Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 01:16 pm GMT

PDB ID	:	6ET7
Title	:	Activated heterodimer of the bacteriophytochrome regulated diguanylyl cyclase variant - S505V A526V - from Idiomarina species A28L
Authors	:	Gourinchas, G.; Winkler, A.
Deposited on	:	2017-10-25
Resolution	:	2.85 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:

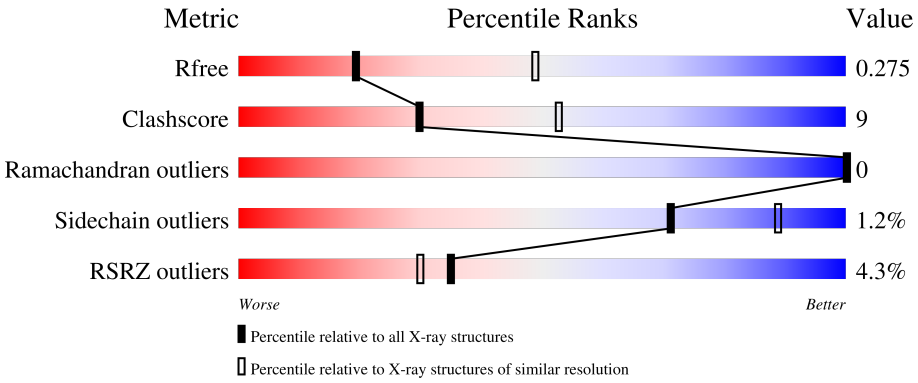
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	685	3% 74% 20% 6%
1	B	685	5% 72% 22% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10522 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.

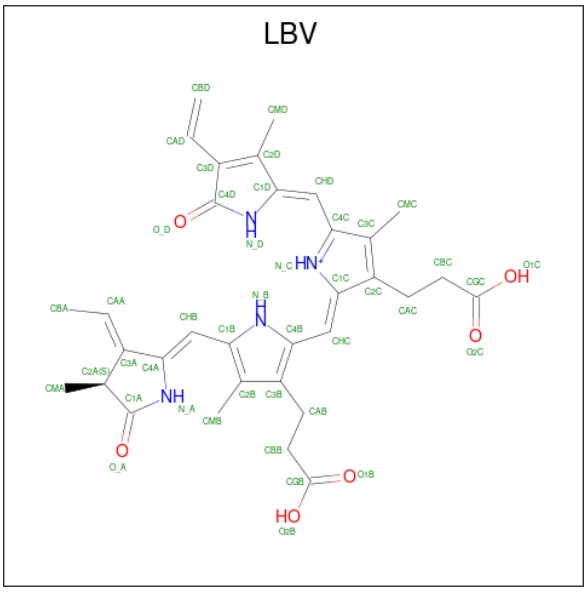
- Molecule 1 is a protein called Diguanylate cyclase (GGDEF) domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	646	Total	C	N	O	S	0	0	0
			5221	3294	933	971	23			
1	B	645	Total	C	N	O	S	0	0	0
			5207	3281	930	973	23			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP F7RW09
A	0	ALA	-	expression tag	UNP F7RW09
A	1	MET	-	expression tag	UNP F7RW09
A	2	ALA	-	expression tag	UNP F7RW09
A	505	VAL	SER	engineered mutation	UNP F7RW09
A	526	VAL	ALA	engineered mutation	UNP F7RW09
B	-1	GLY	-	expression tag	UNP F7RW09
B	0	ALA	-	expression tag	UNP F7RW09
B	1	MET	-	expression tag	UNP F7RW09
B	2	ALA	-	expression tag	UNP F7RW09
B	505	VAL	SER	engineered mutation	UNP F7RW09
B	526	VAL	ALA	engineered mutation	UNP F7RW09

- Molecule 2 is 3-[2-[(Z)-[3-(2-carboxyethyl)-5-[(Z)-(4-ethenyl-3-methyl-5-oxidanylidene-pyrrol-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 (three-letter code: LBV) (formula: $C_{33}H_{37}N_4O_6$).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is water.

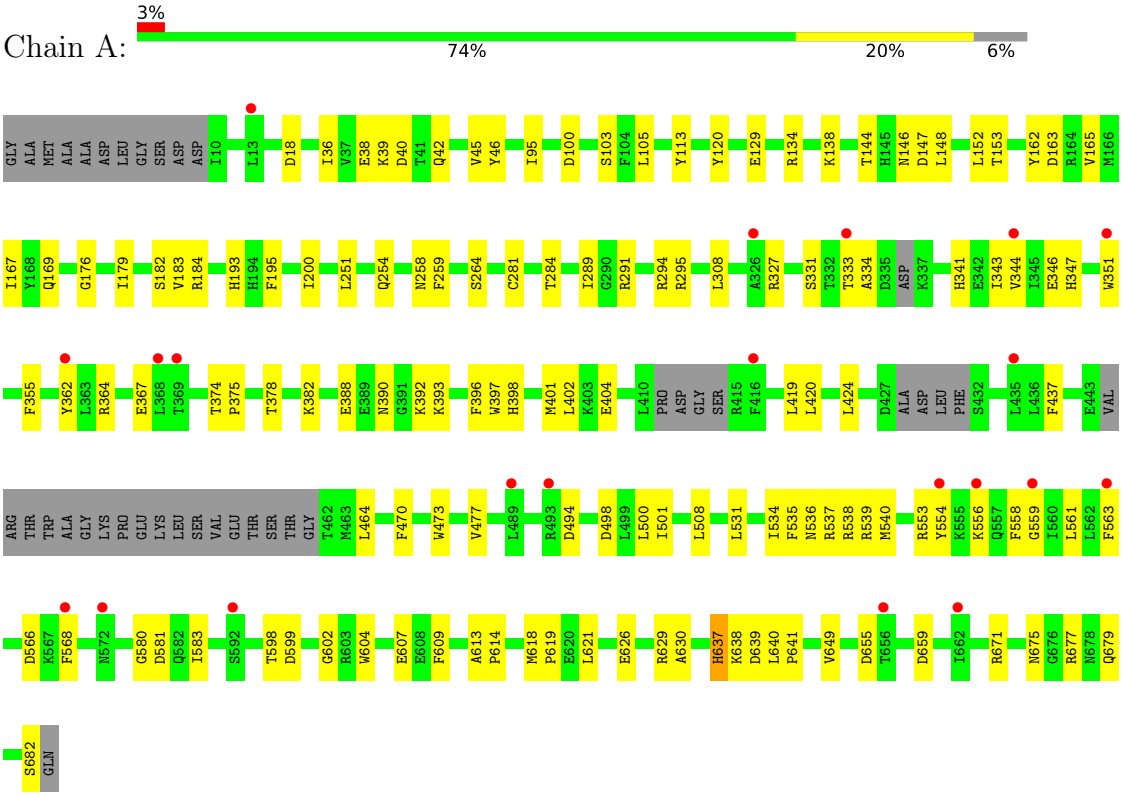
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	5	Total O 5 5	0	0

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.

