



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:35 PM UTC

PDB ID : 1RP7 / pdb_00001rp7
Title : E. COLI PYRUVATE DEHYDROGENASE INHIBITOR COMPLEX
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Deposited on : 2003-12-03
Resolution : 2.09 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

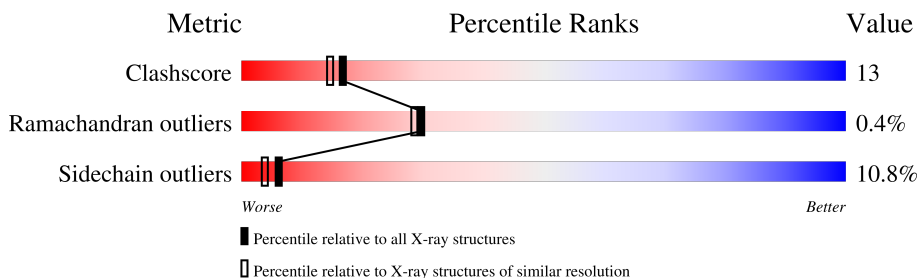
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	886	
1	B	886	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13237 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.

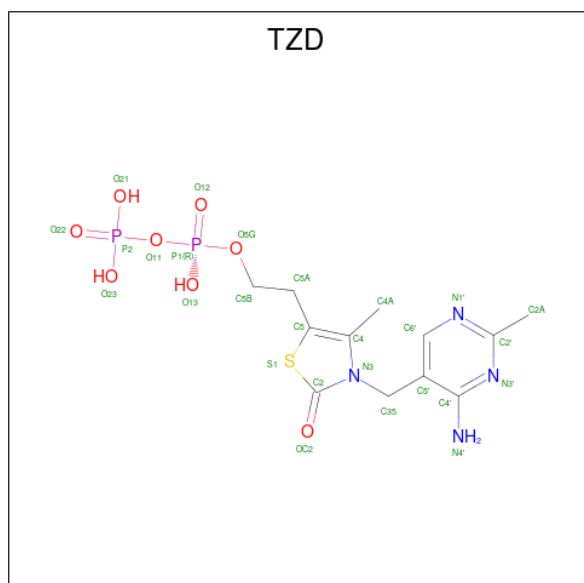
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

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 2-{3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-4-METHYL-2-OXO-2,3-DIHYDRO-1,3-THIAZOL-5-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (CCD ID: TZD) (formula: C₁₂H₁₈N₄O₈P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		

- Molecule 4 is water.

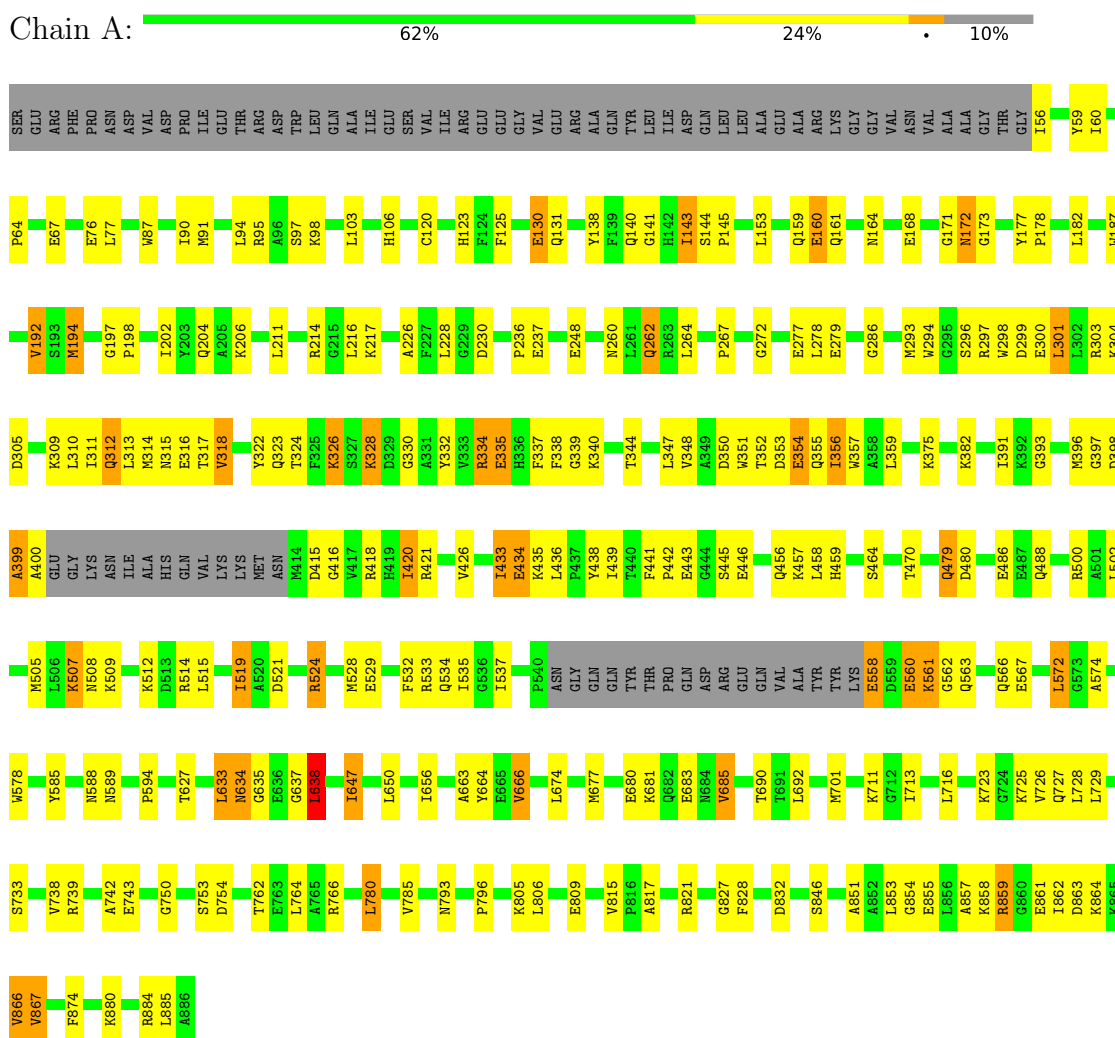
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	223	Total	O	0	0
			223	223		
4	B	276	Total	O	0	0
			276	276		

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. 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. 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.

Note EDS was not executed.

