



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:35 AM UTC

PDB ID : 6FTD / pdb_00006ftd
Title : Deinococcus radiodurans BphP PAS-GAF H290T mutant
Authors : Edlund, P.; Takala, H.; Westenhoff, S.; Ihalainen, J.A.
Deposited on : 2018-02-21
Resolution : 1.40 Å(reported)

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

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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

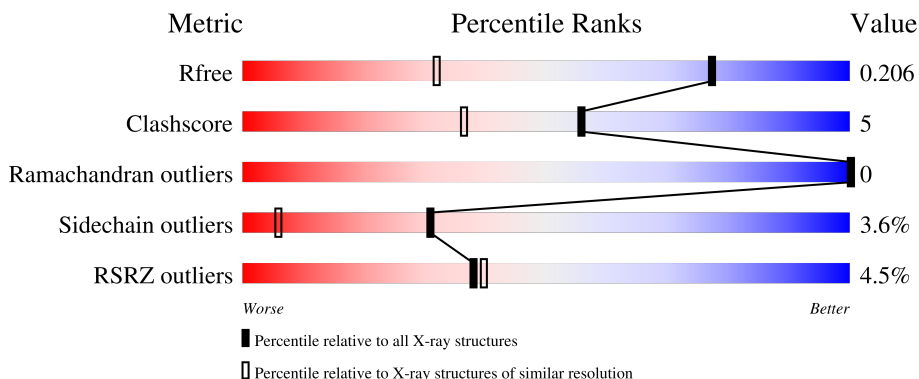
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	343	
1	B	343	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	403	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5741 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 Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2526	1611	442	463	10	0	19	0
1	B	314	2516	1608	436	461	11	0	17	0

There are 46 discrepancies between the modelled and reference sequences:

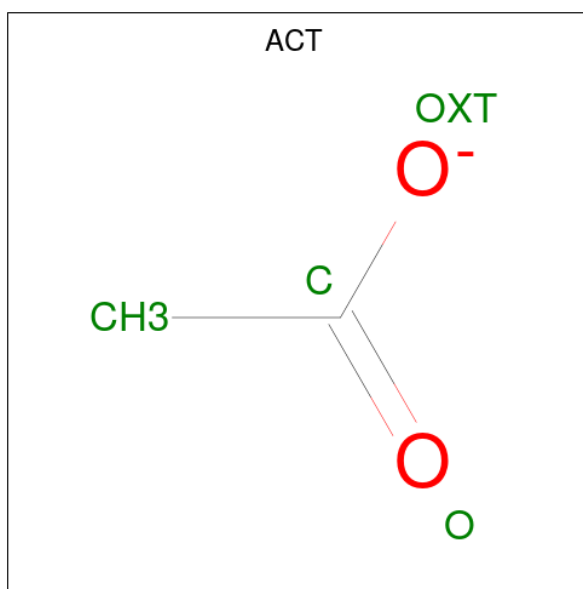
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q9RZA4
A	-12	ALA	-	expression tag	UNP Q9RZA4
A	-11	SER	-	expression tag	UNP Q9RZA4
A	-10	MET	-	expression tag	UNP Q9RZA4
A	-9	THR	-	expression tag	UNP Q9RZA4
A	-8	GLY	-	expression tag	UNP Q9RZA4
A	-7	GLY	-	expression tag	UNP Q9RZA4
A	-6	GLN	-	expression tag	UNP Q9RZA4
A	-5	GLN	-	expression tag	UNP Q9RZA4
A	-4	MET	-	expression tag	UNP Q9RZA4
A	-3	GLY	-	expression tag	UNP Q9RZA4
A	-2	ARG	-	expression tag	UNP Q9RZA4
A	-1	GLY	-	expression tag	UNP Q9RZA4
A	0	SER	-	expression tag	UNP Q9RZA4
A	290	THR	HIS	engineered mutation	UNP Q9RZA4
A	322	LEU	-	expression tag	UNP Q9RZA4
A	323	GLU	-	expression tag	UNP Q9RZA4
A	324	HIS	-	expression tag	UNP Q9RZA4
A	325	HIS	-	expression tag	UNP Q9RZA4
A	326	HIS	-	expression tag	UNP Q9RZA4
A	327	HIS	-	expression tag	UNP Q9RZA4
A	328	HIS	-	expression tag	UNP Q9RZA4
A	329	HIS	-	expression tag	UNP Q9RZA4
B	-13	MET	-	initiating methionine	UNP Q9RZA4
B	-12	ALA	-	expression tag	UNP Q9RZA4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	SER	-	expression tag	UNP Q9RZA4
B	-10	MET	-	expression tag	UNP Q9RZA4
B	-9	THR	-	expression tag	UNP Q9RZA4
B	-8	GLY	-	expression tag	UNP Q9RZA4
B	-7	GLY	-	expression tag	UNP Q9RZA4
B	-6	GLN	-	expression tag	UNP Q9RZA4
B	-5	GLN	-	expression tag	UNP Q9RZA4
B	-4	MET	-	expression tag	UNP Q9RZA4
B	-3	GLY	-	expression tag	UNP Q9RZA4
B	-2	ARG	-	expression tag	UNP Q9RZA4
B	-1	GLY	-	expression tag	UNP Q9RZA4
B	0	SER	-	expression tag	UNP Q9RZA4
B	290	THR	HIS	engineered mutation	UNP Q9RZA4
B	322	LEU	-	expression tag	UNP Q9RZA4
B	323	GLU	-	expression tag	UNP Q9RZA4
B	324	HIS	-	expression tag	UNP Q9RZA4
B	325	HIS	-	expression tag	UNP Q9RZA4
B	326	HIS	-	expression tag	UNP Q9RZA4
B	327	HIS	-	expression tag	UNP Q9RZA4
B	328	HIS	-	expression tag	UNP Q9RZA4
B	329	HIS	-	expression tag	UNP Q9RZA4

