



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:06 AM UTC

PDB ID : 2QTC / pdb_00002qtc
Title : E. coli Pyruvate dehydrogenase E1 component E401K mutant with phosphonolactylthiamin diphosphate
Authors : Furey, W.; Arjunan, P.; Chandrasekhar, K.
Deposited on : 2007-08-01
Resolution : 1.77 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

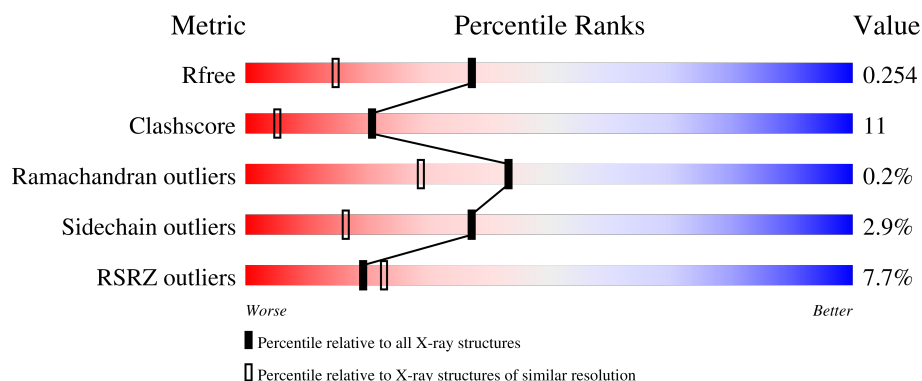
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	886	9% 70% 18% • 10%
1	B	886	5% 72% 16% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13146 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 dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6341	4018	1093	1204	26			
1	B	801	Total	C	N	O	S	0	0	0
			6341	4018	1093	1204	26			

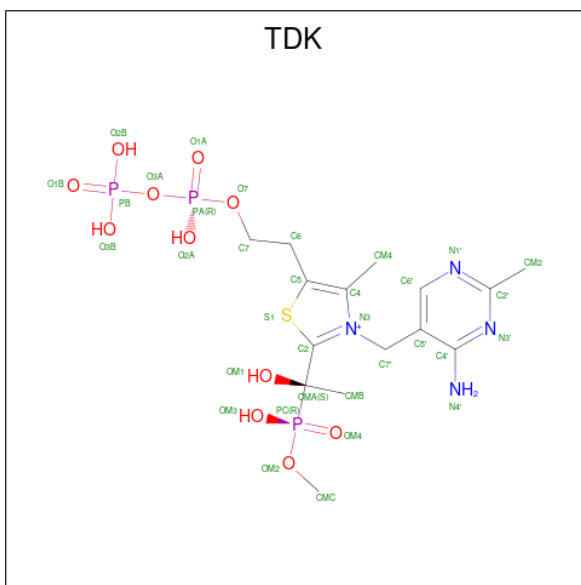
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	LYS	GLU	engineered mutation	UNP P0AFG8
B	401	LYS	GLU	engineered mutation	UNP P0AFG8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-[(1S)-1-HYDROXY-1-[(R)-HYDROXY(METHOXY)PHOSPHORYL]ETHYL]-5-(2-[(S)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY)ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (CCD ID: TDK) (formula: C₁₅H₂₆N₄O₁₁P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 34	C 15	N 4	O 11	P 3	S 1	0	0
3	B	1	Total 34	C 15	N 4	O 11	P 3	S 1	0	0

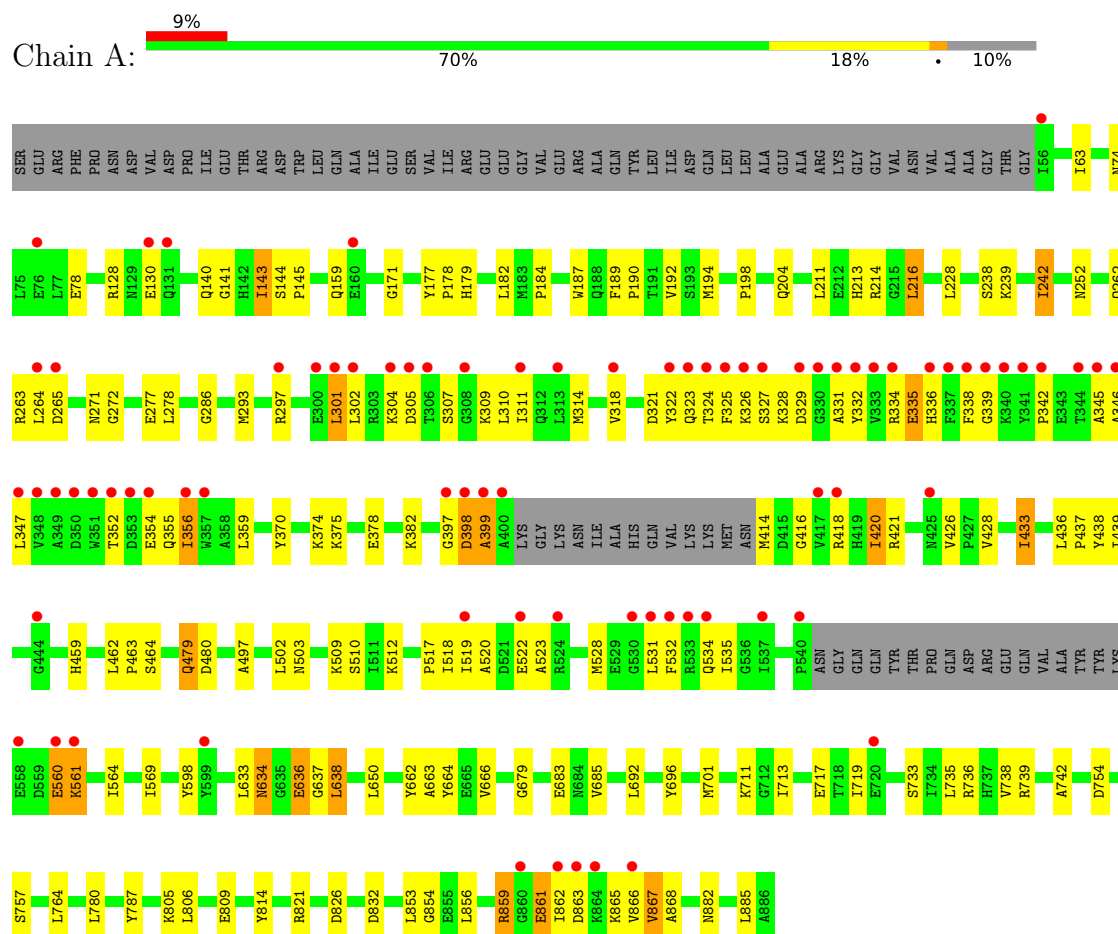
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	186	Total O 186 186	0	0
4	B	208	Total O 208 208	0	0

