WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:03 PM GMT

PDB ID	:	4E04
Title	:	RpBphP2 chromophore-binding domain crystallized by homologue-directed mutagenesis.
Authors	:	Bellini, D.; Papiz, M.Z.
Deposited on	:	2012-03-02
Resolution	:	1.79 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865
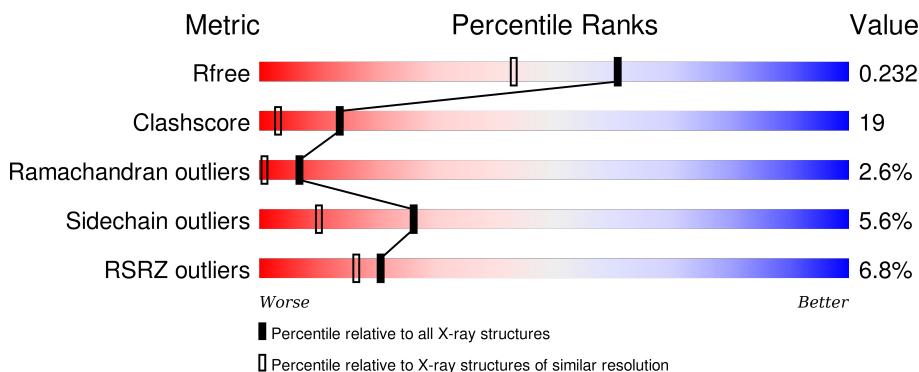
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
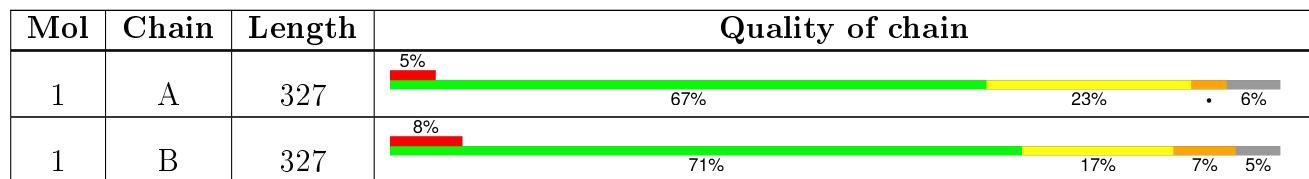
The reported resolution of this entry is 1.79 Å.

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	Percentile Ranks	Value
Rfree		0.232
Clashscore		19
Ramachandran outliers		2.6%
Sidechain outliers		5.6%
RSRZ outliers		6.8%

Worse → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	327	5% 67% 23% • 6%
1	B	327	8% 71% 17% 7% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5439 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 (Light-regulated signal transduction histidine kinase), PhyB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	5	0
			2423	1529	441	441	12			
1	B	310	Total	C	N	O	S	0	2	0
			2415	1524	435	444	12			

