



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:39 AM UTC

PDB ID : 8GK8 / pdb_00008gk8
Title : R21A Staphylococcus aureus pyruvate carboxylase
Authors : Laseke, A.J.; St.Maurice, M.
Deposited on : 2023-03-17
Resolution : 2.68 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

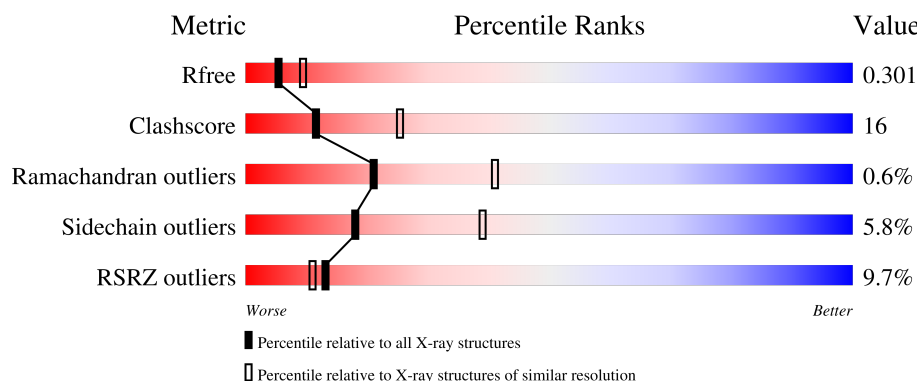
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	1151	
1	B	1151	
1	C	1151	
1	D	1151	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BTI	C	1204	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31053 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.

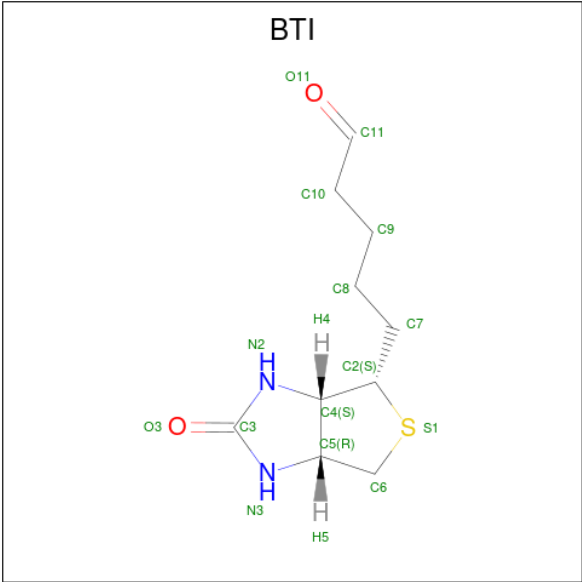
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	993	Total	C	N	O	S	0	2	0
			7687	4881	1290	1488	28			
1	B	1053	Total	C	N	O	S	0	0	0
			8029	5102	1348	1551	28			
1	D	950	Total	C	N	O	S	0	0	0
			7205	4585	1213	1381	26			
1	A	1041	Total	C	N	O	S	0	0	0
			7691	4883	1298	1484	26			

There are 12 discrepancies between the modelled and reference sequences:

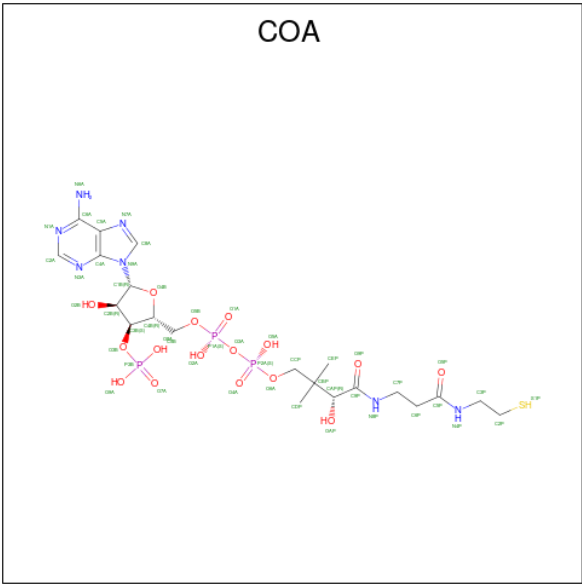
Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ALA	ARG	engineered mutation	UNP A0A3A5LTU8
C	1150	ASN	-	expression tag	UNP A0A3A5LTU8
C	1151	CYS	-	expression tag	UNP A0A3A5LTU8
B	21	ALA	ARG	engineered mutation	UNP A0A3A5LTU8
B	1150	ASN	-	expression tag	UNP A0A3A5LTU8
B	1151	CYS	-	expression tag	UNP A0A3A5LTU8
D	21	ALA	ARG	engineered mutation	UNP A0A3A5LTU8
D	1150	ASN	-	expression tag	UNP A0A3A5LTU8
D	1151	CYS	-	expression tag	UNP A0A3A5LTU8
A	21	ALA	ARG	engineered mutation	UNP A0A3A5LTU8
A	1150	ASN	-	expression tag	UNP A0A3A5LTU8
A	1151	CYS	-	expression tag	UNP A0A3A5LTU8

- Molecule 2 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
2	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).

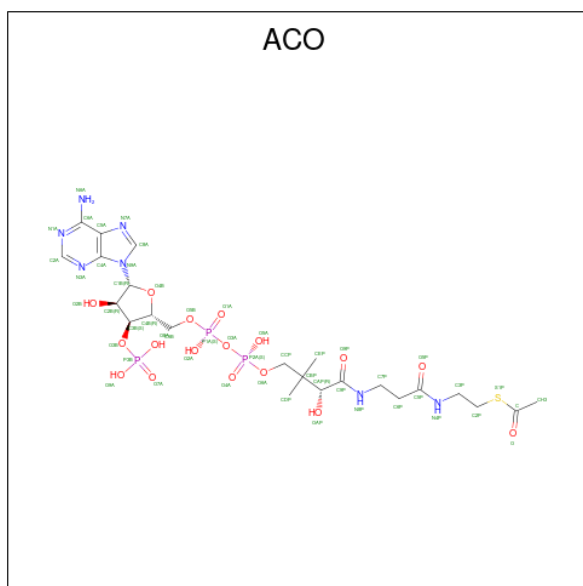


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	
								0	0

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 5 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			51	23	7	17	3	1	
								0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	85	Total	O	0	0
			85	85		

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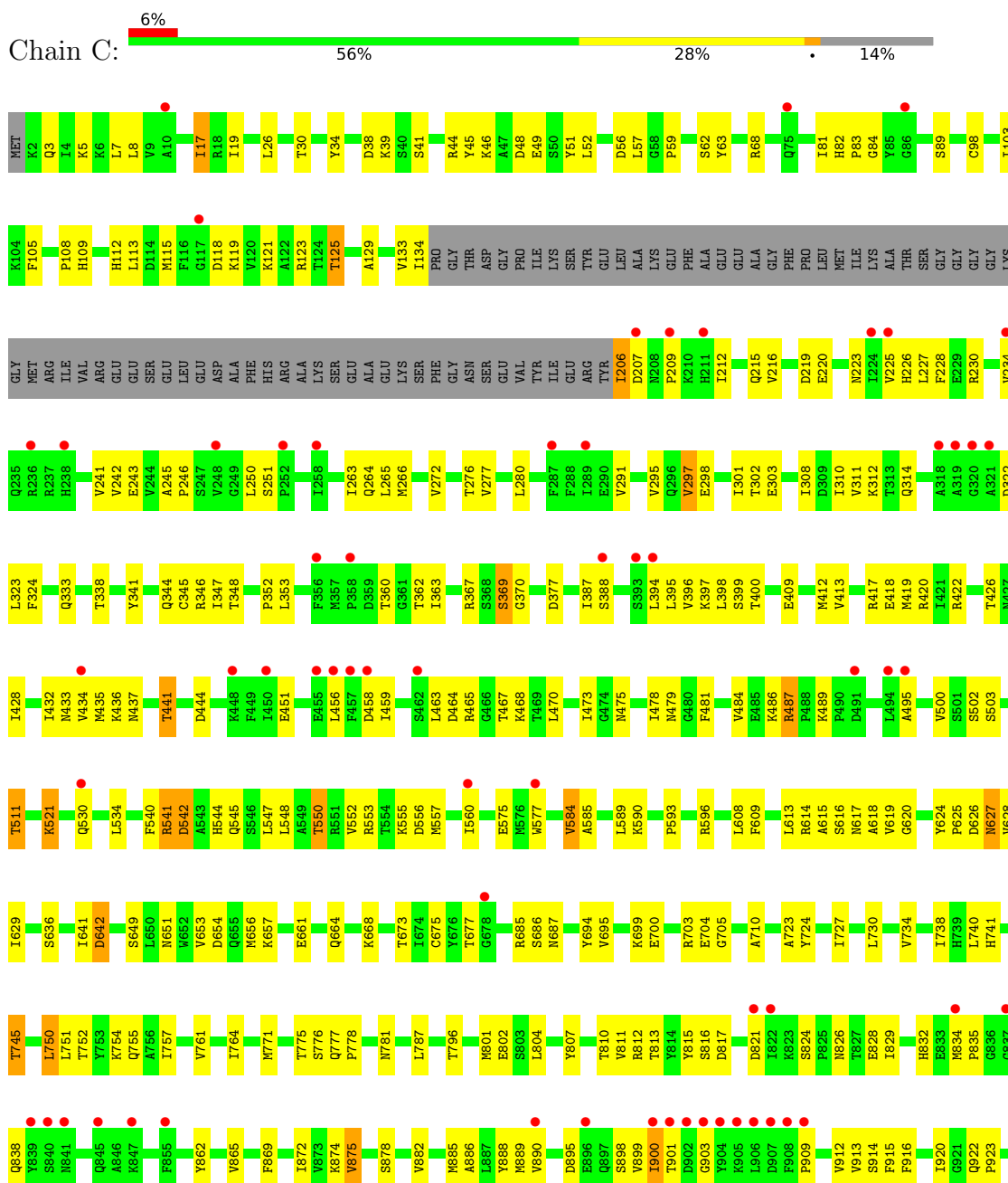
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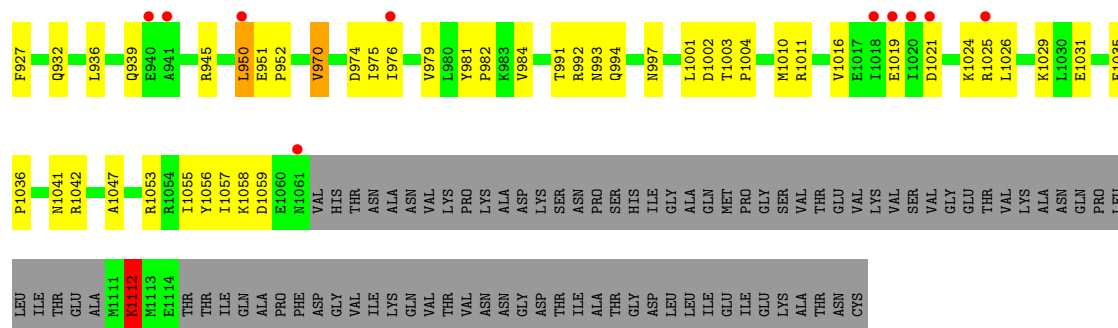
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	89	Total 89	O 89	0	0
6	D	44	Total 44	O 44	0	0
6	A	60	Total 60	O 60	0	0

3 Residue-property plots

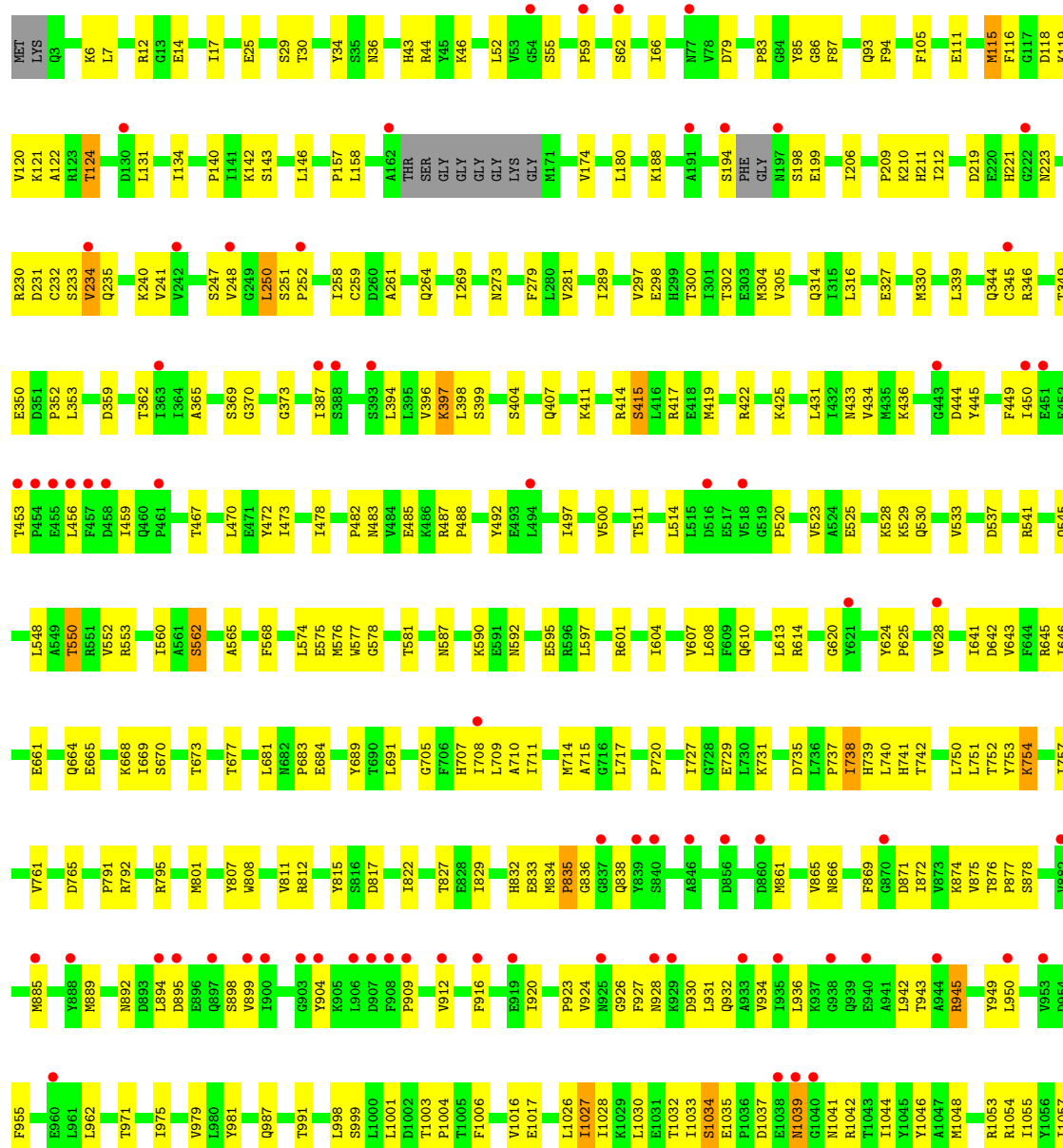
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

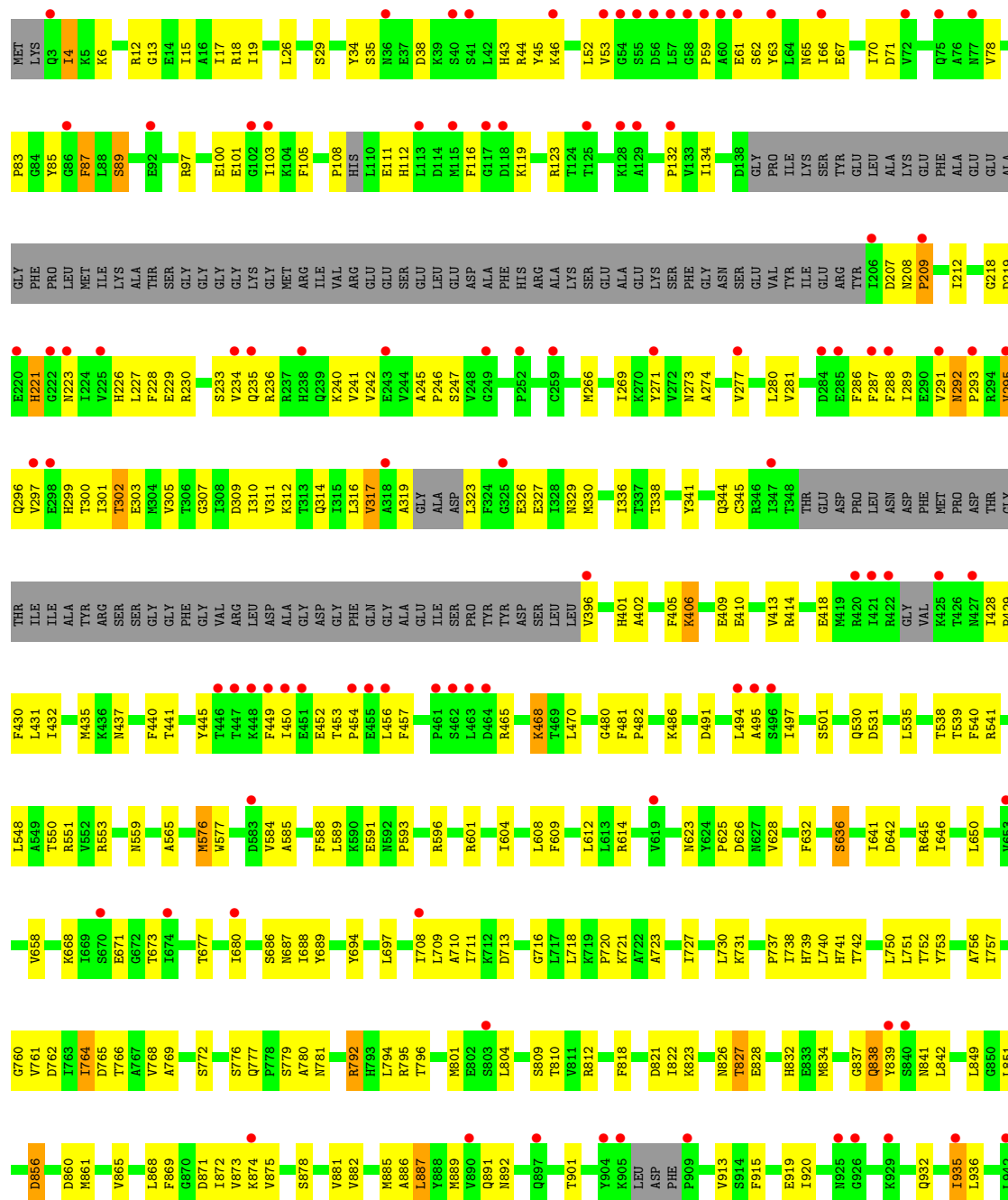
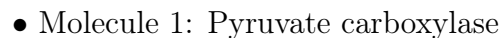
• Molecule 1: Pyruvate carboxylase

