



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:24 AM UTC

PDB ID : 3HBL / pdb_00003hbl
Title : Crystal Structure of S. aureus Pyruvate Carboxylase T908A Mutant
Authors : Tong, L.; Yu, L.P.C.
Deposited on : 2009-05-04
Resolution : 2.71 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

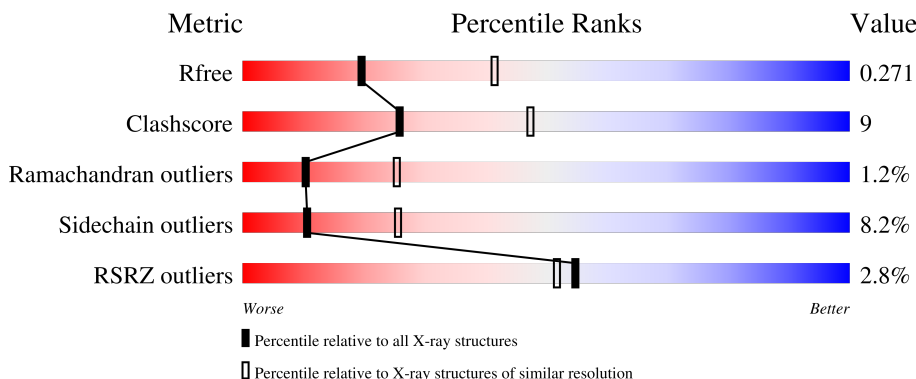
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	 3% 75% 19% • •
1	B	1150	 3% 71% 19% • 7%
1	C	1150	 2% 71% 19% • 7%
1	D	1150	 3% 67% 22% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34327 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.

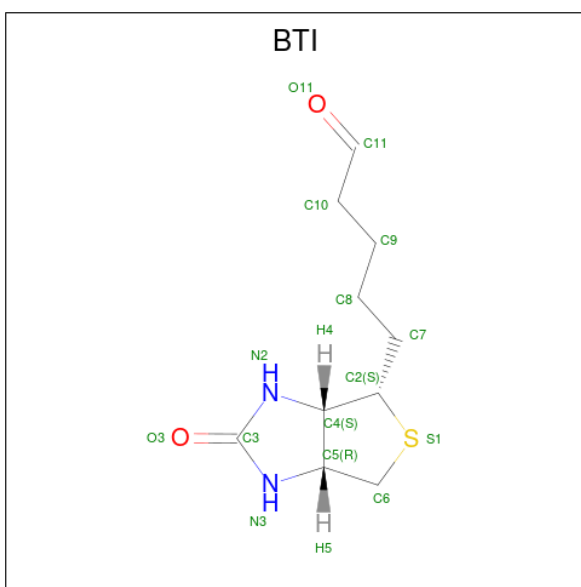
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1131	Total	C	N	O	S	0	0	0
			8923	5654	1502	1737	30			
1	B	1074	Total	C	N	O	S	0	0	0
			8463	5364	1427	1643	29			
1	C	1067	Total	C	N	O	S	0	0	0
			8439	5349	1421	1639	30			
1	D	1067	Total	C	N	O	S	0	0	0
			8411	5333	1416	1633	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	908	ALA	THR	engineered mutation	UNP Q99UY8
B	908	ALA	THR	engineered mutation	UNP Q99UY8
C	908	ALA	THR	engineered mutation	UNP Q99UY8
D	908	ALA	THR	engineered mutation	UNP Q99UY8

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

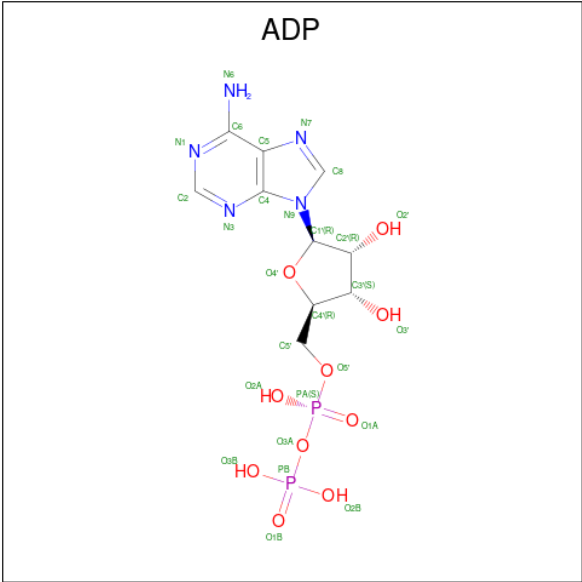


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	D	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

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

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

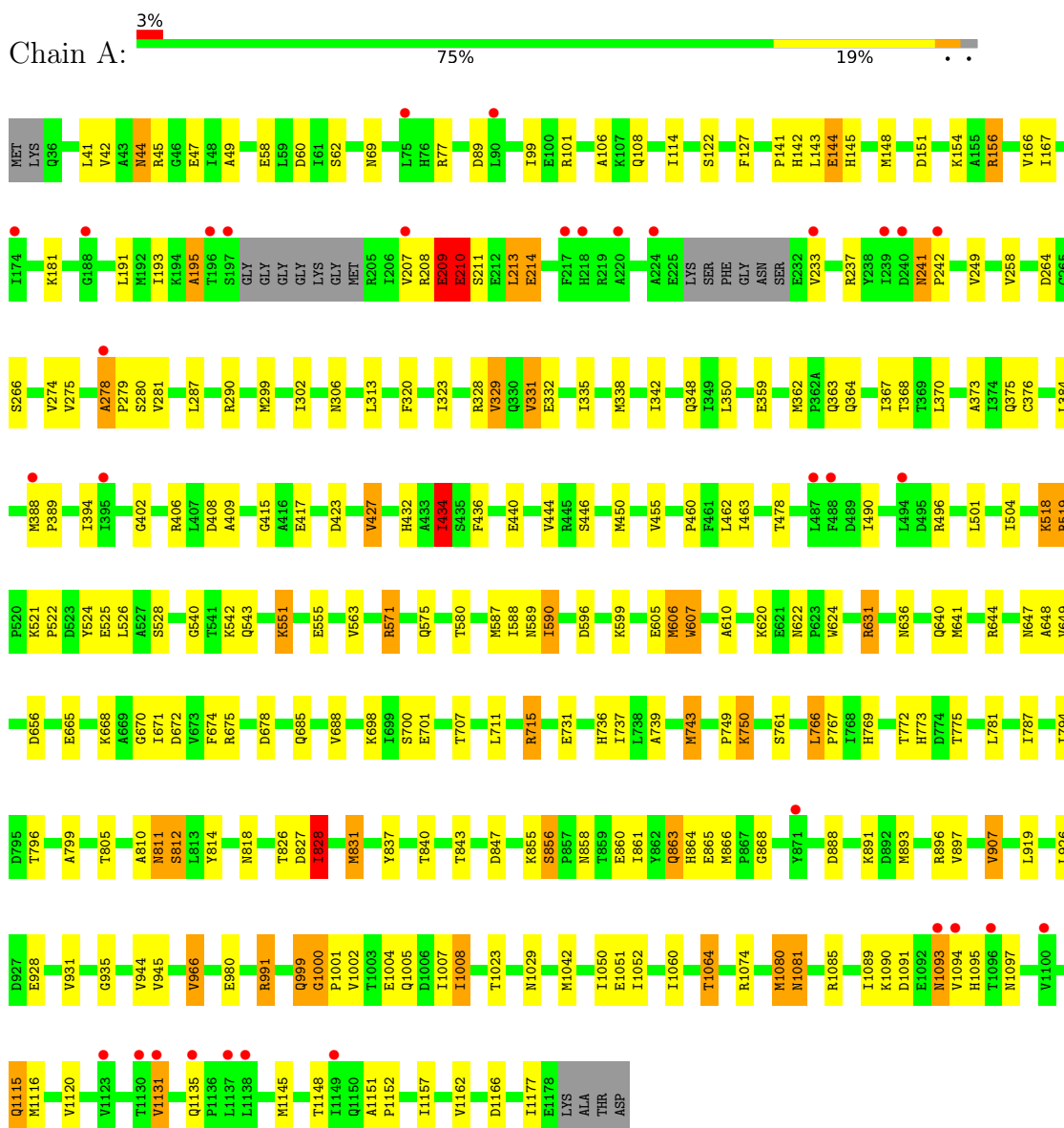


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots

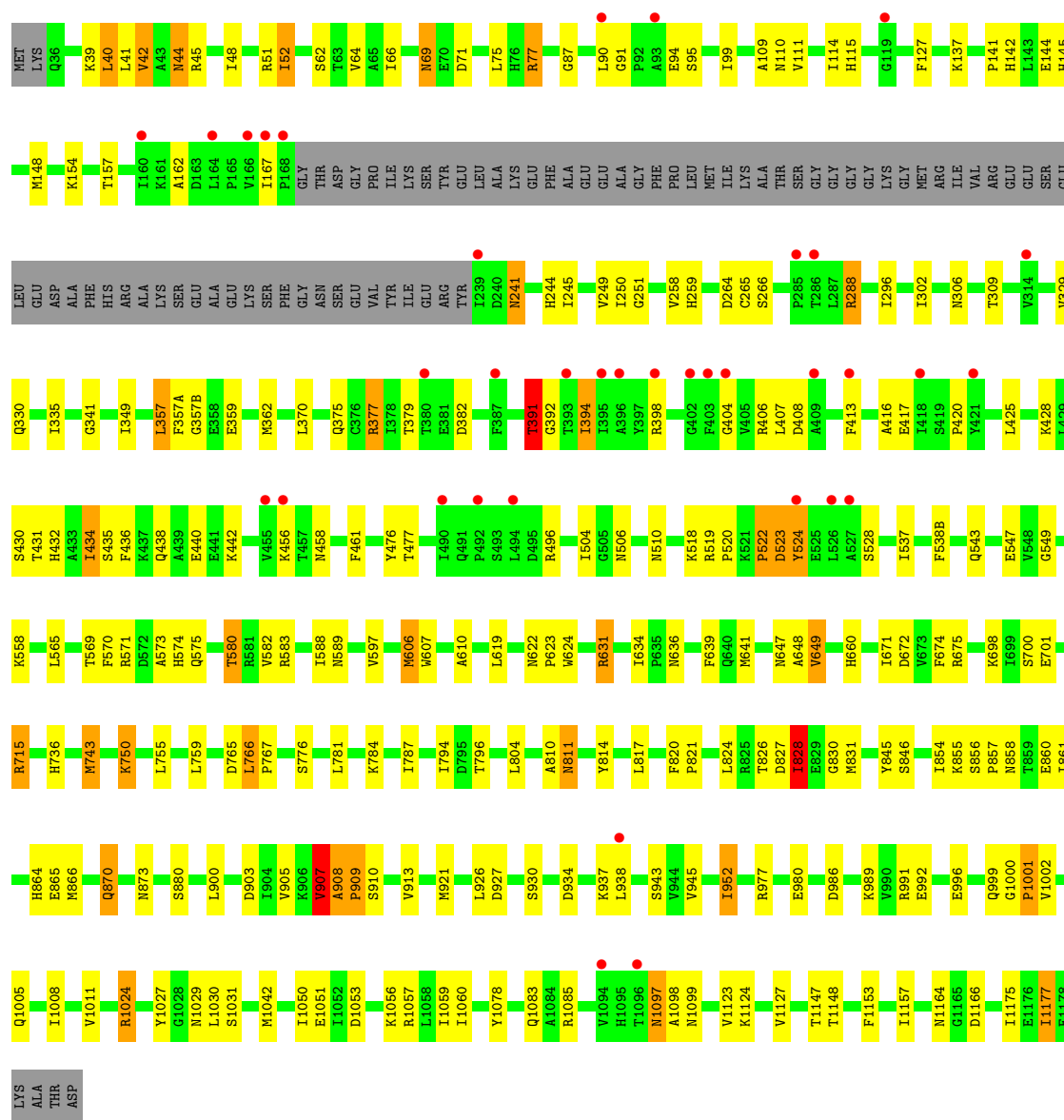
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