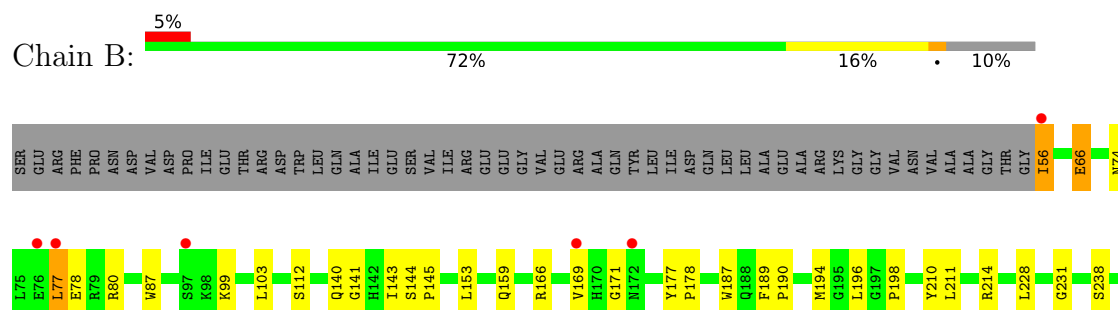
3 Residue-property plots

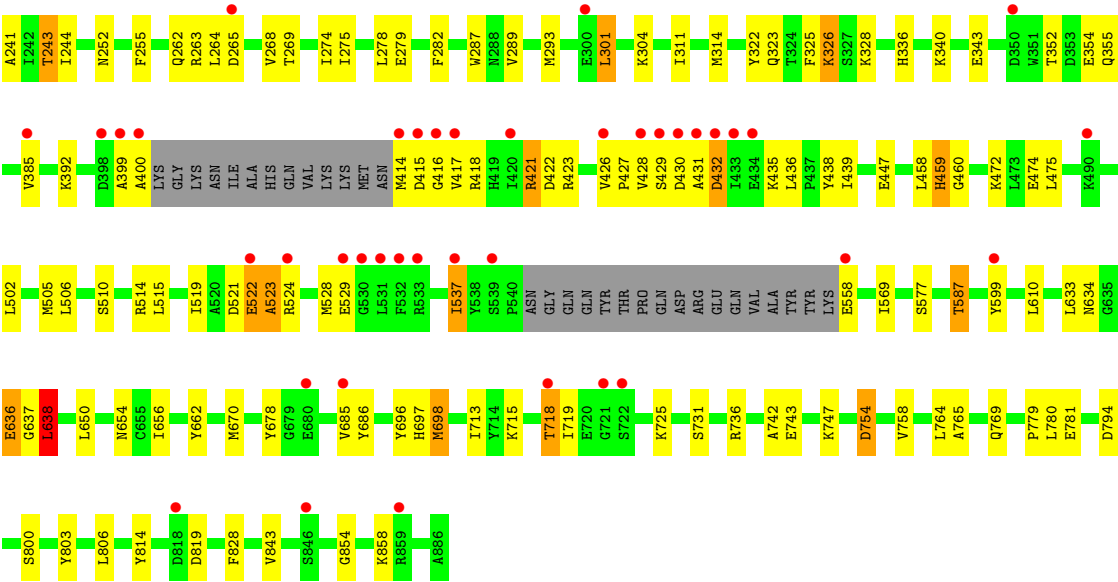
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Pyruvate dehydrogenase E1 component



• Molecule 1: Pyruvate dehydrogenase E1 component





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.61Å 142.11Å 82.14Å 90.00° 102.68° 90.00°	Depositor
Resolution (Å)	47.53 – 1.77 47.53 – 1.77	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.53-1.77) 90.7 (47.53-1.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 1.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.255 0.225 , 0.254	Depositor DCC
R_{free} test set	8037 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13146	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: MG, TDK

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	0.63	0/6484	1.04	24/8766 (0.3%)
1	B	0.68	1/6484 (0.0%)	1.05	26/8766 (0.3%)
All	All	0.66	1/12968 (0.0%)	1.04	50/17532 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	698	MET	SD-CE	-10.11	1.54	1.79

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	634	ASN	N-CA-C	9.82	122.06	111.36
1	B	634	ASN	N-CA-C	9.52	121.66	111.28
1	B	171	GLY	N-CA-C	9.27	127.26	115.21
1	A	171	GLY	N-CA-C	9.25	126.95	114.92
1	A	638	LEU	N-CA-C	8.65	121.80	111.33
1	B	633	LEU	N-CA-C	-8.14	98.23	109.71
1	A	633	LEU	N-CA-C	-8.03	98.39	109.71
1	B	141	GLY	N-CA-C	8.02	122.34	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	638	LEU	N-CA-C	7.91	120.60	111.11
1	B	238	SER	N-CA-C	6.90	118.45	111.07
1	B	263	ARG	N-CA-C	-6.62	99.95	109.29
1	B	523	ALA	N-CA-C	-6.41	104.65	113.18
1	B	169	VAL	N-CA-C	6.30	117.80	110.62
1	B	636	GLU	N-CA-C	6.23	119.05	111.82
1	A	141	GLY	N-CA-C	6.19	120.13	112.64
1	A	535	ILE	N-CA-C	6.13	119.05	113.10
1	B	430	ASP	N-CA-C	-6.02	105.65	112.87
1	B	754	ASP	N-CA-C	-5.97	99.45	109.07
1	A	662	TYR	N-CA-C	5.87	119.12	109.85
1	B	459	HIS	N-CA-C	5.87	120.39	113.23
1	B	794	ASP	N-CA-C	5.86	120.12	112.92
1	A	263	ARG	N-CA-C	-5.84	101.06	109.29
1	B	460	GLY	N-CA-C	5.80	117.42	111.56
1	B	328	LYS	N-CA-C	5.73	113.48	108.78
1	B	781	GLU	N-CA-C	5.71	118.90	110.46
1	A	184	PRO	N-CA-C	5.70	121.25	113.84
1	A	510	SER	N-CA-C	5.69	117.56	111.36
1	A	867	VAL	N-CA-C	-5.66	105.21	110.53
1	A	637	GLY	N-CA-C	5.63	122.44	112.53
1	B	514	ARG	N-CA-C	-5.61	106.44	113.28
1	A	143	ILE	N-CA-C	-5.53	107.09	112.29
1	B	416	GLY	N-CA-C	-5.49	100.17	113.18
1	A	754	ASP	N-CA-C	-5.45	100.29	109.07
1	B	637	GLY	N-CA-C	5.44	122.10	112.53
1	A	636	GLU	N-CA-C	5.43	118.11	111.82
1	A	242	ILE	N-CA-C	5.42	117.83	111.05
1	B	293	MET	N-CA-C	5.41	119.83	112.04
1	B	528	MET	N-CA-C	-5.41	106.85	113.50
1	A	679	GLY	N-CA-C	-5.39	104.33	112.41
1	B	252	ASN	N-CA-C	-5.38	106.02	112.59
1	A	293	MET	N-CA-C	5.33	119.72	112.04
1	A	459	HIS	N-CA-C	5.17	120.75	113.56
1	A	204	GLN	N-CA-C	-5.14	105.76	111.36
1	A	433	ILE	N-CA-C	5.13	116.47	110.62
1	B	336	HIS	N-CA-C	5.08	119.19	112.89
1	A	757	SER	N-CA-C	-5.07	101.04	109.46
1	A	252	ASN	N-CA-C	-5.05	106.36	112.88
1	B	577	SER	N-CA-C	-5.02	105.71	111.14
1	B	510	SER	N-CA-C	5.02	116.83	111.36
1	A	238	SER	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	598	TYR	Sidechain
1	A	814	TYR	Sidechain
1	B	678	TYR	Sidechain
1	B	803	TYR	Sidechain
1	B	814	TYR	Sidechain

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	6341	0	6179	158	0
1	B	6341	0	6179	137	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	34	0	22	8	0
3	B	34	0	22	6	0
4	A	186	0	0	1	0
4	B	208	0	0	4	0
All	All	13146	0	12402	278	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 11.