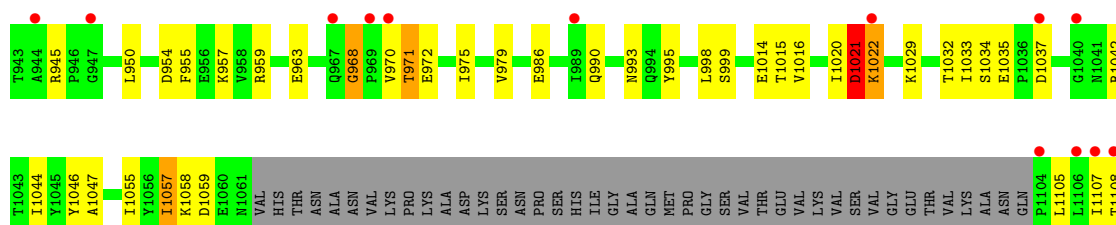




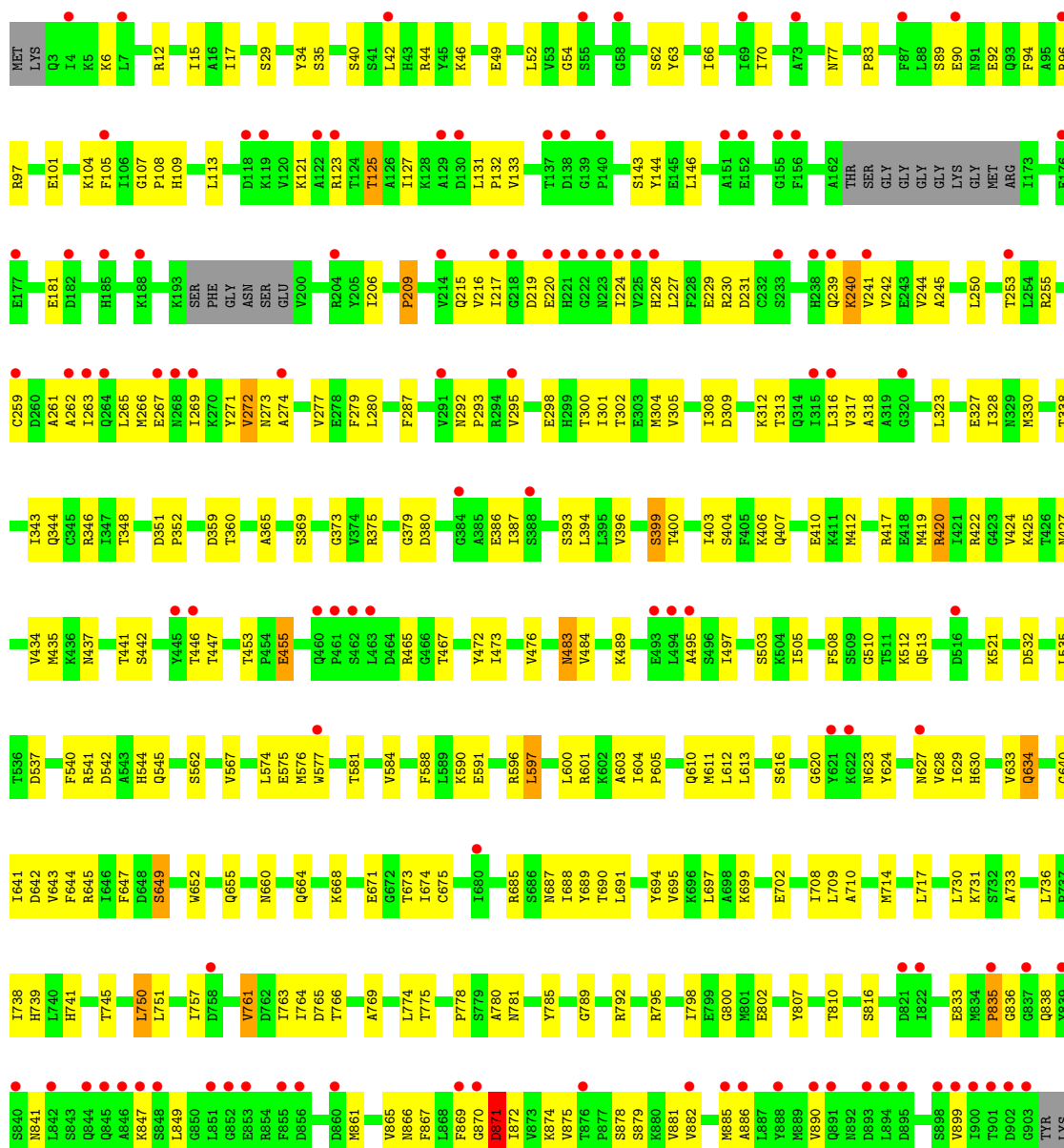
• Molecule 1: Pyruvate carboxylase

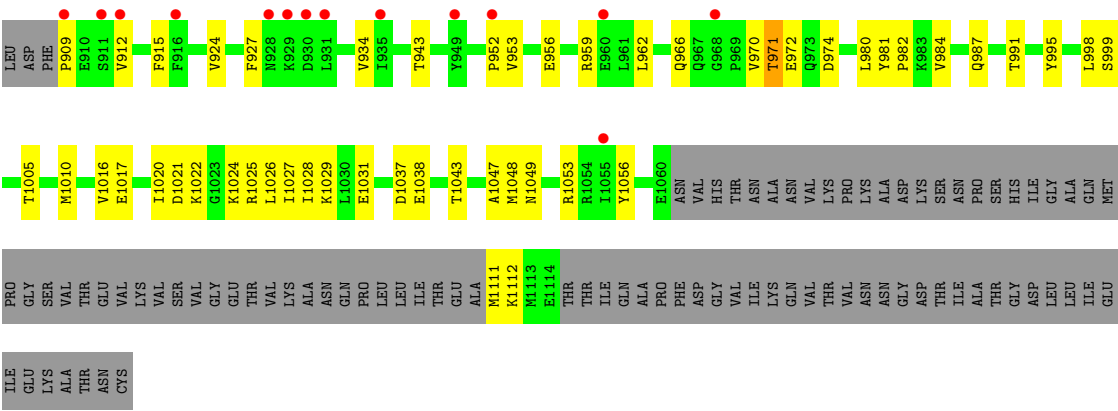






• Molecule 1: Pyruvate carboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.98Å 253.67Å 125.66Å 90.00° 110.99° 90.00°	Depositor
Resolution (Å)	60.62 – 2.68 60.62 – 2.68	Depositor EDS
% Data completeness (in resolution range)	70.7 (60.62-2.68) 71.0 (60.62-2.68)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.248 , 0.301 0.248 , 0.301	Depositor DCC
R_{free} test set	5562 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	31053	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, ACO, BTI, MN

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	0.16	0/7839	0.41	3/10674 (0.0%)
1	B	0.16	0/8183	0.41	3/11110 (0.0%)
1	C	0.17	0/7842	0.42	2/10633 (0.0%)
1	D	0.20	0/7339	0.45	5/9966 (0.1%)
All	All	0.17	0/31203	0.42	13/42383 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	GLY	N-CA-C	13.88	133.26	115.21
1	D	1021	ASP	CB-CA-C	8.29	126.91	110.42
1	C	542	ASP	N-CA-C	-7.38	104.42	113.50
1	A	871	ASP	CA-C-N	-7.24	114.52	122.27
1	A	871	ASP	C-N-CA	-7.24	114.52	122.27
1	C	541	ARG	N-CA-C	6.37	124.37	110.80
1	D	576	MET	CB-CA-C	6.28	118.78	109.29
1	B	87	PHE	N-CA-C	-6.14	97.72	110.80
1	D	292	ASN	CA-C-N	6.01	133.97	120.56
1	D	292	ASN	C-N-CA	6.01	133.97	120.56
1	D	1022	LYS	N-CA-C	5.30	122.08	110.80
1	B	87	PHE	N-CA-CB	5.29	119.44	110.49
1	A	542	ASP	N-CA-C	-5.01	107.01	113.23

There are no chirality outliers.

There are no planarity outliers.

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	7691	0	7118	236	0
1	B	8029	0	7697	230	0
1	C	7687	0	7443	256	0
1	D	7205	0	6868	261	0
2	A	15	0	16	6	0
2	B	15	0	15	2	0
2	C	30	0	31	10	0
3	C	48	0	32	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	51	0	34	4	0
6	A	60	0	0	5	0
6	B	89	0	0	12	0
6	C	85	0	0	23	0
6	D	44	0	0	3	0
All	All	31053	0	29254	961	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 16.

