



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:38 PM UTC

PDB ID : 3HB9 / pdb_00003hb9
Title : Crystal Structure of S. aureus Pyruvate Carboxylase A610T Mutant
Authors : Tong, L.; Yu, L.P.C.
Deposited on : 2009-05-04
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

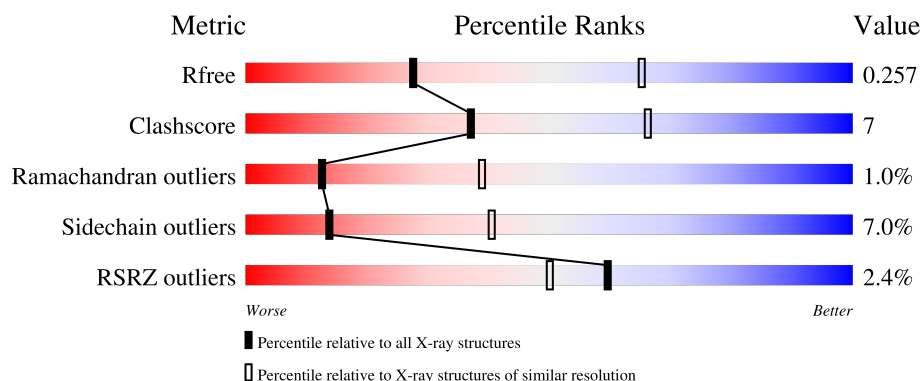
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1150	3% 78% 19% ..
1	B	1150	3% 74% 17% 7%
1	C	1150	% 74% 17% 7%
1	D	1150	2% 70% 15% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33840 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.

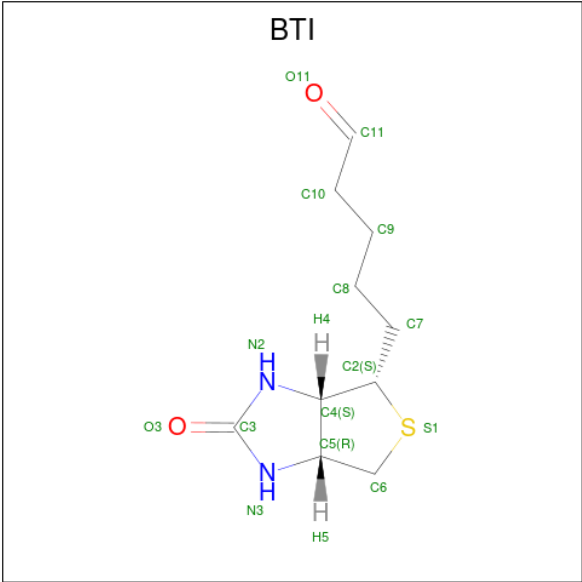
- Molecule 1 is a protein called Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1133	Total	C	N	O	S	0	0	0
			8942	5665	1505	1742	30			
1	B	1074	Total	C	N	O	S	0	0	0
			8467	5366	1427	1645	29			
1	C	1067	Total	C	N	O	S	0	0	0
			8443	5351	1421	1641	30			
1	D	993	Total	C	N	O	S	0	0	0
			7870	4995	1326	1521	28			

There are 4 discrepancies between the modelled and reference sequences:

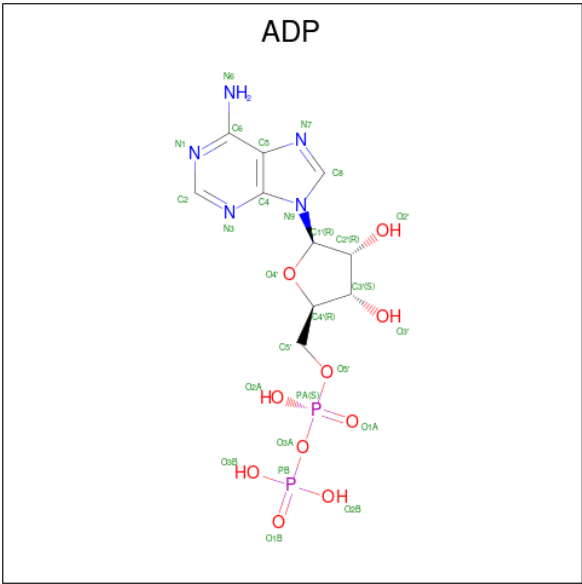
Chain	Residue	Modelled	Actual	Comment	Reference
A	610	THR	ALA	engineered mutation	UNP Q99UY8
B	610	THR	ALA	engineered mutation	UNP Q99UY8
C	610	THR	ALA	engineered mutation	UNP Q99UY8
D	610	THR	ALA	engineered mutation	UNP Q99UY8

- 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	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

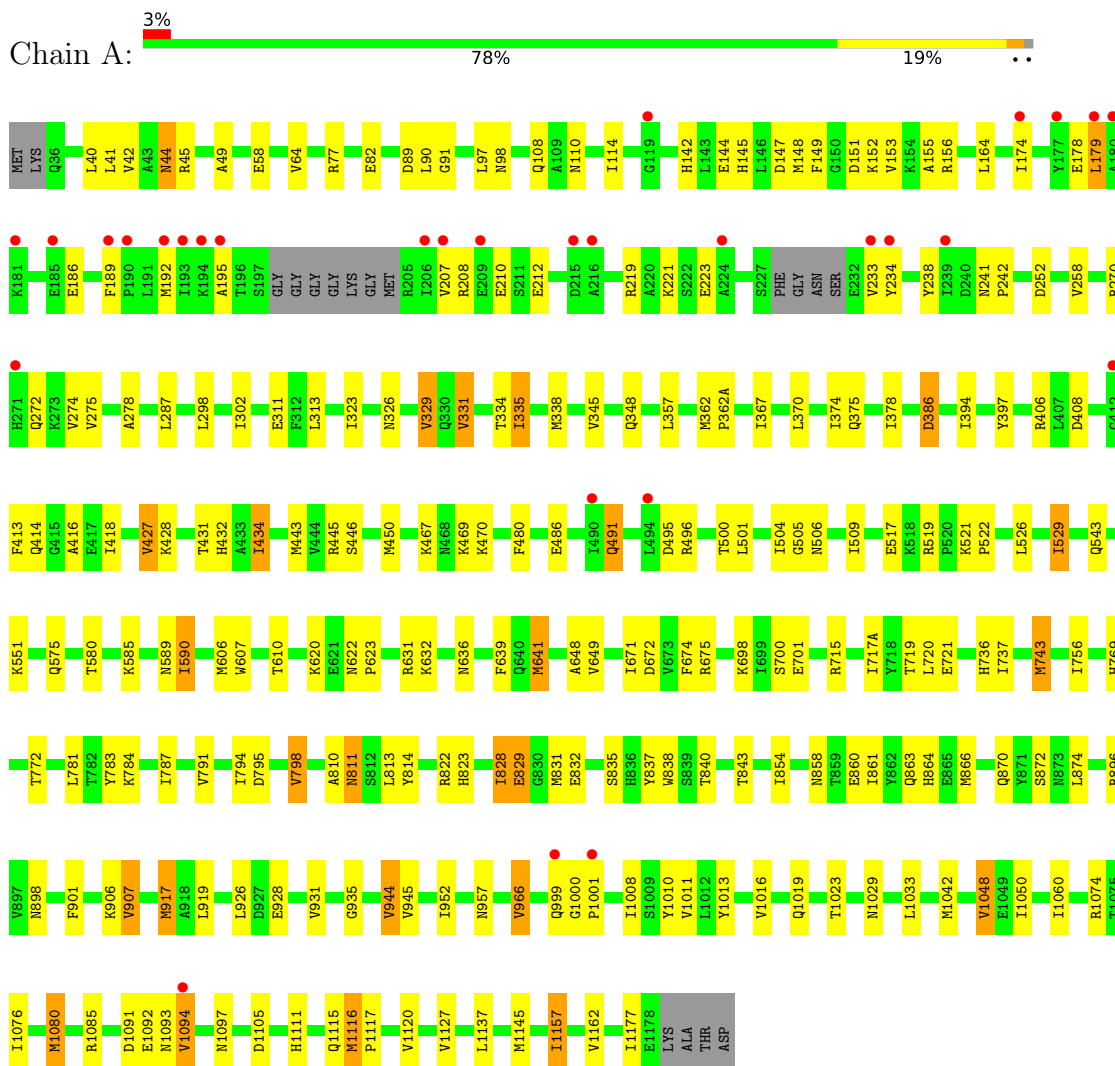
- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

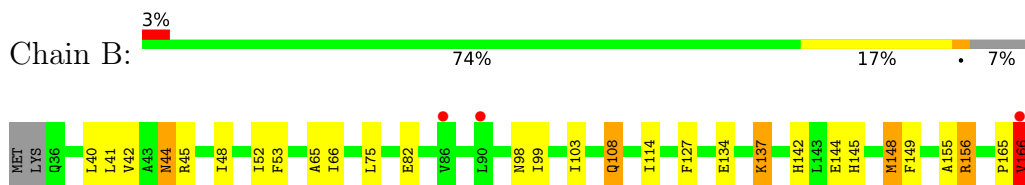
3 Residue-property plots [i](#)

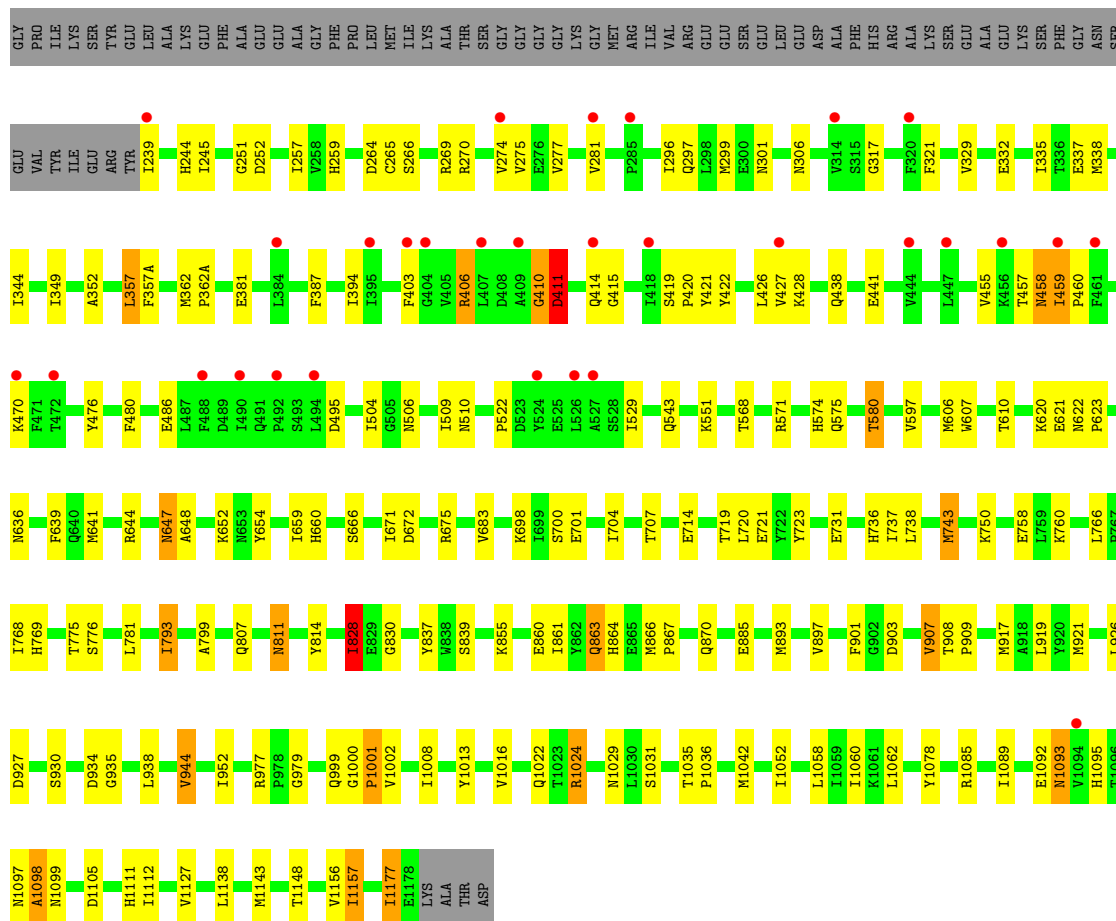
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Pyruvate carboxylase