There are 48 discrepancies between the modelled and reference sequences:
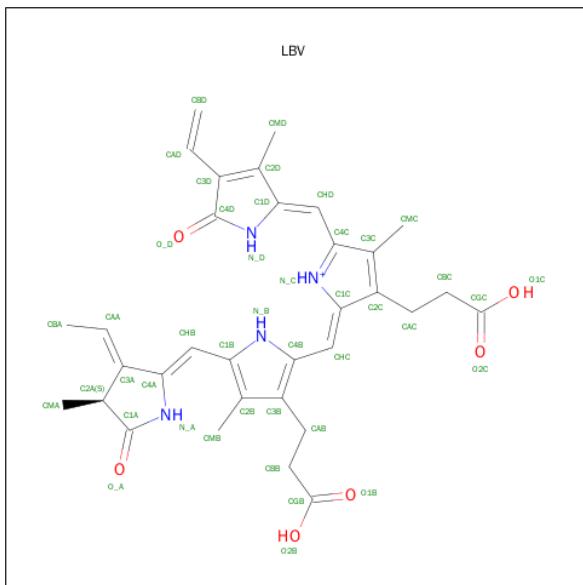
Chain	Residue	Modelled	Actual	Comment	Reference
A	98	PRO	ARG	ENGINEERED MUTATION	UNP Q6N5G3
A	99	ASP	LYS	ENGINEERED MUTATION	UNP Q6N5G3
A	100	GLY	ASP	ENGINEERED MUTATION	UNP Q6N5G3
A	101	GLU	ALA	ENGINEERED MUTATION	UNP Q6N5G3
A	102	ARG	GLY	ENGINEERED MUTATION	UNP Q6N5G3
A	103	ALA	PHE	ENGINEERED MUTATION	UNP Q6N5G3
A	104	PHE	VAL	ENGINEERED MUTATION	UNP Q6N5G3
A	105	ASN	-	INSERTION	UNP Q6N5G3
A	127	ARG	ALA	ENGINEERED MUTATION	UNP Q6N5G3
A	128	TYR	GLU	ENGINEERED MUTATION	UNP Q6N5G3
A	135	SER	ARG	ENGINEERED MUTATION	UNP Q6N5G3
A	136	VAL	THR	ENGINEERED MUTATION	UNP Q6N5G3
A	137	ARG	ASN	ENGINEERED MUTATION	UNP Q6N5G3
A	237	ARG	VAL	ENGINEERED MUTATION	UNP Q6N5G3
A	296	GLU	ASP	ENGINEERED MUTATION	UNP Q6N5G3
A	297	VAL	GLY	ENGINEERED MUTATION	UNP Q6N5G3
A	320	LEU	-	EXPRESSION TAG	UNP Q6N5G3
A	321	GLU	-	EXPRESSION TAG	UNP Q6N5G3
A	322	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	323	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	324	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	325	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	326	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	327	HIS	-	EXPRESSION TAG	UNP Q6N5G3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	98	PRO	ARG	ENGINEERED MUTATION	UNP Q6N5G3
B	99	ASP	LYS	ENGINEERED MUTATION	UNP Q6N5G3
B	100	GLY	ASP	ENGINEERED MUTATION	UNP Q6N5G3
B	101	GLU	ALA	ENGINEERED MUTATION	UNP Q6N5G3
B	102	ARG	GLY	ENGINEERED MUTATION	UNP Q6N5G3
B	103	ALA	PHE	ENGINEERED MUTATION	UNP Q6N5G3
B	104	PHE	VAL	ENGINEERED MUTATION	UNP Q6N5G3
B	105	ASN	-	INSERTION	UNP Q6N5G3
B	127	ARG	ALA	ENGINEERED MUTATION	UNP Q6N5G3
B	128	TYR	GLU	ENGINEERED MUTATION	UNP Q6N5G3
B	135	SER	ARG	ENGINEERED MUTATION	UNP Q6N5G3
B	136	VAL	THR	ENGINEERED MUTATION	UNP Q6N5G3
B	137	ARG	ASN	ENGINEERED MUTATION	UNP Q6N5G3
B	237	ARG	VAL	ENGINEERED MUTATION	UNP Q6N5G3
B	296	GLU	ASP	ENGINEERED MUTATION	UNP Q6N5G3
B	297	VAL	GLY	ENGINEERED MUTATION	UNP Q6N5G3
B	320	LEU	-	EXPRESSION TAG	UNP Q6N5G3
B	321	GLU	-	EXPRESSION TAG	UNP Q6N5G3
B	322	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	323	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	324	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	325	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	326	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	327	HIS	-	EXPRESSION TAG	UNP Q6N5G3

- Molecule 2 is 3-[2-[(Z)-[3-(2-CARBOXYETHYL)-5-[(Z)-(4-ETHENYL-3-METHYL-5-OX IDANYLIDENE-PYRROL-2-YLIDENE)METHYL]-4-METHYL-PYRROL-1-IUM-2-YLI DENE]METHYL]-5-[(Z)-[(3E)-3-ETHYLIDENE-4-METHYL-5-OXIDANYLIDENE-PYR ROLIDIN-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	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		
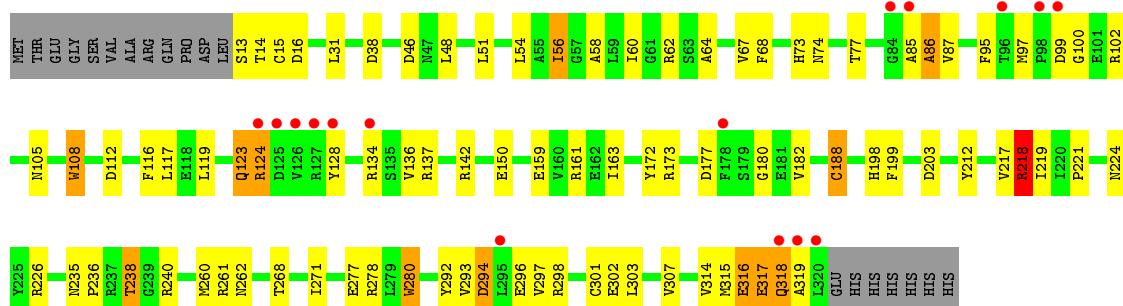
• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	277	Total	O	0	0
			277	277		
3	B	238	Total	O	0	0
			238	238		
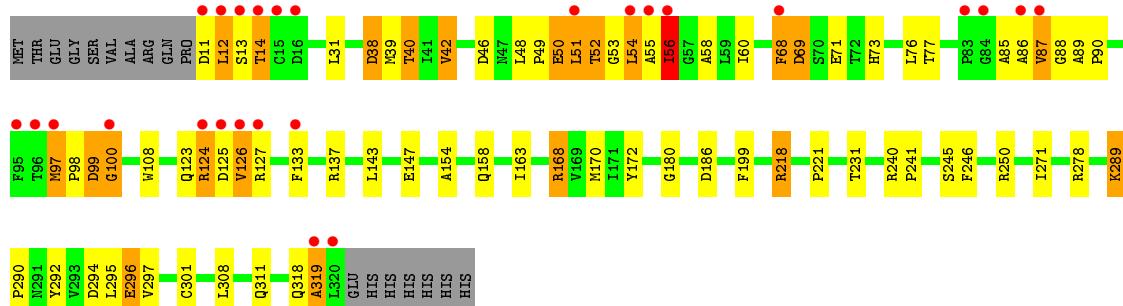
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 (Light-regulated signal transduction histidine kinase), PhyB1