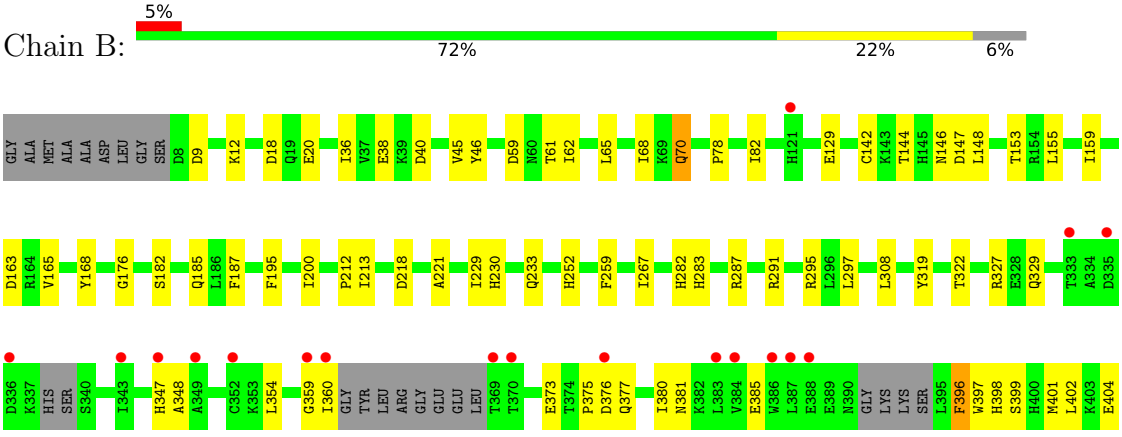
• Molecule 1: Diguanylate cyclase (GGDEF) domain-containing protein

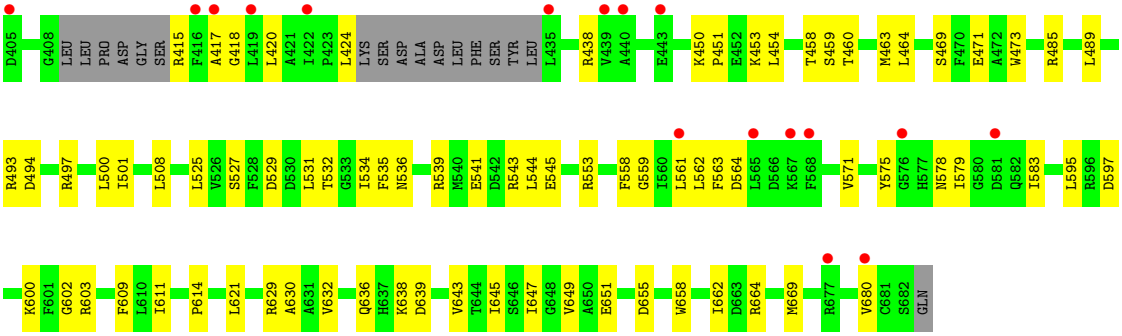
Chain A:



• Molecule 1: Diguanylate cyclase (GGDEF) domain-containing protein

Chain B:




D405 G408 LEU LEU PRO ASP GLY SER R415 F416 A417 G418 L419 L420 A421 I422 P423 L424 LYS SER ASP ALA ASP LEU PHE SER TYR LEU L435 R438 V439 A440 E443 K450 P451 E452 K453 L454 T458 S459 T460 M463 L464 S469 F470 E471 A472 W473 R485 L489
R493 D494 R497 L500 I501 L508 L525 V526 S527 F528 D529 D530 L531 T532 G533 I534 F535 N536 R539 M540 E541 D542 R543 L544 E545 R553 F558 G559 I560 L561 L562 F563 D564 L565 D566 K567 F568 V571 Y575 G576 H577 N578 I579 G580 D581 Q582 I583 L595 R596 D597
K600 F601 G602 R603 F609 L610 I611 P614 L621 R629 A630 A631 V632 Q636 H637 K638 D639 V643 T644 I645 S646 I647 G648 V649 A650 E651 D655 W658 I662 D663 R664 M669 R677 V680 C681 S682 GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.46Å 78.42Å 443.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 2.85 58.77 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.31-2.85) 99.9 (58.77-2.85)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.216 , 0.275 0.216 , 0.275	Depositor DCC
R_{free} test set	2089 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 71.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10522	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: LBV, CL

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	0.40	0/5329	0.63	0/7212
1	B	0.42	1/5314 (0.0%)	0.66	0/7196
All	All	0.41	1/10643 (0.0%)	0.65	0/14408

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	CYS	CB-SG	-5.11	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5221	0	5141	93	3
1	B	5207	0	5114	112	3
2	A	43	0	33	3	0
2	B	43	0	33	6	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
4	A	1	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10522	0	10321	196	3

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 9.

