Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:58 PM GMT

PDB ID	:	1RGB
Title	:	Phospholipase A2 from Vipera ammodytes meridionalis
Authors	:	Georgieva, D.N.
Deposited on	:	2003-11-12
Resolution	:	3.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

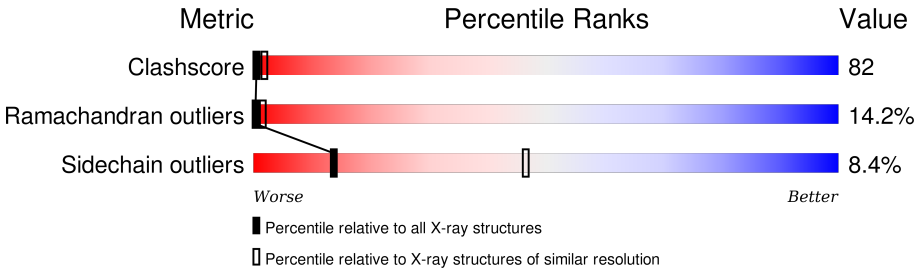
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	122	18% 70% 11%
1	B	122	20% 64% 16%
1	K	122	23% 63% 12%
1	L	122	17% 64% 19%

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	ELD	B	134	-	-	X	-
2	ELD	L	134	-	-	X	-

2 Entry composition

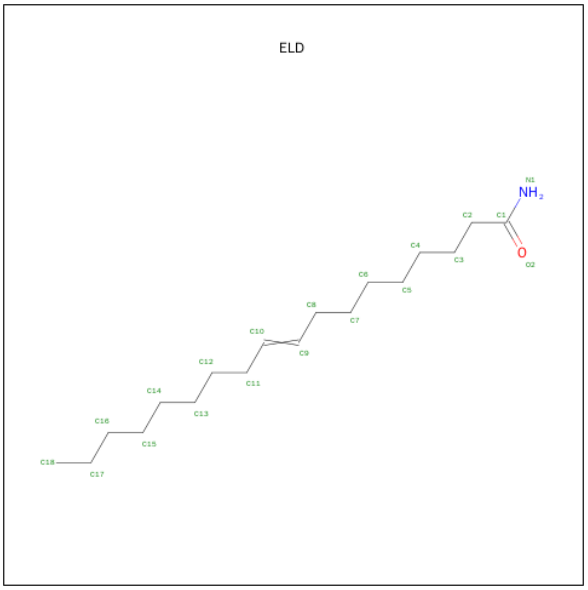
There are 2 unique types of molecules in this entry. The entry contains 3892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospholipase A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	84	0	0
			963	598	176	174	15			
1	B	122	Total	C	N	O	S	65	0	0
			963	598	176	174	15			
1	K	122	Total	C	N	O	S	87	0	0
			963	598	176	174	15			
1	L	122	Total	C	N	O	S	81	0	0
			963	598	176	174	15			

- Molecule 2 is (9E)-OCTADEC-9-ENAMIDE (three-letter code: ELD) (formula: $C_{18}H_{35}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			20	18	1	1		
2	L	1	Total	C	N	O	0	0
			20	18	1	1		

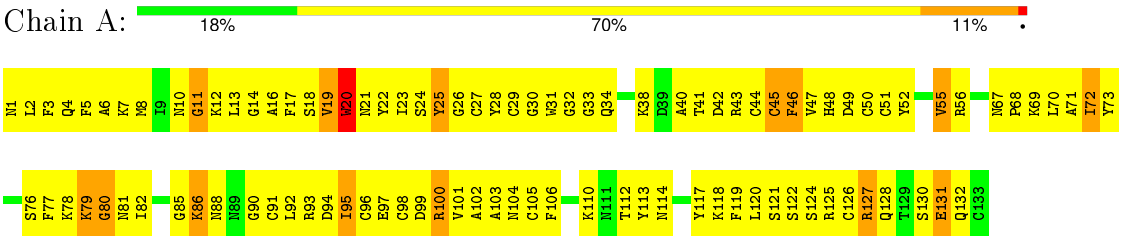
3 Residue-property plots (i)

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.

Note EDS was not executed.

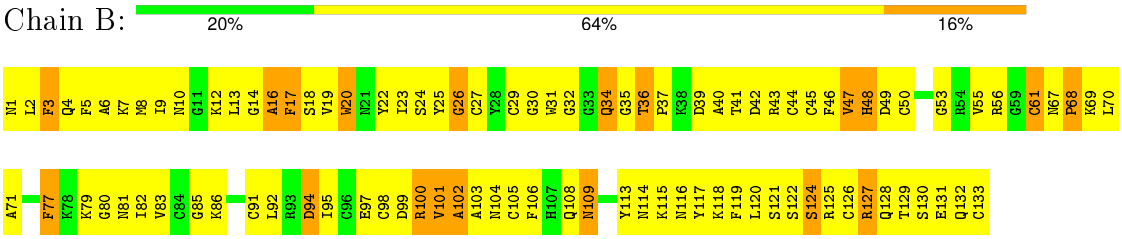
- Molecule 1: Phospholipase A2

Chain A:



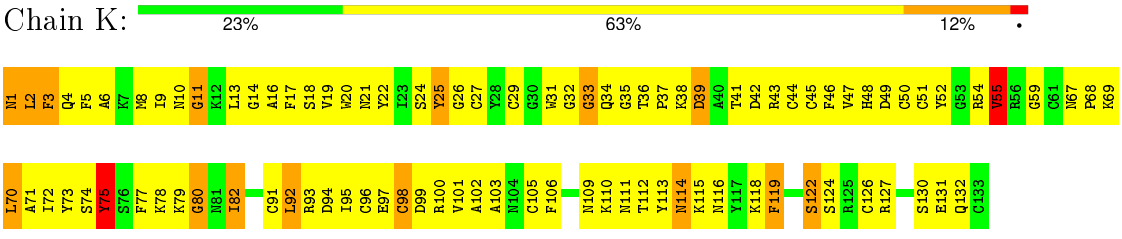
- Molecule 1: Phospholipase A2

Chain B:



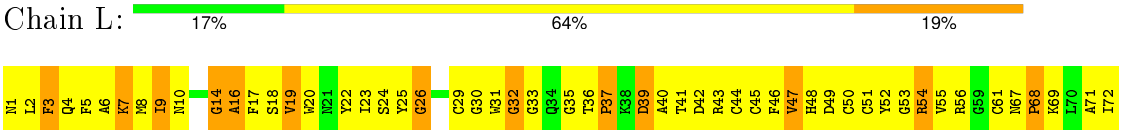
- Molecule 1: Phospholipase A2

Chain K:



- Molecule 1: Phospholipase A2

Chain L:




Y73
S74
Y75
S76
F77
N81
I82
V83
C84
G85
K86
N88
N89
G90
C91
L92
R93
D94
I95
C96
E97
C98
D99
R100
Y101
A102
A103
N104
C105
F106
H107
Q108
N109
K110
N111
T112
Y113
N114
K115
N116
Y117
K118
F119
L120
S121
S122
S124
R125
C126
R127
Q128
T129
S130
C133

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.57Å 82.67Å 119.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.53 – 3.30	Depositor
% Data completeness (in resolution range)	94.5 (19.53-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3892	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.52	0/985	0.75	0/1320
1	B	0.55	0/985	0.78	0/1320
1	K	0.52	0/985	0.74	0/1320
1	L	0.48	0/985	0.71	0/1320
All	All	0.52	0/3940	0.75	0/5280

There are no bond length outliers.