- Molecule 1: Pyruvate dehydrogenase E1 component



- Molecule 1: Pyruvate dehydrogenase E1 component



G724	A574	K490	D398	E300	M194	E66	SER
K725	G575	I496	A399	L301	G195	E67	GLU
R736	C576		A400	L302	L196	Q68	ARG
H737	S577	R500	GLU	R303	G197	P69	PHE
H738			GLY	K304	P198	E70	PRO
R739	Y585		LYS		Y71	Y71	ASN
	S586	M505	ASN	K309	Y203		ASP
	T587	L506	ILE			E76	VAL
G752	N588	F507	ALA	T317	K206	L77	ASP
	N589		HIS		F207	E78	PRO
L764	L590	K509	GLN	Y322	L208	R79	ILE
	P591	S510	VAL	Q323	K209		GLU
H778	I511	I511	LYS		Y210	R82	THR
P779	K512	K512	LYS	K326	L211		ARG
L790			MET	S327	E212	W87	ASP
	L610	L515	ASN	K328	H213		TRP
R794	L623	D521	M414	D329	K221	I90	LEU
S800		E522	G416	G330	Q222	M91	GLN
	G626		V417	K340		R95	ALA
Y803	T627	G527	R418	Y341	L228	A96	ILE
M804		M528	H419	P342	G229	S97	GLU
K805	L633	E529	I420	E343	D230		SER
L806	N634	G530	R421	T344	E231	L103	VAL
F807	G635	I531	D422		E232		ILE
A808	E636	F532		V348	K239	H106	ARG
B809	G637	R533	V426	A349		M107	GLU
Q810	L638		P427	D350			GLY
V811		F537	V428	W351	I242	S112	VAL
	L650	Y538	S429	T352	T243		GLU
V815		S539		D353	E248	F125	ARG
	L656	P540	D432	E584			ALA
D818	Y664	ASN	I433	Q355	N260	G134	GLN
F828		GLY	E434	I356	L261	Q140	TYR
	V668	GLN	K435				LEU
V843	I669	TYR	I439	L359	Q262	I143	ILE
	M670	THR		N360	R263	S144	ASP
S846		PRO	P442	D365	L264	P145	GLN
E855	E680	GLN	E443		D265		LEU
L856	K681	ASP	G444	S445	G266	N164	LEU
	V685	ARG	E446	K368	P267		ALA
R859		GLU			V268		GLU
G860	E694	GLN	Y450	K374	K273	V169	ALA
B861		VAL		K375	I274	H170	ARG
K864	M698	ALA	Q454	A376		G171	LYS
		TYR		Q377	L278	N172	GLY
I871	M701	LYS	L458	E378		L174	VAL
	I713		E471	K380	F282	S175	ASN
F874	L716	D558			W287	S176	VAL
D877	E717	E560	L475	V385	R288	Y177	ALA
	T718	I564	L478	T390	V289	W187	GLY
K880	I719	L565		I391		Q188	THR
V881	E720	Q566	L484	K392	M293	F189	GLY
	G721	E567		G393	W294	P190	VAL
A886	S722	N570	Q488	Y394	R297	T191	ASN
	K723		S489	G397	W298	V192	VAL
					D299	S193	ALA
							GLY
							THR
							GLY
							I56
							I63
							P64
							V65

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.55Å 141.84Å 82.17Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	8.00 – 2.09	Depositor
% Data completeness (in resolution range)	84.5 (8.00-2.09)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.192 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13237	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TZD, MG

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	0.43	0/6484	0.95	20/8766 (0.2%)
1	B	0.46	0/6484	0.96	20/8766 (0.2%)
All	All	0.44	0/12968	0.95	40/17532 (0.2%)

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	B	0	1

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	634	ASN	N-CA-C	10.42	122.63	111.28
1	A	634	ASN	N-CA-C	10.09	123.54	111.33
1	A	171	GLY	N-CA-C	10.01	126.61	114.69
1	B	171	GLY	N-CA-C	9.29	123.52	113.58
1	B	633	LEU	N-CA-C	-7.84	97.86	109.62
1	A	143	ILE	N-CA-C	-6.60	106.08	112.29
1	A	633	LEU	N-CA-C	-6.48	101.68	110.68
1	B	778	HIS	CA-C-N	6.40	126.32	119.28
1	B	778	HIS	C-N-CA	6.40	126.32	119.28
1	A	415	ASP	N-CA-C	-6.27	104.33	112.23
1	B	328	LYS	N-CA-C	6.26	113.92	108.78
1	A	433	ILE	N-CA-C	6.25	117.74	110.62
1	A	805	LYS	N-CA-C	6.20	118.84	111.33
1	B	577	SER	N-CA-C	-6.11	104.70	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	GLY	N-CA-C	5.94	119.82	112.64
1	B	636	GLU	N-CA-C	5.84	118.43	111.71
1	B	416	GLY	N-CA-C	-5.83	108.25	114.67
1	B	805	LYS	N-CA-C	5.81	118.36	111.33
1	A	677	MET	N-CA-C	5.72	117.59	111.36
1	A	293	MET	N-CA-C	5.71	120.25	112.04
1	B	293	MET	N-CA-C	5.67	120.23	111.56
1	A	785	VAL	N-CA-C	5.64	114.08	107.77
1	B	478	LEU	N-CA-C	-5.59	105.27	111.36
1	B	63	ILE	N-CA-C	5.48	113.91	107.77
1	B	71	TYR	CA-C-N	5.42	125.12	119.64
1	B	71	TYR	C-N-CA	5.42	125.12	119.64
1	A	328	LYS	CB-CA-C	-5.41	109.28	117.07
1	B	623	LEU	N-CA-C	-5.38	99.75	108.52
1	A	638	LEU	N-CA-C	5.37	120.17	111.37
1	A	328	LYS	CA-C-O	5.20	120.95	117.94
1	B	511	ILE	N-CA-C	5.13	118.08	113.10
1	A	637	GLY	N-CA-C	5.13	121.56	112.53
1	B	328	LYS	CB-CA-C	-5.12	109.69	117.07
1	A	123	HIS	N-CA-C	5.12	121.29	113.61
1	A	470	THR	N-CA-C	5.11	117.98	111.69
1	B	637	GLY	N-CA-C	5.11	121.77	112.37
1	A	647	ILE	N-CA-C	-5.10	105.44	111.00
1	A	103	LEU	N-CA-C	5.05	116.86	111.36
1	B	860	GLY	N-CA-C	-5.04	108.04	115.30
1	A	204	GLN	N-CA-C	-5.03	105.50	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	803	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	169	0
1	B	6341	0	6179	164	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	15	0	0
3	B	27	0	15	1	0
4	A	223	0	0	2	0
4	B	276	0	0	10	0
All	All	13237	0	12388	321	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 13.