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



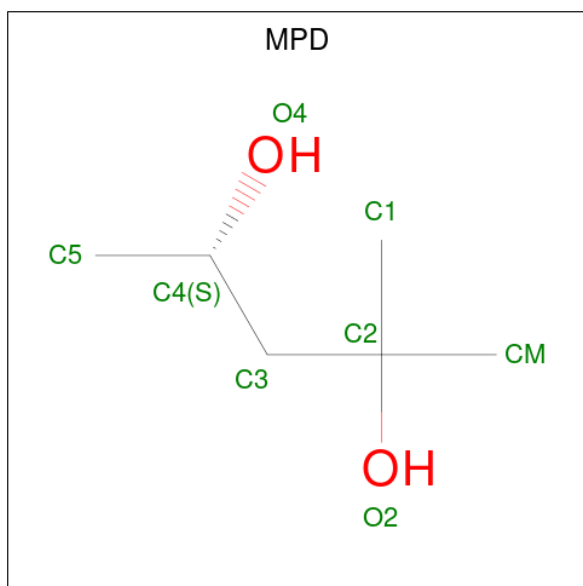
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total	0	0
			C		
			4	2	2

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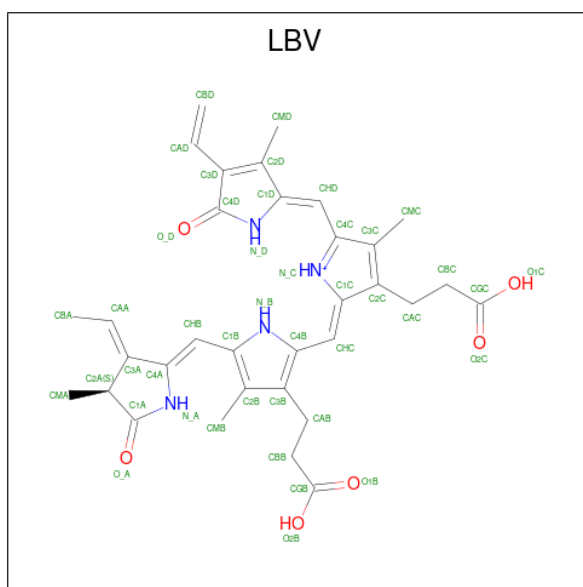
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is 3-[2-[(Z)-[3-(2-carboxyethyl)-5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrro l-2-ylidene)methyl]-4-methyl-pyrrol-1-ium -2-ylidene]methyl]-5-[(Z)-[(3E)-3-ethylidene-4-methyl-5-oxidanylidene-pyrrolidin-2-ylidene]methyl]-4-methyl-1H-pyrrol-3-yl]propanoic acid (CCD ID: LBV) (formula: C₃₃H₃₇N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	43	33	4	6	0	0
4	B	1	43	33	4	6	0	0

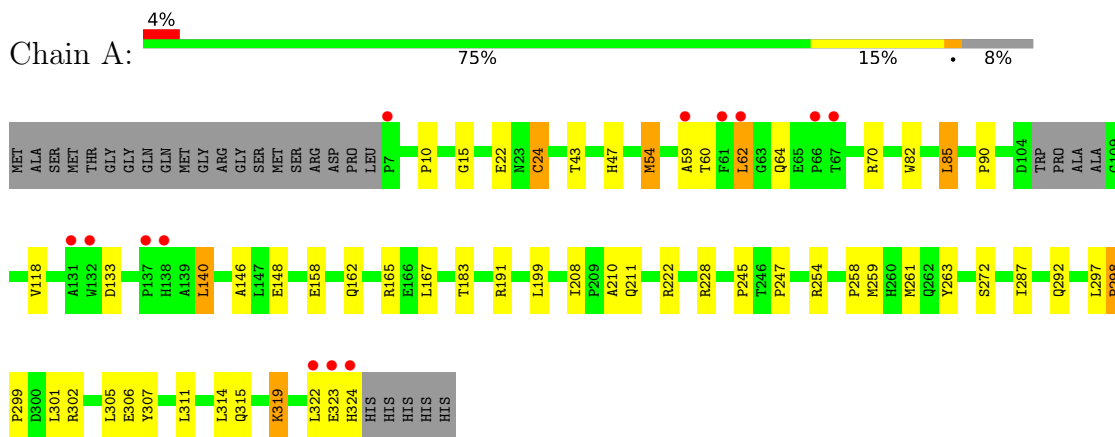
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	274	274	274	0	0
5	B	299	299	299	0	0

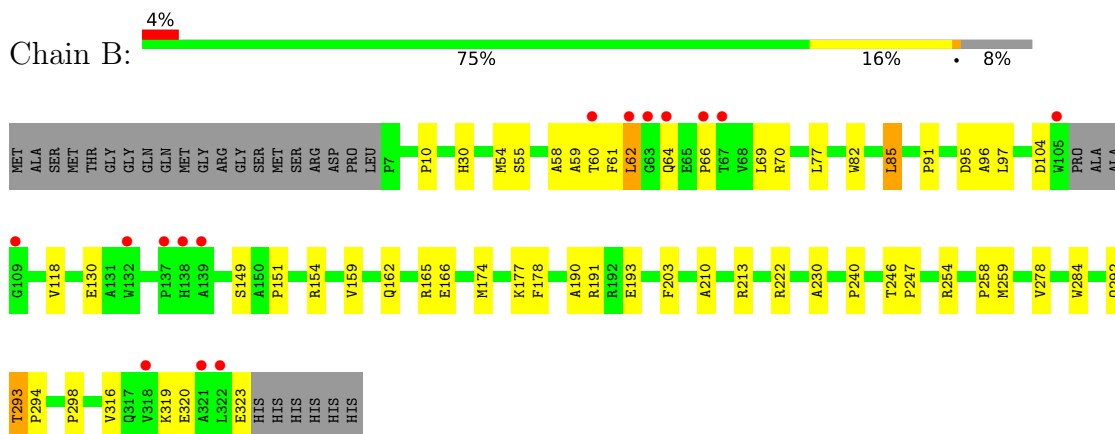
3 Residue-property plots [i](#)