All (196) 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:168:TYR:CZ	1:B:176:GLY:HA3	2.23	0.73
1:B:527:SER:OG	1:B:539:ARG:NH1	2.24	0.70
1:B:401:MET:HB2	1:B:417:ALA:HB1	1.72	0.69
1:B:398:HIS:HB3	1:B:420:LEU:HD13	1.76	0.68
1:A:295:ARG:NH1	3:A:702:CL:CL	2.64	0.68
1:B:376:ASP:OD1	1:B:377:GLN:N	2.26	0.68
1:A:144:THR:HB	1:A:147:ASP:OD2	1.93	0.68
1:B:558:PHE:HB2	1:B:614:PRO:HA	1.76	0.67
1:A:163:ASP:OD2	1:A:284:THR:HG22	1.94	0.66
1:B:40:ASP:OD2	1:B:233:GLN:NE2	2.27	0.66
1:A:566:ASP:HB3	1:A:677:ARG:HD3	1.77	0.66
1:A:538:ARG:NH2	1:B:525:LEU:O	2.28	0.66
1:A:568:PHE:CD2	1:A:607:GLU:HG2	2.31	0.65
1:B:9:ASP:HB3	1:B:453:LYS:HE3	1.79	0.65
1:B:348:ALA:HB1	1:B:360:ILE:HD12	1.79	0.64
1:B:559:GLY:HA3	1:B:621:LEU:HD21	1.79	0.64
1:B:527:SER:O	1:B:536:ASN:ND2	2.30	0.62
1:B:229:ILE:HG22	1:B:230:HIS:HD2	1.64	0.62
1:B:399:SER:OG	1:B:402:LEU:HG	2.01	0.61
1:B:632:VAL:HG11	1:B:645:ILE:HG23	1.83	0.60
1:A:424:LEU:HB3	1:A:500:LEU:HD13	1.84	0.60
1:B:59:ASP:HB3	1:B:62:ILE:HG12	1.83	0.60
1:B:148:LEU:HD22	1:B:308:LEU:HD13	1.84	0.59
1:B:20:GLU:HB2	1:B:460:THR:HG21	1.84	0.59
1:B:544:LEU:HG	1:B:658:TRP:HB2	1.85	0.59
1:A:536:ASN:OD1	1:A:537:ARG:N	2.35	0.59
1:A:153:THR:HG23	1:A:165:VAL:HG12	1.86	0.58
1:B:381:ASN:O	1:B:385:GLU:HG3	2.02	0.58
1:B:401:MET:N	1:B:417:ALA:O	2.32	0.58
1:B:450:LYS:HB2	1:B:473:TRP:CD1	2.37	0.58
1:A:388:GLU:HA	1:A:393:LYS:HB3	1.86	0.58
1:B:329:GLN:HG3	1:B:347:HIS:CE1	2.38	0.58
1:A:134:ARG:HH11	1:A:138:LYS:NZ	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:GLU:O	1:B:664:ARG:NH2	2.38	0.57
1:A:398:HIS:HB3	1:A:420:LEU:HD13	1.86	0.57
1:A:659:ASP:OD2	1:B:578:ASN:HB2	2.04	0.57
1:B:59:ASP:OD1	1:B:61:THR:OG1	2.20	0.57
1:B:636:GLN:HB2	1:B:638:LYS:HE3	1.87	0.57
1:B:396:PHE:HD2	1:B:493:ARG:HH11	1.53	0.56
1:A:390:ASN:HB3	1:A:392:LYS:HG3	1.88	0.56
1:A:501:ILE:HD13	1:B:501:ILE:HG21	1.87	0.56
1:B:534:ILE:HG22	1:B:602:GLY:HA2	1.86	0.56
1:B:558:PHE:CB	1:B:614:PRO:HA	2.36	0.56
1:A:401:MET:HG3	1:A:404:GLU:HB2	1.88	0.56
1:A:675:ASN:O	1:A:679:GLN:NE2	2.39	0.56
1:A:531:LEU:HD21	1:A:581:ASP:HB3	1.88	0.55
1:A:36:ILE:HB	1:A:46:TYR:HB2	1.89	0.55
1:A:346:GLU:HG2	1:A:347:HIS:CE1	2.41	0.54
1:A:334:ALA:HA	1:A:343:ILE:HD11	1.88	0.54
1:A:637:HIS:HB3	1:A:640:LEU:O	2.07	0.54
1:A:134:ARG:HH11	1:A:138:LYS:HZ2	1.54	0.54
1:B:375:PRO:HB2	1:B:380:ILE:HG13	1.90	0.54
1:A:289:ILE:HG22	1:A:294:ARG:HG3	1.89	0.54
1:B:541:GLU:HG2	1:B:658:TRP:CH2	2.44	0.53
1:B:571:VAL:HG11	1:B:583:ILE:HD12	1.89	0.53
1:B:543:ARG:HG2	1:B:600:LYS:HD3	1.90	0.53
1:A:18:ASP:OD2	1:A:18:ASP:N	2.42	0.53
1:B:595:LEU:HD21	1:B:611:ILE:HD13	1.89	0.53
1:A:144:THR:HG22	1:A:146:ASN:H	1.73	0.53
1:A:598:THR:HB	1:A:614:PRO:HG2	1.91	0.52
2:B:701:LBV:HHC1	2:B:701:LBV:HBB1	1.91	0.52
1:A:291:ARG:O	1:A:295:ARG:HG2	2.10	0.52
1:A:39:LYS:HG3	1:A:113:TYR:CZ	2.44	0.52
1:B:168:TYR:CD1	2:B:701:LBV:HBD1	2.45	0.52
1:B:200:ILE:HG12	2:B:701:LBV:C4C	2.39	0.52
1:B:144:THR:HG22	1:B:146:ASN:H	1.75	0.52
1:A:162:TYR:HE1	1:A:289:ILE:HD11	1.74	0.52
1:A:640:LEU:HB3	1:A:641:PRO:HD2	1.92	0.52
1:A:251:LEU:HD21	2:A:701:LBV:HMA2	1.91	0.51
1:B:163:ASP:OD1	1:B:185:GLN:HG3	2.10	0.51
1:A:374:THR:HG22	1:A:375:PRO:O	2.10	0.51
1:B:373:GLU:OE1	1:B:415:ARG:NH2	2.41	0.51
1:A:103:SER:HB2	1:A:120:TYR:HB2	1.92	0.51
1:A:327:ARG:NH1	1:B:327:ARG:HH22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLY:HA2	1:A:583:ILE:HD12	1.93	0.51
1:B:144:THR:HB	1:B:147:ASP:OD1	2.11	0.51
1:A:333:THR:HG22	1:A:343:ILE:HG12	1.93	0.50
1:B:295:ARG:NH1	3:B:702:CL:CL	2.77	0.50
1:B:396:PHE:HD2	1:B:396:PHE:H	1.59	0.50
1:A:134:ARG:HD2	1:A:138:LYS:HZ2	1.77	0.50
1:A:327:ARG:NH1	1:B:327:ARG:NH2	2.60	0.50
1:A:638:LYS:O	1:A:639:ASP:HB2	2.11	0.50
1:B:532:THR:O	1:B:534:ILE:HG13	2.11	0.50
1:A:152:LEU:HD23	1:A:167:ILE:HD11	1.94	0.50
1:B:471:GLU:OE1	1:B:471:GLU:HA	2.11	0.50
1:B:282:HIS:NE2	2:B:701:LBV:O_D	2.45	0.49
1:B:359:GLY:HA3	1:B:373:GLU:O	2.12	0.49
1:B:485:ARG:O	1:B:489:LEU:HG	2.12	0.49
1:A:148:LEU:HD22	1:A:308:LEU:HB2	1.93	0.49
1:A:559:GLY:HA3	1:A:621:LEU:HD21	1.93	0.49
1:B:575:TYR:O	1:B:579:ILE:HD12	2.13	0.48
1:A:254:GLN:NE2	1:A:258:ASN:OD1	2.44	0.48
1:B:563:PHE:CZ	1:B:609:PHE:HB2	2.49	0.48
1:B:65:LEU:HD12	1:B:68:ILE:HD12	1.94	0.48
1:B:545:GLU:HG3	1:B:658:TRP:HD1	1.78	0.48
1:A:327:ARG:HH12	1:B:327:ARG:NH2	2.12	0.48
1:B:144:THR:HG22	1:B:146:ASN:N	2.28	0.48
1:B:148:LEU:HD22	1:B:308:LEU:HB2	1.96	0.47
1:B:36:ILE:HB	1:B:46:TYR:HB2	1.96	0.47