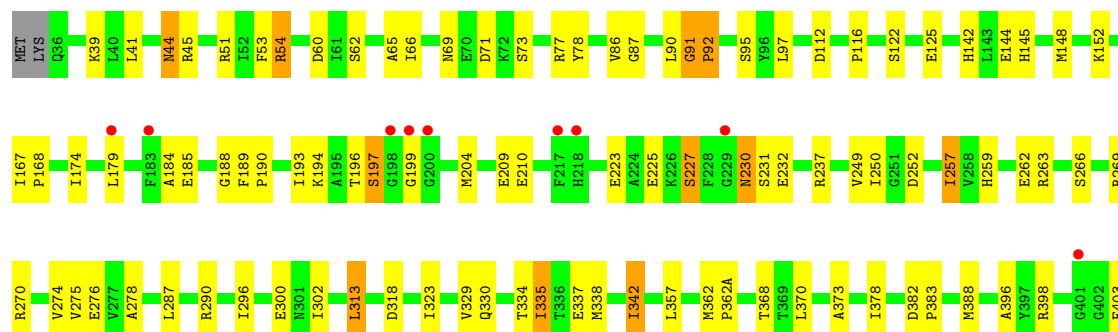


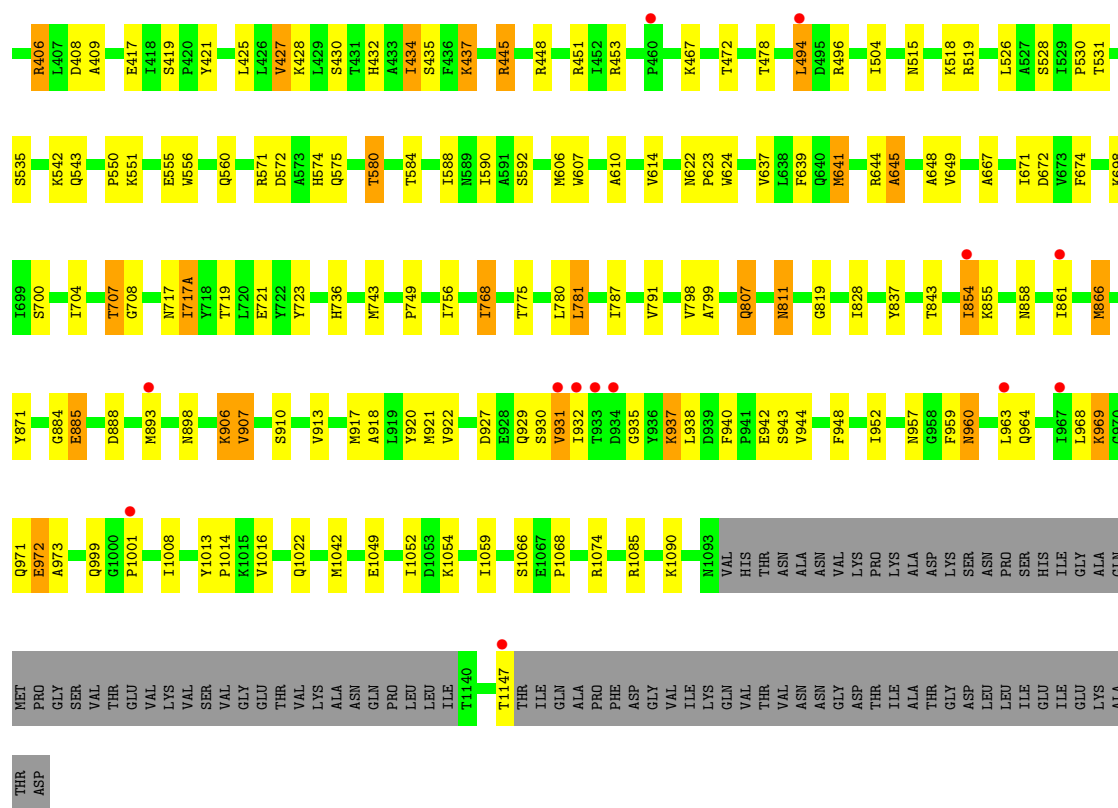
• Molecule 1: Pyruvate carboxylase



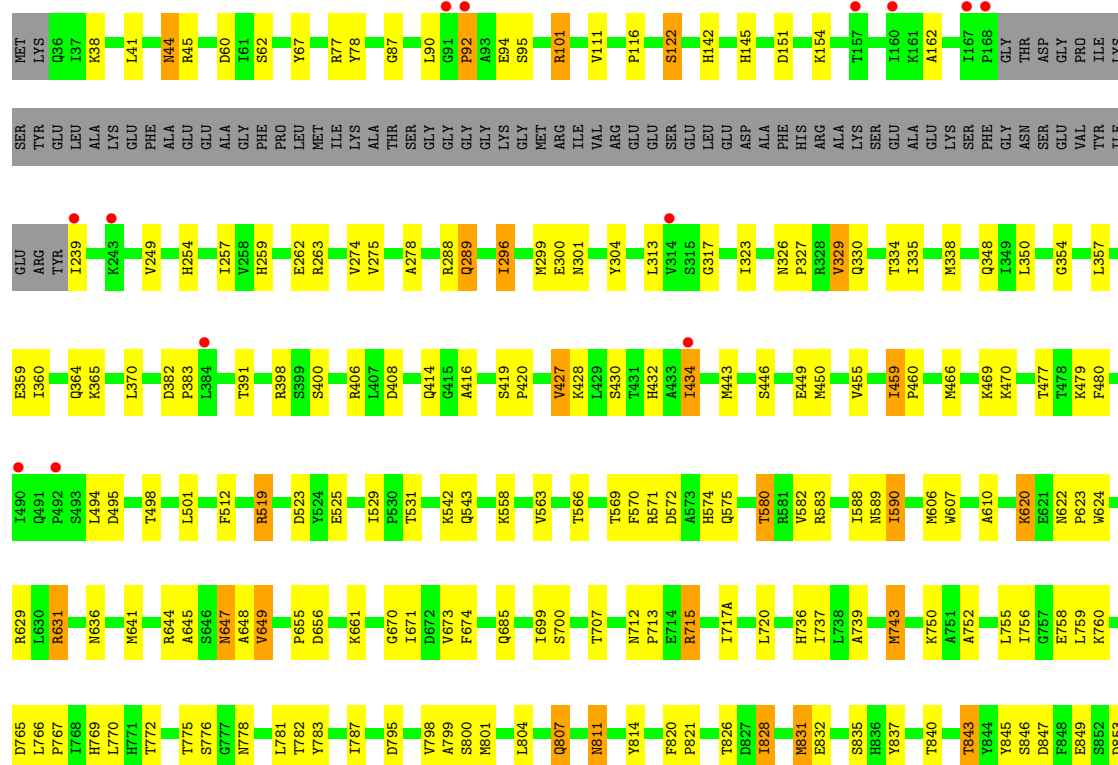


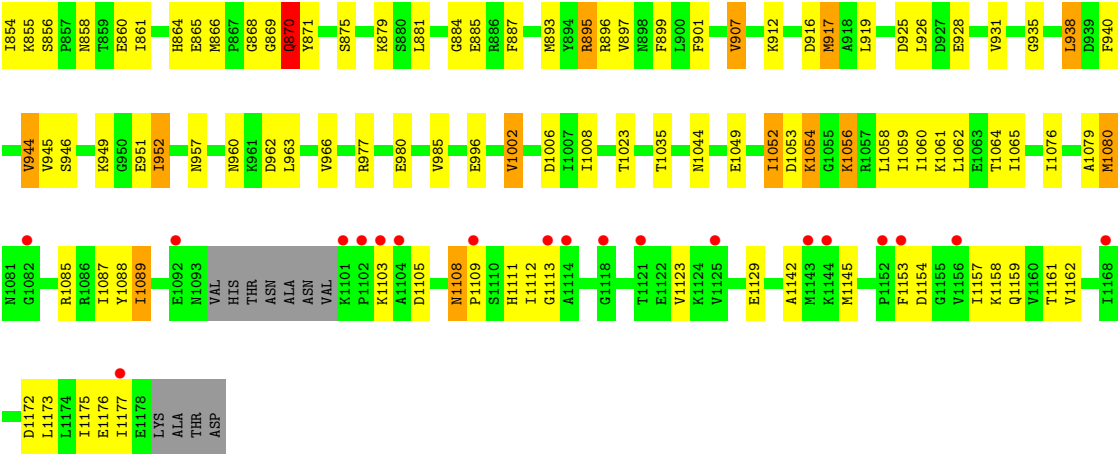
• Molecule 1: Pyruvate carboxylase





• 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	96.53Å 257.15Å 130.32Å 90.00° 114.35° 90.00°	Depositor
Resolution (Å)	29.95 – 2.71 29.95 – 2.71	Depositor EDS
% Data completeness (in resolution range)	86.2 (29.95-2.71) 86.3 (29.95-2.71)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.279 0.222 , 0.271	Depositor DCC
R_{free} test set	6799 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34327	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: BTI, MN, ADP

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	0.52	0/9091	0.85	2/12299 (0.0%)
1	B	0.47	0/8623	0.82	8/11672 (0.1%)
1	C	0.46	0/8601	0.81	1/11624 (0.0%)
1	D	0.52	1/8569 (0.0%)	0.83	3/11595 (0.0%)
All	All	0.49	1/34884 (0.0%)	0.83	14/47190 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	459	ILE	CA-CB	6.04	1.57	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	GLY	N-CA-C	8.48	117.93	110.21
1	B	908	ALA	CA-C-N	8.41	130.36	119.84
1	B	908	ALA	C-N-CA	8.41	130.36	119.84
1	A	828	ILE	CB-CA-C	-6.98	103.03	111.97
1	D	649	VAL	N-CA-C	-6.62	106.85	113.20
1	D	938	LEU	N-CA-C	6.28	117.93	111.14
1	B	91	GLY	CA-C-N	6.06	127.42	119.84
1	B	91	GLY	C-N-CA	6.06	127.42	119.84
1	B	828	ILE	CB-CA-C	-5.45	104.88	112.02
1	B	549	GLY	CA-C-N	5.34	124.98	119.05
1	B	549	GLY	C-N-CA	5.34	124.98	119.05
1	D	416	ALA	N-CA-C	5.31	118.17	110.42
1	C	69	ASN	N-CA-C	5.07	116.62	111.14
1	B	524	TYR	N-CA-C	-5.06	105.42	112.45

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	8923	0	8850	169	0
1	B	8463	0	8410	165	0
1	C	8439	0	8348	144	0
1	D	8411	0	8360	180	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
2	C	15	0	15	1	0
2	D	15	0	15	0	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	C	27	0	12	1	0
All	All	34327	0	34040	648	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 9.

