



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:40 AM UTC

PDB ID : 2G28 / pdb_00002g28
Title : E. Coli Pyruvate Dehydrogenase H407A variant Phosphonolactylthiamin Diphosphate Complex
Authors : Furey, W.; Arjunan, P.; Chandrasekhar, K.
Deposited on : 2006-02-15
Resolution : 1.85 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

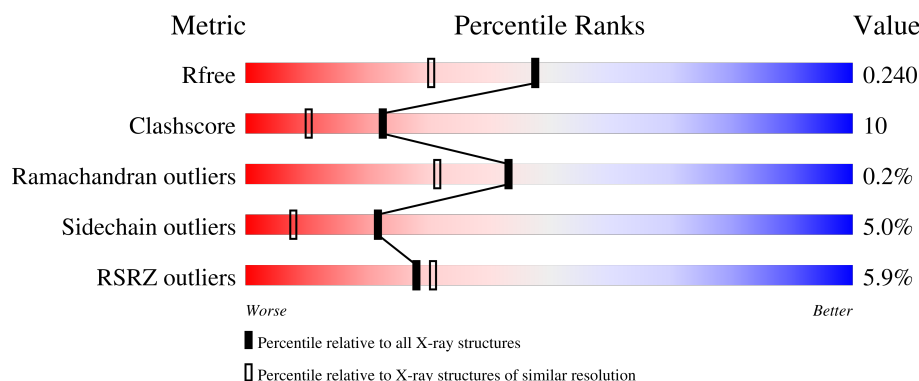
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	6% 70% 17% •• 10%
1	B	886	5% 73% 15% • 10%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13301 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.

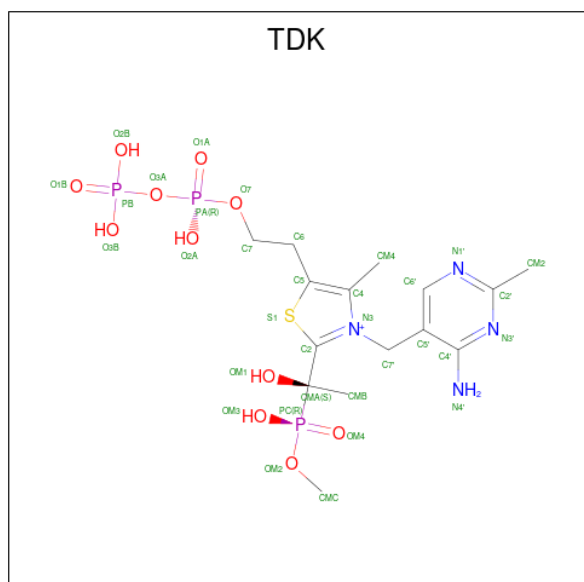
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

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			

- 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(PHOSPHONOXY)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

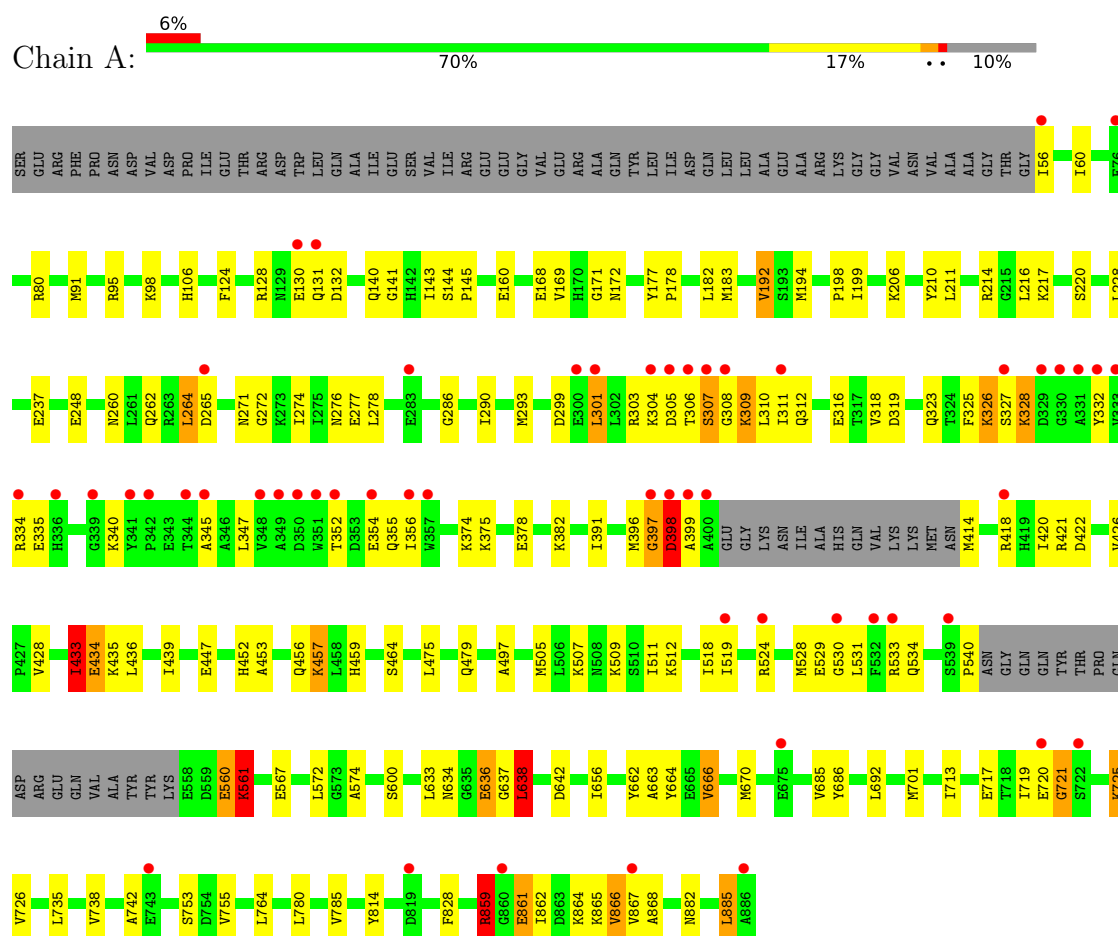
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	278	Total 278	O 278	0	0
4	B	271	Total 271	O 271	0	0

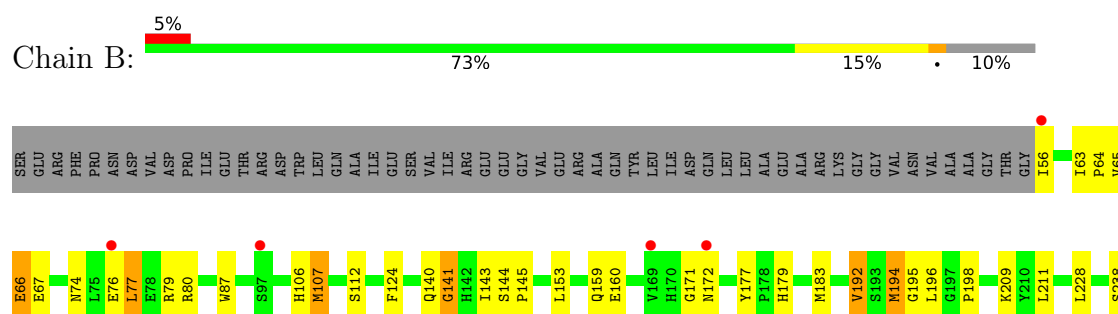
3 Residue-property plots [i](#)