1:B:638:LYS:O	1:B:639:ASP:HB2	2.13	0.47
1:A:134:ARG:NH1	1:A:138:LYS:NZ	2.62	0.47
1:B:319:TYR:O	1:B:322:THR:OG1	2.26	0.47
1:B:583:ILE:CG2	1:B:643:VAL:HG21	2.44	0.47
1:B:78:PRO:O	1:B:82:ILE:HG13	2.15	0.47
1:B:397:TRP:HA	1:B:397:TRP:CE3	2.50	0.47
1:B:559:GLY:HA3	1:B:621:LEU:CD2	2.45	0.47
1:B:40:ASP:N	1:B:40:ASP:OD1	2.45	0.47
1:A:144:THR:HG22	1:A:146:ASN:N	2.29	0.47
1:A:327:ARG:HH12	1:B:327:ARG:CZ	2.28	0.47
1:A:39:LYS:HG3	1:A:113:TYR:CE1	2.50	0.46
1:A:540:MET:SD	1:A:602:GLY:HA3	2.55	0.46
1:A:331:SER:HB2	1:B:497:ARG:NH2	2.30	0.46
1:A:554:TYR:HB2	1:A:556:LYS:HG3	1.98	0.46
1:A:561:LEU:HG	1:A:649:VAL:HG22	1.98	0.46
1:B:562:LEU:HD12	1:B:609:PHE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD22	1:A:308:LEU:HD13	1.98	0.45
1:A:626:GLU:HA	1:A:629:ARG:HG2	1.98	0.45
1:A:40:ASP:N	1:A:40:ASP:OD1	2.49	0.45
1:B:129:GLU:OE1	1:B:129:GLU:N	2.46	0.45
1:B:396:PHE:HD2	1:B:493:ARG:NH1	2.14	0.45
1:B:531:LEU:O	1:B:532:THR:OG1	2.26	0.45
1:A:38:GLU:HG3	1:A:45:VAL:HG11	1.98	0.45
1:A:344:VAL:HG21	1:A:362:TYR:CD2	2.51	0.45
1:A:535:PHE:HB3	1:A:539:ARG:HB2	1.99	0.45
1:B:450:LYS:HG3	1:B:451:PRO:HD2	1.98	0.45
1:A:563:PHE:CZ	1:A:609:PHE:HB2	2.52	0.45
1:B:354:LEU:HD12	1:B:354:LEU:HA	1.82	0.45
1:A:200:ILE:HD11	2:A:701:LBV:HMC3	1.99	0.44
1:B:38:GLU:HG3	1:B:45:VAL:HG11	1.98	0.44
1:A:341:HIS:NE2	1:A:364:ARG:HB3	2.33	0.44
1:A:378:THR:O	1:A:382:LYS:HG3	2.18	0.44
1:A:473:TRP:CH2	1:A:477:VAL:HG21	2.52	0.44
1:A:671:ARG:NH2	1:A:682:SER:O	2.51	0.44
1:B:153:THR:HG22	1:B:182:SER:CB	2.48	0.44
1:B:267:ILE:HD11	1:B:297:LEU:HB3	2.00	0.44
1:A:134:ARG:NH1	1:A:138:LYS:HZ2	2.16	0.44
1:A:534:ILE:HG22	1:A:602:GLY:HA2	2.00	0.44
1:B:252:HIS:NE2	2:B:701:LBV:HBC1	2.32	0.44
1:A:327:ARG:CZ	1:B:327:ARG:HH22	2.31	0.44
1:A:508:LEU:HD23	1:B:508:LEU:HB3	1.99	0.44
1:B:153:THR:HG22	1:B:182:SER:HB2	1.99	0.44
1:A:169:GLN:HB2	1:A:179:ILE:HD13	1.99	0.43
1:A:351:TRP:HB3	1:A:355:PHE:CE2	2.53	0.43
1:B:453:LYS:O	1:B:453:LYS:HG2	2.18	0.43
1:B:212:PRO:O	1:B:267:ILE:HA	2.17	0.43
1:B:153:THR:HG23	1:B:165:VAL:HG12	2.01	0.43
1:B:402:LEU:HB3	1:B:404:GLU:HG3	2.00	0.43
1:B:397:TRP:HA	1:B:397:TRP:HE3	1.83	0.43
1:B:418:GLY:HA3	1:B:438:ARG:HB2	2.00	0.43
1:B:629:ARG:NH2	1:B:630:ALA:HB2	2.33	0.43
1:B:454:LEU:O	1:B:464:LEU:HD12	2.19	0.43
1:A:100:ASP:OD1	1:A:100:ASP:N	2.52	0.43
1:A:341:HIS:NE2	1:A:367:GLU:HB2	2.34	0.43
1:A:374:THR:HG23	1:A:437:PHE:CE2	2.54	0.43
1:A:193:HIS:ND1	1:A:470:PHE:HB2	2.34	0.42
1:B:283:HIS:CD2	1:B:287:ARG:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASP:HB3	1:B:221:ALA:HB2	2.01	0.42
1:B:291:ARG:O	1:B:295:ARG:HG2	2.19	0.42
1:A:129:GLU:OE1	1:A:129:GLU:N	2.43	0.42
1:A:392:LYS:HD3	1:A:397:TRP:CD1	2.54	0.42
1:B:155:LEU:O	1:B:159:ILE:HG13	2.19	0.42
1:B:564:ASP:HB2	1:B:669:MET:SD	2.60	0.42
2:B:701:LBV:N_D	2:B:701:LBV:HMC1	2.35	0.42
1:B:460:THR:HG23	1:B:463:MET:HE1	2.01	0.42
2:A:701:LBV:HMD3	2:A:701:LBV:CMC	2.50	0.42
1:B:229:ILE:HG22	1:B:230:HIS:CD2	2.49	0.42
1:B:583:ILE:HG21	1:B:643:VAL:HG21	2.00	0.42
1:A:176:GLY:HA3	1:A:195:PHE:CE2	2.54	0.42
1:A:153:THR:HG22	1:A:182:SER:CB	2.50	0.41
1:A:659:ASP:CG	1:B:578:ASN:HB2	2.40	0.41
1:B:561:LEU:HG	1:B:649:VAL:HG22	2.01	0.41
1:A:401:MET:CG	1:A:404:GLU:HB2	2.50	0.41
1:B:70:GLN:H	1:B:70:GLN:HG2	1.45	0.41
1:B:424:LEU:HD13	1:B:500:LEU:HD22	2.01	0.41
1:A:327:ARG:NH2	1:A:498:ASP:OD1	2.42	0.41
1:B:454:LEU:HA	1:B:454:LEU:HD12	1.79	0.41
1:B:529:ASP:OD2	1:B:603:ARG:HD3	2.21	0.41
1:B:168:TYR:OH	1:B:195:PHE:HB2	2.21	0.41
1:B:213:ILE:HD12	1:B:267:ILE:HG12	2.02	0.41
1:A:183:VAL:HG22	1:A:184:ARG:O	2.21	0.41
1:A:618:MET:N	1:A:619:PRO:HD2	2.36	0.41
1:A:629:ARG:NH1	1:A:630:ALA:HB2	2.35	0.41
1:B:545:GLU:HG3	1:B:658:TRP:CD1	2.55	0.41
1:B:647:ILE:HB	1:B:680:VAL:HG22	2.03	0.41
1:B:662:ILE:HD13	1:B:662:ILE:HA	1.95	0.41
1:A:264:SER:HA	1:A:281:CYS:O	2.21	0.40
1:A:398:HIS:HA	1:A:419:LEU:O	2.21	0.40
1:A:402:LEU:HD11	1:A:419:LEU:HB2	2.03	0.40
1:A:537:ARG:HD3	1:A:604:TRP:O	2.22	0.40
1:B:458:THR:HG22	1:B:459:SER:H	1.86	0.40
1:B:463:MET:HE2	1:B:463:MET:HB3	1.84	0.40
1:A:251:LEU:HD11	1:A:464:LEU:HD11	2.04	0.40
1:A:498:ASP:OD2	1:B:497:ARG:NH1	2.51	0.40
1:B:534:ILE:HG22	1:B:535:PHE:N	2.36	0.40
1:A:95:ILE:O	1:A:105:LEU:HA	2.22	0.40
1:A:558:PHE:HB2	1:A:613:ALA:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ARG:NH1	1:B:597:ASP:OD1[3_547]	2.05	0.15
1:A:599:ASP:O	1:B:553:ARG:NH1[3_647]	2.17	0.03
1:A:42:GLN:OE1	1:B:12:LYS:NZ[1_565]	2.19	0.01