All (961) 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:A:1112:LYS:HZ3	2:A:1201:BTI:C11	1.08	1.60
2:C:1204:BTI:H11	1:D:1112:LYS:NZ	1.02	1.33
2:C:1204:BTI:C11	1:D:1112:LYS:NZ	1.98	1.27
2:C:1204:BTI:C11	1:D:1112:LYS:HZ1	1.55	1.19
1:A:1112:LYS:NZ	2:A:1201:BTI:H11	0.86	1.19
1:D:288:PHE:CZ	1:D:291:VAL:HG23	1.84	1.11
1:A:1112:LYS:NZ	2:A:1201:BTI:C11	1.81	1.08
1:D:288:PHE:CE1	1:D:291:VAL:HG23	1.89	1.07
1:D:626:ASP:OD2	1:D:945:ARG:NH2	1.90	1.05
1:C:609:PHE:HB3	6:C:1342:HOH:O	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:MET:HE1	1:D:291:VAL:HG11	1.39	0.98
1:A:689:TYR:HE2	1:A:871:ASP:HB3	1.33	0.94
2:C:1204:BTI:C11	1:D:1112:LYS:HZ2	1.73	0.92
1:A:216:VAL:HG21	1:A:266:MET:HG3	1.51	0.91
1:D:288:PHE:CE1	1:D:291:VAL:CG2	2.55	0.90
1:C:754:LYS:NZ	6:C:1302:HOH:O	2.05	0.89
1:C:216:VAL:HG21	1:C:266:MET:HG3	1.55	0.89
1:C:345:CYS:SG	6:C:1375:HOH:O	2.32	0.88
1:A:1112:LYS:HZ2	2:A:1201:BTI:H11	1.33	0.87
1:C:1019:GLU:HG3	1:C:1025:ARG:HG2	1.58	0.86
1:D:591:GLU:OE2	1:D:596:ARG:NH2	2.08	0.86
1:A:1112:LYS:HZ1	2:A:1201:BTI:H11	1.37	0.85
1:D:266:MET:CE	1:D:291:VAL:HG11	2.08	0.84
1:A:689:TYR:OH	1:A:871:ASP:O	1.95	0.83
1:A:83:PRO:HB2	1:A:89:SER:HA	1.60	0.83
1:C:243:GLU:OE2	1:C:346:ARG:NH2	2.13	0.82
1:D:491:ASP:OD1	6:D:1301:HOH:O	1.98	0.81
1:D:230:ARG:HD3	1:D:301:ILE:HD11	1.60	0.81
1:B:673:THR:HG22	1:B:710:ALA:HB3	1.63	0.81
1:C:82:HIS:HD2	1:C:84:GLY:H	1.30	0.80
1:D:288:PHE:HE1	1:D:291:VAL:CG2	1.95	0.80
1:A:838:GLN:NE2	1:A:879:SER:OG	2.15	0.80
1:C:226:HIS:HB3	1:C:263:ILE:HD11	1.63	0.80
1:D:731:LYS:NZ	1:D:760:GLY:O	2.14	0.80
1:A:584:VAL:HG13	1:A:588:PHE:HD2	1.46	0.80
1:B:548:LEU:HD11	1:B:812:ARG:HG3	1.63	0.79
1:C:302:THR:OG1	6:C:1301:HOH:O	2.01	0.79
1:C:39:LYS:HG3	1:A:1027:ILE:HD13	1.64	0.79
1:A:241:VAL:HG23	1:A:242:VAL:HG23	1.62	0.79
1:D:277:VAL:HG13	1:D:291:VAL:HG22	1.63	0.79
1:C:553:ARG:NH2	1:C:1001:LEU:O	2.16	0.78
1:B:541:ARG:NH1	1:B:545:GLN:OE1	2.16	0.78
1:A:673:THR:HG22	1:A:710:ALA:HB3	1.64	0.78
1:D:1022:LYS:O	1:D:1022:LYS:HD3	1.83	0.78
1:B:895:ASP:H	1:B:898:SER:HB3	1.48	0.78
1:A:143:SER:HB3	1:A:146:LEU:HD12	1.65	0.78
2:C:1204:BTI:H11	1:D:1112:LYS:HZ2	0.97	0.77
1:C:463:LEU:HD12	1:C:465:ARG:HG3	1.68	0.75
1:D:531:ASP:O	1:D:792:ARG:NH1	2.19	0.75
1:A:645:ARG:HG3	1:A:673:THR:HG21	1.69	0.74
1:C:81:ILE:HG13	1:C:103:ILE:HG21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:GLN:HB3	1:D:240:LYS:HA	1.70	0.74
1:C:129:ALA:O	1:C:264:GLN:NE2	2.20	0.74
1:C:241:VAL:HG23	1:C:242:VAL:HG23	1.69	0.74
1:B:1111:MET:HG3	1:A:483:ASN:HA	1.70	0.74
1:D:209:PRO:HB2	1:D:280:LEU:HD22	1.70	0.74
1:D:288:PHE:CZ	1:D:291:VAL:CG2	2.68	0.73
1:C:426:THR:HG22	1:C:428:ILE:H	1.52	0.73
1:A:343:ILE:HG21	1:A:435:MET:HE1	1.69	0.73
1:A:1112:LYS:CE	2:A:1201:BTI:H11	2.12	0.73
1:C:641:ILE:HD13	6:C:1342:HOH:O	1.87	0.72
1:B:892:ASN:HB2	1:B:894:LEU:HD11	1.70	0.72
1:C:745:THR:HG22	1:C:775:THR:HA	1.70	0.72
1:D:266:MET:HE1	1:D:291:VAL:CG1	2.19	0.72
1:C:420:ARG:NH2	3:C:1202:COA:O5P	2.22	0.72
1:D:673:THR:HG22	1:D:710:ALA:HB3	1.73	0.71
1:C:694:TYR:OH	6:C:1303:HOH:O	2.08	0.71
1:B:592:ASN:HB3	1:B:595:GLU:HB2	1.72	0.71
1:C:398:LEU:HG	1:C:412:MET:HE1	1.72	0.71
1:A:699:LYS:HE2	1:A:733:ALA:HB1	1.71	0.71
1:D:1035:GLU:OE2	1:D:1035:GLU:N	2.17	0.70
1:B:212:ILE:HD12	1:B:281:VAL:HG21	1.73	0.70
1:D:236:ARG:HH12	1:D:457:PHE:HE1	1.40	0.70
1:C:832:HIS:CD2	1:C:834:MET:HE2	2.26	0.69
1:A:717:LEU:HD11	1:A:833:GLU:HB3	1.72	0.69
1:C:557:MET:HE1	1:C:596:ARG:HD3	1.73	0.69
1:D:235:GLN:HA	1:D:241:VAL:HG22	1.73	0.69
1:C:123:ARG:HH11	1:C:133:VAL:HG13	1.57	0.69
1:B:866:ASN:ND2	1:B:871:ASP:HA	2.07	0.69
3:C:1202:COA:HN8	3:C:1202:COA:H132	1.58	0.69
1:D:327:GLU:N	1:D:327:GLU:OE1	2.25	0.69
1:A:412:MET:HG2	1:A:435:MET:HE2	1.74	0.69
1:C:82:HIS:CD2	1:C:84:GLY:H	2.10	0.69
1:C:495:ALA:HB2	1:C:810:THR:HG21	1.75	0.69
1:A:645:ARG:HA	1:A:671:GLU:HB2	1.74	0.69
1:B:259:CYS:SG	6:B:1316:HOH:O	2.50	0.69
1:D:108:PRO:HG2	1:D:293:PRO:HB2	1.73	0.69
1:D:708:ILE:HG23	1:D:737:PRO:HG2	1.73	0.69
1:B:500:VAL:H	1:B:562:SER:HB2	1.59	0.69
1:C:451:GLU:N	1:C:451:GLU:OE1	2.26	0.68
1:B:876:THR:O	6:B:1301:HOH:O	2.10	0.68
1:C:219:ASP:OD2	1:C:323:LEU:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:MET:HE1	1:A:909:PRO:HG2	1.76	0.68
1:A:689:TYR:CE2	1:A:871:ASP:HB3	2.23	0.68
1:C:530:GLN:HG3	1:C:534:LEU:HD11	1.76	0.68
1:C:1042:ARG:NH1	1:C:1059:ASP:OD2	2.27	0.68
1:B:829:ILE:HD12	1:B:832:HIS:HE1	1.58	0.67
1:B:834:MET:HB3	1:B:838:GLN:HB3	1.74	0.67
1:B:514:LEU:HD23	1:B:523:VAL:HG22	1.75	0.67
1:B:740:LEU:HD12	1:B:741:HIS:H	1.58	0.67
1:B:1042:ARG:NH1	1:B:1059:ASP:OD2	2.27	0.67
1:C:654:ASP:OD1	1:C:657:LYS:NZ	2.27	0.67
1:D:288:PHE:HZ	1:D:291:VAL:HG23	1.53	0.67
1:B:829:ILE:HD12	1:B:832:HIS:CE1	2.29	0.67
1:A:453:THR:HG23	1:A:455:GLU:OE2	1.93	0.67
1:A:505:ILE:HA	1:A:508:PHE:HD2	1.59	0.67
1:C:265:LEU:HG	1:C:266:MET:HE2	1.77	0.66
1:B:467:THR:OG1	1:B:1053:ARG:NH2	2.19	0.66
1:A:262:ALA:HB2	1:A:279:PHE:HE2	1.61	0.66
1:C:83:PRO:HB2	1:C:89:SER:HA	1.75	0.66
1:C:754:LYS:HD3	1:B:751:LEU:HD21	1.78	0.66
1:B:230:ARG:HE	1:B:298:GLU:HG3	1.61	0.66
1:B:14:GLU:OE2	1:B:397:LYS:NZ	2.27	0.66
1:B:34:TYR:CD1	1:B:44:ARG:HG3	2.31	0.66
1:D:623:ASN:ND2	1:D:919:GLU:O	2.29	0.66
1:C:297:VAL:HG12	1:C:397:LYS:HE2	1.78	0.66
1:B:417:ARG:NH2	6:B:1305:HOH:O	2.28	0.66
1:D:645:ARG:HA	1:D:671:GLU:HB2	1.77	0.66
1:D:913:VAL:HG12	1:D:935:ILE:HG22	1.78	0.66
1:B:835:PRO:HD2	1:B:838:GLN:HG2	1.78	0.66
1:C:303:GLU:HG3	1:C:310:ILE:HG13	1.78	0.65
1:A:365:ALA:HB3	1:A:422:ARG:HB2	1.78	0.65
1:C:781:ASN:HB3	1:B:827:THR:HG21	1.78	0.65
1:D:301:ILE:O	1:D:305:VAL:HG23	1.97	0.65
1:B:449:PHE:O	1:B:453:THR:OG1	2.08	0.65
1:A:685:ARG:NH2	1:A:833:GLU:OE2	2.26	0.65
1:A:674:ILE:HG23	1:A:697:LEU:HD23	1.79	0.65
1:C:487:ARG:HH22	1:C:817:ASP:CG	2.05	0.65
1:B:450:ILE:H	1:B:450:ILE:HD12	1.62	0.64
1:B:923:PRO:HD3	1:B:927:PHE:CZ	2.32	0.64
1:A:266:MET:HE3	1:A:277:VAL:HG22	1.79	0.64
1:D:872:ILE:O	1:D:874:LYS:NZ	2.30	0.64
1:D:495:ALA:HB2	1:D:810:THR:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1108:THR:N	1:D:1115:THR:O	2.29	0.64
1:A:12:ARG:HH22	1:A:380:ASP:CG	2.05	0.64
1:C:677:THR:O	6:C:1303:HOH:O	2.14	0.64
1:D:1042:ARG:HD2	1:D:1059:ASP:OD2	1.98	0.64
1:A:15:ILE:HG12	6:A:1323:HOH:O	1.97	0.64
1:C:895:ASP:H	1:C:898:SER:HB3	1.62	0.64
1:D:409:GLU:OE2	1:D:441:THR:OG1	2.16	0.64
1:A:647:PHE:HE2	1:A:875:VAL:HG21	1.63	0.64
1:C:548:LEU:HD11	1:C:812:ARG:HG3	1.80	0.64
1:A:866:ASN:O	1:A:870:GLY:O	2.16	0.63
1:B:211:HIS:H	1:B:233:SER:HB3	1.64	0.63
1:B:904:TYR:HA	1:B:934:VAL:HG23	1.80	0.63
1:D:741:HIS:ND1	1:D:765:ASP:OD2	2.25	0.63
1:C:834:MET:HG2	1:C:862:TYR:CE2	2.33	0.63
1:D:277:VAL:HG13	1:D:291:VAL:CG2	2.28	0.63
1:B:553:ARG:HD3	1:B:1003:THR:HG23	1.81	0.63
1:A:541:ARG:NH2	1:A:575:GLU:OE1	2.22	0.63
1:B:470:LEU:HD13	1:B:1046:TYR:CD2	2.34	0.63
1:A:627:ASN:HD22	1:A:953:VAL:H	1.47	0.63
1:D:437:ASN:HD22	1:D:456:LEU:HD21	1.64	0.62
1:D:626:ASP:HB3	1:D:658:VAL:HG21	1.81	0.62
1:A:17:ILE:HG23	1:A:46:LYS:HG3	1.81	0.62
1:C:627[B]:ASN:ND2	1:C:952:PRO:HA	2.14	0.62
1:C:548:LEU:HB2	6:C:1367:HOH:O	1.99	0.62
1:C:951:GLU:HG3	1:C:952:PRO:HD2	1.80	0.62
1:A:576:MET:HE1	1:A:597:LEU:HD13	1.80	0.62
1:A:866:ASN:ND2	1:A:871:ASP:OD2	2.27	0.62
1:A:1029:LYS:HB3	1:A:1047:ALA:HB3	1.81	0.62
1:C:17:ILE:HG23	1:C:46:LYS:HG3	1.81	0.62
1:D:881:VAL:HG21	1:D:915:PHE:HB2	1.80	0.62
1:C:17:ILE:HD13	1:C:46:LYS:HG3	1.81	0.62
1:C:115:MET:HG2	1:C:125:THR:HG21	1.82	0.62
1:C:922:GLN:HG3	1:C:927:PHE:HE1	1.64	0.62
1:A:104:LYS:HG2	1:A:318:ALA:HB1	1.80	0.62
1:B:478:ILE:HD11	1:B:1044:ILE:HD11	1.82	0.61
1:C:585:ALA:HB3	1:C:593:PRO:HG3	1.82	0.61
2:C:1204:BTI:H11	1:D:1112:LYS:HZ1	0.79	0.61
1:D:266:MET:CE	1:D:291:VAL:CG1	2.77	0.61
1:C:422:ARG:HG3	1:C:1053:ARG:HH21	1.65	0.61
1:A:417:ARG:O	1:A:420:ARG:NH1	2.33	0.61
1:C:832:HIS:HD2	1:C:834:MET:HG3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:GLN:HA	1:B:241:VAL:HG22	1.82	0.61
1:B:436:LYS:NZ	6:B:1305:HOH:O	2.33	0.61
1:A:273:ASN:ND2	6:A:1306:HOH:O	2.32	0.61
1:C:363:ILE:HD12	1:C:387:ILE:HD11	1.83	0.61
1:C:685:ARG:HH21	1:C:686:SER:HB2	1.64	0.61
1:B:415:SER:O	1:B:419:MET:HG3	2.00	0.61
1:A:750:LEU:HD12	1:A:778:PRO:HB3	1.81	0.61
1:D:796:THR:HG21	1:D:801:MET:HE2	1.81	0.61
1:A:230:ARG:HD2	1:A:298:GLU:HG3	1.82	0.61
1:C:550:THR:HB	1:C:584:VAL:HG11	1.83	0.61
1:D:614:ARG:NH2	6:D:1306:HOH:O	2.33	0.61
1:C:821:ASP:OD2	1:C:821:ASP:N	2.33	0.61
1:B:923:PRO:HD2	1:B:926:GLY:HA2	1.83	0.61
1:B:553:ARG:NH2	1:B:1001:LEU:O	2.33	0.60
1:D:832:HIS:HD2	1:D:834:MET:H	1.48	0.60
1:B:434:VAL:HA	1:B:456:LEU:HD22	1.83	0.60
1:D:535:LEU:HD23	1:D:794:LEU:HD11	1.84	0.60
1:B:497:ILE:HG12	1:B:807:TYR:HE1	1.66	0.59
1:B:909:PRO:HB2	1:B:912:VAL:HG23	1.82	0.59
1:A:348:THR:HG22	1:A:394:LEU:HA	1.84	0.59
1:D:601:ARG:NH2	1:D:642:ASP:OD2	2.34	0.59
1:A:590:LYS:HG2	1:A:991:THR:HG21	1.83	0.59
1:C:560:ILE:HG12	1:C:807:TYR:CE2	2.37	0.59
1:C:727:ILE:HD12	1:C:738:ILE:HG21	1.84	0.59
1:B:339:LEU:HD21	1:D:307:GLY:HA3	1.84	0.59
1:B:613:LEU:HD23	1:B:646:ILE:HG12	1.84	0.59
1:C:787:LEU:O	6:C:1304:HOH:O	2.16	0.59
1:A:396:VAL:HG11	1:A:419:MET:HE2	1.85	0.59
1:C:750:LEU:HD22	1:C:778:PRO:HB3	1.85	0.59
1:A:1053:ARG:NH2	5:A:1202:ACO:O9A	2.36	0.59
1:C:541:ARG:NH1	1:C:545:GLN:OE1	2.36	0.59
1:B:470:LEU:HG	1:B:1048:MET:HE2	1.84	0.59
1:D:440:PHE:CD1	1:D:445:TYR:HE2	2.20	0.59
1:B:829:ILE:HD11	1:B:834:MET:O	2.03	0.59
1:B:861:MET:O	1:B:865:VAL:HG23	2.03	0.59
1:D:35:SER:HB2	1:D:63:TYR:CE2	2.38	0.59
1:B:212:ILE:CD1	1:B:250:LEU:HD21	2.32	0.59
1:C:475:ASN:OD1	1:C:479:ASN:ND2	2.35	0.59
1:D:85:TYR:CE2	1:D:297:VAL:HG22	2.38	0.59
1:C:219:ASP:OD2	1:C:223:ASN:HB2	2.03	0.58
1:C:872:ILE:HG22	1:C:923:PRO:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ARG:NH2	6:C:1317:HOH:O	2.35	0.58
1:C:388:SER:OG	6:C:1305:HOH:O	2.17	0.58
1:C:434:VAL:HG22	1:C:456:LEU:HD13	1.85	0.58
1:D:762:ASP:OD2	6:D:1302:HOH:O	2.16	0.58
1:D:83:PRO:HG2	1:D:105:PHE:CE1	2.38	0.58
1:D:856:ASP:OD1	1:D:856:ASP:N	2.36	0.58
1:C:377:ASP:HB2	1:C:397:LYS:HB2	1.85	0.58
1:C:541:ARG:C	1:C:541:ARG:HD2	2.28	0.58
1:D:680:ILE:HD11	1:D:694:TYR:CE2	2.39	0.58
1:A:541:ARG:NH1	1:A:545:GLN:OE1	2.35	0.58
1:A:591:GLU:HB2	1:A:999:SER:HB3	1.86	0.58
1:B:134:ILE:HD11	1:B:289:ILE:HD13	1.85	0.58
1:B:300:THR:O	1:B:304:MET:HG3	2.04	0.58
1:B:369:SER:OG	1:B:370:GLY:N	2.35	0.58
1:A:422:ARG:HE	5:A:1202:ACO:P3B	2.26	0.58
1:C:1035:GLU:HG3	1:C:1036:PRO:HD2	1.86	0.58
1:A:219:ASP:HB3	1:A:323:LEU:HD13	1.84	0.58
2:C:1201:BTI:H5	1:D:481:PHE:CZ	2.38	0.58
1:C:227:LEU:HD22	1:C:308:ILE:HD13	1.85	0.57
1:B:212:ILE:HD11	1:B:250:LEU:HD21	1.85	0.57
1:B:1054:ARG:O	6:B:1302:HOH:O	2.17	0.57
1:B:625:PRO:HD3	1:B:950:LEU:HD22	1.86	0.57
1:B:916:PHE:HD2	1:B:932:GLN:HB2	1.68	0.57
1:B:1033:ILE:HG12	1:B:1044:ILE:HG12	1.86	0.57
1:A:833:GLU:OE1	1:A:874:LYS:NZ	2.36	0.57
1:D:828:GLU:HB3	1:A:802:GLU:OE2	2.04	0.57
1:C:108:PRO:HA	1:C:272:VAL:HG13	1.87	0.57
1:B:210:LYS:HE2	1:B:231:ASP:OD2	2.04	0.57
1:B:485:GLU:HB2	1:A:1111:MET:HE2	1.86	0.57
1:C:577:TRP:HZ3	1:C:636:SER:HG	1.52	0.57
1:B:894:LEU:HD22	1:B:899:VAL:HG23	1.85	0.57
1:C:544:HIS:HB2	6:C:1367:HOH:O	2.05	0.57
1:B:866:ASN:C	1:B:866:ASN:HD22	2.11	0.57
1:A:66:ILE:H	1:A:66:ILE:HD12	1.70	0.57
1:A:671:GLU:HG2	1:A:708:ILE:HB	1.87	0.57
1:C:541:ARG:HD2	1:C:541:ARG:O	2.05	0.56
1:D:288:PHE:O	1:D:289:ILE:HD13	2.05	0.56
1:D:826:ASN:OD1	1:D:828:GLU:HG2	2.05	0.56
1:D:780:ALA:HB1	1:D:801:MET:HE1	1.87	0.56
1:C:426:THR:CG2	1:C:428:ILE:HG13	2.36	0.56
1:D:565:ALA:HB2	1:D:604:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:642:ASP:OD1	1:D:668:LYS:NZ	2.31	0.56
1:A:107:GLY:O	1:A:273:ASN:ND2	2.38	0.56
1:A:316:LEU:HD22	1:A:327:GLU:HB3	1.87	0.56
1:B:643:VAL:HG22	1:B:669:ILE:HB	1.86	0.56
1:C:552:VAL:HG23	6:C:1367:HOH:O	2.05	0.56
1:B:231:ASP:OD1	1:B:233:SER:OG	2.21	0.56
1:B:251:SER:HB2	1:B:252:PRO:HD2	1.88	0.56
1:A:630:HIS:O	1:A:634:GLN:HG2	2.06	0.56
1:C:464:ASP:CG	1:C:467:THR:HB	2.30	0.56
1:C:826:ASN:OD1	1:C:828:GLU:N	2.39	0.56
1:B:6:LYS:HG3	1:B:29:SER:HB2	1.87	0.56
1:A:875:VAL:O	1:A:879:SER:N	2.38	0.56
1:A:601:ARG:NH2	1:A:604:ILE:O	2.38	0.56
1:C:468:LYS:NZ	1:C:993:ASN:O	2.39	0.56
1:A:242:VAL:HG21	1:A:434:VAL:HG11	1.87	0.56
1:C:1029:LYS:HB3	1:C:1047:ALA:HB3	1.86	0.56
1:D:646:ILE:O	1:D:673:THR:OG1	2.22	0.56
1:D:868:LEU:HD13	1:D:889:MET:HE1	1.86	0.56
1:C:981:TYR:HB3	1:C:984:VAL:HB	1.87	0.55
1:D:6:LYS:HG2	1:D:78:VAL:HG12	1.88	0.55
1:C:1112:LYS:HE3	1:D:482:PRO:HD3	1.88	0.55
1:D:226:HIS:CD2	1:D:228:PHE:H	2.25	0.55
1:A:123:ARG:O	1:A:127:ILE:HG13	2.07	0.55
1:A:872:ILE:HD11	1:A:882:VAL:HG22	1.87	0.55
1:C:829:ILE:HA	1:C:832:HIS:CE1	2.42	0.55
1:B:25:GLU:HG3	1:D:414:ARG:HG2	1.88	0.55
1:B:273:ASN:OD1	1:B:314:GLN:HG2	2.06	0.55
1:D:83:PRO:HB2	1:D:89:SER:OG	2.06	0.55
1:A:437:ASN:HD21	1:A:453:THR:HG21	1.71	0.55
1:B:511:THR:OG1	1:B:608:LEU:HG	2.07	0.55
1:D:576:MET:HE1	1:D:641:ILE:HD13	1.88	0.55
1:D:1033:ILE:HG13	1:D:1044:ILE:HG23	1.88	0.55
1:A:83:PRO:HG3	1:A:105:PHE:CE2	2.42	0.55
1:A:865:VAL:HG21	1:A:886:ALA:HA	1.88	0.55
1:B:66:ILE:HG23	1:B:94:PHE:HD1	1.71	0.55
1:B:661:GLU:O	1:B:665:GLU:HB2	2.07	0.55
1:D:959:ARG:HA	1:D:975:ILE:HD11	1.88	0.55
1:B:866:ASN:HD21	1:B:871:ASP:HA	1.69	0.55
1:D:230:ARG:NH1	1:D:302:THR:OG1	2.39	0.55
1:D:769:ALA:HB2	1:D:781:ASN:HB2	1.89	0.55
1:D:861:MET:O	1:D:865:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:832:HIS:CD2	1:C:834:MET:HG3	2.42	0.55
1:C:541:ARG:NH2	1:C:575:GLU:OE1	2.39	0.54
1:C:614:ARG:HB3	1:C:617:ASN:O	2.07	0.54
1:B:414:ARG:HG3	1:B:415:SER:N	2.22	0.54
1:B:601:ARG:NH2	1:B:604:ILE:O	2.35	0.54
1:B:866:ASN:HD21	1:B:872:ILE:H	1.55	0.54
1:D:832:HIS:CD2	1:D:834:MET:H	2.24	0.54
1:D:686:SER:HB2	1:D:871:ASP:OD2	2.08	0.54
1:D:1022:LYS:O	1:D:1022:LYS:CD	2.54	0.54
1:B:247:SER:HB3	1:B:250:LEU:HD22	1.90	0.54
1:D:295:VAL:HG22	1:D:314:GLN:HE22	1.72	0.54
1:A:959:ARG:NH1	1:A:972:GLU:OE2	2.40	0.54
1:B:578:GLY:O	1:B:581:THR:OG1	2.25	0.54
1:B:720:PRO:HA	1:B:752:THR:HA	1.88	0.54
1:A:131:LEU:HD21	1:A:261:ALA:HB1	1.89	0.54
1:D:1108:THR:HG23	1:D:1115:THR:HB	1.88	0.54
1:D:405:PHE:HE2	1:D:441:THR:HA	1.73	0.54
1:D:776:SER:OG	1:D:777:GLN:N	2.40	0.54
1:C:108:PRO:HG2	1:C:113:LEU:HD21	1.89	0.54
1:A:92:GLU:O	1:A:96:ARG:N	2.36	0.54
1:D:34:TYR:CD2	1:D:44:ARG:HD2	2.44	0.53
1:D:865:VAL:HG22	1:D:889:MET:HE3	1.90	0.53
1:C:230:ARG:HD3	6:C:1301:HOH:O	2.08	0.53