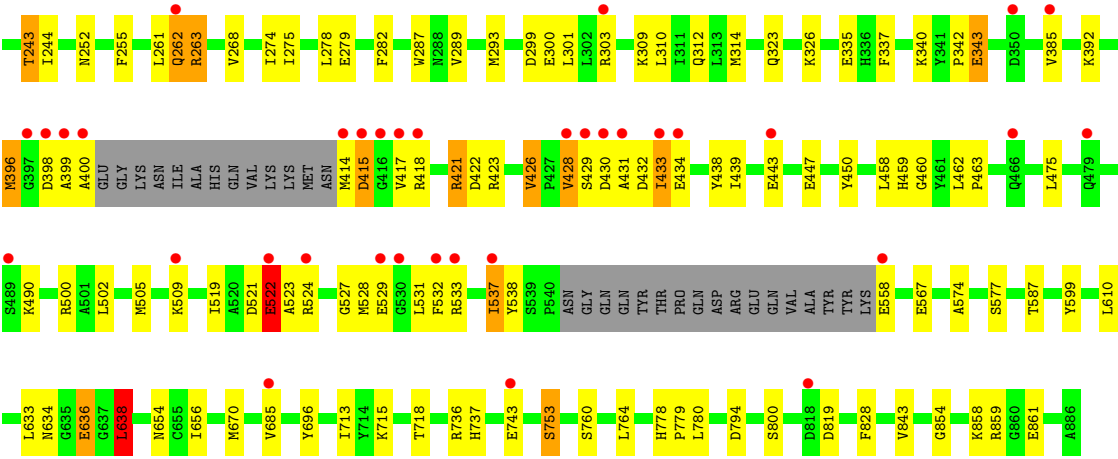
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Pyruvate 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	81.99Å 143.20Å 82.53Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	41.77 – 1.85 41.77 – 1.85	Depositor EDS
% Data completeness (in resolution range)	95.2 (41.77-1.85) 95.2 (41.77-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.68 (at 1.55Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.240 0.216 , 0.240	Depositor DCC
R_{free} test set	7535 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13301	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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	0.57	0/6484	1.02	33/8766 (0.4%)
1	B	0.57	1/6484 (0.0%)	1.02	28/8766 (0.3%)
All	All	0.57	1/12968 (0.0%)	1.02	61/17532 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	MET	SD-CE	-5.09	1.66	1.79

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	634	ASN	N-CA-C	9.88	122.05	111.28
1	A	634	ASN	N-CA-C	9.85	123.25	111.33
1	A	633	LEU	N-CA-C	-8.82	99.54	110.65
1	A	171	GLY	N-CA-C	8.63	127.23	115.32
1	B	638	LEU	N-CA-C	8.27	121.03	111.11
1	B	417	VAL	N-CA-C	-7.88	101.55	112.50
1	A	459	HIS	N-CA-C	7.66	122.34	113.38
1	A	433	ILE	N-CA-C	7.44	118.21	110.62
1	A	534	GLN	N-CA-C	7.18	118.80	110.97
1	B	141	GLY	N-CA-C	6.92	121.01	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	633	LEU	N-CA-C	-6.91	99.25	109.62
1	B	426	VAL	CA-C-N	6.88	128.44	119.84
1	B	426	VAL	C-N-CA	6.88	128.44	119.84
1	B	523	ALA	N-CA-C	-6.82	103.99	112.72
1	A	662	TYR	N-CA-C	6.80	120.68	110.14
1	A	636	GLU	N-CA-C	6.76	119.67	111.82
1	B	124	PHE	N-CA-C	6.65	121.23	112.72
1	A	859	ARG	NE-CZ-NH1	-6.61	114.89	121.50
1	B	396	MET	N-CA-C	-6.41	105.50	113.38
1	A	299	ASP	N-CA-C	6.23	117.73	111.07
1	A	220	SER	N-CA-C	6.09	119.81	112.38
1	B	753	SER	N-CA-C	6.03	117.40	108.60
1	A	307	SER	N-CA-C	-5.98	105.06	112.90
1	B	636	GLU	N-CA-C	5.97	118.75	111.82
1	A	169	VAL	N-CA-C	5.96	116.70	110.62
1	B	335	GLU	N-CA-C	5.92	118.62	111.40
1	A	183	MET	CA-C-N	5.91	125.61	119.82
1	A	183	MET	C-N-CA	5.91	125.61	119.82
1	B	171	GLY	N-CA-C	5.89	122.58	114.92
1	A	692	LEU	N-CA-C	5.89	119.27	110.14
1	B	460	GLY	N-CA-C	5.86	117.48	111.56
1	B	778	HIS	CA-C-N	5.83	125.50	119.56
1	B	778	HIS	C-N-CA	5.83	125.50	119.56
1	B	238	SER	N-CA-C	5.72	117.19	111.07
1	B	183	MET	CA-C-N	5.70	125.37	119.56
1	B	183	MET	C-N-CA	5.70	125.37	119.56
1	A	637	GLY	N-CA-C	5.69	122.84	112.37
1	A	293	MET	N-CA-C	5.66	120.19	112.04
1	A	475	LEU	N-CA-C	5.65	117.70	109.84
1	A	785	VAL	N-CA-C	5.60	114.66	108.05
1	A	345	ALA	N-CA-C	-5.55	105.31	111.36
1	A	124	PHE	N-CA-C	5.47	119.73	112.72
1	A	168	GLU	N-CA-C	5.44	120.08	113.38
1	B	63	ILE	N-CA-C	5.40	112.90	107.55
1	A	642	ASP	N-CA-C	5.39	117.48	107.99
1	B	522	GLU	N-CA-C	5.34	122.18	110.80
1	A	600	SER	N-CA-C	5.34	117.79	111.33
1	B	794	ASP	N-CA-C	5.31	119.45	112.92
1	A	561	LYS	N-CA-C	-5.27	106.90	113.38
1	B	262	GLN	N-CA-C	5.27	117.83	109.50
1	A	511	ILE	N-CA-C	5.24	118.77	113.47
1	A	306	THR	N-CA-C	-5.13	105.79	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	GLY	N-CA-C	-5.11	108.27	115.32
1	B	293	MET	N-CA-C	5.11	119.39	112.04
1	A	721	GLY	N-CA-C	-5.11	101.08	113.18
1	A	753	SER	N-CA-C	5.09	116.58	108.79
1	B	760	SER	N-CA-C	5.08	115.70	107.32
1	A	260	ASN	N-CA-C	-5.06	106.95	113.02
1	A	638	LEU	N-CA-C	5.04	119.69	111.37
1	B	577	SER	N-CA-C	-5.03	105.88	111.36
1	B	431	ALA	N-CA-C	-5.00	106.95	113.16

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	686	TYR	Sidechain
1	A	814	TYR	Sidechain

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	6341	0	6179	142	0
1	B	6341	0	6179	128	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	34	0	22	5	0
3	B	34	0	22	3	0
4	A	278	0	0	3	0
4	B	271	0	0	5	0
All	All	13301	0	12402	264	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 10.