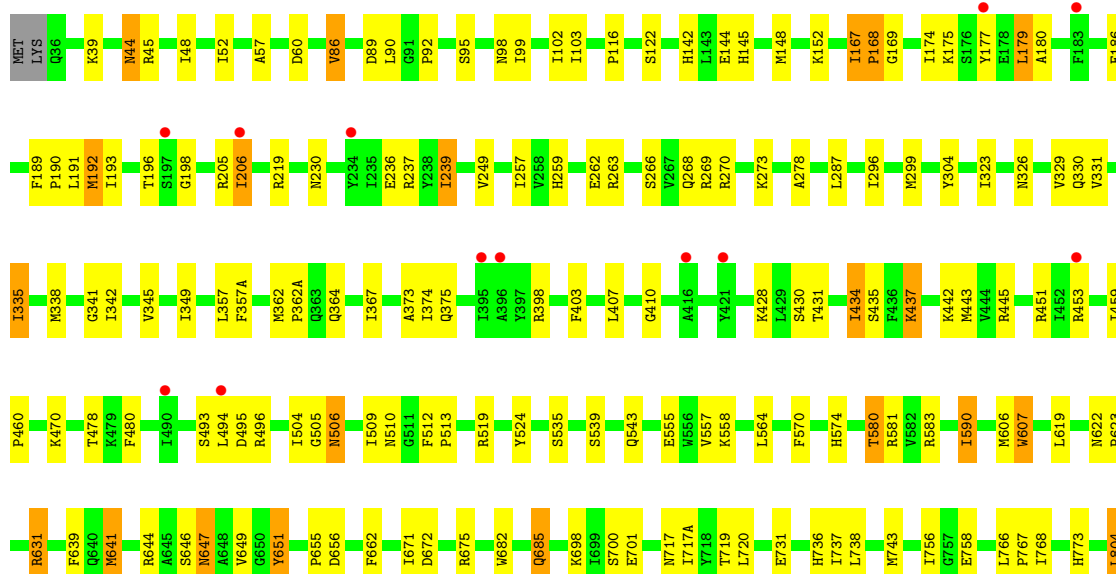
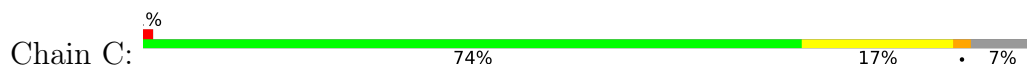


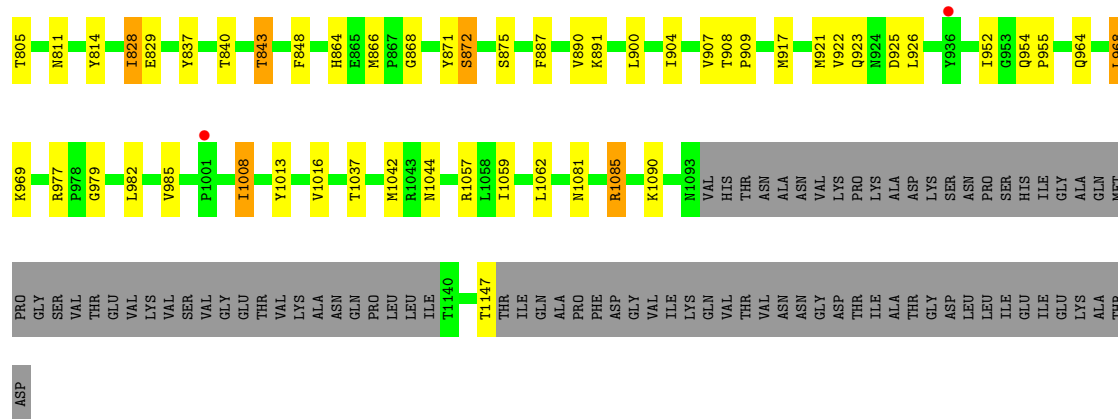
- Molecule 1: Pyruvate carboxylase



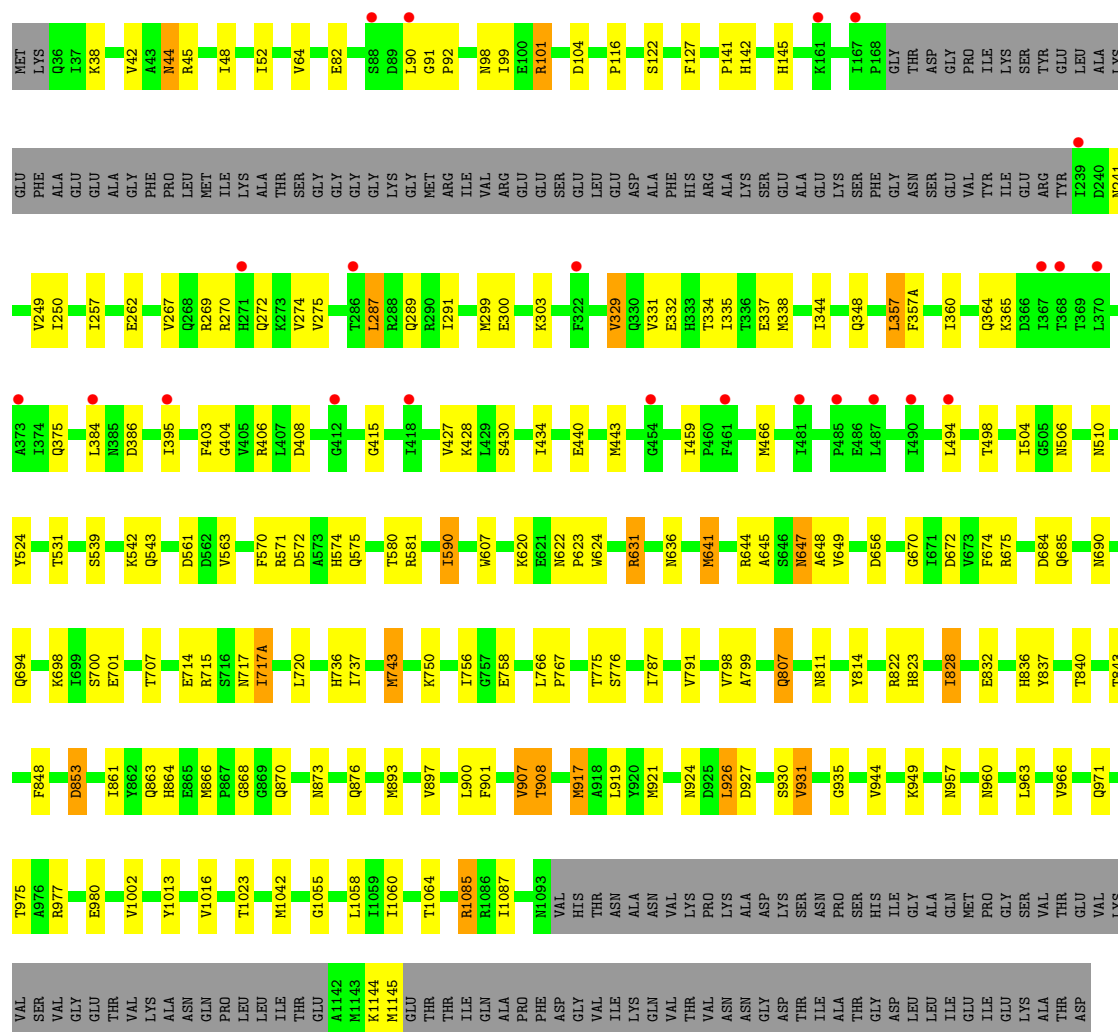


• Molecule 1: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.57Å 256.76Å 126.48Å 90.00° 109.65° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.8 (30.00-2.90) 92.7 (30.00-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.266 0.213 , 0.257	Depositor DCC
R_{free} test set	6262 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	33840	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.44	0/9110	0.78	2/12324 (0.0%)
1	B	0.44	1/8627 (0.0%)	0.78	1/11678 (0.0%)
1	C	0.43	0/8605	0.79	2/11630 (0.0%)
1	D	0.43	1/8021 (0.0%)	0.79	0/10848
All	All	0.43	2/34363 (0.0%)	0.78	5/46480 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	459	ILE	CA-CB	5.45	1.56	1.54
1	B	459	ILE	CA-CB	5.17	1.56	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	ILE	CA-C-N	5.99	127.33	119.84
1	C	167	ILE	C-N-CA	5.99	127.33	119.84
1	A	91	GLY	CA-C-N	5.29	125.10	119.28
1	A	91	GLY	C-N-CA	5.29	125.10	119.28
1	B	828	ILE	CB-CA-C	-5.18	105.23	112.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8942	0	8872	131	0
1	B	8467	0	8413	120	0
1	C	8443	0	8352	127	0
1	D	7870	0	7808	112	0
2	A	15	0	15	1	0
2	B	15	0	15	1	0
2	C	30	0	31	1	0
3	A	27	0	12	0	0
3	C	27	0	12	1	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
All	All	33840	0	33530	479	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 7.

