80	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:773:HIS:C	1:B:775:THR:H	2.07	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:606:MET:HE1	1:C:671:ILE:CD1	2.32	0.60
1:C:438:GLN:O	1:C:442:LYS:HG3	2.02	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:240:ASP:C	1:D:242:PRO:HD3	2.26	0.59
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:A:968:LEU:C	1:A:970:GLY:H	2.08	0.59
1:C:1044:ASN:H	1:C:1044:ASN:ND2	1.92	0.59
1:B:1092:GLU:O	1:B:1093:ASN:CB	2.49	0.59
1:A:144:GLU:CD	1:A:144:GLU:H	2.09	0.59
1:A:335:ILE:HD11	1:A:374:ILE:CA	2.33	0.59
1:C:1042:MET:HE1	1:C:1060:ILE:CG2	2.33	0.59
1:B:772:THR:HG22	1:B:783:TYR:CE2	2.38	0.59
1:A:99:ILE:HG12	1:A:127:PHE:HB2	1.85	0.59
1:B:606:MET:HE1	1:B:671:ILE:CD1	2.32	0.59
1:A:626:ARG:O	1:A:630:LEU:HB2	2.03	0.58
1:B:606:MET:HE1	1:B:671:ILE:HD11	1.86	0.58
1:C:359:GLU:H	1:C:359:GLU:CD	2.10	0.58
1:B:512:PHE:CD2	1:B:513:PRO:HD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:430:SER:HA	1:B:443:MET:HE1	1.86	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: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: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:C:504:ILE:HG21	1:C:1042:MET:HE2	1.86	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:D:360:ILE:O	1:D:361:ASN:C	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:820:PHE:HB3	1:C:821:PRO:HD2	1.87	0.56
1:B:952:ILE:HG22	1:B:952:ILE:O	2.03	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:HE2	2.46	0.55
1:D:783:TYR:O	1:D:786:ALA:N	2.35	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: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:D:1042:MET:HE3	1:D:1062:LEU:HB2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:330:GLN:O	1:D:333:HIS:ND1	2.32	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:D:343:ASP:CG	1:D:346:LYS:HB2	2.33	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:338:MET:HE3	1:D:373:ALA:HB1	1.90	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:144:GLU:H	1:B:144:GLU:CD	2.17	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: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:C:287:LEU:C	1:C:289:GLN:H	2.18	0.52
1:C:606:MET:HE2	1:C:639:PHE:CB	2.14	0.52
1:A:299:MET:HE1	1:A:325:VAL:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:MET:SD	1:D:606:MET:C	2.92	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
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: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:360:ILE:C	1:C:362:MET:H	2.18	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:88:SER:C	1:D:90:LEU:H	2.18	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:148:MET:HE1	1:B:302:ILE:HB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:571:ARG:HE	1:B:605:GLU:CD	2.18	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
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:D:1042:MET:HE1	1:D:1060:ILE:HG22	1.92	0.50
1:C:955:PRO:O	1:C:956:VAL:C	2.53	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:C:881:LEU:C	1:C:883:LEU:H	2.18	0.50
1:A:898:ASN:ND2	1:A:904:ILE:H	2.09	0.50
1:D:641:MET:HE2	1:D:671:ILE:HG13	1.94	0.50
1:D:1013:TYR:HB3	1:D:1016:VAL:HB	1.94	0.50
1:C:269:ARG:O	1:C:270:ARG:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:993:LEU:C	1:D:995:GLU:H	2.20	0.50
1:C:566:THR:HG1	1:C:603:SER:HG	1.56	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
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: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:C:422:TYR:O	1:C:423:ASP:C	2.56	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:A:968:LEU:C	1:A:970:GLY:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:85:LEU:HD21	1:B:88:SER:HB3	1.95	0.48
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: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:A:771:HIS:C	1:A:771:HIS:CD2	2.91	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: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:641:MET:HE3	1:C:674:PHE:CE1	2.49	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:D:490:ILE:O	1:D:491:GLN:C	2.58	0.47
1:C:47:GLU:OE1	1:C:428:LYS:NZ	2.47	0.47
1:C:287:LEU:C	1:C:289:GLN:N	2.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:45:ARG:HH22	1:B:411:ASP:CG	2.22	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:D:783:TYR:O	1:D:784:LYS:C	2.57	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
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:299:MET:HE1	1:A:325:VAL:HG11	1.97	0.46
1:A:940:PHE:CE2	1:A:967:ILE:HA	2.50	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:A:422:TYR:O	1:A:423:ASP:C	2.57	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: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:D:845:TYR:O	1:D:846:SER:C	2.58	0.46
1:D:1078:TYR:HB2	1:D:1085:ARG:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:773:HIS:C	1:B:775:THR:N	2.74	0.46
1:A:275:VAL:HG11	1:A:466:MET:HE1	1.98	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:890:VAL:O	1:C:891:LYS:C	2.59	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
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: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:B:867:PRO:O	1:B:868:GLY:C	2.59	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:D:286:THR:O	1:D:287:LEU:C	2.58	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: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:C:810:ALA:HB1	1:C:831:MET:HE1	1.99	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:A:504:ILE:HG21	1:A:1042:MET:CE	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:571:ARG:C	1:C:571:ARG:CD	2.88	0.45
1:C:778:ASN:ND2	1:B:816:ALA:HB2	2.33	0.45
1:C:866:MET:HE3	1:C:870:GLN:HG2	1.98	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: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:C:700:SER:H	1:C:736:HIS:CD2	2.33	0.44
1:C:927:ASP:OD1	1:C:927:ASP:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:952:ILE:HG22	1:D:952:ILE:O	2.17	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
1:B:46:GLY:O	1:B:47:GLU:C	2.59	0.44
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:A:300:GLU:C	1:A:302:ILE:H	2.25	0.44
1:A:641:MET:HE2	1:A:671:ILE:HG13	1.99	0.44
1:A:861:ILE:HD11	1:A:866:MET:O	2.18	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:108:GLN:O	1:C:108:GLN:HG3	2.16	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:B:566:THR:OG1	1:B:603:SER:OG	2.31	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:C:771:HIS:CD2	1:C:771:HIS:C	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:385:ASN:O	1:C:386:ASP:C	2.61	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
1:B:394:ILE:HG13	1:B:418:ILE:CD1	2.48	0.43
1:B:864:HIS:CD2	1:B:866:MET:HE3	2.53	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:D:88:SER:C	1:D:90:LEU:N	2.76	0.43
1:D:964:GLN:C	1:D:966:VAL:H	2.26	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:119:GLY:O	1:B:120:PHE:C	2.60	0.43
1:B:871:TYR:CD1	1:B:871:TYR:C	2.95	0.43
1:B:927:ASP:O	1:B:931:VAL:HG23	2.18	0.43
1:A:41:LEU:C	1:A:41:LEU:HD23	2.43	0.43
1:A:338:MET:HE3	1:A:373:ALA:HB1	2.00	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:622:ASN:HD22	1:B:622:ASN:C	2.26	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:673:VAL:O	1:A:674:PHE:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:ILE:HD13	1:A:755:LEU:HD23	2.01	0.43
1:D:90:LEU:HD21	1:D:101:ARG:NH2	2.34	0.43
1:C:503:TYR:C	1:C:503:TYR:CD1	2.96	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:343:ASP:CG	1:C:346:LYS:HB3	2.44	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:A:38:LYS:HB2	1:A:112:ASP:OD1	2.19	0.43
1:A:413:PHE:O	1:A:414:GLN:C	2.61	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:606:MET:HE1	1:C:671:ILE:HD11	2.01	0.43
1:C:609:GLY:HA2	1:C:644:ARG:NH1	2.34	0.43
1:C:869:GLY:O	1:C:870:GLN:C	2.62	0.43
1:C:902:GLY:O	1:C:903:ASP:HB3	2.19	0.43
1:B:71:ASP:O	1:B:72:LYS:C	2.62	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
1:D:267:VAL:HG12	1:D:274:VAL:HB	2.00	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:C:329:VAL:HG13	1:C:348:GLN:CD	2.44	0.42
1:B:332:GLU:H	1:B:332:GLU:CD	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:86:VAL:O	1:D:87:GLY:C	2.61	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:C:647:ASN:O	1:C:649:VAL:N	2.47	0.42
1:C:881:LEU:C	1:C:883:LEU:N	2.78	0.42
1:B:281:VAL:HG22	1:B:372:TYR:HE2	1.84	0.42
1:B:479:LYS:O	1:B:480:PHE:C	2.62	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:582:VAL:HG12	1:C:587:MET:HE3	2.01	0.42
1:C:750:LYS:HE2	1:B:820:PHE:CE2	2.54	0.42
1:B:343:ASP:CG	1:B:346:LYS:HB3	2.45	0.42
1:B:571:ARG:NE	1:B:605:GLU:OE2	2.52	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:827:ASP:OD2	1:B:827:ASP:C	2.61	0.42
1:B:1000:GLY:N	1:B:1001:PRO:CD	2.76	0.42
1:A:606:MET:HE1	1:A:671:ILE:HD13	2.02	0.42
1:A:615:ALA:HB3	1:A:623:PRO:HG3	2.00	0.42
1:D:485:PRO:C	1:D:487:LEU:H	2.26	0.42
1:D:598:PHE:CE2	1:D:831:MET:HE1	2.55	0.42
1:C:444:VAL:CG1	1:C:445:ARG:N	2.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:656:ASP:O	1:B:659:ILE:N	2.50	0.42
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: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:299:MET:HE1	1:A:325:VAL:HG13	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:71:ASP:C	1:D:73:SER:N	2.79	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:THR:CG2	1:B:720:LEU:N	2.83	0.41
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:504:ILE:HD13	1:A:1042:MET:HE2	2.03	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:94:GLU:C	1:D:96:TYR:H	2.29	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:622:ASN:HD21	1:B:624:TRP:CD1	2.39	0.41
1:B:641:MET:HE3	1:B:671:ILE:HG21	2.03	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: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: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:71:ASP:O	1:A:72:LYS:C	2.64	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:459:ILE:O	1:D:460:PRO:C	2.64	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
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:HE1	1:B:671:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:ASN:ND2	1:B:831:MET:HG2	2.36	0.41
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:485:PRO:C	1:D:487:LEU:N	2.79	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:C:606:MET:HE1	1:C:671:ILE:HD13	2.02	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:622:ASN:HD21	1:C:624:TRP:CD1	2.39	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: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
1:B:571:ARG:HD2	1:B:571:ARG:C	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	990/1150 (86%)	862 (87%)	105 (11%)	23 (2%)	5	19
1	B	985/1150 (86%)	875 (89%)	89 (9%)	21 (2%)	5	21
1	C	991/1150 (86%)	887 (90%)	79 (8%)	25 (2%)	4	17
1	D	924/1150 (80%)	777 (84%)	123 (13%)	24 (3%)	4	17
All	All	3890/4600 (85%)	3401 (87%)	396 (10%)	93 (2%)	4	18