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	963	0	904	149	0
1	B	963	0	904	154	0
1	K	963	0	904	131	0
1	L	963	0	904	159	0
2	B	20	0	35	13	0
2	L	20	0	35	16	0
All	All	3892	0	3686	556	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 82.

All (556) 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:L:114:ASN:HD22	1:L:116:ASN:HB3	1.14	1.11
1:B:124:SER:HB3	1:B:127:ARG:HH21	1.20	1.06
1:A:25:TYR:O	1:A:29:CYS:HB2	1.52	1.05
1:L:20:TRP:HA	1:L:23:ILE:HG12	1.34	1.04
1:B:82:ILE:HG21	1:B:100:ARG:HG3	1.41	1.01
1:K:2:LEU:HD12	1:L:31:TRP:HA	1.45	0.99
1:K:69:LYS:HG2	1:L:49:ASP:OD1	1.66	0.95
1:L:41:THR:O	1:L:44:CYS:HB2	1.67	0.95
1:A:11:GLY:HA3	1:A:77:PHE:CZ	2.02	0.95
1:B:25:TYR:HB3	1:B:29:CYS:HB2	1.52	0.92
1:L:101:VAL:HA	1:L:104:ASN:HB2	1.53	0.91
1:K:1:ASN:HB2	1:L:33:GLY:HA3	1.49	0.91
1:K:43:ARG:O	1:K:47:VAL:HG23	1.68	0.90
1:A:69:LYS:HG3	1:A:70:LEU:HD12	1.54	0.90
1:L:114:ASN:ND2	1:L:116:ASN:HB3	1.88	0.88
1:L:5:PHE:CE1	1:L:99:ASP:HA	2.09	0.87
1:L:25:TYR:O	1:L:29:CYS:HB2	1.75	0.86
1:L:45:CYS:SG	2:L:134:ELD:H151	2.16	0.85
1:K:35:GLY:H	1:K:130:SER:HA	1.41	0.85
1:K:1:ASN:HD21	1:K:4:GLN:HG3	1.39	0.85
1:K:118:LYS:HG3	1:K:119:PHE:CD2	2.13	0.84
1:A:24:SER:HA	1:A:30:GLY:HA3	1.59	0.83
1:K:1:ASN:CB	1:L:33:GLY:HA3	2.08	0.83
1:A:23:ILE:HG12	1:B:23:ILE:HD11	1.62	0.81
1:B:25:TYR:HB3	1:B:29:CYS:CB	2.11	0.81
1:L:128:GLN:H	1:L:128:GLN:CD	1.82	0.81
1:A:131:GLU:HG3	1:A:132:GLN:H	1.47	0.80
1:A:11:GLY:HA3	1:A:77:PHE:HZ	1.43	0.80
1:A:122:SER:HA	1:B:3:PHE:CZ	2.17	0.79
1:B:8:MET:SD	1:B:99:ASP:HB3	2.21	0.79
1:L:19:VAL:HG13	1:L:20:TRP:H	1.47	0.79
1:A:100:ARG:O	1:A:103:ALA:HB3	1.83	0.79
1:B:124:SER:HB3	1:B:127:ARG:NH2	1.96	0.78
1:K:25:TYR:O	1:K:29:CYS:HB2	1.82	0.78
1:K:100:ARG:NH2	1:K:101:VAL:HG22	1.98	0.78
1:A:101:VAL:HA	1:A:104:ASN:HD22	1.50	0.77
1:A:41:THR:O	1:A:44:CYS:HB2	1.85	0.76
1:L:48:HIS:O	1:L:51:CYS:HB3	1.85	0.76
1:A:120:LEU:HB3	1:A:125:ARG:HB2	1.67	0.76
1:B:82:ILE:CG2	1:B:100:ARG:HG3	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:VAL:HG13	1:B:20:TRP:CE3	2.20	0.76
1:L:5:PHE:HD1	1:L:99:ASP:CG	1.88	0.76
1:L:20:TRP:HA	1:L:23:ILE:CG1	2.15	0.75
1:A:48:HIS:HB3	2:B:134:ELD:HN11	1.51	0.75
1:A:122:SER:HA	1:B:3:PHE:CE1	2.21	0.75
1:L:36:THR:HG23	1:L:37:PRO:HD2	1.67	0.75
1:A:90:GLY:O	1:A:93:ARG:HB3	1.86	0.74
1:A:1:ASN:HB3	1:A:71:ALA:O	1.88	0.74
1:B:45:CYS:SG	2:B:134:ELD:H172	2.28	0.74
1:L:5:PHE:HE1	1:L:99:ASP:HA	1.51	0.74
1:L:94:ASP:O	1:L:97:GLU:HB2	1.88	0.74
1:B:23:ILE:O	1:B:30:GLY:HA3	1.87	0.74
1:K:49:ASP:OD1	1:L:69:LYS:HG2	1.88	0.74
1:K:29:CYS:SG	1:K:42:ASP:HA	2.28	0.74
1:K:3:PHE:CE1	1:L:32:GLY:HA2	2.23	0.73
1:B:103:ALA:O	1:B:106:PHE:HB2	1.88	0.73
1:L:18:SER:HB3	1:L:22:TYR:HE2	1.53	0.73
1:L:20:TRP:CA	1:L:23:ILE:HG12	2.17	0.73
1:B:117:TYR:C	1:B:120:LEU:HD21	2.09	0.73
1:B:94:ASP:O	1:B:97:GLU:HB2	1.87	0.73
1:A:25:TYR:HD2	1:A:118:LYS:HG2	1.52	0.73
1:B:102:ALA:HB1	2:B:134:ELD:H183	1.70	0.73
1:B:132:GLN:HG2	1:B:133:CYS:N	2.04	0.73
1:K:45:CYS:O	1:K:48:HIS:HB3	1.88	0.72
1:L:91:CYS:SG	1:L:92:LEU:N	2.63	0.72
1:L:118:LYS:HB3	1:L:119:PHE:CD2	2.24	0.72
1:B:47:VAL:O	1:B:50:CYS:N	2.22	0.72
1:A:49:ASP:OD1	1:B:69:LYS:HG2	1.90	0.72
1:K:72:ILE:O	1:K:92:LEU:HD11	1.89	0.72
1:B:45:CYS:HA	2:B:134:ELD:H172	1.72	0.71
1:A:43:ARG:O	1:A:47:VAL:HG23	1.90	0.71
1:A:8:MET:SD	1:A:82:ILE:HD13	2.31	0.71
1:L:88:ASN:ND2	1:L:93:ARG:HB2	2.06	0.70
1:K:51:CYS:O	1:K:55:VAL:HG12	1.92	0.70
1:B:16:ALA:O	1:B:17:PHE:HB2	1.91	0.70
1:K:59:GLY:HA3	1:K:91:CYS:HB3	1.73	0.70
1:A:71:ALA:O	1:A:72:ILE:HG13	1.92	0.70
1:B:41:THR:O	1:B:44:CYS:HB2	1.92	0.69
1:A:26:GLY:HA3	1:A:42:ASP:OD1	1.92	0.69
1:A:47:VAL:O	1:A:51:CYS:N	2.21	0.69
1:K:35:GLY:N	1:K:130:SER:HA	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:44:CYS:HB3	2:L:134:ELD:H181	1.75	0.69
1:K:27:CYS:O	1:K:33:GLY:HA2	1.92	0.68
1:K:91:CYS:C	1:K:93:ARG:H	1.95	0.68
1:L:54:ARG:CZ	1:L:54:ARG:HA	2.23	0.68
1:K:67:ASN:O	1:K:71:ALA:N	2.27	0.68
1:K:71:ALA:O	1:K:72:ILE:HG13	1.93	0.68
1:K:124:SER:O	1:K:127:ARG:HG2	1.93	0.68
1:A:102:ALA:O	1:A:105:CYS:HB3	1.93	0.68
1:K:91:CYS:O	1:K:93:ARG:N	2.25	0.68
1:L:19:VAL:HG13	1:L:20:TRP:N	2.08	0.68
1:A:28:TYR:HE2	1:A:34:GLN:N	1.92	0.68
1:B:29:CYS:SG	1:B:42:ASP:HA	2.34	0.68
1:B:122:SER:O	1:B:125:ARG:N	2.27	0.67
1:B:5:PHE:CE1	1:B:99:ASP:HA	2.30	0.67
1:A:3:PHE:CE2	1:B:32:GLY:HA2	2.29	0.67
1:B:24:SER:HB3	1:B:119:PHE:CD1	2.29	0.67
1:A:126:CYS:O	1:A:128:GLN:N	2.29	0.66
1:A:82:ILE:HG22	1:A:100:ARG:HG3	1.76	0.66
1:B:48:HIS:CG	2:B:134:ELD:H161	2.29	0.66
1:B:47:VAL:HG12	1:B:48:HIS:N	2.10	0.66
1:A:28:TYR:HE2	1:A:33:GLY:C	1.99	0.66
1:K:114:ASN:C	1:K:116:ASN:H	1.97	0.66
1:K:71:ALA:C	1:K:72:ILE:HG13	2.16	0.66
1:L:26:GLY:HA3	1:L:42:ASP:CG	2.16	0.66