1:C:776:SER:OG	1:C:777:GLN:N	2.41	0.53
1:A:675:CYS:HB3	1:A:714:MET:HE1	1.90	0.53
1:A:610:GLN:HB2	1:A:643:VAL:HB	1.89	0.53
1:B:885:MET:HE3	1:B:889:MET:HE2	1.89	0.53
1:D:246:PRO:HD2	1:D:341:TYR:CD1	2.43	0.53
1:A:12:ARG:NH2	1:A:380:ASP:OD1	2.35	0.53
1:A:601:ARG:HH21	1:A:605:PRO:HA	1.74	0.53
1:A:446:THR:OG1	1:A:447:THR:N	2.41	0.53
1:C:344:GLN:OE1	1:C:346:ARG:NH1	2.42	0.53
1:B:17:ILE:HG12	1:B:46:LYS:HG3	1.91	0.53
1:B:398:LEU:HD21	1:B:415:SER:HB3	1.91	0.53
1:D:494:LEU:HD23	1:D:494:LEU:H	1.74	0.53
1:D:584:VAL:HG13	1:D:588:PHE:HD2	1.74	0.53
1:D:642:ASP:HA	1:D:668:LYS:HD2	1.91	0.53
1:C:348:THR:HG22	1:C:394:LEU:HA	1.91	0.52
1:C:865:VAL:HG11	1:C:885:MET:HB3	1.90	0.52
1:B:720:PRO:HG3	1:B:751:LEU:HB3	1.91	0.52
1:A:437:ASN:ND2	1:A:453:THR:HG21	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:ILE:HD13	1:B:807:TYR:CE2	2.44	0.52
1:B:975:ILE:O	1:B:979:VAL:HG23	2.09	0.52
1:C:109:HIS:HB2	1:C:112:HIS:ND1	2.24	0.52
1:A:674:ILE:HG21	1:A:694:TYR:HD1	1.73	0.52
1:D:671:GLU:OE2	1:D:739:HIS:CD2	2.62	0.52
1:B:568:PHE:CZ	1:B:801:MET:HE3	2.44	0.52
1:D:26:LEU:HD22	1:D:316:LEU:HD21	1.90	0.52
1:B:529:LYS:HD3	1:B:530:GLN:NE2	2.25	0.52
1:D:865:VAL:HG11	1:D:885:MET:HB3	1.91	0.52
1:C:56:ASP:OD1	1:C:68:ARG:NH2	2.37	0.52
1:C:298:GLU:HA	1:C:344:GLN:NE2	2.24	0.52
1:B:670:SER:HB3	1:B:707:HIS:HD2	1.75	0.52
1:B:684:GLU:O	1:B:684:GLU:HG2	2.10	0.52
1:D:228:PHE:HE2	1:D:336:ILE:HG22	1.75	0.52
1:D:245:ALA:HB2	1:D:301:ILE:HD12	1.92	0.52
1:A:596:ARG:NH1	6:A:1310:HOH:O	2.43	0.52
1:C:553:ARG:NH1	6:C:1310:HOH:O	2.28	0.52
1:D:650:LEU:HD11	1:D:920:ILE:HG13	1.91	0.52
1:B:111:GLU:O	1:B:115:MET:HG3	2.10	0.51
1:B:120:VAL:O	1:B:124:THR:HG22	2.09	0.51
1:B:1058:LYS:H	1:B:1058:LYS:HD3	1.75	0.51
1:D:764:ILE:HG13	1:D:766:THR:HG23	1.93	0.51
1:D:539:THR:OG1	1:D:768:VAL:HG23	2.11	0.51
1:D:713:ASP:OD2	1:D:718:LEU:HB3	2.10	0.51
1:D:470:LEU:HD13	1:D:1046:TYR:CD2	2.44	0.51
1:A:265:LEU:HG	1:A:266:MET:HE2	1.93	0.51
1:A:540:PHE:O	1:A:544:HIS:NE2	2.37	0.51
1:C:463:LEU:HD23	1:C:463:LEU:H	1.76	0.51
1:C:865:VAL:HG22	1:C:889:MET:HE2	1.93	0.51
1:B:916:PHE:HA	1:B:927:PHE:CD1	2.46	0.51
1:B:916:PHE:HA	1:B:927:PHE:CE1	2.46	0.51
1:D:309:ASP:OD2	1:D:312:LYS:HB2	2.11	0.51
1:A:596:ARG:O	1:A:600:LEU:HB2	2.11	0.51
1:A:709:LEU:HB2	1:A:736:LEU:HD12	1.91	0.51
1:B:434:VAL:HG22	1:B:456:LEU:HD13	1.93	0.51
1:D:274:ALA:HB3	1:D:314:GLN:HE21	1.76	0.51
1:D:873:VAL:HG12	1:D:875:VAL:HG12	1.92	0.51
1:C:266:MET:HE3	1:C:277:VAL:HG22	1.92	0.51
1:C:975:ILE:O	1:C:979:VAL:HG23	2.10	0.51
1:D:869:PHE:CZ	1:D:885:MET:HG2	2.46	0.51
1:A:360:THR:OG1	1:A:387:ILE:O	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:TYR:O	1:B:757:ILE:HG13	2.10	0.51
1:A:673:THR:HA	1:A:710:ALA:O	2.11	0.51
1:B:530:GLN:OE1	1:B:795:ARG:NH2	2.43	0.51
1:C:412:MET:HE2	1:C:412:MET:HA	1.92	0.51
1:D:273:ASN:HA	1:D:317:VAL:HG11	1.93	0.51
1:D:414:ARG:HH11	1:D:418:GLU:HG2	1.75	0.51
1:D:963:GLU:HG2	1:D:968:GLY:O	2.11	0.51
1:C:57:LEU:HD13	1:C:62:SER:HA	1.92	0.50
1:C:301:ILE:HG13	6:C:1301:HOH:O	2.11	0.50
1:C:369:SER:OG	1:C:370:GLY:N	2.43	0.50
1:C:654:ASP:HA	1:C:657:LYS:HD2	1.93	0.50
1:A:313:THR:HG23	1:A:328:ILE:HD13	1.92	0.50
1:B:1017:GLU:HG3	1:B:1027:ILE:HD12	1.92	0.50
1:A:642:ASP:O	1:A:668:LYS:HB3	2.11	0.50
1:B:877:PRO:HG2	1:B:920:ILE:HG23	1.93	0.50
1:D:218:GLY:HA2	1:D:223:ASN:O	2.11	0.50
1:A:861:MET:O	1:A:865:VAL:N	2.29	0.50
1:A:874:LYS:HD3	1:A:882:VAL:HG21	1.92	0.50
1:C:832:HIS:HD2	1:C:834:MET:HE2	1.77	0.50
1:C:34:TYR:O	1:C:52:LEU:HD12	2.12	0.50
1:C:899:VAL:O	1:C:903:GLY:HA3	2.12	0.50
1:D:418:GLU:N	1:D:418:GLU:OE1	2.44	0.50
1:A:1005:THR:HG23	6:A:1312:HOH:O	2.11	0.50
1:C:49:GLU:OE1	1:C:51:TYR:OH	2.26	0.50
1:C:909:PRO:HB2	1:C:912:VAL:HG23	1.94	0.50
1:A:109:HIS:HE1	1:A:220:GLU:OE2	1.94	0.50
1:C:834:MET:HB3	1:C:838:GLN:HB2	1.93	0.50
1:B:869:PHE:HZ	1:B:885:MET:HG2	1.76	0.50
1:D:34:TYR:HD1	1:D:35:SER:O	1.94	0.50
1:D:553:ARG:NH2	1:D:998:LEU:O	2.45	0.50
1:A:739:HIS:CD2	1:A:763:ILE:HB	2.46	0.50
1:C:45:TYR:CE2	1:A:1049:ASN:HB3	2.46	0.50
1:B:52:LEU:HD21	1:B:55:SER:N	2.27	0.50
1:B:387:ILE:O	1:B:387:ILE:HG13	2.11	0.50
1:C:1055:ILE:HD12	1:C:1056:TYR:H	1.77	0.50
1:D:718:LEU:HD21	1:D:723:ALA:HB2	1.94	0.50
1:A:512:LYS:HE2	1:A:601:ARG:NH1	2.27	0.50
1:A:627:ASN:ND2	1:A:952:PRO:HB3	2.27	0.50
1:C:409:GLU:O	1:C:413:VAL:HG22	2.12	0.49
1:A:271:TYR:OH	1:A:293:PRO:HA	2.12	0.49
1:A:346:ARG:HB3	1:A:394:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ASP:HA	1:A:668:LYS:HD2	1.93	0.49
1:D:761:VAL:O	1:D:792:ARG:NH2	2.44	0.49
1:A:301:ILE:O	1:A:305:VAL:HG22	2.13	0.49
1:A:652:TRP:CE3	1:A:655:GLN:HG3	2.47	0.49
1:A:885:MET:HE3	1:A:912:VAL:HG11	1.93	0.49
1:A:956:GLU:HA	1:A:959:ARG:HB3	1.94	0.49
1:C:26:LEU:HD11	1:C:312:LYS:HG3	1.95	0.49
1:D:233:SER:HB2	1:D:445:TYR:CE1	2.48	0.49
1:D:738:ILE:HG22	1:D:761:VAL:HG23	1.94	0.49
1:D:932:GLN:O	1:D:936:LEU:HD23	2.12	0.49
1:B:614:ARG:NH2	6:B:1315:HOH:O	2.45	0.49
1:D:291:VAL:O	1:D:291:VAL:HG12	2.12	0.49
1:D:406:LYS:O	1:D:410:GLU:HG3	2.12	0.49
1:C:664:GLN:NE2	1:C:705:GLY:O	2.46	0.49
1:A:144:TYR:HE1	1:A:181:GLU:HA	1.77	0.49
1:A:227:LEU:HD21	1:A:308:ILE:HG21	1.95	0.49
1:C:3:GLN:HG2	1:C:5:LYS:HG2	1.94	0.49
1:C:541:ARG:NE	1:C:575:GLU:OE1	2.44	0.49
1:B:345:CYS:SG	1:B:431:LEU:HD13	2.52	0.49
1:B:971:THR:O	1:B:975:ILE:HG13	2.13	0.49
1:B:482:PRO:HD3	1:A:1112:LYS:NZ	2.27	0.49
1:B:590:LYS:HG3	1:B:991:THR:HG21	1.94	0.49
1:B:620:GLY:HA2	1:B:981:TYR:CE1	2.48	0.49
1:A:351:ASP:OD2	1:A:425:LYS:HG3	2.13	0.49
1:C:834:MET:HG2	1:C:862:TYR:CZ	2.48	0.49
1:C:992[B]:ARG:HH21	1:C:997:ASN:HD22	1.59	0.49
1:B:118:ASP:HB3	1:B:121:LYS:HB2	1.95	0.49
1:B:349:THR:HG21	1:B:387:ILE:HD13	1.94	0.49
1:D:18:ARG:NH2	1:D:309:ASP:OD1	2.46	0.49
1:C:322:ASP:OD2	1:C:323:LEU:N	2.45	0.49
1:B:433:ASN:HB3	1:B:456:LEU:HA	1.95	0.49
1:A:741:HIS:HB2	1:A:765:ASP:OD2	2.13	0.49
1:C:1041:ASN:HA	1:C:1058:LYS:HA	1.95	0.48
1:B:359:ASP:OD2	1:B:425:LYS:HG3	2.12	0.48
1:B:497:ILE:HG12	1:B:807:TYR:CE1	2.46	0.48
1:D:548:LEU:HD11	1:D:812:ARG:HG3	1.94	0.48
1:A:714:MET:HE2	1:A:875:VAL:HG13	1.95	0.48
1:C:360:THR:OG1	1:C:387:ILE:O	2.30	0.48
1:C:869:PHE:CE1	1:C:916:PHE:HE2	2.31	0.48
1:B:807:TYR:CZ	1:B:811:VAL:HG21	2.48	0.48
1:D:954:ASP:HB3	1:D:957:LYS:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ASN:ND2	6:A:1301:HOH:O	2.21	0.48
1:B:670:SER:HB3	1:B:707:HIS:CD2	2.48	0.48
1:A:406:LYS:O	1:A:410:GLU:HG3	2.12	0.48
1:B:235:GLN:HB2	1:B:240:LYS:HA	1.94	0.48
1:B:708:ILE:N	6:B:1303:HOH:O	2.44	0.48
1:D:470:LEU:HB3	1:D:1055:ILE:HG13	1.94	0.48
1:D:842:LEU:HD21	1:D:887:LEU:HD21	1.95	0.48
1:D:887:LEU:O	1:D:891:GLN:N	2.46	0.48
1:A:229:GLU:OE2	1:A:255:ARG:NH1	2.47	0.48
1:A:652:TRP:HE3	1:A:655:GLN:HG3	1.78	0.48
1:A:1021:ASP:HB3	1:A:1024:LYS:HB2	1.96	0.48
1:A:1021:ASP:OD1	1:A:1022:LYS:N	2.44	0.48
1:C:627[B]:ASN:HD21	1:C:952:PRO:HA	1.79	0.48
1:C:723:ALA:HB2	1:C:752:THR:HG23	1.95	0.48
1:C:754:LYS:NZ	1:B:751:LEU:HD21	2.29	0.48
1:D:465:ARG:O	1:D:468:LYS:N	2.45	0.48
1:C:333:GLN:NE2	6:C:1325:HOH:O	2.46	0.48
1:C:419:MET:HA	6:C:1334:HOH:O	2.14	0.48
1:C:547:LEU:C	1:C:548:LEU:HD23	2.39	0.48
1:C:624:TYR:HB3	1:C:628:VAL:HG21	1.95	0.48
1:B:1044:ILE:HB	1:B:1055:ILE:HG22	1.96	0.48
1:D:208:ASN:N	1:D:209:PRO:HD3	2.29	0.48
1:A:465:ARG:NE	5:A:1202:ACO:O1A	2.46	0.48
1:C:685:ARG:NH2	1:C:686:SER:HB2	2.28	0.48
1:C:886:ALA:O	1:C:890:VAL:HG23	2.14	0.48
1:B:174:VAL:HG11	1:B:180:LEU:HA	1.95	0.48
1:B:349:THR:HB	1:B:359:ASP:HB3	1.95	0.48
1:D:827:THR:HG23	1:A:785:TYR:HE2	1.77	0.48
1:A:660:ASN:O	1:A:664:GLN:HG2	2.13	0.48
1:A:869:PHE:N	1:A:869:PHE:CD2	2.82	0.48
1:C:807:TYR:O	1:C:811:VAL:HG23	2.13	0.48
1:D:625:PRO:HD3	1:D:950:LEU:HD13	1.96	0.48
1:D:720:PRO:HG3	1:D:751:LEU:HB3	1.95	0.48
1:D:837:GLY:O	1:D:841:ASN:HB2	2.13	0.48
1:A:52:LEU:HG	1:A:54:GLY:H	1.78	0.48
1:C:322:ASP:OD2	1:C:324:PHE:N	2.44	0.48
2:C:1201:BTI:H5	1:D:481:PHE:CE2	2.49	0.48
1:B:565:ALA:HB2	1:B:604:ILE:HG12	1.95	0.48
1:D:13:GLY:O	1:D:17:ILE:HG12	2.14	0.48
1:D:15:ILE:HG13	1:D:19:ILE:CD1	2.44	0.48
1:C:642:ASP:OD2	1:C:668:LYS:NZ	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:875:VAL:O	1:C:878:SER:N	2.46	0.47
1:C:1025:ARG:O	1:A:44:ARG:NH2	2.36	0.47
1:B:610:GLN:HG3	1:B:643:VAL:HB	1.96	0.47
1:B:832:HIS:ND1	1:B:834:MET:HG3	2.29	0.47
1:D:242:VAL:HA	1:D:344:GLN:O	2.14	0.47
1:C:1031:GLU:OE2	1:C:1047:ALA:HB2	2.13	0.47
1:C:409:GLU:OE1	1:C:436:LYS:HA	2.14	0.47
1:B:459:ILE:HG13	1:B:459:ILE:O	2.15	0.47
1:D:986:GLU:O	1:D:990:GLN:HG2	2.13	0.47
1:A:265:LEU:O	1:A:269:ILE:HG13	2.14	0.47
1:A:745:THR:HG22	1:A:775:THR:HA	1.97	0.47
1:A:757:ILE:HA	1:A:761:VAL:HG12	1.96	0.47
1:C:246:PRO:HD2	1:C:341:TYR:CE1	2.49	0.47
1:C:703:ARG:HG2	1:C:703:ARG:HH11	1.78	0.47
1:B:642:ASP:O	1:B:668:LYS:HB3	2.15	0.47
1:D:229:GLU:OE1	1:D:229:GLU:N	2.43	0.47
1:D:709:LEU:O	1:D:738:ILE:HA	2.15	0.47
1:A:473:ILE:HD13	1:A:1010:MET:HE2	1.97	0.47
1:A:971:THR:HG23	1:A:974:ASP:OD2	2.15	0.47
2:C:1204:BTI:H11	1:D:1112:LYS:CE	2.23	0.47
1:B:66:ILE:HG23	1:B:94:PHE:CD1	2.49	0.47
1:D:12:ARG:HD3	1:D:38:ASP:OD2	2.15	0.47
1:C:295:VAL:HG23	1:C:314:GLN:NE2	2.30	0.47
1:C:653:VAL:HG21	1:C:700:GLU:HG2	1.96	0.47
1:C:810:THR:O	1:C:813:THR:HB	2.15	0.47
1:B:472:TYR:OH	1:B:1006:PHE:O	2.32	0.47
1:D:15:ILE:HB	1:D:85:TYR:CE2	2.50	0.47
1:D:19:ILE:HD12	1:D:19:ILE:H	1.80	0.47
1:D:551:ARG:HG3	1:D:818:PHE:CD2	2.50	0.47
1:A:6:LYS:HG3	1:A:29:SER:HB3	1.97	0.47
1:C:521:LYS:HB2	1:C:521:LYS:HE2	1.57	0.47
1:B:869:PHE:CZ	1:B:885:MET:HG2	2.49	0.47
1:A:231:ASP:N	1:A:244:VAL:O	2.46	0.47
1:A:352:PRO:HG3	1:A:427:ASN:HA	1.97	0.47
1:C:626:ASP:OD1	1:C:945:ARG:NH2	2.48	0.47
1:C:807:TYR:CZ	1:C:811:VAL:HG21	2.49	0.47
1:B:664:GLN:NE2	1:B:705:GLY:O	2.48	0.47
1:A:577:TRP:CE3	1:A:641:ILE:HG13	2.49	0.47
1:C:34:TYR:HA	1:C:63:TYR:OH	2.15	0.47
1:C:475:ASN:CG	2:C:1204:BTI:H103	2.40	0.47
1:D:821:ASP:N	1:D:821:ASP:OD2	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:548:LEU:HD13	1:C:815:TYR:HB2	1.97	0.46
1:C:657:LYS:O	1:C:661:GLU:HG3	2.13	0.46
6:C:1302:HOH:O	1:B:754:LYS:HB3	2.14	0.46
1:B:709:LEU:O	1:B:738:ILE:HA	2.14	0.46
1:D:721:LYS:HG2	1:A:789:GLY:HA3	1.97	0.46
1:C:426:THR:HG21	1:C:428:ILE:HG13	1.98	0.46
1:C:865:VAL:HG12	1:C:882:VAL:HG13	1.97	0.46
1:D:15:ILE:HB	1:D:85:TYR:CZ	2.50	0.46
1:D:234:VAL:HG22	1:D:449:PHE:HD2	1.80	0.46
1:D:406:LYS:HE2	1:D:406:LYS:HB2	1.75	0.46
1:C:541:ARG:NH1	1:C:542:ASP:OD1	2.48	0.46
1:C:486:LYS:HA	1:C:486:LYS:HD2	1.76	0.46
1:B:365:ALA:HB3	1:B:422:ARG:HB2	1.97	0.46
1:B:761:VAL:O	1:B:792:ARG:NH2	2.40	0.46
1:A:209:PRO:HB2	1:A:280:LEU:HG	1.96	0.46
1:A:962:LEU:O	1:A:966:GLN:HG3	2.16	0.46
1:B:83:PRO:HG3	1:B:105:PHE:CZ	2.50	0.46
1:B:470:LEU:HA	6:B:1330:HOH:O	2.15	0.46
1:B:689:TYR:OH	1:B:871:ASP:O	2.15	0.46
1:B:1030:LEU:HD21	1:B:1033:ILE:HG13	1.96	0.46
1:D:281:VAL:HG22	1:D:286:PHE:HB3	1.96	0.46
1:D:303:GLU:OE1	1:D:310:ILE:HB	2.15	0.46
1:A:121:LYS:O	1:A:125:THR:HG23	2.15	0.46
1:A:624:TYR:OH	1:A:980:LEU:O	2.32	0.46
1:A:885:MET:HE1	1:A:909:PRO:CG	2.44	0.46
1:C:428:ILE:O	1:C:432:ILE:HG13	2.16	0.46
1:C:435:MET:HE3	6:C:1375:HOH:O	2.15	0.46
1:B:146:LEU:HD12	1:B:146:LEU:HA	1.78	0.46
1:D:235:GLN:CB	1:D:240:LYS:HA	2.42	0.46
1:D:753:TYR:O	1:D:757:ILE:HD12	2.15	0.46
1:C:437:ASN:O	1:C:441:THR:HG23	2.16	0.46
1:C:1036:PRO:HD3	1:C:1042:ARG:CZ	2.46	0.46
1:B:815:TYR:CZ	1:B:1003:THR:HG21	2.50	0.46
1:B:928:ASN:OD1	1:B:930:ASP:N	2.48	0.46
1:C:118:ASP:C	1:C:118:ASP:OD1	2.59	0.46
1:B:433:ASN:CB	1:B:456:LEU:HA	2.45	0.46
1:D:228:PHE:CE2	1:D:336:ILE:HG22	2.50	0.46
1:D:452:GLU:OE2	1:D:452:GLU:C	2.59	0.46
1:A:66:ILE:HG23	1:A:94:PHE:HD1	1.81	0.46
1:A:97:ARG:HA	1:A:97:ARG:HD2	1.68	0.46
1:A:387:ILE:HD12	1:A:387:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:PHE:N	1:A:869:PHE:HD2	2.13	0.46
1:D:123:ARG:NH2	1:D:134:ILE:O	2.45	0.46
1:D:959:ARG:NH1	1:D:970:VAL:O	2.49	0.46
1:C:478:ILE:HD12	1:C:1057:ILE:HB	1.98	0.46
1:B:560:ILE:HD11	1:B:808:TRP:CZ2	2.51	0.46
1:D:66:ILE:O	1:D:70:ILE:HD12	2.16	0.46
1:D:345:CYS:HB3	1:D:431:LEU:HD13	1.98	0.46
1:A:403:ILE:HG22	1:A:407:GLN:OE1	2.14	0.46
1:A:532:ASP:HB2	1:A:795:ARG:HH21	1.81	0.46
1:A:620:GLY:HA2	1:A:981:TYR:CE2	2.51	0.46
1:C:625:PRO:HB3	1:C:950:LEU:HB3	1.97	0.45
1:C:916:PHE:HA	1:C:927:PHE:CE2	2.51	0.45
1:B:211:HIS:ND1	1:B:232:CYS:HB2	2.31	0.45
1:B:590:LYS:HA	1:B:590:LYS:HD3	1.71	0.45
1:B:942:LEU:HB2	1:B:949:TYR:CZ	2.52	0.45
1:B:1032:THR:HG21	1:D:1034:SER:HB2	1.98	0.45
1:D:4:ILE:HG13	1:D:319:ALA:HB2	1.98	0.45
1:A:766:THR:OG1	1:A:780:ALA:HB2	2.15	0.45
1:A:1043:THR:HG1	1:A:1056:TYR:HE1	1.62	0.45
1:B:711:ILE:HB	1:B:740:LEU:HD13	1.98	0.45
1:B:715:ALA:HB3	1:B:717:LEU:HG	1.98	0.45
1:D:234:VAL:HB	1:D:242:VAL:HB	1.97	0.45
1:A:92:GLU:HA	1:A:113:LEU:HD12	1.98	0.45
1:C:206:ILE:HG22	1:C:207:ASP:H	1.82	0.45
1:C:625:PRO:O	1:C:628:VAL:HG22	2.16	0.45
1:B:833:GLU:HB2	1:B:874:LYS:HE2	1.98	0.45
1:D:530:GLN:HG3	1:D:795:ARG:HH22	1.81	0.45
1:A:108:PRO:HA	1:A:272:VAL:HG23	1.97	0.45
1:A:312:LYS:O	1:A:316:LEU:HD12	2.16	0.45
1:C:673:THR:HA	1:C:710:ALA:O	2.16	0.45
1:C:807:TYR:CE2	1:C:811:VAL:HG21	2.51	0.45
1:B:344:GLN:HE21	1:B:346:ARG:HH11	1.64	0.45
1:B:473:ILE:HB	6:B:1330:HOH:O	2.15	0.45
1:D:15:ILE:HD13	1:D:85:TYR:CD2	2.50	0.45
1:B:116:PHE:CZ	1:B:269:ILE:HD11	2.52	0.45
1:B:487:ARG:NH2	1:B:817:ASP:OD2	2.49	0.45
1:D:292:ASN:HA	1:D:293:PRO:HD3	1.56	0.45
1:D:822:ILE:HD13	1:D:839:TYR:CZ	2.51	0.45
1:B:116:PHE:HA	1:B:122:ALA:HB2	1.98	0.45
1:D:116:PHE:HZ	1:D:269:ILE:CD1	2.30	0.45
1:D:658:VAL:HG12	1:D:945:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1058:LYS:HB3	1:D:1058:LYS:HE3	1.72	0.45
1:A:611:MET:HG3	1:A:612:LEU:N	2.32	0.45
1:A:833:GLU:HB2	1:A:874:LYS:NZ	2.32	0.45
1:C:695:VAL:HG22	1:C:730:LEU:HD23	1.99	0.45
1:D:12:ARG:HB2	1:D:43:HIS:CE1	2.51	0.45
1:D:673:THR:CG2	1:D:710:ALA:HB3	2.46	0.45
1:A:46:LYS:HD2	1:A:46:LYS:HA	1.74	0.45
1:A:473:ILE:HG21	1:A:1010:MET:CE	2.47	0.45
1:A:687:ASN:OD1	1:A:687:ASN:N	2.41	0.45
1:A:1017:GLU:OE1	1:A:1025:ARG:HD3	2.17	0.45
1:C:615:ALA:HB1	1:C:656:MET:HA	1.99	0.45
1:C:624:TYR:HB3	1:C:628:VAL:CG2	2.47	0.45
1:C:932:GLN:HG2	1:C:936:LEU:HD11	1.98	0.45
1:B:742:THR:HG22	1:B:753:TYR:CE1	2.52	0.45
1:C:225:VAL:HG22	1:C:323:LEU:HD21	1.98	0.45
1:C:547:LEU:HD22	1:C:812:ARG:HH22	1.81	0.45
1:C:804:LEU:HD23	1:C:804:LEU:HA	1.86	0.45
1:D:409:GLU:OE2	1:D:435:MET:O	2.35	0.45
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.78	0.45