• Molecule 1: Bacteriophytochrome (Light-regulated signal transduction histidine kinase), PhyB1

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.35Å 79.86Å 149.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.79 74.94 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-1.79) 99.7 (74.94-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.02	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.181 , 0.232 0.181 , 0.232	Depositor DCC
R_{free} test set	3024 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 59842 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5439	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	1.00	3/2492 (0.1%)	1.07	6/3391 (0.2%)
1	B	0.97	1/2475 (0.0%)	1.24	10/3371 (0.3%)
All	All	0.98	4/4967 (0.1%)	1.16	16/6762 (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	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	TRP	CD2-CE2	6.11	1.48	1.41
1	B	245	SER	CB-OG	5.57	1.49	1.42
1	A	292	TYR	CE1-CZ	5.57	1.45	1.38
1	A	108	TRP	CD2-CE2	5.25	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	ARG	NE-CZ-NH1	-27.80	106.40	120.30
1	B	218	ARG	NE-CZ-NH2	24.53	132.57	120.30
1	A	218	ARG	NE-CZ-NH1	14.00	127.30	120.30
1	B	168	ARG	NE-CZ-NH1	13.44	127.02	120.30
1	B	168	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	A	46	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	218	ARG	NE-CZ-NH2	-6.94	116.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	ARG	CD-NE-CZ	6.84	133.18	123.60
1	A	46	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	B	42	VAL	CG1-CB-CG2	6.16	120.76	110.90
1	A	177	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	38	ASP	CB-CG-OD1	5.64	123.37	118.30
1	B	69	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	B	186	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	117	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	B	250	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	GLU	Peptide

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	2423	0	2420	98	0
1	B	2415	0	2398	85	2
2	A	43	0	33	3	0
2	B	43	0	33	2	0
3	A	277	0	0	18	0
3	B	238	0	0	15	2
All	All	5439	0	4884	182	2

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 19.