1:K:51:CYS:HA	1:K:54:ARG:HE	1.61	0.65
1:K:103:ALA:O	1:K:106:PHE:HB2	1.96	0.65
1:K:69:LYS:HG3	1:K:70:LEU:HD13	1.78	0.65
1:L:91:CYS:SG	1:L:92:LEU:HG	2.37	0.65
1:A:19:VAL:HG13	1:A:20:TRP:H	1.60	0.65
1:K:11:GLY:HA3	1:K:77:PHE:CZ	2.32	0.65
1:K:1:ASN:ND2	1:K:4:GLN:HG3	2.11	0.65
1:L:101:VAL:CA	1:L:104:ASN:HB2	2.26	0.64
1:K:102:ALA:O	1:K:105:CYS:HB3	1.97	0.64
1:K:70:LEU:HD11	1:L:49:ASP:HB3	1.79	0.64
1:K:3:PHE:HE1	1:L:32:GLY:HA2	1.63	0.64
1:B:121:SER:O	1:B:125:ARG:HB2	1.98	0.64
1:A:1:ASN:CG	1:A:4:GLN:HG3	2.17	0.64
1:B:25:TYR:O	1:B:26:GLY:O	2.16	0.64
1:K:24:SER:O	1:K:25:TYR:HB2	1.98	0.64
1:K:10:ASN:HD21	1:K:19:VAL:CG1	2.12	0.63
1:A:8:MET:HE3	1:A:99:ASP:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PHE:HB2	1:B:99:ASP:OD2	1.99	0.63
1:A:38:LYS:HB3	1:A:117:TYR:CE1	2.34	0.63
1:L:29:CYS:SG	1:L:42:ASP:HA	2.39	0.63
1:L:77:PHE:HD2	1:L:81:ASN:O	1.82	0.63
1:A:82:ILE:CG2	1:A:100:ARG:HG3	2.29	0.63
1:A:25:TYR:HA	1:A:118:LYS:HA	1.81	0.62
1:L:10:ASN:HB3	1:L:16:ALA:HA	1.81	0.62
1:K:67:ASN:CG	1:K:70:LEU:HD22	2.19	0.62
1:L:46:PHE:CE1	1:L:50:CYS:SG	2.93	0.62
1:L:88:ASN:ND2	1:L:90:GLY:H	1.97	0.62
1:K:10:ASN:HA	1:K:14:GLY:O	1.99	0.62
1:K:37:PRO:O	1:K:39:ASP:N	2.32	0.62
1:L:67:ASN:O	1:L:71:ALA:N	2.33	0.62
1:L:47:VAL:O	1:L:48:HIS:C	2.38	0.62
1:A:28:TYR:HD1	1:A:46:PHE:HB2	1.65	0.62
1:A:3:PHE:CD2	1:B:32:GLY:HA2	2.35	0.62
1:B:105:CYS:O	1:B:108:GLN:HB2	2.00	0.62
1:B:26:GLY:HA3	1:B:42:ASP:CG	2.20	0.61
1:L:98:CYS:O	1:L:102:ALA:CB	2.48	0.61
1:B:122:SER:O	1:B:126:CYS:N	2.32	0.61
1:L:56:ARG:HA	1:L:56:ARG:HE	1.65	0.61
1:K:52:TYR:O	1:K:55:VAL:HG13	2.00	0.61
1:A:100:ARG:NH2	1:A:101:VAL:HG22	2.15	0.61
1:A:19:VAL:O	1:A:21:ASN:N	2.34	0.60
1:B:67:ASN:O	1:B:71:ALA:HB2	2.00	0.60
1:B:67:ASN:ND2	1:B:70:LEU:HD12	2.17	0.60
1:K:97:GLU:O	1:K:101:VAL:HG23	2.01	0.60
1:A:5:PHE:CD1	1:A:99:ASP:HB3	2.35	0.60
1:L:61:CYS:SG	1:L:95:ILE:HD12	2.42	0.60
1:B:122:SER:C	1:B:125:ARG:H	2.04	0.60
1:B:41:THR:HG22	1:B:109:ASN:HB2	1.82	0.60
1:L:36:THR:CG2	1:L:37:PRO:HD2	2.31	0.60
1:A:88:ASN:CG	1:A:93:ARG:HA	2.22	0.60
1:A:126:CYS:O	1:A:127:ARG:C	2.40	0.60
1:A:70:LEU:HD13	1:B:49:ASP:HB3	1.83	0.59
1:K:74:SER:O	1:K:75:TYR:HB3	2.02	0.59
1:B:39:ASP:O	1:B:43:ARG:N	2.35	0.59
1:B:16:ALA:O	1:B:17:PHE:CB	2.50	0.59
1:L:5:PHE:CD1	1:L:99:ASP:HA	2.36	0.59
1:L:6:ALA:O	1:L:9:ILE:N	2.35	0.59
1:A:2:LEU:O	1:A:5:PHE:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:16:ALA:O	1:L:17:PHE:HB2	2.02	0.59
1:L:51:CYS:O	1:L:55:VAL:HG23	2.01	0.59
1:K:17:PHE:CD2	1:K:20:TRP:HD1	2.21	0.59
1:L:126:CYS:HA	1:L:128:GLN:OE1	2.03	0.59
1:L:67:ASN:OD1	1:L:67:ASN:C	2.40	0.58
1:B:1:ASN:N	1:B:4:GLN:OE1	2.35	0.58
1:L:128:GLN:H	1:L:128:GLN:NE2	2.00	0.58
1:A:16:ALA:C	1:A:18:SER:H	2.07	0.58
1:K:2:LEU:CD1	1:L:31:TRP:HA	2.27	0.58
1:B:101:VAL:O	1:B:105:CYS:N	2.33	0.58
1:B:129:THR:HG22	1:B:130:SER:O	2.03	0.58
1:B:18:SER:O	1:B:22:TYR:HD2	1.87	0.58
1:A:118:LYS:O	1:A:119:PHE:HB2	2.04	0.58
1:B:91:CYS:SG	1:B:92:LEU:HD12	2.44	0.58
1:K:77:PHE:CE2	1:K:82:ILE:HG23	2.38	0.58
1:L:1:ASN:O	1:L:5:PHE:N	2.30	0.58
1:A:8:MET:HE3	1:A:99:ASP:CB	2.34	0.57
1:B:45:CYS:HA	2:B:134:ELD:C17	2.34	0.57
1:L:114:ASN:HD22	1:L:116:ASN:CB	2.04	0.57
1:A:1:ASN:OD1	1:A:3:PHE:HB2	2.04	0.57
1:A:94:ASP:O	1:A:97:GLU:N	2.37	0.57
1:B:45:CYS:O	1:B:46:PHE:C	2.43	0.57
1:L:56:ARG:HA	1:L:56:ARG:NE	2.20	0.57
1:B:8:MET:SD	1:B:100:ARG:N	2.78	0.57
1:B:8:MET:SD	1:B:99:ASP:CB	2.91	0.57
1:K:114:ASN:O	1:K:116:ASN:N	2.37	0.57
1:K:78:LYS:C	1:K:80:GLY:H	2.07	0.57
1:K:110:LYS:O	1:K:113:TYR:HB2	2.04	0.57
1:A:46:PHE:O	1:A:49:ASP:HB2	2.05	0.57
1:B:114:ASN:O	1:B:117:TYR:HB2	2.04	0.56
1:B:23:ILE:HG23	1:B:24:SER:N	2.20	0.56
1:A:23:ILE:HG12	1:B:23:ILE:CD1	2.35	0.56
1:A:49:ASP:HB3	1:B:70:LEU:HD11	1.87	0.56
1:L:98:CYS:O	1:L:102:ALA:HB3	2.06	0.56
1:B:69:LYS:NZ	2:B:134:ELD:H22	2.20	0.55
1:K:111:ASN:O	1:K:113:TYR:N	2.36	0.55
1:L:92:LEU:O	1:L:93:ARG:C	2.43	0.55
1:B:18:SER:O	1:B:22:TYR:CD2	2.59	0.55
1:A:45:CYS:O	1:A:48:HIS:N	2.38	0.55
1:L:100:ARG:O	1:L:104:ASN:N	2.27	0.55
1:K:6:ALA:O	1:K:9:ILE:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:128:GLN:CD	1:L:128:GLN:N	2.59	0.55
1:L:25:TYR:C	1:L:29:CYS:HB2	2.26	0.55
1:K:29:CYS:HA	2:L:134:ELD:O2	2.06	0.55
1:K:68:PRO:HG3	1:K:95:ILE:HD11	1.87	0.55
1:A:71:ALA:C	1:A:72:ILE:HG13	2.27	0.55
1:K:1:ASN:C	1:K:3:PHE:N	2.60	0.55
1:K:130:SER:O	1:K:131:GLU:HB3	2.06	0.55
1:B:122:SER:C	1:B:125:ARG:N	2.60	0.55
1:A:4:GLN:HE22	1:A:73:TYR:N	2.05	0.55
1:K:3:PHE:CE2	1:L:122:SER:HA	2.42	0.55
1:K:1:ASN:N	1:K:1:ASN:HD22	2.04	0.54
1:L:45:CYS:O	1:L:48:HIS:HB3	2.07	0.54
1:B:132:GLN:HG2	1:B:133:CYS:O	2.07	0.54
1:A:47:VAL:O	1:A:50:CYS:N	2.41	0.54
1:B:34:GLN:HG2	1:B:126:CYS:HB2	1.90	0.54