All (278) 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:656:ILE:HG12	1:B:685:VAL:HG21	1.37	1.03
1:A:182:LEU:HD11	1:B:638:LEU:HD23	1.45	0.97
1:B:800:SER:OG	1:B:843:VAL:HG13	1.71	0.91
1:A:311:ILE:HA	1:A:314:MET:HE3	1.49	0.91
1:A:418:ARG:HD2	1:A:433:ILE:HD13	1.52	0.90
1:A:194:MET:HE2	3:A:887:TDK:C4'	2.04	0.88
1:B:698:MET:HE2	1:B:698:MET:HA	1.54	0.88
1:B:656:ILE:CG1	1:B:685:VAL:HG21	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ILE:HG12	1:B:685:VAL:CG2	2.06	0.84
1:A:882:ASN:HB3	1:A:885:LEU:HD23	1.59	0.83
1:B:287:TRP:CE3	1:B:385:VAL:HG13	2.13	0.82
1:A:497:ALA:HB1	1:A:666:VAL:HG11	1.60	0.82
1:A:194:MET:HE1	3:A:887:TDK:HM42	1.61	0.82
1:B:311:ILE:HA	1:B:314:MET:CE	2.11	0.81
1:B:654:ASN:O	1:B:685:VAL:HG23	1.80	0.81
1:A:182:LEU:CD1	1:B:638:LEU:HD23	2.12	0.79
1:A:497:ALA:CB	1:A:666:VAL:HG11	2.14	0.78
1:B:638:LEU:HD22	1:B:828:PHE:HB3	1.65	0.78
1:B:255:PHE:HB2	1:B:385:VAL:HG12	1.66	0.78
1:A:301:LEU:HD12	1:A:310:LEU:HD22	1.67	0.76
1:A:328:LYS:HG3	1:A:332:TYR:CD1	2.22	0.75
1:A:859:ARG:HH11	1:A:859:ARG:HB3	1.51	0.74
1:A:519:ILE:HD11	1:A:528:MET:HE2	1.68	0.74
1:B:198:PRO:HG3	1:B:228:LEU:HD22	1.70	0.72
1:A:277:GLU:OE2	1:B:243:THR:HG21	1.89	0.72
1:A:636:GLU:OE1	3:B:887:TDK:HMC1	1.91	0.70
1:A:503:ASN:OD1	1:A:534:GLN:NE2	2.18	0.70
1:B:311:ILE:HA	1:B:314:MET:HE3	1.72	0.70
1:A:286:GLY:O	1:A:382:LYS:HE3	1.93	0.69
1:A:418:ARG:HD2	1:A:433:ILE:CD1	2.23	0.68
1:A:735:LEU:O	1:A:738:VAL:HG22	1.93	0.68
1:A:502:LEU:HD23	1:A:531:LEU:HD11	1.76	0.68
1:B:159:GLN:HG3	1:B:438:TYR:CD2	2.30	0.67
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.25	0.67
1:A:310:LEU:HG	1:A:314:MET:HE2	1.76	0.67
1:A:418:ARG:HE	1:A:421:ARG:NH2	1.93	0.66
1:A:867:VAL:HG12	1:B:779:PRO:HG3	1.77	0.66
1:B:282:PHE:CD2	1:B:385:VAL:HG11	2.30	0.66
1:A:696:TYR:CG	1:A:736:ARG:HD2	2.31	0.66
1:B:854:GLY:O	1:B:858:LYS:HG3	1.98	0.64
1:A:335:GLU:HB3	1:A:336:HIS:HD2	1.62	0.64
1:A:636:GLU:CD	3:B:887:TDK:HMC1	2.22	0.64
1:B:537:ILE:HG23	1:B:558:GLU:HG3	1.78	0.64
1:B:662:TYR:HD1	1:B:698:MET:HE1	1.63	0.64
1:A:271:ASN:C	1:A:318:VAL:HG21	2.22	0.64
1:A:194:MET:HE1	3:A:887:TDK:CM4	2.27	0.63
1:A:179:HIS:HB3	1:A:182:LEU:HD13	1.79	0.63
1:A:302:LEU:HD21	1:A:314:MET:HE1	1.79	0.63
1:B:472:LYS:HE3	1:B:474:GLU:OE2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:ARG:HB3	1:A:859:ARG:NH1	2.15	0.62
1:B:843:VAL:O	1:B:843:VAL:HG12	2.01	0.61
1:A:328:LYS:HB3	1:A:332:TYR:HB3	1.82	0.61
1:B:696:TYR:CD1	1:B:698:MET:HE3	2.35	0.61
1:A:416:GLY:O	1:A:420:ILE:HD12	2.00	0.61
1:B:414:MET:O	1:B:414:MET:HG2	2.01	0.61
1:A:663:ALA:O	1:A:666:VAL:CG1	2.48	0.61
1:A:374:LYS:O	1:A:378:GLU:HG3	2.01	0.61
1:B:80:ARG:HD2	1:B:447:GLU:OE2	2.01	0.61
1:A:194:MET:HE1	3:A:887:TDK:C4	2.31	0.60
1:B:587:THR:HG22	4:B:905:HOH:O	2.01	0.60
1:B:719:ILE:HD12	1:B:742:ALA:HB1	1.83	0.60
1:B:587:THR:HG21	4:B:1054:HOH:O	2.01	0.60
1:A:272:GLY:O	1:A:318:VAL:HG22	2.02	0.60
1:B:519:ILE:HD12	1:B:523:ALA:HB2	1.84	0.60
1:B:279:GLU:HG3	1:B:289:VAL:HG21	1.83	0.60
1:A:301:LEU:HD12	1:A:310:LEU:CD2	2.30	0.59
3:A:887:TDK:HMC1	1:B:636:GLU:CD	2.27	0.59
1:A:717:GLU:CD	1:A:739:ARG:HH21	2.09	0.59
1:B:282:PHE:CE2	1:B:385:VAL:HG11	2.37	0.59
1:A:329:ASP:OD1	1:A:331:ALA:HB3	2.02	0.59
1:A:522:GLU:CD	1:B:264:LEU:HD22	2.27	0.59
1:B:56:ILE:N	1:B:56:ILE:HD13	2.18	0.59
1:A:518:ILE:C	1:A:519:ILE:HD12	2.27	0.59
1:A:307:SER:OG	1:A:309:LYS:HB2	2.03	0.58
1:A:302:LEU:CD2	1:A:314:MET:HE1	2.34	0.58
1:B:429:SER:HB3	1:B:432:ASP:OD1	2.03	0.58
1:A:302:LEU:HD23	1:A:310:LEU:HD23	1.86	0.58
1:B:268:VAL:HB	1:B:274:ILE:HG21	1.86	0.58
1:A:859:ARG:HH11	1:A:859:ARG:CB	2.16	0.58
1:A:418:ARG:HH21	1:A:421:ARG:HH21	1.52	0.58
1:A:418:ARG:HG3	1:A:418:ARG:HH11	1.69	0.57
1:A:523:ALA:N	1:B:265:ASP:OD2	2.35	0.57
1:A:265:ASP:OD2	1:B:523:ALA:N	2.37	0.57
1:B:399:ALA:O	1:B:400:ALA:HB3	2.04	0.56
1:B:421:ARG:NH1	1:B:422:ASP:OD1	2.38	0.56
1:A:418:ARG:HB3	1:A:418:ARG:CZ	2.35	0.56
1:A:339:GLY:HA2	1:A:345:ALA:HB2	1.87	0.56
1:A:128:ARG:NH1	1:A:464:SER:OG	2.38	0.56
1:A:370:TYR:OH	1:A:374:LYS:HE3	2.06	0.56
1:B:505:MET:HE3	1:B:670:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:HG2	1:A:297:ARG:HH11	1.70	0.55
1:A:194:MET:HE2	3:A:887:TDK:C5'	2.36	0.55
1:A:311:ILE:HA	1:A:314:MET:CE	2.29	0.55
1:A:198:PRO:HD3	1:A:228:LEU:CD2	2.37	0.55
1:A:426:VAL:HG12	1:A:428:VAL:HG23	1.88	0.55
1:A:561:LYS:HZ2	1:A:561:LYS:HB2	1.72	0.55
1:A:304:LYS:NZ	1:A:347:LEU:O	2.40	0.55
1:A:663:ALA:O	1:A:666:VAL:HG12	2.06	0.55
1:B:194:MET:HE1	3:B:887:TDK:S1	2.46	0.55
1:A:334:ARG:HB3	1:A:356:ILE:HD13	1.89	0.55
1:A:194:MET:HE3	1:B:569:ILE:CG2	2.37	0.54
1:B:843:VAL:O	1:B:843:VAL:CG1	2.55	0.54
1:A:264:LEU:HD12	1:B:522:GLU:OE1	2.07	0.54
1:A:418:ARG:NE	1:A:421:ARG:NH2	2.55	0.54
1:A:305:ASP:OD1	1:A:305:ASP:C	2.49	0.54
1:A:334:ARG:HB3	1:A:356:ILE:CD1	2.37	0.54
1:B:301:LEU:HD12	1:B:304:LYS:HE2	1.90	0.54
1:B:696:TYR:HE1	1:B:698:MET:HE1	1.73	0.54
1:A:140:GLN:O	1:A:143:ILE:HG13	2.08	0.54
1:A:328:LYS:HG3	1:A:332:TYR:CG	2.43	0.53
1:A:194:MET:HE3	1:B:569:ILE:HG21	1.91	0.53
1:B:650:LEU:HD12	1:B:650:LEU:C	2.33	0.53
1:B:587:THR:CG2	4:B:1054:HOH:O	2.55	0.53
1:B:311:ILE:HA	1:B:314:MET:HE2	1.90	0.53
1:B:696:TYR:HB3	1:B:736:ARG:NH1	2.23	0.53
1:B:654:ASN:O	1:B:685:VAL:CG2	2.56	0.53
1:A:311:ILE:HD13	1:A:314:MET:CE	2.39	0.53
1:A:561:LYS:HB2	1:A:561:LYS:NZ	2.24	0.53
1:B:66:GLU:CD	1:B:66:GLU:H	2.16	0.53
1:B:506:LEU:HD23	1:B:515:LEU:HD12	1.90	0.52
1:A:859:ARG:NH1	1:A:861:GLU:OE2	2.42	0.52
1:A:868:ALA:HB2	1:B:780:LEU:HD11	1.90	0.52
1:B:696:TYR:HB3	1:B:736:ARG:HH11	1.75	0.52
1:B:198:PRO:HG3	1:B:228:LEU:CD2	2.40	0.52
1:A:182:LEU:N	1:A:182:LEU:HD12	2.26	0.51
1:B:685:VAL:HG22	1:B:686:TYR:N	2.25	0.51
1:B:244:ILE:HD12	1:B:244:ILE:H	1.76	0.51
1:B:262:GLN:HG2	1:B:323:GLN:HE21	1.75	0.51
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.92	0.51
1:A:663:ALA:O	1:A:666:VAL:HG13	2.11	0.51
1:A:634:ASN:HB2	1:A:832:ASP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:TYR:CE1	1:B:698:MET:HE1	2.46	0.51
1:A:863:ASP:O	1:A:866:VAL:HG22	2.11	0.51
1:A:414:MET:O	1:A:418:ARG:HG2	2.11	0.51
1:B:428:VAL:HG13	1:B:428:VAL:O	2.11	0.51
1:B:432:ASP:OD1	1:B:432:ASP:N	2.43	0.51
1:A:522:GLU:OE1	1:B:264:LEU:HD22	2.11	0.50
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.92	0.50
1:B:352:THR:OG1	1:B:355:GLN:HG3	2.12	0.50
1:B:524:ARG:HD2	1:B:529:GLU:OE2	2.12	0.50
1:B:241:ALA:HB1	1:B:244:ILE:HD13	1.94	0.50
1:A:272:GLY:O	1:A:318:VAL:CG2	2.60	0.50
1:A:638:LEU:C	1:A:638:LEU:HD23	2.37	0.50