All (182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASP:HB3	3:A:518:HOH:O	1.43	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:HG21	1:B:231:THR:HG23	1.31	1.07
1:A:318:GLN:HG3	1:A:319:ALA:H	1.18	1.07
1:B:123:GLN:HG3	1:B:124:ARG:H	1.24	1.01
1:B:231:THR:HB	3:B:519:HOH:O	0.82	0.99
1:B:97:MET:HB3	1:B:98:PRO:HD2	1.46	0.96
1:A:56:ILE:H	1:A:56:ILE:HD12	1.31	0.95
1:A:318:GLN:HG3	1:A:319:ALA:N	1.85	0.91
1:A:319:ALA:HB2	3:B:584:HOH:O	1.73	0.89
1:A:224:ASN:HD21	1:A:261:ARG:HE	1.18	0.89
1:A:316:GLU:O	1:A:317[B]:GLU:HB2	1.72	0.88
1:A:150:GLU:HG2	3:A:734:HOH:O	1.73	0.88
1:B:56:ILE:H	1:B:56:ILE:HD12	1.35	0.88
1:A:56:ILE:HG22	1:A:60:ILE:HD11	1.57	0.87
1:A:293:VAL:O	3:A:651:HOH:O	1.93	0.85
1:A:56:ILE:CG2	1:A:60:ILE:HD11	2.08	0.84
1:B:38:ASP:OD1	1:B:40:THR:HG23	1.81	0.80
1:B:99:ASP:HB2	1:B:100:GLY:CA	2.11	0.80
1:B:87:VAL:HA	3:B:573:HOH:O	1.79	0.80
1:B:168:ARG:HD3	1:B:170:MET:SD	2.23	0.78
1:A:15:CYS:HB2	3:A:698:HOH:O	1.83	0.78
1:B:55:ALA:H	1:B:58:ALA:HB3	1.50	0.77
1:A:219:ILE:HD11	1:A:298[B]:ARG:HG3	1.65	0.76
1:B:55:ALA:HB1	3:B:728:HOH:O	1.87	0.74
1:B:56:ILE:HD12	1:B:56:ILE:N	2.02	0.74
1:A:212:TYR:CE1	1:A:218:ARG:HD2	2.23	0.74
1:B:123:GLN:HG3	1:B:124:ARG:N	2.02	0.74
1:A:97:MET:HG3	1:A:100:GLY:O	1.88	0.74
1:B:56:ILE:HG21	1:B:231:THR:CG2	2.13	0.73
1:B:126:VAL:HA	1:B:127:ARG:HB2	1.71	0.72
1:B:73:HIS:O	1:B:77:THR:HG23	1.89	0.72
1:B:88:GLY:N	3:B:573:HOH:O	2.23	0.72
1:B:54:LEU:HD12	1:B:55:ALA:HB2	1.72	0.72
1:B:123:GLN:HB3	1:B:294:ASP:OD1	1.89	0.71
1:B:289:LYS:HB2	1:B:290:PRO:HD2	1.71	0.71
1:A:218:ARG:HD3	3:A:521:HOH:O	1.91	0.70
1:A:238:THR:HG23	1:A:240[A]:ARG:H	1.57	0.69
1:A:224:ASN:ND2	1:A:261:ARG:HE	1.89	0.69
1:A:217:VAL:HG21	1:A:302:GLU:CD	2.12	0.69
1:A:56:ILE:H	1:A:56:ILE:CD1	2.05	0.68
1:A:163:ILE:HG22	1:A:297:VAL:HG13	1.76	0.68
1:B:99:ASP:HB2	1:B:100:GLY:HA2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:MET:CE	1:B:76:LEU:HD23	2.24	0.67
1:B:12:LEU:HD21	1:B:14:THR:HG22	1.78	0.66
1:B:289:LYS:HB2	1:B:290:PRO:CD	2.25	0.66
1:A:238:THR:HG23	1:A:240[B]:ARG:H	1.60	0.66
1:B:69:ASP:OD2	3:B:626:HOH:O	2.14	0.65
1:B:12:LEU:CD2	1:B:14:THR:HG22	2.27	0.65
1:B:97:MET:HB3	1:B:98:PRO:CD	2.25	0.65
1:A:316:GLU:O	1:A:317[A]:GLU:HB2	1.92	0.64
1:A:14:THR:HG23	1:A:15:CYS:N	2.13	0.64
1:B:123:GLN:O	1:B:125:ASP:N	2.21	0.64
1:A:73:HIS:O	1:A:77:THR:HG23	1.97	0.64
1:A:68:PHE:O	3:A:631:HOH:O	2.15	0.63
2:A:400:LBV:N_D	2:A:400:LBV:HMC1	2.13	0.63
1:A:128:TYR:OH	1:B:71:GLU:OE1	2.12	0.63
1:A:142:ARG:HD3	1:A:159:GLU:OE2	1.98	0.62
1:A:318:GLN:CG	1:A:319:ALA:H	1.95	0.62
1:A:238:THR:CG2	1:A:240[A]:ARG:H	2.12	0.62
1:A:315:MET:O	1:A:317[A]:GLU:HG3	1.99	0.61