All (321) 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:309:LYS:HG3	1:B:343:GLU:HG3	1.34	1.09
1:A:64:PRO:HG2	1:A:67:GLU:HG3	1.47	0.96
1:B:509:LYS:H	1:B:509:LYS:HD2	1.30	0.95
1:B:198:PRO:HG3	1:B:228:LEU:HD22	1.52	0.91
1:B:490:LYS:HE2	1:B:500:ARG:HH22	1.35	0.90
1:B:194:MET:HB3	1:B:232:GLU:HG3	1.55	0.86
1:B:90:ILE:HG12	1:B:107:MET:HE3	1.56	0.86
1:B:309:LYS:CG	1:B:343:GLU:HG3	2.11	0.80
1:B:432:ASP:HA	1:B:435:LYS:HD2	1.63	0.80
1:B:587:THR:HG21	4:B:923:HOH:O	1.83	0.79
1:A:326:LYS:HD2	1:A:391:ILE:HG23	1.62	0.78
1:B:309:LYS:HG3	1:B:343:GLU:CG	2.13	0.77
1:A:297:ARG:HB3	1:A:359:LEU:HD23	1.65	0.77
1:A:334:ARG:HB3	1:A:356:ILE:HD13	1.65	0.77
1:B:352:THR:OG1	1:B:355:GLN:HG3	1.86	0.75
1:A:638:LEU:HD22	1:A:828:PHE:HB3	1.69	0.74
1:B:300:GLU:HG3	1:B:301:LEU:N	2.02	0.74
1:A:867:VAL:HG22	1:B:779:PRO:HG3	1.70	0.72
1:B:326:LYS:HE2	1:B:391:ILE:HG23	1.71	0.72
1:A:277:GLU:OE2	1:B:243:THR:HG21	1.90	0.72
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.74	0.70
1:A:160:GLU:HG2	1:A:161:GLN:N	2.07	0.70
4:A:1079:HOH:O	1:B:522:GLU:HG3	1.92	0.69
1:B:301:LEU:HD12	1:B:304:LYS:HE2	1.74	0.69
1:B:509:LYS:H	1:B:509:LYS:CD	2.05	0.69
1:A:627:THR:HB	1:A:633:LEU:HD13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.22	0.69
1:A:262:GLN:HA	1:A:267:PRO:HA	1.75	0.68
1:B:638:LEU:HD22	1:B:828:PHE:HB3	1.74	0.68
1:A:393:GLY:HA3	1:A:400:ALA:HB3	1.74	0.68
1:B:414:MET:O	1:B:433:ILE:HG23	1.94	0.67
1:B:490:LYS:HE2	1:B:500:ARG:NH2	2.08	0.66
1:B:90:ILE:HG23	1:B:107:MET:HE3	1.76	0.66
1:B:361:ARG:HD2	1:B:391:ILE:HG13	1.77	0.66
1:A:348:VAL:O	1:A:351:TRP:HB2	1.96	0.66
1:A:140:GLN:O	1:A:143:ILE:HG13	1.95	0.65
1:B:323:GLN:HA	1:B:326:LYS:HD3	1.78	0.65
1:B:374:LYS:HE3	1:B:377:GLN:OE1	1.96	0.65
1:B:87:TRP:CD1	1:B:439:ILE:HG13	2.32	0.64
1:A:237:GLU:HG2	1:A:572:LEU:HD11	1.79	0.64
1:B:287:TRP:CE3	1:B:385:VAL:HG22	2.33	0.64
1:A:508:ASN:O	1:A:512:LYS:HB3	1.99	0.63
1:B:656:ILE:HD11	1:B:685:VAL:HG21	1.79	0.63
1:A:328:LYS:HG3	1:A:332:TYR:CD1	2.35	0.62
1:A:334:ARG:HG3	1:A:335:GLU:N	2.14	0.62
1:B:800:SER:OG	1:B:843:VAL:HG22	1.99	0.62
1:A:796:PRO:HG3	1:A:859:ARG:NE	2.15	0.61
1:B:415:ASP:OD1	1:B:433:ILE:HG21	1.99	0.61
1:A:334:ARG:HA	1:A:338:PHE:HB2	1.83	0.61
1:B:846:SER:OG	1:B:874:PHE:HB3	2.01	0.60
1:A:324:THR:HG23	1:A:328:LYS:HE3	1.82	0.60
1:A:298:TRP:CE2	1:A:359:LEU:HB3	2.37	0.60
1:A:98:LYS:HE2	1:A:436:LEU:HD12	1.82	0.60
1:B:90:ILE:HG12	1:B:107:MET:CE	2.32	0.59
1:A:313:LEU:HD21	1:A:337:PHE:O	2.02	0.59
1:B:112:SER:HB3	1:B:392:LYS:HA	1.85	0.59
1:A:418:ARG:HG2	1:A:433:ILE:HD13	1.84	0.59
1:A:561:LYS:HB2	1:A:561:LYS:NZ	2.17	0.59
1:A:867:VAL:CG2	1:B:779:PRO:HG3	2.32	0.59
1:A:344:THR:HA	1:A:347:LEU:HD12	1.85	0.59
1:A:192:VAL:HG22	4:A:1062:HOH:O	2.01	0.58
1:A:857:ALA:HA	1:A:862:ILE:HG13	1.84	0.58
1:B:522:GLU:HG2	1:B:599:TYR:OH	2.02	0.58
1:A:854:GLY:O	1:A:858:LYS:HG3	2.04	0.58
1:A:91:MET:O	1:A:95:ARG:HG3	2.03	0.58
1:B:505:MET:CE	1:B:670:MET:HE2	2.34	0.58
1:B:694:GLU:CD	1:B:736:ARG:HH12	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ILE:HG13	1:B:421:ARG:N	2.18	0.58
1:B:77:LEU:HD11	1:B:446:GLU:HG2	1.85	0.57
1:A:821:ARG:HH11	1:A:851:ALA:HA	1.69	0.57
1:A:832:ASP:OD2	1:B:169:VAL:HB	2.04	0.57
1:A:335:GLU:O	1:A:339:GLY:HA3	2.04	0.57
1:A:853:LEU:O	1:A:862:ILE:HD11	2.05	0.56
1:B:681:LYS:HB2	4:B:1075:HOH:O	2.05	0.56
1:B:177:TYR:HB3	1:B:178:PRO:CD	2.35	0.56
1:B:509:LYS:HD2	1:B:509:LYS:N	2.12	0.56
1:A:859:ARG:NH1	1:A:861:GLU:OE1	2.39	0.56
1:A:294:TRP:HB3	1:A:298:TRP:CD1	2.41	0.56
1:B:195:GLY:C	1:B:198:PRO:HD2	2.32	0.55
1:B:505:MET:HE3	1:B:670:MET:HE2	1.88	0.55
1:B:76:GLU:CD	1:B:76:GLU:H	2.15	0.55
1:B:627:THR:HB	1:B:633:LEU:HD22	1.88	0.55
1:A:153:LEU:HD21	1:A:441:PHE:CE2	2.41	0.55
1:A:863:ASP:O	1:A:866:VAL:HG22	2.07	0.55
1:B:489:SER:HB2	1:B:490:LYS:NZ	2.22	0.55
1:A:352:THR:OG1	1:A:354:GLU:HG2	2.07	0.55
1:B:664:TYR:O	1:B:668:VAL:HG23	2.07	0.54
1:A:663:ALA:O	1:A:666:VAL:HG13	2.07	0.54
1:A:806:LEU:HD11	1:B:806:LEU:HD11	1.88	0.54
1:A:656:ILE:HG12	1:A:685:VAL:HG13	1.89	0.54
1:B:294:TRP:HB3	1:B:298:TRP:CD1	2.43	0.54
1:A:519:ILE:CD1	1:A:528:MET:HE2	2.37	0.54
1:A:177:TYR:CG	1:A:192:VAL:HG11	2.43	0.54
1:B:426:VAL:HG12	1:B:428:VAL:HG12	1.89	0.54
1:A:524:ARG:HA	1:A:529:GLU:OE1	2.08	0.53
1:B:106:HIS:HD2	4:B:1161:HOH:O	1.90	0.53
1:A:396:MET:HE2	1:A:399:ALA:CB	2.38	0.53
1:B:537:ILE:HG22	1:B:558:GLU:HA	1.91	0.53
1:B:297:ARG:HB2	1:B:359:LEU:HD23	1.90	0.53
1:A:585:TYR:O	1:A:589:ASN:HA	2.08	0.53
1:B:213:HIS:HB3	1:B:560:GLU:O	2.09	0.53
1:B:532:PHE:HD1	1:B:564:ILE:HD12	1.73	0.53
1:A:177:TYR:CD2	1:A:192:VAL:HG11	2.44	0.52
1:B:323:GLN:O	1:B:326:LYS:HG2	2.08	0.52
1:B:490:LYS:CE	1:B:500:ARG:HH22	2.17	0.52
1:B:64:PRO:HB2	1:B:66:GLU:OE2	2.09	0.52
1:A:434:GLU:H	1:A:434:GLU:CD	2.16	0.52
1:A:507:LYS:HE3	1:A:507:LYS:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASN:HB3	1:B:173:GLY:HA2	1.91	0.52