1:B:117:TYR:CA	1:B:120:LEU:HD21	2.38	0.54
1:L:20:TRP:HE3	1:L:23:ILE:HG13	1.73	0.54
1:A:8:MET:SD	1:A:100:ARG:HA	2.48	0.54
1:K:69:LYS:HG2	1:L:49:ASP:CG	2.29	0.54
1:K:105:CYS:O	1:K:109:ASN:OD1	2.25	0.54
1:L:103:ALA:HA	1:L:106:PHE:CD2	2.43	0.54
1:L:46:PHE:O	1:L:47:VAL:C	2.45	0.54
1:A:23:ILE:CG2	1:A:24:SER:N	2.71	0.53
1:B:106:PHE:CZ	2:B:134:ELD:H171	2.44	0.53
1:B:67:ASN:OD1	1:B:70:LEU:N	2.37	0.53
1:A:10:ASN:HA	1:A:14:GLY:O	2.08	0.53
1:A:70:LEU:CD1	1:B:49:ASP:HB3	2.39	0.53
1:L:121:SER:O	1:L:122:SER:C	2.44	0.53
1:L:18:SER:O	1:L:19:VAL:C	2.46	0.53
1:B:99:ASP:O	1:B:103:ALA:N	2.41	0.53
1:A:97:GLU:O	1:A:100:ARG:HB3	2.08	0.53
1:K:97:GLU:HA	1:K:100:ARG:NH1	2.24	0.53
1:K:1:ASN:O	1:K:3:PHE:N	2.42	0.53
1:L:82:ILE:CG2	1:L:100:ARG:HG3	2.38	0.53
1:L:48:HIS:O	1:L:51:CYS:CB	2.55	0.53
1:L:96:CYS:O	1:L:100:ARG:N	2.35	0.53
1:A:48:HIS:HB3	2:B:134:ELD:N1	2.24	0.52
1:K:94:ASP:O	1:K:97:GLU:HB2	2.09	0.52
1:B:24:SER:HB3	1:B:119:PHE:HD1	1.73	0.52
1:A:101:VAL:O	1:A:105:CYS:N	2.28	0.52
1:B:67:ASN:OD1	1:B:67:ASN:C	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:CYS:HB3	1:B:34:GLN:O	2.08	0.52
1:L:88:ASN:HD22	1:L:93:ARG:HB2	1.74	0.52
1:L:94:ASP:O	1:L:97:GLU:N	2.43	0.52
1:L:96:CYS:O	1:L:99:ASP:HB2	2.10	0.52
1:K:3:PHE:CD1	1:L:32:GLY:HA2	2.44	0.52
1:L:48:HIS:O	1:L:52:TYR:N	2.41	0.52
1:B:25:TYR:CD1	1:B:26:GLY:N	2.71	0.52
1:L:20:TRP:O	1:L:23:ILE:HG12	2.10	0.52
1:A:47:VAL:HA	1:A:50:CYS:HB2	1.92	0.52
1:A:23:ILE:HD12	1:B:31:TRP:NE1	2.25	0.52
1:A:28:TYR:CE2	1:A:33:GLY:C	2.83	0.52
1:K:45:CYS:SG	1:K:106:PHE:HZ	2.33	0.52
1:A:22:TYR:OH	1:A:106:PHE:HB3	2.09	0.52
1:A:32:GLY:HA2	1:B:3:PHE:CG	2.46	0.51
1:B:22:TYR:CD2	1:B:22:TYR:N	2.78	0.51
1:A:45:CYS:O	1:A:46:PHE:C	2.47	0.51
1:B:98:CYS:O	1:B:102:ALA:N	2.38	0.51
1:K:73:TYR:HA	1:K:92:LEU:HD11	1.91	0.51
1:A:38:LYS:HB3	1:A:117:TYR:HE1	1.75	0.51
1:B:9:ILE:HG22	1:B:10:ASN:N	2.24	0.51
1:K:122:SER:HA	1:L:3:PHE:CZ	2.45	0.51
1:L:122:SER:O	1:L:124:SER:C	2.48	0.51
1:A:13:LEU:O	1:A:18:SER:HB3	2.09	0.51
1:L:3:PHE:O	1:L:7:LYS:HG3	2.11	0.51
1:A:77:PHE:O	1:A:79:LYS:N	2.43	0.51
1:K:54:ARG:O	1:K:55:VAL:C	2.49	0.51
1:K:111:ASN:C	1:K:113:TYR:H	2.14	0.51
1:K:45:CYS:SG	1:K:106:PHE:CZ	3.04	0.51
1:L:10:ASN:OD1	1:L:19:VAL:HG12	2.11	0.50
1:B:102:ALA:O	1:B:103:ALA:C	2.48	0.50
1:B:6:ALA:O	1:B:9:ILE:HB	2.11	0.50
1:K:1:ASN:O	1:K:4:GLN:N	2.44	0.50
1:K:46:PHE:O	1:K:49:ASP:HB2	2.11	0.50
1:L:4:GLN:NE2	1:L:75:TYR:HE1	2.09	0.50
1:A:55:VAL:CG1	1:A:56:ARG:N	2.74	0.50
1:A:49:ASP:CG	2:B:134:ELD:HN12	2.15	0.50
1:K:114:ASN:C	1:K:116:ASN:N	2.64	0.50
1:K:78:LYS:O	1:K:80:GLY:N	2.43	0.50
1:A:1:ASN:ND2	1:A:4:GLN:HG3	2.27	0.50
1:A:10:ASN:O	1:A:14:GLY:O	2.29	0.50
1:A:25:TYR:HD2	1:A:118:LYS:CG	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:HIS:NE2	1:L:52:TYR:CZ	2.80	0.50
1:K:35:GLY:CA	1:K:130:SER:HA	2.41	0.50
1:B:34:GLN:HG3	1:B:35:GLY:N	2.26	0.50
1:A:67:ASN:OD1	1:A:69:LYS:HB3	2.11	0.50
1:B:46:PHE:O	1:B:47:VAL:C	2.50	0.50
1:A:67:ASN:O	1:A:71:ALA:N	2.45	0.50
1:B:117:TYR:HA	1:B:120:LEU:HD21	1.94	0.50
1:A:101:VAL:O	1:A:102:ALA:C	2.50	0.50
1:B:5:PHE:O	1:B:9:ILE:HG13	2.11	0.50
1:K:1:ASN:ND2	1:K:4:GLN:H	2.10	0.50
1:K:2:LEU:HB3	1:L:31:TRP:CE3	2.47	0.50
1:K:91:CYS:C	1:K:93:ARG:N	2.64	0.50
1:L:24:SER:OG	1:L:119:PHE:HA	2.12	0.49
1:B:25:TYR:CD1	1:B:42:ASP:HB2	2.46	0.49
1:A:5:PHE:O	1:A:8:MET:HB2	2.13	0.49
1:L:5:PHE:CE1	1:L:48:HIS:CD2	3.00	0.49
1:A:95:ILE:O	1:A:98:CYS:HB2	2.12	0.49
1:K:1:ASN:N	1:K:1:ASN:ND2	2.60	0.49
1:K:18:SER:O	1:K:21:ASN:N	2.40	0.49
1:L:30:GLY:H	2:L:134:ELD:H122	1.78	0.49
1:L:6:ALA:O	1:L:7:LYS:C	2.49	0.49
1:B:82:ILE:HD12	1:B:104:ASN:ND2	2.28	0.49
1:B:97:GLU:O	1:B:101:VAL:HG23	2.12	0.49
1:A:23:ILE:O	1:A:30:GLY:HA2	2.12	0.49
1:A:49:ASP:OD2	1:B:69:LYS:NZ	2.44	0.49
1:K:3:PHE:HE2	1:L:122:SER:HA	1.78	0.49
1:B:39:ASP:OD2	1:B:40:ALA:N	2.46	0.49
1:B:4:GLN:O	1:B:7:LYS:N	2.46	0.49
1:A:23:ILE:HG22	1:A:24:SER:N	2.27	0.49
1:A:19:VAL:HG13	1:A:20:TRP:N	2.27	0.49
1:A:25:TYR:CD1	1:A:25:TYR:C	2.86	0.48
1:L:39:ASP:C	1:L:39:ASP:OD2	2.52	0.48
1:B:115:LYS:C	1:B:117:TYR:H	2.16	0.48
1:L:40:ALA:O	1:L:43:ARG:HB2	2.13	0.48
1:A:94:ASP:O	1:A:95:ILE:C	2.50	0.48
1:A:2:LEU:O	1:A:6:ALA:N	2.30	0.48
1:A:4:GLN:NE2	1:A:73:TYR:O	2.47	0.48
1:L:102:ALA:O	1:L:105:CYS:HB3	2.13	0.48
1:L:73:TYR:HB3	1:L:92:LEU:HD22	1.95	0.48
1:A:1:ASN:O	1:A:2:LEU:C	2.49	0.48
1:L:19:VAL:HG22	1:L:23:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LYS:HD2	1:B:69:LYS:O	2.14	0.48
1:K:2:LEU:HB2	1:L:31:TRP:CA	2.43	0.48
1:K:16:ALA:C	1:K:18:SER:H	2.15	0.48
1:A:92:LEU:O	1:A:93:ARG:C	2.51	0.48
1:K:24:SER:O	1:K:25:TYR:CB	2.62	0.48
1:K:42:ASP:O	1:K:45:CYS:HB2	2.14	0.48
1:L:45:CYS:HA	2:L:134:ELD:H151	1.96	0.48