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

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Mol	Chain	Res	Type
1	A	434	ILE
1	A	674	PHE
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

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Mol	Chain	Res	Type
1	A	433	ALA
1	A	494	LEU
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 ⓘ

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	860/987 (87%)	761 (88%)	99 (12%)	5	18
1	B	856/987 (87%)	746 (87%)	110 (13%)	4	13
1	C	861/987 (87%)	754 (88%)	107 (12%)	4	15
1	D	806/987 (82%)	709 (88%)	97 (12%)	5	16
All	All	3383/3948 (86%)	2970 (88%)	413 (12%)	5	16

All (413) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	70	GLU
1	A	83	SER
1	A	88	SER
1	A	98	ASN
1	A	107	LYS
1	A	108	GLN
1	A	122	SER
1	A	123	GLU
1	A	126	GLN
1	A	136	ILE
1	A	144	GLU
1	A	151	ASP
1	A	170	THR
1	A	241	ASN
1	A	249	VAL
1	A	269	ARG
1	A	274	VAL
1	A	284	SER
1	A	287	LEU
1	A	299	MET
1	A	302	ILE
1	A	326	ASN
1	A	329	VAL
1	A	331	VAL
1	A	335	ILE
1	A	366	ASP
1	A	375	GLN
1	A	393	THR
1	A	399	SER

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Mol	Chain	Res	Type
1	A	418	ILE
1	A	427	VAL
1	A	434	ILE
1	A	440	GLU
1	A	442	LYS
1	A	446	SER
1	A	455	VAL
1	A	472	THR
1	A	481	ILE
1	A	486	GLU
1	A	491	GLN
1	A	493	SER
1	A	494	LEU
1	A	506	ASN
1	A	518	LYS
1	A	523	ASP
1	A	526	LEU
1	A	548	VAL
1	A	559	LYS
1	A	565	LEU
1	A	567	ASP
1	A	580	THR
1	A	588	ILE
1	A	590	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	707	THR
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

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Mol	Chain	Res	Type
1	A	793	ILE
1	A	804	LEU
1	A	805	THR
1	A	807	GLN
1	A	813	LEU
1	A	828	ILE
1	A	839	SER
1	A	855	LYS
1	A	861	ILE
1	A	870	GLN
1	A	885	GLU
1	A	907	VAL
1	A	924	ASN
1	A	932	ILE
1	A	934	ASP
1	A	952	ILE
1	A	962	ASP
1	A	966	VAL
1	A	969	LYS
1	A	991	ARG
1	A	1048	VAL
1	A	1058	LEU
1	A	1062	LEU
1	A	1064	THR
1	A	1071	ASN
1	A	1085	ARG
1	A	1089	ILE
1	D	36	GLN
1	D	44	ASN
1	D	69	ASN
1	D	70	GLU
1	D	90	LEU
1	D	99	ILE
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	245	ILE