1:A:235:ASN:HB3	1:A:238:THR:HG22	1.83	0.61
1:A:238:THR:CG2	1:A:240[B]:ARG:H	2.13	0.60
1:A:102:ARG:HG2	3:A:630:HOH:O	2.01	0.60
1:A:100:GLY:HA2	3:A:641:HOH:O	2.02	0.60
1:B:87:VAL:HG11	1:B:246:PHE:CD2	2.37	0.59
1:A:14:THR:HG23	1:A:15:CYS:H	1.68	0.58
1:B:296:GLU:HG2	1:B:297:VAL:N	2.17	0.57
1:B:39:MET:HE1	1:B:76:LEU:HD23	1.85	0.57
1:A:224:ASN:HD22	1:A:261:ARG:HH21	1.50	0.57
1:A:277:GLU:HG3	3:A:584:HOH:O	2.04	0.57
1:A:235:ASN:HB3	1:A:238:THR:CG2	2.35	0.57
1:B:231:THR:CB	3:B:519:HOH:O	1.70	0.57
1:B:127:ARG:HD2	1:B:296:GLU:OE2	2.04	0.57
1:A:260:MET:CE	1:A:268:THR:HG21	2.35	0.57
1:B:124:ARG:NH2	1:B:292:TYR:O	2.34	0.57
1:B:87:VAL:CG1	1:B:87:VAL:O	2.53	0.56
2:B:400:LBV:HMC1	2:B:400:LBV:N_D	2.18	0.56
1:A:31:LEU:HD11	1:A:119:LEU:HD12	1.88	0.56
1:A:105:ASN:ND2	3:A:671:HOH:O	2.38	0.56
1:A:13:SER:HA	1:A:16:ASP:HB2	1.87	0.55
1:A:64:ALA:HA	1:A:67:VAL:HG12	1.88	0.55
1:B:318:GLN:O	1:B:319:ALA:HB3	2.07	0.55
1:A:87:VAL:HG13	3:A:696:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:HD11	1:B:311[A]:GLN:HE22	1.71	0.54
1:A:238:THR:HG23	1:A:240[B]:ARG:HB2	1.88	0.54
1:B:99:ASP:HB2	1:B:100:GLY:HA3	1.87	0.54
1:B:318:GLN:HB2	3:B:661:HOH:O	2.07	0.53
1:A:13:SER:HA	1:A:16:ASP:OD2	2.09	0.53
1:A:212:TYR:CE1	1:A:218:ARG:CD	2.91	0.53
1:B:126:VAL:HA	1:B:127:ARG:CB	2.34	0.53
1:B:39:MET:HE1	1:B:68:PHE:HZ	1.73	0.53
1:B:318:GLN:O	1:B:319:ALA:CB	2.56	0.52
1:A:319:ALA:CB	3:B:584:HOH:O	2.43	0.52
1:B:124:ARG:NH2	3:B:623:HOH:O	2.42	0.52
1:B:154:ALA:O	1:B:158:GLN:HG3	2.09	0.52
1:A:136:VAL:HG11	1:A:303:LEU:HD23	1.92	0.52
1:B:55:ALA:H	1:B:58:ALA:CB	2.19	0.52
1:A:123:GLN:HG3	1:A:123:GLN:O	2.10	0.52
1:B:87:VAL:HG12	1:B:87:VAL:O	2.08	0.51
1:B:88:GLY:HA3	1:B:108:TRP:O	2.11	0.51
1:B:53:GLY:O	1:B:54:LEU:HB3	2.10	0.51
1:A:95:PHE:HB2	1:A:97:MET:CE	2.41	0.51
1:B:168:ARG:CD	1:B:170:MET:SD	2.98	0.50
1:B:143:LEU:CD1	1:B:311[A]:GLN:HE22	2.25	0.50
1:A:226:ARG:NH2	3:A:548:HOH:O	2.45	0.50
1:A:95:PHE:HB2	1:A:97:MET:HE2	1.92	0.50
1:B:240[B]:ARG:HB3	1:B:241:PRO:HD2	1.94	0.50
1:B:53:GLY:O	1:B:54:LEU:CB	2.60	0.49
1:B:271:ILE:CD1	1:B:301:CYS:HB3	2.42	0.49
1:A:296:GLU:HG3	1:B:133:PHE:CE2	2.47	0.49
1:B:221:PRO:O	1:B:290:PRO:HA	2.13	0.49
1:A:56:ILE:N	1:A:56:ILE:HD12	2.15	0.49
1:B:89:ALA:HB1	1:B:90:PRO:HD2	1.93	0.49
1:B:31:LEU:HD21	1:B:51:LEU:HB2	1.95	0.49
1:B:48:LEU:N	1:B:49:PRO:HD2	2.28	0.49
1:B:56:ILE:CD1	1:B:56:ILE:N	2.73	0.48
1:B:56:ILE:C	1:B:58:ALA:N	2.66	0.48
1:B:50:GLU:O	1:B:52:THR:N	2.46	0.48
1:A:137:ARG:HD2	3:A:713:HOH:O	2.12	0.48
1:A:108:TRP:HA	1:A:116:PHE:O	2.14	0.48
1:B:289:LYS:CB	1:B:290:PRO:CD	2.89	0.47
1:A:271:ILE:HD11	1:A:301:CYS:HB3	1.97	0.47