All (264) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:LYS:HB2	1:A:561:LYS:NZ	1.77	0.99
1:B:177:TYR:HB3	1:B:192:VAL:HG21	1.43	0.97
1:B:490:LYS:HE2	1:B:500:ARG:HH22	1.29	0.96
1:A:868:ALA:HB2	1:B:780:LEU:HD11	1.46	0.95
1:A:418:ARG:HH21	1:A:421:ARG:HH21	1.13	0.94
1:A:326:LYS:HB3	1:A:326:LYS:NZ	1.82	0.92
1:A:561:LYS:HB2	1:A:561:LYS:HZ2	1.32	0.92
1:A:326:LYS:HB3	1:A:326:LYS:HZ2	1.32	0.91
1:A:540:PRO:HB3	1:A:560:GLU:HB3	1.53	0.91
1:B:177:TYR:CB	1:B:192:VAL:HG21	2.00	0.91
1:A:177:TYR:CB	1:A:192:VAL:HG21	2.05	0.86
1:A:326:LYS:HD2	1:A:391:ILE:HG23	1.58	0.85
1:A:862:ILE:HD12	1:A:866:VAL:HG22	1.59	0.83
1:B:490:LYS:HE2	1:B:500:ARG:NH2	1.93	0.82
1:A:859:ARG:CB	1:A:859:ARG:HH11	1.93	0.82
1:A:177:TYR:HB3	1:A:192:VAL:HG21	1.64	0.79
1:B:414:MET:O	1:B:414:MET:HG2	1.81	0.79
1:B:177:TYR:HB3	1:B:192:VAL:CG2	2.12	0.79
1:A:418:ARG:NH2	1:A:421:ARG:HH21	1.80	0.78
1:A:290:ILE:HD11	1:A:375:LYS:HD2	1.65	0.78
1:B:287:TRP:CE3	1:B:385:VAL:HG13	2.19	0.77
1:B:192:VAL:HG23	4:B:903:HOH:O	1.84	0.77
1:B:262:GLN:HG3	1:B:323:GLN:HE21	1.50	0.77
1:B:255:PHE:HB2	1:B:385:VAL:HG12	1.67	0.76
1:A:352:THR:OG1	1:A:355:GLN:HG3	1.86	0.75
1:B:859:ARG:NH1	1:B:861:GLU:OE1	2.20	0.75
1:B:490:LYS:CE	1:B:500:ARG:HH22	1.99	0.75
1:A:414:MET:HE2	1:A:434:GLU:HA	1.69	0.74
1:B:421:ARG:NH1	1:B:422:ASP:OD1	2.19	0.74
1:B:656:ILE:HG12	1:B:685:VAL:CG2	2.17	0.74
1:A:638:LEU:HD22	1:A:828:PHE:HB3	1.68	0.73
1:B:426:VAL:HG12	1:B:428:VAL:HG12	1.70	0.73
1:A:862:ILE:HD12	1:A:866:VAL:CG2	2.18	0.73
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.19	0.73
1:A:540:PRO:CB	1:A:560:GLU:HB3	2.19	0.72
1:A:326:LYS:O	1:A:326:LYS:HG2	1.89	0.72
1:B:421:ARG:HG3	1:B:421:ARG:HH11	1.54	0.72
1:A:530:GLY:HA2	1:A:533:ARG:NH1	2.05	0.71
1:A:859:ARG:NH1	1:A:861:GLU:OE1	2.22	0.71
1:A:720:GLU:HG2	1:A:721:GLY:N	2.06	0.71
1:B:656:ILE:HG12	1:B:685:VAL:HG21	1.73	0.70
1:B:522:GLU:N	1:B:522:GLU:OE1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.72	0.70
1:A:374:LYS:O	1:A:378:GLU:HG3	1.92	0.70
1:A:352:THR:HG23	1:A:355:GLN:CD	2.17	0.70
1:A:312:GLN:O	1:A:316:GLU:HG2	1.93	0.69
1:A:177:TYR:HB3	1:A:192:VAL:CG2	2.21	0.69
1:B:177:TYR:CG	1:B:192:VAL:HG21	2.27	0.69
1:B:656:ILE:CG1	1:B:685:VAL:HG21	2.23	0.69
1:B:715:LYS:HD3	1:B:718:THR:HG22	1.76	0.68
1:B:198:PRO:HG3	1:B:228:LEU:HD22	1.75	0.67
1:A:418:ARG:HE	1:A:421:ARG:NH2	1.91	0.67
1:A:307:SER:OG	1:A:309:LYS:HB2	1.94	0.67
1:A:656:ILE:HG12	1:A:685:VAL:CG2	2.25	0.67
1:A:868:ALA:HB2	1:B:780:LEU:CD1	2.25	0.66
1:B:268:VAL:HB	1:B:274:ILE:HG21	1.77	0.66
1:B:262:GLN:HG3	1:B:323:GLN:NE2	2.10	0.66
1:A:277:GLU:OE2	1:B:243:THR:HG21	1.95	0.66
1:A:518:ILE:C	1:A:519:ILE:HD12	2.20	0.65
1:A:859:ARG:HH11	1:A:859:ARG:HB2	1.62	0.65
1:B:194:MET:HE1	4:B:1005:HOH:O	1.95	0.65
1:B:282:PHE:CD2	1:B:385:VAL:HG11	2.32	0.65
1:B:141:GLY:HA3	1:B:192:VAL:HG22	1.76	0.65
1:B:800:SER:OG	1:B:843:VAL:HG13	1.95	0.65
1:A:418:ARG:NH2	1:A:422:ASP:OD2	2.29	0.65
1:A:128:ARG:NH1	4:A:1074:HOH:O	2.26	0.64
1:A:177:TYR:CG	1:A:192:VAL:HG21	2.31	0.64
1:A:636:GLU:OE1	3:A:887:TDK:HMC1	1.98	0.64
1:A:140:GLN:O	1:A:143:ILE:HG13	1.99	0.63
1:A:262:GLN:HG2	1:A:323:GLN:NE2	2.13	0.63
1:A:274:ILE:O	1:A:278:LEU:HD13	1.99	0.63
1:A:528:MET:HE2	1:A:531:LEU:HD12	1.80	0.63
1:A:264:LEU:HG	1:B:522:GLU:OE2	1.98	0.62
1:A:271:ASN:C	1:A:318:VAL:HG21	2.25	0.62
1:B:587:THR:HG22	4:B:951:HOH:O	2.00	0.62
1:A:56:ILE:HD13	1:A:276:ASN:HB3	1.82	0.62
1:A:326:LYS:CD	1:A:391:ILE:HG23	2.30	0.61
1:A:199:ILE:HD13	1:A:572:LEU:HD22	1.81	0.61
1:A:397:GLY:O	1:A:399:ALA:N	2.34	0.61
1:A:859:ARG:NH1	1:A:859:ARG:HB3	2.15	0.60
1:A:663:ALA:O	1:A:666:VAL:HG13	2.00	0.60
1:A:859:ARG:CB	1:A:859:ARG:NH1	2.64	0.60
1:B:587:THR:HG21	4:B:954:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ARG:HG2	1:B:268:VAL:HG22	1.82	0.60
1:B:421:ARG:HG2	1:B:433:ILE:HD11	1.84	0.60
1:A:453:ALA:O	1:A:457:LYS:HD3	2.02	0.60
1:A:418:ARG:NE	1:A:421:ARG:NH2	2.49	0.60
1:B:107:MET:HE3	1:B:396:MET:HE1	1.84	0.60
1:A:636:GLU:CD	3:A:887:TDK:HMC1	2.27	0.59