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Mol	Chain	Res	Type
1	D	249	VAL
1	D	253	GLU
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	329	VAL
1	D	331	VAL
1	D	339	VAL
1	D	342	ILE
1	D	346	LYS
1	D	358	GLU
1	D	360	ILE
1	D	365	LYS
1	D	368	THR
1	D	374	ILE
1	D	375	GLN
1	D	417	GLU
1	D	427	VAL
1	D	434	ILE
1	D	440	GLU
1	D	442	LYS
1	D	451	ARG
1	D	455	VAL
1	D	482	GLU
1	D	517	GLU
1	D	519	ARG
1	D	525	GLU
1	D	541	THR
1	D	543	GLN
1	D	544	LEU
1	D	551	LYS
1	D	558	LYS
1	D	569	THR
1	D	575	GLN
1	D	580	THR
1	D	588	ILE

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Mol	Chain	Res	Type
1	D	590	ILE
1	D	592	SER
1	D	607	TRP
1	D	628	GLU
1	D	631	ARG
1	D	636	ASN
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	732	ARG
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	822	ARG
1	D	827	ASP
1	D	839	SER
1	D	840	THR
1	D	856	SER
1	D	861	ILE
1	D	891	LYS
1	D	892	ASP
1	D	949	LYS
1	D	956	VAL
1	D	971	GLN
1	D	983	GLU
1	D	1003	THR
1	D	1019	GLN
1	D	1048	VAL
1	D	1052	ILE
1	D	1059	ILE
1	D	1064	THR
1	D	1083	GLN
1	D	1086	ARG
1	C	36	GLN
1	C	45	ARG

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Mol	Chain	Res	Type
1	C	48	ILE
1	C	52	ILE
1	C	60	ASP
1	C	73	SER
1	C	75	LEU
1	C	82	GLU
1	C	83	SER
1	C	90	LEU
1	C	100	GLU
1	C	103	ILE
1	C	107	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	319	GLU
1	C	323	ILE
1	C	336	THR
1	C	346	LYS
1	C	359	GLU
1	C	360	ILE
1	C	363	GLN
1	C	365	LYS
1	C	368	THR
1	C	370	LEU
1	C	411	ASP
1	C	426	LEU
1	C	427	VAL
1	C	434	ILE
1	C	437	LYS
1	C	445	ARG
1	C	478	THR
1	C	484	THR
1	C	493	SER
1	C	494	LEU
1	C	498	THR

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Mol	Chain	Res	Type
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	580	THR
1	C	588	ILE
1	C	590	ILE
1	C	604	LEU
1	C	607	TRP
1	C	613	ASP
1	C	641	MET
1	C	644	ARG
1	C	649	VAL
1	C	671	ILE
1	C	704	ILE
1	C	707	THR
1	C	717	ASN
1	C	717(A)	ILE
1	C	728	LYS
1	C	743	MET
1	C	766	LEU
1	C	781	LEU
1	C	784	LYS
1	C	794	ILE
1	C	796	THR
1	C	809	SER
1	C	828	ILE
1	C	834	LEU
1	C	855	LYS
1	C	866	MET
1	C	881	LEU
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	945	VAL
1	C	949	LYS

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Mol	Chain	Res	Type
1	C	952	ILE
1	C	961	LYS
1	C	968	LEU
1	C	969	LYS
1	C	971	GLN
1	C	982	LEU
1	C	983	GLU
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	1044	ASN
1	C	1048	VAL
1	C	1050	ILE
1	C	1058	LEU
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	50	ILE
1	B	58	GLU
1	B	89	ASP
1	B	90	LEU
1	B	98	ASN
1	B	101	ARG
1	B	156	ARG
1	B	157	THR
1	B	167	ILE
1	B	239	ILE
1	B	250	ILE
1	B	253	GLU
1	B	270	ARG
1	B	272	GLN
1	B	274	VAL
1	B	281	VAL
1	B	286	THR
1	B	287	LEU

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Mol	Chain	Res	Type
1	B	288	ARG
1	B	306	ASN
1	B	310	VAL
1	B	313	LEU
1	B	318	ASP
1	B	329	VAL
1	B	334	THR
1	B	342	ILE
1	B	351	VAL
1	B	384	LEU
1	B	393	THR
1	B	399	SER
1	B	408	ASP
1	B	426	LEU
1	B	427	VAL
1	B	429	LEU
1	B	434	ILE
1	B	435	SER
1	B	444	VAL
1	B	473	SER
1	B	479	LYS
1	B	487	LEU
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	566	THR
1	B	580	THR
1	B	581	ARG
1	B	588	ILE
1	B	589	ASN
1	B	596	ASP
1	B	605	GLU
1	B	606	MET
1	B	607	TRP
1	B	631	ARG
1	B	647	ASN
1	B	649	VAL
1	B	657	ASN

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Mol	Chain	Res	Type
1	B	684	ASP
1	B	715	ARG
1	B	717	ASN
1	B	717(A)	ILE
1	B	719	THR
1	B	743	MET
1	B	766	LEU
1	B	771	HIS
1	B	781	LEU
1	B	784	LYS
1	B	794	ILE
1	B	798	VAL
1	B	806	SER
1	B	809	SER
1	B	825	ARG
1	B	828	ILE
1	B	833	SER
1	B	863	GLN
1	B	866	MET
1	B	871	TYR
1	B	872	SER
1	B	873	ASN
1	B	874	LEU
1	B	879	LYS
1	B	881	LEU
1	B	888	ASP
1	B	906	LYS
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	989	LYS
1	B	990	VAL
1	B	1008	ILE
1	B	1009	SER
1	B	1019	GLN
1	B	1029	ASN
1	B	1048	VAL

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Mol	Chain	Res	Type
1	B	1063	GLU
1	B	1077	TYR
1	B	1081	ASN
1	B	1092	GLU
1	B	1093	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) 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	491	GLN
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	589	ASN
1	A	617	ASN
1	A	685	GLN
1	A	736	HIS
1	A	778	ASN
1	A	811	ASN
1	A	864	HIS
1	A	898	ASN
1	A	924	ASN
1	A	960	ASN
1	A	1005	GLN
1	A	1025	ASN
1	A	1081	ASN
1	D	44	ASN
1	D	145	HIS
1	D	330	GLN
1	D	364	GLN
1	D	375	GLN
1	D	414	GLN