1:L:4:GLN:HA	1:L:7:LYS:HG3	1.95	0.48
1:L:115:LYS:HA	1:L:118:LYS:HG3	1.96	0.48
1:B:121:SER:O	1:B:125:ARG:N	2.41	0.48
1:A:3:PHE:O	1:A:6:ALA:HB3	2.14	0.48
1:B:36:THR:CG2	1:B:131:GLU:HB2	2.44	0.48
1:K:41:THR:O	1:K:44:CYS:HB2	2.13	0.48
1:B:101:VAL:O	1:B:104:ASN:HB2	2.12	0.47
1:B:9:ILE:HG12	1:B:106:PHE:HE2	1.79	0.47
1:L:3:PHE:O	1:L:7:LYS:CG	2.62	0.47
1:A:19:VAL:C	1:A:21:ASN:N	2.67	0.47
1:A:110:LYS:O	1:A:113:TYR:HB2	2.14	0.47
1:A:85:GLY:O	1:A:86:LYS:C	2.51	0.47
1:K:95:ILE:O	1:K:96:CYS:C	2.51	0.47
1:L:52:TYR:CD2	1:L:68:PRO:HB3	2.49	0.47
1:A:25:TYR:CD2	1:A:118:LYS:HG2	2.42	0.47
1:A:1:ASN:N	1:A:4:GLN:OE1	2.46	0.47
1:L:97:GLU:O	1:L:98:CYS:C	2.51	0.47
1:A:1:ASN:OD1	1:A:4:GLN:HG3	2.14	0.47
1:L:6:ALA:C	1:L:8:MET:N	2.66	0.47
1:A:73:TYR:HB3	1:A:92:LEU:HB3	1.97	0.47
1:A:78:LYS:O	1:A:80:GLY:N	2.41	0.47
1:K:70:LEU:HD11	1:L:49:ASP:CB	2.45	0.47
1:A:121:SER:HB3	1:A:124:SER:HB3	1.96	0.47
1:A:118:LYS:O	1:A:119:PHE:CB	2.62	0.47
1:B:100:ARG:O	1:B:101:VAL:C	2.53	0.47
1:A:3:PHE:O	1:A:4:GLN:C	2.53	0.46
1:K:20:TRP:C	1:K:22:TYR:N	2.67	0.46
1:L:107:HIS:O	1:L:110:LYS:HG2	2.15	0.46
1:B:9:ILE:HG12	1:B:106:PHE:CE2	2.50	0.46
1:L:106:PHE:CE2	2:L:134:ELD:H183	2.49	0.46
1:L:106:PHE:CD2	2:L:134:ELD:H183	2.51	0.46
1:A:23:ILE:CG1	1:B:23:ILE:HD11	2.41	0.46
1:A:25:TYR:O	1:A:29:CYS:CB	2.44	0.46
1:L:19:VAL:HA	1:L:22:TYR:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:O	1:A:48:HIS:C	2.54	0.46
1:B:91:CYS:HA	1:B:94:ASP:OD1	2.16	0.46
1:B:121:SER:O	1:B:125:ARG:CB	2.64	0.46
1:L:102:ALA:O	1:L:105:CYS:CB	2.64	0.46
1:L:118:LYS:HB3	1:L:119:PHE:CE2	2.49	0.46
1:B:1:ASN:OD1	1:B:2:LEU:N	2.48	0.46
1:A:31:TRP:CZ2	2:B:134:ELD:H121	2.51	0.46
1:K:5:PHE:O	1:K:8:MET:HB3	2.16	0.46
1:L:31:TRP:CE2	2:L:134:ELD:H62	2.51	0.46
1:L:46:PHE:HE1	1:L:50:CYS:SG	2.35	0.46
1:B:26:GLY:HA3	1:B:42:ASP:OD1	2.16	0.46
1:B:104:ASN:C	1:B:106:PHE:N	2.69	0.46
1:B:97:GLU:HA	1:B:97:GLU:OE1	2.13	0.46
1:B:20:TRP:CE3	1:B:20:TRP:HA	2.52	0.46
1:A:19:VAL:C	1:A:21:ASN:H	2.18	0.46
1:A:69:LYS:HG3	1:A:70:LEU:CD1	2.37	0.45
1:B:41:THR:CG2	1:B:109:ASN:HB2	2.45	0.45
1:B:9:ILE:O	1:B:10:ASN:C	2.54	0.45
1:K:24:SER:HB3	1:K:119:PHE:CD1	2.51	0.45
1:L:94:ASP:O	1:L:95:ILE:C	2.54	0.45
1:L:26:GLY:HA3	1:L:42:ASP:OD1	2.16	0.45
1:A:1:ASN:OD1	1:A:4:GLN:N	2.42	0.45
1:A:27:CYS:O	1:A:28:TYR:CD2	2.68	0.45
1:B:47:VAL:O	1:B:48:HIS:C	2.53	0.45
1:A:23:ILE:O	1:A:30:GLY:CA	2.64	0.45
1:L:10:ASN:HD21	1:L:19:VAL:CG1	2.29	0.45
1:K:75:TYR:N	1:K:75:TYR:CD1	2.85	0.45
1:A:2:LEU:HB2	1:B:32:GLY:H	1.82	0.45
1:A:91:CYS:O	1:A:94:ASP:N	2.49	0.45
1:K:67:ASN:ND2	1:K:70:LEU:CD2	2.79	0.45
1:B:99:ASP:O	1:B:100:ARG:C	2.53	0.45
1:K:94:ASP:HA	1:K:97:GLU:HG2	1.99	0.45
1:B:25:TYR:HD1	1:B:42:ASP:HB2	1.80	0.45
1:B:47:VAL:O	1:B:49:ASP:N	2.50	0.45
1:L:30:GLY:H	2:L:134:ELD:C12	2.30	0.45
1:K:31:TRP:CH2	2:L:134:ELD:H121	2.52	0.45
1:K:32:GLY:H	1:L:2:LEU:HB2	1.81	0.45
1:K:50:CYS:O	1:K:54:ARG:HG3	2.17	0.45
1:B:4:GLN:O	1:B:5:PHE:C	2.55	0.45
1:K:5:PHE:O	1:K:5:PHE:CD1	2.70	0.45
1:A:46:PHE:O	1:A:49:ASP:N	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:VAL:O	1:B:102:ALA:C	2.55	0.45
1:K:2:LEU:HB2	1:L:31:TRP:O	2.17	0.45
1:A:28:TYR:OH	1:A:130:SER:HA	2.16	0.44
1:L:47:VAL:O	1:L:50:CYS:N	2.50	0.44
1:L:8:MET:SD	1:L:99:ASP:HB3	2.57	0.44
1:K:36:THR:HA	1:K:37:PRO:HD3	1.70	0.44
1:A:97:GLU:CD	1:A:100:ARG:HE	2.19	0.44
1:L:68:PRO:O	1:L:69:LYS:C	2.53	0.44
1:A:121:SER:C	1:A:124:SER:N	2.69	0.44
1:B:1:ASN:OD1	1:B:3:PHE:N	2.47	0.44
1:L:111:ASN:C	1:L:113:TYR:H	2.21	0.44
1:L:19:VAL:CG1	1:L:20:TRP:H	2.26	0.44
1:A:27:CYS:O	1:A:28:TYR:HD2	2.00	0.44
1:B:4:GLN:O	1:B:6:ALA:N	2.51	0.44
1:K:25:TYR:HE2	1:K:114:ASN:O	2.01	0.44
1:L:113:TYR:C	1:L:113:TYR:CD1	2.91	0.44
1:A:94:ASP:O	1:A:96:CYS:N	2.51	0.44
1:B:104:ASN:O	1:B:105:CYS:C	2.53	0.44
1:K:1:ASN:O	1:K:1:ASN:ND2	2.48	0.44
1:B:46:PHE:O	1:B:49:ASP:HB2	2.18	0.44
1:A:52:TYR:CE2	1:A:68:PRO:HB2	2.52	0.44
1:B:13:LEU:HB3	1:B:18:SER:CB	2.48	0.44
1:A:2:LEU:O	1:A:3:PHE:C	2.56	0.44
1:L:124:SER:O	1:L:126:CYS:N	2.51	0.44
1:B:102:ALA:O	1:B:104:ASN:N	2.51	0.44
1:K:2:LEU:HD23	1:K:2:LEU:N	2.32	0.44
1:L:14:GLY:O	1:L:16:ALA:O	2.36	0.43
1:L:19:VAL:CG1	1:L:20:TRP:N	2.79	0.43
1:K:48:HIS:HE1	1:K:99:ASP:OD2	2.01	0.43
1:B:23:ILE:CG2	1:B:24:SER:N	2.81	0.43
1:A:43:ARG:O	1:A:44:CYS:C	2.55	0.43
1:L:26:GLY:HA3	1:L:42:ASP:HB2	1.99	0.43
1:K:95:ILE:O	1:K:98:CYS:N	2.52	0.43
1:A:131:GLU:HG3	1:A:132:GLN:N	2.25	0.43
1:A:121:SER:C	1:A:124:SER:H	2.21	0.43
1:K:37:PRO:C	1:K:39:ASP:N	2.72	0.43
1:B:94:ASP:N	1:B:94:ASP:OD2	2.51	0.43
1:K:1:ASN:C	1:K:3:PHE:H	2.21	0.43
1:L:45:CYS:HA	2:L:134:ELD:H172	2.00	0.43
1:L:26:GLY:HA3	1:L:42:ASP:CB	2.48	0.43
1:B:34:GLN:HG3	1:B:126:CYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PHE:CD1	1:B:99:ASP:HA	2.52	0.43