All (648) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:ALA:HB1	1:B:909:PRO:HD2	1.35	1.09
1:B:504:ILE:HG21	1:B:1042:MET:HE3	1.36	1.04
1:B:288:ARG:HG3	1:B:288:ARG:HH11	1.24	1.01
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.26	1.00
1:B:44:ASN:HD22	1:B:45:ARG:H	1.03	0.98
1:A:810:ALA:HB1	1:A:831:MET:HE1	1.45	0.94
1:D:44:ASN:HD22	1:D:45:ARG:H	1.12	0.92
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.35	0.90
1:B:826:THR:HG21	1:B:831:MET:HE2	1.52	0.90
1:C:606:MET:HE2	1:C:639:PHE:HB3	1.54	0.89
1:A:278:ALA:HB1	1:A:279:PRO:HD2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ARG:HH11	1:B:377:ARG:HG2	1.38	0.88
1:A:44:ASN:HD22	1:A:45:ARG:H	1.21	0.88
1:A:504:ILE:HG21	1:A:1042:MET:HE3	1.57	0.87
1:C:44:ASN:HD22	1:C:45:ARG:H	1.16	0.87
1:D:338:MET:HE1	1:D:430:SER:HB2	1.56	0.86
1:C:504:ILE:HG21	1:C:1042:MET:CE	2.06	0.85
1:D:259:HIS:H	1:D:364:GLN:HE22	1.22	0.85
1:A:278:ALA:CB	1:A:279:PRO:HD2	2.07	0.84
1:A:278:ALA:HB1	1:A:279:PRO:CD	2.07	0.84
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.41	0.83
1:D:101:ARG:HG2	1:D:101:ARG:HH21	1.43	0.83
1:D:700:SER:H	1:D:736:HIS:HD2	1.28	0.82
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.62	0.81
1:A:620:LYS:HG2	1:A:1023:THR:HG21	1.60	0.81
1:A:504:ILE:HD13	1:A:1042:MET:HE2	1.60	0.81
1:B:700:SER:H	1:B:736:HIS:HD2	1.29	0.81
1:A:700:SER:H	1:A:736:HIS:HD2	1.27	0.81
1:C:54:ARG:CG	1:C:54:ARG:HH11	1.93	0.80
1:D:644:ARG:HH11	1:D:647:ASN:HD21	1.30	0.79
1:A:258:VAL:HG21	1:A:362:MET:HE2	1.64	0.78
1:D:960:ASN:HD22	1:D:963:LEU:H	1.29	0.78
1:B:77:ARG:HH11	1:B:77:ARG:CG	1.99	0.76
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.49	0.76
1:C:362:MET:HE3	1:C:362(A):PRO:HD2	1.68	0.76
1:A:896:ARG:HD2	1:A:928:GLU:OE2	1.86	0.76
1:A:406:ARG:HD3	1:C:403:PHE:HA	1.67	0.76
1:B:48:ILE:O	1:B:52:ILE:HG12	1.86	0.76
1:B:44:ASN:ND2	1:B:45:ARG:H	1.83	0.75
1:C:700:SER:H	1:C:736:HIS:HD2	1.33	0.75
1:C:504:ILE:HG21	1:C:1042:MET:HE3	1.66	0.74
1:D:1108:ASN:HB2	1:D:1109:PRO:HD3	1.70	0.73
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.72	0.72
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.20	0.72
1:C:504:ILE:HG21	1:C:1042:MET:HE2	1.72	0.71
1:A:363:GLN:HE21	1:A:364:GLN:H	1.39	0.71
1:A:313:LEU:HD13	1:A:323:ILE:HG13	1.72	0.71
1:A:1000:GLY:H	1:A:1001:PRO:HD2	1.55	0.71
1:B:814:TYR:CZ	1:B:828:ILE:HG12	2.25	0.71
1:B:908:ALA:O	1:B:910:SER:N	2.24	0.71
1:D:313:LEU:HB2	1:D:323:ILE:HD11	1.71	0.71
1:D:570:PHE:O	1:D:574:HIS:HE1	1.74	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:908:ALA:CB	1:B:909:PRO:HD2	2.15	0.71
1:A:1093:ASN:HB2	1:A:1095:HIS:O	1.92	0.70
1:C:866:MET:HE1	1:C:871:TYR:HA	1.72	0.70
1:C:116:PRO:HB2	1:C:122:SER:HA	1.74	0.70
1:D:329:VAL:HG22	1:D:348:GLN:NE2	2.02	0.70
1:C:700:SER:H	1:C:736:HIS:CD2	2.08	0.70
1:C:54:ARG:HH11	1:C:54:ARG:HG2	1.56	0.69
1:C:152:LYS:HG3	1:C:197:SER:H	1.55	0.69
1:D:840:THR:O	1:D:843:THR:HB	1.91	0.69
1:A:641:MET:HE2	1:A:671:ILE:HG13	1.75	0.69
1:B:39:LYS:HB3	1:B:62:SER:HB3	1.75	0.69
1:A:840:THR:O	1:A:843:THR:HB	1.92	0.69
1:B:675:ARG:HA	1:B:701:GLU:HB3	1.75	0.69
1:A:278:ALA:CB	1:A:279:PRO:CD	2.68	0.68
1:A:99:ILE:HG23	1:A:127:PHE:HD1	1.58	0.68
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.28	0.68
1:C:437:LYS:H	1:C:437:LYS:HD3	1.57	0.67
1:D:142:HIS:H	1:D:145:HIS:HD2	1.43	0.67
1:D:572:ASP:HB3	1:D:807:GLN:NE2	2.10	0.67
1:A:715:ARG:HH12	1:A:865:GLU:CD	2.02	0.67
1:B:506:ASN:ND2	1:B:510:ASN:HD22	1.93	0.67
1:C:811:ASN:HD22	1:C:811:ASN:H	1.42	0.67
1:B:927:ASP:H	1:B:930:SER:HB3	1.59	0.66
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.60	0.66
1:D:350:LEU:HD22	1:D:359:GLU:HB3	1.77	0.66
1:B:504:ILE:HG21	1:B:1042:MET:CE	2.22	0.66
1:A:1064:THR:HG21	1:C:1066:SER:HA	1.76	0.66
1:B:811:ASN:H	1:B:811:ASN:HD22	1.43	0.66
1:D:101:ARG:HH21	1:D:101:ARG:CG	2.09	0.66
1:B:435:SER:HB3	1:B:438:GLN:HB2	1.78	0.66
1:C:269:ARG:HG3	1:C:270:ARG:H	1.59	0.66
1:D:558:LYS:HD2	1:D:765:ASP:O	1.96	0.66
1:D:743:MET:HG3	1:D:907:VAL:HG13	1.78	0.66
1:A:209:GLU:HG2	1:A:210:GLU:N	2.11	0.65
1:C:338:MET:HE3	1:C:373:ALA:HB1	1.78	0.65
1:D:470:LYS:HB2	1:D:480:PHE:HE1	1.61	0.65
1:A:810:ALA:CB	1:A:831:MET:HE1	2.23	0.65
1:B:750:LYS:HG3	1:C:819:GLY:HA3	1.76	0.65
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.32	0.65
1:A:1081:ASN:HB2	1:C:78:TYR:CE2	2.32	0.65
1:A:209:GLU:CG	1:A:210:GLU:H	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.62	0.64
1:A:799:ALA:H	1:A:811:ASN:ND2	1.96	0.64
1:D:647:ASN:HD22	1:D:647:ASN:C	2.03	0.64
1:D:338:MET:HE1	1:D:430:SER:CB	2.28	0.64
1:A:209:GLU:CG	1:A:210:GLU:N	2.60	0.64
1:A:328:ARG:HD2	1:A:329:VAL:O	1.98	0.64
1:C:51:ARG:NH2	1:C:337:GLU:OE2	2.31	0.64
1:D:563:VAL:HG21	1:D:787:ILE:HG12	1.79	0.63
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.32	0.63
1:D:87:GLY:HA3	1:D:90:LEU:HD12	1.80	0.63
1:C:90:LEU:HB3	1:C:95:SER:HB3	1.79	0.63
1:C:313:LEU:HB2	1:C:323:ILE:HD11	1.81	0.63
1:A:641:MET:CE	1:A:671:ILE:HG13	2.28	0.63
1:D:543:GLN:HE22	1:D:636:ASN:HA	1.64	0.63
1:C:54:ARG:HG2	1:C:54:ARG:NH1	2.13	0.62
1:A:143:LEU:HD12	1:A:143:LEU:H	1.64	0.62
1:D:443:MET:HG2	1:D:466:MET:HE3	1.82	0.62
1:C:606:MET:HE1	1:C:671:ILE:HD13	1.81	0.62
1:C:866:MET:CE	1:C:871:TYR:HA	2.29	0.62
1:A:144:GLU:O	1:A:148:MET:HB2	2.00	0.61
1:D:259:HIS:H	1:D:364:GLN:NE2	1.96	0.61
1:C:435:SER:HB2	1:C:437:LYS:HE3	1.82	0.61
1:D:893:MET:O	1:D:897:VAL:HG23	2.00	0.61
1:A:811:ASN:HD22	1:A:811:ASN:H	1.48	0.61
1:B:1057:ARG:HD3	1:B:1059:ILE:HD11	1.82	0.61
1:A:290:ARG:HG2	1:A:320:PHE:HE1	1.64	0.61
1:B:864:HIS:HD2	1:B:866:MET:H	1.49	0.61
1:D:400:SER:OG	1:D:449:GLU:HB3	2.00	0.61
1:D:620:LYS:HG2	1:D:1023:THR:HG21	1.83	0.61
1:B:288:ARG:HG3	1:B:288:ARG:NH1	2.01	0.61
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.66	0.61
1:D:814:TYR:CE2	1:D:828:ILE:HG12	2.36	0.61
1:B:631:ARG:NH2	1:B:672:ASP:OD1	2.34	0.60
1:C:342:ILE:HG12	1:C:362:MET:HE1	1.82	0.60
1:C:940:PHE:HB3	1:C:944:VAL:CG1	2.31	0.60
1:A:504:ILE:HD13	1:A:1042:MET:CE	2.30	0.60
1:C:269:ARG:HG3	1:C:270:ARG:N	2.16	0.60
1:A:864:HIS:CD2	1:A:866:MET:HG3	2.36	0.60
1:B:41:LEU:O	1:B:64:VAL:O	2.20	0.60
1:B:142:HIS:H	1:B:145:HIS:HD2	1.50	0.60
1:B:504:ILE:HD13	1:B:1042:MET:CE	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:856:SER:HB2	1:B:857:PRO:HD2	1.84	0.60
1:C:858:ASN:O	1:C:861:ILE:HG12	2.02	0.60
1:D:357:LEU:HA	1:D:360:ILE:HD13	1.83	0.60
1:C:768:ILE:HG22	1:C:791:VAL:HG23	1.83	0.60
1:D:519:ARG:NH2	1:D:847:ASP:OD2	2.31	0.60
1:B:927:ASP:HB3	1:B:930:SER:H	1.67	0.59
1:D:1065:ILE:HG12	1:D:1076:ILE:HG12	1.84	0.59
1:A:575:GLN:NE2	1:A:610:ALA:H	2.00	0.59
1:A:504:ILE:HG21	1:A:1042:MET:CE	2.31	0.59
1:B:934:ASP:O	1:B:938:LEU:HG	2.02	0.59
1:B:1177:ILE:HD13	1:B:1177:ILE:H	1.67	0.59
1:D:249:VAL:HG21	1:D:299:MET:HG3	1.84	0.59
1:A:524:TYR:CD2	1:A:843:THR:HG22	2.36	0.59
1:B:408:ASP:HB2	1:B:428:LYS:HB3	1.84	0.59
1:A:700:SER:H	1:A:736:HIS:CD2	2.15	0.59
1:B:1000:GLY:N	1:B:1001:PRO:HD3	2.16	0.59
1:C:606:MET:HE1	1:C:671:ILE:CD1	2.32	0.59
1:A:814:TYR:CZ	1:A:828:ILE:HG12	2.38	0.59
1:A:278:ALA:O	1:A:279:PRO:C	2.44	0.58
1:A:675:ARG:HA	1:A:701:GLU:HB3	1.85	0.58
1:A:264:ASP:HB2	1:A:280:SER:HB3	1.84	0.58
1:A:737:ILE:HG12	1:A:767:PRO:HG2	1.84	0.58
1:A:991:ARG:NH2	1:A:1004:GLU:OE1	2.35	0.58
1:B:99:ILE:HG23	1:B:127:PHE:HD1	1.68	0.58
1:D:572:ASP:HB3	1:D:807:GLN:HE22	1.66	0.58
1:A:151:ASP:HB3	1:A:154:LYS:HB2	1.85	0.58
1:A:1081:ASN:HB2	1:C:78:TYR:CD2	2.39	0.58
1:B:41:LEU:HB2	1:B:111:VAL:HG11	1.85	0.58
1:D:151:ASP:HB3	1:D:154:LYS:HG3	1.85	0.58
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.86	0.58
1:D:811:ASN:H	1:D:811:ASN:HD22	1.49	0.58
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.68	0.58
1:C:278:ALA:HB3	1:C:335:ILE:HG23	1.86	0.58
1:D:960:ASN:ND2	1:D:963:LEU:H	2.00	0.57
1:B:42:VAL:HA	1:B:115:HIS:O	2.05	0.57
1:D:826:THR:HG21	1:D:831:MET:HE1	1.86	0.57
1:D:935:GLY:HA3	1:D:966:VAL:HG11	1.85	0.57
1:D:641:MET:HE3	1:D:674:PHE:CE1	2.40	0.57
1:C:920:TYR:OH	1:C:938:LEU:HB3	2.04	0.57
1:D:1103:LYS:O	1:D:1173:LEU:HB2	2.05	0.57
1:C:41:LEU:HD11	1:C:66:ILE:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:MET:HG3	1:B:907:VAL:HG13	1.86	0.56
1:C:71:ASP:C	1:C:73:SER:H	2.11	0.56
1:D:647:ASN:C	1:D:647:ASN:ND2	2.63	0.56
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.69	0.56
1:D:1049:GLU:HG2	1:D:1059:ILE:HD12	1.86	0.56
1:B:622:ASN:HD21	1:B:624:TRP:HD1	1.53	0.56
1:A:306:ASN:OD1	1:A:348:GLN:HG2	2.06	0.56
1:B:244:HIS:HD2	1:B:265:CYS:HB2	1.70	0.56
1:D:631:ARG:HG2	1:D:670:GLY:HA3	1.87	0.56
1:D:645:ALA:HB1	1:D:685:GLN:O	2.04	0.56
1:D:656:ASP:OD2	1:D:977:ARG:NH2	2.39	0.56
1:A:370:LEU:O	1:A:432:HIS:HE1	1.87	0.56
1:B:1157:ILE:HA	1:B:1177:ILE:HG22	1.86	0.56
1:D:1061:LYS:HB3	1:D:1079:ALA:HB3	1.87	0.56
1:C:787:ILE:HA	1:C:791:VAL:HG12	1.87	0.56
1:A:145:HIS:HE1	1:A:302:ILE:O	1.87	0.56
1:B:377:ARG:HG2	1:B:377:ARG:NH1	2.15	0.56
1:B:504:ILE:HD13	1:B:1042:MET:HE2	1.88	0.56
1:D:935:GLY:HA2	1:D:938:LEU:HD12	1.88	0.56
1:B:506:ASN:HD22	1:B:510:ASN:HD22	1.53	0.56
1:D:529:ILE:HD13	1:D:589:ASN:HB3	1.88	0.56
1:D:583:ARG:HD3	1:D:1035:THR:HG23	1.87	0.55
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.88	0.55
1:D:1112:ILE:HD12	1:D:1175:ILE:HB	1.88	0.55
1:C:504:ILE:HD13	1:C:1042:MET:HE2	1.88	0.55
1:A:864:HIS:HD2	1:A:866:MET:H	1.54	0.55
1:B:900:LEU:HD23	1:B:921:MET:HE1	1.89	0.55
1:C:225:GLU:HB2	1:C:231:SER:HB3	1.89	0.55
1:A:335:ILE:HD11	1:A:375:GLN:HB3	1.89	0.55
1:D:1142:ALA:HB3	1:D:1145:MET:HB3	1.87	0.55
1:B:370:LEU:O	1:B:432:HIS:HE1	1.89	0.55
1:D:866:MET:CE	1:D:871:TYR:HA	2.36	0.55
1:C:528:SER:O	1:C:530:PRO:HD3	2.07	0.55
1:A:338:MET:HE3	1:A:373:ALA:HB1	1.89	0.55
1:B:309:THR:HG21	1:B:330:GLN:HE21	1.72	0.55
1:B:519:ARG:HB2	1:B:520:PRO:HD2	1.88	0.55
1:D:90:LEU:HD13	1:D:95:SER:HA	1.89	0.55
1:D:864:HIS:HD2	1:D:866:MET:H	1.54	0.55
1:A:860:GLU:HA	1:A:863:GLN:HE21	1.71	0.54
1:D:408:ASP:HB2	1:D:428:LYS:HB3	1.88	0.54
1:A:864:HIS:HD2	1:A:866:MET:HG3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:GLY:HA3	1:C:237:ARG:HH12	1.71	0.54
1:B:1097:ASN:HB2	1:B:1166:ASP:HA	1.89	0.54
1:A:58:GLU:HG3	1:C:445:ARG:HD3	1.90	0.54
1:A:519:ARG:HH22	1:A:847:ASP:CG	2.14	0.54
1:D:1053:ASP:OD2	1:D:1054:LYS:N	2.41	0.54
1:A:893:MET:O	1:A:897:VAL:HG23	2.07	0.54
1:D:575:GLN:NE2	1:D:610:ALA:H	2.05	0.54
1:B:398:ARG:HG2	1:B:1083:GLN:HE22	1.73	0.54
1:C:53:PHE:CZ	1:C:65:ALA:HB2	2.43	0.54
1:D:1159:GLN:HG2	1:D:1176:GLU:HG2	1.89	0.54
1:C:266:SER:O	1:C:478:THR:HA	2.08	0.54
1:C:717(A):ILE:HG12	1:C:957:ASN:HD21	1.73	0.53
1:C:575:GLN:HE22	1:C:610:ALA:H	1.55	0.53
1:A:44:ASN:ND2	1:A:45:ARG:H	1.99	0.53
1:B:606:MET:HE2	1:B:639:PHE:HB3	1.90	0.53
1:C:39:LYS:HG2	1:C:62:SER:HB3	1.89	0.53
1:D:1053:ASP:HB3	1:D:1056:LYS:HG2	1.90	0.53
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.18	0.53
1:C:167:ILE:HD11	1:C:323:ILE:HD13	1.91	0.53
1:C:396:ALA:HB3	1:C:453:ARG:HH12	1.73	0.53
1:D:846:SER:HA	1:D:849:GLU:HG2	1.90	0.53
1:B:999:GLN:HG2	1:B:1001:PRO:HD3	1.91	0.53
1:C:898:ASN:ND2	1:C:906:LYS:HE3	2.24	0.53
1:B:1053:ASP:HB3	1:B:1056:LYS:HG3	1.90	0.53
1:D:952:ILE:CG2	1:D:952:ILE:O	2.56	0.53
1:D:977:ARG:HG3	1:D:980:GLU:HG3	1.91	0.53
1:B:375:GLN:HG3	1:B:430:SER:HB3	1.89	0.53
1:D:917:MET:HG2	1:D:944:VAL:HG11	1.90	0.53
1:A:446:SER:O	1:A:450:MET:HG2	2.09	0.53
1:A:47:GLU:HB2	1:A:408:ASP:HB3	1.91	0.52
1:A:278:ALA:HB3	1:A:279:PRO:HD2	1.91	0.52
1:A:524:TYR:HD2	1:A:843:THR:CG2	2.22	0.52
1:B:44:ASN:HD22	1:B:45:ARG:N	1.87	0.52
1:B:341:GLY:O	1:D:434:ILE:HG12	2.09	0.52
1:B:435:SER:HB3	1:B:438:GLN:CB	2.39	0.52
1:D:44:ASN:ND2	1:D:45:ARG:H	1.94	0.52
1:D:391:THR:HG21	1:D:420:PRO:HG3	1.91	0.52
1:B:259:HIS:HB3	1:B:296:ILE:HD11	1.91	0.52
1:B:543:GLN:O	1:B:547:GLU:HG2	2.09	0.52
1:C:811:ASN:H	1:C:811:ASN:ND2	2.08	0.52
1:D:772:THR:HG22	1:D:783:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:GLU:HG2	1:C:210:GLU:H	1.75	0.52
1:C:948:PHE:HD2	1:C:964:GLN:HG3	1.75	0.52
1:D:257:ILE:HD12	1:D:300:GLU:HG3	1.92	0.52
1:D:575:GLN:HE22	1:D:610:ALA:H	1.57	0.52
1:D:1002:VAL:HG13	1:D:1006:ASP:HB2	1.92	0.52
1:B:574:HIS:HD2	1:B:580:THR:HA	1.75	0.52
1:B:905:VAL:HG12	1:B:907:VAL:HG23	1.91	0.52
1:C:644:ARG:O	1:C:645:ALA:C	2.52	0.52
1:D:717(A):ILE:HG13	1:D:957:ASN:HD21	1.75	0.52
1:C:929:GLN:HG2	1:C:932:ILE:HD12	1.92	0.52
1:D:446:SER:O	1:D:450:MET:HG2	2.10	0.52
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.08	0.52
1:D:715:ARG:HH12	1:D:865:GLU:CD	2.18	0.52
1:D:866:MET:HE2	1:D:871:TYR:HA	1.92	0.52
1:B:641:MET:HE3	1:B:674:PHE:CE1	2.45	0.51
1:A:44:ASN:HD22	1:A:45:ARG:N	1.99	0.51
1:A:641:MET:HG2	1:A:671:ILE:HG21	1.91	0.51
1:C:194:LYS:HB2	1:C:204:MET:HG2	1.92	0.51
1:C:409:ALA:HA	1:C:427:VAL:HG12	1.92	0.51
1:C:574:HIS:HD2	1:C:580:THR:HA	1.76	0.51
1:A:266:SER:O	1:A:478:THR:HA	2.10	0.51
1:A:606:MET:HE3	1:A:606:MET:H	1.76	0.51
1:A:622:ASN:ND2	1:A:624:TRP:H	2.08	0.51
1:C:884:GLY:O	1:C:885:GLU:HB3	2.11	0.51
1:A:402:GLY:HA3	1:C:54:ARG:HE	1.76	0.51
1:B:266:SER:HB2	1:B:476:TYR:CE2	2.45	0.51
1:C:1068:PRO:HG3	1:C:1074:ARG:HH11	1.76	0.51
1:B:41:LEU:O	1:B:42:VAL:HB	2.11	0.51
1:D:869:GLY:O	1:D:871:TYR:N	2.44	0.51
1:B:1042:MET:HE1	1:B:1060:ILE:HG21	1.92	0.51
1:A:856:SER:OG	1:D:800:SER:HA	2.11	0.51
1:B:672:ASP:HA	1:B:698:LYS:HD2	1.92	0.51
1:D:798:VAL:CG1	1:D:835:SER:HA	2.40	0.51
1:B:715:ARG:HE	1:B:715:ARG:C	2.19	0.50
1:C:913:VAL:HG22	1:C:943:SER:HB2	1.93	0.50
1:D:254:HIS:NE2	1:D:354:GLY:O	2.45	0.50
1:D:756:ILE:HD11	1:D:770:LEU:HD22	1.93	0.50
1:D:917:MET:HE1	1:D:940:PHE:HD2	1.75	0.50
1:A:665:GLU:OE1	1:A:668:LYS:HE3	2.12	0.50
1:B:404:GLY:O	1:B:431:THR:HA	2.11	0.50
1:B:776:SER:HB3	1:B:861:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:TYR:CD2	1:A:843:THR:CG2	2.95	0.50
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.44	0.50
1:B:90:LEU:HG	1:B:94:GLU:HB2	1.93	0.50
1:B:606:MET:HE1	1:B:671:ILE:CD1	2.41	0.50
1:D:470:LYS:HB2	1:D:480:PHE:CE1	2.44	0.50
1:D:879:LYS:HG3	1:D:884:GLY:HA3	1.94	0.50
1:B:811:ASN:HD22	1:B:811:ASN:N	2.09	0.50
1:C:257:ILE:HD13	1:C:300:GLU:HG3	1.94	0.50
1:C:1049:GLU:HG2	1:C:1059:ILE:HD12	1.93	0.50
1:D:606:MET:HE2	1:D:606:MET:O	2.11	0.50
1:B:570:PHE:O	1:B:574:HIS:HE1	1.94	0.50
1:B:755:LEU:O	1:B:759:LEU:HG	2.12	0.50
1:B:1153:PHE:CE1	1:B:1177:ILE:HG12	2.46	0.50
1:C:574:HIS:CD2	1:C:580:THR:HA	2.47	0.50
1:D:38:LYS:HA	1:D:38:LYS:HE2	1.92	0.50
1:C:396:ALA:HB3	1:C:453:ARG:NH1	2.26	0.50
1:C:707:THR:HG22	1:C:708:GLY:H	1.77	0.50
1:D:370:LEU:O	1:D:432:HIS:HE1	1.95	0.50
1:B:574:HIS:CD2	1:B:580:THR:HA	2.46	0.49
1:A:1093:ASN:ND2	1:A:1093:ASN:H	2.10	0.49
1:A:1005:GLN:HA	1:A:1008:ILE:HD11	1.92	0.49
1:C:622:ASN:HD21	1:C:624:TRP:HD1	1.59	0.49
1:C:223:GLU:O	1:C:227:SER:HB2	2.11	0.49
1:C:580:THR:HB	1:C:614:VAL:HG21	1.95	0.49
1:A:191:LEU:HD23	1:A:237:ARG:HA	1.93	0.49
1:D:574:HIS:CD2	1:D:580:THR:HA	2.47	0.49
1:D:1129:GLU:HB3	1:D:1157:ILE:HD12	1.93	0.49