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.93	0.50
1:A:735:LEU:HD12	1:A:738:VAL:CG2	2.42	0.49
1:B:112:SER:HB3	1:B:392:LYS:HA	1.94	0.49
1:B:244:ILE:HD12	1:B:244:ILE:N	2.26	0.49
1:A:321:ASP:O	1:A:324:THR:HB	2.12	0.49
1:B:262:GLN:CG	1:B:323:GLN:NE2	2.75	0.49
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.43	0.49
1:A:502:LEU:HD23	1:A:531:LEU:CD1	2.42	0.49
1:A:806:LEU:HD11	1:B:806:LEU:HD11	1.95	0.49
1:A:853:LEU:O	1:A:862:ILE:HD11	2.12	0.49
1:B:323:GLN:O	1:B:326:LYS:HG3	2.13	0.48
1:A:311:ILE:HD13	1:A:314:MET:HE1	1.94	0.48
1:B:255:PHE:CB	1:B:385:VAL:HG12	2.40	0.48
1:B:656:ILE:CD1	1:B:685:VAL:HG21	2.43	0.48
1:B:269:THR:OG1	1:B:274:ILE:HG23	2.13	0.48
1:A:178:PRO:HA	1:A:187:TRP:CG	2.48	0.48
1:A:497:ALA:HB1	1:A:666:VAL:CG1	2.39	0.48
1:B:765:ALA:O	1:B:769:GLN:HG3	2.14	0.48
1:A:867:VAL:CG1	1:B:779:PRO:HG3	2.44	0.48
3:A:887:TDK:OM1	3:A:887:TDK:H7'1	2.14	0.48
1:B:177:TYR:HB3	1:B:178:PRO:CD	2.43	0.48
1:A:322:TYR:HA	1:A:325:PHE:CD2	2.49	0.48
1:A:569:ILE:HD12	1:B:231:GLY:C	2.39	0.48
1:B:262:GLN:HB2	1:B:392:LYS:HD2	1.96	0.48
1:B:506:LEU:CD2	1:B:515:LEU:HD12	2.44	0.48
1:B:143:ILE:HD12	1:B:143:ILE:C	2.39	0.47
1:A:663:ALA:HA	1:A:666:VAL:HG12	1.96	0.47
3:B:887:TDK:H7'1	3:B:887:TDK:OM1	2.14	0.47
1:B:696:TYR:CD2	1:B:736:ARG:NH1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:ARG:HG3	4:A:955:HOH:O	2.14	0.47
1:B:522:GLU:OE1	1:B:522:GLU:CA	2.63	0.47
1:A:342:PRO:O	1:A:346:ALA:HB2	2.15	0.47
1:A:352:THR:HG1	1:A:355:GLN:CD	2.23	0.47
1:B:140:GLN:O	1:B:143:ILE:HG13	2.15	0.47
1:B:696:TYR:HD2	1:B:736:ARG:NH1	2.13	0.47
1:A:517:PRO:HB2	1:A:564:ILE:HG12	1.96	0.47
1:B:697:HIS:O	1:B:698:MET:HE2	2.15	0.47
1:B:698:MET:HE2	1:B:698:MET:CA	2.36	0.47
1:A:144:SER:OG	1:A:145:PRO:HD3	2.15	0.47
1:A:509:LYS:HA	1:A:512:LYS:HE3	1.97	0.46
1:B:435:LYS:O	1:B:436:LEU:C	2.59	0.46
1:B:189:PHE:HA	1:B:190:PRO:HD3	1.85	0.46
1:A:262:GLN:CG	1:A:323:GLN:NE2	2.79	0.46
1:A:262:GLN:CG	1:A:323:GLN:HE21	2.29	0.45
1:B:392:LYS:HE2	3:B:887:TDK:O2B	2.16	0.45
1:B:458:LEU:O	1:B:459:HIS:HB2	2.17	0.45
1:B:522:GLU:HG2	1:B:599:TYR:CZ	2.51	0.45
1:B:537:ILE:HG23	1:B:558:GLU:HA	1.98	0.45
1:B:696:TYR:CE1	1:B:698:MET:CE	2.99	0.45
1:B:696:TYR:HD2	1:B:736:ARG:HH11	1.60	0.45
1:A:265:ASP:OD2	1:B:521:ASP:O	2.34	0.45
1:A:418:ARG:HH11	1:A:418:ARG:CG	2.29	0.45
1:B:77:LEU:HD21	1:B:447:GLU:HA	1.98	0.45
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.97	0.45
1:A:328:LYS:HD2	1:A:332:TYR:CD2	2.52	0.45
1:B:522:GLU:OE1	1:B:522:GLU:HA	2.17	0.45
1:A:277:GLU:OE2	1:B:243:THR:CG2	2.63	0.45
1:A:301:LEU:CD1	1:A:310:LEU:HD22	2.42	0.45
1:A:868:ALA:HB2	1:B:780:LEU:CD1	2.47	0.45
1:B:144:SER:N	1:B:145:PRO:CD	2.80	0.45
1:B:731:SER:HB2	1:B:758:VAL:O	2.16	0.45
1:A:522:GLU:OE2	1:B:264:LEU:CD2	2.64	0.45
1:A:352:THR:C	1:A:354:GLU:N	2.75	0.45
1:B:423:ARG:O	1:B:423:ARG:HD3	2.17	0.44
1:A:214:ARG:HB2	1:A:216:LEU:HD22	2.00	0.44
1:A:328:LYS:HG3	1:A:332:TYR:CE1	2.52	0.44
1:A:692:LEU:HD13	1:A:733:SER:HB3	1.99	0.44
1:B:287:TRP:CZ3	1:B:385:VAL:HG13	2.52	0.44
1:B:662:TYR:HD1	1:B:698:MET:CE	2.29	0.44
1:B:274:ILE:HG13	1:B:275:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:ASN:C	1:B:685:VAL:HG23	2.42	0.44
1:A:297:ARG:HB2	1:A:359:LEU:HD23	1.99	0.44
1:B:429:SER:C	1:B:431:ALA:N	2.75	0.44
1:B:354:GLU:CD	1:B:354:GLU:H	2.26	0.44
1:A:332:TYR:CD1	1:A:332:TYR:O	2.71	0.43
1:A:522:GLU:CD	1:B:264:LEU:CD2	2.90	0.43
1:A:821:ARG:HH12	1:A:854:GLY:HA3	1.82	0.43
3:B:887:TDK:OM1	3:B:887:TDK:N4'	2.47	0.43
1:B:74:ASN:O	1:B:78:GLU:HG3	2.19	0.43
1:B:262:GLN:CG	1:B:323:GLN:HE21	2.31	0.43
1:A:74:ASN:O	1:A:78:GLU:HG3	2.18	0.43
1:A:189:PHE:HA	1:A:190:PRO:HD3	1.88	0.43
1:B:178:PRO:HA	1:B:187:TRP:CG	2.54	0.43
1:B:696:TYR:CD1	1:B:698:MET:CE	3.02	0.43
1:A:334:ARG:HA	1:A:338:PHE:HB2	2.00	0.43
1:B:725:LYS:HE3	1:B:754:ASP:OD2	2.19	0.43
1:A:262:GLN:HG3	1:A:323:GLN:NE2	2.34	0.43
1:B:289:VAL:O	1:B:289:VAL:HG23	2.17	0.43
1:B:715:LYS:HD3	1:B:718:THR:HG22	2.01	0.43
1:A:497:ALA:HB3	1:A:666:VAL:HG11	1.98	0.43
1:A:805:LYS:HG3	1:A:826:ASP:OD1	2.19	0.43
1:A:462:LEU:HB2	1:A:463:PRO:HA	2.01	0.42
1:B:696:TYR:HD1	1:B:698:MET:HE3	1.83	0.42
1:A:479:GLN:HG2	1:A:480:ASP:N	2.34	0.42
1:A:663:ALA:HA	1:A:666:VAL:CG1	2.50	0.42
1:A:664:TYR:CG	1:A:701:MET:HB2	2.53	0.42
1:A:711:LYS:HD2	1:A:787:TYR:CE1	2.54	0.42
1:A:711:LYS:HD2	1:A:787:TYR:CZ	2.53	0.42
1:A:198:PRO:HD3	1:A:228:LEU:HD22	2.00	0.42
1:B:262:GLN:HE21	1:B:323:GLN:HE22	1.67	0.42
1:B:301:LEU:HD12	1:B:301:LEU:HA	1.90	0.42
1:A:213:HIS:HB3	1:A:560:GLU:HB2	2.01	0.42
1:A:63:ILE:HD11	1:A:375:LYS:HD2	2.01	0.42
1:A:663:ALA:C	1:A:666:VAL:HG12	2.44	0.42
1:A:159:GLN:HG3	1:A:438:TYR:CD2	2.55	0.42
1:A:397:GLY:O	1:A:398:ASP:C	2.64	0.41
1:A:436:LEU:N	1:A:437:PRO:CD	2.82	0.41
1:A:650:LEU:C	1:A:650:LEU:HD12	2.45	0.41
1:B:743:GLU:O	1:B:747:LYS:HG2	2.20	0.41
1:A:329:ASP:CG	1:A:331:ALA:H	2.28	0.41
1:A:532:PHE:N	1:A:532:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:LEU:HB2	1:A:862:ILE:HG12	2.02	0.41
1:B:415:ASP:OD1	1:B:418:ARG:HD3	2.21	0.41
1:A:336:HIS:CD2	1:A:336:HIS:N	2.89	0.41
1:A:352:THR:O	1:A:355:GLN:N	2.52	0.41
1:B:427:PRO:HG2	1:B:439:ILE:HD13	2.02	0.41
1:A:865:LYS:HE3	1:A:865:LYS:HB2	1.76	0.41
1:B:399:ALA:O	1:B:400:ALA:CB	2.68	0.41
1:A:239:LYS:O	1:A:242:ILE:HG12	2.20	0.41
1:A:398:ASP:CG	1:A:399:ALA:H	2.28	0.41
1:A:519:ILE:CG2	1:A:520:ALA:N	2.81	0.41
1:A:806:LEU:HA	1:A:809:GLU:HB2	2.03	0.41
3:A:887:TDK:H62	1:B:569:ILE:HD11	2.03	0.40
1:B:429:SER:C	1:B:431:ALA:H	2.29	0.40
1:A:178:PRO:HA	1:A:187:TRP:CD2	2.56	0.40
1:B:87:TRP:CD2	1:B:426:VAL:HG11	2.56	0.40
1:B:103:LEU:O	1:B:166:ARG:HD3	2.22	0.40
1:B:153:LEU:HD12	1:B:153:LEU:HA	1.93	0.40
1:A:304:LYS:HE2	1:A:347:LEU:CD2	2.50	0.40
1:B:322:TYR:HA	1:B:325:PHE:CD2	2.56	0.40
1:A:325:PHE:C	1:A:327:SER:H	2.29	0.40
1:A:418:ARG:CG	1:A:418:ARG:NH1	2.84	0.40
1:A:683:GLU:HG2	1:A:685:VAL:HG13	2.02	0.40
1:B:99:LYS:HE3	4:B:1087:HOH:O	2.22	0.40
1:B:210:TYR:CZ	1:B:214:ARG:HD3	2.57	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	795/886 (90%)	762 (96%)	30 (4%)	3 (0%)	30 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	795/886 (90%)	762 (96%)	33 (4%)	0	100	100
All	All	1590/1772 (90%)	1524 (96%)	63 (4%)	3 (0%)	43	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ASP
1	A	399	ALA
1	A	326	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	665/735 (90%)	650 (98%)	15 (2%)	44	25
1	B	665/735 (90%)	642 (96%)	23 (4%)	32	11
All	All	1330/1470 (90%)	1292 (97%)	38 (3%)	37	16