1:L:75:TYR:CD2	1:L:76:SER:N	2.87	0.43
1:B:113:TYR:CD1	1:B:113:TYR:C	2.91	0.43
1:B:77:PHE:HA	1:B:81:ASN:O	2.19	0.43
1:L:117:TYR:O	1:L:120:LEU:HG	2.19	0.43
1:A:28:TYR:CD1	1:A:46:PHE:HB2	2.48	0.43
1:B:5:PHE:CE1	1:B:102:ALA:HB3	2.54	0.43
1:K:93:ARG:O	1:K:96:CYS:N	2.52	0.43
1:L:85:GLY:O	1:L:88:ASN:N	2.52	0.43
1:L:61:CYS:SG	1:L:92:LEU:HD23	2.59	0.43
1:B:36:THR:HG23	1:B:131:GLU:HB2	2.01	0.43
1:B:68:PRO:C	1:B:70:LEU:N	2.72	0.43
1:K:111:ASN:C	1:K:113:TYR:N	2.73	0.43
1:B:121:SER:O	1:B:122:SER:C	2.56	0.43
1:K:34:GLN:O	1:K:126:CYS:HB3	2.19	0.43
1:K:43:ARG:O	1:K:44:CYS:C	2.55	0.43
1:B:50:CYS:O	1:B:53:GLY:N	2.52	0.42
1:B:91:CYS:O	1:B:94:ASP:HB2	2.19	0.42
1:B:95:ILE:C	1:B:97:GLU:N	2.72	0.42
1:B:115:LYS:C	1:B:117:TYR:N	2.73	0.42
1:B:13:LEU:HB3	1:B:18:SER:OG	2.19	0.42
1:B:101:VAL:O	1:B:104:ASN:N	2.52	0.42
1:K:43:ARG:O	1:K:46:PHE:HB3	2.19	0.42
1:L:104:ASN:HD22	1:L:104:ASN:HA	1.62	0.42
1:L:126:CYS:HA	1:L:128:GLN:HE22	1.84	0.42
1:K:18:SER:O	1:K:19:VAL:C	2.58	0.42
1:A:91:CYS:O	1:A:92:LEU:C	2.57	0.42
1:B:67:ASN:HA	1:B:68:PRO:HD3	1.81	0.42
1:L:31:TRP:O	1:L:32:GLY:O	2.36	0.42
1:B:29:CYS:O	1:B:30:GLY:C	2.58	0.42
1:B:34:GLN:CG	1:B:126:CYS:HB2	2.49	0.42
1:A:7:LYS:HA	1:A:10:ASN:HD22	1.83	0.42
1:L:35:GLY:CA	1:L:128:GLN:OE1	2.67	0.42
1:A:119:PHE:O	1:A:120:LEU:HD23	2.20	0.42
1:B:79:LYS:O	1:B:81:ASN:N	2.53	0.42
1:A:49:ASP:CG	1:B:69:LYS:NZ	2.73	0.42
1:B:106:PHE:CE1	2:B:134:ELD:H171	2.55	0.42
1:K:68:PRO:O	1:K:69:LYS:C	2.57	0.42
1:A:44:CYS:SG	1:A:105:CYS:O	2.77	0.42
1:A:40:ALA:O	1:A:43:ARG:N	2.53	0.42
1:L:45:CYS:HA	2:L:134:ELD:C15	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:46:PHE:O	1:L:49:ASP:HB2	2.20	0.42
1:L:95:ILE:HG22	1:L:96:CYS:N	2.34	0.42
1:A:88:ASN:HB3	1:A:93:ARG:HB2	2.02	0.41
1:K:70:LEU:N	1:K:70:LEU:HD13	2.35	0.41
1:L:101:VAL:HA	1:L:104:ASN:CB	2.38	0.41
1:K:8:MET:O	1:K:9:ILE:C	2.59	0.41
1:A:80:GLY:O	1:A:81:ASN:ND2	2.53	0.41
1:B:67:ASN:O	1:B:71:ALA:N	2.53	0.41
1:L:105:CYS:O	1:L:106:PHE:C	2.59	0.41
1:A:112:THR:O	1:A:112:THR:HG22	2.20	0.41
1:B:61:CYS:O	1:B:68:PRO:HD3	2.20	0.41
1:K:100:ARG:NH2	1:K:101:VAL:CG2	2.75	0.41
1:K:68:PRO:HG3	1:K:95:ILE:CD1	2.50	0.41
1:K:52:TYR:O	1:K:55:VAL:CG1	2.67	0.41
1:B:125:ARG:HD2	1:B:125:ARG:HA	1.88	0.41
1:A:124:SER:HB2	1:A:127:ARG:CZ	2.50	0.41
1:B:99:ASP:O	1:B:100:ARG:O	2.38	0.41
1:K:26:GLY:HA3	1:K:42:ASP:HB2	2.03	0.41
1:L:45:CYS:SG	2:L:134:ELD:H131	2.60	0.41
1:L:5:PHE:CE1	1:L:48:HIS:HD2	2.38	0.41
1:B:115:LYS:O	1:B:117:TYR:N	2.53	0.41
1:K:5:PHE:O	1:K:5:PHE:HD1	2.04	0.41
1:A:8:MET:HB3	1:A:82:ILE:HD11	2.01	0.41
1:A:78:LYS:C	1:A:80:GLY:H	2.24	0.41
1:A:52:TYR:CE1	1:A:68:PRO:HB3	2.55	0.41
1:A:4:GLN:HE22	1:A:72:ILE:C	2.24	0.41
1:K:101:VAL:O	1:K:102:ALA:C	2.59	0.41
1:L:98:CYS:O	1:L:102:ALA:N	2.48	0.41
1:A:16:ALA:C	1:A:18:SER:N	2.73	0.41
1:B:69:LYS:HZ1	2:B:134:ELD:H22	1.86	0.41
1:L:102:ALA:O	2:L:134:ELD:H182	2.20	0.41
1:K:16:ALA:C	1:K:18:SER:N	2.73	0.41
1:K:10:ASN:HD21	1:K:19:VAL:HB	1.86	0.41
1:A:12:LYS:HB3	1:A:13:LEU:HD12	2.03	0.41
1:B:46:PHE:CZ	1:B:131:GLU:O	2.74	0.41
1:B:92:LEU:N	1:B:92:LEU:HD12	2.36	0.41
1:K:116:ASN:C	1:K:118:LYS:H	2.24	0.41
1:A:88:ASN:CB	1:A:93:ARG:HB2	2.51	0.41
1:A:5:PHE:O	1:A:6:ALA:C	2.58	0.41
1:B:105:CYS:O	1:B:109:ASN:OD1	2.37	0.41
1:K:2:LEU:HB2	1:L:31:TRP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:106:PHE:CZ	2:L:134:ELD:H162	2.56	0.41
1:K:19:VAL:HG13	1:K:20:TRP:N	2.35	0.41
1:K:13:LEU:HD12	1:K:13:LEU:N	2.36	0.41
1:L:10:ASN:O	1:L:14:GLY:N	2.53	0.41
1:B:98:CYS:O	1:B:99:ASP:C	2.59	0.41
1:L:39:ASP:OD2	1:L:41:THR:N	2.54	0.41
1:L:2:LEU:HA	1:L:5:PHE:HB3	2.03	0.41
1:A:52:TYR:CZ	1:A:68:PRO:HB3	2.56	0.41
1:K:4:GLN:NE2	1:K:73:TYR:CD1	2.89	0.40
1:K:67:ASN:HD22	1:L:53:GLY:HA3	1.86	0.40
1:A:44:CYS:SG	1:A:105:CYS:C	3.00	0.40
1:K:109:ASN:O	1:K:110:LYS:C	2.59	0.40
1:L:5:PHE:CZ	1:L:48:HIS:CD2	3.08	0.40
1:L:72:ILE:HG23	1:L:72:ILE:O	2.22	0.40
1:A:101:VAL:C	1:A:103:ALA:N	2.74	0.40
1:B:104:ASN:HA	1:B:104:ASN:HD22	1.68	0.40
1:B:8:MET:SD	1:B:99:ASP:C	2.99	0.40
1:K:72:ILE:C	1:K:92:LEU:HD11	2.42	0.40
1:L:20:TRP:C	1:L:23:ILE:HG12	2.41	0.40
1:A:31:TRP:N	1:A:31:TRP:CD1	2.90	0.40
1:K:44:CYS:SG	1:K:105:CYS:C	3.00	0.40
1:L:44:CYS:HB3	2:L:134:ELD:C18	2.49	0.40
1:L:82:ILE:HG22	1:L:83:VAL:N	2.37	0.40
1:B:68:PRO:HA	1:B:71:ALA:HB3	2.03	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	120/122 (98%)	72 (60%)	33 (28%)	15 (12%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	120/122 (98%)	69 (58%)	33 (28%)	18 (15%)	0 1
1	K	120/122 (98%)	70 (58%)	34 (28%)	16 (13%)	0 2
1	L	120/122 (98%)	66 (55%)	35 (29%)	19 (16%)	0 1
All	All	480/488 (98%)	277 (58%)	135 (28%)	68 (14%)	0 1