All (479) 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:1024:ARG:HG3	1:B:1024:ARG:HH11	1.13	1.14
1:D:1085:ARG:HG2	1:D:1085:ARG:HH11	1.21	1.05
1:C:44:ASN:HD22	1:C:45:ARG:H	1.00	0.99
1:B:1000:GLY:H	1:B:1001:PRO:HD3	1.28	0.94
1:C:700:SER:H	1:C:736:HIS:HD2	1.16	0.94
1:A:44:ASN:HD22	1:A:45:ARG:H	1.13	0.93
1:B:1024:ARG:HG3	1:B:1024:ARG:NH1	1.90	0.85
1:D:44:ASN:HD22	1:D:45:ARG:H	1.24	0.84
1:A:700:SER:H	1:A:736:HIS:HD2	1.27	0.82
1:D:644:ARG:HH21	1:D:908:THR:HB	1.44	0.81
1:B:700:SER:H	1:B:736:HIS:HD2	1.25	0.81
1:D:700:SER:H	1:D:736:HIS:HD2	1.28	0.81
1:D:101:ARG:HG2	1:D:101:ARG:HH21	1.46	0.81
1:C:606:MET:HE2	1:C:639:PHE:HB3	1.62	0.80
1:B:606:MET:HE2	1:B:639:PHE:HB3	1.64	0.79
1:A:329:VAL:HG22	1:A:348:GLN:HE22	1.47	0.79
1:A:606:MET:HE2	1:A:639:PHE:HB3	1.63	0.79
1:A:590:ILE:HG12	1:A:837:TYR:CE2	2.18	0.78
1:A:1115:GLN:CD	1:A:1115:GLN:H	1.92	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:ARG:HH11	1:B:647:ASN:HD21	1.32	0.77
1:C:362:MET:HE3	1:C:362(A):PRO:HD2	1.64	0.77
1:B:410:GLY:O	1:B:411:ASP:HB2	1.83	0.77
1:C:98:ASN:O	1:C:102:ILE:HG12	1.86	0.76
1:A:811:ASN:HD22	1:A:811:ASN:H	1.31	0.76
1:B:917:MET:HG2	1:B:944:VAL:HG11	1.66	0.76
1:C:700:SER:H	1:C:736:HIS:CD2	2.03	0.76
1:B:1024:ARG:HH11	1:B:1024:ARG:CG	1.94	0.76
1:A:864:HIS:HD2	1:A:866:MET:H	1.34	0.75
1:A:164:LEU:HD11	1:A:298:LEU:HB2	1.68	0.74
1:C:504:ILE:HG21	1:C:1042:MET:HE3	1.69	0.73
1:A:866:MET:HE2	1:A:870:GLN:HG2	1.70	0.73
1:B:48:ILE:O	1:B:52:ILE:HG12	1.89	0.73
1:B:44:ASN:HD22	1:B:45:ARG:H	1.35	0.72
1:C:44:ASN:ND2	1:C:45:ARG:H	1.82	0.72
1:D:743:MET:HG3	1:D:907:VAL:HG13	1.72	0.72
1:B:156:ARG:HE	1:B:166:VAL:HG21	1.53	0.71
1:B:551:LYS:HD3	1:B:551:LYS:H	1.54	0.71
1:B:644:ARG:HD2	1:B:647:ASN:HD21	1.52	0.71
1:D:644:ARG:HH11	1:D:647:ASN:HD21	1.38	0.71
1:D:720:LEU:HD21	1:D:758:GLU:HG3	1.71	0.71
1:D:504:ILE:HG21	1:D:1042:MET:HE2	1.72	0.70
1:A:335:ILE:HD13	1:A:375:GLN:HB2	1.74	0.70
1:C:590:ILE:HG12	1:C:837:TYR:CE2	2.27	0.70
1:A:999:GLN:HG2	1:A:1001:PRO:HD2	1.74	0.69
1:D:864:HIS:HD2	1:D:866:MET:H	1.40	0.69
1:C:672:ASP:HA	1:C:698:LYS:HD2	1.74	0.69
1:D:776:SER:HB3	1:D:861:ILE:HD11	1.73	0.69
1:C:48:ILE:O	1:C:52:ILE:HG12	1.91	0.69
1:D:48:ILE:O	1:D:52:ILE:HG12	1.92	0.69
1:B:811:ASN:H	1:B:811:ASN:HD22	1.40	0.69
1:B:1042:MET:HE3	1:B:1062:LEU:HB2	1.75	0.68
1:B:1000:GLY:N	1:B:1001:PRO:HD3	2.06	0.68
1:D:917:MET:HG2	1:D:944:VAL:HG21	1.76	0.68
1:D:44:ASN:HD22	1:D:45:ARG:N	1.91	0.68
1:A:258:VAL:HG21	1:A:362:MET:HE2	1.77	0.67
1:B:458:ASN:HD22	1:B:458:ASN:H	1.42	0.66
1:C:607:TRP:HE3	1:C:641:MET:HE3	1.60	0.66
1:D:90:LEU:HD11	1:D:98:ASN:HD22	1.59	0.66
1:C:864:HIS:HD2	1:C:866:MET:H	1.43	0.66
1:D:644:ARG:NH2	1:D:908:THR:HB	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1085:ARG:HH11	1:D:1085:ARG:CG	2.05	0.66
1:A:44:ASN:ND2	1:A:45:ARG:H	1.90	0.65
1:A:898:ASN:ND2	1:A:906:LYS:HE3	2.11	0.65
1:A:701:GLU:HG2	1:A:737:ILE:HB	1.78	0.65
1:A:144:GLU:O	1:A:148:MET:HB2	1.98	0.64
1:A:491:GLN:H	1:A:491:GLN:HE21	1.45	0.64
1:B:142:HIS:H	1:B:145:HIS:HD2	1.46	0.64
1:B:864:HIS:HD2	1:B:866:MET:H	1.47	0.63
1:A:606:MET:HE1	1:A:671:ILE:CD1	2.29	0.63
1:C:326:ASN:HD22	1:C:330:GLN:NE2	1.97	0.63
1:D:1085:ARG:HG2	1:D:1085:ARG:NH1	2.01	0.63
1:C:641:MET:HG2	1:C:671:ILE:HG21	1.81	0.62
1:A:313:LEU:HD13	1:A:323:ILE:HG13	1.81	0.62
1:B:672:ASP:HA	1:B:698:LYS:HD2	1.82	0.62
1:A:620:LYS:HG2	1:A:1023:THR:HG21	1.81	0.62
1:A:901:PHE:HZ	1:A:917:MET:HG3	1.65	0.62
1:D:269:ARG:HD2	1:D:270:ARG:HG3	1.82	0.62
1:C:574:HIS:HD2	1:C:580:THR:HA	1.65	0.61
1:A:935:GLY:HA3	1:A:966:VAL:HG13	1.82	0.61
1:B:675:ARG:HA	1:B:701:GLU:HB2	1.82	0.61
1:B:901:PHE:HZ	1:B:917:MET:HG3	1.66	0.61
1:D:250:ILE:HD11	1:D:344:ILE:HG23	1.83	0.61
1:D:647:ASN:HD22	1:D:647:ASN:C	2.07	0.61
1:C:434:ILE:HD13	1:C:434:ILE:H	1.66	0.61
1:D:329:VAL:HG22	1:D:348:GLN:HE22	1.66	0.60
1:D:814:TYR:CE2	1:D:828:ILE:HG12	2.36	0.60
1:B:1105:ASP:H	1:B:1111:HIS:HD2	1.49	0.60
1:D:960:ASN:HD22	1:D:963:LEU:H	1.46	0.60
1:C:814:TYR:CE2	1:C:828:ILE:HG12	2.35	0.60
1:D:935:GLY:HA3	1:D:966:VAL:HG13	1.83	0.60
1:A:606:MET:HE1	1:A:671:ILE:HD13	1.84	0.60
1:C:335:ILE:HD13	1:C:375:GLN:HB2	1.84	0.60
1:A:641:MET:HE3	1:A:674:PHE:CE1	2.37	0.59
1:B:644:ARG:HD2	1:B:647:ASN:ND2	2.16	0.59
1:D:337:GLU:HG2	1:D:344:ILE:HG12	1.82	0.59
1:A:64:VAL:HG22	1:A:82:GLU:HB2	1.85	0.59
1:B:1105:ASP:H	1:B:1111:HIS:CD2	2.19	0.59
1:B:337:GLU:HG2	1:B:344:ILE:HG12	1.84	0.59
1:C:403:PHE:O	1:C:442:LYS:HE3	2.03	0.59
1:B:543:GLN:HE22	1:B:636:ASN:HA	1.68	0.59
1:D:901:PHE:HZ	1:D:917:MET:HG3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:MET:HE3	3:C:2100:ADP:C5	2.38	0.59
1:D:539:SER:HA	1:D:543:GLN:HG3	1.84	0.59
1:A:145:HIS:HE1	1:A:302:ILE:O	1.85	0.58
1:A:311:GLU:OE1	1:A:326:ASN:ND2	2.36	0.58
1:D:1058:LEU:HD23	1:D:1060:ILE:HD11	1.85	0.58
1:B:743:MET:HG3	1:B:907:VAL:HG13	1.85	0.58
1:C:871:TYR:O	1:C:872:SER:HB2	2.03	0.58
1:A:901:PHE:CZ	1:A:917:MET:HG3	2.38	0.58
1:C:647:ASN:OD1	1:C:647:ASN:N	2.37	0.58
1:C:86:VAL:HG11	1:C:102:ILE:HD13	1.85	0.58
1:C:606:MET:HE1	1:C:671:ILE:HD13	1.84	0.58
1:C:44:ASN:HD22	1:C:45:ARG:N	1.85	0.58
1:B:1000:GLY:H	1:B:1001:PRO:CD	2.11	0.58
1:D:543:GLN:HE21	1:D:636:ASN:HA	1.67	0.58
1:D:949:LYS:HE3	1:D:971:GLN:OE1	2.04	0.58
1:C:1059:ILE:H	1:C:1081:ASN:HD21	1.52	0.57
1:A:142:HIS:H	1:A:145:HIS:HD2	1.51	0.57
1:A:641:MET:HE2	1:A:671:ILE:HG13	1.86	0.57
1:B:144:GLU:O	1:B:148:MET:HB3	2.04	0.57
1:A:622:ASN:HD22	1:A:623:PRO:HD2	1.70	0.57
1:A:672:ASP:HA	1:A:698:LYS:HD2	1.86	0.57
1:D:935:GLY:HA3	1:D:966:VAL:CG1	2.35	0.57
1:C:398:ARG:HB3	1:C:451:ARG:HB2	1.85	0.57
1:D:901:PHE:CZ	1:D:917:MET:HG3	2.40	0.57
1:C:656:ASP:OD1	1:C:977:ARG:NH2	2.37	0.57
1:D:590:ILE:HG12	1:D:837:TYR:CE2	2.39	0.57
1:B:252:ASP:HB3	1:B:357:LEU:HD23	1.86	0.56
1:B:1095:HIS:HB3	1:B:1098:ALA:HB3	1.85	0.56
1:A:675:ARG:HA	1:A:701:GLU:HB2	1.87	0.56
1:C:606:MET:HE1	1:C:671:ILE:CD1	2.35	0.56
1:C:644:ARG:HD2	1:C:647:ASN:OD1	2.04	0.56
1:D:900:LEU:CD2	1:D:921:MET:HE1	2.35	0.56
1:B:935:GLY:HA2	1:B:938:LEU:HD12	1.86	0.56
1:D:622:ASN:ND2	1:D:624:TRP:H	2.04	0.56
1:A:575:GLN:NE2	1:A:610:THR:H	2.02	0.56
1:B:622:ASN:HD22	1:B:623:PRO:HD2	1.70	0.56
1:C:335:ILE:HD11	1:C:374:ILE:C	2.30	0.56
1:D:357:LEU:HA	1:D:360:ILE:HB	1.88	0.56
1:A:1105:ASP:H	1:A:1111:HIS:HD2	1.53	0.56
1:C:174:ILE:HG21	1:C:180:ALA:HB2	1.87	0.56
1:D:287:LEU:HD22	1:D:291:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:ASN:ND2	1:D:510:ASN:HD22	2.04	0.56
1:D:44:ASN:ND2	1:D:45:ARG:H	2.00	0.55
1:D:101:ARG:HH21	1:D:101:ARG:CG	2.18	0.55
1:A:77:ARG:HH22	1:C:1057:ARG:HD2	1.71	0.55
1:A:446:SER:O	1:A:450:MET:HG2	2.05	0.55
1:C:152:LYS:H	1:C:196:THR:HG23	1.71	0.55
1:C:811:ASN:HD22	1:C:811:ASN:H	1.54	0.55
1:C:871:TYR:O	1:C:872:SER:CB	2.54	0.55
1:B:149:PHE:HA	1:B:155:ALA:HB2	1.88	0.55
1:C:622:ASN:HD22	1:C:623:PRO:HD2	1.70	0.55
1:C:651:TYR:HD1	1:C:651:TYR:H	1.53	0.55
1:D:408:ASP:HB2	1:D:428:LYS:HB3	1.89	0.55
1:D:701:GLU:HG2	1:D:737:ILE:HB	1.89	0.55
1:C:191:LEU:HD23	1:C:237:ARG:HA	1.87	0.54
1:D:675:ARG:HA	1:D:701:GLU:HB2	1.89	0.54
1:B:299:MET:HA	1:B:299:MET:HE2	1.90	0.54
1:B:738:LEU:HD23	1:B:768:ILE:HG12	1.89	0.54
1:B:769:HIS:CD2	1:B:793:ILE:HB	2.42	0.54
1:C:169:GLY:HA2	1:C:236:GLU:HA	1.88	0.54
1:D:338:MET:HE1	1:D:430:SER:HB3	1.89	0.54
1:B:41:LEU:HB3	1:B:114:ILE:HG12	1.88	0.54
1:C:375:GLN:NE2	1:C:428:LYS:HD3	2.23	0.54
1:D:622:ASN:C	1:D:622:ASN:HD22	2.15	0.54
1:C:453:ARG:HH11	1:C:453:ARG:HB2	1.73	0.54
1:A:791:VAL:O	1:A:822:ARG:NH2	2.36	0.54
1:C:607:TRP:CE3	1:C:641:MET:HE3	2.42	0.54
1:C:917:MET:O	1:C:921:MET:HB2	2.07	0.53
1:D:828:ILE:O	1:D:832:GLU:HG2	2.08	0.53
1:C:700:SER:N	1:C:736:HIS:HD2	1.97	0.53
1:B:40:LEU:HD11	1:B:349:ILE:HD12	1.90	0.53
1:D:1013:TYR:HB3	1:D:1016:VAL:HB	1.89	0.53
1:A:811:ASN:H	1:A:811:ASN:ND2	2.02	0.53
1:D:571:ARG:HH11	1:D:575:GLN:NE2	2.06	0.53
1:D:900:LEU:HD22	1:D:921:MET:HE1	1.89	0.53
1:B:1029:ASN:C	1:B:1029:ASN:HD22	2.17	0.53
1:D:840:THR:O	1:D:843:THR:HB	2.09	0.53
1:D:690:ASN:O	1:D:694:GLN:HG2	2.08	0.53
1:C:655:PRO:HG2	1:C:985:VAL:HG23	1.91	0.52
1:D:561:ASP:O	1:D:822:ARG:HD2	2.10	0.52
1:A:90:LEU:HD12	1:A:98:ASN:HD22	1.74	0.52
1:A:149:PHE:HA	1:A:155:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ALA:HB3	1:A:335:ILE:HG23	1.91	0.52
1:C:338:MET:HE3	1:C:373:ALA:HB1	1.91	0.52
1:C:494:LEU:HB3	1:C:496:ARG:NH1	2.24	0.52
1:A:345:VAL:O	1:A:348:GLN:HB2	2.10	0.52
1:C:570:PHE:O	1:C:574:HIS:HE1	1.92	0.52
1:A:828:ILE:HD12	1:A:829:GLU:H	1.74	0.52
1:B:1127:VAL:HA	1:B:1157:ILE:HG22	1.91	0.52
1:C:828:ILE:HD12	1:C:828:ILE:H	1.73	0.52
1:A:174:ILE:HD12	1:A:179:LEU:HD11	1.91	0.52
1:B:1052:ILE:HD11	1:B:1058:LEU:HG	1.92	0.52
1:B:1078:TYR:HB2	1:B:1085:ARG:HB3	1.91	0.52
1:C:606:MET:HE2	1:C:639:PHE:CB	2.36	0.52
1:C:144:GLU:O	1:C:148:MET:HB2	2.10	0.52
1:B:867:PRO:O	1:B:870:GLN:HB2	2.10	0.52
1:B:1177:ILE:HD13	1:B:1177:ILE:N	2.25	0.52
1:C:890:VAL:HG22	1:C:922:VAL:HG21	1.92	0.52
1:B:860:GLU:O	1:B:863:GLN:HG2	2.11	0.51
1:C:539:SER:HA	1:C:543:GLN:HG3	1.92	0.51
1:A:575:GLN:HE22	1:A:610:THR:H	1.58	0.51
1:D:631:ARG:NH2	1:D:672:ASP:OD1	2.43	0.51
1:C:574:HIS:CD2	1:C:580:THR:HA	2.44	0.51
1:A:866:MET:HE3	1:A:874:LEU:HD22	1.92	0.51
1:B:99:ILE:HG23	1:B:127:PHE:HD1	1.76	0.51
1:B:406:ARG:HD3	1:D:404:GLY:H	1.75	0.51
1:C:871:TYR:HE1	1:C:891:LYS:HD3	1.74	0.51
1:A:274:VAL:HG12	1:A:275:VAL:HG23	1.93	0.51
1:B:1022:GLN:HE21	1:B:1022:GLN:HA	1.75	0.51
1:A:192:MET:HB2	1:A:238:TYR:HB2	1.91	0.51
1:A:717(A):ILE:HG12	1:A:957:ASN:OD1	2.11	0.51
1:D:334:THR:HB	1:D:375:GLN:NE2	2.25	0.51
1:B:814:TYR:CZ	1:B:828:ILE:HG12	2.46	0.51
1:D:64:VAL:HG22	1:D:82:GLU:HB2	1.93	0.51
1:D:641:MET:HE3	1:D:674:PHE:CE1	2.46	0.51
1:D:977:ARG:HG3	1:D:980:GLU:HG3	1.93	0.51
1:A:207:VAL:HG13	1:A:212:GLU:HB3	1.92	0.51
1:C:505:GLY:O	1:C:509:ILE:HG12	2.10	0.50
1:B:909:PRO:HG2	1:B:952:ILE:HD12	1.93	0.50
1:C:701:GLU:HG2	1:C:737:ILE:HB	1.94	0.50
1:C:342:ILE:HG13	1:C:362:MET:HE1	1.93	0.50
1:A:606:MET:HE2	1:A:639:PHE:CB	2.37	0.50
1:B:266:SER:HB2	1:B:476:TYR:HE2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ASP:HB3	1:B:426:LEU:HD23	1.94	0.50
1:B:244:HIS:HD2	1:B:265:CYS:HB2	1.77	0.50
1:C:116:PRO:HB2	1:C:122:SER:HA	1.94	0.50
1:A:329:VAL:HG22	1:A:348:GLN:NE2	2.20	0.50
1:B:381:GLU:HB3	1:B:387:PHE:HA	1.94	0.50
1:B:927:ASP:H	1:B:930:SER:HB2	1.77	0.50
1:D:275:VAL:HG11	1:D:466:MET:HE1	1.92	0.50
1:B:406:ARG:HD3	1:D:403:PHE:HA	1.94	0.49
1:D:581:ARG:HG3	1:D:848:PHE:CG	2.47	0.49
1:D:921:MET:HE2	1:D:931:VAL:HG21	1.94	0.49
1:A:370:LEU:O	1:A:432:HIS:HE1	1.95	0.49
1:B:42:VAL:HG12	1:B:44:ASN:H	1.77	0.49
1:A:504:ILE:HG21	1:A:1042:MET:HE3	1.94	0.49
1:B:720:LEU:HD21	1:B:758:GLU:HG3	1.95	0.49
1:B:1035:THR:HB	1:B:1036:PRO:HD3	1.94	0.49
1:C:1042:MET:HB3	1:C:1062:LEU:HD13	1.94	0.49
1:A:858:ASN:HD21	1:A:860:GLU:HB2	1.77	0.49
1:C:364:GLN:HA	1:C:367:ILE:HD12	1.93	0.49
1:B:652:LYS:HG2	1:B:654:TYR:CZ	2.48	0.49