1:A:249:VAL:HG11	1:A:299:MET:HG3	1.95	0.49
1:B:382:ASP:HB3	1:B:456:LYS:O	2.13	0.49
1:A:142:HIS:H	1:A:145:HIS:HD2	1.60	0.49
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.48	0.49
1:A:1120:VAL:HG23	1:A:1166:ASP:O	2.13	0.49
1:B:858:ASN:HD21	1:B:860:GLU:CG	2.25	0.48
1:C:54:ARG:HH11	1:C:54:ARG:HG3	1.75	0.48
1:A:290:ARG:HG2	1:A:320:PHE:CE1	2.47	0.48
1:C:419:SER:HB2	1:C:421:TYR:HD1	1.78	0.48
1:A:1000:GLY:N	1:A:1001:PRO:HD2	2.26	0.48
1:C:451:ARG:HG3	1:C:453:ARG:HH21	1.79	0.48
1:D:101:ARG:CG	1:D:101:ARG:NH2	2.73	0.48
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.95	0.48
1:D:811:ASN:H	1:D:811:ASN:ND2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ARG:HD3	1:A:605:GLU:OE1	2.12	0.48
1:B:826:THR:HG22	1:B:827:ASP:N	2.28	0.48
1:D:1158:LYS:HB2	1:D:1176:GLU:HG3	1.94	0.48
1:A:1042:MET:HE1	1:A:1060:ILE:CG2	2.44	0.48
1:B:1127:VAL:HA	1:B:1157:ILE:HG22	1.95	0.48
1:C:551:LYS:O	1:C:555:GLU:HG2	2.14	0.48
1:D:259:HIS:HD2	1:D:296:ILE:HD12	1.78	0.48
1:A:278:ALA:O	1:A:280:SER:N	2.47	0.48
1:B:571:ARG:C	1:B:571:ARG:HD2	2.39	0.48
1:B:1029:ASN:ND2	1:B:1031:SER:OG	2.46	0.48
1:C:550:PRO:HB2	1:C:736:HIS:CE1	2.48	0.48
1:C:913:VAL:HG13	1:C:944:VAL:HA	1.95	0.48
1:C:276:GLU:O	1:C:335:ILE:HD11	2.14	0.48
1:C:398:ARG:HH11	1:C:451:ARG:HE	1.62	0.48
1:C:667:ALA:HB1	1:C:698:LYS:HE3	1.95	0.48
1:A:631:ARG:HA	1:A:631:ARG:HD3	1.69	0.48
1:B:820:PHE:HB3	1:B:821:PRO:HD2	1.95	0.48
1:C:259:HIS:HB3	1:C:296:ILE:HD11	1.95	0.48
1:D:574:HIS:HD2	1:D:580:THR:HA	1.79	0.48
1:B:519:ARG:NH2	1:B:846:SER:OG	2.46	0.47
1:C:338:MET:CE	1:C:430:SER:HB3	2.44	0.47
1:C:1013:TYR:HB3	1:C:1016:VAL:HB	1.95	0.47
1:D:799:ALA:H	1:D:811:ASN:ND2	2.12	0.47
1:A:1115:GLN:H	1:A:1115:GLN:NE2	2.12	0.47
1:B:908:ALA:HB1	1:B:909:PRO:CD	2.25	0.47
1:A:812:SER:HB2	1:D:778:ASN:HD21	1.79	0.47
1:B:765:ASP:O	1:B:766:LEU:C	2.57	0.47
1:C:572:ASP:HB3	1:C:807:GLN:HE22	1.80	0.47
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.95	0.47
1:D:804:LEU:HD13	1:D:854:ILE:HG22	1.95	0.47
1:A:631:ARG:NH2	1:A:672:ASP:OD1	2.47	0.47
1:B:1024:ARG:HH11	1:B:1024:ARG:HB2	1.79	0.47
1:C:77:ARG:HD3	1:C:78:TYR:CE2	2.50	0.47
1:C:799:ALA:H	1:C:811:ASN:ND2	2.13	0.47
1:D:41:LEU:HB2	1:D:111:VAL:HG21	1.96	0.47
1:D:661:LYS:HB3	1:D:1008:ILE:HD13	1.95	0.47
1:D:1044:ASN:HD22	1:D:1062:LEU:HD22	1.79	0.47
1:A:409:ALA:HA	1:A:427:VAL:HG13	1.96	0.47
1:A:826:THR:OG1	1:A:827:ASP:N	2.48	0.47
1:B:569:THR:HA	1:B:573:ALA:HB3	1.96	0.47
1:C:71:ASP:C	1:C:73:SER:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:ASN:C	1:D:622:ASN:HD22	2.22	0.47
1:A:384:LEU:HD11	1:A:490:ILE:HD11	1.96	0.47
1:C:263:ARG:HG2	1:C:278:ALA:HB2	1.96	0.47
1:C:263:ARG:HH21	1:C:330:GLN:HE21	1.63	0.47
1:C:494:LEU:HB2	1:C:496:ARG:HH11	1.80	0.47
1:D:928:GLU:O	1:D:931:VAL:HG12	2.14	0.47
1:A:496:ARG:HD2	1:A:1052:ILE:HD13	1.96	0.47
1:B:141:PRO:HB2	1:B:145:HIS:HB2	1.96	0.47
1:D:477:THR:HG23	1:D:479:LYS:H	1.79	0.47
1:D:879:LYS:C	1:D:881:LEU:H	2.22	0.47
1:D:895:ARG:HE	1:D:899:PHE:HE1	1.61	0.47
1:D:912:LYS:NZ	1:D:916:ASP:OD1	2.48	0.47
1:D:1087:ILE:HG22	1:D:1088:TYR:N	2.30	0.47
1:A:596:ASP:O	1:A:599:LYS:HG2	2.15	0.47
1:A:1093:ASN:H	1:A:1093:ASN:HD22	1.63	0.47
1:B:700:SER:H	1:B:736:HIS:CD2	2.20	0.47
1:B:909:PRO:HB2	1:B:952:ILE:HG12	1.97	0.47
1:B:1097:ASN:C	1:B:1099:ASN:H	2.23	0.47
1:D:743:MET:CG	1:D:907:VAL:HG13	2.44	0.47
1:A:460:PRO:HA	1:A:463:ILE:HD12	1.96	0.47
1:A:672:ASP:HA	1:A:698:LYS:HD2	1.97	0.47
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.25	0.46
1:A:521:LYS:HA	1:A:522:PRO:HD3	1.82	0.46
1:B:537:ILE:HA	1:B:538(B):PHE:CD1	2.50	0.46
1:B:558:LYS:HE3	1:B:767:PRO:HD3	1.96	0.46
1:D:566:THR:HB	1:D:795:ASP:OD1	2.16	0.46
1:B:251:GLY:O	1:B:306:ASN:N	2.47	0.46
1:A:1120:VAL:HG21	1:A:1162:VAL:HB	1.97	0.46
1:C:960:ASN:HB3	1:C:963:LEU:HB3	1.96	0.46
1:D:622:ASN:ND2	1:D:624:TRP:H	2.13	0.46
1:A:41:LEU:HD13	1:A:106:ALA:HB2	1.97	0.46
1:B:258:VAL:HG22	1:B:357:LEU:HD11	1.96	0.46
1:C:968:LEU:O	1:C:969:LYS:C	2.58	0.46
1:D:569:THR:HG23	1:D:801:MET:HG3	1.98	0.46
1:D:828:ILE:O	1:D:832:GLU:HG2	2.16	0.46
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.80	0.46
1:B:583:ARG:HG2	1:B:619:LEU:HD22	1.97	0.46
1:C:290:ARG:NH2	1:C:318:ASP:O	2.49	0.46
1:A:644:ARG:HG2	1:A:647:ASN:OD1	2.16	0.46
1:A:711:LEU:HD21	1:A:750:LYS:HB3	1.98	0.46
1:C:44:ASN:ND2	1:C:45:ARG:H	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1108:ASN:CB	1:D:1109:PRO:HD3	2.44	0.46
1:A:606:MET:HE3	1:A:640:GLN:O	2.16	0.46
1:D:631:ARG:HA	1:D:631:ARG:HD3	1.72	0.46
1:A:1029:ASN:C	1:A:1029:ASN:HD22	2.23	0.46
1:A:1042:MET:HE1	1:A:1060:ILE:HG21	1.98	0.46
1:B:864:HIS:CD2	1:B:866:MET:H	2.31	0.46
1:C:313:LEU:HD13	1:C:323:ILE:HG13	1.98	0.46
1:A:436:PHE:O	1:A:440:GLU:HB2	2.15	0.45
1:A:749:PRO:HG3	1:A:781:LEU:HB3	1.98	0.45
1:B:624:TRP:HB3	1:B:1005:GLN:NE2	2.31	0.45
1:C:931:VAL:HA	1:C:935:GLY:H	1.81	0.45
1:A:214:GLU:O	1:A:214:GLU:HG2	2.16	0.45
1:B:244:HIS:CD2	1:B:265:CYS:HB2	2.50	0.45
1:B:1123:VAL:HG12	1:B:1164:ASN:OD1	2.15	0.45
1:D:398:ARG:HH21	1:D:449:GLU:HG2	1.81	0.45
1:A:274:VAL:HG12	1:A:275:VAL:HG23	1.97	0.45
1:B:558:LYS:NZ	1:B:765:ASP:HB3	2.32	0.45
1:B:1053:ASP:HB3	1:B:1056:LYS:CG	2.45	0.45
1:A:739:ALA:HA	1:A:769:HIS:O	2.17	0.45
1:B:1177:ILE:HD13	1:B:1177:ILE:N	2.31	0.45
1:D:145:HIS:CE1	1:D:304:TYR:HA	2.51	0.45
1:A:209:GLU:HG3	1:A:210:GLU:H	1.79	0.45
1:B:357(B):GLY:C	1:B:359:GLU:H	2.24	0.45
1:B:606:MET:HE1	1:B:671:ILE:HD13	1.98	0.45
1:A:563:VAL:HG21	1:A:787:ILE:HG12	1.98	0.45
1:B:144:GLU:O	1:B:148:MET:HB2	2.16	0.45
1:B:804:LEU:HD13	1:B:854:ILE:HG22	1.99	0.45
1:A:278:ALA:HB3	1:A:373:ALA:H	1.80	0.45
1:B:575:GLN:HE22	1:B:610:ALA:H	1.63	0.45
1:C:575:GLN:NE2	1:C:610:ALA:H	2.14	0.45
1:C:927:ASP:O	1:C:930:SER:HB2	2.17	0.45
1:D:67:TYR:CD1	1:D:77:ARG:HG3	2.52	0.45
1:A:589:ASN:HD22	1:A:589:ASN:HA	1.61	0.45
1:A:606:MET:HE1	1:A:671:ILE:CD1	2.47	0.45
1:B:796:THR:HB	1:B:810:ALA:HB2	1.99	0.45
1:D:875:SER:HA	1:D:887:PHE:CE1	2.51	0.45
1:A:141:PRO:HB2	1:A:145:HIS:HB2	1.99	0.45
1:A:799:ALA:H	1:A:811:ASN:HD21	1.63	0.45
1:B:51:ARG:HD3	1:B:406:ARG:HH22	1.82	0.45
1:A:331:VAL:HG23	1:A:332:GLU:OE2	2.17	0.45
1:B:141:PRO:HB2	1:B:145:HIS:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:GLY:H	1:A:543:GLN:HE21	1.64	0.44
1:C:342:ILE:HG12	1:C:362:MET:CE	2.46	0.44
1:C:641:MET:HB3	1:C:671:ILE:HD12	1.99	0.44
1:D:263:ARG:HH21	1:D:330:GLN:HE21	1.64	0.44
1:D:858:ASN:HD21	1:D:860:GLU:HB2	1.81	0.44
1:B:413:PHE:HE1	1:B:416:ALA:HB3	1.82	0.44
1:C:749:PRO:HG3	1:C:781:LEU:HB3	2.00	0.44
1:D:162:ALA:HB2	1:D:301:ASN:HD22	1.82	0.44
1:B:41:LEU:HB3	1:B:114:ILE:HG12	1.99	0.44
1:C:893:MET:HE2	1:C:921:MET:HB2	1.99	0.44
1:D:896:ARG:HD2	1:D:928:GLU:OE1	2.17	0.44
1:A:731:GLU:HG3	1:A:766:LEU:HD13	2.00	0.44
1:A:888:ASP:HA	1:A:891:LYS:HE3	2.00	0.44
1:B:522:PRO:HB2	1:B:523:ASP:H	1.66	0.44
1:B:641:MET:HE3	1:B:674:PHE:HE1	1.82	0.44
1:B:858:ASN:HD21	1:B:860:GLU:HG2	1.83	0.44
1:C:313:LEU:HD11	4:C:2100:ADP:H2'	2.00	0.44
1:D:116:PRO:HB2	1:D:122:SER:HA	2.00	0.44
1:A:144:GLU:CD	1:A:144:GLU:H	2.25	0.44
1:B:391:THR:HG23	1:B:420:PRO:HD3	1.98	0.44
1:B:597:VAL:HG22	1:B:830:GLY:HA3	1.99	0.44
1:B:631:ARG:HA	1:B:631:ARG:HD3	1.47	0.44
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.50	0.44
1:A:551:LYS:O	1:A:555:GLU:HG2	2.18	0.44
1:C:854:ILE:H	1:C:854:ILE:HG13	1.63	0.44
1:D:700:SER:H	1:D:736:HIS:CD2	2.19	0.44
1:A:350:LEU:HD13	1:A:359:GLU:HB3	2.00	0.44
1:B:40:LEU:HD11	1:B:349:ILE:HD12	2.00	0.44
1:D:641:MET:HB3	1:D:671:ILE:HD12	1.99	0.44
1:A:631:ARG:HG2	1:A:670:GLY:HA3	2.00	0.44
1:C:152:LYS:HG3	1:C:197:SER:N	2.30	0.44
1:A:195:ALA:HA	1:A:233:VAL:HG12	1.99	0.43
1:A:501:LEU:HD21	1:A:1080:MET:HG3	2.00	0.43
1:B:715:ARG:NH1	1:B:865:GLU:OE2	2.47	0.43
1:C:378:ILE:HB	1:C:427:VAL:HG23	2.00	0.43
1:C:606:MET:HE2	1:C:639:PHE:CB	2.38	0.43
1:C:918:ALA:O	1:C:922:VAL:HG23	2.19	0.43
1:D:739:ALA:HA	1:D:769:HIS:O	2.19	0.43
1:A:376:CYS:HB2	1:A:462:LEU:HD22	1.99	0.43
1:A:622:ASN:HD22	1:A:622:ASN:C	2.25	0.43
1:B:357:LEU:O	1:B:362:MET:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:775:THR:HG22	1:C:861:ILE:HG13	2.00	0.43
1:D:752:ALA:HB2	1:D:782:THR:HG23	2.00	0.43
1:A:434:ILE:H	1:A:434:ILE:HG13	1.56	0.43
1:C:580:THR:O	1:C:614:VAL:HG11	2.18	0.43
1:A:647:ASN:O	1:A:649:VAL:N	2.52	0.43
1:B:506:ASN:ND2	1:B:510:ASN:ND2	2.65	0.43
1:B:907:VAL:HB	1:B:908:ALA:H	1.58	0.43
1:C:1090:LYS:HE2	1:C:1090:LYS:HB3	1.77	0.43
1:B:241:ASN:HB2	1:B:477:THR:HG21	2.01	0.43
1:B:565:LEU:HD23	1:B:824:LEU:HD22	2.00	0.43
1:B:828:ILE:O	1:B:831:MET:HB2	2.19	0.43
1:B:1029:ASN:C	1:B:1029:ASN:HD22	2.26	0.43
1:D:655:PRO:HG3	1:D:985:VAL:HG23	1.99	0.43
1:B:913:VAL:HG22	1:B:943:SER:HB2	2.01	0.43
1:C:144:GLU:O	1:C:148:MET:HB2	2.19	0.43
1:C:704:ILE:HG21	1:C:723:TYR:HD2	1.84	0.43
1:C:434:ILE:H	1:C:434:ILE:HG13	1.67	0.43
1:D:655:PRO:CG	1:D:985:VAL:HG23	2.48	0.43
1:A:641:MET:HE3	1:A:674:PHE:CE1	2.54	0.43
1:B:245:ILE:HD13	1:B:264:ASP:HA	2.00	0.43
1:B:631:ARG:NH1	1:B:634:ILE:O	2.52	0.43
1:B:1078:TYR:HB2	1:B:1085:ARG:HB3	2.01	0.43
1:B:989:LYS:HA	1:B:992:GLU:HB2	2.01	0.43
1:C:960:ASN:CB	1:C:963:LEU:HB3	2.49	0.43
2:C:2000:BTI:H5	1:D:512:PHE:CZ	2.54	0.43
1:D:1052:ILE:HD13	1:D:1058:LEU:HB2	2.00	0.43
1:A:42:VAL:HG11	1:A:49:ALA:HA	2.01	0.42
1:B:1027:TYR:HB3	1:B:1030:LEU:HD21	2.00	0.42
1:C:142:HIS:H	1:C:145:HIS:HD2	1.67	0.42
1:C:584:THR:O	1:C:588:ILE:HG12	2.19	0.42
1:D:501:LEU:CD1	1:D:1085:ARG:HG2	2.49	0.42
1:A:656:ASP:OD1	1:A:688:VAL:HG21	2.19	0.42
1:A:811:ASN:ND2	1:A:811:ASN:H	2.12	0.42
1:D:326:ASN:HA	1:D:327:PRO:HD3	1.91	0.42
1:A:406:ARG:HA	1:A:406:ARG:NE	2.34	0.42
1:B:558:LYS:HG3	1:B:767:PRO:HG3	2.01	0.42
1:B:828:ILE:H	1:B:828:ILE:HG13	1.37	0.42
1:D:1113:GLY:HA2	1:D:1172:ASP:O	2.19	0.42
1:A:313:LEU:HB2	1:A:323:ILE:HD11	2.02	0.42
1:B:39:LYS:HD2	1:B:109:ALA:O	2.19	0.42
1:C:382:ASP:HA	1:C:383:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1153:PHE:HB3	1:D:1154:ASP:H	1.60	0.42
1:A:1060:ILE:HG12	1:A:1080:MET:HG2	2.02	0.42
1:C:937:LYS:H	1:C:937:LYS:HG3	1.64	0.42
1:D:641:MET:HG2	1:D:671:ILE:HG21	2.01	0.42
1:A:607:TRP:HE3	1:A:641:MET:HE2	1.83	0.42
1:A:678:ASP:OD2	1:A:685:GLN:NE2	2.51	0.42
1:A:1050:ILE:HD12	1:A:1060:ILE:HD12	2.02	0.42
1:B:69:ASN:HD22	1:B:69:ASN:HA	1.67	0.42
1:B:379:THR:HG22	1:B:425:LEU:HA	2.02	0.42
1:C:302:ILE:H	1:C:302:ILE:HG13	1.77	0.42
1:C:917:MET:SD	1:C:944:VAL:HG21	2.60	0.42
1:A:796:THR:HB	1:A:810:ALA:HB2	2.02	0.42
1:A:935:GLY:HA3	1:A:966:VAL:HG13	2.01	0.42
1:B:391:THR:HB	1:B:392:GLY:H	1.65	0.42
1:B:787:ILE:HD13	1:B:817:LEU:HD11	2.01	0.42
1:D:737:ILE:HG12	1:D:767:PRO:HG2	2.01	0.42
1:A:41:LEU:HB3	1:A:114:ILE:HG12	2.02	0.42
1:C:370:LEU:O	1:C:432:HIS:HE1	2.02	0.42
1:D:77:ARG:HD3	1:D:78:TYR:CE2	2.55	0.42
1:D:92:PRO:HD2	1:D:94:GLU:HG2	2.02	0.42
1:D:1060:ILE:HG12	1:D:1080:MET:HG2	2.01	0.42
1:A:1131:VAL:HB	1:A:1135:GLN:CD	2.45	0.42
1:D:712:ASN:HA	1:D:713:PRO:HD2	1.95	0.42
1:A:1151:ALA:HA	1:A:1152:PRO:HD3	1.89	0.42
1:B:870:GLN:HA	1:B:873:ASN:HD22	1.84	0.42
1:C:408:ASP:HB2	1:C:428:LYS:HB3	2.01	0.42
1:A:773:HIS:ND1	1:A:805:THR:O	2.39	0.41
1:B:436:PHE:O	1:B:440:GLU:HB2	2.19	0.41
1:C:338:MET:HE1	1:C:430:SER:HB3	2.02	0.41
1:D:622:ASN:HD22	1:D:623:PRO:N	2.18	0.41
1:B:39:LYS:HG3	1:B:111:VAL:HA	2.02	0.41
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.85	0.41
1:A:622:ASN:HD21	1:A:624:TRP:HD1	1.68	0.41
1:A:828:ILE:H	1:A:828:ILE:HG13	1.60	0.41
1:A:1004:GLU:HA	1:A:1007:ILE:HD12	2.01	0.41
1:B:434:ILE:H	1:B:434:ILE:HG13	1.67	0.41
1:C:972:GLU:HB2	1:C:973:ALA:H	1.58	0.41
1:A:364:GLN:HA	1:A:367:ILE:HD12	2.02	0.41
1:A:606:MET:HE1	1:A:671:ILE:HD12	2.01	0.41
1:B:77:ARG:HG2	1:B:77:ARG:NH1	2.15	0.41
1:B:309:THR:HG21	1:B:330:GLN:NE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:934:ASP:HB2	1:B:937:LYS:HE2	2.03	0.41
1:C:641:MET:HE3	1:C:674:PHE:CE1	2.55	0.41
1:D:263:ARG:HG2	1:D:278:ALA:HB2	2.01	0.41
1:D:1105:ASP:HB3	1:D:1111:HIS:ND1	2.35	0.41
1:A:89:ASP:HB2	1:A:101:ARG:HH12	1.84	0.41
1:A:818:ASN:N	1:A:818:ASN:HD22	2.18	0.41
1:D:334:THR:HB	1:D:338:MET:HE3	2.03	0.41
1:D:570:PHE:O	1:D:574:HIS:CE1	2.62	0.41
1:D:582:VAL:HA	1:D:845:TYR:CZ	2.56	0.41
1:D:622:ASN:HD22	1:D:623:PRO:CD	2.34	0.41
1:A:1115:GLN:H	1:A:1115:GLN:CD	2.27	0.41
1:B:45:ARG:HD2	1:B:71:ASP:OD2	2.21	0.41
1:B:145:HIS:HE1	1:B:302:ILE:O	2.03	0.41
1:C:44:ASN:HD22	1:C:45:ARG:N	1.98	0.41
1:C:334:THR:O	1:C:338:MET:HG3	2.21	0.41
1:D:946:SER:OG	1:D:951:GLU:OE1	2.31	0.41
1:D:951:GLU:O	1:D:952:ILE:HD13	2.20	0.41
1:A:1157:ILE:HG13	1:A:1177:ILE:HG12	2.03	0.41
1:B:622:ASN:HD21	1:B:624:TRP:CD1	2.34	0.41
1:C:274:VAL:HG12	1:C:275:VAL:HG23	2.01	0.41
1:C:798:VAL:O	1:C:799:ALA:C	2.63	0.41
1:A:388:MET:HA	1:A:389:PRO:HD3	1.81	0.41
1:B:66:ILE:O	1:B:66:ILE:HG13	2.20	0.41
1:B:137:LYS:HA	1:B:137:LYS:HD2	1.84	0.41
1:B:349:ILE:H	1:B:349:ILE:HG12	1.73	0.41
1:B:977:ARG:NH1	1:B:980:GLU:HB3	2.35	0.41
1:C:91:GLY:HA3	1:C:92:PRO:HD3	1.78	0.41
1:C:252:ASP:HB3	1:C:357:LEU:HD13	2.03	0.41
1:C:406:ARG:NH1	1:C:408:ASP:OD1	2.54	0.41
1:C:556:TRP:O	1:C:560:GLN:HG2	2.21	0.41
1:C:571:ARG:HH11	1:C:575:GLN:NE2	2.18	0.41
1:D:382:ASP:HA	1:D:383:PRO:HD2	1.87	0.41
1:D:406:ARG:NH2	1:D:408:ASP:OD1	2.53	0.41
1:D:427:VAL:HG21	1:D:450:MET:HE1	2.03	0.41
1:D:866:MET:HE1	1:D:871:TYR:HA	2.02	0.41
1:D:869:GLY:O	1:D:870:GLN:C	2.63	0.41
1:D:960:ASN:HD21	1:D:962:ASP:HB2	1.86	0.41
1:D:1076:ILE:HD12	1:D:1089:ILE:HD13	2.03	0.41
1:A:241:ASN:N	1:A:242:PRO:HD3	2.36	0.41
1:A:524:TYR:CE2	1:A:843:THR:HG22	2.56	0.41
1:B:647:ASN:O	1:B:649:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:LYS:H	1:D:365:LYS:HG2	1.66	0.41
1:D:459:ILE:HB	1:D:460:PRO:HD3	2.03	0.41
1:D:1087:ILE:CG2	1:D:1088:TYR:N	2.84	0.41
1:A:524:TYR:HD2	1:A:843:THR:HG21	1.85	0.40
1:C:230:ASN:HD22	1:C:232:GLU:H	1.68	0.40
1:C:907:VAL:O	1:C:910:SER:N	2.55	0.40
1:D:263:ARG:HH21	1:D:330:GLN:NE2	2.19	0.40
1:D:289:GLN:HE21	1:D:289:GLN:HA	1.85	0.40
1:A:587:MET:O	1:A:590:ILE:HD12	2.21	0.40
1:C:448:ARG:HH22	1:C:467:LYS:HE3	1.86	0.40
1:D:870:GLN:O	1:D:871:TYR:C	2.64	0.40
1:B:394:ILE:H	1:B:394:ILE:HG13	1.76	0.40
1:D:755:LEU:O	1:D:759:LEU:HG	2.20	0.40
1:D:820:PHE:HB3	1:D:821:PRO:CD	2.52	0.40
1:D:885:GLU:HA	1:D:885:GLU:OE2	2.22	0.40
1:A:156:ARG:HB3	1:A:156:ARG:HH11	1.86	0.40
1:D:494:LEU:HD23	1:D:495:ASP:N	2.37	0.40
1:D:673:VAL:HG22	1:D:699:ILE:HD12	2.03	0.40
1:D:828:ILE:H	1:D:828:ILE:HG13	1.57	0.40
1:A:99:ILE:HG23	1:A:127:PHE:CD1	2.45	0.40
1:B:582:VAL:HA	1:B:845:TYR:CZ	2.56	0.40
1:B:1050:ILE:HD12	1:B:1060:ILE:HD12	2.04	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	1125/1150 (98%)	1034 (92%)	76 (7%)	15 (1%)	9	23
1	B	1070/1150 (93%)	981 (92%)	75 (7%)	14 (1%)	9	23
1	C	1063/1150 (92%)	968 (91%)	79 (7%)	16 (2%)	8	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1061/1150 (92%)	985 (93%)	70 (7%)	6 (1%)	21	42
All	All	4319/4600 (94%)	3968 (92%)	300 (7%)	51 (1%)	10	25