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PHE
1	A	55	VAL
1	A	127	ARG
1	B	16	ALA
1	B	17	PHE
1	B	26	GLY
1	B	47	VAL
1	K	25	TYR
1	K	92	LEU
1	K	115	LYS
1	L	16	ALA
1	L	19	VAL
1	L	76	SER
1	L	86	LYS
1	L	100	ARG
1	A	20	TRP
1	A	45	CYS
1	A	79	LYS
1	A	86	LYS
1	A	95	ILE
1	B	100	ARG
1	B	102	ALA
1	B	124	SER
1	K	38	LYS
1	K	119	PHE
1	K	122	SER
1	L	32	GLY
1	L	47	VAL
1	L	124	SER
1	L	125	ARG
1	L	130	SER
1	A	11	GLY
1	A	25	TYR

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Mol	Chain	Res	Type
1	A	131	GLU
1	B	86	LYS
1	K	11	GLY
1	K	75	TYR
1	K	79	LYS
1	K	98	CYS
1	K	112	THR
1	L	37	PRO
1	L	89	ASN
1	L	108	GLN
1	B	48	HIS
1	B	116	ASN
1	K	2	LEU
1	K	55	VAL
1	L	95	ILE
1	A	76	SER
1	B	37	PRO
1	B	80	GLY
1	B	85	GLY
1	B	101	VAL
1	K	132	GLN
1	L	120	LEU
1	A	100	ARG
1	B	127	ARG
1	L	14	GLY
1	A	80	GLY
1	B	55	VAL
1	L	26	GLY
1	A	72	ILE
1	K	33	GLY
1	L	9	ILE
1	L	68	PRO
1	K	80	GLY
1	B	14	GLY
1	B	68	PRO