1:A:313:LEU:HB2	1:A:323:ILE:HD11	1.94	0.49
1:D:622:ASN:HD22	1:D:623:PRO:N	2.11	0.49
1:A:1116:MET:HB2	1:A:1117:PRO:CD	2.43	0.48
1:B:811:ASN:H	1:B:811:ASN:ND2	2.07	0.48
1:C:99:ILE:O	1:C:103:ILE:HG12	2.13	0.48
1:C:583:ARG:HG2	1:C:619:LEU:HD22	1.95	0.48
1:A:335:ILE:HD12	1:A:338:MET:HE2	1.96	0.48
1:A:1013:TYR:HB3	1:A:1016:VAL:HB	1.94	0.48
1:D:99:ILE:HG23	1:D:127:PHE:HD1	1.77	0.48
1:D:811:ASN:H	1:D:811:ASN:HD22	1.61	0.48
1:A:814:TYR:CE2	1:A:828:ILE:HG12	2.48	0.48
1:A:278:ALA:CB	1:A:335:ILE:HG23	2.44	0.48
1:A:413:PHE:HE1	1:A:416:ALA:HB3	1.77	0.48
1:A:434:ILE:HG12	1:C:341:GLY:O	2.13	0.48
1:A:1033:LEU:HD23	1:A:1050:ILE:HD12	1.95	0.48
1:B:1013:TYR:HB3	1:B:1016:VAL:HB	1.94	0.48
1:D:572:ASP:HB3	1:D:807:GLN:NE2	2.27	0.48
1:D:672:ASP:HA	1:D:698:LYS:HD2	1.95	0.48
1:A:431:THR:HG21	1:A:443:MET:HA	1.96	0.48
1:A:590:ILE:HD11	1:A:838:TRP:CZ2	2.48	0.48
1:B:266:SER:HB2	1:B:476:TYR:CE2	2.49	0.48
1:D:631:ARG:HG2	1:D:670:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LYS:HE2	1:A:589:ASN:HD21	1.78	0.48
1:A:41:LEU:HB3	1:A:114:ILE:HG12	1.95	0.48
1:B:529:ILE:HG12	1:B:837:TYR:HE1	1.79	0.48
1:A:42:VAL:HG11	1:A:49:ALA:HA	1.96	0.47
1:B:893:MET:O	1:B:897:VAL:HG23	2.14	0.47
1:C:504:ILE:CG2	1:C:1042:MET:HE3	2.40	0.47
1:D:274:VAL:HG12	1:D:275:VAL:HG23	1.96	0.47
1:A:394:ILE:HD11	1:A:418:ILE:HD11	1.95	0.47
1:A:219:ARG:HB3	1:A:223:GLU:HB2	1.95	0.47
1:C:174:ILE:HG23	1:C:179:LEU:HB3	1.96	0.47
1:D:787:ILE:HA	1:D:791:VAL:HG12	1.96	0.47
1:A:1029:ASN:C	1:A:1029:ASN:HD22	2.22	0.47
1:B:1042:MET:HE1	1:B:1060:ILE:HG22	1.96	0.47
1:A:470:LYS:HB3	1:A:480:PHE:HE1	1.80	0.47
1:C:331:VAL:HG12	1:C:428:LYS:HE2	1.97	0.47
1:D:563:VAL:HG21	1:D:787:ILE:HG12	1.96	0.47
1:A:189:PHE:HB3	1:A:208:ARG:HE	1.79	0.47
1:A:743:MET:HG3	1:A:907:VAL:HG13	1.97	0.47
1:C:142:HIS:HB2	1:C:145:HIS:CD2	2.49	0.47
1:C:1059:ILE:H	1:C:1081:ASN:ND2	2.13	0.47
1:A:378:ILE:HB	1:A:427:VAL:HG23	1.97	0.46
1:C:506:ASN:ND2	1:C:510:ASN:HD22	2.12	0.46
1:D:799:ALA:H	1:D:811:ASN:ND2	2.13	0.46
1:A:1060:ILE:HG12	1:A:1080:MET:HG2	1.96	0.46
1:C:1085:ARG:CG	1:C:1085:ARG:HH11	2.27	0.46
1:B:799:ALA:H	1:B:811:ASN:ND2	2.13	0.46
1:A:505:GLY:O	1:A:509:ILE:HG12	2.16	0.46
1:C:875:SER:HA	1:C:887:PHE:CE1	2.50	0.46
1:A:620:LYS:HB2	2:B:2000:BTI:H63	1.97	0.46
1:B:506:ASN:ND2	1:B:510:ASN:HD22	2.14	0.46
1:B:977:ARG:HG2	1:B:979:GLY:H	1.81	0.46
1:C:263:ARG:HG2	1:C:278:ALA:HB2	1.97	0.46
1:B:666:SER:HB3	1:B:671:ILE:HD13	1.98	0.46
1:A:917:MET:HG2	1:A:944:VAL:HG11	1.97	0.46
1:D:395:ILE:HD12	1:D:1085:ARG:HH22	1.81	0.46
1:D:645:ALA:HB1	1:D:685:GLN:O	2.16	0.46
1:A:1127:VAL:HA	1:A:1157:ILE:HG22	1.98	0.46
1:C:675:ARG:HA	1:C:701:GLU:HB2	1.97	0.46
1:A:787:ILE:HA	1:A:791:VAL:HG12	1.97	0.46
2:A:2000:BTI:H63	1:B:620:LYS:CG	2.46	0.46
1:C:167:ILE:HG12	1:C:239:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:ARG:HD2	1:A:928:GLU:OE2	2.16	0.45
1:C:682:TRP:CE3	1:C:685:GLN:HG3	2.51	0.45
1:A:1115:GLN:CD	1:A:1115:GLN:N	2.68	0.45
1:B:731:GLU:HG3	1:B:766:LEU:HD13	1.98	0.45
1:C:1013:TYR:HB3	1:C:1016:VAL:HB	1.99	0.45
1:B:406:ARG:HA	1:B:406:ARG:CZ	2.46	0.45
1:B:701:GLU:HG2	1:B:737:ILE:HB	1.98	0.45
1:D:543:GLN:NE2	1:D:636:ASN:HA	2.31	0.45
1:B:99:ILE:H	1:B:99:ILE:HD12	1.81	0.45
1:B:165:PRO:HG2	1:B:321:PHE:HA	1.99	0.45
1:B:1092:GLU:O	1:B:1093:ASN:C	2.59	0.45
1:C:662:PHE:HA	1:C:1008:ILE:HD13	1.98	0.45
1:C:921:MET:HG3	1:C:926:LEU:HD23	1.98	0.45
1:A:543:GLN:HE22	1:A:636:ASN:HA	1.81	0.45
1:B:335:ILE:HA	1:B:338:MET:HE2	1.99	0.45
1:B:700:SER:H	1:B:736:HIS:CD2	2.17	0.45
1:C:504:ILE:HD12	1:C:1037:THR:HG22	1.99	0.45
1:D:332:GLU:O	1:D:335:ILE:HG22	2.15	0.45
1:A:362(A):PRO:HG2	1:A:367:ILE:HG12	1.98	0.45
1:B:1097:ASN:C	1:B:1099:ASN:H	2.25	0.45
1:C:152:LYS:HE3	1:C:198:GLY:H	1.81	0.45
1:A:641:MET:HE3	1:A:674:PHE:HE1	1.82	0.45
1:A:1120:VAL:HG21	1:A:1162:VAL:HB	1.99	0.45
1:A:811:ASN:ND2	1:A:811:ASN:N	2.65	0.45
1:A:335:ILE:HD11	1:A:374:ILE:C	2.42	0.44
1:A:1042:MET:HE2	1:A:1048:VAL:HG11	1.98	0.44
1:D:924:ASN:HB2	1:D:926:LEU:HD22	1.97	0.44
1:A:840:THR:O	1:A:843:THR:HB	2.17	0.44
1:B:459:ILE:N	1:B:460:PRO:HD2	2.32	0.44
1:D:927:ASP:HB3	1:D:930:SER:H	1.82	0.44
1:A:521:LYS:HA	1:A:522:PRO:HD3	1.86	0.44
1:A:935:GLY:HA3	1:A:966:VAL:CG1	2.46	0.44
1:D:524:TYR:CD2	1:D:843:THR:HG22	2.52	0.44
1:B:814:TYR:CE2	1:B:828:ILE:HG12	2.52	0.44
1:D:116:PRO:HB2	1:D:122:SER:HA	1.98	0.44
1:D:717(A):ILE:HG13	1:D:957:ASN:OD1	2.17	0.44
1:A:500:THR:O	1:A:504:ILE:HG12	2.17	0.44
1:B:504:ILE:HG21	1:B:1042:MET:HE2	1.98	0.44
1:B:53:PHE:CZ	1:B:65:ALA:HB2	2.53	0.44
1:B:251:GLY:O	1:B:306:ASN:N	2.46	0.44
1:B:704:ILE:HG21	1:B:723:TYR:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:HIS:CD2	1:B:866:MET:HG3	2.52	0.44
1:C:206:ILE:HD13	1:C:206:ILE:H	1.83	0.44
1:B:571:ARG:HH11	1:B:575:GLN:NE2	2.16	0.44
1:C:453:ARG:HB2	1:C:453:ARG:NH1	2.31	0.44
1:C:335:ILE:HD12	1:C:338:MET:HE2	1.99	0.44
1:D:249:VAL:HG21	1:D:299:MET:HG3	2.00	0.44
1:D:443:MET:HG2	1:D:466:MET:SD	2.58	0.44
1:D:622:ASN:HD22	1:D:623:PRO:CD	2.30	0.44
1:D:622:ASN:HD22	1:D:623:PRO:HD2	1.83	0.44
1:A:810:ALA:HB1	1:A:831:MET:HE1	2.00	0.44
2:C:2000:BTI:H63	1:D:620:LYS:HB2	2.00	0.44
1:A:828:ILE:O	1:A:832:GLU:HG2	2.18	0.43
1:A:1074:ARG:NH1	1:A:1091:ASP:OD2	2.47	0.43
1:C:459:ILE:HB	1:C:460:PRO:HD3	1.99	0.43
1:B:760:LYS:HG2	1:B:768:ILE:HD12	2.00	0.43
1:C:375:GLN:HG3	1:C:430:SER:OG	2.18	0.43
1:C:435:SER:HB2	1:C:437:LYS:HE3	2.00	0.43
1:D:257:ILE:HD13	1:D:300:GLU:HA	2.00	0.43
1:D:498:THR:OG1	1:D:1085:ARG:NH2	2.50	0.43
1:A:270:ARG:C	1:A:272:GLN:H	2.26	0.43
1:C:890:VAL:HA	1:C:922:VAL:HG21	2.00	0.43
1:C:964:GLN:O	1:C:968:LEU:HG	2.19	0.43
1:D:494:LEU:HD23	1:D:494:LEU:H	1.83	0.43
1:A:866:MET:CE	1:A:870:GLN:HG2	2.45	0.43
1:B:568:THR:OG1	1:B:807:GLN:HG3	2.18	0.43
1:A:719:THR:HG22	1:A:721:GLU:H	1.83	0.43
1:C:89:ASP:HB2	1:C:90:LEU:HD12	2.01	0.43
1:C:249:VAL:HG11	1:C:299:MET:HG3	2.00	0.43
1:C:773:HIS:ND1	1:C:805:THR:O	2.47	0.43
1:D:334:THR:HB	1:D:375:GLN:HE22	1.84	0.43
1:D:620:LYS:HG2	1:D:1023:THR:HG21	2.00	0.43
1:A:331:VAL:HG12	1:A:428:LYS:HD2	2.00	0.43
1:A:406:ARG:HA	1:A:406:ARG:NE	2.34	0.43
1:A:772:THR:HG22	1:A:783:TYR:CZ	2.54	0.43
1:B:621:GLU:HB2	1:B:1031:SER:HB3	2.01	0.43
1:C:259:HIS:HB3	1:C:296:ILE:HD11	2.00	0.43
1:C:437:LYS:H	1:C:437:LYS:HD3	1.83	0.43
1:C:335:ILE:HD11	1:C:374:ILE:O	2.19	0.43
1:A:769:HIS:NE2	1:A:795:ASP:OD1	2.52	0.43
1:C:814:TYR:CZ	1:C:828:ILE:HG12	2.54	0.43
1:A:811:ASN:HD22	1:A:811:ASN:N	2.08	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:HIS:CD2	1:B:296:ILE:HD11	2.54	0.43
1:B:574:HIS:CD2	1:B:580:THR:HA	2.54	0.43
1:C:558:LYS:HG3	1:C:767:PRO:HG3	2.01	0.43
1:C:840:THR:O	1:C:843:THR:HG22	2.19	0.43
1:A:58:GLU:HG3	1:C:445:ARG:HD3	2.01	0.42
1:A:864:HIS:CD2	1:A:866:MET:HG3	2.54	0.42
1:B:644:ARG:HH11	1:B:647:ASN:ND2	2.10	0.42
1:B:917:MET:O	1:B:921:MET:HB2	2.18	0.42
1:C:512:PHE:HA	1:C:513:PRO:HD2	1.85	0.42
1:C:738:LEU:HD23	1:C:768:ILE:HD12	2.01	0.42
1:D:622:ASN:ND2	1:D:622:ASN:C	2.76	0.42
1:D:893:MET:O	1:D:897:VAL:HG23	2.20	0.42
1:A:152:LYS:O	1:A:156:ARG:HB2	2.20	0.42
1:A:794:ILE:CD1	1:A:813:LEU:HD21	2.49	0.42
1:C:731:GLU:HG3	1:C:766:LEU:HD13	2.01	0.42
1:B:606:MET:HE1	1:B:671:ILE:HG13	2.01	0.42
1:C:720:LEU:HD21	1:C:758:GLU:HG3	2.00	0.42
1:A:195:ALA:HA	1:A:233:VAL:HA	2.01	0.42
1:A:854:ILE:HD11	1:A:872:SER:HB2	2.02	0.42
1:B:438:GLN:HA	1:B:441:GLU:HG2	2.00	0.42
1:B:776:SER:HB3	1:B:861:ILE:HD11	2.01	0.42
1:C:470:LYS:HB2	1:C:480:PHE:CE1	2.55	0.42
1:C:979:GLY:HA2	1:C:982:LEU:HD12	2.02	0.42
1:A:252:ASP:HB3	1:A:357:LEU:HG	2.00	0.42
1:A:445:ARG:HD3	1:C:57:ALA:HB1	2.00	0.42
1:A:860:GLU:CD	1:D:836:HIS:HE2	2.26	0.42
1:B:470:LYS:HB2	1:B:480:PHE:HE1	1.84	0.42
1:C:145:HIS:CE1	1:C:304:TYR:HA	2.55	0.42
1:C:345:VAL:O	1:C:349:ILE:HG12	2.20	0.42
1:C:631:ARG:NH2	1:C:672:ASP:OD1	2.52	0.42
1:C:923:GLN:C	1:C:925:ASP:H	2.28	0.42
1:D:570:PHE:O	1:D:574:HIS:HE1	2.03	0.42
1:D:631:ARG:HA	1:D:631:ARG:HD3	1.71	0.42
1:A:408:ASP:HB2	1:A:428:LYS:HB3	2.02	0.42
1:B:103:ILE:HG21	1:B:134:GLU:HG3	2.01	0.42
1:B:297:GLN:O	1:B:301:ASN:HB2	2.20	0.42
1:B:458:ASN:H	1:B:458:ASN:ND2	2.12	0.42
1:B:597:VAL:HG22	1:B:830:GLY:HA3	2.02	0.42
1:B:251:GLY:HA3	1:B:257:ILE:HG13	2.02	0.41
1:B:403:PHE:HB2	1:D:406:ARG:NH1	2.34	0.41
1:B:574:HIS:HD2	1:B:580:THR:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:GLN:HA	1:B:1022:GLN:NE2	2.35	0.41
1:C:954:GLN:HA	1:C:955:PRO:HD3	1.92	0.41
1:D:334:THR:HG23	1:D:406:ARG:NH1	2.35	0.41
1:D:737:ILE:HG12	1:D:767:PRO:HG2	2.02	0.41
1:B:274:VAL:HG12	1:B:275:VAL:HG23	2.03	0.41
1:C:555:GLU:HA	1:C:558:LYS:HE3	2.02	0.41
1:B:332:GLU:O	1:B:335:ILE:HG22	2.20	0.41
1:A:529:ILE:HG21	1:A:589:ASN:HB3	2.03	0.41
1:C:167:ILE:HA	1:C:168:PRO:HD2	1.83	0.41
1:C:268:GLN:HG2	1:C:273:LYS:HA	2.02	0.41
1:C:431:THR:HG21	1:C:443:MET:HA	2.01	0.41
1:D:853:ASP:OD2	1:D:853:ASP:N	2.53	0.41
1:A:151:ASP:C	1:A:153:VAL:H	2.29	0.41
1:A:631:ARG:O	1:A:631:ARG:HD3	2.20	0.41
1:B:44:ASN:ND2	1:B:45:ARG:H	2.08	0.41
1:C:557:VAL:HG13	1:C:564:LEU:HD12	2.02	0.41
1:A:719:THR:HG22	1:A:720:LEU:N	2.36	0.41
1:A:798:VAL:CG1	1:A:835:SER:HA	2.50	0.41
1:A:828:ILE:H	1:A:828:ILE:HG13	1.62	0.41
1:C:335:ILE:HD12	1:C:335:ILE:HA	1.78	0.41
1:C:524:TYR:CD2	1:C:843:THR:HG23	2.56	0.41
1:C:908:THR:HA	1:C:909:PRO:HA	1.82	0.41
1:D:101:ARG:CG	1:D:101:ARG:NH2	2.80	0.41
1:A:58:GLU:OE2	1:C:445:ARG:NH1	2.53	0.41
1:B:82:GLU:HA	1:D:1055:GLY:O	2.21	0.41
1:B:108:GLN:HE21	1:B:108:GLN:HB3	1.72	0.41
1:B:264:ASP:HB3	1:B:277:VAL:HB	2.02	0.41
1:B:362:MET:HA	1:B:362(A):PRO:HD3	1.94	0.41
1:C:266:SER:O	1:C:478:THR:HA	2.21	0.41
1:C:513:PRO:HD3	1:D:1144:LYS:HZ2	1.86	0.41
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.82	0.40
1:D:828:ILE:H	1:D:828:ILE:HG13	1.59	0.40
1:A:501:LEU:HD21	1:A:1080:MET:HG3	2.03	0.40
1:C:1085:ARG:CG	1:C:1085:ARG:NH1	2.85	0.40
1:B:509:ILE:HD12	1:B:1089:ILE:HB	2.04	0.40
1:D:641:MET:HE3	1:D:674:PHE:HE1	1.85	0.40
1:D:647:ASN:C	1:D:647:ASN:ND2	2.78	0.40
1:A:174:ILE:HG12	1:A:234:TYR:HA	2.04	0.40
1:A:866:MET:CE	1:A:874:LEU:HD22	2.51	0.40
1:A:1010:TYR:O	1:A:1011:VAL:C	2.64	0.40
1:A:1105:ASP:H	1:A:1111:HIS:CD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:SER:HA	1:B:420:PRO:HD3	1.90	0.40
1:C:581:ARG:HG3	1:C:848:PHE:CD2	2.56	0.40
1:D:141:PRO:HB2	1:D:145:HIS:HB2	2.02	0.40
1:D:142:HIS:H	1:D:145:HIS:HD2	1.69	0.40
1:D:656:ASP:OD2	1:D:977:ARG:NH2	2.54	0.40
1:B:137:LYS:HG2	1:B:352:ALA:HB1	2.03	0.40
1:C:269:ARG:HG3	1:C:270:ARG:N	2.36	0.40
1:D:42:VAL:HG21	1:D:52:ILE:HB	2.03	0.40
1:D:590:ILE:H	1:D:590:ILE:HG13	1.79	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	1127/1150 (98%)	1044 (93%)	74 (7%)	9 (1%)	16	44
1	B	1070/1150 (93%)	995 (93%)	60 (6%)	15 (1%)	9	30
1	C	1063/1150 (92%)	983 (92%)	69 (6%)	11 (1%)	12	39
1	D	987/1150 (86%)	928 (94%)	52 (5%)	7 (1%)	18	48
All	All	4247/4600 (92%)	3950 (93%)	255 (6%)	42 (1%)	12	39