1:B:442:PRO:HG2	1:B:445:SER:HB3	1.90	0.52
1:A:396:MET:HB3	1:A:399:ALA:HB3	1.93	0.51
1:A:130:GLU:HG3	1:A:131:GLN:NE2	2.25	0.51
1:A:537:ILE:O	1:A:558:GLU:HA	2.11	0.51
1:B:144:SER:OG	1:B:145:PRO:HD3	2.10	0.51
1:A:827:GLY:CA	1:A:884:ARG:HA	2.40	0.51
1:B:140:GLN:O	1:B:143:ILE:HG13	2.10	0.51
1:A:314:MET:HA	1:A:322:TYR:OH	2.11	0.51
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.91	0.51
1:B:91:MET:O	1:B:95:ARG:HG3	2.10	0.51
1:B:506:LEU:HD23	1:B:515:LEU:HD12	1.92	0.50
1:B:537:ILE:HD11	1:B:566:GLN:HB3	1.92	0.50
1:A:396:MET:HE2	1:A:399:ALA:HB3	1.93	0.50
1:B:721:GLY:HA3	1:B:752:GLY:N	2.27	0.50
1:B:177:TYR:CD2	1:B:192:VAL:HG11	2.46	0.50
1:B:178:PRO:HA	1:B:187:TRP:CG	2.47	0.50
1:B:309:LYS:HD2	1:B:341:TYR:CD2	2.46	0.50
1:A:304:LYS:HE2	1:A:347:LEU:HD23	1.93	0.50
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.93	0.50
1:B:509:LYS:HD3	4:B:1145:HOH:O	2.12	0.50
1:B:736:ARG:NH1	4:B:1081:HOH:O	2.44	0.50
1:A:317:THR:HB	1:A:322:TYR:CE2	2.47	0.50
1:B:273:LYS:HG2	4:B:1042:HOH:O	2.11	0.50
1:A:324:THR:O	1:A:328:LYS:HG2	2.11	0.49
1:A:420:ILE:HG13	1:A:421:ARG:N	2.26	0.49
1:B:195:GLY:O	1:B:198:PRO:HD2	2.12	0.49
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.42	0.49
1:A:352:THR:OG1	1:A:355:GLN:HG3	2.12	0.49
1:B:164:ASN:CB	1:B:173:GLY:HA2	2.42	0.49
1:B:415:ASP:OD1	1:B:418:ARG:HB3	2.13	0.49
1:A:638:LEU:CD2	1:A:828:PHE:HB3	2.42	0.49
1:A:304:LYS:NZ	1:A:347:LEU:O	2.45	0.49
1:A:418:ARG:HG2	1:A:433:ILE:CD1	2.42	0.49
1:A:304:LYS:HE2	1:A:347:LEU:CD2	2.43	0.49
1:A:519:ILE:HD13	1:A:528:MET:HE2	1.94	0.49
1:A:197:GLY:N	1:A:198:PRO:HD2	2.28	0.49
1:B:317:THR:HB	1:B:322:TYR:CE2	2.47	0.49
1:B:881:VAL:HG12	4:B:1147:HOH:O	2.11	0.49
1:A:153:LEU:HD21	1:A:441:PHE:HE2	1.78	0.49
1:A:120:CYS:HB3	1:A:125:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:TRP:CZ2	1:A:359:LEU:HB3	2.48	0.49
1:B:508:ASN:O	1:B:512:LYS:HB3	2.13	0.48
1:B:856:LEU:HB3	1:B:861:GLU:HB3	1.93	0.48
1:B:397:GLY:O	1:B:398:ASP:C	2.56	0.48
1:A:578:TRP:CD1	1:A:594:PRO:HB2	2.48	0.48
1:A:130:GLU:HG3	1:A:131:GLN:HE22	1.79	0.48
1:A:330:GLY:HA3	1:A:353:ASP:O	2.14	0.48
1:A:821:ARG:NH1	1:A:851:ALA:HA	2.28	0.48
1:B:87:TRP:CZ2	1:B:428:VAL:HG11	2.48	0.48
1:A:780:LEU:HD12	1:B:864:LYS:HB3	1.95	0.48
1:B:567:GLU:HG3	1:B:574:ALA:HA	1.96	0.48
1:B:585:TYR:O	1:B:589:ASN:HA	2.14	0.48
1:B:811:VAL:O	1:B:815:VAL:HG23	2.14	0.48
1:A:567:GLU:HG3	1:A:574:ALA:HA	1.95	0.48
1:B:638:LEU:CD2	1:B:828:PHE:HB3	2.43	0.48
1:A:635:GLY:HA3	1:B:103:LEU:O	2.14	0.47
1:A:95:ARG:HD2	1:A:438:TYR:OH	2.14	0.47
1:B:134:GLY:O	1:B:222:GLN:HG2	2.14	0.47
1:B:807:PHE:O	1:B:810:GLN:HG2	2.14	0.47
1:A:206:LYS:HD2	1:A:248:GLU:HG3	1.95	0.47
1:A:535:ILE:HB	1:A:563:GLN:HB3	1.97	0.47
1:A:821:ARG:HD2	1:A:855:GLU:CG	2.45	0.47
1:B:489:SER:HB2	1:B:490:LYS:HZ1	1.79	0.47
1:B:877:ASP:O	1:B:880:LYS:HG2	2.13	0.47
1:A:300:GLU:O	1:A:304:LYS:HB2	2.14	0.47
1:B:262:GLN:HA	1:B:267:PRO:HA	1.96	0.47
1:B:421:ARG:HA	1:B:426:VAL:CG2	2.44	0.47
1:B:528:MET:C	1:B:530:GLY:H	2.23	0.47
1:A:664:TYR:CG	1:A:701:MET:HB2	2.49	0.47
1:B:106:HIS:CD2	4:B:1161:HOH:O	2.68	0.47
1:B:421:ARG:HG2	1:B:433:ILE:HD11	1.97	0.47
1:B:87:TRP:CD2	1:B:426:VAL:HG11	2.50	0.46
1:B:230:ASP:OD1	1:B:230:ASP:N	2.47	0.46
1:B:414:MET:HE3	1:B:434:GLU:HG2	1.97	0.46
1:A:144:SER:N	1:A:145:PRO:CD	2.79	0.46
1:B:194:MET:H	1:B:194:MET:HG2	1.52	0.46
1:B:207:PHE:O	1:B:210:TYR:HB3	2.16	0.46
1:B:720:GLU:OE1	1:B:720:GLU:HA	2.15	0.46
1:B:855:GLU:O	1:B:859:ARG:HG3	2.15	0.46
1:A:729:LEU:N	1:A:729:LEU:HD12	2.30	0.46
1:A:272:GLY:O	1:A:318:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:TYR:HB2	1:B:344:THR:OG1	2.16	0.46
1:A:138:TYR:HB2	1:A:226:ALA:HA	1.97	0.46
1:A:286:GLY:O	1:A:382:LYS:HE3	2.15	0.46
1:A:634:ASN:HB2	1:A:832:ASP:O	2.15	0.46
1:A:726:VAL:O	1:A:753:SER:HA	2.16	0.46
1:B:239:LYS:HA	1:B:242:ILE:HG23	1.97	0.46
1:A:505:MET:HB3	1:A:515:LEU:HD11	1.97	0.46
1:A:77:LEU:CD2	1:A:446:GLU:HG2	2.46	0.45
1:A:806:LEU:HA	1:A:809:GLU:HB2	1.98	0.45
1:A:143:ILE:C	1:A:143:ILE:HD12	2.41	0.45
1:B:421:ARG:HG3	1:B:422:ASP:N	2.31	0.45
1:B:528:MET:C	1:B:530:GLY:N	2.74	0.45
1:A:479:GLN:HG2	1:A:480:ASP:N	2.31	0.45
1:B:274:ILE:O	1:B:278:LEU:HB2	2.15	0.45
1:B:418:ARG:O	1:B:421:ARG:HG3	2.16	0.45
1:A:160:GLU:CD	1:A:172:ASN:OD1	2.60	0.45
1:A:762:THR:O	1:A:766:ARG:HG3	2.16	0.45
1:A:864:LYS:O	1:A:867:VAL:HG13	2.17	0.45
1:B:626:GLY:O	1:B:627:THR:C	2.60	0.45
1:B:808:ALA:O	1:B:811:VAL:HG22	2.16	0.45
1:A:144:SER:OG	1:A:145:PRO:HD3	2.17	0.45
1:A:647:ILE:O	1:A:650:LEU:HG	2.17	0.45
1:B:125:PHE:O	1:B:458:LEU:HB3	2.17	0.44
1:B:716:LEU:HD13	1:B:739:ARG:CZ	2.47	0.44
1:A:90:ILE:HG22	1:A:91:MET:HE2	1.98	0.44
1:A:426:VAL:HG13	1:A:439:ILE:CD1	2.46	0.44
1:A:827:GLY:HA2	1:A:884:ARG:HA	1.99	0.44
1:B:194:MET:CB	1:B:232:GLU:HG3	2.38	0.44
1:B:330:GLY:HA3	1:B:353:ASP:O	2.17	0.44