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: Bacteriophytochrome



- Molecule 1: Bacteriophytochrome



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.81Å 53.03Å 135.88Å 90.00° 93.30° 90.00°	Depositor
Resolution (Å)	47.33 – 1.40 47.33 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.33-1.40) 99.7 (47.33-1.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.148 , 0.198 0.158 , 0.206	Depositor DCC
R_{free} test set	6620 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtrriage
Anisotropy	0.184	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5741	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9659e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, MPD, LBV

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	1.71	25/2603 (1.0%)	1.44	14/3560 (0.4%)
1	B	1.73	22/2594 (0.8%)	1.46	13/3548 (0.4%)
All	All	1.72	47/5197 (0.9%)	1.45	27/7108 (0.4%)

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	2
All	All	0	4

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	PRO	CA-C	9.46	1.57	1.51
1	A	59	ALA	CA-C	9.13	1.65	1.52
1	A	133	ASP	C-O	-8.89	1.13	1.23
1	A	64	GLN	CA-C	7.69	1.63	1.52
1	B	82	TRP	N-CA	7.65	1.53	1.46
1	A	82	TRP	N-CA	7.46	1.53	1.46
1	B	193	GLU	CA-C	-7.37	1.43	1.52
1	B	85	LEU	N-CA	7.15	1.54	1.46
1	A	146	ALA	C-O	7.13	1.32	1.24
1	B	97	LEU	CA-C	7.09	1.62	1.52
1	A	315	GLN	CA-C	-6.94	1.43	1.52
1	A	59	ALA	N-CA	6.89	1.54	1.46
1	A	140	LEU	CA-C	6.87	1.61	1.52
1	B	91	PRO	CA-C	-6.85	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	THR	CA-C	6.78	1.60	1.52
1	B	97	LEU	N-CA	-6.41	1.37	1.46
1	B	60	THR	C-O	6.33	1.31	1.24
1	B	104	ASP	N-CA	6.03	1.53	1.46
1	A	263	TYR	C-O	-6.03	1.17	1.24
1	B	230	ALA	N-CA	-6.02	1.38	1.46
1	A	62	LEU	CA-C	5.72	1.59	1.52
1	A	211	GLN	CA-C	5.71	1.60	1.52
1	A	60	THR	C-O	-5.57	1.17	1.24
1	A	287	ILE	CA-C	5.51	1.58	1.53
1	A	302	ARG	N-CA	5.49	1.53	1.46
1	A	47	HIS	CA-C	5.47	1.59	1.52
1	B	240	PRO	C-O	5.47	1.30	1.24
1	B	254	ARG	CZ-NH2	-5.46	1.26	1.33
1	A	199	LEU	CA-C	-5.38	1.45	1.52
1	B	55	SER	C-O	5.36	1.30	1.23
1	A	10	PRO	N-CA	-5.35	1.39	1.46
1	A	15	GLY	N-CA	5.35	1.52	1.45
1	A	208	ILE	CA-C	5.32	1.58	1.52
1	B	178	PHE	N-CA	5.29	1.52	1.46
1	B	30	HIS	CA-C	5.25	1.60	1.52
1	B	298	PRO	CA-CB	-5.22	1.46	1.54
1	A	314	LEU	N-CA	5.16	1.52	1.46
1	B	298	PRO	CA-C	-5.15	1.47	1.52
1	B	190	ALA	CA-C	-5.13	1.46	1.52
1	B	174	MET	CA-C	-5.11	1.46	1.52
1	B	278	VAL	C-O	-5.09	1.18	1.24
1	A	272[A]	SER	C-O	5.05	1.29	1.23
1	A	272[B]	SER	C-O	5.05	1.29	1.23
1	B	254	ARG	C-O	5.04	1.29	1.23
1	A	245	PRO	N-CA	5.02	1.53	1.47
1	A	43	THR	N-CA	5.00	1.52	1.46
1	B	151	PRO	C-O	5.00	1.30	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	CYS	CB-CA-C	-10.59	93.21	110.79
1	B	213	ARG	NE-CZ-NH1	8.35	129.85	121.50
1	B	104	ASP	N-CA-C	8.20	122.27	109.07
1	B	316	VAL	N-CA-C	-7.33	103.64	110.53
1	B	10	PRO	O-C-N	7.19	124.62	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	PRO	O-C-N	7.17	124.61	121.31
1	A	59	ALA	N-CA-C	7.00	119.80	111.33
1	A	64	GLN	N-CA-C	6.88	121.25	110.32
1	A	254	ARG	NE-CZ-NH2	6.84	125.35	119.20
1	B	203	PHE	CA-C-N	-6.55	113.24	119.85
1	B	203	PHE	C-N-CA	-6.55	113.24	119.85
1	A	302	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	B	203	PHE	O-C-N	6.08	126.20	121.88
1	A	183	THR	N-CA-C	-6.07	102.52	110.53
1	A	298	PRO	CA-C-N	6.04	125.52	119.24
1	A	298	PRO	C-N-CA	6.04	125.52	119.24
1	A	85	LEU	CA-CB-CG	6.02	137.38	116.30
1	B	58	ALA	N-CA-C	5.97	117.66	111.03
1	B	210	ALA	N-CA-C	5.68	118.24	111.71
1	A	322	LEU	N-CA-C	5.54	117.17	111.03
1	B	58	ALA	O-C-N	5.52	127.99	122.03
1	B	77	LEU	N-CA-C	5.45	117.30	111.36
1	B	149	SER	CA-CB-OG	-5.26	100.57	111.10
1	A	297	LEU	CA-C-N	-5.19	115.04	120.38
1	A	297	LEU	C-N-CA	-5.19	115.04	120.38
1	B	85	LEU	CB-CA-C	-5.13	102.83	110.88
1	A	210	ALA	N-CA-C	5.02	117.48	111.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	A	191	ARG	Sidechain
1	B	165	ARG	Sidechain
1	B	191	ARG	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	2526	0	2545	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2516	0	2531	29	0
2	A	12	0	9	1	0
2	B	12	0	9	2	0
3	A	8	0	14	0	0
3	B	8	0	14	0	0
4	A	43	0	33	1	0
4	B	43	0	34	0	0
5	A	274	0	0	7	0
5	B	299	0	0	8	0
All	All	5741	0	5189	49	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 5.