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	ASP
1	A	1094	VAL
1	B	522	PRO
1	B	1001	PRO
1	B	1093	ASN
1	C	804	LEU

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Mol	Chain	Res	Type
1	C	872	SER
1	D	870	GLN
1	A	397	TYR
1	A	648	ALA
1	B	411	ASP
1	B	415	GLY
1	C	92	PRO
1	C	168	PRO
1	C	868	GLY
1	C	969	LYS
1	D	364	GLN
1	D	868	GLY
1	A	178	GLU
1	A	1093	ASN
1	B	156	ARG
1	B	648	ALA
1	C	177	TYR
1	C	189	PHE
1	C	410	GLY
1	D	648	ALA
1	B	166	VAL
1	B	269	ARG
1	B	1098	ALA
1	C	493	SER
1	D	92	PRO
1	B	903	ASP
1	B	1002	VAL
1	A	210	GLU
1	A	242	PRO
1	B	270	ARG
1	B	410	GLY
1	A	1000	GLY
1	C	190	PRO
1	D	415	GLY
1	B	317	GLY
1	D	91	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	978/988 (99%)	905 (92%)	73 (8%)	12	37
1	B	929/988 (94%)	863 (93%)	66 (7%)	13	40
1	C	918/988 (93%)	859 (94%)	59 (6%)	16	44
1	D	860/988 (87%)	799 (93%)	61 (7%)	13	40
All	All	3685/3952 (93%)	3426 (93%)	259 (7%)	14	40

