Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 02:36 PM EDT

PDB ID	:	1JS9
Title	:	Brome Mosaic Virus
Authors	:	Lucas, R.W.; Larson, S.B.; McPherson, A.
Deposited on	:	2001-08-16
Resolution	:	3.40 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:

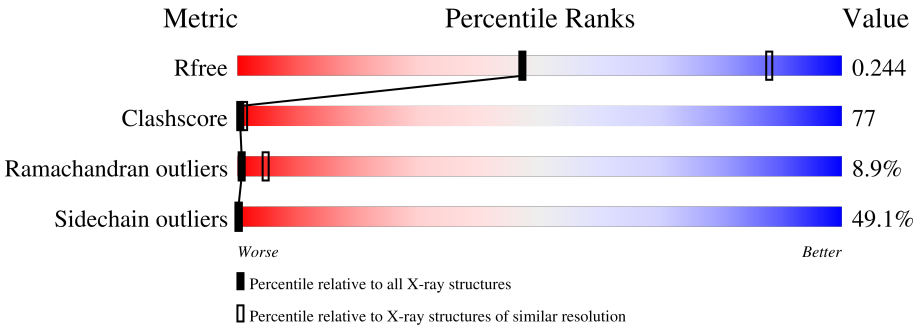
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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%

Mol	Chain	Length	Quality of chain
1	A	189	13% 37% 26% • 21%
1	B	189	13% 41% 33% • 13%
1	C	189	24% 43% 31% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3762 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.

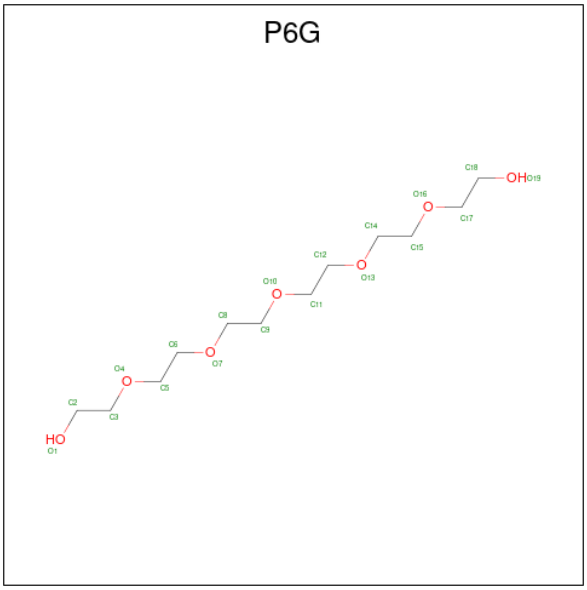
- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	8	0	0
			1133	728	190	212	3			
1	B	165	Total	C	N	O	S	4	0	0
			1245	799	211	232	3			
1	C	189	Total	C	N	O	S	4	0	0
			1363	869	235	256	3			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



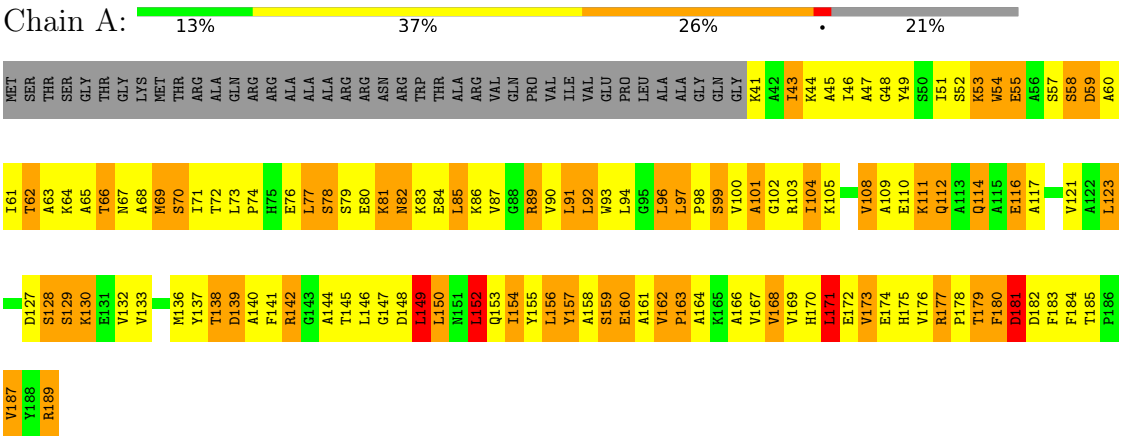
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			19	12	7		

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

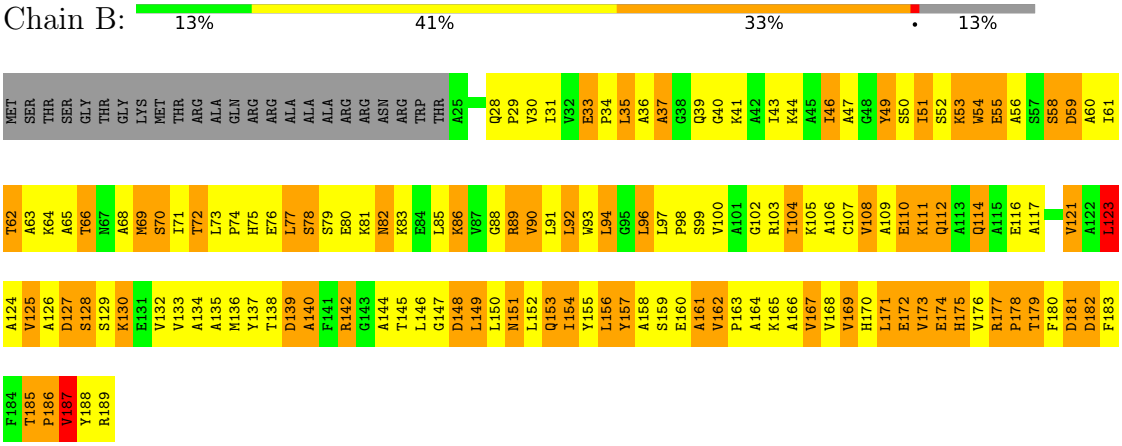
• Molecule 1: Coat protein

Chain A:



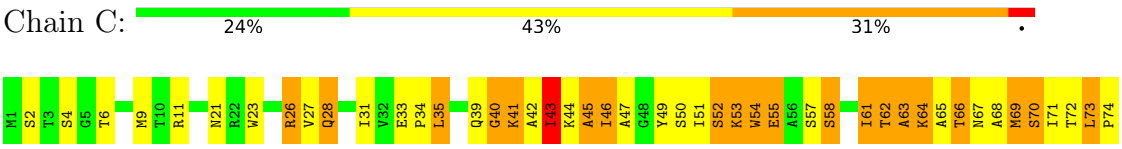
• Molecule 1: Coat protein

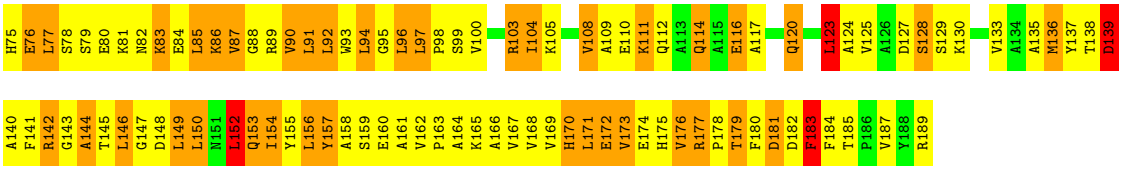
Chain B:



• Molecule 1: Coat protein

Chain C:




H75 E76 L77 S78 S79 E80 K81 N82 K83 E84 L85 K86 V87 G88 R89 V90 L91 L92 W93 L94 G95 L96 L97 P98 S99 V100 R103 I104 K105 V108 A109 E110 K111 Q112 A113 Q114 A115 E116 A117 Q120 L123 A124 V125 A126 D127 S128 S129 K130 V133 A134 A135 M136 Y137 T138 D139
A140 F141 R142 G143 A144 T145 L146 G147 D148 L149 L150 N151 L152 Q153 I154 Y155 L156 Y157 A158 S159 E160 A161 V162 P163 A164 K165 A166 V167 V168 V169 H170 L171 E172 V173 E174 H175 V176 R177 P178 T179 F180 D181 D182 F183 F184 T185 P186 V187 Y188 R189

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	269.24Å 269.24Å 638.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.70 – 3.40 39.79 – 3.40	Depositor EDS
% Data completeness (in resolution range)	50.3 (39.70-3.40) 69.2 (39.79-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	0.59 (at 3.40Å)	Xtriage
Refinement program	X-PLOR 3.851, CNS 1.1	Depositor
R, R_{free}	0.238 , 0.250 0.231 , 0.244	Depositor DCC
R_{free} test set	5118 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å^2)	80.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 301.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.007 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.009 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.005 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.008 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.006 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.019 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	3762	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: MG, P6G

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	0.45	0/1154	0.71	1/1566 (0.1%)
1	B	0.42	0/1268	0.70	1/1723 (0.1%)
1	C	0.42	0/1386	0.70	1/1887 (0.1%)
All	All	0.43	0/3808	0.70	3/5176 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	123	LEU	CA-CB-CG	7.35	132.20	115.30
1	C	123	LEU	CA-CB-CG	6.62	130.53	115.30
1	A	171	LEU	CA-CB-CG	-5.11	103.54	115.30

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	1133	0	1159	178	0
1	B	1245	0	1278	212	0
1	C	1363	0	1343	200	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	0	26	0	0
All	All	3762	0	3806	581	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 77.