1:C:34:TYR:HE2	1:C:39:LYS:HD3	1.81	0.44
1:C:312:LYS:HB2	1:C:312:LYS:HE3	1.59	0.44
1:C:540:PHE:CD1	1:C:557:MET:HG2	2.52	0.44
1:C:751:LEU:HD11	1:B:750:LEU:HB3	1.98	0.44
3:C:1202:COA:H2A	1:A:44:ARG:NH2	2.32	0.44
1:D:227:LEU:HD21	1:D:330:MET:HE3	1.99	0.44
1:D:430:PHE:HZ	1:D:450:ILE:HD12	1.82	0.44
1:D:689:TYR:OH	1:D:871:ASP:O	2.18	0.44
1:D:709:LEU:HD23	1:D:738:ILE:HG12	1.98	0.44
1:D:1107:ILE:HA	1:D:1116:THR:HA	1.99	0.44
1:A:42:LEU:HD23	1:A:379:GLY:O	2.17	0.44
1:A:108:PRO:HG2	1:A:293:PRO:HB2	1.99	0.44
1:A:645:ARG:CG	1:A:673:THR:HG21	2.44	0.44
1:A:710:ALA:HB2	1:A:739:HIS:HB3	1.99	0.44
1:A:1037:ASP:OD2	1:A:1037:ASP:C	2.60	0.44
1:C:420:ARG:HA	1:C:420:ARG:HD3	1.64	0.44
1:B:681:LEU:O	1:B:683:PRO:HD3	2.18	0.44
1:D:219:ASP:OD1	1:D:223:ASN:N	2.48	0.44
1:D:753:TYR:O	1:D:756:ALA:N	2.51	0.44
1:A:537:ASP:HB3	1:A:574:LEU:HD22	1.99	0.44
1:C:234:VAL:HG12	1:C:241:VAL:HG22	2.00	0.44
1:C:362:THR:HG21	1:C:1056:TYR:OH	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:LYS:HG2	1:C:1002:ASP:HA	1.99	0.44
1:B:350:GLU:O	1:B:352:PRO:HD3	2.17	0.44
1:B:587:ASN:O	1:B:590:LYS:HE3	2.17	0.44
1:B:1027:ILE:HG12	1:D:45:TYR:OH	2.17	0.44
1:D:52:LEU:HD12	1:D:53:VAL:N	2.32	0.44
1:D:108:PRO:HB2	1:D:112:HIS:HB2	1.98	0.44
1:D:838:GLN:O	1:D:842:LEU:HB2	2.16	0.44
1:A:603:ALA:O	1:A:605:PRO:HD3	2.17	0.44
1:A:731:LYS:HD2	1:A:731:LYS:HA	1.85	0.44
1:C:298:GLU:HA	1:C:344:GLN:HE22	1.81	0.44
1:C:481:PHE:HB3	1:C:484:VAL:HB	1.99	0.44
1:B:955:PHE:HE1	1:B:979:VAL:HG21	1.82	0.44
1:D:230:ARG:NH2	1:D:296:GLN:OE1	2.51	0.44
1:A:35:SER:HB2	1:A:62:SER:HB2	1.99	0.44
1:A:245:ALA:O	1:A:305:VAL:HG11	2.17	0.44
1:C:771:MET:HE3	1:C:771:MET:HB3	1.91	0.44
1:D:541:ARG:HD2	1:D:541:ARG:C	2.43	0.44
1:D:601:ARG:HA	1:D:601:ARG:HD3	1.81	0.44
1:D:632:PHE:O	1:D:636:SER:OG	2.36	0.44
1:D:1057:ILE:HD13	1:D:1057:ILE:HA	1.82	0.44
1:A:131:LEU:HD22	1:A:132:PRO:HD2	1.99	0.44
1:A:847:LYS:C	1:A:849:LEU:H	2.26	0.44
1:B:874:LYS:NZ	6:B:1312:HOH:O	2.47	0.44
1:D:97:ARG:NH1	1:D:100:GLU:OE1	2.50	0.44
1:D:713:ASP:OD1	1:D:716:GLY:N	2.51	0.44
1:A:473:ILE:HG21	1:A:1010:MET:HE3	2.00	0.44
1:A:645:ARG:HG3	1:A:673:THR:CG2	2.45	0.44
1:A:702:GLU:HG3	1:A:736:LEU:HD21	1.99	0.44
1:C:835:PRO:HG3	1:C:874:LYS:O	2.18	0.44
1:B:691:LEU:HD21	1:B:729:GLU:HG3	1.99	0.44
1:A:497:ILE:HG12	1:A:807:TYR:HE1	1.81	0.44
1:A:833:GLU:HB2	1:A:874:LYS:HZ2	1.82	0.44
1:C:590:LYS:HG3	1:C:991:THR:HG21	2.00	0.44
1:C:1021:ASP:OD1	1:C:1024:LYS:NZ	2.46	0.44
1:B:1041:ASN:HA	1:B:1058:LYS:HA	1.99	0.44
1:D:288:PHE:C	1:D:289:ILE:HD13	2.43	0.44
1:A:34:TYR:HA	1:A:63:TYR:OH	2.16	0.44
1:A:216:VAL:HA	1:A:226:HIS:HA	2.00	0.44
1:A:304:MET:HE1	1:A:399:SER:HB2	2.00	0.44
1:B:234:VAL:HG22	1:B:445:TYR:CE1	2.52	0.44
1:B:575:GLU:HA	1:B:610:GLN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740:LEU:HD12	1:B:741:HIS:N	2.31	0.44
1:D:132:PRO:HB2	1:D:287:PHE:HA	1.98	0.44
1:D:995:TYR:HB3	1:D:998:LEU:HD21	2.00	0.44
1:A:437:ASN:O	1:A:441:THR:HG23	2.18	0.44
1:C:641:ILE:HA	6:C:1342:HOH:O	2.18	0.43
1:C:699:LYS:HG2	1:C:734:VAL:HG13	1.99	0.43
1:C:900:ILE:HG13	1:C:901:THR:H	1.82	0.43
1:B:470:LEU:HD23	1:B:1028:ILE:HD13	1.99	0.43
1:B:822:ILE:HD12	1:B:822:ILE:H	1.83	0.43
1:B:875:VAL:O	1:B:878:SER:N	2.51	0.43
1:D:428:ILE:HB	1:D:429:PRO:HD3	1.99	0.43
1:D:1109:GLU:HG2	1:D:1114:GLU:HA	1.99	0.43
1:C:44:ARG:NH1	1:A:1027:ILE:HD12	2.33	0.43
1:C:741:HIS:CE1	1:C:777:GLN:HE21	2.36	0.43
1:D:975:ILE:HD13	1:D:975:ILE:HA	1.81	0.43
1:A:495:ALA:HB2	1:A:810:THR:HG21	1.99	0.43
1:C:796:THR:HG21	1:C:801:MET:HE1	2.00	0.43
1:B:904:TYR:CA	1:B:934:VAL:HG23	2.46	0.43
1:B:1037:ASP:OD2	1:B:1039:ASN:N	2.51	0.43
1:D:326:GLU:HA	1:D:329:ASN:OD1	2.17	0.43
1:D:453:THR:CG2	1:D:456:LEU:HG	2.47	0.43
1:D:541:ARG:HB2	1:D:576:MET:HA	2.00	0.43
1:D:1014:GLU:HG2	1:D:1015:THR:N	2.33	0.43
1:A:224:ILE:CD1	1:A:271:TYR:HB3	2.49	0.43
1:A:915:PHE:CE2	1:A:927:PHE:HE1	2.36	0.43
1:B:34:TYR:CE2	1:B:52:LEU:HB2	2.53	0.43
1:B:373:GLY:HA3	1:B:411:LYS:HD3	2.00	0.43
1:D:1029:LYS:HB3	1:D:1047:ALA:HB3	2.01	0.43
1:A:70:ILE:HD13	1:A:70:ILE:HA	1.90	0.43
1:A:867:PHE:HA	1:A:870:GLY:O	2.18	0.43
1:C:553:ARG:HG2	1:C:589:LEU:HD22	1.99	0.43
1:C:556:ASP:HB3	1:C:811:VAL:HG11	1.99	0.43
1:B:206:ILE:HD13	1:B:206:ILE:HA	1.79	0.43
1:D:401:HIS:CD2	1:D:402:ALA:N	2.87	0.43
1:A:97:ARG:NH1	1:A:101:GLU:OE2	2.34	0.43
1:A:298:GLU:HA	1:A:344:GLN:NE2	2.33	0.43
1:A:691:LEU:O	1:A:695:VAL:HG23	2.18	0.43
1:A:872:ILE:HD11	1:A:882:VAL:CG2	2.48	0.43
1:C:295:VAL:HG23	1:C:314:GLN:HE22	1.84	0.43
1:C:347:ILE:HD12	1:C:347:ILE:N	2.34	0.43
1:C:367:ARG:NH1	1:C:420:ARG:HG2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:THR:HB	1:C:608:LEU:HG	1.99	0.43
1:C:757:ILE:HA	1:C:761:VAL:HG12	2.01	0.43
1:B:330:MET:HE2	1:B:330:MET:HB2	1.83	0.43
1:B:487:ARG:HG3	1:B:488:PRO:O	2.19	0.43
1:B:861:MET:HB2	1:B:861:MET:HE2	1.73	0.43
1:D:221:HIS:ND1	1:D:221:HIS:N	2.66	0.43
1:D:585:ALA:HB3	1:D:593:PRO:HG3	2.00	0.43
1:A:1026:LEU:HD13	1:A:1028:ILE:HD11	2.00	0.43
1:C:470:LEU:HD23	1:C:470:LEU:HA	1.84	0.43
1:C:651:ASN:OD1	1:C:675:CYS:HB2	2.18	0.43
1:B:85:TYR:CZ	1:B:297:VAL:HG22	2.53	0.43
1:B:219:ASP:OD1	1:B:223:ASN:HB2	2.19	0.43
1:A:219:ASP:HA	1:A:317:VAL:HG13	2.00	0.43
1:C:547:LEU:HD22	1:C:812:ARG:NH2	2.34	0.43
1:C:1112:LYS:HE2	1:D:480:GLY:O	2.18	0.43
1:B:12:ARG:HA	1:B:43:HIS:CD2	2.53	0.43
1:B:316:LEU:HD22	1:B:327:GLU:HB3	1.99	0.43
1:B:836:GLY:HA3	6:B:1327:HOH:O	2.19	0.43
1:D:288:PHE:HE1	1:D:291:VAL:HG21	1.81	0.43
1:D:589:LEU:H	1:D:589:LEU:HG	1.68	0.43
1:D:1020:ILE:O	1:D:1021:ASP:HB2	2.17	0.43
1:C:134:ILE:HD11	1:C:280:LEU:HD12	2.00	0.43
1:B:739:HIS:NE2	1:B:765:ASP:OD1	2.52	0.43
1:D:1105:LEU:HD12	1:D:1117:ILE:HG22	2.01	0.43
1:A:1024:LYS:HE3	5:A:1202:ACO:OAP	2.19	0.43
1:C:473:ILE:HD13	1:C:1010:MET:HE2	2.01	0.43
1:B:708:ILE:HG23	1:B:737:PRO:HG2	2.01	0.43
1:D:17:ILE:CD1	1:D:46:LYS:HG3	2.49	0.43
1:D:409:GLU:O	1:D:413:VAL:HG23	2.19	0.43
1:D:990:GLN:HG2	1:D:990:GLN:H	1.68	0.43
1:A:229:GLU:HG2	1:A:230:ARG:N	2.34	0.43
1:A:359:ASP:OD1	1:A:424:VAL:HB	2.19	0.43
1:C:19:ILE:HD13	1:C:82:HIS:CG	2.54	0.42
1:C:422:ARG:HH21	3:C:1202:COA:P3B	2.42	0.42
1:B:140:PRO:HB2	1:B:199:GLU:CB	2.49	0.42
1:B:751:LEU:HD23	1:B:751:LEU:HA	1.61	0.42
1:D:804:LEU:HD23	1:D:804:LEU:HA	1.77	0.42
1:A:240:LYS:H	1:A:240:LYS:HG3	1.59	0.42
1:C:83:PRO:HG3	1:C:105:PHE:CZ	2.54	0.42
1:C:347:ILE:HG22	1:C:395:LEU:HD12	2.01	0.42
1:B:188:LYS:HG2	1:B:198:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:LEU:HD11	1:B:833:GLU:HB3	2.01	0.42
1:D:687:ASN:C	1:D:688:ILE:HD13	2.45	0.42
1:B:116:PHE:HZ	1:B:269:ILE:HD11	1.84	0.42
1:B:230:ARG:HD3	1:B:302:THR:OG1	2.19	0.42
1:B:936:LEU:HD23	1:B:936:LEU:HA	1.91	0.42
1:B:1113:MET:HE3	1:A:483:ASN:OD1	2.18	0.42
1:D:296:GLN:O	1:D:299:HIS:ND1	2.51	0.42
1:A:259:CYS:O	1:A:263:ILE:HG22	2.19	0.42
1:A:472:TYR:CD2	1:A:998:LEU:HD21	2.53	0.42
1:B:645:ARG:HG3	1:B:673:THR:HG21	2.02	0.42
1:B:866:ASN:HD21	1:B:872:ILE:N	2.18	0.42
1:A:309:ASP:HB3	1:A:312:LYS:HB3	2.00	0.42
1:C:936:LEU:O	1:C:939:GLN:HB2	2.20	0.42
3:C:1202:COA:H132	3:C:1202:COA:N8P	2.31	0.42
1:D:212:ILE:HD12	1:D:281:VAL:HG21	2.01	0.42
1:D:608:LEU:HD22	1:D:642:ASP:HB2	2.01	0.42
1:A:472:TYR:HD2	1:A:995:TYR:CD2	2.36	0.42
1:C:228:PHE:CD2	1:C:338:THR:HG23	2.55	0.42
1:B:520:PRO:HB2	1:B:707:HIS:CE1	2.54	0.42
1:D:87:PHE:H	1:D:87:PHE:HD1	1.65	0.42
1:D:288:PHE:CE1	1:D:291:VAL:HG21	2.51	0.42
1:D:727:ILE:HD11	1:D:740:LEU:HD22	2.00	0.42
1:D:842:LEU:CD2	1:D:887:LEU:HD21	2.50	0.42
1:A:215:GLN:O	1:A:227:LEU:N	2.52	0.42
1:C:121:LYS:O	1:C:125:THR:HG23	2.19	0.42
1:C:298:GLU:O	1:C:301:ILE:HG12	2.19	0.42
1:C:473:ILE:HG21	1:C:1010:MET:HE2	2.00	0.42
1:A:613:LEU:HD22	1:A:644:PHE:HD2	1.83	0.42
1:B:7:LEU:O	1:B:30:THR:HA	2.20	0.42
1:A:273:ASN:HB3	1:A:274:ALA:H	1.59	0.42
1:A:567:VAL:HG22	1:A:800:GLY:HA3	2.00	0.42
1:A:861:MET:HG3	1:A:890:VAL:CG2	2.49	0.42
1:C:352:PRO:HG2	1:C:459:ILE:CD1	2.49	0.42
1:B:620:GLY:HA3	1:B:624:TYR:CE1	2.54	0.42
1:B:942:LEU:HD12	1:B:943:THR:N	2.35	0.42
1:A:262:ALA:HB2	1:A:279:PHE:CE2	2.49	0.42
1:A:300:THR:HB	1:A:375:ARG:CZ	2.50	0.42
1:A:577:TRP:CZ3	1:A:641:ILE:HG13	2.54	0.42
1:C:276:THR:O	1:C:291:VAL:HG13	2.19	0.42
1:B:344:GLN:HE21	1:B:346:ARG:NH1	2.17	0.42
1:B:576:MET:HE1	1:B:597:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ASN:HB2	1:B:894:LEU:CD1	2.44	0.42
1:B:962:LEU:HD23	1:B:962:LEU:HA	1.84	0.42
1:B:1026:LEU:C	1:B:1027:ILE:HD13	2.45	0.42
1:D:576:MET:HE2	1:D:609:PHE:HB3	2.02	0.42
1:A:798:ILE:O	1:A:802:GLU:HG2	2.19	0.42
1:C:724:TYR:HB2	1:C:755:GLN:HB3	2.02	0.41
1:C:888:TYR:CG	1:C:909:PRO:HG3	2.54	0.41
1:C:970:VAL:HG13	1:C:974:ASP:HB2	2.02	0.41
1:B:118:ASP:OD2	1:B:119:LYS:N	2.53	0.41
1:B:545:GLN:HG3	1:B:550:THR:OG1	2.20	0.41
1:D:428:ILE:O	1:D:432:ILE:HG13	2.20	0.41
1:D:497:ILE:HG21	1:D:559:ASN:O	2.20	0.41
1:C:657:LYS:HE3	1:C:704:GLU:OE1	2.19	0.41
1:B:157:PRO:O	1:B:158:LEU:HD23	2.21	0.41
1:B:219:ASP:OD2	1:B:221:HIS:N	2.45	0.41
1:B:548:LEU:HD22	1:B:815:TYR:HB2	2.02	0.41
1:B:727:ILE:O	1:B:731:LYS:HB2	2.20	0.41
1:D:61:GLU:O	1:D:65:ASN:ND2	2.44	0.41
1:D:207:ASP:OD1	1:D:208:ASN:N	2.51	0.41
1:A:489:LYS:HB2	1:A:489:LYS:HE3	1.78	0.41
1:C:48:ASP:O	1:A:1024:LYS:NZ	2.53	0.41
1:C:468:LYS:HG2	1:C:994:GLN:O	2.20	0.41
1:C:552:VAL:HA	1:C:815:TYR:CE2	2.55	0.41
1:C:835:PRO:O	1:C:838:GLN:HG2	2.20	0.41
1:C:1024:LYS:HZ2	1:C:1024:LYS:HG3	1.76	0.41
1:B:131:LEU:HD11	1:B:261:ALA:O	2.20	0.41
1:B:576:MET:SD	1:B:577:TRP:HB2	2.60	0.41
1:D:959:ARG:HD2	1:D:963:GLU:OE1	2.21	0.41
1:A:90:GLU:C	1:A:113:LEU:HD13	2.45	0.41
1:A:510:GLY:N	1:A:513:GLN:OE1	2.48	0.41
1:C:242:VAL:HG22	6:C:1375:HOH:O	2.20	0.41
1:C:246:PRO:HD2	1:C:341:TYR:CD1	2.55	0.41
1:D:541:ARG:HH22	1:D:612:LEU:HD13	1.85	0.41
1:D:673:THR:HA	1:D:710:ALA:O	2.20	0.41
1:A:304:MET:CE	1:A:399:SER:HB2	2.50	0.41
1:A:373:GLY:O	1:A:400:THR:HA	2.21	0.41
1:C:927:PHE:CD1	1:C:927:PHE:N	2.88	0.41
1:D:861:MET:HB3	1:D:886:ALA:HB1	2.03	0.41
1:A:230:ARG:NH1	1:A:302:THR:OG1	2.52	0.41
1:A:404:SER:HB3	1:A:407:GLN:CD	2.46	0.41
1:A:761:VAL:O	1:A:792:ARG:NH1	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:832:HIS:HD2	1:C:834:MET:CG	2.32	0.41
1:B:188:LYS:HB3	1:B:188:LYS:HE3	1.77	0.41
1:B:577:TRP:CE3	1:B:641:ILE:HG13	2.56	0.41
1:A:330:MET:HE2	1:A:330:MET:HB2	1.95	0.41
1:C:38:ASP:HB3	1:C:41:SER:HG	1.86	0.41
1:C:547:LEU:O	1:C:548:LEU:HD23	2.20	0.41
1:C:754:LYS:CD	1:B:751:LEU:HD21	2.47	0.41
1:D:711:ILE:HD11	1:D:730:LEU:HD13	2.02	0.41
1:C:489:LYS:HB3	1:C:1011:ARG:NH2	2.35	0.41
1:C:869:PHE:CE1	1:C:916:PHE:CE2	3.08	0.41
1:B:1044:ILE:HD12	1:B:1057:ILE:HD12	2.03	0.41
1:D:101:GLU:HB2	1:D:103:ILE:HD12	2.03	0.41
1:D:772:SER:OG	1:D:779:SER:HB2	2.20	0.41
1:C:215:GLN:NE2	6:C:1307:HOH:O	2.25	0.41
1:C:353:LEU:HD23	1:C:353:LEU:HA	1.73	0.41
1:C:920:ILE:O	1:C:920:ILE:HG12	2.19	0.41
1:C:1003:THR:HB	1:C:1004:PRO:HD3	2.03	0.41
1:B:118:ASP:OD2	1:B:118:ASP:C	2.64	0.41
1:B:404:SER:OG	1:B:407:GLN:HG3	2.21	0.41
1:B:537:ASP:HB3	1:B:574:LEU:CD2	2.51	0.41
1:B:834:MET:HE1	6:B:1355:HOH:O	2.20	0.41
2:B:1201:BTI:H82	1:A:476:VAL:HG22	2.03	0.41
1:D:53:VAL:HG11	1:D:62:SER:HA	2.03	0.41
1:D:540:PHE:HB2	1:D:576:MET:HB3	2.02	0.41
1:D:710:ALA:HB2	1:D:739:HIS:HB3	2.03	0.41
1:D:860:ASP:OD2	1:D:860:ASP:C	2.63	0.41
1:D:872:ILE:HD11	1:D:882:VAL:CG2	2.50	0.41
1:D:975:ILE:O	1:D:979:VAL:HG23	2.20	0.41
1:D:1112:LYS:O	1:D:1113:MET:HE2	2.21	0.41
1:A:215:GLN:HB2	1:A:230:ARG:HH12	1.86	0.41
1:A:279:PHE:HD1	1:A:287:PHE:O	2.03	0.41
1:A:629:ILE:O	1:A:633:VAL:HG23	2.21	0.41
1:A:769:ALA:HB2	1:A:781:ASN:HB2	2.02	0.41
1:C:915:PHE:HA	1:C:920:ILE:HG22	2.02	0.41
1:B:552:VAL:HA	1:B:815:TYR:CZ	2.56	0.41
1:B:714:MET:SD	1:B:714:MET:N	2.92	0.41
1:B:931:LEU:HA	1:B:934:VAL:CG1	2.51	0.41
1:D:67:GLU:O	1:D:71:ASP:HB2	2.21	0.41
1:D:614:ARG:HE	1:D:614:ARG:HB2	1.55	0.41
1:D:713:ASP:HB3	1:D:742:THR:HA	2.03	0.41
1:D:971:THR:OG1	1:D:972:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:THR:OG1	1:A:1053:ARG:NH1	2.54	0.41
1:C:118:ASP:OD1	1:C:119:LYS:N	2.54	0.40
1:C:369:SER:HB2	1:C:418:GLU:CD	2.46	0.40
1:B:258:ILE:HG23	1:B:279:PHE:CD1	2.56	0.40
1:B:444:ASP:OD1	1:B:444:ASP:N	2.54	0.40
1:D:689:TYR:HE2	1:D:871:ASP:HB3	1.85	0.40
1:D:750:LEU:HB3	1:A:751:LEU:HD11	2.01	0.40
1:D:950:LEU:HD23	1:D:950:LEU:HA	1.97	0.40
1:A:709:LEU:HD12	1:A:738:ILE:HD13	2.03	0.40
1:A:835:PRO:HD2	1:A:838:GLN:HB2	2.03	0.40
1:C:616:SER:O	1:C:629:ILE:HD11	2.21	0.40
1:C:620:GLY:HA2	1:C:981:TYR:CE1	2.56	0.40
1:C:740:LEU:O	1:C:764:ILE:HA	2.21	0.40
1:B:525:GLU:HA	1:B:528:LYS:HE3	2.04	0.40
1:B:1058:LYS:H	1:B:1058:LYS:CD	2.35	0.40
1:D:271:TYR:OH	1:D:274:ALA:O	2.39	0.40
1:A:217:ILE:O	1:A:224:ILE:HA	2.20	0.40
1:A:226:HIS:HB3	1:A:263:ILE:HB	2.03	0.40
1:A:688:ILE:O	1:A:690:THR:N	2.54	0.40
1:C:245:ALA:HA	1:C:246:PRO:HA	1.95	0.40
1:C:422:ARG:NE	3:C:1202:COA:O8A	2.45	0.40
1:B:206:ILE:CG2	1:B:209:PRO:HB3	2.52	0.40
1:B:714:MET:HG3	1:B:875:VAL:HB	2.02	0.40
1:B:931:LEU:HA	1:B:934:VAL:HG12	2.02	0.40
2:B:1201:BTI:HN3	1:A:590:LYS:HD3	1.86	0.40
1:D:406:LYS:O	1:D:409:GLU:HB3	2.21	0.40
1:D:431:LEU:O	1:D:435:MET:HG2	2.21	0.40
1:A:649:SER:HB2	1:A:878:SER:HB3	2.03	0.40
1:C:311:VAL:O	1:C:314:GLN:HB2	2.21	0.40
1:C:413:VAL:O	1:C:417:ARG:HG3	2.21	0.40
1:C:577:TRP:CE3	1:C:641:ILE:HD11	2.56	0.40
1:C:613:LEU:HD11	1:C:618:ALA:HB1	2.03	0.40
1:C:802:GLU:H	1:C:802:GLU:HG2	1.74	0.40
1:B:492:TYR:CE1	1:B:1004:PRO:HB3	2.55	0.40
1:D:34:TYR:CE2	1:D:44:ARG:HD2	2.56	0.40
1:D:219:ASP:CG	1:D:223:ASN:HD22	2.29	0.40
1:D:288:PHE:HZ	1:D:291:VAL:CG2	2.23	0.40
1:D:440:PHE:CD1	1:D:440:PHE:C	2.99	0.40
1:D:468:LYS:NZ	1:D:993:ASN:O	2.51	0.40
1:D:766:THR:HB	1:D:780:ALA:HB2	2.02	0.40
1:D:873:VAL:O	1:D:878:SER:OG	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:955:PHE:CE1	1:D:979:VAL:HG21	2.56	0.40
1:A:541:ARG:HG2	1:A:581:THR:HG21	2.03	0.40
1:A:1031:GLU:OE2	1:A:1047:ALA:HB2	2.21	0.40
1:C:223:ASN:O	1:C:323:LEU:HD22	2.22	0.40
1:B:1034:SER:OG	1:B:1035:GLU:N	2.55	0.40
1:D:18:ARG:HG2	1:D:311:VAL:HG21	2.02	0.40
1:D:849:LEU:HB2	1:D:851:LEU:HD13	2.03	0.40
1:A:671:GLU:OE2	1:A:708:ILE:HG21	2.22	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	1031/1151 (90%)	958 (93%)	66 (6%)	7 (1%)	18	37
1	B	1045/1151 (91%)	972 (93%)	68 (6%)	5 (0%)	24	45
1	C	989/1151 (86%)	928 (94%)	56 (6%)	5 (0%)	24	45
1	D	934/1151 (81%)	872 (93%)	54 (6%)	8 (1%)	14	31
All	All	3999/4604 (87%)	3730 (93%)	244 (6%)	25 (1%)	21	41