All (49) 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:162[A]:GLN:HE21	1:B:166[A]:GLU:HG3	1.32	0.94
1:B:54[B]:MET:HE1	1:B:69:LEU:HB2	1.63	0.79
1:A:167[B]:LEU:HD23	1:A:305[B]:LEU:HD21	1.71	0.71
1:A:167[B]:LEU:HD23	1:A:305[B]:LEU:CD2	2.21	0.71
1:B:293[A]:THR:HG23	1:B:294:PRO:HD2	1.74	0.70
1:A:162[B]:GLN:HG2	5:A:503:HOH:O	1.91	0.68
1:B:54[B]:MET:HE1	1:B:69:LEU:CB	2.27	0.63
1:A:118:VAL:HG11	1:A:247[B]:PRO:CG	2.29	0.63
1:B:54[B]:MET:SD	1:B:66:PRO:HB3	2.40	0.62
1:B:162[B]:GLN:HG2	5:B:519:HOH:O	2.00	0.61
1:A:307:TYR:CE2	1:A:311[B]:LEU:HD11	2.36	0.61
1:B:247[B]:PRO:HB3	5:B:772:HOH:O	2.02	0.59
1:A:158:GLU:O	1:A:162[B]:GLN:HG3	2.03	0.59
1:A:118:VAL:HG11	1:A:247[B]:PRO:HG3	1.84	0.58
1:B:54[A]:MET:HE1	1:B:70:ARG:HG3	1.87	0.57
1:A:54:MET:HE1	1:A:70:ARG:HD2	1.88	0.56
1:B:162[B]:GLN:CG	5:B:519:HOH:O	2.54	0.56
1:A:228[B]:ARG:NH2	5:A:505:HOH:O	2.39	0.55
1:B:61:PHE:HD2	1:B:62:LEU:HD22	1.71	0.55
1:A:258[A]:PRO:HG2	5:A:683:HOH:O	2.08	0.54
1:B:54[B]:MET:SD	1:B:66:PRO:CB	2.96	0.53
1:B:159[A]:VAL:HG23	5:B:686:HOH:O	2.08	0.53
1:B:54[A]:MET:SD	1:B:70:ARG:HB2	2.49	0.53
1:B:258[A]:PRO:HG2	5:B:720:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:VAL:HG11	1:B:247[A]:PRO:CG	2.41	0.51
1:A:167[B]:LEU:HG	1:A:301:LEU:HD22	1.92	0.51
1:B:177[B]:LYS:HE2	1:B:284:TRP:CE2	2.46	0.51
1:A:259:MET:HG2	5:A:683:HOH:O	2.15	0.47
1:B:320:GLU:O	1:B:323:GLU:HB2	2.15	0.46
1:A:292[B]:GLN:HG3	2:A:403:ACT:H1	1.98	0.46
1:B:292[B]:GLN:CG	2:B:403:ACT:H1	2.46	0.46
1:B:96:ALA:HA	5:B:748:HOH:O	2.16	0.45
1:B:162[A]:GLN:HE21	1:B:166[A]:GLU:CG	2.16	0.45
1:B:292[A]:GLN:HG2	1:B:292[A]:GLN:O	2.16	0.45
1:B:154:ARG:HD2	5:B:736:HOH:O	2.16	0.45
1:B:259:MET:HG2	5:B:720:HOH:O	2.17	0.45
1:A:167[B]:LEU:HD23	1:A:305[B]:LEU:HD23	1.96	0.44
1:A:292[A]:GLN:O	1:A:292[A]:GLN:HG2	2.17	0.44
1:B:292[B]:GLN:HG3	2:B:403:ACT:H1	2.01	0.43
1:A:90:PRO:HA	5:A:620:HOH:O	2.19	0.42
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.86	0.42
1:A:306:GLU:HG3	5:A:729:HOH:O	2.18	0.42
1:B:59:ALA:HB2	1:B:66:PRO:HA	2.01	0.42
1:B:61:PHE:CD2	1:B:62:LEU:HD22	2.53	0.42
1:B:293[A]:THR:HG22	1:B:294:PRO:O	2.19	0.41
1:B:54[B]:MET:HE3	1:B:54[B]:MET:HB3	1.55	0.41
1:A:24:CYS:HB3	4:A:405:LBV:HAA1	1.94	0.41
1:A:319:LYS:HE2	5:A:525:HOH:O	2.20	0.41
1:A:298:PRO:HA	1:A:299:PRO:HD3	1.95	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	329/343 (96%)	324 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	327/343 (95%)	324 (99%)	3 (1%)	0	100	100
All	All	656/686 (96%)	648 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	272/275 (99%)	260 (96%)	12 (4%)	25	4
1	B	270/275 (98%)	262 (97%)	8 (3%)	36	8
All	All	542/550 (98%)	522 (96%)	20 (4%)	31	5

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	54	MET
1	A	62	LEU
1	A	85	LEU
1	A	140	LEU
1	A	148	GLU
1	A	222	ARG
1	A	261[A]	MET
1	A	261[B]	MET
1	A	319	LYS
1	A	323	GLU
1	A	324	HIS
1	B	62	LEU
1	B	64	GLN
1	B	95	ASP
1	B	130	GLU
1	B	222	ARG
1	B	293[A]	THR