All (581) 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:123:LEU:HD22	1:A:123:LEU:H	1.16	1.05
1:B:53:LYS:HG2	1:B:172:GLU:HG3	1.38	1.01
1:B:35:LEU:HD12	1:B:35:LEU:H	1.22	1.00
1:C:69:MET:HG3	1:C:154:ILE:HD11	1.43	1.00
1:B:123:LEU:HD11	1:B:137:TYR:HA	1.43	0.97
1:B:85:LEU:HB3	1:B:86:LYS:HZ1	1.29	0.96
1:B:145:THR:HG22	1:B:147:GLY:H	1.28	0.95
1:B:85:LEU:O	1:B:145:THR:HA	1.68	0.94
1:B:53:LYS:HB3	1:B:172:GLU:HA	1.50	0.94
1:A:85:LEU:HD13	1:A:176:VAL:HG23	1.52	0.91
1:A:87:VAL:HG12	1:A:146:LEU:HD23	1.49	0.91
1:B:149:LEU:O	1:B:152:LEU:HB2	1.70	0.91
1:A:108:VAL:HG23	1:A:152:LEU:HD11	1.52	0.90
1:C:35:LEU:HD23	1:C:35:LEU:H	1.33	0.90
1:B:73:LEU:HG	1:B:74:PRO:HD2	1.54	0.89
1:C:139:ASP:HA	1:C:142:ARG:HB2	1.52	0.89
1:C:103:ARG:HE	1:C:129:SER:HB2	1.35	0.89
1:A:76:GLU:H	1:A:76:GLU:CD	1.76	0.87
1:C:82:ASN:HA	1:C:85:LEU:HD13	1.57	0.87
1:B:46:ILE:HG22	1:B:89:ARG:NH1	1.89	0.86
1:A:89:ARG:HB2	1:A:138:THR:HA	1.57	0.86
1:B:187:VAL:HG13	1:B:188:TYR:H	1.39	0.86
1:B:91:LEU:HB3	1:B:172:GLU:HB3	1.58	0.86
1:C:82:ASN:O	1:C:85:LEU:HB2	1.76	0.85
1:B:85:LEU:HD13	1:B:176:VAL:HG22	1.58	0.85
1:B:90:VAL:HG23	1:B:137:TYR:HB2	1.58	0.85
1:A:80:GLU:HA	1:A:83:LYS:HE3	1.57	0.85
1:A:145:THR:HG22	1:A:147:GLY:H	1.38	0.84
1:C:146:LEU:HA	1:C:149:LEU:HD21	1.59	0.84
1:B:86:LYS:H	1:B:86:LYS:CE	1.90	0.83
1:A:53:LYS:HG2	1:A:172:GLU:HA	1.60	0.83
1:B:164:ALA:C	1:B:166:ALA:H	1.82	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ILE:HD12	1:A:44:LYS:H	1.43	0.83
1:C:94:LEU:N	1:C:94:LEU:HD22	1.94	0.82
1:C:45:ALA:HB2	1:C:51:ILE:HG12	1.62	0.82
1:A:91:LEU:HD22	1:A:92:LEU:N	1.95	0.82
1:B:146:LEU:O	1:B:149:LEU:HG	1.80	0.81
1:A:46:ILE:HG22	1:A:47:ALA:N	1.96	0.80
1:C:104:ILE:HB	1:C:157:TYR:O	1.81	0.80
1:A:123:LEU:H	1:A:123:LEU:CD2	1.94	0.80
1:C:94:LEU:HD22	1:C:94:LEU:H	1.47	0.80
1:B:51:ILE:HA	1:B:174:GLU:HA	1.63	0.80
1:B:49:TYR:HA	1:B:175:HIS:O	1.82	0.79
1:A:63:ALA:HB2	1:A:161:ALA:H	1.47	0.79
1:B:94:LEU:N	1:B:94:LEU:HD12	1.97	0.79
1:B:55:GLU:HG3	1:B:168:VAL:CG2	2.13	0.79
1:C:108:VAL:HG23	1:C:152:LEU:HD11	1.64	0.78
1:B:60:ALA:H	1:B:164:ALA:HB2	1.47	0.78
1:B:86:LYS:H	1:B:86:LYS:NZ	1.81	0.78
1:A:101:ALA:HB1	1:A:160:GLU:HB2	1.66	0.77
1:B:85:LEU:HB3	1:B:86:LYS:NZ	1.99	0.77
1:B:110:GLU:OE2	1:C:80:GLU:HB2	1.86	0.76
1:B:54:TRP:CZ2	1:B:171:LEU:HD12	2.21	0.75
1:C:145:THR:C	1:C:147:GLY:H	1.88	0.75
1:C:103:ARG:NE	1:C:129:SER:HB2	2.02	0.75
1:A:58:SER:HB3	1:A:167:VAL:O	1.87	0.74
1:B:145:THR:HG22	1:B:147:GLY:N	2.02	0.73
1:A:123:LEU:HD23	1:A:137:TYR:CE2	2.23	0.73
1:A:44:LYS:HD2	1:A:45:ALA:H	1.53	0.73
1:A:51:ILE:HD13	1:A:174:GLU:HA	1.69	0.73
1:A:69:MET:O	1:A:154:ILE:HD12	1.89	0.73
1:B:89:ARG:HD3	1:B:174:GLU:OE1	1.89	0.73
1:B:55:GLU:HG3	1:B:168:VAL:HG21	1.70	0.72
1:A:67:ASN:HB2	1:A:156:LEU:HD21	1.71	0.72
1:C:92:LEU:C	1:C:92:LEU:HD22	2.10	0.72
1:C:96:LEU:HD13	1:C:96:LEU:N	2.04	0.71
1:A:43:ILE:HD12	1:A:44:LYS:N	2.04	0.71
1:B:90:VAL:HG12	1:B:173:VAL:HB	1.70	0.71
1:A:87:VAL:HG13	1:A:144:ALA:O	1.90	0.71
1:B:30:VAL:HG22	1:B:31:ILE:H	1.56	0.71
1:C:35:LEU:HD23	1:C:35:LEU:N	2.05	0.70
1:C:146:LEU:O	1:C:149:LEU:HD11	1.90	0.70
1:A:123:LEU:HD22	1:A:123:LEU:N	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:H	1:B:150:LEU:HD22	1.55	0.70
1:A:110:GLU:O	1:A:112:GLN:N	2.25	0.70
1:A:96:LEU:HB3	1:A:167:VAL:HG23	1.74	0.70
1:A:145:THR:HB	1:A:148:ASP:CG	2.11	0.70
1:A:149:LEU:HD23	1:A:149:LEU:H	1.55	0.70
1:C:61:ILE:HD12	1:C:62:THR:H	1.56	0.70
1:A:139:ASP:HA	1:A:142:ARG:HB2	1.72	0.70
1:A:46:ILE:HG13	1:A:174:GLU:OE1	1.92	0.69
1:A:63:ALA:HB2	1:A:161:ALA:N	2.07	0.69
1:B:114:GLN:HB3	1:B:117:ALA:HB2	1.74	0.69
1:A:156:LEU:HD13	1:A:156:LEU:N	2.07	0.69
1:B:79:SER:HB3	1:B:82:ASN:ND2	2.08	0.69
1:C:110:GLU:O	1:C:112:GLN:N	2.26	0.68
1:B:46:ILE:HG13	1:B:47:ALA:N	2.06	0.68
1:B:151:ASN:OD1	1:B:151:ASN:N	2.27	0.68
1:B:35:LEU:HD12	1:B:35:LEU:N	2.02	0.68
1:B:73:LEU:HG	1:B:74:PRO:CD	2.22	0.68
1:C:67:ASN:HB2	1:C:156:LEU:HD11	1.73	0.68
1:C:74:PRO:HD2	1:C:77:LEU:HD11	1.75	0.68
1:B:163:PRO:HG2	1:B:166:ALA:HB2	1.76	0.68
1:A:46:ILE:CG2	1:A:47:ALA:N	2.56	0.68
1:B:61:ILE:HD11	1:B:162:VAL:HB	1.76	0.68
1:C:46:ILE:HG13	1:C:47:ALA:H	1.59	0.68
1:B:35:LEU:H	1:B:35:LEU:CD1	2.03	0.68
1:B:60:ALA:N	1:B:164:ALA:HB2	2.09	0.67
1:B:91:LEU:HD12	1:B:92:LEU:H	1.58	0.67
1:A:180:PHE:O	1:A:182:ASP:N	2.26	0.67
1:C:51:ILE:HD11	1:C:174:GLU:HG3	1.76	0.67
1:A:46:ILE:CG2	1:A:47:ALA:H	2.06	0.67
1:A:73:LEU:HG	1:A:74:PRO:HD2	1.75	0.67
1:C:77:LEU:HD23	1:C:77:LEU:H	1.60	0.67
1:C:124:ALA:HB3	1:C:135:ALA:HB1	1.77	0.67
1:B:28:GLN:NE2	1:B:29:PRO:HD2	2.09	0.66
1:B:61:ILE:HD12	1:B:61:ILE:O	1.95	0.66
1:B:61:ILE:HD13	1:B:158:ALA:HB3	1.78	0.66
1:C:50:SER:O	1:C:51:ILE:HD13	1.95	0.66
1:C:123:LEU:HD11	1:C:136:MET:O	1.95	0.66
1:B:36:ALA:O	1:B:39:GLN:HB2	1.96	0.66
1:B:66:THR:HG23	1:B:116:GLU:OE2	1.96	0.66
1:B:136:MET:HG3	1:B:138:THR:HG23	1.77	0.66
1:C:123:LEU:HD13	1:C:124:ALA:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:HG22	1:C:28:GLN:N	2.11	0.65
1:B:179:THR:HA	1:B:182:ASP:OD2	1.95	0.65