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	636/685 (93%)	615 (97%)	21 (3%)	0	100	100
1	B	633/685 (92%)	611 (96%)	22 (4%)	0	100	100
All	All	1269/1370 (93%)	1226 (97%)	43 (3%)	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	563/592 (95%)	558 (99%)	5 (1%)	78	92
1	B	562/592 (95%)	554 (99%)	8 (1%)	67	86
All	All	1125/1184 (95%)	1112 (99%)	13 (1%)	71	89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	PHE
1	A	396	PHE
1	A	494	ASP
1	A	637	HIS
1	A	655	ASP
1	B	18	ASP
1	B	70	GLN
1	B	187	PHE
1	B	259	PHE
1	B	396	PHE
1	B	469	SER
1	B	494	ASP
1	B	655	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	157	GLN
1	A	519	ASN
1	A	653	GLN
1	B	92	ASN
1	B	230	HIS
1	B	519	ASN
1	B	578	ASN

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 monosaccharides 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	$\#\|Z\| > 2$
2	LBV	B	701	1	42,46,46	3.14	19 (45%)	47,67,67	1.74	7 (14%)
2	LBV	A	701	1	42,46,46	2.96	17 (40%)	47,67,67	1.53	7 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LBV	B	701	1	-	10/26/74/74	0/4/4/4
2	LBV	A	701	1	-	16/26/74/74	0/4/4/4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	LBV	C2A-C1A	-8.98	1.40	1.51
2	A	701	LBV	C2A-C1A	-8.65	1.41	1.51
2	A	701	LBV	CHC-C1C	7.85	1.41	1.35
2	B	701	LBV	CHC-C1C	7.25	1.41	1.35
2	B	701	LBV	C2A-C3A	-7.13	1.42	1.51
2	A	701	LBV	C2A-C3A	-6.55	1.43	1.51
2	B	701	LBV	CMB-C2B	-6.30	1.38	1.51
2	B	701	LBV	CAB-C3B	-4.80	1.45	1.52
2	B	701	LBV	CMC-C3C	-4.72	1.40	1.50
2	A	701	LBV	CAB-C3B	-4.69	1.45	1.52
2	B	701	LBV	CMD-C2D	-4.40	1.41	1.50
2	A	701	LBV	CHB-C4A	4.26	1.43	1.34
2	A	701	LBV	CMB-C2B	-4.18	1.42	1.51
2	B	701	LBV	CMA-C2A	-3.89	1.41	1.53
2	A	701	LBV	CMC-C3C	-3.83	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	LBV	CMD-C2D	-3.83	1.42	1.50
2	B	701	LBV	CHB-C4A	3.58	1.41	1.34
2	A	701	LBV	CMA-C2A	-3.56	1.42	1.53
2	B	701	LBV	C3D-C4D	-3.31	1.38	1.47
2	A	701	LBV	CBC-CGC	-3.19	1.43	1.50
2	B	701	LBV	CAC-C2C	-3.00	1.43	1.51
2	A	701	LBV	CAC-C2C	-2.82	1.44	1.51
2	B	701	LBV	CHD-C4C	2.76	1.46	1.40
2	B	701	LBV	CBC-CGC	-2.75	1.44	1.50
2	A	701	LBV	C2C-C3C	2.74	1.42	1.36
2	A	701	LBV	CAA-C3A	2.58	1.40	1.33
2	A	701	LBV	C3B-C2B	2.56	1.45	1.37
2	B	701	LBV	CBC-CAC	-2.45	1.44	1.52
2	B	701	LBV	CAA-C3A	2.30	1.39	1.33
2	B	701	LBV	O1C-CGC	-2.30	1.23	1.30
2	B	701	LBV	C3D-C2D	2.23	1.41	1.37
2	A	701	LBV	CBC-CAC	-2.22	1.45	1.52
2	B	701	LBV	CAD-C3D	-2.19	1.41	1.47
2	B	701	LBV	CBB-CGB	-2.17	1.45	1.50
2	A	701	LBV	C3D-C4D	-2.16	1.41	1.47
2	A	701	LBV	CAB-CBB	-2.01	1.42	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	LBV	C4B-CHC-C1C	7.77	138.09	128.81
2	A	701	LBV	CHC-C1C-N-C	-5.05	121.82	128.83
2	A	701	LBV	O-A-C1A-N-A	-3.01	121.30	124.94
2	A	701	LBV	C1C-N-C-C4C	2.83	111.84	106.51
2	A	701	LBV	CHC-C1C-C2C	2.76	131.69	125.32
2	B	701	LBV	O-A-C1A-N-A	-2.61	121.78	124.94
2	B	701	LBV	C2C-C1C-N-C	-2.53	106.37	110.05
2	A	701	LBV	C2C-C1C-N-C	-2.46	106.47	110.05
2	A	701	LBV	O2C-CGC-CBC	-2.25	115.87	123.08
2	A	701	LBV	CHD-C4C-C3C	2.24	130.66	124.90
2	B	701	LBV	C1D-N-D-C4D	2.18	113.44	110.67
2	B	701	LBV	C1C-N-C-C4C	2.18	110.62	106.51
2	B	701	LBV	O1B-CGB-CBB	-2.13	116.24	123.08
2	B	701	LBV	O-D-C4D-N-D	-2.02	120.38	125.08