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	GLU
1	A	192	VAL
1	A	211	LEU
1	A	216	LEU
1	A	278	LEU
1	A	301	LEU
1	A	335	GLU
1	A	356	ILE
1	A	420	ILE
1	A	479	GLN
1	A	560	GLU
1	A	561	LYS
1	A	780	LEU

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Mol	Chain	Res	Type
1	A	859	ARG
1	A	861	GLU
1	B	56	ILE
1	B	66	GLU
1	B	77	LEU
1	B	196	LEU
1	B	211	LEU
1	B	243	THR
1	B	278	LEU
1	B	301	LEU
1	B	326	LYS
1	B	340	LYS
1	B	343	GLU
1	B	417	VAL
1	B	421	ARG
1	B	432	ASP
1	B	475	LEU
1	B	502	LEU
1	B	522	GLU
1	B	537	ILE
1	B	587	THR
1	B	610	LEU
1	B	638	LEU
1	B	718	THR
1	B	819	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	323	GLN
1	A	336	HIS
1	A	377	GLN
1	A	588	ASN
1	A	695	ASN
1	A	793	ASN
1	A	810	GLN
1	B	122	ASN
1	B	323	GLN
1	B	695	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	TDK	B	887	2	31,35,35	1.54	5 (16%)	41,55,55	1.18	4 (9%)
3	TDK	A	887	2	31,35,35	1.56	4 (12%)	41,55,55	1.25	5 (12%)