1:C:146:LEU:CA	1:C:149:LEU:HD21	2.27	0.65
1:B:89:ARG:HG3	1:B:142:ARG:HH12	1.62	0.65
1:B:145:THR:O	1:B:148:ASP:HB2	1.96	0.65
1:C:162:VAL:HG22	1:C:163:PRO:HD2	1.77	0.65
1:B:46:ILE:HG23	1:B:49:TYR:HB3	1.78	0.65
1:B:123:LEU:CD1	1:B:137:TYR:HA	2.25	0.65
1:A:139:ASP:HA	1:A:142:ARG:CB	2.27	0.65
1:B:49:TYR:CG	1:B:175:HIS:O	2.50	0.65
1:C:94:LEU:N	1:C:94:LEU:CD2	2.59	0.65
1:A:55:GLU:HG3	1:A:168:VAL:HG21	1.77	0.65
1:A:96:LEU:HB3	1:A:167:VAL:CG2	2.27	0.65
1:B:55:GLU:HB2	1:B:169:VAL:O	1.97	0.65
1:A:55:GLU:HB2	1:A:168:VAL:HG22	1.78	0.65
1:C:66:THR:HG23	1:C:116:GLU:OE2	1.97	0.65
1:B:74:PRO:HB2	1:B:76:GLU:OE1	1.97	0.64
1:B:164:ALA:C	1:B:166:ALA:N	2.48	0.64
1:C:138:THR:C	1:C:140:ALA:H	2.00	0.64
1:A:130:LYS:HG2	1:B:189:ARG:HH22	1.61	0.64
1:C:96:LEU:HB3	1:C:167:VAL:HG23	1.80	0.64
1:C:145:THR:HG22	1:C:147:GLY:H	1.63	0.64
1:C:58:SER:HB3	1:C:167:VAL:O	1.98	0.64
1:A:62:THR:HG23	1:A:65:ALA:HB3	1.80	0.64
1:C:52:SER:HB2	1:C:175:HIS:NE2	2.13	0.64
1:A:91:LEU:O	1:A:171:LEU:HD13	1.98	0.63
1:A:112:GLN:HE21	1:A:112:GLN:HA	1.63	0.63
1:C:85:LEU:HA	1:C:86:LYS:NZ	2.12	0.63
1:C:124:ALA:CB	1:C:135:ALA:HB1	2.28	0.63
1:B:96:LEU:HB3	1:B:167:VAL:HG23	1.80	0.63
1:C:96:LEU:HB3	1:C:167:VAL:CG2	2.26	0.63
1:A:53:LYS:HD3	1:A:172:GLU:OE1	2.00	0.62
1:B:51:ILE:HB	1:B:174:GLU:HB2	1.80	0.62
1:B:162:VAL:HG22	1:B:163:PRO:HD2	1.81	0.62
1:A:104:ILE:HB	1:A:157:TYR:O	1.99	0.62
1:B:79:SER:HB3	1:B:82:ASN:HD21	1.64	0.62
1:B:68:ALA:HA	1:B:154:ILE:O	1.99	0.62
1:B:46:ILE:HG23	1:B:49:TYR:CB	2.30	0.62
1:B:164:ALA:O	1:B:166:ALA:N	2.33	0.61
1:C:54:TRP:CD2	1:C:171:LEU:HD11	2.35	0.61
1:B:33:GLU:OE1	1:B:34:PRO:HD2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:THR:HG22	1:C:150:LEU:HD11	1.82	0.61
1:C:111:LYS:H	1:C:152:LEU:HA	1.63	0.61
1:C:55:GLU:HG2	1:C:170:HIS:CD2	2.36	0.61
1:C:61:ILE:HD11	1:C:65:ALA:O	1.99	0.61
1:C:164:ALA:C	1:C:166:ALA:N	2.52	0.61
1:B:53:LYS:HG2	1:B:172:GLU:CG	2.21	0.61
1:B:74:PRO:HB2	1:B:76:GLU:CD	2.21	0.61
1:B:121:VAL:HG22	1:B:121:VAL:O	1.99	0.61
1:C:74:PRO:HG2	1:C:77:LEU:HD21	1.83	0.61
1:A:71:ILE:HD11	1:A:152:LEU:O	2.01	0.60
1:B:46:ILE:HG22	1:B:89:ARG:HH12	1.64	0.60
1:B:85:LEU:HB2	1:B:146:LEU:HD22	1.81	0.60
1:B:94:LEU:HD13	1:B:133:VAL:HG22	1.83	0.60
1:A:123:LEU:HD23	1:A:137:TYR:HE2	1.64	0.60
1:B:46:ILE:HD12	1:B:47:ALA:H	1.66	0.60
1:A:180:PHE:CE1	1:A:185:THR:HG22	2.36	0.60
1:B:145:THR:HB	1:B:148:ASP:CG	2.21	0.60
1:B:150:LEU:HD22	1:B:150:LEU:N	2.16	0.60
1:A:91:LEU:CD1	1:A:172:GLU:HG3	2.31	0.60
1:A:108:VAL:CG2	1:A:152:LEU:HD11	2.28	0.60
1:B:150:LEU:H	1:B:150:LEU:CD2	2.14	0.60
1:C:46:ILE:CG1	1:C:47:ALA:H	2.14	0.60
1:C:73:LEU:HD13	1:C:78:SER:OG	2.01	0.60
1:B:88:GLY:HA2	1:B:142:ARG:HD3	1.83	0.60
1:C:31:ILE:HG23	1:C:31:ILE:O	2.01	0.60
1:C:69:MET:HG3	1:C:154:ILE:CD1	2.27	0.60
1:C:164:ALA:C	1:C:166:ALA:H	2.05	0.59
1:B:49:TYR:HD2	1:B:174:GLU:HG2	1.67	0.59
1:C:39:GLN:O	1:C:40:GLY:O	2.20	0.59
1:B:50:SER:HB2	1:B:177:ARG:HH11	1.67	0.59
1:B:58:SER:HB3	1:B:167:VAL:O	2.01	0.59
1:B:110:GLU:O	1:B:111:LYS:C	2.40	0.59
1:C:87:VAL:HG23	1:C:88:GLY:N	2.17	0.59
1:C:51:ILE:CD1	1:C:174:GLU:HA	2.33	0.59
1:A:53:LYS:HA	1:A:171:LEU:O	2.02	0.59
1:A:103:ARG:NE	1:A:129:SER:HA	2.18	0.59
1:C:51:ILE:CD1	1:C:174:GLU:HG3	2.33	0.59
1:B:54:TRP:CZ2	1:B:74:PRO:HD3	2.38	0.58
1:B:123:LEU:HD13	1:B:124:ALA:N	2.18	0.58
1:A:52:SER:O	1:A:173:VAL:HG13	2.03	0.58
1:A:73:LEU:HD22	1:A:78:SER:OG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ALA:O	1:A:162:VAL:HG23	2.03	0.58
1:B:86:LYS:H	1:B:86:LYS:HZ2	1.50	0.58
1:B:171:LEU:N	1:B:171:LEU:HD23	2.18	0.58
1:C:167:VAL:HG22	1:C:168:VAL:O	2.03	0.58
1:C:86:LYS:HD3	1:C:86:LYS:N	2.17	0.58
1:A:164:ALA:C	1:A:166:ALA:N	2.54	0.58
1:B:156:LEU:HD23	1:B:156:LEU:N	2.19	0.58
1:A:89:ARG:CB	1:A:138:THR:HA	2.33	0.57
1:B:66:THR:HG22	1:B:157:TYR:HB2	1.86	0.57
1:C:92:LEU:HD13	1:C:92:LEU:O	2.04	0.57
1:C:111:LYS:HA	1:C:153:GLN:HG2	1.86	0.57
1:C:53:LYS:O	1:C:54:TRP:HB3	2.04	0.57
1:A:187:VAL:O	1:A:189:ARG:HG2	2.04	0.57
1:B:85:LEU:HD13	1:B:86:LYS:HZ1	1.70	0.57
1:C:52:SER:O	1:C:173:VAL:HG13	2.05	0.57
1:C:73:LEU:HD12	1:C:73:LEU:H	1.69	0.57
1:A:82:ASN:O	1:A:85:LEU:HB2	2.05	0.57
1:B:82:ASN:O	1:B:85:LEU:HG	2.04	0.57
1:C:50:SER:HB2	1:C:177:ARG:HD3	1.85	0.57
1:C:90:VAL:HG23	1:C:172:GLU:O	2.05	0.57
1:B:88:GLY:HA2	1:B:142:ARG:HA	1.86	0.57
1:C:57:SER:HB3	1:C:165:LYS:HD3	1.87	0.57
1:C:87:VAL:HG12	1:C:144:ALA:O	2.05	0.57
1:C:104:ILE:CG2	1:C:158:ALA:HA	2.35	0.57
1:A:138:THR:O	1:A:140:ALA:N	2.38	0.56
1:C:177:ARG:HG3	1:C:178:PRO:HD2	1.87	0.56
1:A:49:TYR:CD2	1:A:174:GLU:HG2	2.40	0.56
1:A:104:ILE:HB	1:A:158:ALA:HA	1.87	0.56
1:A:109:ALA:C	1:A:152:LEU:HD13	2.26	0.56
1:B:104:ILE:HG12	1:B:105:LYS:N	2.19	0.56
1:C:74:PRO:HD2	1:C:77:LEU:CG	2.35	0.56
1:C:138:THR:O	1:C:140:ALA:N	2.38	0.56
1:A:46:ILE:HG22	1:A:47:ALA:H	1.62	0.56
1:C:74:PRO:HD2	1:C:77:LEU:CD1	2.35	0.56
1:C:45:ALA:HB2	1:C:51:ILE:CG1	2.32	0.56
1:A:128:SER:HA	1:A:133:VAL:HG12	1.88	0.56
1:B:46:ILE:CG1	1:B:47:ALA:N	2.68	0.56