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Mol	Chain	Res	Type
1	B	293[B]	THR
1	B	319	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	B	401	-	3,3,3	0.79	0	3,3,3	0.90	0
2	ACT	A	401	-	3,3,3	0.60	0	3,3,3	1.48	0
4	LBV	B	405	1	46,46,46	2.02	15 (32%)	58,67,67	2.14	20 (34%)
2	ACT	B	403	-	3,3,3	0.94	0	3,3,3	1.08	0
3	MPD	A	404	-	7,7,7	0.69	0	9,10,10	1.89	2 (22%)
2	ACT	B	402	-	3,3,3	1.46	1 (33%)	3,3,3	0.74	0
2	ACT	A	402	-	3,3,3	0.99	0	3,3,3	1.23	0
3	MPD	B	404	-	7,7,7	0.76	0	9,10,10	1.28	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	403	-	3,3,3	1.04	0	3,3,3	1.91	2 (66%)
4	LBV	A	405	1	46,46,46	1.97	15 (32%)	58,67,67	1.96	19 (32%)

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	MPD	A	404	-	-	0/5/5/5	-
4	LBV	A	405	1	-	6/26/74/74	0/4/4/4
3	MPD	B	404	-	-	3/5/5/5	-
4	LBV	B	405	1	-	7/26/74/74	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	405	LBV	C2A-C3A	-5.44	1.44	1.51
4	B	405	LBV	C2C-C3C	4.74	1.47	1.36
4	A	405	LBV	O1B-CGB	4.09	1.35	1.22
4	A	405	LBV	C2A-C3A	-4.02	1.46	1.51
4	A	405	LBV	CAA-C3A	3.84	1.43	1.33
4	B	405	LBV	C2A-C1A	-3.80	1.47	1.52
4	A	405	LBV	C4C-C3C	-3.46	1.38	1.45
4	A	405	LBV	CHC-C4B	3.06	1.47	1.40
4	B	405	LBV	O1B-CGB	3.03	1.32	1.22
4	A	405	LBV	C4A-N_A	2.99	1.42	1.37
4	B	405	LBV	O1C-CGC	-2.98	1.21	1.30
4	B	405	LBV	CMB-C2B	2.94	1.56	1.50
4	A	405	LBV	CHB-C1B	2.93	1.47	1.40
4	B	405	LBV	CHC-C1C	2.93	1.44	1.38
4	B	405	LBV	CHC-C4B	2.91	1.46	1.40
4	A	405	LBV	C1C-N_C	-2.86	1.32	1.38
4	B	405	LBV	O_D-C4D	2.76	1.28	1.23
4	A	405	LBV	C1C-C2C	-2.75	1.41	1.45
4	A	405	LBV	C1D-N_D	-2.71	1.33	1.37
4	B	405	LBV	C1B-C2B	-2.63	1.35	1.41
4	B	405	LBV	C1C-N_C	-2.52	1.33	1.38
4	B	405	LBV	CAA-C3A	2.45	1.39	1.33
4	B	405	LBV	CHD-C4C	2.45	1.46	1.40
4	A	405	LBV	C1B-C2B	-2.33	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	ACT	OXT-C	-2.31	1.20	1.30
4	B	405	LBV	O_A-C1A	2.27	1.27	1.23
4	A	405	LBV	C1D-C2D	-2.19	1.41	1.45
4	B	405	LBV	C4A-C3A	2.11	1.48	1.45
4	A	405	LBV	CHD-C4C	2.10	1.45	1.40
4	A	405	LBV	C2C-C3C	2.08	1.41	1.36
4	A	405	LBV	C3B-C2B	2.05	1.44	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	LBV	C4B-C3B-C2B	-5.03	101.77	107.62
4	B	405	LBV	O_A-C1A-N_A	-4.61	119.49	124.93
4	A	405	LBV	CMD-C2D-C1D	4.18	129.24	124.16
4	B	405	LBV	C2D-C1D-N_D	4.15	113.02	106.97
4	B	405	LBV	C3D-C2D-C1D	-4.12	103.33	107.92
4	A	405	LBV	C3D-C2D-C1D	-4.08	103.37	107.92
4	B	405	LBV	CAA-C3A-C4A	-4.08	121.44	126.36
4	A	405	LBV	CHC-C4B-C3B	-3.96	118.71	127.22
4	B	405	LBV	C1B-C2B-C3B	3.96	112.70	107.76
4	B	405	LBV	CMC-C3C-C4C	3.91	131.16	125.10
3	A	404	MPD	O2-C2-C1	3.89	120.12	107.99
4	A	405	LBV	C4C-C3C-C2C	3.77	110.75	106.48
4	A	405	LBV	C4B-C3B-C2B	-3.72	103.29	107.62
4	B	405	LBV	CHC-C4B-C3B	-3.70	119.27	127.22
4	B	405	LBV	C1D-N_D-C4D	-3.65	106.18	110.66
4	A	405	LBV	CAA-C3A-C4A	-3.09	122.63	126.36
4	B	405	LBV	CAB-C3B-C4B	3.06	130.62	125.77
4	A	405	LBV	CHD-C4C-C3C	3.03	132.66	124.87
4	B	405	LBV	O2C-CGC-CBC	-2.91	113.88	123.09
4	A	405	LBV	CAC-C2C-C1C	2.87	130.07	125.02
4	A	405	LBV	O2B-CGB-CBB	2.83	122.93	114.00
4	A	405	LBV	C2D-C1D-N_D	2.82	111.08	106.97
3	A	404	MPD	CM-C2-C1	-2.80	104.36	110.63
4	A	405	LBV	C3C-C4C-N_C	-2.77	104.54	110.58
4	B	405	LBV	CHD-C1D-C2D	-2.74	121.51	126.97
3	B	404	MPD	O2-C2-C1	-2.71	99.53	107.99
4	B	405	LBV	C1C-C2C-C3C	-2.71	103.79	106.73
4	A	405	LBV	CAB-C3B-C4B	2.71	130.07	125.77
4	B	405	LBV	C3B-C4B-N_B	2.60	110.83	107.57
4	A	405	LBV	CHD-C1D-C2D	-2.58	121.82	126.97
4	A	405	LBV	C1C-N_C-C4C	2.58	111.25	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	LBV	CHC-C4B-N_B	2.54	131.03	125.29
4	A	405	LBV	O2C-CGC-CBC	-2.53	115.06	123.09
4	A	405	LBV	C1C-C2C-C3C	-2.50	104.02	106.73
4	B	405	LBV	C1C-N_C-C4C	2.45	111.01	106.52
4	A	405	LBV	CHC-C1C-N_C	2.41	129.65	124.60
2	A	403	ACT	O-C-CH3	-2.37	112.80	122.53
2	A	403	ACT	OXT-C-CH3	2.30	124.71	115.05
4	B	405	LBV	O1C-CGC-CBC	2.28	121.20	114.00
4	B	405	LBV	CMB-C2B-C3B	-2.25	120.86	125.62
4	B	405	LBV	O_D-C4D-N_D	-2.25	119.82	125.08
4	B	405	LBV	CMD-C2D-C1D	2.21	126.85	124.16
4	B	405	LBV	O1B-CGB-CBB	-2.19	116.16	123.09
4	A	405	LBV	O2B-CGB-O1B	-2.16	117.79	123.33