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	LBV	C-N-C1C-CHC-C4B
2	A	701	LBV	C2D-C1D-CHD-C4C
2	A	701	LBV	D-N-C1D-CHD-C4C
2	A	701	LBV	C1C-C2C-CAC-CBC
2	A	701	LBV	C3C-C2C-CAC-CBC
2	A	701	LBV	A-N-C4A-CHB-C1B
2	A	701	LBV	C3C-C4C-CHD-C1D
2	A	701	LBV	C-N-C4C-CHD-C1D
2	B	701	LBV	C-N-C4C-CHD-C1D
2	B	701	LBV	C3C-C4C-CHD-C1D
2	A	701	LBV	C4D-C3D-CAD-CBD
2	A	701	LBV	C2D-C3D-CAD-CBD
2	A	701	LBV	C2C-C1C-CHC-C4B
2	B	701	LBV	D-N-C1D-CHD-C4C
2	B	701	LBV	C2D-C1D-CHD-C4C
2	B	701	LBV	C2D-C3D-CAD-CBD
2	A	701	LBV	CAC-CBC-CGC-O2C
2	B	701	LBV	CAB-CBB-CGB-O1B
2	B	701	LBV	CAC-CBC-CGC-O2C
2	B	701	LBV	CAB-CBB-CGB-O2B
2	A	701	LBV	CAC-CBC-CGC-O1C
2	B	701	LBV	CAC-CBC-CGC-O1C
2	B	701	LBV	C4D-C3D-CAD-CBD
2	A	701	LBV	CAB-CBB-CGB-O1B
2	A	701	LBV	CAB-CBB-CGB-O2B
2	A	701	LBV	C3A-C4A-CHB-C1B

There are no ring outliers.

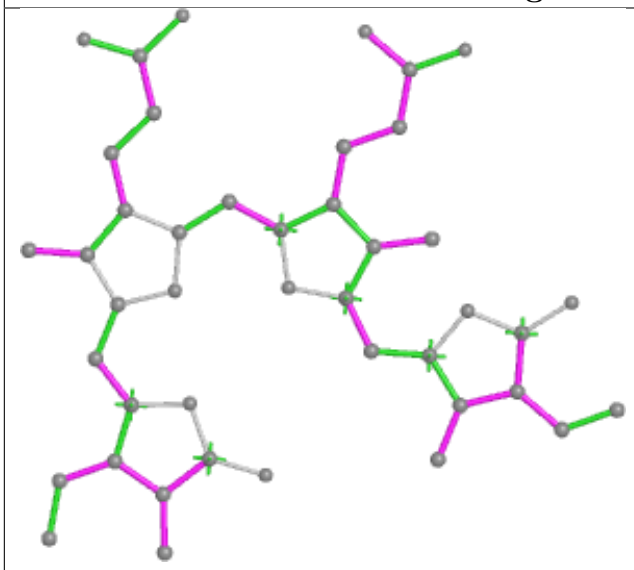
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	LBV	6	0
2	A	701	LBV	3	0

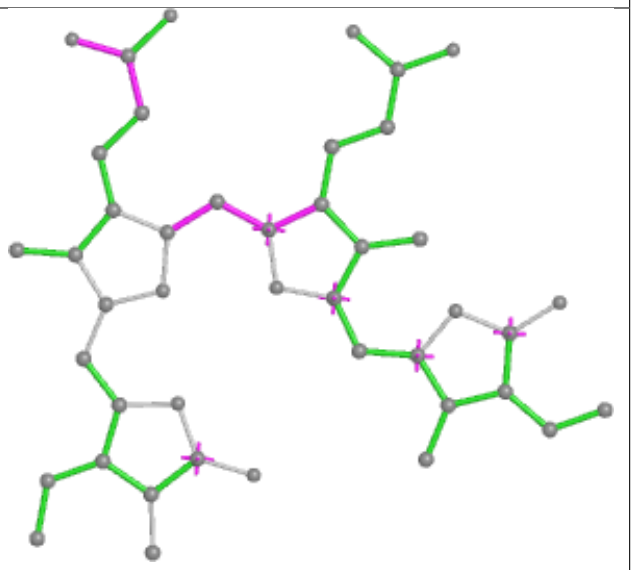
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