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Mol	Chain	Res	Type
1	D	464	ASN
1	D	491	GLN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	660	HIS
1	D	690	ASN
1	D	694	GLN
1	D	717	ASN
1	D	736	HIS
1	D	778	ASN
1	D	811	ASN
1	D	818	ASN
1	D	864	HIS
1	D	971	GLN
1	D	1005	GLN
1	D	1025	ASN
1	D	1029	ASN
1	C	69	ASN
1	C	98	ASN
1	C	126	GLN
1	C	145	HIS
1	C	256	ASN
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	589	ASN
1	C	622	ASN
1	C	717	ASN
1	C	736	HIS
1	C	771	HIS
1	C	773	HIS
1	C	778	ASN
1	C	811	ASN
1	C	818	ASN
1	C	823	HIS

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Mol	Chain	Res	Type
1	C	864	HIS
1	C	870	GLN
1	C	873	ASN
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	B	44	ASN
1	B	142	HIS
1	B	145	HIS
1	B	289	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	506	ASN
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	863	GLN
1	B	864	HIS
1	B	873	ASN
1	B	877	GLN
1	B	923	GLN

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Mol	Chain	Res	Type
1	B	924	ASN
1	B	960	ASN
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 oligosaccharides 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	-	47,50,50	1.17	4 (8%)	69,75,75	1.61	12 (17%)
2	COA	B	2001	-	47,50,50	1.36	7 (14%)	69,75,75	1.63	12 (17%)
4	BTI	C	2000	-	15,16,16	1.70	2 (13%)	20,21,21	2.23	3 (15%)
2	COA	A	2001	-	47,50,50	1.44	5 (10%)	69,75,75	1.65	13 (18%)
4	BTI	B	2000	-	15,16,16	1.62	2 (13%)	20,21,21	1.95	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	D	2001	-	47,50,50	1.15	2 (4%)	69,75,75	1.68	11 (15%)

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	-	-	14/48/64/64	0/3/3/3
2	COA	B	2001	-	-	17/48/64/64	0/3/3/3
4	BTI	C	2000	-	-	5/6/27/27	0/2/2/2
2	COA	A	2001	-	-	16/48/64/64	0/3/3/3
4	BTI	B	2000	-	-	3/6/27/27	0/2/2/2
2	COA	D	2001	-	-	4/48/64/64	0/3/3/3

All (22) 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
2	B	2001	COA	C5A-N7A	-3.50	1.32	1.39
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	C	2001	COA	C5A-N7A	-3.34	1.33	1.39
2	A	2001	COA	P3B-O7A	3.29	1.60	1.50
2	A	2001	COA	C5A-N7A	-3.06	1.33	1.39
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	D	2001	COA	C5A-N7A	-2.89	1.33	1.39
2	B	2001	COA	P3B-O3B	2.83	1.64	1.59
2	B	2001	COA	C4A-N9A	-2.47	1.32	1.37
2	C	2001	COA	C4A-N9A	-2.37	1.32	1.37
2	C	2001	COA	C8A-N9A	-2.37	1.33	1.37
2	B	2001	COA	C8A-N9A	-2.18	1.33	1.37
2	A	2001	COA	C4A-N9A	-2.12	1.33	1.37
2	B	2001	COA	P3B-O9A	-2.04	1.47	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	D	2001	COA	C5A-C4A-N3A	-5.61	119.00	126.72
2	A	2001	COA	C5A-C4A-N3A	-5.13	119.66	126.72
2	D	2001	COA	O4B-C1B-N9A	-5.12	98.26	108.09
2	C	2001	COA	C5A-C4A-N3A	-5.09	119.71	126.72
2	B	2001	COA	C5A-C4A-N3A	-4.82	120.07	126.72
2	D	2001	COA	N3A-C2A-N1A	-4.77	121.36	128.58
2	A	2001	COA	N3A-C2A-N1A	-4.64	121.55	128.58
4	B	2000	BTI	C2-C4-N2	-4.45	108.63	113.34
2	C	2001	COA	N3A-C2A-N1A	-4.41	121.91	128.58
2	B	2001	COA	N3A-C2A-N1A	-4.07	122.42	128.58
2	D	2001	COA	C2A-N3A-C4A	3.97	121.53	111.83
2	A	2001	COA	O4B-C1B-N9A	-3.93	100.54	108.09
2	A	2001	COA	N3A-C4A-N9A	3.78	133.60	127.17
2	C	2001	COA	N9A-C8A-N7A	-3.75	108.62	113.94
2	D	2001	COA	N3A-C4A-N9A	3.72	133.49	127.17
2	B	2001	COA	O4B-C4B-C5B	-3.70	97.48	109.33
2	B	2001	COA	O4B-C1B-N9A	-3.55	101.27	108.09
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	B	2001	COA	N3A-C4A-N9A	3.45	133.03	127.17
2	A	2001	COA	C2A-N3A-C4A	3.44	120.22	111.83
2	C	2001	COA	C4A-C5A-N7A	-3.42	106.67	110.58
2	C	2001	COA	C5A-N7A-C8A	3.39	108.78	103.45
2	D	2001	COA	N9A-C8A-N7A	-3.33	109.21	113.94
2	C	2001	COA	C2A-N3A-C4A	3.31	119.90	111.83
2	C	2001	COA	N3A-C4A-N9A	3.28	132.75	127.17
2	B	2001	COA	C2A-N3A-C4A	3.05	119.27	111.83
2	C	2001	COA	O4B-C1B-N9A	-3.00	102.32	108.09
2	A	2001	COA	N9A-C8A-N7A	-2.98	109.71	113.94
2	D	2001	COA	C5A-N7A-C8A	2.70	107.69	103.45
2	A	2001	COA	O8A-P3B-O7A	-2.65	100.52	110.83
2	B	2001	COA	N9A-C8A-N7A	-2.56	110.30	113.94
2	C	2001	COA	C4A-N9A-C8A	2.52	108.38	105.74
2	D	2001	COA	C4A-C5A-N7A	-2.51	107.71	110.58
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	A	2001	COA	C5A-N7A-C8A	2.34	107.12	103.45
2	A	2001	COA	C4A-N9A-C8A	2.29	108.14	105.74
2	B	2001	COA	CEP-CBP-CCP	2.27	111.97	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	COA	C4B-O4B-C1B	-2.25	104.50	109.47
2	B	2001	COA	O8A-P3B-O7A	-2.21	102.23	110.83
2	B	2001	COA	O9A-P3B-O7A	2.18	119.33	110.83
2	B	2001	COA	C4B-O4B-C1B	-2.12	104.78	109.47
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	C4A-N9A-C8A	2.03	107.87	105.74
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
2	A	2001	COA	C4A-C5A-N7A	-2.01	108.28	110.58

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

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Mol	Chain	Res	Type	Atoms
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
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:

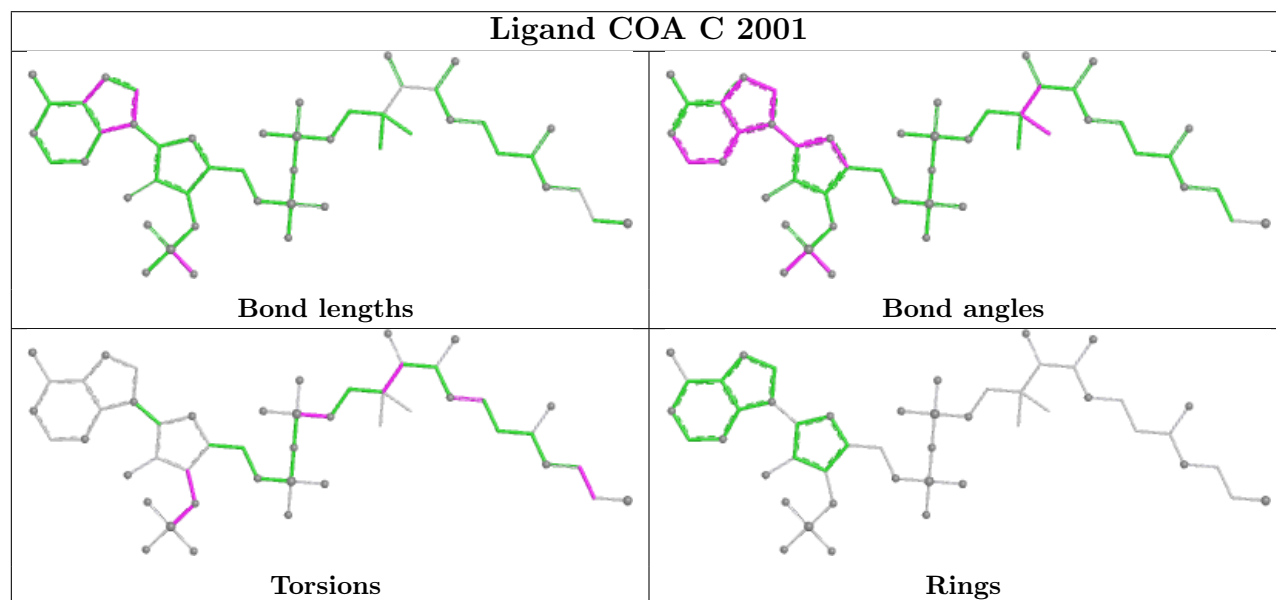
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	COA	2	0
2	B	2001	COA	1	0
4	C	2000	BTI	3	0

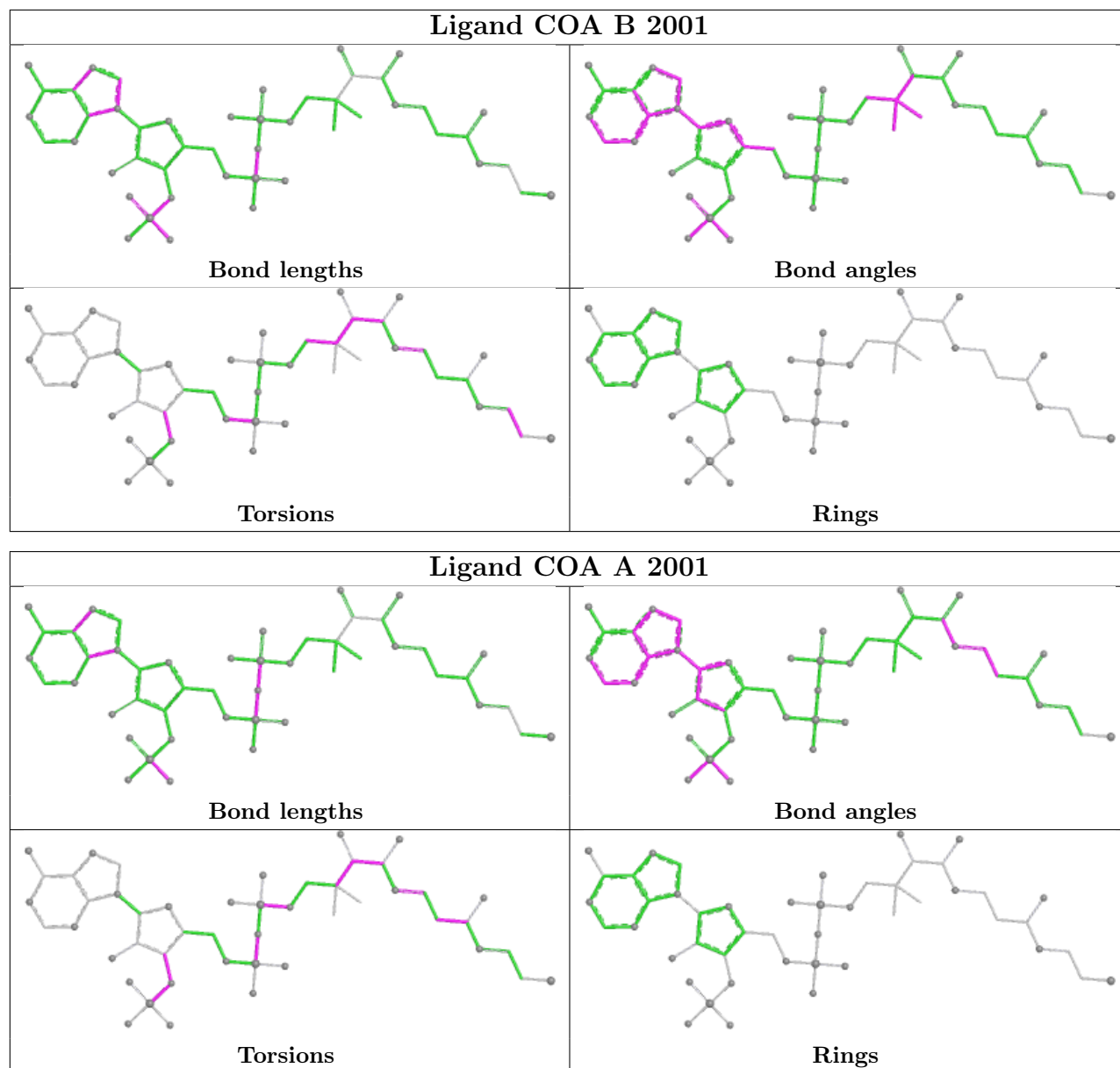
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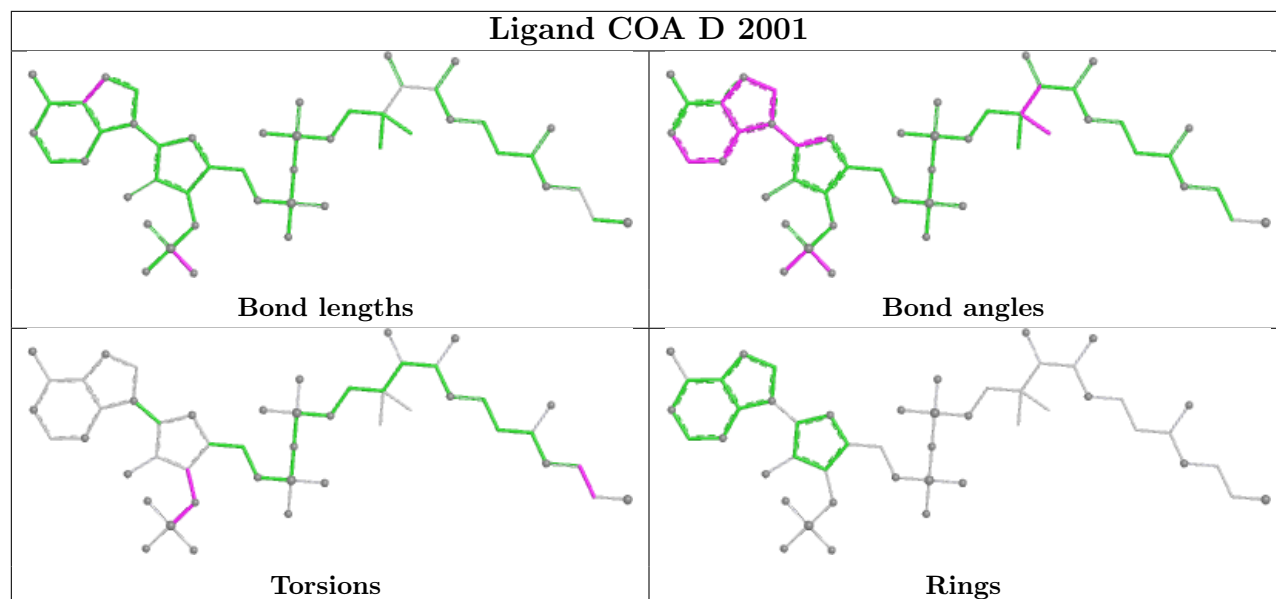
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2001	COA	6	0