1:A:59:TYR:N	1:A:315:ASN:OD1	2.40	0.44
1:A:198:PRO:O	1:A:202:ILE:HG13	2.17	0.44
1:A:236:PRO:HD3	1:B:570:ASN:OD1	2.17	0.44
1:A:334:ARG:NH2	1:A:351:TRP:O	2.51	0.44
1:B:421:ARG:HG3	1:B:421:ARG:HH11	1.82	0.44
1:A:328:LYS:HD2	1:A:332:TYR:CD2	2.53	0.44
1:B:488:GLN:HB2	1:B:698:MET:HB2	2.00	0.44
1:A:519:ILE:HD11	1:A:528:MET:HG3	1.99	0.44
1:A:521:ASP:N	1:A:566:GLN:OE1	2.44	0.44
1:B:144:SER:N	1:B:145:PRO:CD	2.81	0.44
1:B:309:LYS:HD2	1:B:341:TYR:CG	2.53	0.44
1:A:859:ARG:HD3	1:A:861:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:PRO:HA	1:B:560:GLU:HB2	2.00	0.43
1:B:650:LEU:HD12	1:B:650:LEU:C	2.43	0.43
1:A:723:LYS:HG2	1:A:750:GLY:HA3	2.00	0.43
1:B:529:GLU:OE1	1:B:529:GLU:N	2.51	0.43
1:A:561:LYS:HB2	1:A:561:LYS:HZ3	1.82	0.43
1:A:862:ILE:HD12	1:A:866:VAL:HG22	1.98	0.43
1:B:309:LYS:CB	1:B:343:GLU:HG3	2.48	0.43
1:B:532:PHE:CD1	1:B:564:ILE:HD12	2.53	0.43
1:A:328:LYS:HD2	1:A:332:TYR:CE2	2.53	0.43
1:B:274:ILE:H	1:B:274:ILE:HG13	1.54	0.43
1:A:309:LYS:HB3	1:A:344:THR:HG23	2.01	0.43
1:A:416:GLY:O	1:A:420:ILE:HG23	2.18	0.43
1:A:656:ILE:HG12	1:A:685:VAL:CG1	2.49	0.43
1:B:496:ILE:O	1:B:500:ARG:HG3	2.19	0.43
1:B:558:GLU:O	1:B:558:GLU:HG2	2.18	0.43
1:A:681:LYS:HD3	1:A:683:GLU:HB2	1.99	0.43
1:B:326:LYS:HE3	4:B:1063:HOH:O	2.19	0.43
1:A:521:ASP:O	1:B:265:ASP:HB2	2.18	0.43
1:A:532:PHE:N	1:A:532:PHE:CD1	2.86	0.43
1:A:560:GLU:H	1:A:560:GLU:HG3	1.53	0.43
1:A:728:LEU:HD12	1:A:742:ALA:HB2	2.01	0.43
1:B:471:GLU:OE2	1:B:591:PRO:HD2	2.18	0.43
1:A:348:VAL:HA	1:A:351:TRP:CD1	2.53	0.42
1:A:458:LEU:O	1:A:459:HIS:HB2	2.18	0.42
1:A:692:LEU:HD13	1:A:733:SER:HB3	1.99	0.42
1:B:177:TYR:HB3	1:B:178:PRO:HD2	1.99	0.42
1:B:450:TYR:O	1:B:454:GLN:HG2	2.20	0.42
1:B:421:ARG:HH11	1:B:421:ARG:CG	2.32	0.42
1:A:301:LEU:HD23	1:A:351:TRP:CZ2	2.55	0.42
1:A:524:ARG:HD3	1:B:265:ASP:OD2	2.19	0.42
1:B:263:ARG:HE	1:B:263:ARG:HB2	1.44	0.42
1:B:263:ARG:HG3	1:B:268:VAL:HG22	2.01	0.42
1:B:415:ASP:C	1:B:417:VAL:H	2.26	0.42
1:A:716:LEU:HD13	1:A:739:ARG:CZ	2.50	0.42
1:A:815:VAL:HG12	1:A:817:ALA:H	1.84	0.42
1:A:867:VAL:HG22	1:B:779:PRO:CG	2.47	0.42
1:B:348:VAL:HB	1:B:356:ILE:HD11	2.02	0.42
1:A:296:SER:O	1:A:299:ASP:HB2	2.18	0.42
1:B:79:ARG:HG2	1:B:82:ARG:NH2	2.35	0.42
1:A:312:GLN:NE2	1:A:316:GLU:OE1	2.52	0.42
1:B:350:ASP:OD1	1:B:350:ASP:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HG21	1:A:311:ILE:HD12	2.01	0.42
1:A:194:MET:H	1:A:194:MET:HG2	1.56	0.42
1:A:442:PRO:HG2	1:A:445:SER:HB3	2.02	0.42
1:B:260:ASN:HA	1:B:390:THR:O	2.20	0.42
1:B:365:ASP:HB3	1:B:368:LYS:HB2	2.01	0.42
1:B:415:ASP:C	1:B:417:VAL:N	2.77	0.42
1:A:77:LEU:HD22	1:A:446:GLU:HG2	2.01	0.42
1:B:737:HIS:HE1	4:B:1081:HOH:O	2.02	0.42
1:A:87:TRP:HE3	1:A:420:ILE:HD11	1.85	0.42
1:A:262:GLN:HG2	1:A:323:GLN:NE2	2.34	0.42
1:B:203:TYR:HB2	1:B:576:CYS:HB3	2.02	0.42
1:A:352:THR:O	1:A:355:GLN:N	2.50	0.41
1:A:857:ALA:CA	1:A:862:ILE:HG13	2.50	0.41
1:B:90:ILE:CG2	1:B:107:MET:HE3	2.45	0.41
1:A:328:LYS:HG3	1:A:332:TYR:CG	2.55	0.41
1:A:505:MET:CB	1:A:515:LEU:HD11	2.50	0.41
1:B:206:LYS:HD3	1:B:248:GLU:OE1	2.20	0.41
1:A:106:HIS:CD2	1:A:106:HIS:N	2.88	0.41
1:A:164:ASN:CB	1:A:173:GLY:HA2	2.50	0.41
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.92	0.41
1:A:846:SER:HB2	1:A:874:PHE:HB3	2.01	0.41
1:B:79:ARG:HG2	1:B:82:ARG:HH21	1.85	0.41
1:B:189:PHE:HA	1:B:190:PRO:HD3	1.80	0.41
1:A:178:PRO:HA	1:A:187:TRP:CG	2.54	0.41
1:A:356:ILE:HG22	1:A:357:TRP:N	2.35	0.41
1:A:862:ILE:HD12	1:A:866:VAL:CG2	2.50	0.41
1:B:558:GLU:O	1:B:558:GLU:CG	2.68	0.41
1:A:177:TYR:HB3	1:A:178:PRO:HD2	2.03	0.41
1:A:217:LYS:NZ	1:A:588:ASN:HB3	2.36	0.41
1:A:230:ASP:OD1	1:A:230:ASP:N	2.51	0.41
1:A:537:ILE:C	1:A:562:GLY:HA3	2.46	0.41
1:B:90:ILE:HG22	1:B:91:MET:HE2	2.03	0.41
1:B:282:PHE:CD2	1:B:385:VAL:HG21	2.56	0.41
1:A:56:ILE:HG23	1:A:279:GLU:OE1	2.21	0.41
1:A:260:ASN:O	1:A:262:GLN:HG3	2.21	0.41
1:A:864:LYS:HD3	1:B:779:PRO:O	2.21	0.41
1:B:506:LEU:CD2	1:B:515:LEU:HD12	2.50	0.41
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.86	0.41
1:A:638:LEU:CD1	1:A:638:LEU:C	2.94	0.41
1:A:727:GLN:HG2	1:A:754:ASP:HB2	2.03	0.41
1:A:851:ALA:O	1:A:855:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:THR:O	1:A:355:GLN:HB2	2.21	0.40
1:B:343:GLU:H	1:B:343:GLU:HG2	1.55	0.40
1:B:527:GLY:HA2	1:B:529:GLU:OE1	2.21	0.40
1:B:391:ILE:O	1:B:394:TYR:HB2	2.22	0.40
1:B:664:TYR:CG	1:B:701:MET:HB2	2.57	0.40
1:A:488:GLN:OE1	1:A:500:ARG:NH2	2.55	0.40
1:A:674:LEU:HD23	1:A:674:LEU:HA	1.96	0.40
1:B:194:MET:HG2	3:B:887:TZD:N3'	2.36	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%)	752 (95%)	40 (5%)	3 (0%)	30	28
1	B	795/886 (90%)	755 (95%)	37 (5%)	3 (0%)	30	28
All	All	1590/1772 (90%)	1507 (95%)	77 (5%)	6 (0%)	30	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	GLY
1	A	305	ASP
1	B	627	THR
1	B	398	ASP
1	A	399	ALA
1	B	521	ASP