1:A:271:ILE:CD1	1:A:301:CYS:HB3	2.44	0.47
1:A:260:MET:HE2	1:A:268:THR:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:C	1:B:58:ALA:H	2.18	0.47
1:A:56:ILE:HG23	1:A:60:ILE:HD11	1.94	0.47
1:A:260:MET:CE	1:A:268:THR:CG2	2.93	0.47
1:B:39:MET:HE2	1:B:76:LEU:HD23	1.96	0.47
1:A:173[B]:ARG:HD3	1:A:280:TRP:CZ2	2.49	0.46
1:B:308:LEU:HA	1:B:311[A]:GLN:HE21	1.81	0.46
1:B:172:TYR:CZ	1:B:180:GLY:HA3	2.51	0.46
1:A:182:VAL:CG2	2:A:400:LBV:HBD2	2.45	0.46
1:A:87:VAL:CG1	3:A:696:HOH:O	2.63	0.46
1:A:38:ASP:OD1	1:A:38:ASP:C	2.54	0.46
1:A:307:VAL:CG2	3:B:554:HOH:O	2.64	0.45
1:A:14:THR:CG2	1:A:15:CYS:N	2.78	0.45
1:A:307:VAL:HG23	3:B:554:HOH:O	2.16	0.45
1:A:102:ARG:HB2	1:A:102:ARG:HH11	1.82	0.45
1:A:31:LEU:HB3	1:A:51:LEU:HD12	1.98	0.45
1:A:172:TYR:OH	1:A:199:PHE:HB2	2.17	0.45
1:A:303:LEU:HB2	1:B:137:ARG:HD3	1.99	0.44
1:A:48:LEU:HD12	1:A:56:ILE:HG13	2.00	0.44
1:A:58:ALA:O	1:A:62:ARG:HD2	2.17	0.44
1:A:219:ILE:HG22	1:A:221:PRO:HD3	2.00	0.44
1:B:240[A]:ARG:HB3	1:B:241:PRO:HD2	1.99	0.44
1:A:180:GLY:O	1:A:198:HIS:HA	2.18	0.44
1:A:172:TYR:CZ	1:A:180:GLY:HA3	2.53	0.44
1:A:97:MET:CG	1:A:100:GLY:O	2.64	0.43
1:B:12:LEU:HD21	1:B:14:THR:CG2	2.47	0.43
1:A:217:VAL:HG21	1:A:302:GLU:CG	2.48	0.43
1:A:14:THR:CG2	1:A:15:CYS:H	2.31	0.43
1:A:161:ARG:NH2	1:A:188:CYS:HB3	2.33	0.43
1:A:318:GLN:CG	1:A:319:ALA:N	2.60	0.43
1:B:56:ILE:O	1:B:60:ILE:HG12	2.19	0.43
1:B:11:ASP:HA	1:B:12:LEU:HA	1.76	0.43
1:B:271:ILE:HD13	1:B:301:CYS:HB3	2.01	0.43
1:B:147:GLU:HB3	3:B:584:HOH:O	2.19	0.42
1:A:217:VAL:HG21	1:A:302:GLU:OE1	2.17	0.42
1:B:87:VAL:CA	3:B:573:HOH:O	2.54	0.42
1:A:314:VAL:O	1:A:317[A]:GLU:HA	2.19	0.42
1:A:203:ASP:HB3	2:A:400:LBV:HMD3	2.01	0.42
1:A:260:MET:HE2	1:A:268:THR:HG21	2.02	0.42
1:A:86:ALA:HB3	3:A:617:HOH:O	2.20	0.42
1:A:224:ASN:ND2	1:A:261:ARG:HH21	2.16	0.42
1:B:240[B]:ARG:HB3	1:B:241:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:CA	1:B:127:ARG:HB2	2.46	0.42
1:B:199:PHE:CE2	2:B:400:LBV:HAD1	2.55	0.41
1:A:235:ASN:HA	1:A:236:PRO:HD3	1.74	0.41
1:B:289:LYS:HG2	1:B:289:LYS:H	1.66	0.41
1:B:123:GLN:CG	1:B:124:ARG:H	2.10	0.41
1:B:46:ASP:OD1	1:B:231:THR:CG2	2.69	0.41
1:A:238:THR:HG21	3:A:776:HOH:O	2.20	0.41
1:A:203:ASP:O	3:A:538:HOH:O	2.22	0.41
1:A:161:ARG:HH21	1:A:188:CYS:HB3	1.86	0.41
1:A:124:ARG:C	1:A:124:ARG:HD3	2.41	0.41
1:B:271:ILE:HD11	1:B:301:CYS:HB3	2.03	0.41
1:B:123:GLN:CG	1:B:124:ARG:N	2.75	0.40
1:B:87:VAL:C	3:B:573:HOH:O	2.55	0.40
1:A:298[A]:ARG:NH2	3:A:670:HOH:O	2.50	0.40
1:B:90:PRO:HB3	1:B:295:LEU:HD21	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:MET:CE	3:B:645:HOH:O[3_655]	1.96	0.24
1:B:39:MET:CG	3:B:645:HOH:O[3_655]	1.97	0.23