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
3	TDK	B	887	2	-	3/28/35/35	0/2/2/2
3	TDK	A	887	2	-	4/28/35/35	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	887	TDK	PA-O3A	3.46	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	887	TDK	PC-OM3	-3.41	1.50	1.56
3	B	887	TDK	C6'-C5'	-3.39	1.31	1.37
3	A	887	TDK	C7'-N3	3.32	1.51	1.47
3	B	887	TDK	PA-O3A	3.08	1.62	1.59
3	B	887	TDK	PC-OM3	-3.04	1.50	1.56
3	B	887	TDK	C7'-N3	2.86	1.50	1.47
3	A	887	TDK	C6'-C5'	-2.68	1.32	1.37
3	B	887	TDK	C4-N3	-2.07	1.37	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	887	TDK	OM4-PC-CMA	-3.58	109.83	113.45
3	B	887	TDK	OM4-PC-CMA	-3.14	110.28	113.45
3	A	887	TDK	OM2-PC-OM4	-2.94	108.25	114.62
3	B	887	TDK	OM2-PC-OM4	-2.69	108.79	114.62
3	B	887	TDK	OM3-PC-OM4	2.53	117.55	111.17
3	B	887	TDK	C6'-N1'-C2'	2.50	120.18	116.07
3	A	887	TDK	C6'-N1'-C2'	2.45	120.10	116.07
3	A	887	TDK	OM3-PC-OM4	2.40	117.20	111.17
3	A	887	TDK	S1-C2-N3	-2.03	110.25	112.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

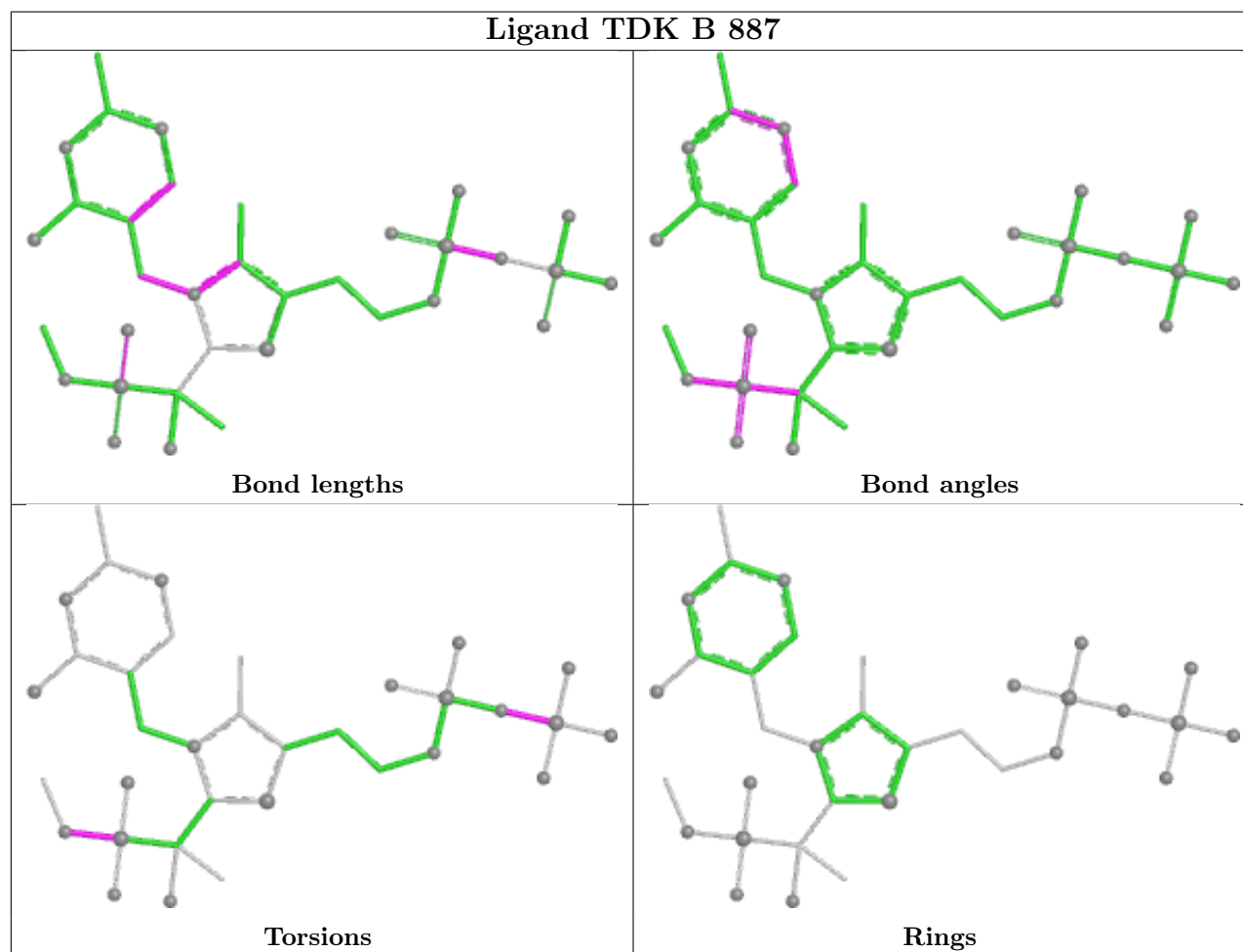
Mol	Chain	Res	Type	Atoms
3	A	887	TDK	PA-O3A-PB-O2B
3	B	887	TDK	PA-O3A-PB-O2B
3	A	887	TDK	CMC-OM2-PC-OM4
3	A	887	TDK	PA-O3A-PB-O3B
3	B	887	TDK	PA-O3A-PB-O3B
3	B	887	TDK	CMC-OM2-PC-OM4
3	A	887	TDK	C5-C6-C7-O7