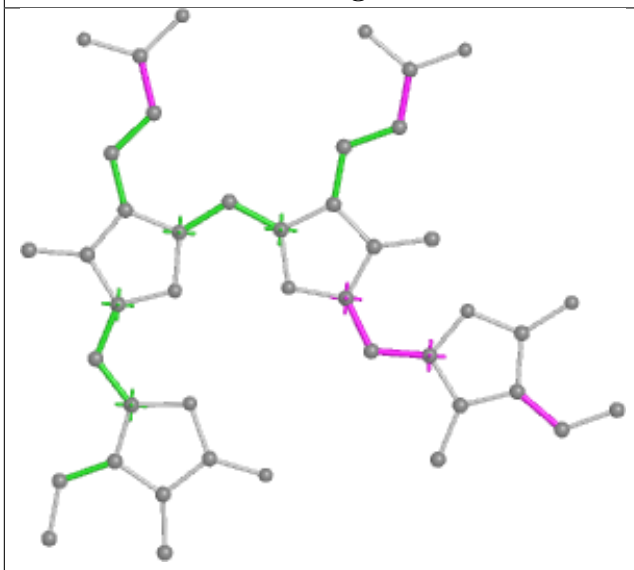
Ligand LBV B 701



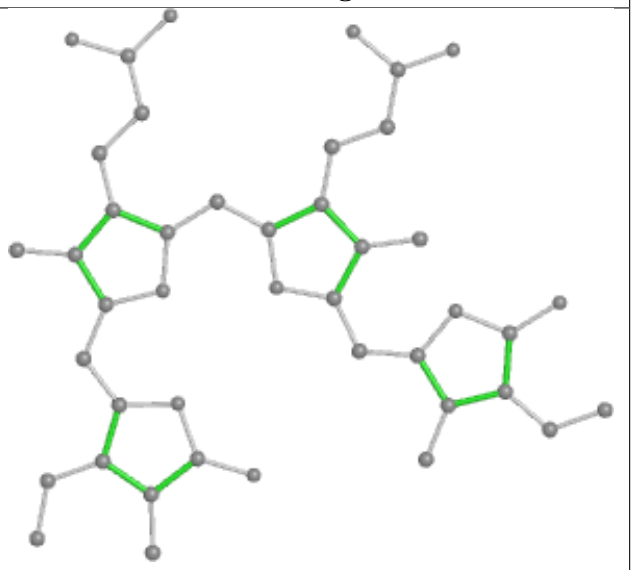
Bond lengths



Bond angles

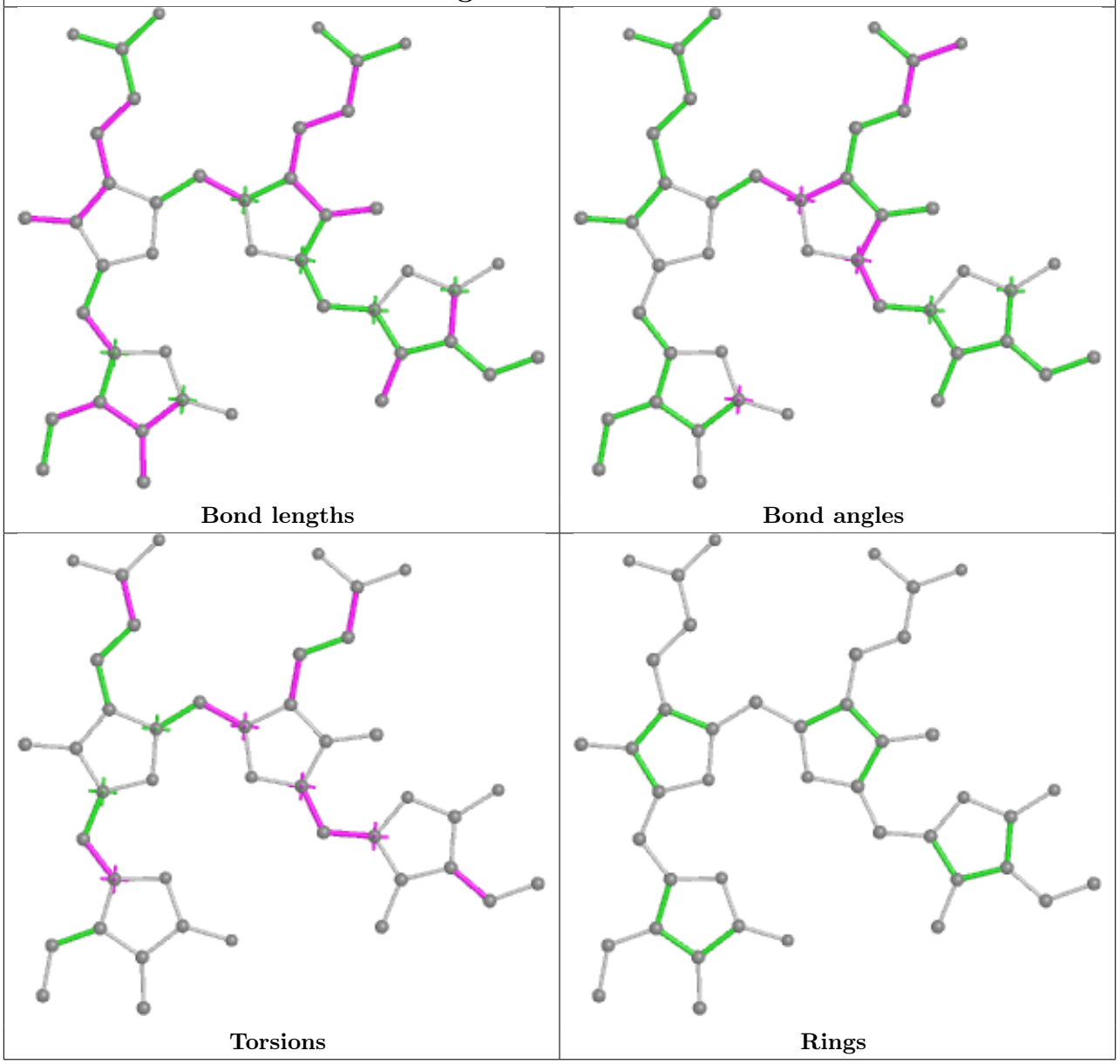


Torsions



Rings

Ligand LBV A 701



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, 95^{th} 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	646/685 (94%)	0.13	21 (3%)	46	41	32, 94, 134, 155	0
1	B	645/685 (94%)	0.19	35 (5%)	25	21	29, 79, 131, 163	0
All	All	1291/1370 (94%)	0.16	56 (4%)	35	30	29, 85, 133, 163	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	567	LYS	5.5
1	B	343	ILE	4.0
1	B	383	LEU	3.8
1	A	368	LEU	3.4
1	B	376	ASP	3.4
1	B	387	LEU	3.3
1	B	360	ILE	3.3
1	A	362	TYR	3.2
1	B	386	TRP	3.1
1	B	347	HIS	3.1
1	B	349	ALA	3.1
1	B	439	VAL	3.0
1	A	493	ARG	2.9
1	B	416	PHE	2.8
1	B	333	THR	2.8
1	B	384	VAL	2.8
1	B	680	VAL	2.7
1	B	359	GLY	2.7
1	B	422	ILE	2.7
1	A	435	LEU	2.6
1	B	568	PHE	2.6
1	B	370	THR	2.6
1	A	559	GLY	2.5
1	B	419	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	556	LYS	2.5
1	B	388	GLU	2.5
1	A	554	TYR	2.5
1	A	662	ILE	2.5
1	B	335	ASP	2.5
1	A	13	LEU	2.4
1	B	677	ARG	2.4
1	A	326	ALA	2.4
1	A	563	PHE	2.4
1	A	489	LEU	2.4
1	A	568	PHE	2.3
1	B	417	ALA	2.3
1	B	440	ALA	2.3
1	A	344	VAL	2.3
1	A	416	PHE	2.3
1	B	121	HIS	2.2
1	B	405	ASP	2.2
1	A	592	SER	2.2
1	B	336	ASP	2.2
1	B	581	ASP	2.2
1	A	572	ASN	2.2
1	B	576	GLY	2.2
1	A	351	TRP	2.2
1	A	656	THR	2.1
1	B	561	LEU	2.1
1	A	333	THR	2.1
1	B	352	CYS	2.1
1	A	369	THR	2.1
1	B	369	THR	2.1
1	B	565	LEU	2.0
1	B	443	GLU	2.0
1	B	435	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