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	PRO
1	D	87	PHE
1	D	1021	ASP
1	C	1112	LYS
1	A	239	GLN
1	C	209	PRO
1	D	59	PRO

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Mol	Chain	Res	Type
1	D	486	LYS
1	A	77	ASN
1	B	115	MET
1	D	209	PRO
1	D	1037	ASP
1	C	982	PRO
1	D	454	PRO
1	A	835	PRO
1	B	835	PRO
1	A	836	GLY
1	C	619	VAL
1	B	791	PRO
1	C	59	PRO
1	B	945	ARG
1	A	209	PRO
1	A	982	PRO
1	D	968	GLY
1	A	640	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	745/987 (76%)	693 (93%)	52 (7%)	14	31
1	B	828/987 (84%)	789 (95%)	39 (5%)	23	47
1	C	810/987 (82%)	763 (94%)	47 (6%)	18	39
1	D	732/987 (74%)	690 (94%)	42 (6%)	18	40
All	All	3115/3948 (79%)	2935 (94%)	180 (6%)	18	39

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	7	LEU
1	C	8	LEU
1	C	17	ILE

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Mol	Chain	Res	Type
1	C	30	THR
1	C	98	CYS
1	C	125	THR
1	C	206	ILE
1	C	212	ILE
1	C	220	GLU
1	C	250	LEU
1	C	251	SER
1	C	297	VAL
1	C	369	SER
1	C	396	VAL
1	C	399	SER
1	C	400	THR
1	C	433	ASN
1	C	441	THR
1	C	444	ASP
1	C	458	ASP
1	C	487	ARG
1	C	500	VAL
1	C	502	SER
1	C	503	SER
1	C	511	THR
1	C	521	LYS
1	C	550	THR
1	C	584	VAL
1	C	627[A]	ASN
1	C	627[B]	ASN
1	C	642	ASP
1	C	649	SER
1	C	687	ASN
1	C	745	THR
1	C	750	LEU
1	C	816	SER
1	C	824	SER
1	C	875	VAL
1	C	900	ILE
1	C	913	VAL
1	C	914	SER
1	C	950	LEU
1	C	970	VAL
1	C	976	ILE
1	C	1016	VAL