1:A:561:LYS:HZ2	1:A:561:LYS:CB	2.11	0.59
1:A:418:ARG:HB3	1:A:418:ARG:CZ	2.31	0.59
1:A:561:LYS:HB2	1:A:561:LYS:HZ3	1.65	0.59
1:A:656:ILE:CG1	1:A:685:VAL:HG21	2.32	0.59
1:B:696:TYR:HB3	1:B:736:ARG:NH1	2.17	0.58
1:A:567:GLU:HG3	1:A:574:ALA:HA	1.85	0.58
1:B:430:ASP:OD1	1:B:430:ASP:O	2.21	0.58
1:B:80:ARG:HD2	1:B:447:GLU:OE2	2.03	0.58
1:B:282:PHE:CE2	1:B:385:VAL:HG11	2.39	0.58
1:A:859:ARG:HH11	1:A:859:ARG:HB3	1.69	0.58
1:B:426:VAL:HG13	1:B:439:ILE:HD11	1.85	0.58
1:A:290:ILE:CD1	1:A:375:LYS:HD2	2.34	0.58
1:A:130:GLU:HG3	1:A:131:GLN:NE2	2.18	0.57
1:B:66:GLU:CD	1:B:66:GLU:H	2.12	0.57
1:B:421:ARG:NH1	1:B:421:ARG:HG3	2.18	0.57
1:B:638:LEU:HD22	1:B:828:PHE:HB3	1.86	0.57
1:A:334:ARG:HB3	1:A:356:ILE:CD1	2.34	0.57
1:B:415:ASP:OD2	1:B:418:ARG:HD3	2.04	0.57
1:B:696:TYR:HB3	1:B:736:ARG:HH11	1.70	0.57
1:A:262:GLN:HG2	1:A:323:GLN:HE21	1.69	0.56
1:B:854:GLY:O	1:B:858:LYS:HG3	2.04	0.56
1:B:261:LEU:HD23	1:B:274:ILE:HD11	1.86	0.56
1:A:206:LYS:HG2	4:A:1128:HOH:O	2.06	0.56
1:A:265:ASP:OD1	1:B:521:ASP:O	2.24	0.56
1:A:323:GLN:HA	1:A:326:LYS:NZ	2.21	0.56
1:A:323:GLN:HA	1:A:326:LYS:HZ1	1.71	0.55
1:B:429:SER:HB3	1:B:432:ASP:OD2	2.05	0.55
1:B:528:MET:O	1:B:532:PHE:HD2	1.90	0.55
1:B:279:GLU:HG3	1:B:289:VAL:HG21	1.88	0.55
1:B:414:MET:O	1:B:414:MET:CG	2.54	0.55
1:A:301:LEU:CD1	1:A:347:LEU:HD13	2.37	0.54
1:A:656:ILE:HG12	1:A:685:VAL:HG22	1.88	0.54
1:B:537:ILE:C	1:B:537:ILE:HD13	2.32	0.54
1:A:656:ILE:HG12	1:A:685:VAL:HG21	1.88	0.54
1:B:522:GLU:OE1	1:B:522:GLU:CA	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:LEU:O	1:A:738:VAL:HG22	2.07	0.54
1:A:352:THR:HG23	1:A:355:GLN:OE1	2.07	0.54
1:A:418:ARG:NH2	1:A:421:ARG:NH2	2.55	0.54
1:A:507:LYS:HA	1:A:507:LYS:HE2	1.90	0.54
1:A:237:GLU:HG2	1:A:572:LEU:HD11	1.90	0.53
1:B:656:ILE:HG12	1:B:685:VAL:HG22	1.87	0.53
1:A:262:GLN:CG	1:A:323:GLN:NE2	2.71	0.53
1:A:426:VAL:HG13	1:A:439:ILE:CD1	2.39	0.53
1:B:636:GLU:CD	3:B:887:TDK:HMC1	2.34	0.53
1:A:396:MET:O	1:A:397:GLY:C	2.51	0.53
1:B:414:MET:HE3	1:B:434:GLU:HG3	1.89	0.53
3:B:887:TDK:H7'1	3:B:887:TDK:OM1	2.08	0.53
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.90	0.53
1:B:342:PRO:HD2	1:B:343:GLU:OE2	2.10	0.52
1:B:140:GLN:O	1:B:143:ILE:HG13	2.09	0.52
1:B:527:GLY:HA2	1:B:529:GLU:OE2	2.09	0.52
1:A:505:MET:HE1	1:A:670:MET:HE2	1.92	0.52
1:B:261:LEU:HA	1:B:274:ILE:CD1	2.38	0.52
1:A:720:GLU:HG2	1:A:721:GLY:H	1.74	0.52
1:A:286:GLY:O	1:A:382:LYS:HE3	2.09	0.51
1:A:426:VAL:HG12	1:A:428:VAL:HG23	1.92	0.51
1:A:509:LYS:HA	1:A:512:LYS:HE3	1.92	0.51
1:A:540:PRO:CA	1:A:560:GLU:HB3	2.40	0.51
1:B:107:MET:HE3	1:B:396:MET:CE	2.39	0.51
1:A:272:GLY:O	1:A:318:VAL:HG23	2.11	0.51
1:A:528:MET:HE2	1:A:531:LEU:CD1	2.40	0.51
1:A:80:ARG:HD2	1:A:447:GLU:OE2	2.11	0.50
1:B:843:VAL:CG1	1:B:843:VAL:O	2.58	0.50
1:A:882:ASN:HB3	1:A:885:LEU:CD2	2.41	0.50
1:B:309:LYS:HE3	1:B:312:GLN:NE2	2.26	0.50
1:B:310:LEU:O	1:B:314:MET:HG3	2.12	0.50
1:A:397:GLY:O	1:A:398:ASP:C	2.55	0.50
1:A:106:HIS:HE1	3:B:887:TDK:OM4	1.93	0.49
1:A:98:LYS:HE2	1:A:436:LEU:HD12	1.95	0.49
1:B:429:SER:HB3	1:B:432:ASP:CG	2.37	0.49
1:B:261:LEU:HA	1:B:274:ILE:HD11	1.93	0.49
1:B:198:PRO:HG3	1:B:228:LEU:CD2	2.42	0.49
1:B:76:GLU:CD	1:B:76:GLU:H	2.21	0.48
3:A:887:TDK:OM1	3:A:887:TDK:H7'1	2.13	0.48
1:B:426:VAL:HG13	1:B:439:ILE:CD1	2.44	0.48
1:B:160:GLU:HG2	1:B:172:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:843:VAL:O	1:B:843:VAL:HG12	2.13	0.48
1:A:326:LYS:O	1:A:326:LYS:CG	2.61	0.47
1:B:195:GLY:C	1:B:198:PRO:HD2	2.39	0.47
1:A:452:HIS:O	1:A:456:GLN:HG2	2.14	0.47
1:B:112:SER:HB3	1:B:392:LYS:HA	1.97	0.47
1:B:64:PRO:HG2	1:B:67:GLU:HG3	1.96	0.46
1:B:610:LEU:C	1:B:610:LEU:HD13	2.40	0.46
1:A:206:LYS:HD2	1:A:248:GLU:HG3	1.96	0.46
1:B:505:MET:CE	1:B:670:MET:HE2	2.45	0.46
1:A:518:ILE:O	1:A:519:ILE:HD12	2.16	0.46
1:B:743:GLU:OE1	1:B:743:GLU:HA	2.16	0.46
1:A:272:GLY:O	1:A:318:VAL:CG2	2.63	0.46
3:A:887:TDK:OM4	1:B:106:HIS:HE1	1.98	0.46
1:B:244:ILE:N	1:B:244:ILE:HD12	2.31	0.46
1:B:398:ASP:C	1:B:400:ALA:H	2.23	0.46