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	311/327 (95%)	302 (97%)	4 (1%)	5 (2%)	12	3
1	B	310/327 (95%)	281 (91%)	17 (6%)	12 (4%)	4	0
All	All	621/654 (95%)	583 (94%)	21 (3%)	17 (3%)	7	1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317[A]	GLU
1	A	317[B]	GLU
1	A	318	GLN
1	B	54	LEU
1	B	56	ILE
1	B	124	ARG
1	B	319	ALA
1	A	85	ALA
1	A	86	ALA
1	B	50	GLU
1	B	51	LEU
1	B	86	ALA
1	B	100	GLY
1	B	85	ALA
1	B	126	VAL
1	B	52	THR
1	B	97	MET

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	256/268 (96%)	242 (94%)	14 (6%)	27	10
1	B	255/268 (95%)	241 (94%)	14 (6%)	27	10
All	All	511/536 (95%)	483 (94%)	28 (6%)	26	10

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	56	ILE
1	A	74	ASN
1	A	99	ASP
1	A	112	ASP
1	A	123	GLN

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Mol	Chain	Res	Type
1	A	124	ARG
1	A	134	ARG
1	A	188	CYS
1	A	218	ARG
1	A	238	THR
1	A	262	ASN
1	A	278	ARG
1	A	294	ASP
1	B	12	LEU
1	B	13	SER
1	B	14	THR
1	B	40	THR
1	B	42	VAL
1	B	56	ILE
1	B	68	PHE
1	B	87	VAL
1	B	99	ASP
1	B	163	ILE
1	B	218	ARG
1	B	278	ARG
1	B	289	LYS
1	B	296	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	224	ASN
1	A	306	GLN
1	A	318	GLN
1	B	318	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	LBV	A	400	1	35,46,46	3.60	16 (45%)	37,67,67	2.64	15 (40%)
2	LBV	B	400	1	35,46,46	4.33	14 (40%)	37,67,67	3.03	21 (56%)

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	A	400	1	-	2/22/74/74	0/4/4/4
2	LBV	B	400	1	-	2/22/74/74	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	LBV	C2A-C1A	-3.29	1.48	1.52
2	A	400	LBV	C4D-N_D	-2.19	1.32	1.37
2	B	400	LBV	CHD-C4C	2.05	1.45	1.40
2	A	400	LBV	C1C-C2C	2.09	1.49	1.45
2	A	400	LBV	C4B-CHC	2.22	1.48	1.40
2	A	400	LBV	C1B-CHB	2.46	1.49	1.40
2	B	400	LBV	C4B-CHC	2.51	1.49	1.40
2	B	400	LBV	C3B-C2B	2.66	1.45	1.37
2	A	400	LBV	C4C-C3C	2.77	1.51	1.45
2	A	400	LBV	O_D-C4D	2.78	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	LBV	C3B-C2B	2.81	1.46	1.37
2	A	400	LBV	CHD-C4C	2.96	1.47	1.40
2	B	400	LBV	C1A-N_A	3.02	1.41	1.37
2	A	400	LBV	O_A-C1A	3.03	1.29	1.23
2	B	400	LBV	C4C-C3C	3.51	1.53	1.45
2	B	400	LBV	O_A-C1A	3.51	1.30	1.23
2	B	400	LBV	O_D-C4D	3.73	1.30	1.23
2	B	400	LBV	CHD-C1D	3.84	1.47	1.37
2	B	400	LBV	C2C-C3C	3.86	1.45	1.36
2	A	400	LBV	C2C-C3C	3.97	1.45	1.36
2	A	400	LBV	CHD-C1D	4.14	1.47	1.37
2	B	400	LBV	CHB-C4A	4.22	1.43	1.34
2	B	400	LBV	C1C-C2C	4.56	1.53	1.45
2	B	400	LBV	C3D-C2D	5.76	1.48	1.36
2	A	400	LBV	C3D-C2D	5.99	1.49	1.36
2	A	400	LBV	CHB-C4A	6.31	1.48	1.34
2	A	400	LBV	CHC-C1C	10.86	1.44	1.35
2	A	400	LBV	CAA-C3A	11.79	1.47	1.33
2	B	400	LBV	CAA-C3A	13.04	1.49	1.33
2	B	400	LBV	CHC-C1C	17.34	1.50	1.35