1:C:88:GLY:HA2	1:C:142:ARG:HG3	1.88	0.56
1:A:79:SER:O	1:A:83:LYS:HB2	2.06	0.56
1:C:145:THR:C	1:C:147:GLY:N	2.56	0.56
1:C:143:GLY:O	1:C:144:ALA:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:HG2	1:B:189:ARG:NH2	2.20	0.55
1:B:90:VAL:H	1:B:136:MET:HE3	1.70	0.55
1:B:114:GLN:OE1	1:B:114:GLN:HA	2.05	0.55
1:B:94:LEU:CD1	1:B:133:VAL:HG22	2.37	0.55
1:A:123:LEU:HD23	1:A:137:TYR:CD2	2.42	0.55
1:B:110:GLU:O	1:B:112:GLN:N	2.40	0.55
1:A:103:ARG:HG2	1:A:128:SER:OG	2.07	0.55
1:B:49:TYR:CE2	1:B:175:HIS:HA	2.42	0.55
1:C:127:ASP:HB3	1:C:130:LYS:HG3	1.88	0.55
1:A:79:SER:OG	1:A:81:LYS:HB2	2.07	0.55
1:A:93:TRP:NE1	1:A:170:HIS:HB2	2.22	0.55
1:C:76:GLU:CD	1:C:76:GLU:H	2.09	0.55
1:C:74:PRO:CD	1:C:77:LEU:HD11	2.37	0.55
1:B:108:VAL:HG23	1:B:152:LEU:HD12	1.89	0.54
1:C:108:VAL:CG2	1:C:152:LEU:HD11	2.33	0.54
1:C:170:HIS:ND1	1:C:170:HIS:N	2.55	0.54
1:B:86:LYS:HA	1:B:144:ALA:O	2.07	0.54
1:B:180:PHE:C	1:B:182:ASP:N	2.58	0.54
1:C:152:LEU:C	1:C:152:LEU:HD12	2.27	0.54
1:C:97:LEU:O	1:C:100:VAL:HG13	2.06	0.54
1:C:125:VAL:O	1:C:125:VAL:HG13	2.07	0.54
1:A:53:LYS:CG	1:A:172:GLU:HA	2.35	0.54
1:A:103:ARG:CD	1:A:129:SER:HA	2.38	0.54
1:B:132:VAL:O	1:B:132:VAL:HG13	2.08	0.54
1:C:161:ALA:O	1:C:162:VAL:HG23	2.07	0.54
1:B:66:THR:HG21	1:B:116:GLU:HG3	1.89	0.54
1:C:87:VAL:CG2	1:C:88:GLY:N	2.71	0.54
1:C:95:GLY:O	1:C:167:VAL:HG23	2.08	0.54
1:C:86:LYS:N	1:C:86:LYS:CD	2.70	0.54
1:C:49:TYR:CD2	1:C:175:HIS:C	2.81	0.54
1:B:78:SER:O	1:B:83:LYS:HD3	2.08	0.54
1:C:146:LEU:C	1:C:149:LEU:HD11	2.28	0.53
1:C:179:THR:HB	1:C:183:PHE:HZ	1.73	0.53
1:A:79:SER:HB3	1:A:82:ASN:HD21	1.73	0.53
1:A:90:VAL:HG22	1:A:174:GLU:H	1.73	0.53
1:A:136:MET:HE3	1:A:137:TYR:N	2.23	0.53
1:B:62:THR:HG23	1:B:65:ALA:HB3	1.89	0.53
1:A:53:LYS:O	1:A:54:TRP:HB3	2.09	0.53
1:B:104:ILE:HD13	1:B:104:ILE:O	2.08	0.53
1:C:73:LEU:H	1:C:73:LEU:CD1	2.22	0.53
1:C:89:ARG:HG2	1:C:174:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:CB	1:B:86:LYS:HZ1	2.11	0.53
1:C:66:THR:HG23	1:C:116:GLU:CD	2.29	0.53
1:C:97:LEU:HG	1:C:98:PRO:HD2	1.90	0.53
1:A:96:LEU:HD12	1:A:96:LEU:H	1.73	0.53
1:B:133:VAL:O	1:B:133:VAL:HG13	2.09	0.53
1:B:106:ALA:O	1:B:125:VAL:HG23	2.09	0.53
1:A:79:SER:HB3	1:A:82:ASN:ND2	2.24	0.53
1:A:43:ILE:CD1	1:A:44:LYS:N	2.71	0.53
1:A:61:ILE:C	1:A:61:ILE:HD12	2.29	0.53
1:A:70:SER:HA	1:A:153:GLN:HG3	1.90	0.53
1:B:47:ALA:C	1:B:49:TYR:H	2.12	0.53
1:B:86:LYS:H	1:B:86:LYS:HE3	1.73	0.53
1:C:68:ALA:C	1:C:69:MET:HG2	2.30	0.53
1:C:145:THR:HG22	1:C:147:GLY:N	2.24	0.52
1:B:149:LEU:O	1:B:152:LEU:N	2.42	0.52
1:C:73:LEU:HD12	1:C:73:LEU:N	2.24	0.52
1:A:145:THR:HG22	1:A:147:GLY:N	2.16	0.52
1:C:91:LEU:HD21	1:C:172:GLU:HG3	1.92	0.52
1:A:87:VAL:HG12	1:A:146:LEU:CD2	2.32	0.52
1:A:163:PRO:HB2	1:A:166:ALA:HB2	1.91	0.52
1:B:94:LEU:N	1:B:94:LEU:CD1	2.69	0.52
1:B:187:VAL:HG22	1:B:188:TYR:N	2.24	0.52
1:C:79:SER:O	1:C:83:LYS:N	2.37	0.52
1:A:73:LEU:HG	1:A:74:PRO:CD	2.38	0.52
1:A:109:ALA:O	1:A:152:LEU:HD13	2.09	0.52
1:B:66:THR:CG2	1:B:116:GLU:HG3	2.40	0.52
1:B:185:THR:HG22	1:B:186:PRO:HD2	1.92	0.52
1:A:170:HIS:O	1:A:171:LEU:HD22	2.11	0.51
1:A:84:GLU:HA	1:A:145:THR:HG23	1.91	0.51
1:C:69:MET:CG	1:C:154:ILE:HD11	2.30	0.51
1:B:88:GLY:CA	1:B:142:ARG:HD3	2.40	0.51
1:B:89:ARG:HB3	1:B:136:MET:HE1	1.92	0.51
1:C:43:ILE:HG12	1:C:43:ILE:O	2.10	0.51
1:A:104:ILE:HD13	1:A:104:ILE:O	2.10	0.51
1:B:49:TYR:CD2	1:B:175:HIS:O	2.64	0.51
1:C:75:HIS:HA	1:C:78:SER:HB2	1.92	0.51
1:A:164:ALA:C	1:A:166:ALA:H	2.14	0.51
1:B:46:ILE:CD1	1:B:47:ALA:H	2.24	0.51
1:C:67:ASN:HB2	1:C:156:LEU:CD1	2.40	0.51
1:B:54:TRP:CZ2	1:B:73:LEU:HA	2.46	0.51
1:B:187:VAL:HG13	1:B:188:TYR:N	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ILE:HD13	1:B:158:ALA:CB	2.41	0.50
1:B:96:LEU:HB3	1:B:167:VAL:CG2	2.39	0.50
1:C:71:ILE:O	1:C:150:LEU:HD13	2.10	0.50
1:C:145:THR:O	1:C:147:GLY:N	2.44	0.50
1:A:53:LYS:HG2	1:A:172:GLU:CA	2.38	0.50
1:B:145:THR:HB	1:B:148:ASP:OD1	2.11	0.50
1:B:107:CYS:HA	1:B:137:TYR:OH	2.12	0.50
1:A:97:LEU:O	1:A:100:VAL:HG23	2.12	0.50
1:A:104:ILE:HG22	1:A:159:SER:H	1.77	0.50
1:A:103:ARG:HD3	1:A:129:SER:HA	1.93	0.50
1:B:109:ALA:O	1:B:152:LEU:HD13	2.11	0.50
1:A:145:THR:O	1:A:148:ASP:HB2	2.11	0.50
1:A:146:LEU:O	1:A:149:LEU:HD11	2.11	0.50
1:C:138:THR:C	1:C:140:ALA:N	2.65	0.50
1:A:91:LEU:HD13	1:A:91:LEU:C	2.32	0.50
1:B:85:LEU:HD13	1:B:176:VAL:CG2	2.36	0.50
1:C:110:GLU:O	1:C:111:LYS:C	2.50	0.50
1:B:149:LEU:N	1:B:149:LEU:HD23	2.27	0.49
1:B:173:VAL:CG2	1:B:174:GLU:N	2.75	0.49
1:C:90:VAL:O	1:C:137:TYR:HB2	2.11	0.49
1:C:94:LEU:H	1:C:94:LEU:CD2	2.19	0.49
1:C:109:ALA:C	1:C:152:LEU:HD13	2.32	0.49
1:C:85:LEU:HA	1:C:86:LYS:HZ3	1.76	0.49
1:A:87:VAL:CG1	1:A:146:LEU:HD23	2.34	0.49
1:B:85:LEU:HB2	1:B:146:LEU:HB2	1.93	0.49
1:B:91:LEU:CD1	1:B:92:LEU:H	2.24	0.49
1:A:68:ALA:HA	1:A:154:ILE:O	2.12	0.49
1:B:71:ILE:HB	1:B:150:LEU:HD13	1.93	0.49
1:C:86:LYS:O	1:C:176:VAL:HG22	2.13	0.49
1:C:91:LEU:HD12	1:C:92:LEU:N	2.27	0.49
1:B:63:ALA:HB2	1:B:161:ALA:H	1.77	0.49
1:B:168:VAL:HG13	1:B:170:HIS:NE2	2.27	0.49