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 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	994/1150 (86%)	0.70	63 (6%) 26 20	39, 76, 117, 151	0
1	B	989/1150 (86%)	0.20	11 (1%) 78 71	26, 52, 83, 102	0
1	C	995/1150 (86%)	0.22	18 (1%) 67 59	29, 52, 83, 107	0
1	D	934/1150 (81%)	0.93	86 (9%) 14 12	41, 83, 128, 173	0
All	All	3912/4600 (85%)	0.50	178 (4%) 37 29	26, 64, 111, 173	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	272	GLN	5.5
1	D	239	ILE	5.4
1	D	890	VAL	5.2
1	B	163	ASP	5.0
1	D	981	TYR	4.6
1	D	887	PHE	4.1
1	B	282	GLY	4.0
1	D	594	THR	4.0
1	D	973	ALA	3.9
1	D	975	THR	3.8
1	C	933	THR	3.8
1	D	967	ILE	3.7
1	D	963	LEU	3.7
1	A	816	ALA	3.7
1	D	1088	TYR	3.6
1	D	684	ASP	3.5
1	A	713	PRO	3.5
1	D	494	LEU	3.5
1	D	490	ILE	3.4
1	A	938	LEU	3.4
1	D	974	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	993	LEU	3.4
1	D	544	LEU	3.3
1	A	875	SER	3.3
1	A	931	VAL	3.3
1	D	770	LEU	3.3
1	D	962	ASP	3.3
1	D	734	GLY	3.3
1	D	959	PHE	3.2
1	C	877	GLN	3.2
1	D	828	ILE	3.2
1	A	993	LEU	3.1
1	D	952	ILE	3.1
1	D	416	ALA	3.1
1	A	940	PHE	3.1
1	D	555	GLU	3.1
1	D	968	LEU	3.0
1	A	888	ASP	3.0
1	D	688	VAL	2.9
1	A	919	LEU	2.9
1	C	271	HIS	2.9
1	A	239	ILE	2.9
1	D	854	ILE	2.9
1	D	947	PHE	2.8
1	A	160	ILE	2.8
1	D	158	THR	2.8
1	A	965	ALA	2.8
1	D	648	ALA	2.8
1	C	80	ALA	2.8
1	D	912	LYS	2.8
1	A	282	GLY	2.8
1	D	287	LEU	2.8
1	C	882	GLY	2.8
1	A	444	VAL	2.7
1	A	815	TYR	2.7
1	D	869	GLY	2.7
1	D	752	ALA	2.7
1	D	913	VAL	2.7
1	D	726	LEU	2.7
1	D	745	GLY	2.6
1	B	167	ILE	2.6
1	A	920	TYR	2.6
1	A	526	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	164	LEU	2.6
1	A	812	SER	2.6
1	A	474	GLY	2.6
1	A	166	VAL	2.6
1	A	167	ILE	2.6
1	D	1007	ILE	2.6
1	D	674	PHE	2.6
1	C	644	ARG	2.5
1	D	679	SER	2.5
1	D	720	LEU	2.5
1	D	790	GLY	2.5
1	A	932	ILE	2.5
1	A	908	THR	2.5
1	B	523	ASP	2.5
1	D	1087	ILE	2.5
1	A	416	ALA	2.5
1	D	881	LEU	2.5
1	A	317	GLY	2.5
1	D	861	ILE	2.5
1	B	524	TYR	2.5
1	B	414	GLN	2.5
1	C	970	GLY	2.5
1	A	1088	TYR	2.5
1	D	863	GLN	2.5
1	D	976	ALA	2.5
1	D	966	VAL	2.4
1	A	612	PHE	2.4
1	D	965	ALA	2.4
1	D	755	LEU	2.4
1	B	239	ILE	2.4
1	D	647	ASN	2.4
1	A	321	PHE	2.4
1	A	307	ALA	2.4
1	A	821	PRO	2.4
1	C	915	GLY	2.4
1	C	416	ALA	2.4
1	C	95	SER	2.4
1	D	802	SER	2.3
1	D	1062	LEU	2.3
1	A	741	LYS	2.3
1	D	489	ASP	2.3
1	A	287	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1027	TYR	2.3
1	D	793	ILE	2.3
1	D	635	PRO	2.3
1	B	165	PRO	2.3
1	A	552	GLY	2.3
1	D	858	ASN	2.3
1	A	899	PHE	2.3
1	C	527	ALA	2.3
1	A	238	TYR	2.3
1	A	981	TYR	2.3
1	B	494	LEU	2.3
1	D	652	LYS	2.3
1	A	244	HIS	2.3
1	D	279	PRO	2.2
1	D	393	THR	2.2
1	D	909	PRO	2.2
1	A	415	GLY	2.2
1	D	549	GLY	2.2
1	C	938	LEU	2.2
1	A	740	ILE	2.2
1	A	929	GLN	2.2
1	D	707	THR	2.2
1	D	512	PHE	2.2
1	A	973	ALA	2.2
1	D	38	LYS	2.2
1	A	871	TYR	2.2
1	A	872	SER	2.2
1	D	761	SER	2.2
1	A	618	PHE	2.2
1	D	291	ILE	2.2
1	A	664	GLN	2.2
1	A	275	VAL	2.2
1	A	922	VAL	2.2
1	D	274	VAL	2.2
1	D	492	PRO	2.2
1	D	985	VAL	2.2
1	D	990	VAL	2.2
1	A	739	ALA	2.2
1	D	167	ILE	2.1
1	D	244	HIS	2.1
1	C	1093	ASN	2.1
1	A	325	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	927	ASP	2.1
1	D	866	MET	2.1
1	D	415	GLY	2.1
1	A	494	LEU	2.1
1	A	726	LEU	2.1
1	B	83	SER	2.1
1	A	242	PRO	2.1
1	A	775	THR	2.1
1	D	883	LEU	2.1
1	D	532	VAL	2.1
1	C	937	LYS	2.1
1	D	370	LEU	2.1
1	D	487	LEU	2.1
1	D	788	ASP	2.1
1	C	238	TYR	2.1
1	D	673	VAL	2.1
1	D	738	LEU	2.1
1	A	570	PHE	2.1
1	D	892	ASP	2.1
1	C	682	TRP	2.1
1	A	683	VAL	2.0
1	A	283	LEU	2.0
1	A	963	LEU	2.0
1	A	975	THR	2.0
1	D	595	ALA	2.0
1	D	797	ALA	2.0
1	C	422	TYR	2.0
1	A	780	LEU	2.0
1	A	650	GLY	2.0
1	A	240	ASP	2.0
1	C	966	VAL	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