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	MPD	O2-C2-C3-C4
3	B	404	MPD	CM-C2-C3-C4
4	A	405	LBV	C3C-C4C-CHD-C1D
4	A	405	LBV	N_C-C4C-CHD-C1D
4	B	405	LBV	C3C-C4C-CHD-C1D
4	B	405	LBV	N_C-C4C-CHD-C1D
4	B	405	LBV	C2A-C3A-CAA-CBA
3	B	404	MPD	C1-C2-C3-C4
4	A	405	LBV	CAB-CBB-CGB-O2B
4	B	405	LBV	CAB-CBB-CGB-O1B
4	A	405	LBV	CAB-CBB-CGB-O1B
4	B	405	LBV	CAB-CBB-CGB-O2B
4	B	405	LBV	CAC-CBC-CGC-O1C
4	A	405	LBV	CAC-CBC-CGC-O1C
4	A	405	LBV	CAC-CBC-CGC-O2C
4	B	405	LBV	CAC-CBC-CGC-O2C

There are no ring outliers.

3 monomers are involved in 4 short contacts:

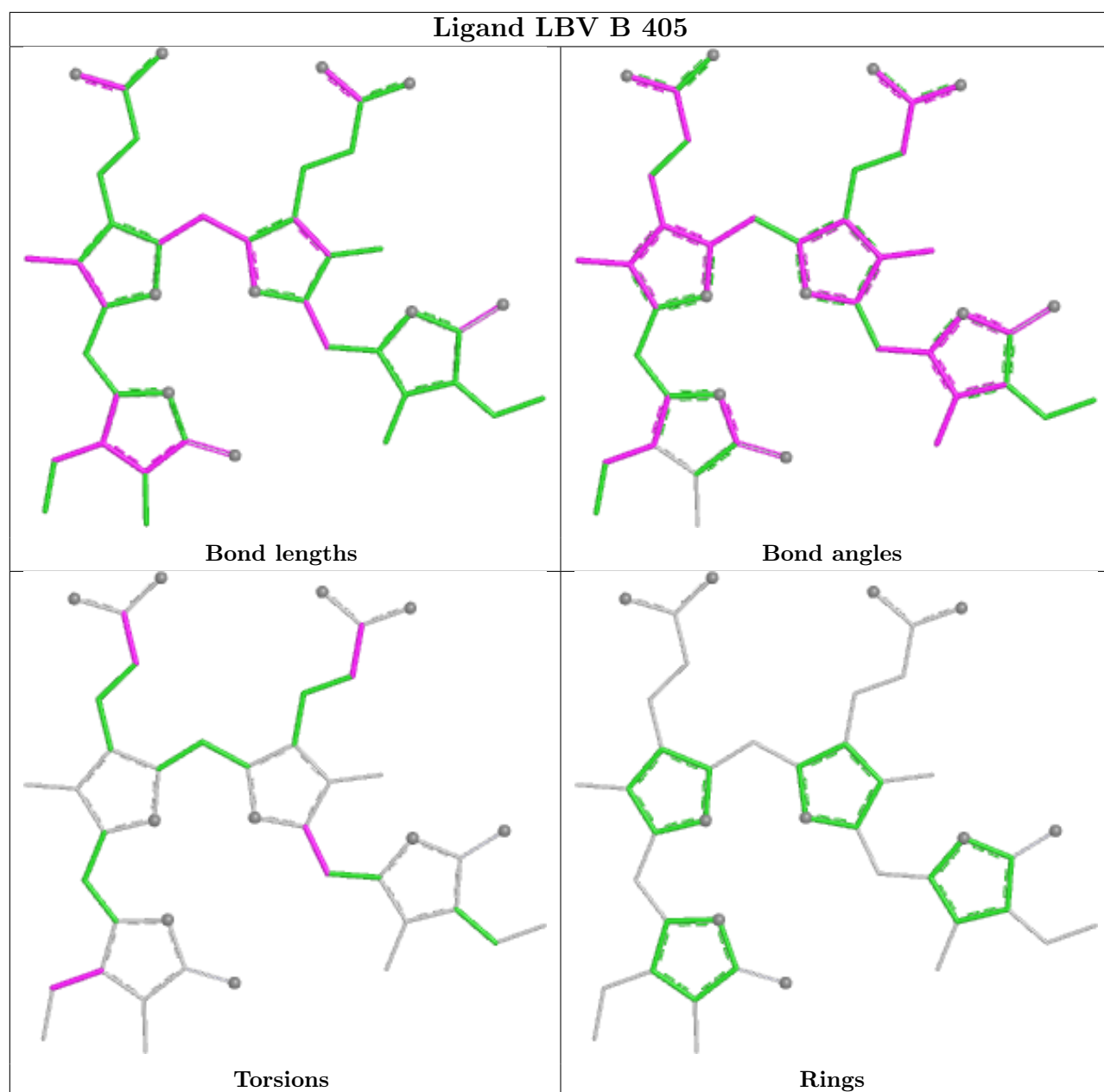
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	ACT	2	0
2	A	403	ACT	1	0