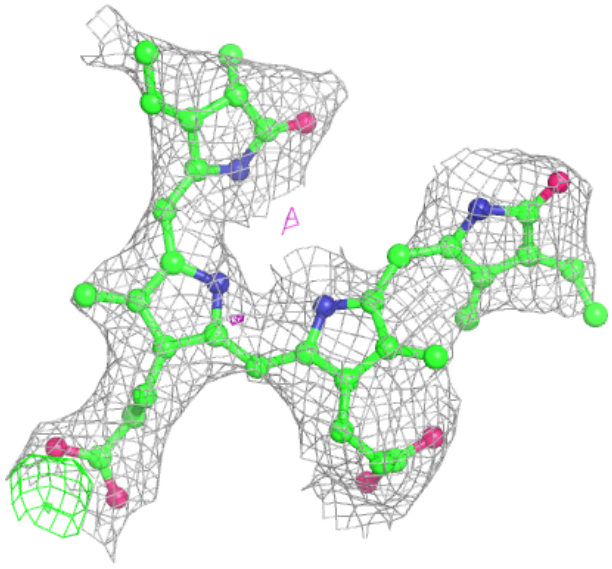
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

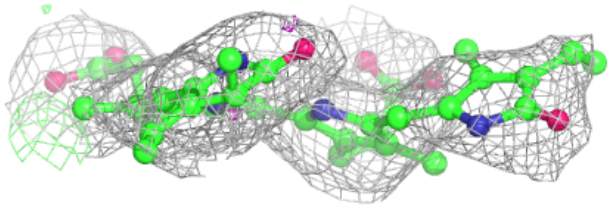
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LBV	A	701	43/43	0.92	0.28	57,72,89,94	0
3	CL	A	702	1/1	0.95	0.11	75,75,75,75	0
3	CL	B	702	1/1	0.95	0.20	71,71,71,71	0
2	LBV	B	701	43/43	0.96	0.19	27,39,59,72	0

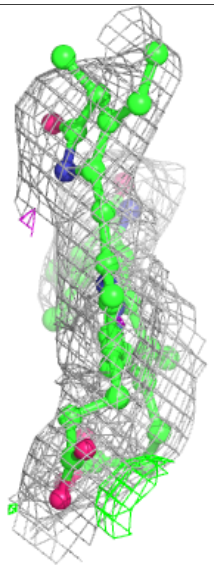
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LBV A 701:

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

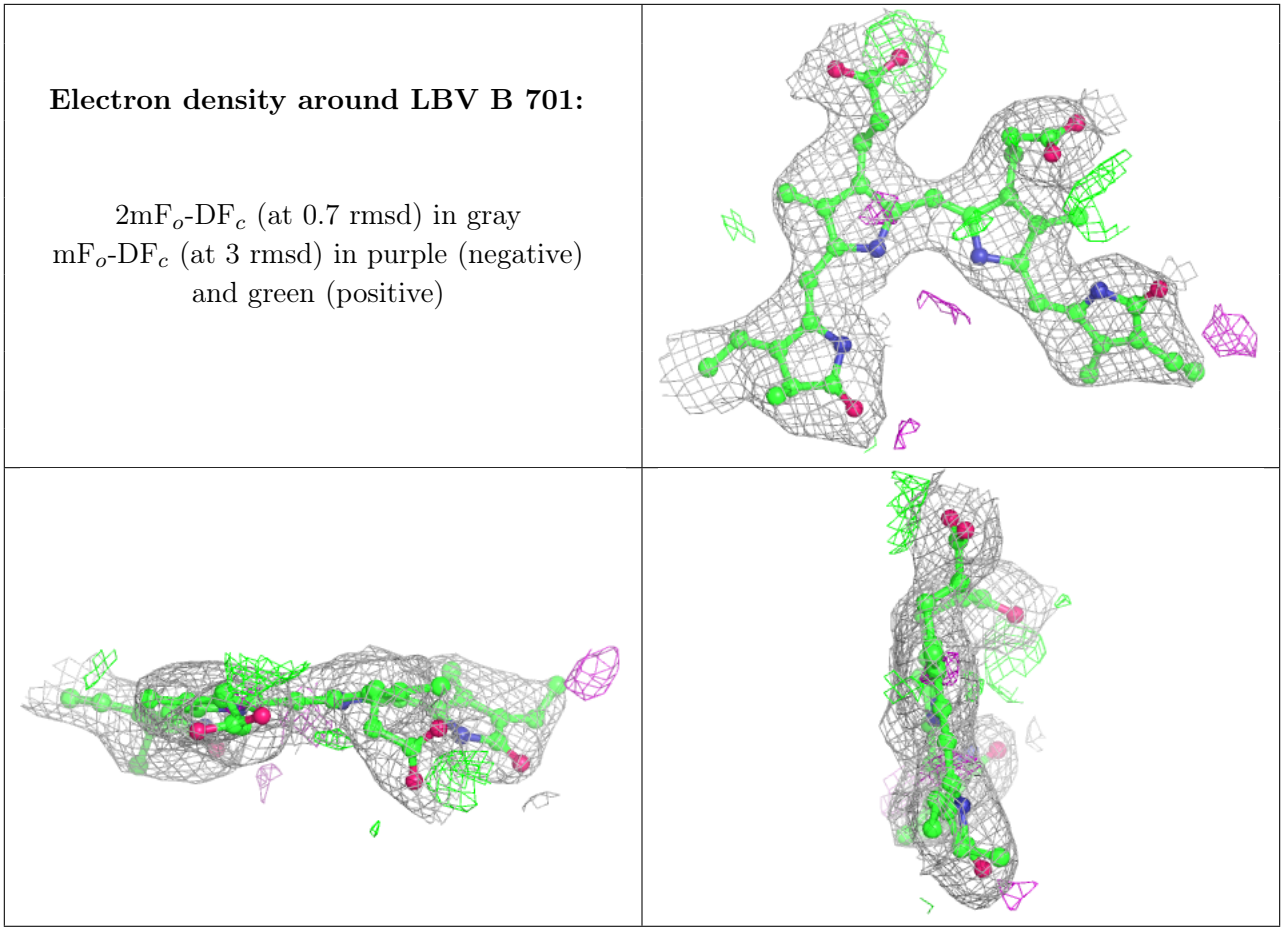






Electron density around LBV B 701:

$2mF_o$-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

There are no such residues in this entry.