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	44	ASN
1	A	89	ASP
1	A	97	LEU
1	A	108	GLN
1	A	110	ASN
1	A	147	ASP
1	A	179	LEU
1	A	186	GLU
1	A	221	LYS
1	A	241	ASN
1	A	287	LEU
1	A	329	VAL
1	A	331	VAL
1	A	334	THR
1	A	335	ILE
1	A	386	ASP
1	A	414	GLN
1	A	427	VAL
1	A	434	ILE
1	A	467	LYS
1	A	469	LYS
1	A	486	GLU
1	A	491	GLN
1	A	495	ASP
1	A	496	ARG
1	A	506	ASN
1	A	517	GLU
1	A	519	ARG
1	A	526	LEU

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Mol	Chain	Res	Type
1	A	529	ILE
1	A	551	LYS
1	A	580	THR
1	A	590	ILE
1	A	607	TRP
1	A	632	LYS
1	A	641	MET
1	A	649	VAL
1	A	715	ARG
1	A	743	MET
1	A	756	ILE
1	A	781	LEU
1	A	784	LYS
1	A	798	VAL
1	A	811	ASN
1	A	823	HIS
1	A	828	ILE
1	A	829	GLU
1	A	861	ILE
1	A	863	GLN
1	A	907	VAL
1	A	917	MET
1	A	919	LEU
1	A	926	LEU
1	A	931	VAL
1	A	944	VAL
1	A	945	VAL
1	A	952	ILE
1	A	966	VAL
1	A	1008	ILE
1	A	1019	GLN
1	A	1048	VAL
1	A	1076	ILE
1	A	1080	MET
1	A	1085	ARG
1	A	1092	GLU
1	A	1094	VAL
1	A	1097	ASN
1	A	1116	MET
1	A	1137	LEU
1	A	1145	MET
1	A	1157	ILE

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Mol	Chain	Res	Type
1	A	1177	ILE
1	B	44	ASN
1	B	66	ILE
1	B	75	LEU
1	B	98	ASN
1	B	108	GLN
1	B	137	LYS
1	B	148	MET
1	B	166	VAL
1	B	239	ILE
1	B	245	ILE
1	B	281	VAL
1	B	329	VAL
1	B	357	LEU
1	B	357(A)	PHE
1	B	394	ILE
1	B	406	ARG
1	B	411	ASP
1	B	414	GLN
1	B	421	TYR
1	B	422	TYR
1	B	427	VAL
1	B	428	LYS
1	B	455	VAL
1	B	457	THR
1	B	458	ASN
1	B	486	GLU
1	B	495	ASP
1	B	580	THR
1	B	607	TRP
1	B	610	THR
1	B	641	MET
1	B	647	ASN
1	B	659	ILE
1	B	660	HIS
1	B	683	VAL
1	B	707	THR
1	B	714	GLU
1	B	719	THR
1	B	721	GLU
1	B	743	MET
1	B	750	LYS

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Mol	Chain	Res	Type
1	B	775	THR
1	B	781	LEU
1	B	793	ILE
1	B	811	ASN
1	B	828	ILE
1	B	839	SER
1	B	855	LYS
1	B	863	GLN
1	B	885	GLU
1	B	907	VAL
1	B	908	THR
1	B	919	LEU
1	B	926	LEU
1	B	934	ASP
1	B	944	VAL
1	B	999	GLN
1	B	1008	ILE
1	B	1024	ARG
1	B	1112	ILE
1	B	1138	LEU
1	B	1143	MET
1	B	1148	THR
1	B	1156	VAL
1	B	1157	ILE
1	B	1177	ILE
1	C	39	LYS
1	C	44	ASN
1	C	60	ASP
1	C	86	VAL
1	C	95	SER
1	C	175	LYS
1	C	179	LEU
1	C	186	GLU
1	C	192	MET
1	C	193	ILE
1	C	205	ARG
1	C	206	ILE
1	C	219	ARG
1	C	230	ASN
1	C	239	ILE
1	C	257	ILE
1	C	262	GLU

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Mol	Chain	Res	Type
1	C	287	LEU
1	C	323	ILE
1	C	329	VAL
1	C	335	ILE
1	C	357	LEU
1	C	357(A)	PHE
1	C	407	LEU
1	C	434	ILE
1	C	437	LYS
1	C	495	ASP
1	C	506	ASN
1	C	519	ARG
1	C	535	SER
1	C	580	THR
1	C	590	ILE
1	C	607	TRP
1	C	631	ARG
1	C	641	MET
1	C	646	SER
1	C	647	ASN
1	C	649	VAL
1	C	651	TYR
1	C	685	GLN
1	C	717	ASN
1	C	717(A)	ILE
1	C	719	THR
1	C	743	MET
1	C	756	ILE
1	C	804	LEU
1	C	828	ILE
1	C	829	GLU
1	C	843	THR
1	C	900	LEU
1	C	904	ILE
1	C	907	VAL
1	C	952	ILE
1	C	968	LEU
1	C	1008	ILE
1	C	1044	ASN
1	C	1085	ARG
1	C	1090	LYS
1	C	1147	THR