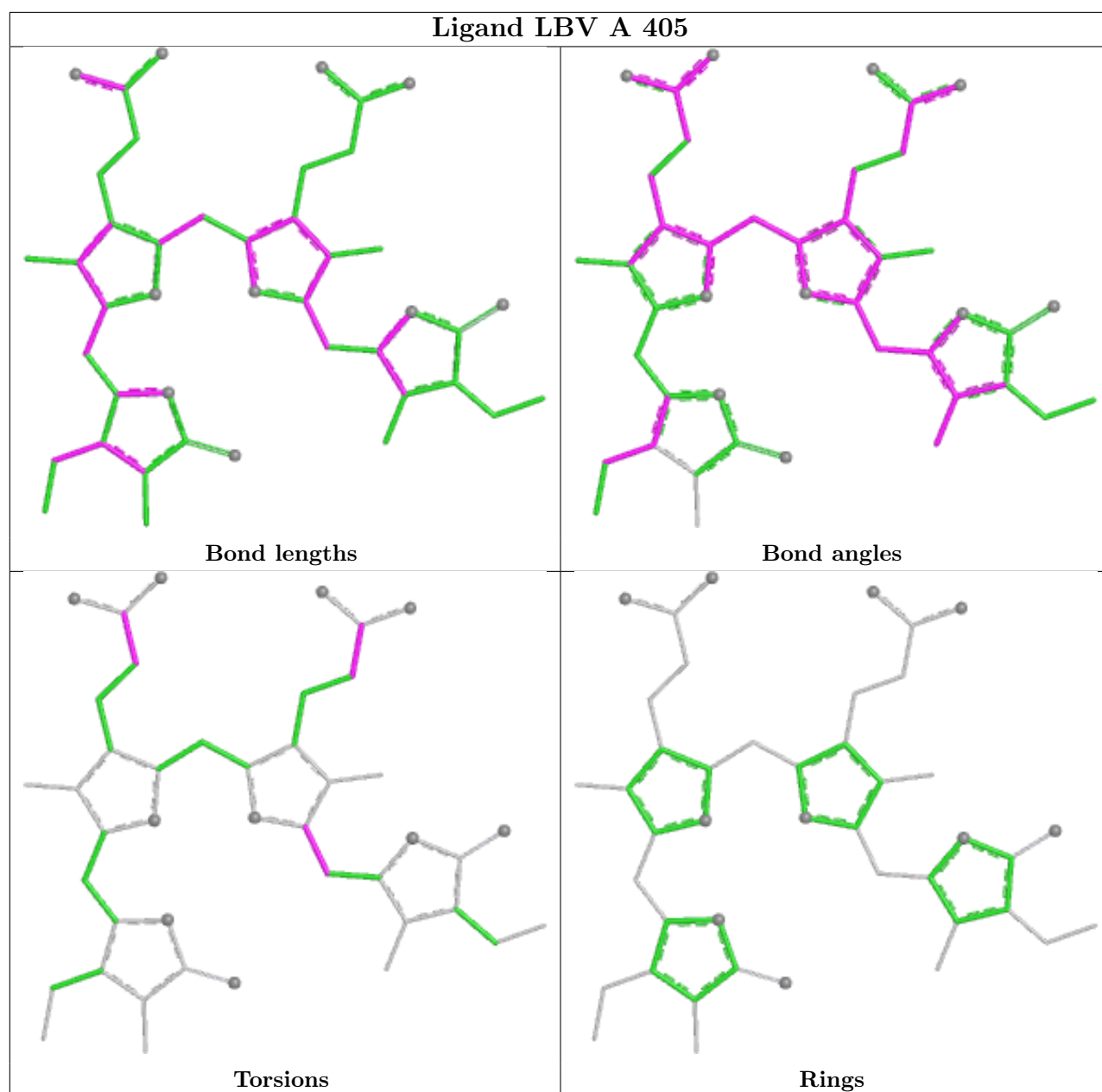
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	LBV	1	0

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





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/343 (91%)	-0.09	13 (4%) 41 43	6, 19, 57, 105	19 (6%)
1	B	314/343 (91%)	-0.18	15 (4%) 35 38	6, 17, 55, 88	17 (5%)
All	All	628/686 (91%)	-0.14	28 (4%) 38 40	6, 18, 55, 105	36 (5%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	TRP	6.3
1	B	105	TRP	6.0
1	B	322	LEU	5.0
1	A	66	PRO	4.3
1	A	132	TRP	4.1
1	B	66	PRO	3.3
1	A	137	PRO	3.2
1	B	321	ALA	3.1
1	A	323	GLU	3.1
1	B	109	GLY	3.0
1	B	318	VAL	3.0
1	A	324	HIS	2.9
1	B	62	LEU	2.7
1	B	139	ALA	2.7
1	A	7	PRO	2.7
1	B	63	GLY	2.6
1	A	62	LEU	2.6
1	A	61	PHE	2.5
1	B	67	THR	2.4
1	B	138	HIS	2.3
1	B	137	PRO	2.3
1	A	59	ALA	2.2
1	A	138	HIS	2.2
1	A	131	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	2.1
1	B	60	THR	2.1
1	A	67	THR	2.0
1	B	64	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](#)