1:B:274:ILE:HG13	1:B:275:ILE:N	2.31	0.46
1:A:328:LYS:HG3	1:A:332:TYR:CD1	2.52	0.45
1:A:656:ILE:HD11	1:A:685:VAL:HG21	1.97	0.45
1:A:91:MET:O	1:A:95:ARG:HG3	2.17	0.45
1:A:328:LYS:HG3	1:A:332:TYR:CG	2.51	0.45
1:B:522:GLU:HG2	1:B:599:TYR:OH	2.16	0.45
1:B:299:ASP:O	1:B:303:ARG:HB3	2.16	0.45
1:B:415:ASP:OD2	1:B:418:ARG:NH1	2.50	0.45
1:A:717:GLU:HG2	1:A:755:VAL:HB	1.97	0.45
1:A:160:GLU:OE1	1:A:172:ASN:OD1	2.35	0.45
1:A:664:TYR:CG	1:A:701:MET:HB2	2.52	0.44
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.47	0.44
1:B:337:PHE:O	1:B:340:LYS:HB2	2.18	0.44
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.99	0.44
1:B:74:ASN:CG	1:B:77:LEU:HB2	2.43	0.44
1:B:399:ALA:O	1:B:400:ALA:O	2.35	0.44
1:A:60:ILE:HG21	1:A:311:ILE:CD1	2.47	0.44
1:B:447:GLU:H	1:B:447:GLU:CD	2.25	0.44
1:B:66:GLU:CD	1:B:66:GLU:N	2.76	0.44
1:B:309:LYS:HE3	1:B:312:GLN:HE22	1.83	0.43
1:B:529:GLU:HA	1:B:532:PHE:CD2	2.53	0.43
1:B:537:ILE:HG23	1:B:558:GLU:HG3	2.00	0.43
1:B:718:THR:HA	1:B:753:SER:O	2.18	0.43
1:A:130:GLU:HG3	1:A:131:GLN:HE22	1.81	0.43
1:A:352:THR:CG2	1:A:355:GLN:HG3	2.49	0.43
1:B:421:ARG:NH1	1:B:421:ARG:CG	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASP:OD1	1:A:398:ASP:N	2.51	0.43
1:A:882:ASN:HB3	1:A:885:LEU:HD23	1.99	0.43
1:B:87:TRP:CZ3	1:B:421:ARG:HB3	2.53	0.43
1:A:128:ARG:NH1	1:A:464:SER:OG	2.47	0.43
1:A:352:THR:HG23	1:A:355:GLN:HG3	2.01	0.43
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.99	0.43
1:B:529:GLU:O	1:B:532:PHE:HB2	2.19	0.43
1:B:656:ILE:CD1	1:B:685:VAL:HG21	2.49	0.43
1:B:398:ASP:C	1:B:400:ALA:N	2.75	0.43
1:B:528:MET:O	1:B:532:PHE:CD2	2.71	0.43
1:B:779:PRO:HG2	1:B:780:LEU:HD12	2.00	0.43
1:B:343:GLU:CD	1:B:343:GLU:H	2.27	0.43
1:B:505:MET:HE3	1:B:670:MET:HE2	2.00	0.43
1:B:737:HIS:HE1	4:B:948:HOH:O	2.01	0.43
1:B:77:LEU:HD13	1:B:450:TYR:CD2	2.53	0.43
1:B:567:GLU:HG3	1:B:574:ALA:HA	2.01	0.43
1:A:60:ILE:HG21	1:A:311:ILE:HD12	2.01	0.42
1:A:328:LYS:HB3	1:A:332:TYR:HB3	2.01	0.42
1:A:132:ASP:HA	1:A:217:LYS:HE3	2.01	0.42
1:A:198:PRO:HD3	1:A:228:LEU:CD2	2.50	0.42
1:A:305:ASP:HB2	1:A:347:LEU:HD11	2.02	0.42
1:B:654:ASN:O	1:B:685:VAL:HG23	2.19	0.42
1:A:497:ALA:CB	1:A:666:VAL:HG11	2.49	0.42
1:A:663:ALA:O	1:A:666:VAL:CG1	2.67	0.42
1:B:779:PRO:HG2	1:B:780:LEU:CD1	2.49	0.42
1:A:325:PHE:C	1:A:327:SER:H	2.28	0.42
1:A:505:MET:CE	1:A:670:MET:HE2	2.49	0.42
1:B:458:LEU:O	1:B:459:HIS:HB2	2.19	0.42
1:A:328:LYS:HB3	1:A:332:TYR:CB	2.50	0.42
4:A:961:HOH:O	1:B:243:THR:HB	2.19	0.42
1:A:352:THR:HG23	1:A:355:GLN:CG	2.49	0.41
1:B:144:SER:N	1:B:145:PRO:CD	2.83	0.41
1:B:656:ILE:HD11	1:B:685:VAL:HG21	2.02	0.41
1:A:210:TYR:O	1:A:214:ARG:HG2	2.19	0.41
1:A:418:ARG:CZ	1:A:421:ARG:NH2	2.84	0.41
1:B:423:ARG:HD3	1:B:423:ARG:O	2.21	0.41
1:B:426:VAL:CG1	1:B:439:ILE:HD11	2.49	0.41
1:A:334:ARG:HB3	1:A:356:ILE:HD12	2.02	0.41
1:A:638:LEU:HB3	1:B:179:HIS:CE1	2.55	0.41
1:A:277:GLU:OE2	1:B:243:THR:CG2	2.65	0.41
1:A:262:GLN:CG	1:A:323:GLN:HE22	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:LYS:O	1:A:867:VAL:HG12	2.21	0.41
1:B:153:LEU:HD12	1:B:153:LEU:HA	1.90	0.41
3:A:887:TDK:N3'	1:B:194:MET:HG3	2.36	0.41
1:A:656:ILE:CD1	1:A:685:VAL:HG21	2.50	0.41
1:B:143:ILE:HD12	1:B:143:ILE:C	2.46	0.41
1:B:262:GLN:CG	1:B:323:GLN:HE21	2.25	0.41
1:A:265:ASP:CG	1:B:521:ASP:O	2.63	0.40
1:A:318:VAL:HG22	1:A:319:ASP:N	2.36	0.40
1:A:418:ARG:HD2	1:A:433:ILE:HD12	2.02	0.40
1:A:725:LYS:HD3	1:A:726:VAL:N	2.36	0.40
1:A:144:SER:N	1:A:145:PRO:CD	2.85	0.40
1:A:144:SER:OG	1:A:145:PRO:HD3	2.22	0.40
1:B:159:GLN:HG3	1:B:438:TYR:CD2	2.56	0.40
1:A:141:GLY:HA3	1:A:192:VAL:HG22	2.02	0.40
1:B:537:ILE:HD13	1:B:538:TYR:C	2.46	0.40
1:B:462:LEU:HB2	1:B:463:PRO:HA	2.03	0.40
1:B:209:LYS:HE2	1:B:252:ASN:CG	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	795/886 (90%)	763 (96%)	29 (4%)	3 (0%)	30	17
1	B	795/886 (90%)	763 (96%)	32 (4%)	0	100	100
All	All	1590/1772 (90%)	1526 (96%)	61 (4%)	3 (0%)	43	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ASP