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%)	598 (90%)	67 (10%)	7	5
1	B	665/735 (90%)	588 (88%)	77 (12%)	5	3
All	All	1330/1470 (90%)	1186 (89%)	144 (11%)	6	4

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	94	LEU
1	A	97	SER
1	A	130	GLU
1	A	159	GLN
1	A	160	GLU
1	A	168	GLU
1	A	172	ASN
1	A	182	LEU
1	A	192	VAL
1	A	194	MET
1	A	211	LEU
1	A	214	ARG
1	A	216	LEU
1	A	228	LEU
1	A	262	GLN
1	A	264	LEU
1	A	278	LEU
1	A	301	LEU
1	A	303	ARG
1	A	310	LEU
1	A	312	GLN
1	A	318	VAL
1	A	326	LYS
1	A	334	ARG
1	A	335	GLU
1	A	340	LYS

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Mol	Chain	Res	Type
1	A	350	ASP
1	A	354	GLU
1	A	356	ILE
1	A	375	LYS
1	A	398	ASP
1	A	420	ILE
1	A	434	GLU
1	A	435	LYS
1	A	443	GLU
1	A	456	GLN
1	A	457	LYS
1	A	464	SER
1	A	479	GLN
1	A	486	GLU
1	A	507	LYS
1	A	509	LYS
1	A	519	ILE
1	A	524	ARG
1	A	533	ARG
1	A	534	GLN
1	A	558	GLU
1	A	560	GLU
1	A	561	LYS
1	A	572	LEU
1	A	638	LEU
1	A	666	VAL
1	A	680	GLU
1	A	685	VAL
1	A	690	THR
1	A	711	LYS
1	A	725	LYS
1	A	738	VAL
1	A	743	GLU
1	A	780	LEU
1	A	793	ASN
1	A	859	ARG
1	A	866	VAL
1	A	867	VAL
1	A	880	LYS
1	A	885	LEU
1	B	65	VAL
1	B	66	GLU