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Mol	Chain	Res	Type
1	D	38	LYS
1	D	44	ASN
1	D	101	ARG
1	D	104	ASP
1	D	241	ASN
1	D	262	GLU
1	D	267	VAL
1	D	272	GLN
1	D	287	LEU
1	D	289	GLN
1	D	303	LYS
1	D	329	VAL
1	D	331	VAL
1	D	357	LEU
1	D	357(A)	PHE
1	D	365	LYS
1	D	384	LEU
1	D	386	ASP
1	D	427	VAL
1	D	434	ILE
1	D	440	GLU
1	D	531	THR
1	D	542	LYS
1	D	580	THR
1	D	590	ILE
1	D	607	TRP
1	D	631	ARG
1	D	641	MET
1	D	647	ASN
1	D	649	VAL
1	D	684	ASP
1	D	707	THR
1	D	714	GLU
1	D	715	ARG
1	D	717	ASN
1	D	717(A)	ILE
1	D	743	MET
1	D	750	LYS
1	D	756	ILE
1	D	766	LEU
1	D	775	THR
1	D	798	VAL

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Mol	Chain	Res	Type
1	D	807	GLN
1	D	823	HIS
1	D	828	ILE
1	D	853	ASP
1	D	863	GLN
1	D	873	ASN
1	D	876	GLN
1	D	907	VAL
1	D	908	THR
1	D	917	MET
1	D	919	LEU
1	D	926	LEU
1	D	931	VAL
1	D	975	THR
1	D	1002	VAL
1	D	1064	THR
1	D	1085	ARG
1	D	1087	ILE
1	D	1145	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	69	ASN
1	A	108	GLN
1	A	145	HIS
1	A	241	ASN
1	A	268	GLN
1	A	297	GLN
1	A	361	ASN
1	A	375	GLN
1	A	432	HIS
1	A	438	GLN
1	A	491	GLN
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

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Mol	Chain	Res	Type
1	A	736	HIS
1	A	778	ASN
1	A	811	ASN
1	A	818	ASN
1	A	858	ASN
1	A	864	HIS
1	A	898	ASN
1	A	929	GLN
1	A	998	GLN
1	A	1005	GLN
1	A	1025	ASN
1	A	1029	ASN
1	A	1044	ASN
1	A	1083	GLN
1	A	1093	ASN
1	A	1099	ASN
1	A	1111	HIS
1	A	1134	ASN
1	A	1150	GLN
1	B	36	GLN
1	B	44	ASN
1	B	69	ASN
1	B	98	ASN
1	B	108	GLN
1	B	126	GLN
1	B	145	HIS
1	B	256	ASN
1	B	326	ASN
1	B	333	HIS
1	B	364	GLN
1	B	385	ASN
1	B	414	GLN
1	B	432	HIS
1	B	458	ASN
1	B	506	ASN
1	B	543	GLN
1	B	574	HIS
1	B	575	GLN
1	B	589	ASN
1	B	617	ASN
1	B	622	ASN
1	B	647	ASN

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Mol	Chain	Res	Type
1	B	736	HIS
1	B	773	HIS
1	B	811	ASN
1	B	818	ASN
1	B	858	ASN
1	B	864	HIS
1	B	876	GLN
1	B	877	GLN
1	B	898	ASN
1	B	924	ASN
1	B	999	GLN
1	B	1005	GLN
1	B	1022	GLN
1	B	1025	ASN
1	B	1029	ASN
1	B	1044	ASN
1	B	1073	ASN
1	B	1111	HIS
1	C	44	ASN
1	C	98	ASN
1	C	145	HIS
1	C	230	ASN
1	C	330	GLN
1	C	361	ASN
1	C	375	GLN
1	C	385	ASN
1	C	432	HIS
1	C	506	ASN
1	C	515	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	660	HIS
1	C	685	GLN
1	C	717	ASN
1	C	736	HIS
1	C	778	ASN
1	C	807	GLN
1	C	811	ASN

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Mol	Chain	Res	Type
1	C	858	ASN
1	C	864	HIS
1	C	870	GLN
1	C	873	ASN
1	C	898	ASN
1	C	923	GLN
1	C	957	ASN
1	C	1005	GLN
1	C	1019	GLN
1	C	1025	ASN
1	C	1026	GLN
1	C	1029	ASN
1	C	1044	ASN
1	C	1073	ASN
1	C	1081	ASN
1	C	1093	ASN
1	D	44	ASN
1	D	98	ASN
1	D	272	GLN
1	D	289	GLN
1	D	326	ASN
1	D	330	GLN
1	D	333	HIS
1	D	361	ASN
1	D	375	GLN
1	D	432	HIS
1	D	491	GLN
1	D	506	ASN
1	D	543	GLN
1	D	574	HIS
1	D	575	GLN
1	D	589	ASN
1	D	617	ASN
1	D	622	ASN
1	D	647	ASN
1	D	685	GLN
1	D	717	ASN
1	D	736	HIS
1	D	778	ASN
1	D	811	ASN
1	D	818	ASN
1	D	858	ASN

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Mol	Chain	Res	Type
1	D	864	HIS
1	D	898	ASN
1	D	929	GLN
1	D	954	GLN
1	D	960	ASN
1	D	998	GLN
1	D	1005	GLN
1	D	1019	GLN
1	D	1025	ASN
1	D	1044	ASN
1	D	1083	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	B	2000	1	15,16,16	1.72	2 (13%)	20,21,21	1.93	4 (20%)
2	BTI	C	2000	1	15,16,16	1.69	2 (13%)	20,21,21	2.01	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	C	2100	-	28,29,29	1.43	4 (14%)	43,45,45	1.84	10 (23%)
2	BTI	A	2000	1	15,16,16	1.72	2 (13%)	20,21,21	2.06	3 (15%)
2	BTI	C	1183	-	15,16,16	1.67	2 (13%)	20,21,21	2.12	5 (25%)
3	ADP	A	2100	-	28,29,29	1.47	5 (17%)	43,45,45	1.83	8 (18%)

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	B	2000	1	-	3/6/27/27	0/2/2/2
2	BTI	C	2000	1	-	5/6/27/27	0/2/2/2
3	ADP	C	2100	-	-	1/16/32/32	0/3/3/3
2	BTI	A	2000	1	-	4/6/27/27	0/2/2/2
2	BTI	C	1183	-	-	5/6/27/27	0/2/2/2
3	ADP	A	2100	-	-	2/16/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2100	ADP	C5-C4	4.89	1.47	1.39
3	C	2100	ADP	C5-C4	4.89	1.47	1.39
2	A	2000	BTI	O3-C3	4.78	1.33	1.23
2	B	2000	BTI	O3-C3	4.73	1.33	1.23
2	C	1183	BTI	O3-C3	4.68	1.33	1.23
2	C	2000	BTI	O3-C3	4.53	1.33	1.23
2	B	2000	BTI	C2-S1	-3.79	1.76	1.82
2	C	2000	BTI	C2-S1	-3.63	1.76	1.82
2	A	2000	BTI	C2-S1	-3.61	1.76	1.82
2	C	1183	BTI	C2-S1	-3.45	1.77	1.82
3	A	2100	ADP	C5-C6	2.92	1.49	1.41
3	C	2100	ADP	C5-C6	2.83	1.48	1.41
3	A	2100	ADP	C8-N7	2.43	1.36	1.31
3	C	2100	ADP	C5-N7	-2.31	1.34	1.39
3	A	2100	ADP	PA-O3A	2.24	1.61	1.59
3	C	2100	ADP	C8-N7	2.23	1.36	1.31
3	A	2100	ADP	C5-N7	-2.17	1.35	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2000	BTI	C6-C5-N3	-6.32	105.04	113.18
2	A	2000	BTI	C2-C4-N2	-6.05	106.94	113.34
2	B	2000	BTI	C6-C5-N3	-5.95	105.52	113.18
3	A	2100	ADP	C5-C4-N3	-5.93	118.55	126.72
3	C	2100	ADP	C5-C4-N3	-5.82	118.70	126.72
2	C	1183	BTI	C6-C5-N3	-5.50	106.10	113.18
2	A	2000	BTI	C6-C5-N3	-5.47	106.13	113.18
2	C	1183	BTI	C2-C4-N2	-5.33	107.69	113.34
2	C	2000	BTI	C2-C4-N2	-5.04	108.00	113.34
3	C	2100	ADP	N3-C4-N9	4.71	135.19	127.17
3	A	2100	ADP	N3-C4-N9	4.61	135.01	127.17
3	A	2100	ADP	C2-N3-C4	3.87	121.27	111.83
3	C	2100	ADP	C2-N3-C4	3.75	120.98	111.83
2	B	2000	BTI	C2-C4-N2	-3.66	109.47	113.34
3	A	2100	ADP	C4-C5-N7	-3.54	106.54	110.58
3	C	2100	ADP	C4-C5-N7	-3.51	106.57	110.58
3	A	2100	ADP	N3-C2-N1	-3.37	123.48	128.58
3	C	2100	ADP	N3-C2-N1	-3.36	123.50	128.58
2	C	1183	BTI	C4-C2-S1	3.06	108.51	105.03
3	C	2100	ADP	C5-N7-C8	2.72	107.73	103.45
3	C	2100	ADP	C4-N9-C8	2.63	108.50	105.74
3	A	2100	ADP	C5-N7-C8	2.55	107.46	103.45
3	A	2100	ADP	C4-N9-C8	2.34	108.19	105.74
3	C	2100	ADP	C2'-C1'-N9	-2.28	107.64	113.30
2	C	1183	BTI	N2-C3-N3	2.27	111.47	108.85
3	A	2100	ADP	C6-C5-N7	2.26	136.44	132.09
2	B	2000	BTI	N2-C3-N3	2.22	111.41	108.85
2	C	1183	BTI	C8-C7-C2	-2.17	109.06	114.04
3	C	2100	ADP	C6-C5-N7	2.15	136.24	132.09
2	A	2000	BTI	C4-C2-S1	2.10	107.42	105.03
2	B	2000	BTI	C5-C6-S1	2.09	108.94	106.06
3	C	2100	ADP	N9-C8-N7	-2.01	111.09	113.94

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	BTI	C9-C10-C11-O11
2	A	2000	BTI	S1-C2-C7-C8
2	A	2000	BTI	C4-C2-C7-C8
2	B	2000	BTI	S1-C2-C7-C8
2	B	2000	BTI	C4-C2-C7-C8
2	C	2000	BTI	C9-C10-C11-O11