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	SER
1	A	278	ALA
1	A	648	ALA
1	B	909	PRO
1	B	1001	PRO
1	C	92	PRO
1	C	168	PRO
1	D	92	PRO
1	D	870	GLN
1	A	209	GLU
1	A	999	GLN
1	A	1000	GLY
1	B	391	THR
1	B	518	LYS
1	B	522	PRO
1	B	766	LEU
1	B	907	VAL
1	C	87	GLY
1	C	199	GLY
1	C	518	LYS
1	C	645	ALA
1	D	868	GLY
1	A	195	ALA
1	A	213	LEU
1	A	518	LYS
1	A	868	GLY
1	A	1081	ASN
1	B	162	ALA
1	B	648	ALA
1	B	903	ASP
1	C	184	ALA
1	C	189	PHE
1	C	197	SER
1	D	1108	ASN
1	A	210	GLU
1	B	42	VAL

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Mol	Chain	Res	Type
1	B	1002	VAL
1	B	1098	ALA
1	C	425	LEU
1	C	885	GLU
1	D	317	GLY
1	D	648	ALA
1	A	1097	ASN
1	C	648	ALA
1	A	1094	VAL
1	C	91	GLY
1	B	87	GLY
1	C	190	PRO
1	C	1014	PRO
1	A	434	ILE
1	C	1001	PRO