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Mol	Chain	Res	Type
1	B	68	GLN
1	B	70	GLU
1	B	77	LEU
1	B	97	SER
1	B	106	HIS
1	B	172	ASN
1	B	175	SER
1	B	192	VAL
1	B	194	MET
1	B	196	LEU
1	B	206	LYS
1	B	209	LYS
1	B	211	LEU
1	B	221	LYS
1	B	228	LEU
1	B	243	THR
1	B	262	GLN
1	B	263	ARG
1	B	264	LEU
1	B	265	ASP
1	B	274	ILE
1	B	278	LEU
1	B	289	VAL
1	B	297	ARG
1	B	300	GLU
1	B	301	LEU
1	B	303	ARG
1	B	309	LYS
1	B	326	LYS
1	B	340	LYS
1	B	343	GLU
1	B	368	LYS
1	B	374	LYS
1	B	375	LYS
1	B	377	GLN
1	B	378	GLU
1	B	380	LYS
1	B	385	VAL
1	B	398	ASP
1	B	417	VAL
1	B	420	ILE
1	B	421	ARG

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Mol	Chain	Res	Type
1	B	428	VAL
1	B	429	SER
1	B	433	ILE
1	B	439	ILE
1	B	443	GLU
1	B	475	LEU
1	B	484	LEU
1	B	488	GLN
1	B	490	LYS
1	B	509	LYS
1	B	512	LYS
1	B	522	GLU
1	B	533	ARG
1	B	537	ILE
1	B	539	SER
1	B	560	GLU
1	B	587	THR
1	B	610	LEU
1	B	638	LEU
1	B	680	GLU
1	B	685	VAL
1	B	718	THR
1	B	723	LYS
1	B	725	LYS
1	B	780	LEU
1	B	784	ARG
1	B	818	ASP
1	B	843	VAL
1	B	846	SER
1	B	861	GLU
1	B	864	LYS
1	B	871	ILE
1	B	880	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	258	ASN
1	A	312	GLN
1	A	336	HIS
1	A	456	GLN

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Mol	Chain	Res	Type
1	A	534	GLN
1	B	106	HIS
1	B	288	ASN
1	B	355	GLN
1	B	419	HIS
1	B	448	HIS
1	B	468	ASN
1	B	737	HIS

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 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	TZD	A	889	2	27,28,28	1.62	6 (22%)	37,42,42	1.11	2 (5%)
3	TZD	B	887	2	27,28,28	1.69	6 (22%)	37,42,42	1.10	2 (5%)

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	TZD	A	889	2	-	2/17/17/17	0/2/2/2
3	TZD	B	887	2	-	4/17/17/17	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	887	TZD	C4'-N3'	4.14	1.40	1.35
3	A	889	TZD	C4'-N3'	3.95	1.40	1.35
3	B	887	TZD	C5'-C4'	3.78	1.49	1.42
3	A	889	TZD	C5'-C4'	3.47	1.48	1.42
3	B	887	TZD	C35-N3	3.09	1.52	1.47
3	B	887	TZD	C2'-N1'	2.80	1.38	1.34
3	A	889	TZD	C35-N3	2.78	1.52	1.47
3	B	887	TZD	C4-N3	2.56	1.43	1.39
3	A	889	TZD	C2'-N1'	2.55	1.38	1.34
3	A	889	TZD	C4-N3	2.44	1.43	1.39
3	B	887	TZD	OC2-C2	2.34	1.25	1.21
3	A	889	TZD	C6'-N1'	2.22	1.38	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	887	TZD	C6'-N1'-C2'	2.62	120.37	116.07
3	A	889	TZD	C6'-N1'-C2'	2.56	120.28	116.07
3	B	887	TZD	C35-N3-C4	-2.26	122.12	124.98
3	A	889	TZD	C35-N3-C4	-2.20	122.19	124.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