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Mol	Chain	Res	Type
1	A	397	GLY
1	A	328	LYS

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	665/735 (90%)	630 (95%)	35 (5%)	20	7
1	B	665/735 (90%)	633 (95%)	32 (5%)	23	8
All	All	1330/1470 (90%)	1263 (95%)	67 (5%)	22	8

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	LEU
1	A	192	VAL
1	A	194	MET
1	A	211	LEU
1	A	216	LEU
1	A	264	LEU
1	A	301	LEU
1	A	303	ARG
1	A	304	LYS
1	A	309	LYS
1	A	310	LEU
1	A	326	LYS
1	A	335	GLU
1	A	340	LYS
1	A	354	GLU
1	A	398	ASP
1	A	420	ILE
1	A	433	ILE
1	A	434	GLU
1	A	435	LYS
1	A	457	LYS

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Mol	Chain	Res	Type
1	A	479	GLN
1	A	524	ARG
1	A	529	GLU
1	A	560	GLU
1	A	561	LYS
1	A	638	LEU
1	A	666	VAL
1	A	725	LYS
1	A	780	LEU
1	A	859	ARG
1	A	861	GLU
1	A	865	LYS
1	A	866	VAL
1	A	885	LEU
1	B	56	ILE
1	B	65	VAL
1	B	66	GLU
1	B	77	LEU
1	B	79	ARG
1	B	192	VAL
1	B	194	MET
1	B	196	LEU
1	B	211	LEU
1	B	243	THR
1	B	263	ARG
1	B	278	LEU
1	B	300	GLU
1	B	301	LEU
1	B	326	LYS
1	B	343	GLU
1	B	415	ASP
1	B	421	ARG
1	B	428	VAL
1	B	433	ILE
1	B	443	GLU
1	B	475	LEU
1	B	502	LEU
1	B	509	LYS
1	B	519	ILE
1	B	522	GLU
1	B	524	ARG
1	B	531	LEU

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Mol	Chain	Res	Type
1	B	533	ARG
1	B	537	ILE
1	B	638	LEU
1	B	819	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	131	GLN
1	A	172	ASN
1	A	262	GLN
1	A	323	GLN
1	A	534	GLN
1	A	618	GLN
1	A	695	ASN
1	A	697	HIS
1	A	810	GLN
1	B	106	HIS
1	B	222	GLN
1	B	312	GLN
1	B	695	ASN
1	B	697	HIS
1	B	737	HIS

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	1.56	4 (12%)	41,55,55	1.32	5 (12%)
3	TDK	A	887	2	31,35,35	1.56	5 (16%)	41,55,55	1.37	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	-	2/28/35/35	0/2/2/2
3	TDK	A	887	2	-	2/28/35/35	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	887	TDK	C7'-N3	3.63	1.51	1.47
3	A	887	TDK	PB-O1B	3.52	1.61	1.50
3	A	887	TDK	PC-OM3	-3.36	1.50	1.56
3	B	887	TDK	PB-O1B	3.18	1.60	1.50
3	B	887	TDK	PC-OM3	-3.12	1.50	1.56
3	A	887	TDK	C6'-C5'	-3.07	1.31	1.37
3	B	887	TDK	C6'-C5'	-2.75	1.32	1.37
3	A	887	TDK	PA-O3A	2.52	1.62	1.59
3	A	887	TDK	C7'-N3	2.42	1.50	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	887	TDK	OM4-PC-CMA	-4.54	108.86	113.45
3	B	887	TDK	OM4-PC-CMA	-3.89	109.52	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	887	TDK	O3B-PB-O2B	2.92	118.74	107.80
3	A	887	TDK	O3B-PB-O2B	2.87	118.55	107.80
3	B	887	TDK	OM2-PC-OM4	-2.69	108.79	114.62
3	A	887	TDK	OM2-PC-OM4	-2.60	109.00	114.62
3	B	887	TDK	C6'-N1'-C2'	2.51	120.19	116.07
3	A	887	TDK	C6'-N1'-C2'	2.50	120.18	116.07
3	A	887	TDK	OM3-PC-OM4	2.38	117.15	111.17
3	B	887	TDK	OM3-PC-OM4	2.35	117.08	111.17

There are no chirality outliers.

All (4) torsion outliers are listed below:

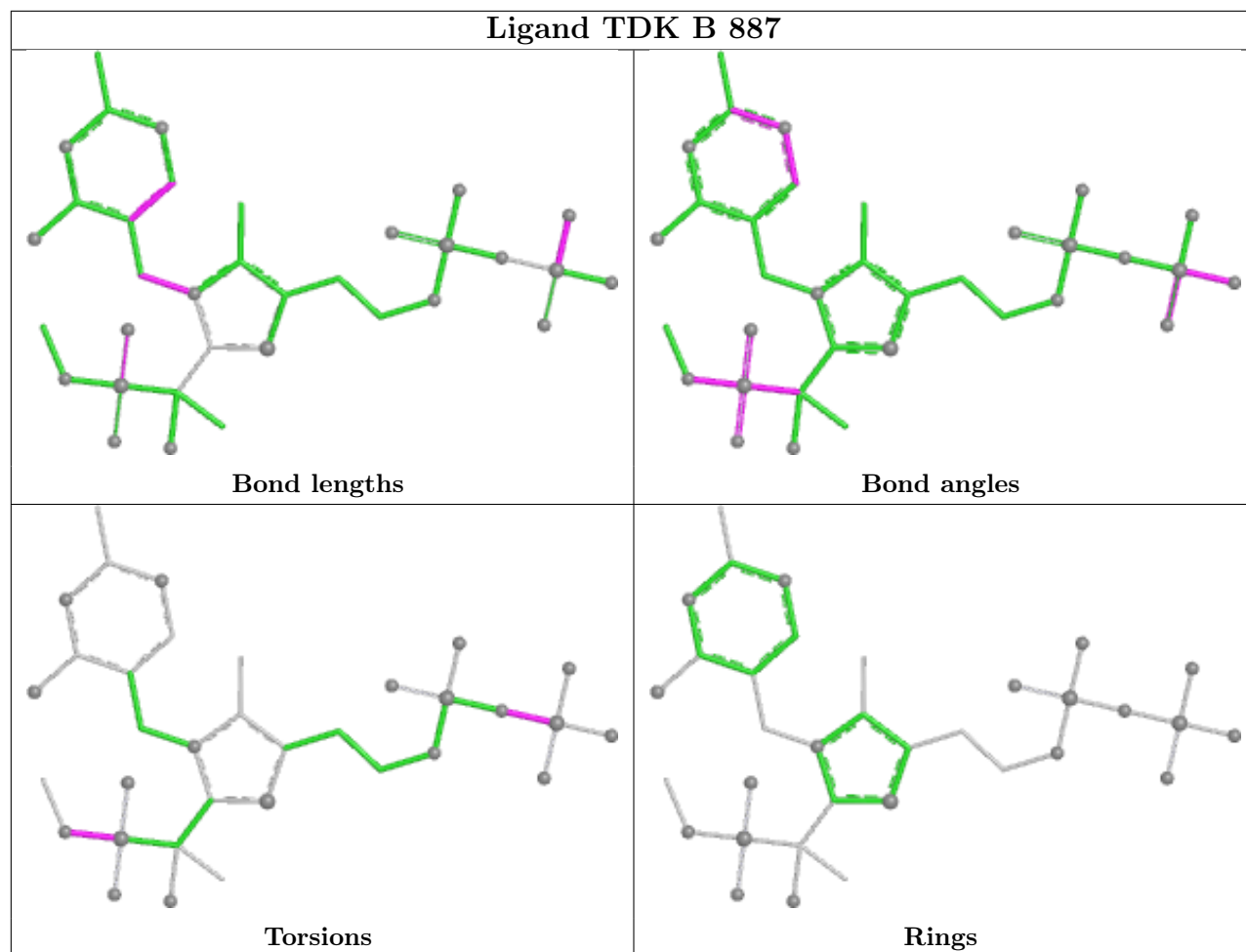
Mol	Chain	Res	Type	Atoms
3	B	887	TDK	CMC-OM2-PC-OM4
3	B	887	TDK	PA-O3A-PB-O2B
3	A	887	TDK	CMC-OM2-PC-OM4
3	A	887	TDK	PA-O3A-PB-O2B