1:C:72:THR:HG22	1:C:150:LEU:CD1	2.43	0.49
1:A:164:ALA:O	1:A:166:ALA:N	2.45	0.49
1:C:85:LEU:HA	1:C:86:LYS:HZ2	1.78	0.49
1:C:147:GLY:O	1:C:150:LEU:HB2	2.12	0.48
1:A:80:GLU:HA	1:A:83:LYS:HB3	1.95	0.48
1:A:127:ASP:OD1	1:A:128:SER:N	2.46	0.48
1:B:180:PHE:O	1:B:181:ASP:C	2.52	0.48
1:C:69:MET:O	1:C:70:SER:C	2.52	0.48
1:C:144:ALA:O	1:C:145:THR:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:H	1:A:164:ALA:HB2	1.79	0.48
1:A:149:LEU:HA	1:A:152:LEU:HD23	1.95	0.48
1:B:70:SER:HA	1:B:153:GLN:HG3	1.94	0.48
1:C:51:ILE:HD12	1:C:174:GLU:HA	1.95	0.48
1:C:92:LEU:HD22	1:C:93:TRP:N	2.29	0.48
1:A:89:ARG:HB3	1:A:142:ARG:NH1	2.28	0.48
1:A:138:THR:C	1:A:140:ALA:H	2.16	0.48
1:B:94:LEU:HD12	1:B:94:LEU:H	1.76	0.48
1:B:138:THR:O	1:B:140:ALA:N	2.45	0.48
1:B:102:GLY:HA3	1:B:160:GLU:OE1	2.13	0.48
1:B:185:THR:CB	1:B:186:PRO:HD2	2.42	0.48
1:A:170:HIS:N	1:A:170:HIS:CD2	2.80	0.48
1:B:142:ARG:O	1:C:81:LYS:HG3	2.14	0.48
1:C:33:GLU:HG3	1:C:34:PRO:HD2	1.95	0.48
1:C:145:THR:O	1:C:148:ASP:HB2	2.14	0.48
1:A:67:ASN:HB2	1:A:156:LEU:CD2	2.43	0.48
1:A:149:LEU:H	1:A:149:LEU:CD2	2.14	0.48
1:C:164:ALA:O	1:C:166:ALA:N	2.46	0.48
1:A:180:PHE:O	1:A:181:ASP:C	2.53	0.47
1:C:96:LEU:N	1:C:96:LEU:CD1	2.76	0.47
1:C:112:GLN:HB2	1:C:155:TYR:CZ	2.48	0.47
1:A:114:GLN:HB3	1:A:117:ALA:HB3	1.96	0.47
1:C:154:ILE:HD13	1:C:154:ILE:O	2.14	0.47
1:A:44:LYS:HG3	1:A:45:ALA:O	2.13	0.47
1:C:93:TRP:CZ2	1:C:170:HIS:CG	3.03	0.47
1:C:136:MET:HG3	1:C:138:THR:HG23	1.97	0.47
1:A:64:LYS:HA	1:A:157:TYR:HE2	1.80	0.47
1:B:53:LYS:CB	1:B:172:GLU:HA	2.33	0.47
1:C:53:LYS:HA	1:C:171:LEU:O	2.14	0.47
1:B:62:THR:OG1	1:B:63:ALA:N	2.46	0.47
1:B:162:VAL:HG13	1:B:163:PRO:HD2	1.96	0.47
1:A:92:LEU:O	1:A:92:LEU:HG	2.14	0.47
1:A:103:ARG:CZ	1:A:129:SER:HA	2.44	0.47
1:B:60:ALA:N	1:B:164:ALA:CB	2.77	0.47
1:B:81:LYS:HZ1	1:B:180:PHE:HB2	1.80	0.47
1:B:130:LYS:NZ	1:B:132:VAL:O	2.44	0.47
1:B:136:MET:HE2	1:B:138:THR:N	2.29	0.47
1:C:68:ALA:HA	1:C:154:ILE:O	2.15	0.47
1:B:93:TRP:HB3	1:B:134:ALA:HB2	1.95	0.47
1:B:114:GLN:HB3	1:B:117:ALA:CB	2.45	0.47
1:C:41:LYS:CE	1:C:41:LYS:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PHE:CZ	1:A:185:THR:HG22	2.50	0.47
1:A:90:VAL:O	1:A:137:TYR:HB2	2.15	0.47
1:B:162:VAL:HG13	1:B:163:PRO:CD	2.45	0.46
1:C:79:SER:HB3	1:C:82:ASN:ND2	2.30	0.46
1:C:79:SER:HB3	1:C:82:ASN:HD22	1.79	0.46
1:A:123:LEU:N	1:A:123:LEU:HD13	2.30	0.46
1:A:102:GLY:O	1:A:104:ILE:HG23	2.16	0.46
1:A:110:GLU:OE2	1:B:80:GLU:HG2	2.15	0.46
1:C:92:LEU:C	1:C:92:LEU:CD2	2.83	0.46
1:A:98:PRO:HG2	1:A:99:SER:H	1.80	0.46
1:B:146:LEU:HA	1:B:146:LEU:HD12	1.60	0.46
1:C:27:VAL:CG2	1:C:28:GLN:N	2.78	0.46
1:B:138:THR:C	1:B:140:ALA:H	2.19	0.46
1:C:27:VAL:HG22	1:C:28:GLN:H	1.78	0.46
1:C:163:PRO:O	1:C:166:ALA:HB2	2.15	0.46
1:A:91:LEU:O	1:A:91:LEU:HD13	2.15	0.46
1:A:130:LYS:CG	1:B:189:ARG:HH22	2.28	0.46
1:B:69:MET:HG2	1:B:154:ILE:HD12	1.96	0.46
1:B:147:GLY:O	1:B:149:LEU:N	2.49	0.46
1:C:149:LEU:H	1:C:149:LEU:HG	1.21	0.46
1:B:90:VAL:H	1:B:136:MET:CE	2.27	0.46
1:B:80:GLU:OE1	1:B:80:GLU:HA	2.16	0.46
1:B:175:HIS:CD2	1:B:175:HIS:N	2.84	0.46
1:C:74:PRO:HD2	1:C:77:LEU:HG	1.98	0.46
1:C:123:LEU:HD13	1:C:124:ALA:CB	2.46	0.46
1:A:43:ILE:CG1	1:A:44:LYS:N	2.79	0.45
1:A:81:LYS:CG	1:C:141:PHE:HA	2.45	0.45
1:C:123:LEU:HD12	1:C:137:TYR:CD2	2.51	0.45
1:A:96:LEU:HD12	1:A:96:LEU:N	2.30	0.45
1:B:28:GLN:HE21	1:B:29:PRO:HD2	1.80	0.45
1:C:44:LYS:NZ	1:C:45:ALA:HB3	2.31	0.45
1:C:94:LEU:O	1:C:94:LEU:HD23	2.17	0.45
1:A:96:LEU:HD12	1:A:96:LEU:O	2.17	0.45
1:B:123:LEU:HD13	1:B:123:LEU:C	2.36	0.45
1:B:127:ASP:CG	1:B:129:SER:H	2.19	0.45
1:B:30:VAL:HG22	1:B:31:ILE:N	2.26	0.45
1:A:112:GLN:HA	1:A:112:GLN:NE2	2.30	0.45
1:A:141:PHE:O	1:A:142:ARG:C	2.53	0.45
1:B:126:ALA:N	1:B:135:ALA:HB2	2.32	0.45
1:C:104:ILE:HG22	1:C:159:SER:H	1.81	0.45
1:A:69:MET:C	1:A:70:SER:O	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LYS:HB3	1:B:171:LEU:O	2.17	0.45
1:C:35:LEU:N	1:C:35:LEU:CD2	2.75	0.45
1:A:64:LYS:HA	1:A:157:TYR:CE2	2.52	0.45
1:B:145:THR:HB	1:B:148:ASP:CB	2.47	0.45
1:B:161:ALA:O	1:B:162:VAL:HG23	2.17	0.45
1:C:156:LEU:O	1:C:156:LEU:HD12	2.17	0.45
1:A:92:LEU:HB2	1:A:171:LEU:HD21	1.99	0.44
1:B:31:ILE:HG23	1:B:31:ILE:O	2.16	0.44
1:B:64:LYS:HA	1:B:157:TYR:CE1	2.51	0.44
1:C:42:ALA:O	1:C:43:ILE:C	2.56	0.44
1:C:61:ILE:HD12	1:C:62:THR:N	2.28	0.44
1:C:128:SER:HA	1:C:133:VAL:HG12	1.99	0.44
1:A:101:ALA:CB	1:A:160:GLU:HB2	2.42	0.44
1:A:138:THR:C	1:A:140:ALA:N	2.71	0.44
1:C:109:ALA:O	1:C:152:LEU:HD13	2.17	0.44
1:A:90:VAL:HG22	1:A:173:VAL:HA	1.99	0.44
1:A:152:LEU:HD12	1:A:152:LEU:C	2.38	0.44
1:B:94:LEU:HD13	1:B:133:VAL:CG2	2.45	0.44
1:B:173:VAL:HG23	1:B:174:GLU:N	2.32	0.44
1:B:180:PHE:O	1:B:182:ASP:N	2.50	0.44
1:C:89:ARG:HB2	1:C:138:THR:HA	2.00	0.44
1:C:152:LEU:HD12	1:C:153:GLN:O	2.18	0.44
1:A:55:GLU:HA	1:A:169:VAL:O	2.18	0.44
1:A:159:SER:HB2	1:A:160:GLU:OE1	2.18	0.44
1:B:162:VAL:HG13	1:B:163:PRO:N	2.32	0.44
1:B:182:ASP:N	1:B:182:ASP:OD1	2.42	0.44
1:C:49:TYR:CD2	1:C:174:GLU:HG2	2.53	0.44