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	974/986 (99%)	887 (91%)	87 (9%)	9	22
1	B	927/986 (94%)	859 (93%)	68 (7%)	13	30
1	C	916/986 (93%)	834 (91%)	82 (9%)	9	21
1	D	921/986 (93%)	850 (92%)	71 (8%)	12	28
All	All	3738/3944 (95%)	3430 (92%)	308 (8%)	10	25

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	60	ASP
1	A	62	SER
1	A	69	ASN
1	A	108	GLN
1	A	122	SER

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Mol	Chain	Res	Type
1	A	144	GLU
1	A	156	ARG
1	A	166	VAL
1	A	167	ILE
1	A	181	LYS
1	A	193	ILE
1	A	207	VAL
1	A	208	ARG
1	A	209	GLU
1	A	210	GLU
1	A	213	LEU
1	A	214	GLU
1	A	241	ASN
1	A	281	VAL
1	A	287	LEU
1	A	329	VAL
1	A	331	VAL
1	A	342	ILE
1	A	368	THR
1	A	394	ILE
1	A	417	GLU
1	A	423	ASP
1	A	427	VAL
1	A	434	ILE
1	A	444	VAL
1	A	455	VAL
1	A	518	LYS
1	A	519	ARG
1	A	525	GLU
1	A	526	LEU
1	A	528	SER
1	A	542	LYS
1	A	551	LYS
1	A	571	ARG
1	A	580	THR
1	A	588	ILE
1	A	590	ILE
1	A	606	MET
1	A	607	TRP
1	A	631	ARG
1	A	707	THR
1	A	715	ARG