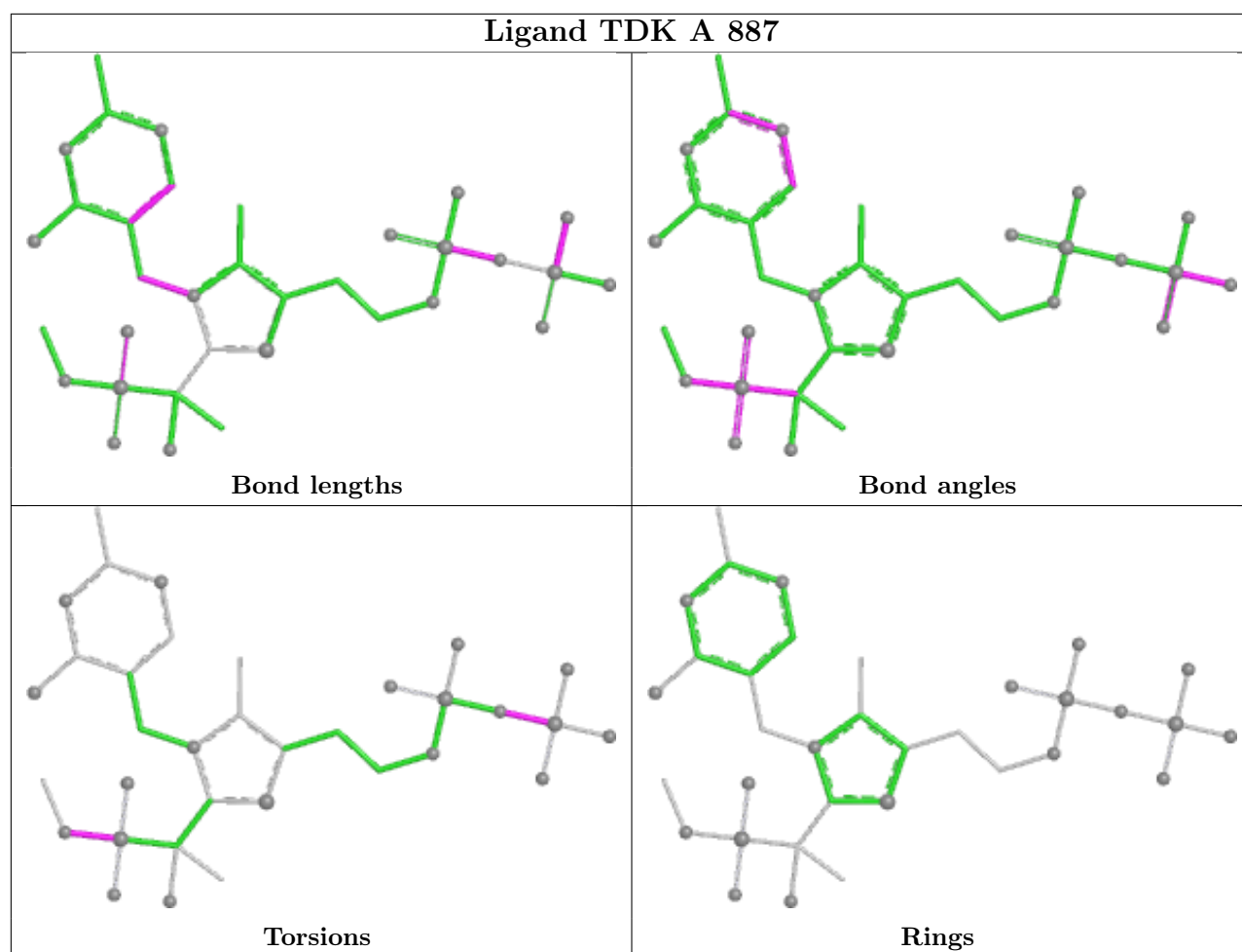
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	887	TDK	3	0
3	A	887	TDK	5	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%)	0.42	54 (6%) 24 26	14, 20, 31, 34	0
1	B	801/886 (90%)	0.28	40 (4%) 34 37	12, 20, 29, 38	0
All	All	1602/1772 (90%)	0.35	94 (5%) 28 31	12, 20, 30, 38	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	ALA	9.7
1	B	399	ALA	7.7
1	B	400	ALA	6.9
1	A	398	ASP	5.6
1	B	398	ASP	5.6
1	A	399	ALA	5.1
1	B	416	GLY	5.1
1	B	414	MET	5.1
1	B	415	ASP	5.0
1	A	397	GLY	4.7
1	B	522	GLU	4.6
1	B	350	ASP	4.2
1	A	341	TYR	4.2
1	B	524	ARG	3.9
1	A	342	PRO	3.9
1	B	532	PHE	3.8
1	A	308	GLY	3.5
1	B	431	ALA	3.2
1	A	339	GLY	3.2
1	A	301	LEU	3.2
1	A	345	ALA	3.2
1	B	303	ARG	3.1
1	A	330	GLY	3.1
1	B	558	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	327	SER	3.1
1	B	533	ARG	3.0
1	B	537	ILE	3.0
1	A	333	VAL	3.0
1	A	329	ASP	3.0
1	B	56	ILE	3.0
1	A	349	ALA	2.9
1	B	430	ASP	2.9
1	A	533	ARG	2.9
1	A	130	GLU	2.9
1	B	417	VAL	2.8
1	A	532	PHE	2.8
1	A	56	ILE	2.8
1	A	348	VAL	2.8
1	A	867	VAL	2.8
1	A	300	GLU	2.8
1	B	530	GLY	2.8
1	A	351	TRP	2.8
1	A	332	TYR	2.8
1	A	720	GLU	2.7
1	A	131	GLN	2.7
1	B	818	ASP	2.7
1	A	352	THR	2.7
1	A	524	ARG	2.7
1	B	418	ARG	2.7
1	A	305	ASP	2.6
1	A	334	ARG	2.6
1	A	350	ASP	2.6
1	B	434	GLU	2.6
1	A	722	SER	2.5
1	B	169	VAL	2.5
1	B	433	ILE	2.5
1	A	539	SER	2.5
1	B	509	LYS	2.5
1	A	743	GLU	2.4
1	A	819	ASP	2.4
1	B	397	GLY	2.4
1	A	306	THR	2.4
1	B	172	ASN	2.4
1	A	265	ASP	2.3
1	A	418	ARG	2.3
1	A	519	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	466	GLN	2.3
1	A	344	THR	2.3
1	A	304	LYS	2.3
1	A	331	ALA	2.3
1	A	530	GLY	2.2
1	A	356	ILE	2.2
1	B	262	GLN	2.2
1	B	428	VAL	2.2
1	A	76	GLU	2.2
1	A	311	ILE	2.2
1	B	385	VAL	2.2
1	A	357	TRP	2.2
1	A	354	GLU	2.2
1	B	529	GLU	2.2
1	B	429	SER	2.2
1	A	886	ALA	2.2
1	B	443	GLU	2.1
1	B	685	VAL	2.1
1	A	307	SER	2.1
1	B	489	SER	2.1
1	A	336	HIS	2.1
1	B	76	GLU	2.1
1	B	743	GLU	2.1
1	A	283	GLU	2.0
1	B	97	SER	2.0
1	A	860	GLY	2.0
1	A	675	GLU	2.0
1	B	479	GLN	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,