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Mol	Chain	Res	Type
1	C	1026	LEU
1	C	1112	LYS
1	B	36	ASN
1	B	62	SER
1	B	79	ASP
1	B	93	GLN
1	B	124	THR
1	B	142	LYS
1	B	143	SER
1	B	194	SER
1	B	234	VAL
1	B	248	VAL
1	B	250	LEU
1	B	264	GLN
1	B	305	VAL
1	B	353	LEU
1	B	362	THR
1	B	394	LEU
1	B	396	VAL
1	B	397	LYS
1	B	399	SER
1	B	415	SER
1	B	483	ASN
1	B	533	VAL
1	B	550	THR
1	B	562	SER
1	B	607	VAL
1	B	628	VAL
1	B	677	THR
1	B	735	ASP
1	B	738	ILE
1	B	754	LYS
1	B	924	VAL
1	B	945	ARG
1	B	987	GLN
1	B	998	LEU
1	B	999	SER
1	B	1016	VAL
1	B	1027	ILE
1	B	1034	SER
1	B	1039	ASN
1	D	4	ILE

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Mol	Chain	Res	Type
1	D	29	SER
1	D	89	SER
1	D	111	GLU
1	D	119	LYS
1	D	221	HIS
1	D	247	SER
1	D	295	VAL
1	D	300	THR
1	D	302	THR
1	D	317	VAL
1	D	323	LEU
1	D	338	THR
1	D	396	VAL
1	D	406	LYS
1	D	468	LYS
1	D	501	SER
1	D	538	THR
1	D	550	THR
1	D	577	TRP
1	D	628	VAL
1	D	636	SER
1	D	677	THR
1	D	697	LEU
1	D	752	THR
1	D	764	ILE
1	D	792	ARG
1	D	809	SER
1	D	823	LYS
1	D	827	THR
1	D	838	GLN
1	D	856	ASP
1	D	887	LEU
1	D	892	ASN
1	D	901	THR
1	D	935	ILE
1	D	971	THR
1	D	999	SER
1	D	1016	VAL
1	D	1032	THR
1	D	1057	ILE
1	D	1117	ILE
1	A	40	SER

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Mol	Chain	Res	Type
1	A	49	GLU
1	A	125	THR
1	A	133	VAL
1	A	206	ILE
1	A	240	LYS
1	A	250	LEU
1	A	253	THR
1	A	267	GLU
1	A	272	VAL
1	A	295	VAL
1	A	338	THR
1	A	369	SER
1	A	386	GLU
1	A	393	SER
1	A	399	SER
1	A	420	ARG
1	A	442	SER
1	A	455	GLU
1	A	483	ASN
1	A	484	VAL
1	A	503	SER
1	A	521	LYS
1	A	535	LEU
1	A	562	SER
1	A	597	LEU
1	A	616	SER
1	A	623	ASN
1	A	628	VAL
1	A	634	GLN
1	A	649	SER
1	A	730	LEU
1	A	750	LEU
1	A	761	VAL
1	A	764	ILE
1	A	774	LEU
1	A	816	SER
1	A	841	ASN
1	A	871	ASP
1	A	881	VAL
1	A	899	VAL
1	A	924	VAL
1	A	934	VAL

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Mol	Chain	Res	Type
1	A	943	THR
1	A	970	VAL
1	A	971	THR
1	A	984	VAL
1	A	987	GLN
1	A	1016	VAL
1	A	1020	ILE
1	A	1038	GLU
1	A	1048	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	GLN
1	C	82	HIS
1	C	208	ASN
1	C	223	ASN
1	C	587	ASN
1	C	630	HIS
1	C	832	HIS
1	B	221	HIS
1	B	223	ASN
1	B	235	GLN
1	B	329	ASN
1	B	344	GLN
1	B	354	ASN
1	B	407	GLN
1	B	630	HIS
1	B	651	ASN
1	B	707	HIS
1	B	788	ASN
1	B	793	HIS
1	B	939	GLN
1	D	407	GLN
1	D	427	ASN
1	D	743	HIS
1	D	832	HIS
1	D	922	GLN
1	A	109	HIS
1	A	256	GLN
1	A	292	ASN
1	A	344	GLN

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Mol	Chain	Res	Type
1	A	437	ASN
1	A	627	ASN
1	A	748	ASN
1	A	838	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	BTI	A	1201	-	15,16,16	1.23	2 (13%)	20,21,21	1.42	3 (15%)
3	COA	C	1202	-	47,50,50	2.58	15 (31%)	69,75,75	1.65	12 (17%)
2	BTI	B	1201	1	15,16,16	1.11	2 (13%)	20,21,21	0.95	0
2	BTI	C	1204	-	15,16,16	1.08	2 (13%)	20,21,21	1.07	1 (5%)
5	ACO	A	1202	-	51,53,53	2.48	14 (27%)	73,79,79	1.41	13 (17%)
2	BTI	C	1201	1	15,16,16	1.11	2 (13%)	20,21,21	1.14	2 (10%)

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	BTI	A	1201	-	-	6/6/27/27	0/2/2/2
3	COA	C	1202	-	-	14/48/64/64	0/3/3/3
2	BTI	B	1201	1	-	3/6/27/27	0/2/2/2
2	BTI	C	1204	-	-	5/6/27/27	0/2/2/2
5	ACO	A	1202	-	-	16/51/67/67	0/3/3/3
2	BTI	C	1201	1	-	4/6/27/27	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1202	ACO	P3B-O3B	13.54	1.83	1.59
3	C	1202	COA	P3B-O3B	12.54	1.81	1.59
3	C	1202	COA	P2A-O6A	4.73	1.77	1.59
3	C	1202	COA	CCP-CBP	4.26	1.59	1.52
3	C	1202	COA	C2B-C3B	3.66	1.61	1.53
5	A	1202	ACO	P2A-O6A	3.65	1.73	1.59
5	A	1202	ACO	C9P-N8P	3.18	1.41	1.33
3	C	1202	COA	C5P-N4P	3.05	1.40	1.33
3	C	1202	COA	C2A-N1A	2.94	1.39	1.33
2	C	1201	BTI	C3-N2	2.92	1.40	1.35
2	A	1201	BTI	C3-N2	2.89	1.40	1.35
3	C	1202	COA	C9P-N8P	2.82	1.40	1.33
5	A	1202	ACO	C2A-N1A	2.82	1.38	1.33
2	A	1201	BTI	C3-N3	2.79	1.40	1.35
2	B	1201	BTI	C3-N2	2.75	1.40	1.35
5	A	1202	ACO	C5P-N4P	2.74	1.39	1.33
2	C	1204	BTI	C3-N2	2.72	1.40	1.35
5	A	1202	ACO	O3B-C3B	-2.70	1.34	1.44
5	A	1202	ACO	C6A-N6A	2.69	1.41	1.34
3	C	1202	COA	O3B-C3B	-2.68	1.34	1.44
2	B	1201	BTI	C3-N3	2.66	1.40	1.35
5	A	1202	ACO	C2B-C3B	2.65	1.58	1.53
2	C	1204	BTI	C3-N3	2.65	1.40	1.35
2	C	1201	BTI	C3-N3	2.58	1.40	1.35
5	A	1202	ACO	C8A-N7A	2.57	1.36	1.31
5	A	1202	ACO	C5A-C4A	2.49	1.43	1.39
3	C	1202	COA	O6A-CCP	-2.45	1.36	1.43
5	A	1202	ACO	C8A-N9A	2.45	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1202	COA	C4A-N3A	2.42	1.38	1.34
3	C	1202	COA	P2A-O3A	-2.42	1.56	1.59
5	A	1202	ACO	C4A-N3A	2.41	1.38	1.34
3	C	1202	COA	C5A-C4A	2.41	1.43	1.39
3	C	1202	COA	C8A-N7A	2.26	1.36	1.31
5	A	1202	ACO	O5B-C5B	-2.25	1.36	1.44
3	C	1202	COA	C8A-N9A	2.20	1.41	1.37
5	A	1202	ACO	CCP-CBP	2.14	1.56	1.52
3	C	1202	COA	O4B-C4B	-2.03	1.40	1.45

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1202	COA	O3A-P1A-O1A	-4.37	97.57	110.70
3	C	1202	COA	C6P-C7P-N8P	-4.00	103.48	112.00
3	C	1202	COA	O5A-P2A-O3A	3.94	117.92	107.27
3	C	1202	COA	O3B-P3B-O7A	-3.93	95.34	109.33
2	A	1201	BTI	C4-C2-S1	3.54	109.05	105.03
3	C	1202	COA	O2A-P1A-O1A	3.05	126.65	112.44
2	A	1201	BTI	C5-C6-S1	2.93	110.10	106.06
3	C	1202	COA	O6A-CCP-CBP	-2.85	105.97	110.55
5	A	1202	ACO	C7P-C6P-C5P	-2.79	107.74	112.39
3	C	1202	COA	O9A-P3B-O7A	2.74	121.53	110.83
5	A	1202	ACO	O3B-P3B-O7A	-2.65	99.88	109.33
5	A	1202	ACO	O2A-P1A-O1A	2.65	124.77	112.44
3	C	1202	COA	O9P-C9P-N8P	-2.47	117.76	122.98
2	C	1201	BTI	C4-C5-N3	2.43	105.13	102.43
5	A	1202	ACO	CEP-CBP-CAP	2.41	112.88	108.77
5	A	1202	ACO	O5A-P2A-O3A	2.41	113.79	107.27
2	C	1204	BTI	C8-C7-C2	-2.37	108.59	114.04
3	C	1202	COA	CDP-CBP-CCP	2.37	112.13	108.22
5	A	1202	ACO	O5A-P2A-O4A	2.35	123.37	112.44
5	A	1202	ACO	O2B-C2B-C3B	2.35	117.76	111.19
5	A	1202	ACO	O3A-P1A-O1A	-2.32	103.73	110.70
5	A	1202	ACO	C2A-N1A-C6A	-2.30	114.96	118.73
5	A	1202	ACO	O2A-P1A-O3A	2.28	113.44	107.27
3	C	1202	COA	O5A-P2A-O4A	2.26	122.94	112.44
5	A	1202	ACO	O6A-CCP-CBP	-2.24	106.94	110.55
3	C	1202	COA	O5P-C5P-C6P	2.19	125.99	122.02
5	A	1202	ACO	C6P-C7P-N8P	-2.08	107.57	112.00
5	A	1202	ACO	O9A-P3B-O3B	-2.07	97.78	105.85
2	A	1201	BTI	C4-C5-N3	2.07	104.72	102.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1202	COA	O6A-P2A-O4A	-2.03	100.88	108.94
2	C	1201	BTI	C5-C6-S1	2.02	108.84	106.06

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1201	BTI	S1-C2-C7-C8
2	C	1201	BTI	C4-C2-C7-C8
2	C	1204	BTI	C9-C10-C11-O11
2	C	1204	BTI	S1-C2-C7-C8
2	C	1204	BTI	C4-C2-C7-C8
2	B	1201	BTI	C4-C2-C7-C8
2	A	1201	BTI	C9-C10-C11-O11
2	A	1201	BTI	S1-C2-C7-C8
2	A	1201	BTI	C4-C2-C7-C8
3	C	1202	COA	O4B-C4B-C5B-O5B
3	C	1202	COA	CCP-O6A-P2A-O3A
3	C	1202	COA	CCP-O6A-P2A-O4A
3	C	1202	COA	CCP-O6A-P2A-O5A
3	C	1202	COA	CDP-CBP-CCP-O6A
3	C	1202	COA	CEP-CBP-CCP-O6A
3	C	1202	COA	CAP-CBP-CCP-O6A
3	C	1202	COA	O9P-C9P-CAP-CBP
3	C	1202	COA	N8P-C9P-CAP-CBP
5	A	1202	ACO	C5B-O5B-P1A-O1A
5	A	1202	ACO	C5B-O5B-P1A-O2A
5	A	1202	ACO	CCP-O6A-P2A-O3A
5	A	1202	ACO	CCP-O6A-P2A-O4A
2	B	1201	BTI	C7-C8-C9-C10
5	A	1202	ACO	C4B-C3B-O3B-P3B
2	A	1201	BTI	C2-C7-C8-C9
3	C	1202	COA	C3B-C4B-C5B-O5B
5	A	1202	ACO	S1P-C2P-C3P-N4P
2	C	1201	BTI	C7-C8-C9-C10
5	A	1202	ACO	C2B-C3B-O3B-P3B
2	C	1204	BTI	C7-C8-C9-C10
3	C	1202	COA	O9P-C9P-CAP-OAP
3	C	1202	COA	N8P-C9P-CAP-OAP
2	B	1201	BTI	S1-C2-C7-C8
3	C	1202	COA	P1A-O3A-P2A-O5A
2	C	1201	BTI	C11-C10-C9-C8

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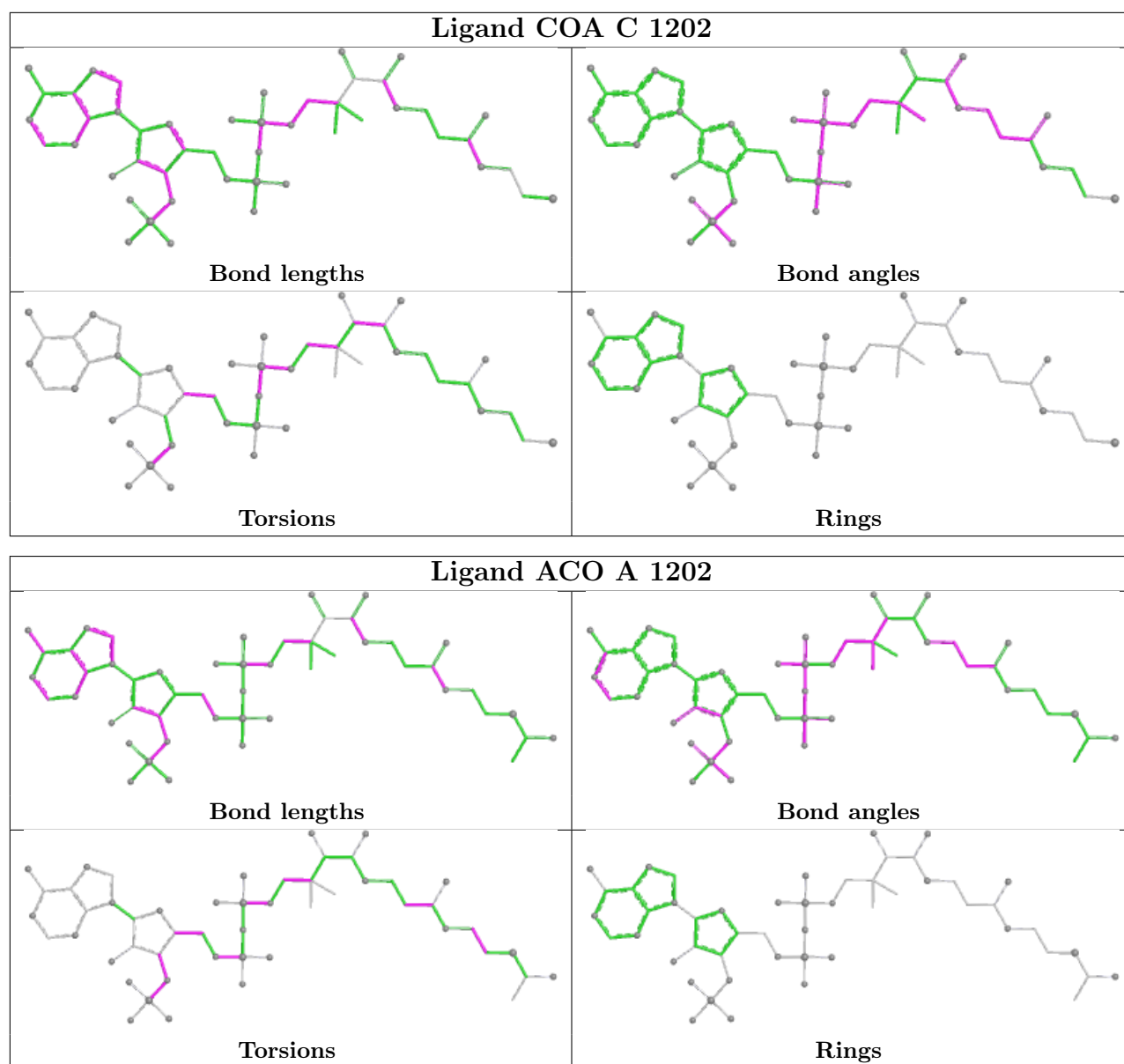
Mol	Chain	Res	Type	Atoms
2	A	1201	BTI	C11-C10-C9-C8
5	A	1202	ACO	CEP-CBP-CCP-O6A
5	A	1202	ACO	C3B-C4B-C5B-O5B
5	A	1202	ACO	O4B-C4B-C5B-O5B
5	A	1202	ACO	C5B-O5B-P1A-O3A
5	A	1202	ACO	CCP-O6A-P2A-O5A
2	A	1201	BTI	C7-C8-C9-C10
2	C	1204	BTI	C2-C7-C8-C9
5	A	1202	ACO	C3B-O3B-P3B-O7A
5	A	1202	ACO	O5P-C5P-C6P-C7P
3	C	1202	COA	C3B-O3B-P3B-O9A
5	A	1202	ACO	C3B-O3B-P3B-O8A
5	A	1202	ACO	N4P-C5P-C6P-C7P

There are no ring outliers.