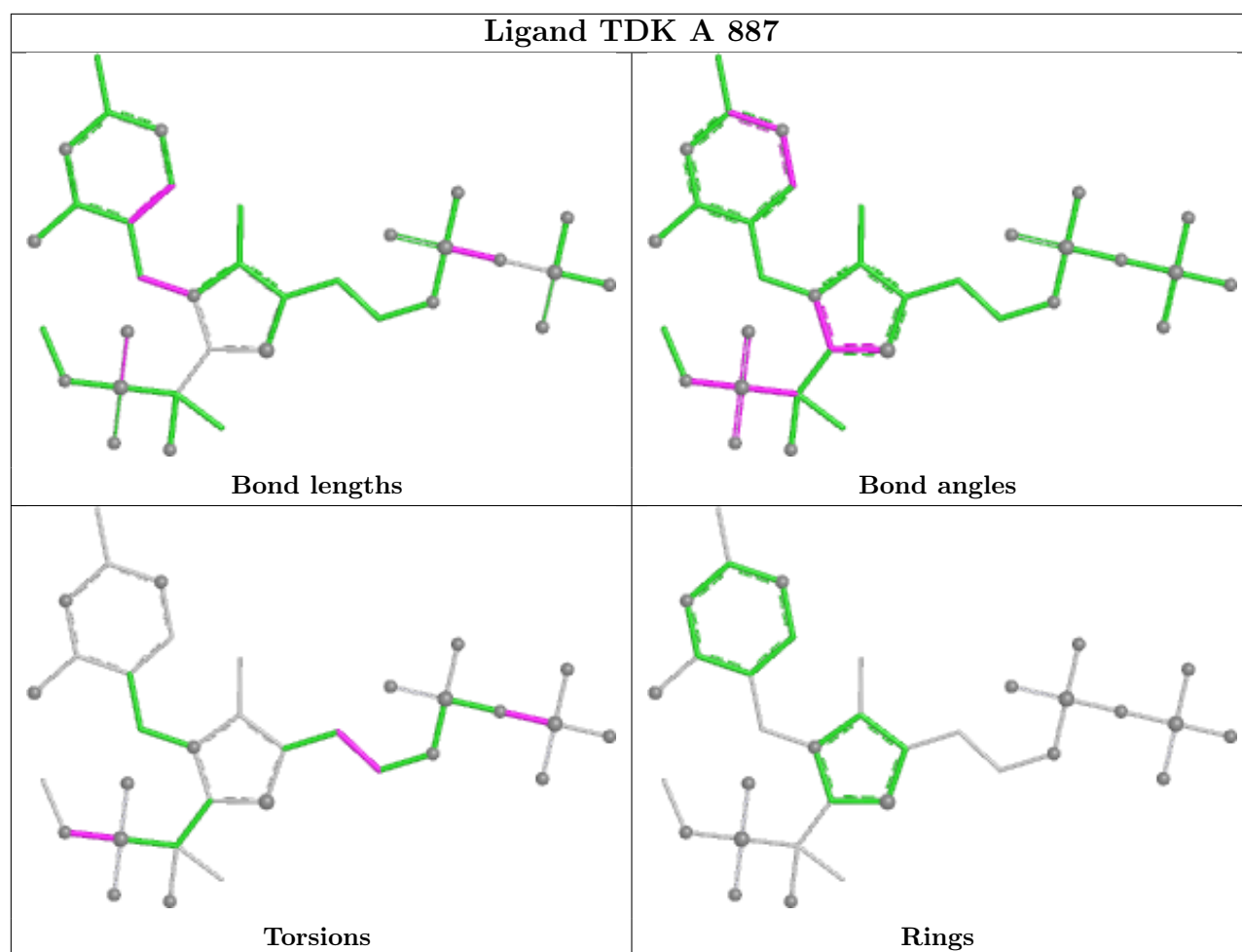
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	887	TDK	6	0
3	A	887	TDK	8	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	801/886 (90%)	0.59	78 (9%) 13 15	14, 22, 37, 42	0
1	B	801/886 (90%)	0.44	46 (5%) 29 35	12, 20, 31, 41	0
All	All	1602/1772 (90%)	0.51	124 (7%) 19 23	12, 21, 35, 42	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	ALA	9.5
1	A	400	ALA	6.6
1	B	400	ALA	6.5
1	B	414	MET	6.4
1	B	415	ASP	5.0
1	A	339	GLY	5.0
1	A	399	ALA	4.7
1	B	56	ILE	4.5
1	B	530	GLY	4.3
1	A	301	LEU	4.3
1	A	349	ALA	4.2
1	A	524	ARG	4.2
1	A	398	ASP	4.2
1	A	333	VAL	4.2
1	A	330	GLY	4.2
1	A	311	ILE	4.2
1	B	522	GLU	4.0
1	A	56	ILE	3.9
1	A	327	SER	3.9
1	B	533	ARG	3.8
1	B	398	ASP	3.8
1	A	351	TRP	3.8
1	A	305	ASP	3.8
1	A	418	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	434	GLU	3.7
1	A	342	PRO	3.7
1	A	331	ALA	3.7
1	A	345	ALA	3.7
1	B	416	GLY	3.7
1	A	306	THR	3.6
1	A	720	GLU	3.6
1	B	532	PHE	3.5
1	B	531	LEU	3.5
1	A	332	TYR	3.5
1	A	341	TYR	3.5
1	B	537	ILE	3.4
1	A	397	GLY	3.3
1	A	325	PHE	3.3
1	B	431	ALA	3.2
1	B	818	ASP	3.2
1	A	354	GLU	3.2
1	A	533	ARG	3.2
1	B	529	GLU	3.2
1	B	428	VAL	3.1
1	A	340	LYS	3.1
1	A	531	LEU	3.1
1	A	337	PHE	3.1
1	A	348	VAL	3.0
1	B	420	ILE	2.9
1	A	860	GLY	2.9
1	B	172	ASN	2.9
1	A	318	VAL	2.9
1	A	329	ASP	2.9
1	B	524	ARG	2.8
1	B	490	LYS	2.8
1	A	522	GLU	2.8
1	A	558	GLU	2.8
1	A	308	GLY	2.8
1	A	866	VAL	2.8
1	B	558	GLU	2.8
1	A	130	GLU	2.7
1	A	338	PHE	2.7
1	A	350	ASP	2.7
1	A	344	THR	2.7
1	A	530	GLY	2.7
1	A	334	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	540	PRO	2.6
1	A	537	ILE	2.6
1	A	862	ILE	2.6
1	A	264	LEU	2.5
1	A	302	LEU	2.5
1	A	560	GLU	2.5
1	B	685	VAL	2.5
1	A	346	ALA	2.5
1	A	324	THR	2.5
1	A	336	HIS	2.5
1	B	300	GLU	2.5
1	A	131	GLN	2.5
1	B	433	ILE	2.5
1	A	352	THR	2.5
1	B	429	SER	2.4
1	B	350	ASP	2.4
1	B	76	GLU	2.4
1	B	680	GLU	2.4
1	A	561	LYS	2.4
1	A	425	ASN	2.4
1	A	265	ASP	2.4
1	A	304	LYS	2.4
1	B	385	VAL	2.4
1	B	97	SER	2.3
1	B	721	GLY	2.3
1	A	300	GLU	2.3
1	A	313	LEU	2.3
1	A	534	GLN	2.3
1	A	356	ILE	2.3
1	A	323	GLN	2.2
1	B	846	SER	2.2
1	B	265	ASP	2.2
1	A	532	PHE	2.2
1	A	519	ILE	2.2
1	B	169	VAL	2.2
1	B	417	VAL	2.2
1	A	347	LEU	2.2
1	B	77	LEU	2.2
1	A	444	GLY	2.2
1	B	599	TYR	2.2
1	A	417	VAL	2.2
1	A	353	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	430	ASP	2.2
1	A	76	GLU	2.2
1	B	539	SER	2.2
1	A	160	GLU	2.1
1	A	297	ARG	2.1
1	A	322	TYR	2.1
1	B	426	VAL	2.1
1	A	864	LYS	2.1
1	B	432	ASP	2.1
1	A	326	LYS	2.1
1	A	863	ASP	2.1
1	A	357	TRP	2.1
1	B	718	THR	2.0
1	A	599	TYR	2.0
1	B	859	ARG	2.0
1	B	722	SER	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.