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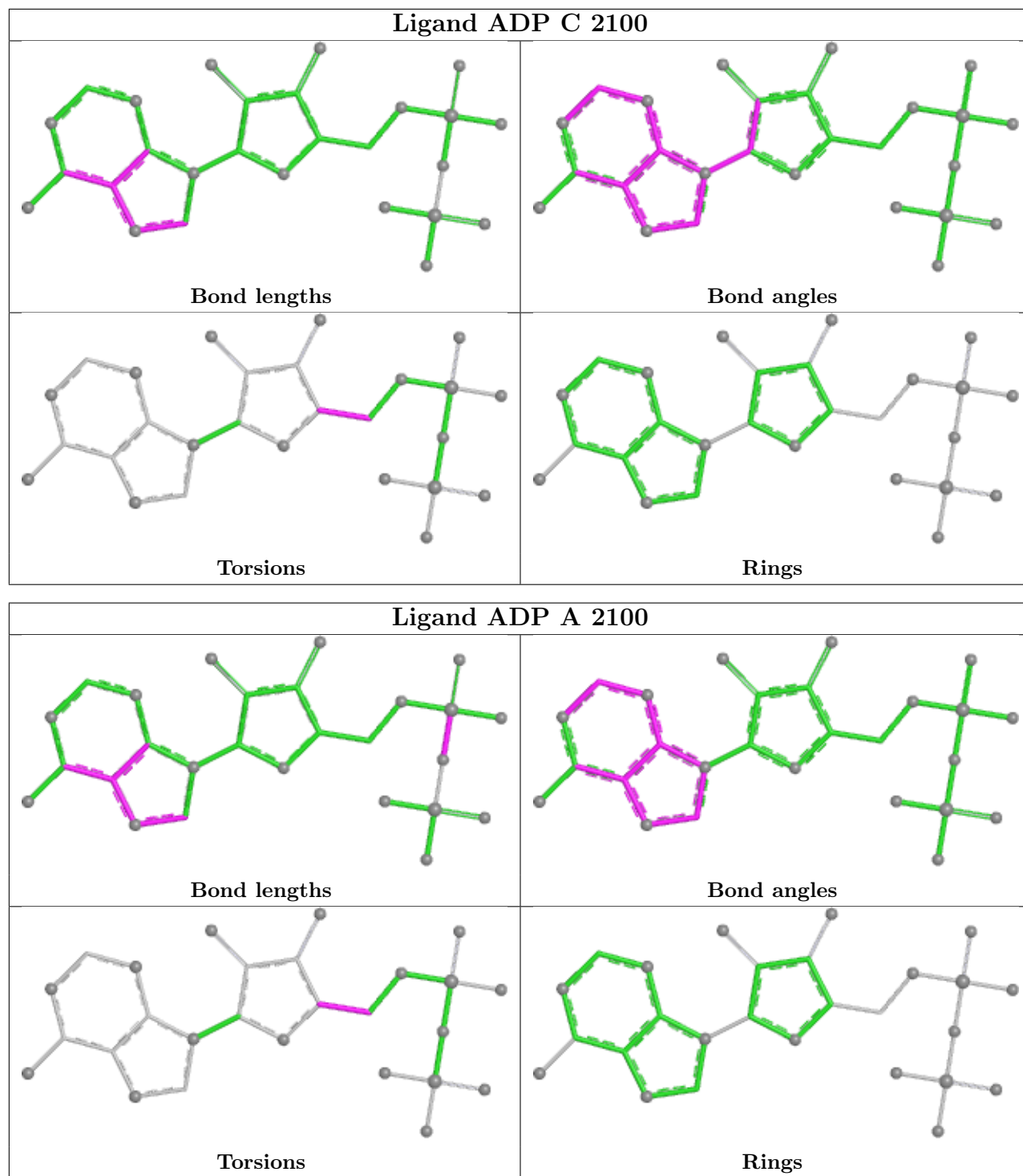
Mol	Chain	Res	Type	Atoms
2	C	2000	BTI	S1-C2-C7-C8
2	C	2000	BTI	C4-C2-C7-C8
2	C	1183	BTI	C9-C10-C11-O11
2	C	1183	BTI	C11-C10-C9-C8
2	C	1183	BTI	S1-C2-C7-C8
2	C	1183	BTI	C4-C2-C7-C8
2	C	1183	BTI	C7-C8-C9-C10
3	A	2100	ADP	O4'-C4'-C5'-O5'
2	B	2000	BTI	C7-C8-C9-C10
3	A	2100	ADP	C3'-C4'-C5'-O5'
2	A	2000	BTI	C11-C10-C9-C8
2	C	2000	BTI	C11-C10-C9-C8
2	C	2000	BTI	C7-C8-C9-C10
3	C	2100	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2000	BTI	1	0
2	C	2000	BTI	1	0
3	C	2100	ADP	1	0
2	A	2000	BTI	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1133/1150 (98%)	-0.07	29 (2%) 57 48	19, 45, 109, 169	0
1	B	1074/1150 (93%)	0.15	35 (3%) 49 40	29, 60, 127, 178	0
1	C	1067/1150 (92%)	0.02	14 (1%) 75 67	29, 61, 102, 147	0
1	D	993/1150 (86%)	-0.06	23 (2%) 61 52	17, 44, 138, 192	0
All	All	4267/4600 (92%)	0.01	101 (2%) 59 50	17, 55, 121, 192	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167	ILE	4.8
1	B	239	ILE	4.4
1	D	494	LEU	4.3
1	B	320	PHE	4.2
1	A	494	LEU	4.0
1	A	206	ILE	3.8
1	A	234	TYR	3.6
1	A	239	ILE	3.5
1	B	395	ILE	3.5
1	B	494	LEU	3.5
1	C	183	PHE	3.5
1	B	527	ALA	3.5
1	A	180	ALA	3.4
1	C	197	SER	3.3
1	D	384	LEU	3.2
1	A	999	GLN	3.2
1	C	206	ILE	3.2
1	B	274	VAL	3.2
1	D	395	ILE	3.2
1	A	195	ALA	3.1
1	A	185	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	322	PHE	2.9
1	A	189	PHE	2.8
1	A	179	LEU	2.8
1	B	409	ALA	2.8
1	D	167	ILE	2.8
1	D	368	THR	2.8
1	A	190	PRO	2.8
1	B	524	TYR	2.8
1	B	166	VAL	2.7
1	D	487	LEU	2.7
1	A	233	VAL	2.7
1	B	1094	VAL	2.7
1	B	447	LEU	2.6
1	B	470	LYS	2.6
1	B	488	PHE	2.6
1	D	90	LEU	2.6
1	A	216	ALA	2.6
1	D	485	PRO	2.6
1	B	418	ILE	2.6
1	A	119	GLY	2.6
1	A	177	TYR	2.6
1	D	370	LEU	2.5
1	D	412	GLY	2.5
1	D	88	SER	2.5
1	D	490	ILE	2.5
1	B	407	LEU	2.5
1	A	174	ILE	2.5
1	B	281	VAL	2.5
1	C	234	TYR	2.5
1	B	403	PHE	2.5
1	B	168	PRO	2.5
1	D	239	ILE	2.5
1	A	224	ALA	2.4
1	A	271	HIS	2.4
1	A	412	GLY	2.4
1	B	472	THR	2.4
1	B	526	LEU	2.4
1	B	459	ILE	2.4
1	A	207	VAL	2.4
1	C	177	TYR	2.4
1	B	490	ILE	2.4
1	B	492	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	86	VAL	2.3
1	B	384	LEU	2.3
1	D	271	HIS	2.3
1	A	193	ILE	2.3
1	C	494	LEU	2.3
1	C	936	TYR	2.3
1	B	444	VAL	2.3
1	D	454	GLY	2.3
1	B	461	PHE	2.3
1	B	456	LYS	2.3
1	C	395	ILE	2.3
1	A	1001	PRO	2.3
1	D	461	PHE	2.3
1	B	404	GLY	2.3
1	B	427	VAL	2.2
1	D	161	LYS	2.2
1	A	490	ILE	2.2
1	C	453	ARG	2.2
1	A	215	ASP	2.2
1	B	285	PRO	2.2
1	A	181	LYS	2.2
1	D	373	ALA	2.2
1	D	481	ILE	2.1
1	A	1094	VAL	2.1
1	B	314	VAL	2.1
1	A	194	LYS	2.1
1	B	90	LEU	2.1
1	C	1001	PRO	2.1
1	D	286	THR	2.1
1	C	490	ILE	2.1
1	A	192	MET	2.1
1	C	421	TYR	2.1
1	B	414	GLN	2.1
1	D	367	ILE	2.1
1	A	209	GLU	2.1
1	C	416	ALA	2.0
1	D	418	ILE	2.0
1	C	396	ALA	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

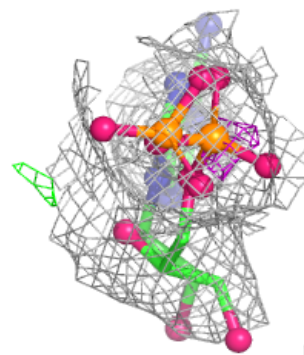
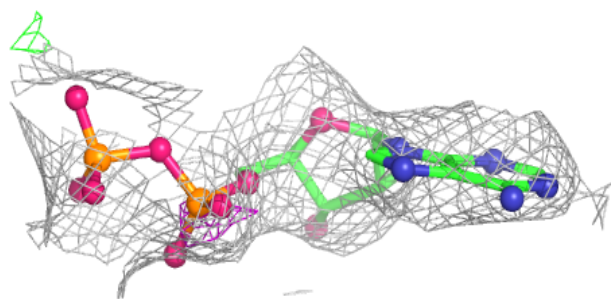
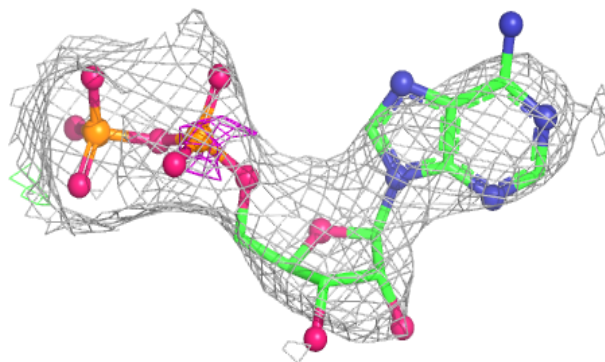
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	ADP	A	2100	27/27	0.84	0.13	99,100,103,103	0
3	ADP	C	2100	27/27	0.92	0.10	78,78,78,79	0
4	MN	B	2002	1/1	0.92	0.06	77,77,77,77	0
2	BTI	C	1183	15/15	0.93	0.10	48,48,49,49	0
4	MN	C	2002	1/1	0.93	0.06	75,75,75,75	0
2	BTI	B	2000	15/15	0.95	0.09	48,48,51,51	0
4	MN	A	2002	1/1	0.95	0.07	63,63,63,63	0
2	BTI	C	2000	15/15	0.96	0.09	45,45,57,57	0
4	MN	D	2002	1/1	0.96	0.06	57,57,57,57	0
2	BTI	A	2000	15/15	0.97	0.07	50,51,53,53	0

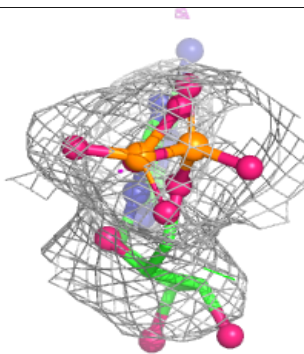
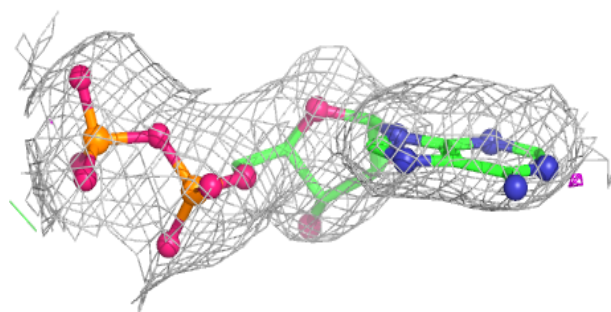
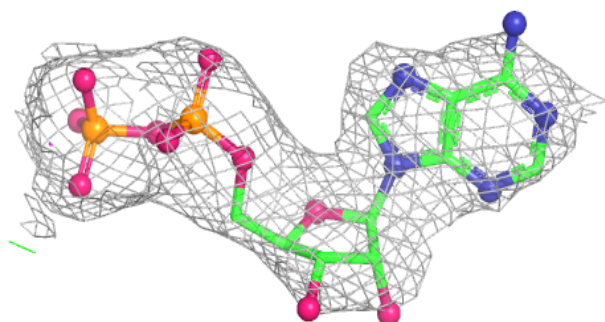
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 2100:

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

**Electron density around ADP C 2100:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.