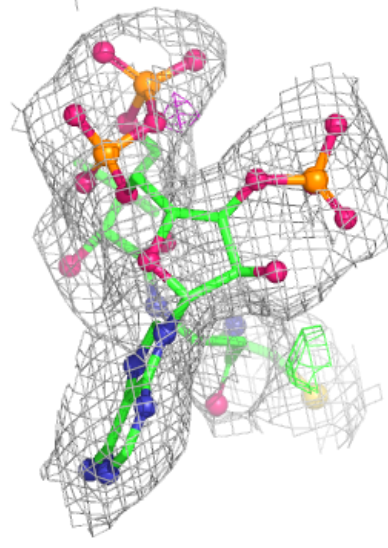
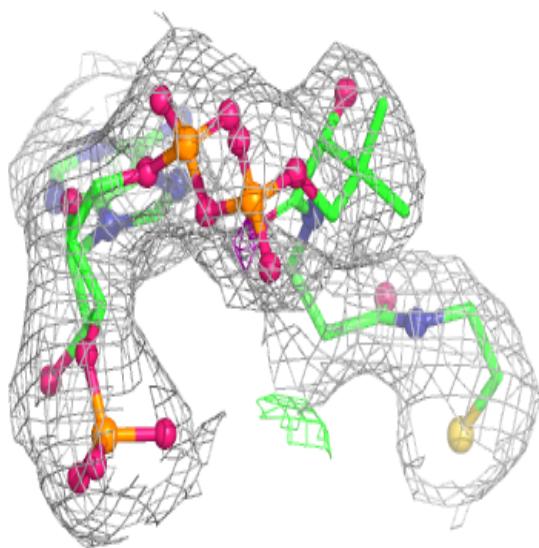
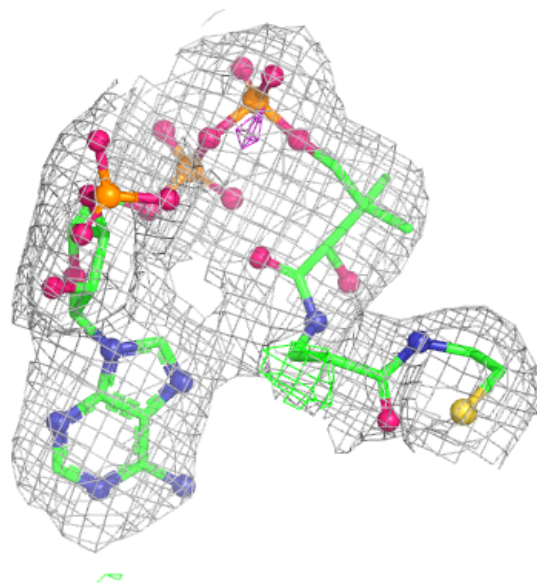
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MN	A	2002	1/1	0.88	0.12	86,86,86,86	0
4	BTI	B	2000	15/15	0.89	0.12	47,53,54,55	0
2	COA	D	2001	48/48	0.92	0.10	45,51,55,56	0
4	BTI	C	2000	15/15	0.93	0.09	36,40,42,43	0
3	MN	B	2002	1/1	0.93	0.09	60,60,60,60	0
2	COA	C	2001	48/48	0.95	0.08	32,36,48,51	0
2	COA	B	2001	48/48	0.95	0.08	37,40,43,45	0
2	COA	A	2001	48/48	0.95	0.08	44,48,57,59	0
3	MN	C	2002	1/1	0.97	0.05	65,65,65,65	0
3	MN	D	2002	1/1	0.98	0.04	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.

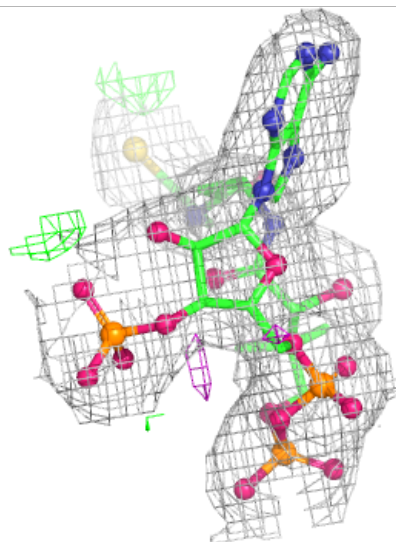
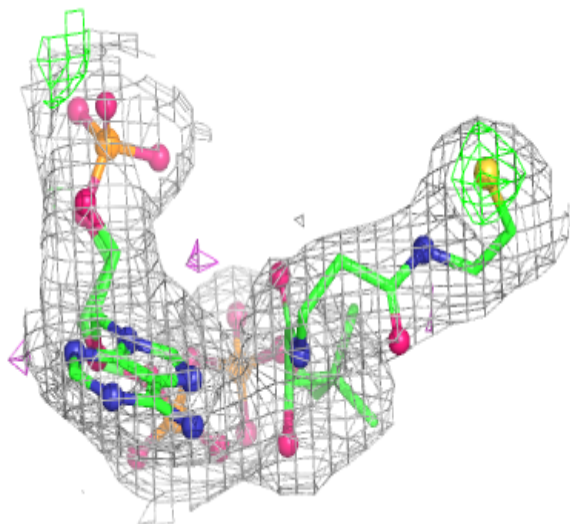
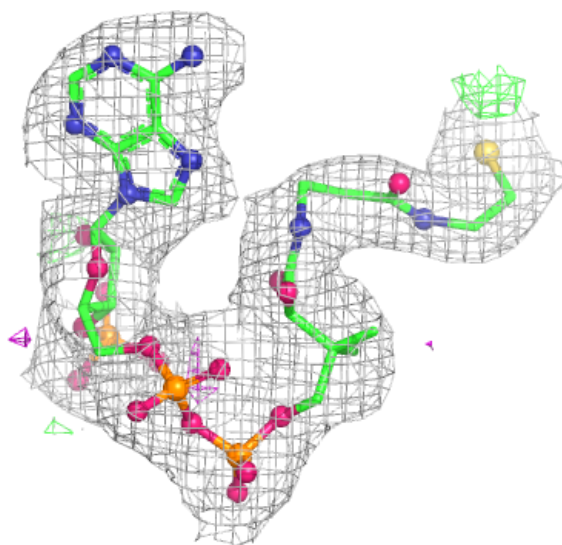
Electron density around COA D 2001:

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



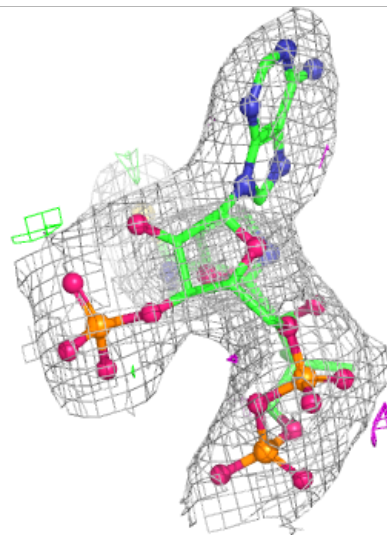
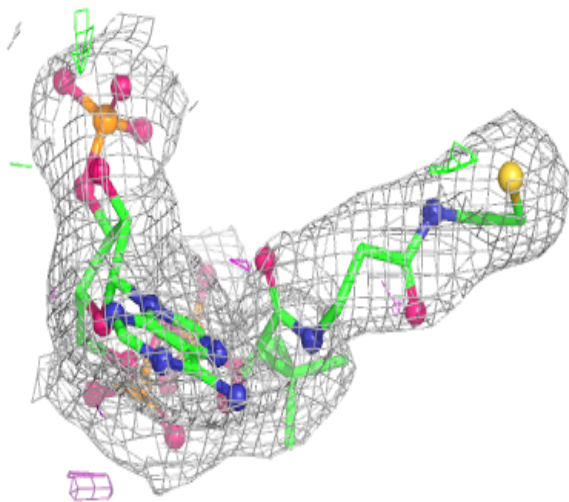
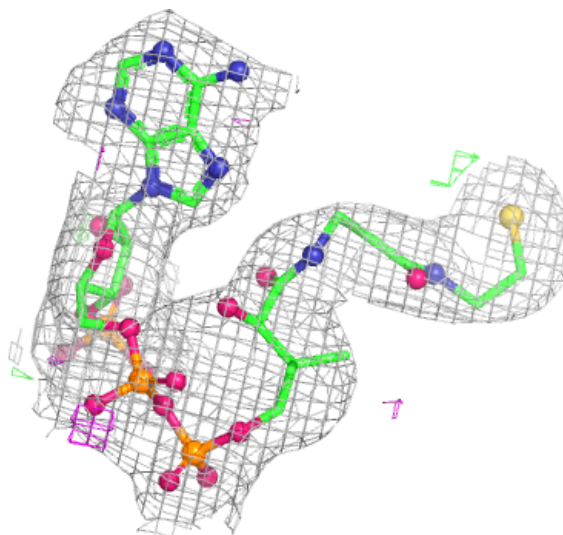
Electron density around COA C 2001:

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



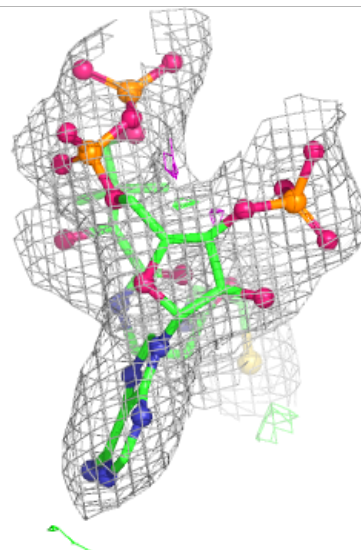
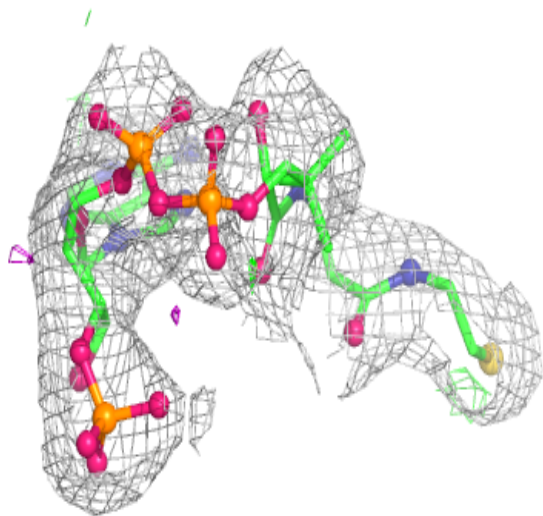
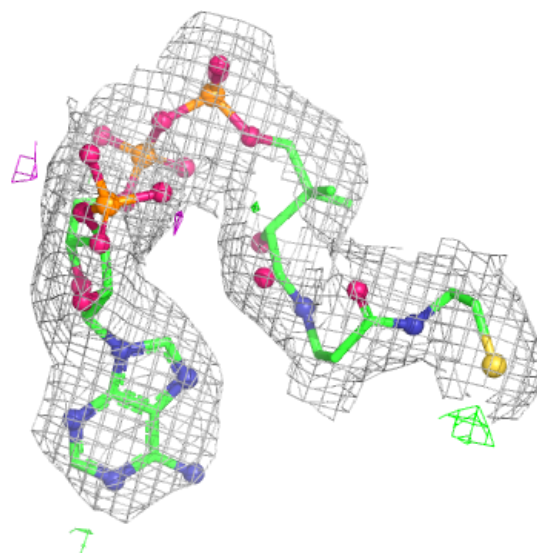
Electron density around COA B 2001:

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



Electron density around COA 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.