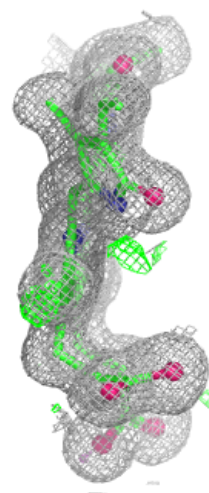
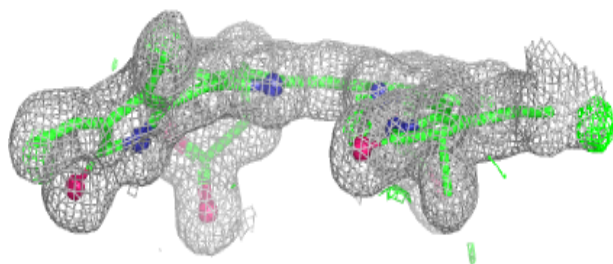
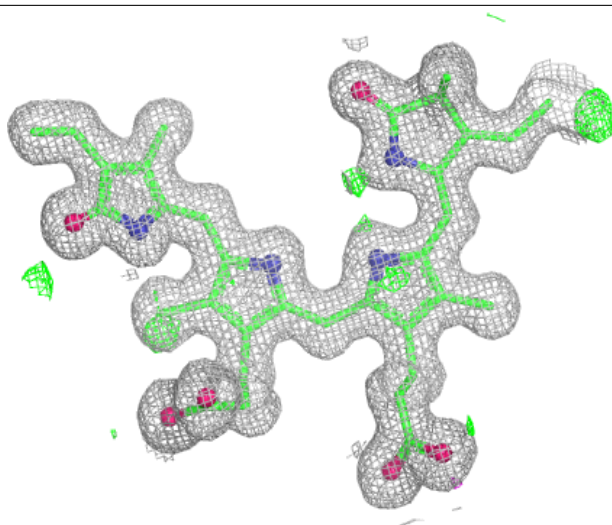
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

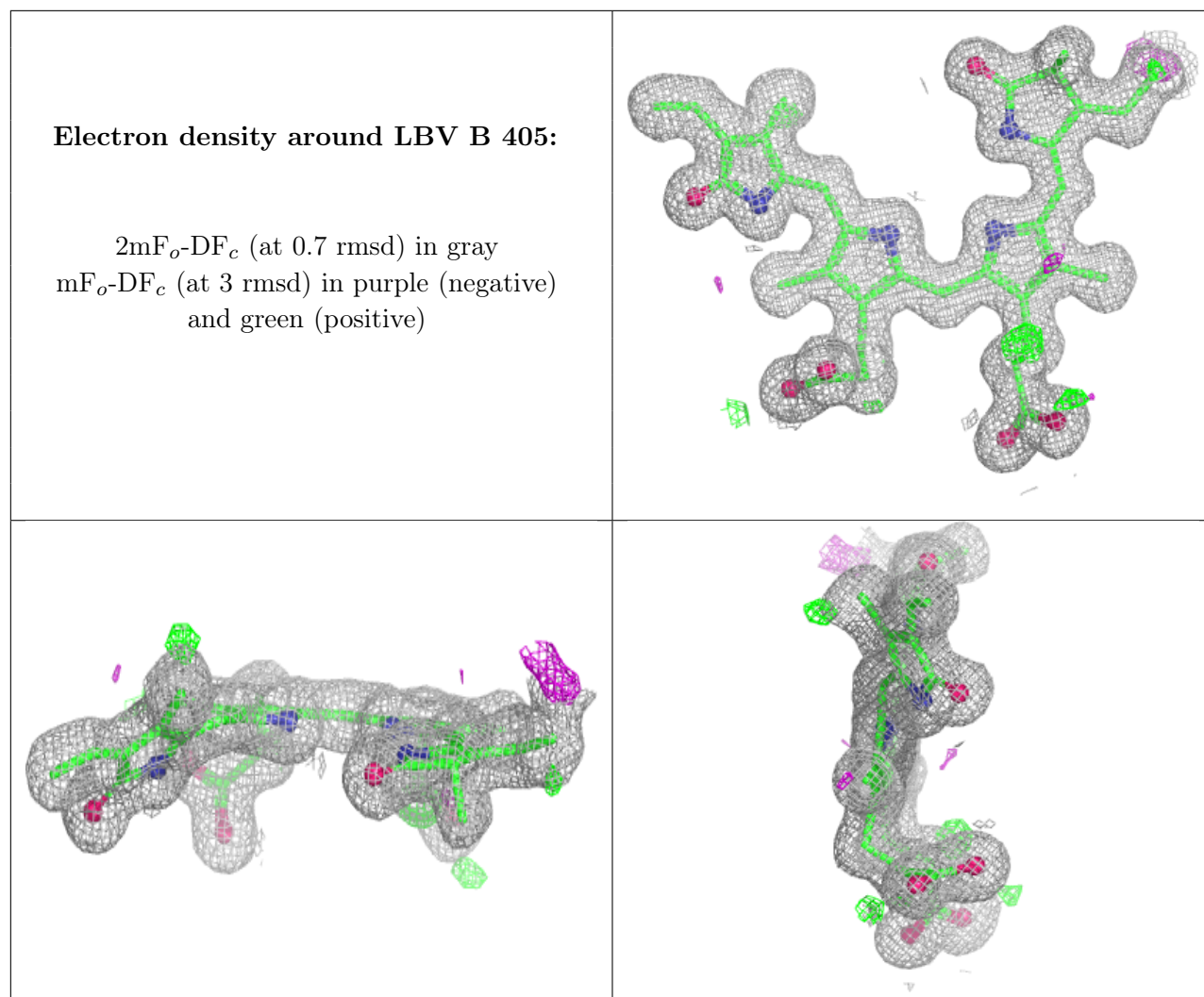
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACT	A	401	4/4	0.85	0.14	41,44,45,54	0
2	ACT	B	401	4/4	0.89	0.16	61,63,64,75	0
2	ACT	A	403	4/4	0.91	0.10	31,36,43,49	0
2	ACT	A	402	4/4	0.92	0.09	28,45,49,49	0
2	ACT	B	402	4/4	0.92	0.10	27,36,39,60	0
2	ACT	B	403	4/4	0.94	0.08	25,26,26,30	0
3	MPD	A	404	8/8	0.94	0.10	22,25,31,32	8
3	MPD	B	404	8/8	0.95	0.08	17,24,28,31	8
4	LBV	A	405	43/43	0.98	0.04	9,11,19,31	0
4	LBV	B	405	43/43	0.99	0.04	8,10,18,24	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 LBV A 405:

$2mF_o-DF_c$ (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.