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Mol	Chain	Res	Type
1	A	743	MET
1	A	750	LYS
1	A	761	SER
1	A	766	LEU
1	A	772	THR
1	A	775	THR
1	A	794	ILE
1	A	811	ASN
1	A	812	SER
1	A	828	ILE
1	A	831	MET
1	A	855	LYS
1	A	856	SER
1	A	861	ILE
1	A	863	GLN
1	A	907	VAL
1	A	919	LEU
1	A	926	LEU
1	A	931	VAL
1	A	944	VAL
1	A	945	VAL
1	A	966	VAL
1	A	980	GLU
1	A	991	ARG
1	A	999	GLN
1	A	1002	VAL
1	A	1008	ILE
1	A	1051	GLU
1	A	1064	THR
1	A	1080	MET
1	A	1085	ARG
1	A	1089	ILE
1	A	1090	LYS
1	A	1093	ASN
1	A	1115	GLN
1	A	1116	MET
1	A	1131	VAL
1	A	1145	MET
1	A	1148	THR
1	B	40	LEU
1	B	44	ASN
1	B	52	ILE

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Mol	Chain	Res	Type
1	B	69	ASN
1	B	75	LEU
1	B	77	ARG
1	B	95	SER
1	B	110	ASN
1	B	154	LYS
1	B	157	THR
1	B	167	ILE
1	B	241	ASN
1	B	249	VAL
1	B	250	ILE
1	B	288	ARG
1	B	329	VAL
1	B	335	ILE
1	B	357	LEU
1	B	357(A)	PHE
1	B	377	ARG
1	B	391	THR
1	B	394	ILE
1	B	407	LEU
1	B	417	GLU
1	B	434	ILE
1	B	442	LYS
1	B	458	ASN
1	B	461	PHE
1	B	496	ARG
1	B	523	ASP
1	B	524	TYR
1	B	528	SER
1	B	580	THR
1	B	588	ILE
1	B	589	ASN
1	B	606	MET
1	B	607	TRP
1	B	631	ARG
1	B	649	VAL
1	B	660	HIS
1	B	715	ARG
1	B	743	MET
1	B	750	LYS
1	B	781	LEU
1	B	784	LYS

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Mol	Chain	Res	Type
1	B	794	ILE
1	B	811	ASN
1	B	828	ILE
1	B	855	LYS
1	B	870	GLN
1	B	880	SER
1	B	907	VAL
1	B	926	LEU
1	B	945	VAL
1	B	952	ILE
1	B	986	ASP
1	B	991	ARG
1	B	996	GLU
1	B	1008	ILE
1	B	1011	VAL
1	B	1024	ARG
1	B	1051	GLU
1	B	1097	ASN
1	B	1124	LYS
1	B	1147	THR
1	B	1148	THR
1	B	1175	ILE
1	B	1177	ILE
1	C	44	ASN
1	C	54	ARG
1	C	60	ASP
1	C	86	VAL
1	C	97	LEU
1	C	112	ASP
1	C	125	GLU
1	C	174	ILE
1	C	179	LEU
1	C	185	GLU
1	C	193	ILE
1	C	196	THR
1	C	227	SER
1	C	230	ASN
1	C	249	VAL
1	C	250	ILE
1	C	257	ILE
1	C	262	GLU
1	C	287	LEU

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Mol	Chain	Res	Type
1	C	313	LEU
1	C	329	VAL
1	C	335	ILE
1	C	342	ILE
1	C	368	THR
1	C	388	MET
1	C	406	ARG
1	C	417	GLU
1	C	427	VAL
1	C	434	ILE
1	C	437	LYS
1	C	445	ARG
1	C	472	THR
1	C	494	LEU
1	C	515	ASN
1	C	519	ARG
1	C	526	LEU
1	C	531	THR
1	C	535	SER
1	C	542	LYS
1	C	543	GLN
1	C	580	THR
1	C	592	SER
1	C	607	TRP
1	C	637	VAL
1	C	641	MET
1	C	649	VAL
1	C	707	THR
1	C	717	ASN
1	C	717(A)	ILE
1	C	719	THR
1	C	721	GLU
1	C	743	MET
1	C	756	ILE
1	C	768	ILE
1	C	780	LEU
1	C	781	LEU
1	C	807	GLN
1	C	811	ASN
1	C	828	ILE
1	C	843	THR
1	C	854	ILE

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Mol	Chain	Res	Type
1	C	855	LYS
1	C	866	MET
1	C	888	ASP
1	C	906	LYS
1	C	907	VAL
1	C	931	VAL
1	C	937	LYS
1	C	942	GLU
1	C	952	ILE
1	C	959	PHE
1	C	960	ASN
1	C	969	LYS
1	C	971	GLN
1	C	972	GLU
1	C	999	GLN
1	C	1008	ILE
1	C	1022	GLN
1	C	1052	ILE
1	C	1054	LYS
1	C	1085	ARG
1	C	1147	THR
1	D	44	ASN
1	D	60	ASP
1	D	62	SER
1	D	101	ARG
1	D	122	SER
1	D	239	ILE
1	D	262	GLU
1	D	288	ARG
1	D	289	GLN
1	D	296	ILE
1	D	329	VAL
1	D	335	ILE
1	D	414	GLN
1	D	419	SER
1	D	427	VAL
1	D	434	ILE
1	D	455	VAL
1	D	469	LYS
1	D	519	ARG
1	D	523	ASP
1	D	525	GLU

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Mol	Chain	Res	Type
1	D	531	THR
1	D	542	LYS
1	D	580	THR
1	D	588	ILE
1	D	590	ILE
1	D	607	TRP
1	D	620	LYS
1	D	629	ARG
1	D	631	ARG
1	D	647	ASN
1	D	649	VAL
1	D	707	THR
1	D	715	ARG
1	D	743	MET
1	D	750	LYS
1	D	760	LYS
1	D	766	LEU
1	D	775	THR
1	D	781	LEU
1	D	807	GLN
1	D	811	ASN
1	D	828	ILE
1	D	831	MET
1	D	843	THR
1	D	853	ASP
1	D	855	LYS
1	D	856	SER
1	D	870	GLN
1	D	895	ARG
1	D	907	VAL
1	D	917	MET
1	D	919	LEU
1	D	925	ASP
1	D	926	LEU
1	D	944	VAL
1	D	945	VAL
1	D	949	LYS
1	D	952	ILE
1	D	996	GLU
1	D	1002	VAL
1	D	1052	ILE
1	D	1054	LYS

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Mol	Chain	Res	Type
1	D	1056	LYS
1	D	1064	THR
1	D	1080	MET
1	D	1089	ILE
1	D	1123	VAL
1	D	1161	THR
1	D	1162	VAL
1	D	1177	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	110	ASN
1	A	145	HIS
1	A	241	ASN
1	A	244	HIS
1	A	254	HIS
1	A	326	ASN
1	A	330	GLN
1	A	361	ASN
1	A	363	GLN
1	A	432	HIS
1	A	506	ASN
1	A	543	GLN
1	A	574	HIS
1	A	575	GLN
1	A	589	ASN
1	A	617	ASN
1	A	622	ASN
1	A	736	HIS
1	A	778	ASN
1	A	807	GLN
1	A	811	ASN
1	A	818	ASN
1	A	823	HIS
1	A	858	ASN
1	A	863	GLN
1	A	864	HIS
1	A	898	ASN
1	A	923	GLN
1	A	957	ASN

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Mol	Chain	Res	Type
1	A	1005	GLN
1	A	1019	GLN
1	A	1025	ASN
1	A	1029	ASN
1	A	1044	ASN
1	A	1093	ASN
1	A	1095	HIS
1	A	1108	ASN
1	A	1135	GLN
1	B	44	ASN
1	B	69	ASN
1	B	145	HIS
1	B	244	HIS
1	B	256	ASN
1	B	297	GLN
1	B	330	GLN
1	B	385	ASN
1	B	414	GLN
1	B	432	HIS
1	B	438	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	736	HIS
1	B	773	HIS
1	B	778	ASN
1	B	811	ASN
1	B	818	ASN
1	B	858	ASN
1	B	864	HIS
1	B	873	ASN
1	B	877	GLN
1	B	898	ASN
1	B	971	GLN
1	B	1005	GLN
1	B	1019	GLN
1	B	1025	ASN
1	B	1029	ASN

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Mol	Chain	Res	Type
1	B	1044	ASN
1	B	1073	ASN
1	B	1081	ASN
1	B	1083	GLN
1	B	1111	HIS
1	C	44	ASN
1	C	69	ASN
1	C	108	GLN
1	C	145	HIS
1	C	230	ASN
1	C	256	ASN
1	C	289	GLN
1	C	326	ASN
1	C	330	GLN
1	C	361	ASN
1	C	432	HIS
1	C	506	ASN
1	C	574	HIS
1	C	575	GLN
1	C	589	ASN
1	C	617	ASN
1	C	622	ASN
1	C	653	ASN
1	C	685	GLN
1	C	690	ASN
1	C	694	GLN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	807	GLN
1	C	811	ASN
1	C	873	ASN
1	C	876	GLN
1	C	877	GLN
1	C	898	ASN
1	C	957	ASN
1	C	971	GLN
1	C	1029	ASN
1	D	44	ASN
1	D	98	ASN
1	D	126	GLN
1	D	145	HIS

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Mol	Chain	Res	Type
1	D	289	GLN
1	D	301	ASN
1	D	326	ASN
1	D	330	GLN
1	D	361	ASN
1	D	364	GLN
1	D	375	GLN
1	D	385	ASN
1	D	432	HIS
1	D	468	ASN
1	D	506	ASN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	589	ASN
1	D	622	ASN
1	D	647	ASN
1	D	736	HIS
1	D	778	ASN
1	D	811	ASN
1	D	818	ASN
1	D	823	HIS
1	D	858	ASN
1	D	863	GLN
1	D	864	HIS
1	D	898	ASN
1	D	957	ASN
1	D	960	ASN
1	D	1005	GLN
1	D	1025	ASN
1	D	1044	ASN
1	D	1083	GLN
1	D	1115	GLN
1	D	1164	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	D	2000	1	15,16,16	1.74	2 (13%)	20,21,21	1.89	3 (15%)
2	BTI	B	2000	1	15,16,16	1.65	2 (13%)	20,21,21	2.00	7 (35%)
2	BTI	C	2000	1	15,16,16	1.73	2 (13%)	20,21,21	1.76	3 (15%)
4	ADP	C	2100	-	28,29,29	1.45	4 (14%)	43,45,45	1.87	8 (18%)
2	BTI	A	2000	1	15,16,16	1.66	2 (13%)	20,21,21	2.13	3 (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	BTI	D	2000	1	-	4/6/27/27	0/2/2/2
2	BTI	B	2000	1	-	4/6/27/27	0/2/2/2
2	BTI	C	2000	1	-	5/6/27/27	0/2/2/2
4	ADP	C	2100	-	-	7/16/32/32	0/3/3/3
2	BTI	A	2000	1	-	4/6/27/27	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2100	ADP	C5-C4	4.79	1.47	1.39
2	A	2000	BTI	O3-C3	4.77	1.33	1.23
2	B	2000	BTI	O3-C3	4.71	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2000	BTI	O3-C3	4.64	1.33	1.23
2	C	2000	BTI	O3-C3	4.59	1.33	1.23
2	D	2000	BTI	C2-S1	-3.88	1.76	1.82
2	C	2000	BTI	C2-S1	-3.77	1.76	1.82
2	B	2000	BTI	C2-S1	-3.49	1.77	1.82
2	A	2000	BTI	C2-S1	-3.25	1.77	1.82
4	C	2100	ADP	C5-C6	2.93	1.49	1.41
4	C	2100	ADP	C5-N7	-2.29	1.34	1.39
4	C	2100	ADP	C8-N7	2.27	1.36	1.31

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	BTI	C2-C4-N2	-6.67	106.28	113.34
4	C	2100	ADP	C5-C4-N3	-6.15	118.25	126.72
2	D	2000	BTI	C6-C5-N3	-5.57	106.00	113.18
2	C	2000	BTI	C6-C5-N3	-5.46	106.14	113.18
2	A	2000	BTI	C6-C5-N3	-5.36	106.27	113.18
4	C	2100	ADP	N3-C4-N9	4.87	135.45	127.17
2	B	2000	BTI	C6-C5-N3	-4.63	107.22	113.18
2	D	2000	BTI	C2-C4-N2	-4.17	108.92	113.34
2	B	2000	BTI	C2-C4-N2	-4.06	109.05	113.34
4	C	2100	ADP	C2-N3-C4	3.97	121.53	111.83
2	C	2000	BTI	C2-C4-N2	-3.63	109.49	113.34
4	C	2100	ADP	N3-C2-N1	-3.45	123.36	128.58
4	C	2100	ADP	C4-C5-N7	-3.42	106.67	110.58
2	B	2000	BTI	C4-C2-S1	3.26	108.73	105.03
2	B	2000	BTI	C5-C6-S1	2.65	109.72	106.06
4	C	2100	ADP	C5-N7-C8	2.55	107.47	103.45
2	B	2000	BTI	N2-C3-N3	2.44	111.67	108.85
2	D	2000	BTI	N2-C3-N3	2.27	111.48	108.85
4	C	2100	ADP	C4-N9-C8	2.27	108.12	105.74
2	C	2000	BTI	N2-C3-N3	2.14	111.33	108.85
2	B	2000	BTI	C6-S1-C2	2.10	94.35	89.98
2	A	2000	BTI	C4-C2-S1	2.10	107.41	105.03
4	C	2100	ADP	C6-C5-N7	2.07	136.09	132.09
2	B	2000	BTI	C8-C7-C2	-2.06	109.31	114.04