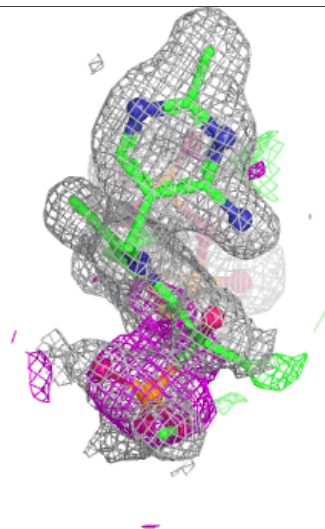
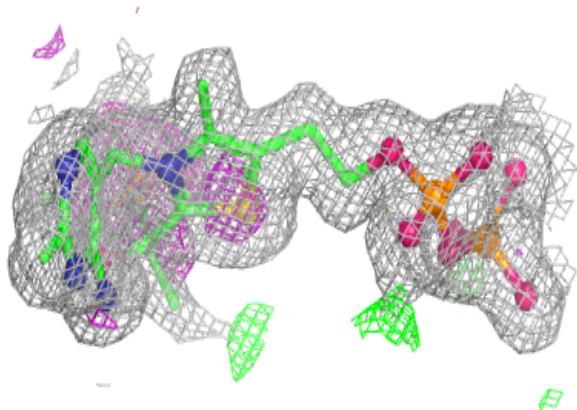
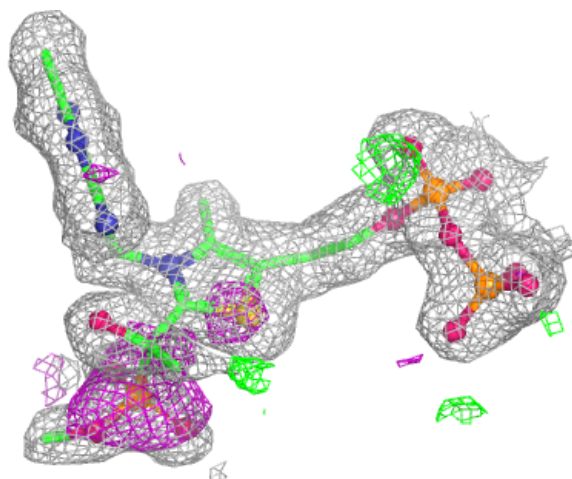
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TDK	A	887	34/34	0.89	0.12	22,25,28,28	0
3	TDK	B	887	34/34	0.89	0.12	20,23,27,27	0
2	MG	A	888	1/1	0.98	0.04	21,21,21,21	0
2	MG	B	888	1/1	0.98	0.04	19,19,19,19	0

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.

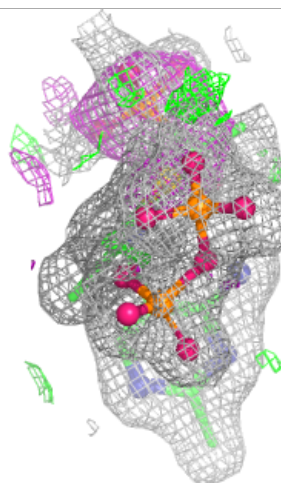
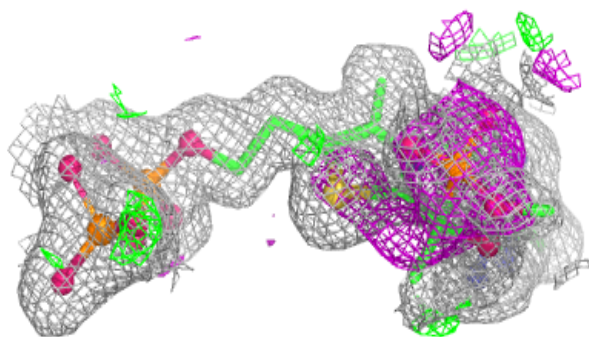
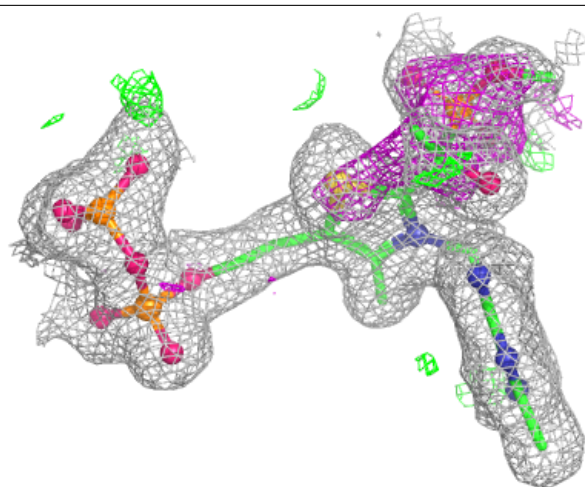
Electron density around TDK A 887:

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



Electron density around TDK B 887:

$2mF_o-DF_c$ (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.