1:C:153:GLN:HG2	1:C:153:GLN:H	1.51	0.44
1:A:51:ILE:HA	1:A:173:VAL:O	2.17	0.44
1:A:73:LEU:C	1:A:73:LEU:HD23	2.38	0.44
1:A:79:SER:C	1:A:81:LYS:N	2.71	0.44
1:A:155:TYR:C	1:A:156:LEU:HD13	2.37	0.44
1:B:112:GLN:HB2	1:B:155:TYR:CZ	2.52	0.44
1:B:83:LYS:HE2	1:B:83:LYS:HB3	1.78	0.44
1:C:93:TRP:CH2	1:C:170:HIS:CE1	3.06	0.44
1:B:73:LEU:HD11	1:B:77:LEU:HD12	2.00	0.44
1:A:180:PHE:HA	1:A:183:PHE:CZ	2.53	0.44
1:A:49:TYR:CD2	1:A:175:HIS:C	2.91	0.43
1:C:64:LYS:HA	1:C:158:ALA:O	2.19	0.43
1:C:87:VAL:HA	1:C:175:HIS:HA	2.00	0.43
1:C:104:ILE:HD13	1:C:104:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LEU:HD22	1:C:96:LEU:O	2.18	0.43
1:A:60:ALA:HA	1:A:163:PRO:O	2.18	0.43
1:A:111:LYS:HA	1:A:153:GLN:NE2	2.33	0.43
1:C:46:ILE:HG23	1:C:47:ALA:N	2.34	0.43
1:A:51:ILE:HD13	1:A:174:GLU:CA	2.43	0.43
1:B:81:LYS:NZ	1:B:180:PHE:HB2	2.33	0.43
1:B:85:LEU:CB	1:B:146:LEU:HD22	2.47	0.43
1:B:175:HIS:CG	1:B:176:VAL:H	2.36	0.43
1:B:86:LYS:HZ2	1:B:86:LYS:N	2.14	0.43
1:C:85:LEU:O	1:C:146:LEU:N	2.51	0.43
1:A:76:GLU:C	1:A:77:LEU:HD23	2.38	0.43
1:A:179:THR:O	1:A:181:ASP:N	2.50	0.43
1:A:83:LYS:HE3	1:A:83:LYS:HB3	1.67	0.43
1:A:162:VAL:HG22	1:A:163:PRO:HD2	2.01	0.43
1:B:123:LEU:HD12	1:B:137:TYR:CD2	2.53	0.43
1:B:127:ASP:OD2	1:B:128:SER:N	2.51	0.43
1:C:54:TRP:O	1:C:171:LEU:CD1	2.66	0.43
1:C:171:LEU:O	1:C:171:LEU:HD12	2.18	0.43
1:A:90:VAL:HG13	1:A:173:VAL:HA	2.01	0.43
1:B:36:ALA:O	1:B:37:ALA:C	2.56	0.43
1:B:86:LYS:NZ	1:B:176:VAL:HG22	2.34	0.43
1:B:63:ALA:O	1:B:64:LYS:HB2	2.18	0.42
1:B:79:SER:O	1:B:83:LYS:HB2	2.20	0.42
1:A:90:VAL:HG13	1:A:172:GLU:O	2.19	0.42
1:A:136:MET:HE3	1:A:137:TYR:H	1.84	0.42
1:C:40:GLY:O	1:C:41:LYS:HD2	2.18	0.42
1:C:61:ILE:CG2	1:C:162:VAL:HG12	2.49	0.42
1:A:44:LYS:HD2	1:A:45:ALA:N	2.29	0.42
1:A:48:GLY:HA2	1:A:177:ARG:CZ	2.49	0.42
1:B:100:VAL:O	1:B:100:VAL:HG13	2.18	0.42
1:C:162:VAL:HG13	1:C:163:PRO:N	2.34	0.42
1:C:179:THR:HB	1:C:183:PHE:CZ	2.54	0.42
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.90	0.42
1:A:156:LEU:N	1:A:156:LEU:CD1	2.79	0.42
1:B:169:VAL:HG22	1:B:171:LEU:CD2	2.49	0.42
1:C:4:SER:C	1:C:6:THR:H	2.23	0.42
1:A:44:LYS:HG3	1:A:45:ALA:N	2.34	0.42
1:A:59:ASP:O	1:A:61:ILE:HG23	2.20	0.42
1:B:50:SER:HB2	1:B:177:ARG:HD3	2.01	0.42
1:B:86:LYS:CE	1:B:86:LYS:N	2.71	0.42
1:C:117:ALA:HA	1:C:120:GLN:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ILE:CG2	1:A:158:ALA:HA	2.50	0.42
1:B:123:LEU:HD13	1:B:124:ALA:CB	2.50	0.42
1:B:148:ASP:O	1:C:80:GLU:HG2	2.20	0.42
1:C:77:LEU:H	1:C:77:LEU:CD2	2.24	0.42
1:A:55:GLU:HB2	1:A:168:VAL:CG2	2.47	0.41
1:C:23:TRP:O	1:C:26:ARG:NH1	2.53	0.41
1:C:41:LYS:HA	1:C:41:LYS:HE2	2.02	0.41
1:A:149:LEU:O	1:A:152:LEU:HB3	2.20	0.41
1:A:157:TYR:CG	1:A:158:ALA:N	2.88	0.41
1:B:49:TYR:CA	1:B:175:HIS:O	2.62	0.41
1:C:53:LYS:HD2	1:C:172:GLU:OE1	2.20	0.41
1:C:104:ILE:O	1:C:128:SER:HB3	2.20	0.41
1:A:127:ASP:O	1:A:133:VAL:HG12	2.20	0.41
1:A:162:VAL:HA	1:A:163:PRO:HD3	1.84	0.41
1:B:46:ILE:HG23	1:B:49:TYR:HB2	2.02	0.41
1:B:85:LEU:O	1:B:146:LEU:N	2.53	0.41
1:A:85:LEU:HB2	1:A:146:LEU:HD12	2.02	0.41
1:C:54:TRP:CD2	1:C:171:LEU:CD1	3.04	0.41
1:C:111:LYS:HB2	1:C:153:GLN:HE21	1.85	0.41
1:C:51:ILE:HA	1:C:173:VAL:O	2.21	0.41
1:C:68:ALA:O	1:C:69:MET:HG2	2.20	0.41
1:C:94:LEU:HD21	1:C:133:VAL:HB	2.02	0.41
1:A:44:LYS:CG	1:A:45:ALA:N	2.83	0.41
1:B:171:LEU:HD23	1:B:171:LEU:H	1.85	0.41
1:C:43:ILE:O	1:C:43:ILE:CG1	2.68	0.41
1:C:50:SER:C	1:C:51:ILE:HD13	2.41	0.41
1:B:56:ALA:HB2	1:B:72:THR:OG1	2.21	0.41
1:B:66:THR:CG2	1:B:157:TYR:HB2	2.49	0.41
1:B:93:TRP:HB3	1:B:134:ALA:CB	2.51	0.41
1:C:62:THR:OG1	1:C:63:ALA:N	2.54	0.41
1:C:103:ARG:HG2	1:C:104:ILE:N	2.36	0.41
1:C:103:ARG:C	1:C:104:ILE:CG2	2.89	0.41
1:C:111:LYS:N	1:C:152:LEU:HA	2.30	0.41
1:A:70:SER:CA	1:A:153:GLN:HG3	2.50	0.41
1:A:76:GLU:CD	1:A:76:GLU:N	2.55	0.41
1:B:54:TRP:CG	1:B:55:GLU:N	2.89	0.41
1:B:160:GLU:O	1:B:161:ALA:O	2.39	0.41
1:C:50:SER:HB3	1:C:175:HIS:CE1	2.56	0.41
1:C:62:THR:C	1:C:161:ALA:HA	2.40	0.40
1:C:146:LEU:C	1:C:149:LEU:HD21	2.42	0.40
1:A:61:ILE:HG22	1:A:67:ASN:CG	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ALA:HA	1:B:163:PRO:C	2.41	0.40
1:B:146:LEU:O	1:B:149:LEU:CG	2.62	0.40
1:C:43:ILE:N	1:C:43:ILE:HD13	2.36	0.40
1:A:139:ASP:HA	1:A:142:ARG:HB3	2.02	0.40
1:B:59:ASP:HA	1:B:164:ALA:HB1	2.03	0.40
1:B:150:LEU:C	1:B:152:LEU:H	2.24	0.40
1:A:59:ASP:O	1:A:60:ALA:C	2.59	0.40
1:A:66:THR:HG23	1:A:116:GLU:OE2	2.22	0.40
1:B:148:ASP:OD2	1:C:84:GLU:HG2	2.21	0.40
1:C:69:MET:CE	1:C:156:LEU:HD21	2.52	0.40
1:C:87:VAL:CG1	1:C:144:ALA:O	2.68	0.40
1:C:112:GLN:HB3	1:C:114:GLN:O	2.21	0.40
1:A:100:VAL:O	1:A:101:ALA:O	2.39	0.40
1:A:150:LEU:HD13	1:A:150:LEU:HA	1.80	0.40
1:B:98:PRO:C	1:B:100:VAL:H	2.24	0.40
1:B:178:PRO:HB2	1:B:179:THR:H	1.59	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	147/189 (78%)	108 (74%)	28 (19%)	11 (8%)	1 7
1	B	163/189 (86%)	117 (72%)	30 (18%)	16 (10%)	0 4
1	C	187/189 (99%)	126 (67%)	44 (24%)	17 (9%)	1 4
All	All	497/567 (88%)	351 (71%)	102 (20%)	44 (9%)	1 5