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	104/104 (100%)	100 (96%)	4 (4%)	40 75
1	B	104/104 (100%)	91 (88%)	13 (12%)	6 24
1	K	104/104 (100%)	96 (92%)	8 (8%)	16 51
1	L	104/104 (100%)	94 (90%)	10 (10%)	10 38
All	All	416/416 (100%)	381 (92%)	35 (8%)	14 46

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	19	VAL
1	A	20	TRP
1	A	114	ASN
1	B	3	PHE
1	B	12	LYS
1	B	20	TRP
1	B	34	GLN
1	B	36	THR
1	B	56	ARG
1	B	61	CYS
1	B	77	PHE
1	B	83	VAL
1	B	94	ASP
1	B	109	ASN
1	B	118	LYS
1	B	128	GLN
1	K	1	ASN
1	K	3	PHE
1	K	39	ASP
1	K	55	VAL
1	K	70	LEU
1	K	75	TYR
1	K	82	ILE
1	K	114	ASN
1	L	3	PHE
1	L	7	LYS
1	L	39	ASP
1	L	54	ARG
1	L	101	VAL
1	L	104	ASN

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Mol	Chain	Res	Type
1	L	108	GLN
1	L	116	ASN
1	L	121	SER
1	L	127	ARG

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

Mol	Chain	Res	Type
1	A	81	ASN
1	A	104	ASN
1	A	107	HIS
1	A	114	ASN
1	B	104	ASN
1	K	1	ASN
1	K	108	GLN
1	K	109	ASN
1	K	114	ASN
1	L	88	ASN
1	L	111	ASN
1	L	114	ASN
1	L	132	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	ELD	B	134	-	19,19,19	0.60	0	19,19,19	1.75	3 (15%)
2	ELD	L	134	-	19,19,19	0.43	0	19,19,19	1.71	3 (15%)

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	ELD	B	134	-	-	0/17/17/17	0/0/0/0
2	ELD	L	134	-	-	0/17/17/17	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	134	ELD	O2-C1-C2	-5.62	104.68	121.05
2	L	134	ELD	O2-C1-C2	-5.44	105.20	121.05
2	B	134	ELD	C4-C3-C2	-3.64	99.94	113.29
2	L	134	ELD	C4-C3-C2	-3.35	101.01	113.29
2	L	134	ELD	C6-C5-C4	-2.89	99.63	114.53
2	B	134	ELD	C6-C5-C4	-2.45	101.88	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	134	ELD	13	0
2	L	134	ELD	16	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.