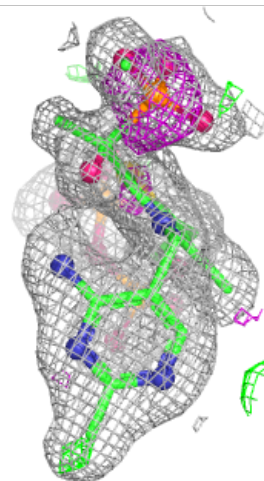
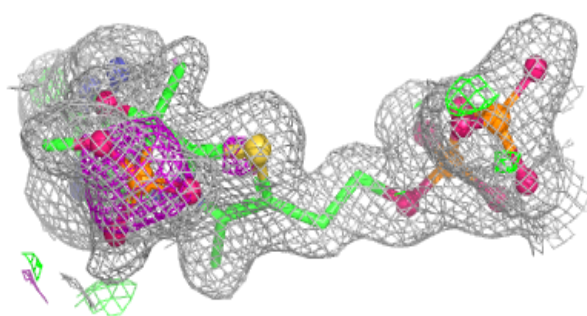
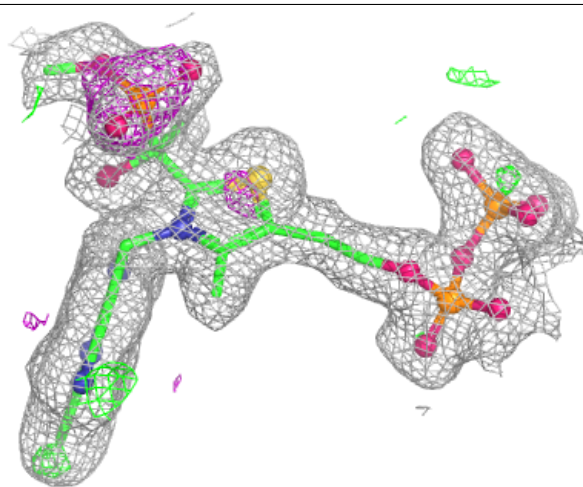
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

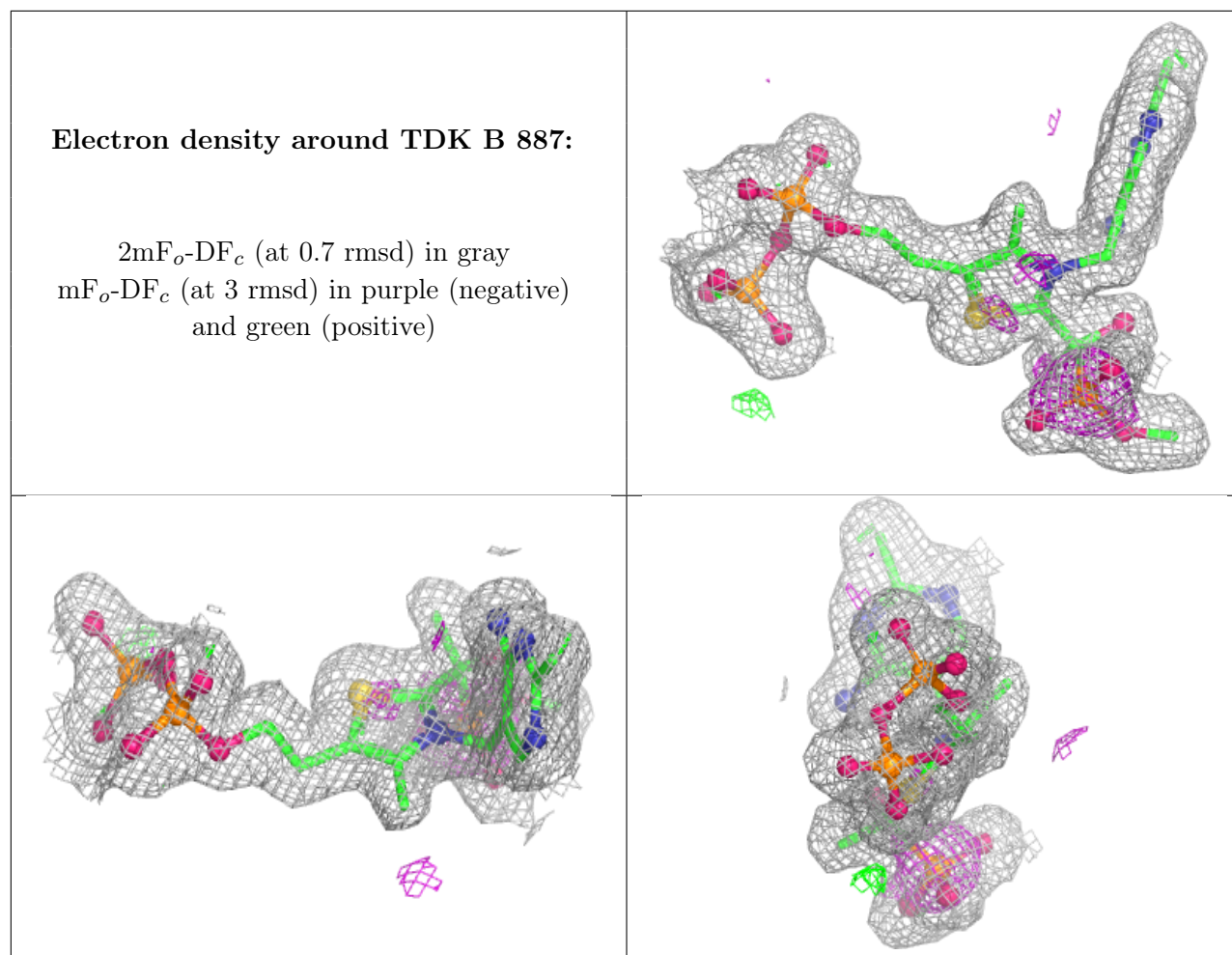
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TDK	A	887	34/34	0.93	0.10	20,23,26,26	0
3	TDK	B	887	34/34	0.93	0.10	19,22,25,25	0
2	MG	A	888	1/1	0.98	0.03	19,19,19,19	0
2	MG	B	888	1/1	0.99	0.05	18,18,18,18	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.