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ALA

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Mol	Chain	Res	Type
1	A	111	LYS
1	A	139	ASP
1	A	181	ASP
1	B	111	LYS
1	B	121	VAL
1	C	11	ARG
1	C	40	GLY
1	C	45	ALA
1	C	63	ALA
1	C	111	LYS
1	C	152	LEU
1	C	183	PHE
1	A	180	PHE
1	B	37	ALA
1	B	139	ASP
1	B	161	ALA
1	B	178	PRO
1	B	186	PRO
1	C	21	ASN
1	C	146	LEU
1	A	149	LEU
1	B	40	GLY
1	B	54	TRP
1	B	148	ASP
1	B	165	LYS
1	B	175	HIS
1	C	2	SER
1	C	43	ILE
1	C	139	ASP
1	C	181	ASP
1	C	184	PHE
1	A	152	LEU
1	A	163	PRO
1	A	178	PRO
1	A	184	PHE
1	B	140	ALA
1	B	187	VAL
1	C	54	TRP
1	C	144	ALA
1	A	54	TRP
1	B	159	SER
1	C	9	MET

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Mol	Chain	Res	Type
1	B	125	VAL

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	117/146 (80%)	61 (52%)	56 (48%)	0 0
1	B	128/146 (88%)	66 (52%)	62 (48%)	0 0
1	C	128/146 (88%)	63 (49%)	65 (51%)	0 0
All	All	373/438 (85%)	190 (51%)	183 (49%)	0 0

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	43	ILE
1	A	53	LYS
1	A	55	GLU
1	A	57	SER
1	A	58	SER
1	A	59	ASP
1	A	62	THR
1	A	66	THR
1	A	69	MET
1	A	70	SER
1	A	72	THR
1	A	77	LEU
1	A	78	SER
1	A	81	LYS
1	A	82	ASN
1	A	85	LEU
1	A	86	LYS
1	A	89	ARG
1	A	91	LEU
1	A	92	LEU

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Mol	Chain	Res	Type
1	A	94	LEU
1	A	96	LEU
1	A	97	LEU
1	A	99	SER
1	A	104	ILE
1	A	105	LYS
1	A	108	VAL
1	A	112	GLN
1	A	114	GLN
1	A	116	GLU
1	A	121	VAL
1	A	123	LEU
1	A	128	SER
1	A	129	SER
1	A	130	LYS
1	A	132	VAL
1	A	138	THR
1	A	142	ARG
1	A	149	LEU
1	A	150	LEU
1	A	152	LEU
1	A	154	ILE
1	A	156	LEU
1	A	157	TYR
1	A	159	SER
1	A	160	GLU
1	A	162	VAL
1	A	168	VAL
1	A	171	LEU
1	A	173	VAL
1	A	177	ARG
1	A	179	THR
1	A	181	ASP
1	A	187	VAL
1	A	189	ARG
1	B	33	GLU
1	B	35	LEU
1	B	41	LYS
1	B	43	ILE
1	B	44	LYS
1	B	46	ILE
1	B	49	TYR