6 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	BTI	6	0
3	C	1202	COA	6	0
2	B	1201	BTI	2	0
2	C	1204	BTI	8	0
5	A	1202	ACO	4	0
2	C	1201	BTI	2	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	1041/1151 (90%)	0.93	126 (12%) 8 7	25, 52, 86, 122	0
1	B	1053/1151 (91%)	0.65	75 (7%) 22 18	23, 43, 79, 141	0
1	C	993/1151 (86%)	0.64	73 (7%) 20 17	19, 41, 74, 140	2 (0%)
1	D	950/1151 (82%)	0.88	116 (12%) 8 7	25, 50, 88, 130	0
All	All	4037/4604 (87%)	0.77	390 (9%) 13 11	19, 46, 83, 141	2 (0%)

All (390) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	ILE	7.8
1	A	493	GLU	7.4
1	A	224	ILE	7.3
1	B	455	GLU	7.3
1	B	456	LEU	6.7
1	D	40	SER	6.4
1	C	457	PHE	6.3
1	C	839	TYR	6.2
1	D	222	GLY	6.1
1	A	268	ASN	5.8
1	A	893	ASP	5.8
1	A	222	GLY	5.8
1	A	845	GLN	5.7
1	A	262	ALA	5.7
1	A	846	ALA	5.6
1	A	839	TYR	5.5
1	A	495	ALA	5.5
1	C	907	ASP	5.4
1	A	218	GLY	5.3
1	D	463	LEU	5.3
1	D	839	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	839	TYR	5.1
1	D	291	VAL	5.1
1	B	904	TYR	4.9
1	D	1106	LEU	4.9
1	D	449	PHE	4.9
1	A	903	GLY	4.9
1	A	225	VAL	4.9
1	D	451	GLU	4.8
1	D	450	ILE	4.6
1	A	494	LEU	4.6
1	A	226	HIS	4.6
1	A	90	GLU	4.5
1	C	908	PHE	4.4
1	D	56	ASP	4.3
1	B	1040	GLY	4.3
1	B	454	PRO	4.3
1	D	235	GLN	4.2
1	A	118	ASP	4.2
1	C	906	LEU	4.2
1	A	151	ALA	4.2
1	A	844	GLN	4.1
1	C	319	ALA	4.1
1	B	907	ASP	4.1
1	A	7	LEU	4.0
1	C	900	ILE	4.0
1	D	238	HIS	4.0
1	A	58	GLY	4.0
1	D	874	LYS	4.0
1	C	902	ASP	3.9
1	B	925	ASN	3.9
1	A	842	LEU	3.9
1	C	321	ALA	3.8
1	A	516	ASP	3.8
1	D	904	TYR	3.8
1	C	494	LEU	3.7
1	B	885	MET	3.7
1	C	901	THR	3.7
1	C	1021	ASP	3.7
1	C	320	GLY	3.7
1	A	968	GLY	3.6
1	D	455	GLU	3.6
1	B	846	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	122	ALA	3.6
1	A	885	MET	3.6
1	A	188	LYS	3.6
1	C	86	GLY	3.6
1	A	105	PHE	3.6
1	C	904	TYR	3.5
1	B	197	ASN	3.5
1	D	59	PRO	3.5
1	B	248	VAL	3.4
1	A	928	ASN	3.4
1	A	851	LEU	3.4
1	D	36	ASN	3.4
1	A	935	ILE	3.4
1	A	388	SER	3.4
1	A	876	THR	3.4
1	C	905	LYS	3.3
1	B	59	PRO	3.3
1	D	57	LEU	3.3
1	C	10	ALA	3.3
1	D	897	GLN	3.3
1	C	840	SER	3.3
1	A	461	PRO	3.3
1	A	870	GLY	3.3
1	D	271	TYR	3.3
1	A	852	GLY	3.3
1	A	320	GLY	3.3
1	A	900	ILE	3.2
1	D	55	SER	3.2
1	A	848	SER	3.2
1	B	234	VAL	3.2
1	D	1110	ALA	3.2
1	D	287	PHE	3.2
1	D	448	LYS	3.2
1	C	950	LEU	3.2
1	A	119	LYS	3.1
1	C	207	ASP	3.1
1	C	1018	ILE	3.1
1	B	457	PHE	3.1
1	D	128	LYS	3.1
1	B	860	ASP	3.1
1	D	61	GLU	3.0
1	C	209	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	123	ARG	3.0
1	C	845	GLN	3.0
1	A	182	ASP	3.0
1	B	837	GLY	3.0
1	B	935	ILE	3.0
1	D	446	THR	3.0
1	D	494	LEU	3.0
1	A	138	ASP	3.0
1	C	434	VAL	3.0
1	B	882	VAL	3.0
1	A	901	THR	2.9
1	A	87	PHE	2.9
1	D	462	SER	2.9
1	D	125	THR	2.9
1	B	194	SER	2.9
1	B	393	SER	2.9
1	C	289	ILE	2.9
1	C	456	LEU	2.9
1	C	940	GLU	2.8
1	D	909	PRO	2.8
1	C	577	TRP	2.8
1	D	925	ASN	2.8
1	D	989	ILE	2.8
1	B	516	ASP	2.8
1	D	947	GLY	2.8
1	D	944	ALA	2.8
1	A	137	THR	2.8
1	B	840	SER	2.8
1	D	347	ILE	2.8
1	B	856	ASP	2.8
1	D	456	LEU	2.8
1	A	295	VAL	2.8
1	D	209	PRO	2.8
1	B	1039	ASN	2.8
1	B	919	GLU	2.8
1	D	234	VAL	2.8
1	D	252	PRO	2.8
1	B	387	ILE	2.8
1	D	288	PHE	2.8
1	C	530	GLN	2.7
1	C	560	ILE	2.7
1	D	1107	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	894	LEU	2.7
1	A	462	SER	2.7
1	C	491	ASP	2.7
1	C	890	VAL	2.7
1	D	60	ALA	2.7
1	D	118	ASP	2.7
1	D	447	THR	2.7
1	D	495	ALA	2.7
1	B	621	TYR	2.7
1	A	622	LYS	2.7
1	C	236	ARG	2.7
1	A	898	SER	2.7
1	B	940	GLU	2.7
1	B	628	VAL	2.7
1	D	129	ALA	2.7
1	C	462	SER	2.7
1	D	840	SER	2.7
1	D	53	VAL	2.7
1	A	241	VAL	2.7
1	B	130	ASP	2.7
1	B	162	ALA	2.6
1	B	458	ASP	2.6
1	D	935	ILE	2.6
1	A	847	LYS	2.6
1	A	929	LYS	2.6
1	B	191	ALA	2.6
1	B	944	ALA	2.6
1	A	909	PRO	2.6
1	A	930	ASP	2.6
1	D	54	GLY	2.6
1	D	249	GLY	2.6
1	A	837	GLY	2.6
1	B	912	VAL	2.6
1	A	223	ASN	2.6
1	A	758	ASP	2.6
1	C	394	LEU	2.6
1	B	888	TYR	2.6
1	D	420	ARG	2.6
1	A	177	GLU	2.6
1	A	890	VAL	2.6
1	A	899	VAL	2.6
1	A	446	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	460	GLN	2.6
1	D	583	ASP	2.5
1	D	113	LEU	2.5
1	A	931	LEU	2.5
1	A	267	GLU	2.5
1	B	222	GLY	2.5
1	B	938	GLY	2.5
1	A	155	GLY	2.5
1	D	293	PRO	2.5
1	D	454	PRO	2.5
1	A	912	VAL	2.5
1	C	855	PHE	2.5
1	A	274	ALA	2.5
1	D	1116	THR	2.5
1	A	856	ASP	2.5
1	B	960	GLU	2.5
1	B	903	GLY	2.5
1	D	102	GLY	2.5
1	C	287	PHE	2.5
1	C	941	ALA	2.5
1	B	388	SER	2.5
1	C	458	ASP	2.5
1	A	895	ASP	2.5
1	C	238	HIS	2.5
1	D	115	MET	2.5
1	B	929	LYS	2.5
1	A	316	LEU	2.5
1	A	840	SER	2.5
1	A	176	GLU	2.5
1	A	960	GLU	2.5
1	A	140	PRO	2.5
1	D	75	GLN	2.5
1	A	239	GLN	2.5
1	A	129	ALA	2.5
1	C	450	ILE	2.4
1	A	259	CYS	2.4
1	A	821	ASP	2.4
1	D	1040	GLY	2.4
1	B	897	GLN	2.4
1	D	72	VAL	2.4
1	D	425	LYS	2.4
1	D	77	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	969	PRO	2.4
1	D	619	VAL	2.4
1	A	949	TYR	2.4
1	A	73	ALA	2.4
1	B	453	THR	2.4
1	A	233	SER	2.4
1	C	448	LYS	2.4
1	B	1058	LYS	2.4
1	C	318	ALA	2.4
1	A	253	THR	2.4
1	D	496	SER	2.4
1	D	670	SER	2.4
1	D	422	ARG	2.4
1	B	908	PHE	2.4
1	B	933	ALA	2.4
1	D	103	ILE	2.3
1	D	421	ILE	2.3
1	D	298	GLU	2.3
1	C	358	PRO	2.3
1	C	117	GLY	2.3
1	C	837	GLY	2.3
1	A	882	VAL	2.3
1	C	495	ALA	2.3
1	A	42	LEU	2.3
1	B	900	ILE	2.3
1	C	834	MET	2.3
1	D	464	ASP	2.3
1	D	1037	ASP	2.3
1	B	870	GLY	2.3
1	A	291	VAL	2.3
1	B	894	LEU	2.3
1	C	822	ILE	2.3
1	A	217	ILE	2.3
1	C	211	HIS	2.3
1	A	185	HIS	2.3
1	D	223	ASN	2.3
1	D	243	GLU	2.3
1	B	909	PRO	2.3
1	A	891	GLN	2.3
1	D	259	CYS	2.3
1	A	156	PHE	2.3
1	B	363	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	66	ILE	2.3
1	A	1055	ILE	2.3
1	A	853	GLU	2.3
1	C	393	SER	2.3
1	C	821	ASP	2.3
1	A	911	SER	2.3
1	C	678	GLY	2.3
1	C	248	VAL	2.3
1	D	295	VAL	2.3
1	D	708	ILE	2.2
1	A	315	ILE	2.2
1	D	220	GLU	2.2
1	D	285	GLU	2.2
1	C	1061	ASN	2.2
1	A	204	ARG	2.2
1	B	461	PRO	2.2
1	D	41	SER	2.2
1	A	55	SER	2.2
1	D	325	GLY	2.2
1	C	234	VAL	2.2
1	B	916	PHE	2.2
1	D	929	LYS	2.2
1	B	345	CYS	2.2
1	B	1038	GLU	2.2
1	D	92	GLU	2.2
1	A	152	GLU	2.2
1	A	445	TYR	2.2
1	A	888	TYR	2.2
1	C	841	ASN	2.2
1	D	86	GLY	2.2
1	A	902	ASP	2.2
1	B	494	LEU	2.2
1	D	653	VAL	2.2
1	B	928	ASN	2.2
1	A	627	ASN	2.2
1	B	252	PRO	2.2
1	D	46	LYS	2.2
1	D	926	GLY	2.2
1	A	860	ASP	2.2
1	B	953	VAL	2.2
1	D	225	VAL	2.2
1	D	277	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	1020	ILE	2.2
1	A	69	ILE	2.2
1	A	238	HIS	2.2
1	A	577	TRP	2.2
1	A	855	PHE	2.2
1	B	451	GLU	2.2
1	A	835	PRO	2.2
1	D	967	GLN	2.2
1	D	905	LYS	2.2
1	B	54	GLY	2.2
1	D	942	LEU	2.2
1	A	463	LEU	2.2
1	C	258	ILE	2.2
1	B	242	VAL	2.2
1	B	518	VAL	2.2
1	A	214	VAL	2.2
1	A	269	ILE	2.2
1	C	356	PHE	2.2
1	D	1108	THR	2.1
1	A	96	ARG	2.1
1	D	1022	LYS	2.1
1	C	903	GLY	2.1
1	A	384	GLY	2.1
1	C	388	SER	2.1
1	B	899	VAL	2.1
1	D	680	ILE	2.1
1	A	130	ASP	2.1
1	A	221	HIS	2.1
1	C	896	GLU	2.1
1	C	1025	ARG	2.1
1	D	1104	PRO	2.1
1	C	75	GLN	2.1
1	A	264	GLN	2.1
1	B	950	LEU	2.1
1	D	63	TYR	2.1
1	D	117	GLY	2.1
1	C	225	VAL	2.1
1	C	976	ILE	2.1
1	D	284	ASP	2.1
1	B	1111	MET	2.1
1	B	77	ASN	2.1
1	C	224	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	297	VAL	2.1
1	D	396	VAL	2.1
1	D	970	VAL	2.1
1	C	1019	GLU	2.1
1	C	909	PRO	2.1
1	D	3	GLN	2.1
1	B	443	GLY	2.1
1	B	708	ILE	2.1
1	A	4	ILE	2.1
1	A	822	ILE	2.1
1	B	895	ASP	2.0
1	A	916	PHE	2.1
1	B	62	SER	2.0
1	D	318	ALA	2.0
1	D	803	SER	2.0
1	C	847	LYS	2.0
1	D	427	ASN	2.0
1	B	450	ILE	2.0
1	D	58	GLY	2.0
1	D	206	ILE	2.0
1	D	674	ILE	2.0
1	A	680	ILE	2.0
1	C	455	GLU	2.0
1	A	220	GLU	2.0
1	A	869	PHE	2.0
1	A	886	ALA	2.0
1	C	252	PRO	2.0
1	D	132	PRO	2.0
1	D	461	PRO	2.0
1	A	952	PRO	2.0
1	B	906	LEU	2.0
1	D	890	VAL	2.0
1	A	621	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

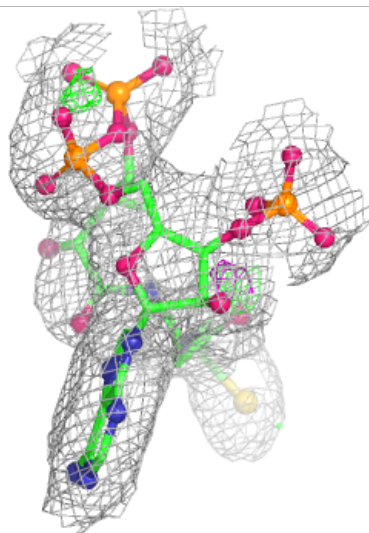
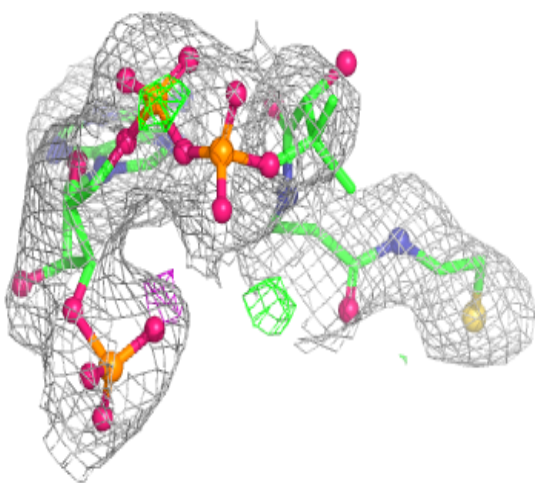
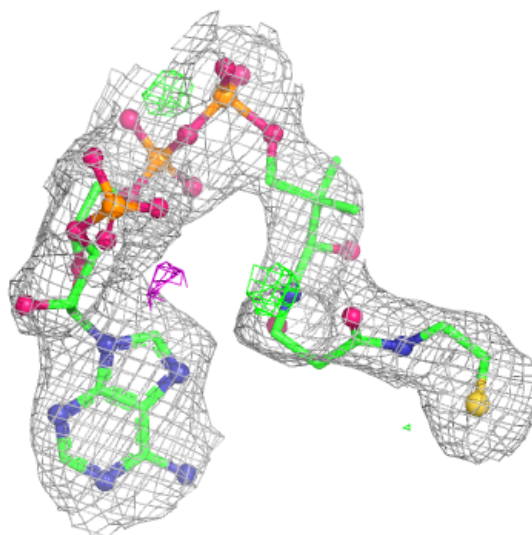
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	MN	D	1201	1/1	0.79	0.22	130,130,130,130	0
4	MN	C	1203	1/1	0.86	0.15	129,129,129,129	0
2	BTI	C	1201	15/15	0.86	0.12	32,37,41,43	0
4	MN	B	1202	1/1	0.87	0.10	74,74,74,74	0
2	BTI	A	1201	15/15	0.88	0.12	48,49,52,54	0
2	BTI	B	1201	15/15	0.89	0.12	44,45,50,51	0
4	MN	A	1203	1/1	0.90	0.10	102,102,102,102	0
2	BTI	C	1204	15/15	0.92	0.10	29,30,33,40	0
3	COA	C	1202	48/48	0.92	0.11	37,45,53,55	0
5	ACO	A	1202	51/51	0.92	0.10	33,38,51,52	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.

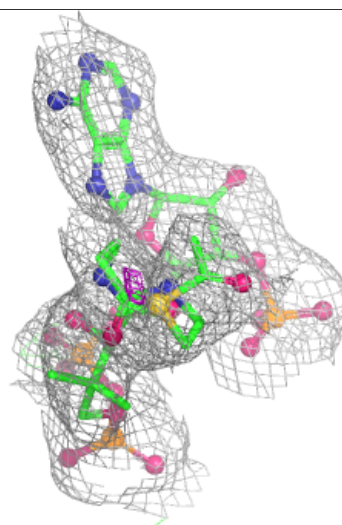
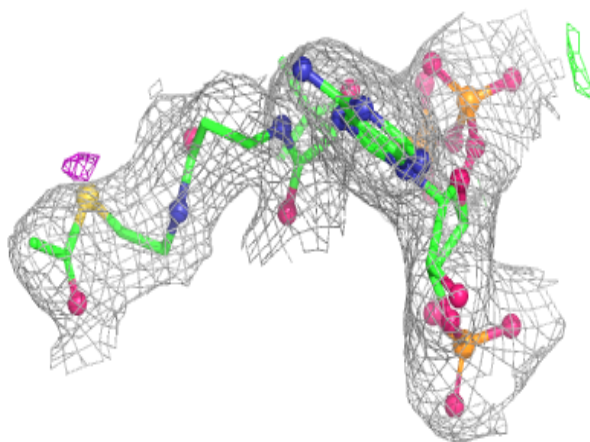
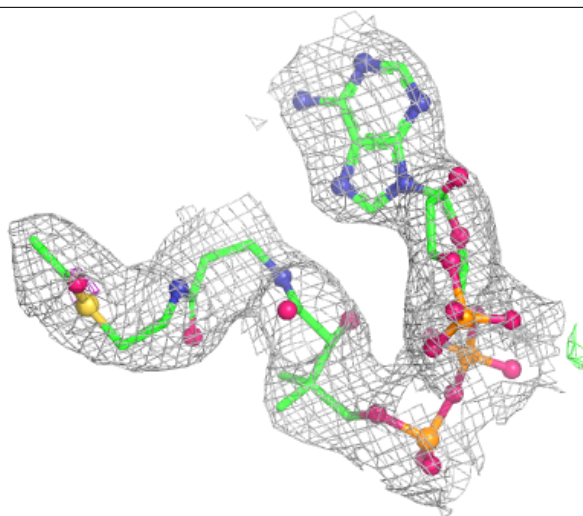
Electron density around COA C 1202:

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



Electron density around ACO A 1202:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.