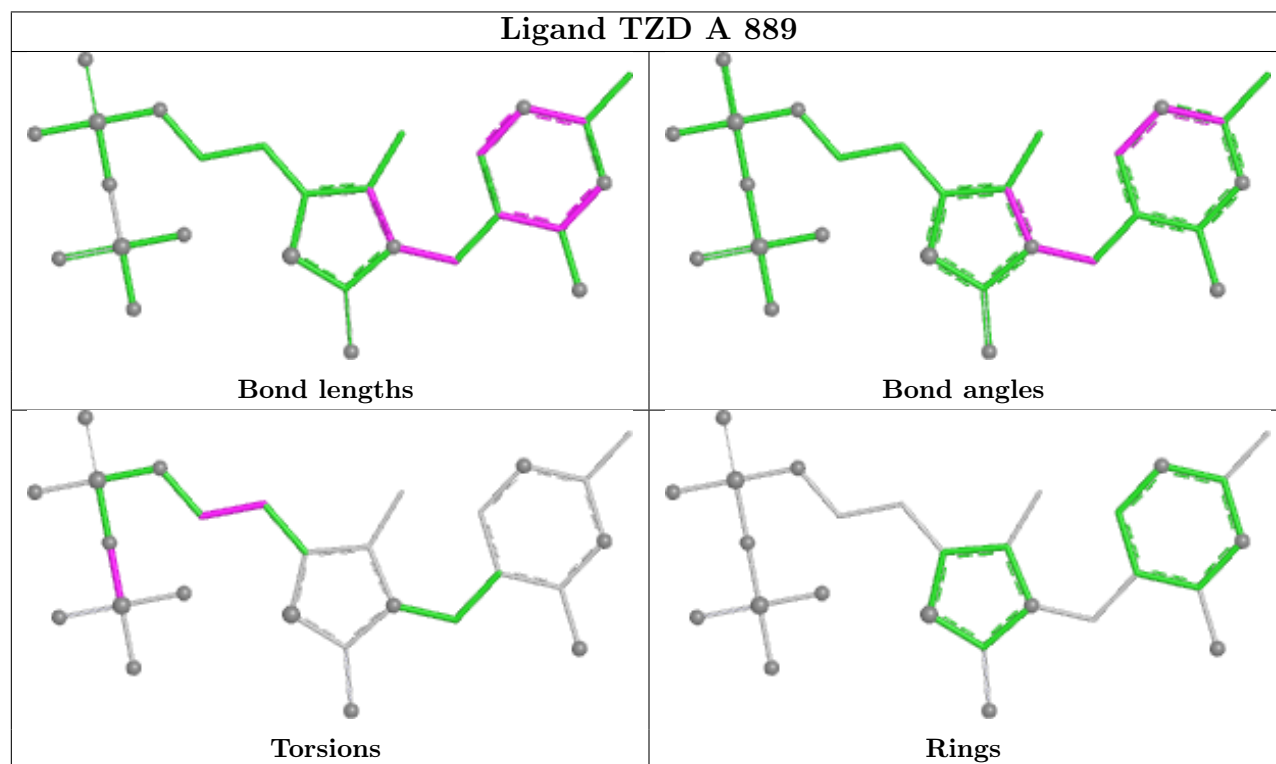
Mol	Chain	Res	Type	Atoms
3	A	889	TZD	P1-O11-P2-O21
3	B	887	TZD	P1-O11-P2-O21
3	B	887	TZD	P1-O11-P2-O23
3	B	887	TZD	C5-C5A-C5B-O5G
3	B	887	TZD	P1-O11-P2-O22
3	A	889	TZD	C5-C5A-C5B-O5G

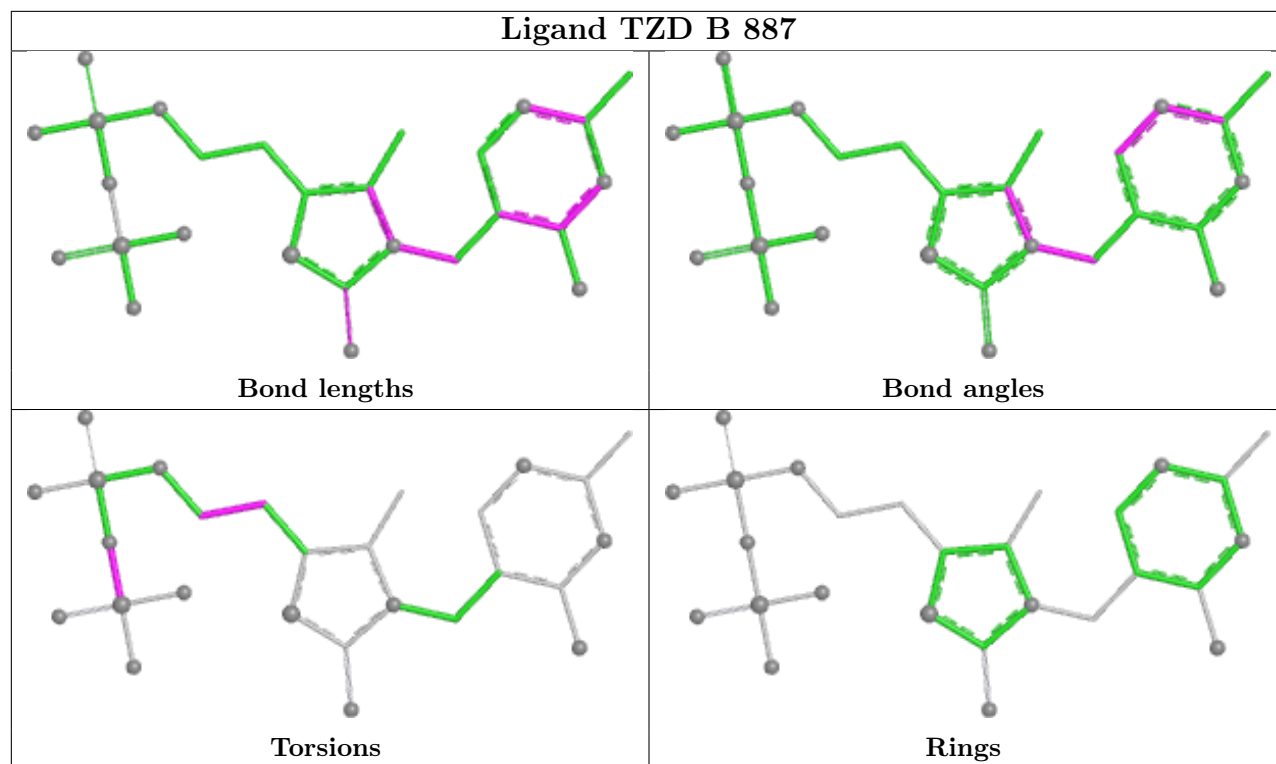
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	887	TZD	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.