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	LBV	O_A-C1A-N_A	-5.82	117.78	124.83
2	A	400	LBV	CAB-CBB-CGB	-5.50	102.67	112.75
2	B	400	LBV	O_A-C1A-N_A	-5.37	118.33	124.83
2	B	400	LBV	CAB-CBB-CGB	-5.01	103.57	112.75
2	B	400	LBV	CHC-C1C-N_C	-4.78	120.12	128.67
2	B	400	LBV	C1C-C2C-C3C	-4.50	101.79	106.81
2	B	400	LBV	C1D-N_D-C4D	-4.22	104.55	110.73
2	A	400	LBV	C1D-N_D-C4D	-3.92	105.00	110.73
2	A	400	LBV	C1C-C2C-C3C	-3.83	102.53	106.81
2	A	400	LBV	O_D-C4D-C3D	-3.81	120.30	129.82
2	B	400	LBV	CHD-C1D-C2D	-3.72	119.16	126.89
2	A	400	LBV	CHC-C1C-N_C	-3.41	122.57	128.67
2	B	400	LBV	CHB-C4A-C3A	-3.41	120.75	127.21
2	A	400	LBV	CHD-C1D-C2D	-3.16	120.33	126.89
2	B	400	LBV	O_D-C4D-C3D	-3.13	122.02	129.82
2	B	400	LBV	CHD-C4C-C3C	-3.00	117.56	124.88
2	B	400	LBV	CBA-CAA-C3A	-2.82	120.57	127.07
2	B	400	LBV	CAC-C2C-C3C	-2.52	123.60	128.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	LBV	CBA-CAA-C3A	-2.16	122.08	127.07
2	B	400	LBV	C1C-N_C-C4C	-2.06	102.44	106.51
2	B	400	LBV	CBB-CAB-C3B	-2.06	108.84	112.53
2	B	400	LBV	CMB-C2B-C3B	2.16	129.76	125.24
2	A	400	LBV	CMD-C2D-C1D	2.25	127.19	124.20
2	A	400	LBV	C2B-C1B-N_B	2.26	113.99	110.29
2	A	400	LBV	CMC-C3C-C4C	2.44	129.03	125.06
2	B	400	LBV	CMD-C2D-C1D	2.50	127.53	124.20
2	B	400	LBV	C3A-C4A-N_A	3.15	111.45	107.32
2	A	400	LBV	CAB-C3B-C4B	3.42	130.72	127.01
2	A	400	LBV	C2C-C1C-N_C	3.73	115.65	109.86
2	B	400	LBV	C2B-C1B-N_B	3.94	116.74	110.29
2	B	400	LBV	C2C-C1C-N_C	4.04	116.14	109.86
2	A	400	LBV	CAC-C2C-C1C	4.28	132.70	125.06
2	B	400	LBV	CMC-C3C-C4C	4.98	133.16	125.06
2	B	400	LBV	CAC-C2C-C1C	5.33	134.59	125.06
2	A	400	LBV	C2D-C1D-N_D	5.71	115.28	107.00
2	B	400	LBV	C2D-C1D-N_D	5.79	115.38	107.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	LBV	C1D-CHD-C4C-C3C
2	A	400	LBV	C1D-CHD-C4C-C3C
2	B	400	LBV	C1D-CHD-C4C-N_C
2	A	400	LBV	C1D-CHD-C4C-N_C

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	LBV	3	0
2	B	400	LBV	2	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	308/327 (94%)	0.29	16 (5%)	31	25	30, 45, 78, 125	0
1	B	310/327 (94%)	0.40	26 (8%)	14	11	29, 43, 99, 135	0
All	All	618/654 (94%)	0.34	42 (6%)	20	16	29, 45, 94, 135	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	VAL	14.6
1	B	51	LEU	11.1
1	A	319	ALA	6.5
1	A	85	ALA	6.5
1	B	54	LEU	6.2
1	A	84	GLY	6.0
1	B	87	VAL	5.9
1	B	97	MET	5.9
1	A	320	LEU	5.8
1	B	125	ASP	5.6
1	B	83	PRO	5.5
1	B	124	ARG	5.4
1	B	320	LEU	4.9
1	A	98	PRO	4.9
1	B	56	ILE	4.8
1	A	318	GLN	4.3
1	A	126	VAL	3.8
1	B	12	LEU	3.7
1	A	128	TYR	3.7
1	A	96	THR	3.6
1	B	14	THR	3.5
1	B	16	ASP	3.5
1	B	13	SER	3.5
1	B	127	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	86	ALA	3.5
1	B	319	ALA	3.4
1	B	100	GLY	3.4
1	A	124	ARG	3.0
1	B	15	CYS	3.0
1	A	99	ASP	2.8
1	B	96	THR	2.7
1	B	11	ASP	2.5
1	A	125	ASP	2.5
1	B	84	GLY	2.4
1	A	127	ARG	2.3
1	A	295	LEU	2.3
1	B	68	PHE	2.3
1	A	134	ARG	2.3
1	B	133	PHE	2.1
1	B	95	PHE	2.1
1	B	55	ALA	2.1
1	A	178	PHE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	LBV	A	400	43/43	0.93	0.12	1.70	37,47,56,60	1
2	LBV	B	400	43/43	0.94	0.09	-0.14	32,43,54,61	1

6.5 Other polymers (i)

There are no such residues in this entry.