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Mol	Chain	Res	Type
1	B	51	ILE
1	B	52	SER
1	B	53	LYS
1	B	55	GLU
1	B	58	SER
1	B	59	ASP
1	B	62	THR
1	B	66	THR
1	B	69	MET
1	B	70	SER
1	B	72	THR
1	B	75	HIS
1	B	77	LEU
1	B	78	SER
1	B	82	ASN
1	B	86	LYS
1	B	89	ARG
1	B	90	VAL
1	B	92	LEU
1	B	94	LEU
1	B	96	LEU
1	B	97	LEU
1	B	99	SER
1	B	103	ARG
1	B	104	ILE
1	B	108	VAL
1	B	110	GLU
1	B	112	GLN
1	B	114	GLN
1	B	123	LEU
1	B	127	ASP
1	B	128	SER
1	B	130	LYS
1	B	139	ASP
1	B	142	ARG
1	B	149	LEU
1	B	151	ASN
1	B	153	GLN
1	B	154	ILE
1	B	156	LEU
1	B	157	TYR
1	B	162	VAL

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Mol	Chain	Res	Type
1	B	167	VAL
1	B	169	VAL
1	B	171	LEU
1	B	172	GLU
1	B	173	VAL
1	B	174	GLU
1	B	177	ARG
1	B	179	THR
1	B	181	ASP
1	B	182	ASP
1	B	183	PHE
1	B	185	THR
1	B	187	VAL
1	C	26	ARG
1	C	28	GLN
1	C	35	LEU
1	C	41	LYS
1	C	43	ILE
1	C	46	ILE
1	C	52	SER
1	C	53	LYS
1	C	55	GLU
1	C	58	SER
1	C	61	ILE
1	C	62	THR
1	C	64	LYS
1	C	66	THR
1	C	69	MET
1	C	70	SER
1	C	73	LEU
1	C	76	GLU
1	C	77	LEU
1	C	83	LYS
1	C	85	LEU
1	C	86	LYS
1	C	87	VAL
1	C	90	VAL
1	C	91	LEU
1	C	92	LEU
1	C	94	LEU
1	C	96	LEU
1	C	97	LEU

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Mol	Chain	Res	Type
1	C	99	SER
1	C	103	ARG
1	C	104	ILE
1	C	105	LYS
1	C	108	VAL
1	C	114	GLN
1	C	116	GLU
1	C	120	GLN
1	C	123	LEU
1	C	128	SER
1	C	136	MET
1	C	139	ASP
1	C	142	ARG
1	C	149	LEU
1	C	150	LEU
1	C	152	LEU
1	C	153	GLN
1	C	154	ILE
1	C	156	LEU
1	C	157	TYR
1	C	160	GLU
1	C	169	VAL
1	C	170	HIS
1	C	171	LEU
1	C	172	GLU
1	C	173	VAL
1	C	176	VAL
1	C	177	ARG
1	C	179	THR
1	C	180	PHE
1	C	181	ASP
1	C	182	ASP
1	C	183	PHE
1	C	185	THR
1	C	187	VAL
1	C	189	ARG

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	82	ASN
1	A	112	GLN

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Mol	Chain	Res	Type
1	A	151	ASN
1	A	153	GLN
1	B	28	GLN
1	C	67	ASN
1	C	82	ASN
1	C	153	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	P6G	B	2001	-	18,18,18	0.73	0	17,17,17	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P6G	B	2001	-	-	4/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

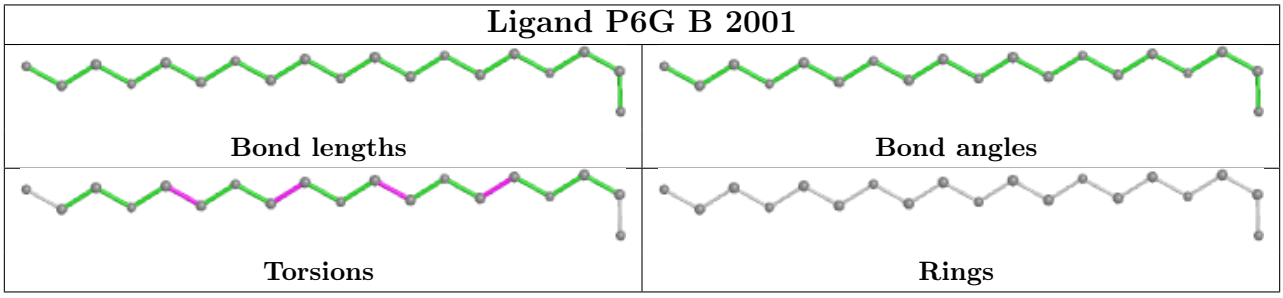
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	P6G	O7-C8-C9-O10
3	B	2001	P6G	O10-C11-C12-O13
3	B	2001	P6G	O4-C5-C6-O7
3	B	2001	P6G	O13-C14-C15-O16

There are no ring outliers.

No monomer is involved in short contacts.

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.



5.7 Other polymers

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

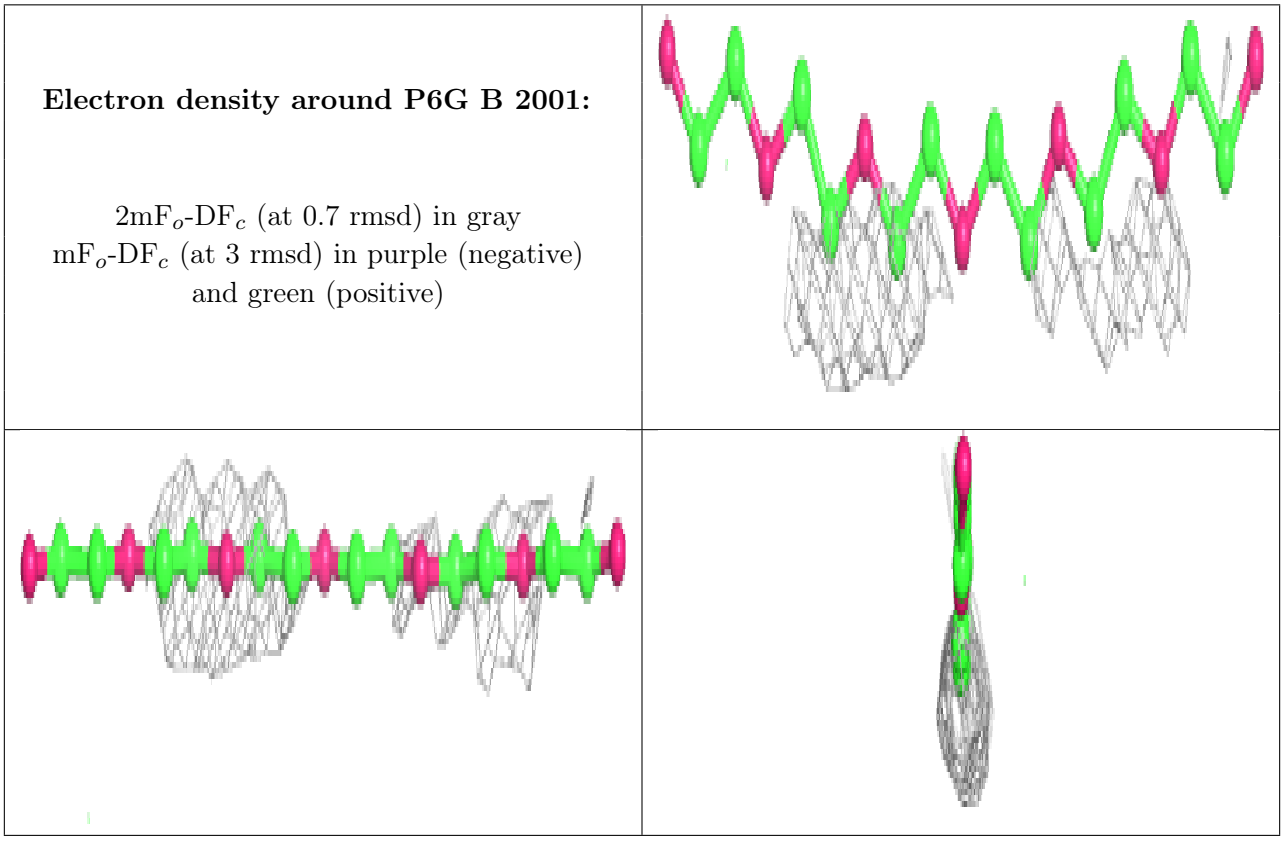
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 P6G B 2001:

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



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.