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	BTI	C9-C10-C11-O11
2	B	2000	BTI	S1-C2-C7-C8
2	B	2000	BTI	C4-C2-C7-C8
2	C	2000	BTI	C9-C10-C11-O11
2	C	2000	BTI	S1-C2-C7-C8
2	C	2000	BTI	C4-C2-C7-C8
2	D	2000	BTI	S1-C2-C7-C8
2	D	2000	BTI	C4-C2-C7-C8
4	C	2100	ADP	PB-O3A-PA-O5'
4	C	2100	ADP	C5'-O5'-PA-O1A
4	C	2100	ADP	C5'-O5'-PA-O3A
4	C	2100	ADP	O4'-C4'-C5'-O5'
4	C	2100	ADP	C3'-C4'-C5'-O5'
2	C	2000	BTI	C7-C8-C9-C10
2	A	2000	BTI	S1-C2-C7-C8
2	A	2000	BTI	C4-C2-C7-C8
2	B	2000	BTI	C7-C8-C9-C10
2	A	2000	BTI	C11-C10-C9-C8
2	C	2000	BTI	C11-C10-C9-C8
2	D	2000	BTI	C11-C10-C9-C8
4	C	2100	ADP	C5'-O5'-PA-O2A
2	D	2000	BTI	C2-C7-C8-C9
4	C	2100	ADP	C4'-C5'-O5'-PA
2	B	2000	BTI	C11-C10-C9-C8

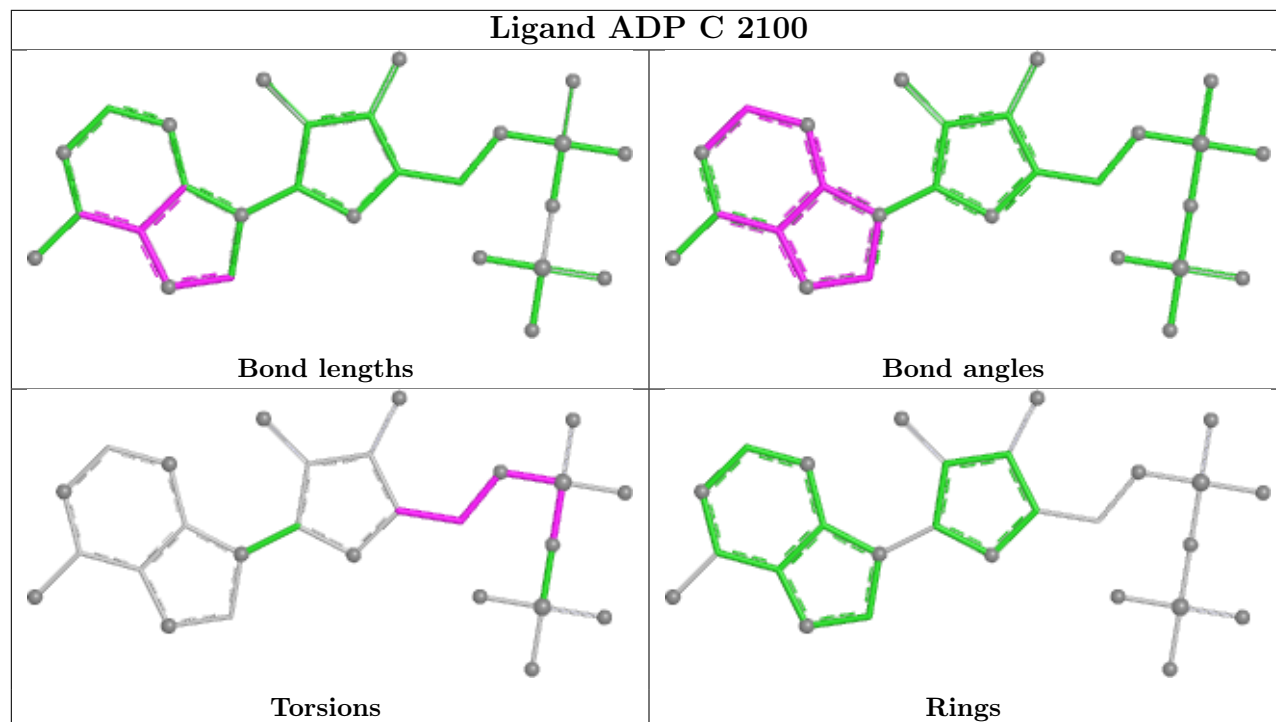
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2000	BTI	1	0
4	C	2100	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1131/1150 (98%)	-0.01	33 (2%) 53 50	25, 52, 127, 194	0
1	B	1074/1150 (93%)	0.28	36 (3%) 48 44	40, 76, 133, 169	0
1	C	1067/1150 (92%)	0.15	22 (2%) 63 60	43, 70, 103, 140	0
1	D	1067/1150 (92%)	-0.01	32 (2%) 52 49	23, 57, 130, 250	0
All	All	4339/4600 (94%)	0.10	123 (2%) 55 52	23, 67, 126, 250	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239	ILE	5.7
1	D	239	ILE	4.5
1	B	167	ILE	4.4
1	C	931	VAL	4.4
1	A	197	SER	3.9
1	B	1094	VAL	3.9
1	C	932	ILE	3.9
1	B	404	GLY	3.9
1	B	403	PHE	3.9
1	D	314	VAL	3.8
1	B	526	LEU	3.7
1	A	1131	VAL	3.5
1	B	494	LEU	3.5
1	A	196	THR	3.4
1	A	1138	LEU	3.4
1	C	199	GLY	3.4
1	D	490	ILE	3.3
1	A	1135	GLN	3.3
1	A	1149	ILE	3.2
1	A	1094	VAL	3.2
1	A	1137	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	174	ILE	3.1
1	D	1152	PRO	3.1
1	A	1123	VAL	3.1
1	A	239	ILE	3.0
1	D	167	ILE	3.0
1	B	456	LYS	2.9
1	B	527	ALA	2.9
1	D	1153	PHE	2.9
1	D	1101	LYS	2.9
1	B	418	ILE	2.9
1	B	524	TYR	2.9
1	B	93	ALA	2.9
1	C	963	LEU	2.9
1	D	1168	ILE	2.9
1	A	90	LEU	2.8
1	A	220	ALA	2.8
1	A	1100	VAL	2.8
1	B	285	PRO	2.8
1	D	92	PRO	2.7
1	C	200	GLY	2.7
1	D	1118	GLY	2.7
1	B	168	PRO	2.7
1	A	395	ILE	2.7
1	A	388	MET	2.7
1	A	207	VAL	2.7
1	B	1096	THR	2.7
1	C	1147	THR	2.7
1	D	1121	THR	2.7
1	D	1109	PRO	2.7
1	D	1082	GLY	2.6
1	A	224	ALA	2.6
1	B	395	ILE	2.6
1	C	893	MET	2.6
1	A	494	LEU	2.6
1	D	384	LEU	2.6
1	B	387	PHE	2.6
1	D	1104	ALA	2.6
1	C	934	ASP	2.6
1	A	188	GLY	2.6
1	B	409	ALA	2.6
1	A	240	ASP	2.6
1	D	243	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	217	PHE	2.6
1	B	402	GLY	2.5
1	B	166	VAL	2.5
1	A	1130	THR	2.5
1	B	90	LEU	2.5
1	A	218	HIS	2.5
1	B	393	THR	2.4
1	B	119	GLY	2.4
1	C	183	PHE	2.4
1	C	861	ILE	2.4
1	D	1103	LYS	2.4
1	D	1156	VAL	2.4
1	D	492	PRO	2.4
1	D	1114	ALA	2.4
1	D	160	ILE	2.3
1	B	380	THR	2.3
1	B	455	VAL	2.3
1	D	1125	VAL	2.3
1	A	233	VAL	2.3
1	B	314	VAL	2.3
1	C	494	LEU	2.3
1	B	396	ALA	2.2
1	B	490	ILE	2.2
1	C	854	ILE	2.2
1	D	1144	LYS	2.2
1	D	1092	GLU	2.2
1	B	492	PRO	2.2
1	D	1102	PRO	2.2
1	C	198	GLY	2.2
1	A	75	LEU	2.2
1	A	487	LEU	2.2
1	C	218	HIS	2.2
1	B	421	TYR	2.2
1	C	1001	PRO	2.2
1	B	938	LEU	2.2
1	D	434	ILE	2.2
1	D	1143	MET	2.2
1	B	160	ILE	2.2
1	A	488	PHE	2.1
1	D	157	THR	2.1
1	D	168	PRO	2.1
1	C	179	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	229	GLY	2.1
1	C	967	ILE	2.1
1	B	286	THR	2.1
1	B	164	LEU	2.1
1	C	401	GLY	2.1
1	D	91	GLY	2.1
1	A	278	ALA	2.1
1	A	1096	THR	2.1
1	C	460	PRO	2.1
1	D	1113	GLY	2.1
1	A	871	TYR	2.1
1	A	217	PHE	2.1
1	C	933	THR	2.0
1	A	1093	ASN	2.0
1	B	398	ARG	2.0
1	B	413	PHE	2.0
1	A	242	PRO	2.0
1	D	1177	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

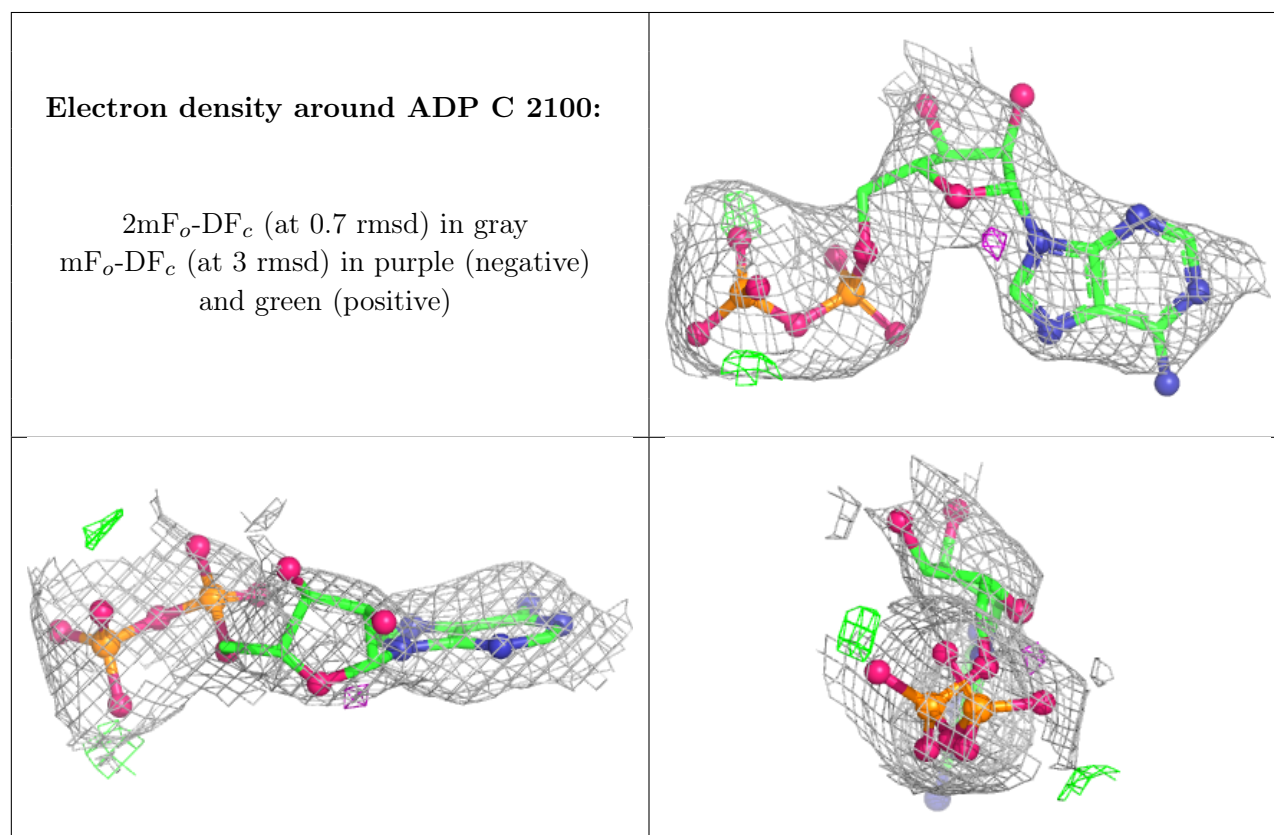
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ADP	C	2100	27/27	0.89	0.10	92,92,94,94	0
3	MN	C	2002	1/1	0.90	0.09	103,103,103,103	0
2	BTI	D	2000	15/15	0.91	0.10	64,66,67,69	0
3	MN	D	2002	1/1	0.92	0.07	54,54,54,54	0
3	MN	A	2002	1/1	0.92	0.07	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BTI	B	2000	15/15	0.94	0.09	50,51,56,57	0
2	BTI	A	2000	15/15	0.94	0.10	65,67,69,69	0
2	BTI	C	2000	15/15	0.96	0.10	58,59,70,70	0
3	MN	B	2002	1/1	0.97	0.04	75,75,75,75	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.