Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 02:54 PM EDT

PDB ID	:	1RZO
Title	:	Agglutinin from Ricinus communis with galactoaza
Authors	:	Gabdoulkhakov, A.G.; Savochkina, Y.; Konareva, N.; Krauspenhaar, R.; Stoeva, S.; Nikonov, S.V.; Voelter, W.; Betzel, C.; Mikhailov, A.M.
Deposited on	:	2003-12-26
Resolution	:	2.63 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:

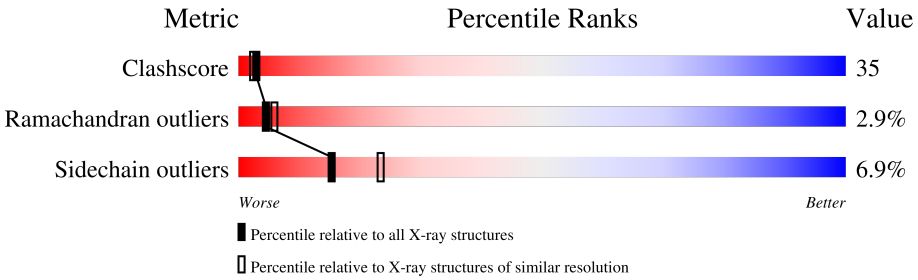
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.63 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	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	262	49% 47% • •
1	C	262	52% 42% 5% •
2	B	262	42% 52% 6%
2	D	262	31% 59% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8759 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.

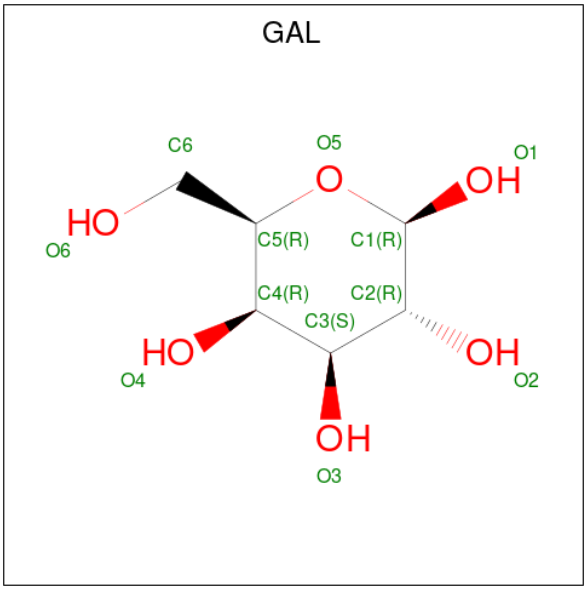
- Molecule 1 is a protein called Agglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2038	1289	356	385	8			
1	C	260	Total	C	N	O	S	0	0	0
			2045	1294	357	386	8			

- Molecule 2 is a protein called Agglutinin.

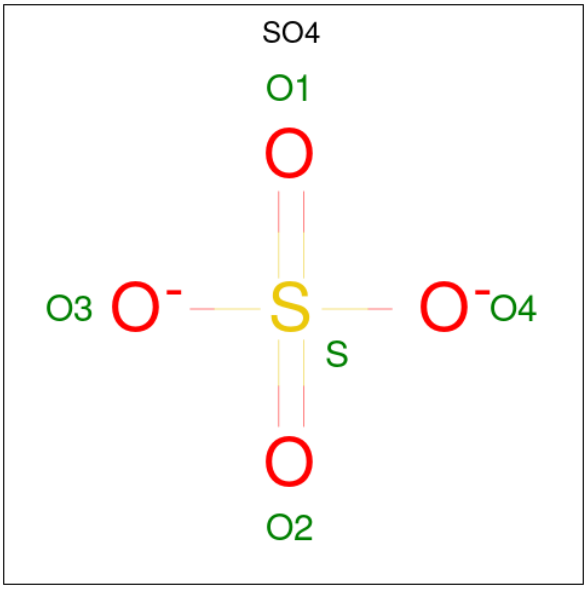
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	0	0
			2044	1284	363	385	12			
2	D	262	Total	C	N	O	S	0	0	0
			2044	1284	363	385	12			

- Molecule 3 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	B	1	Total C O 12 6 6	0	0
3	C	1	Total C O 12 6 6	0	0
3	D	1	Total C O 12 6 6	0	0
3	D	1	Total C O 12 6 6	0	0
3	D	1	Total C O 12 6 6	0	0
3	D	1	Total C O 12 6 6	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	131	Total O 131 131	0	0
5	B	117	Total O 117 117	0	0
5	C	82	Total O 82 82	0	0
5	D	76	Total O 76 76	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

Note EDS was not executed.

• Molecule 1: Agglutinin

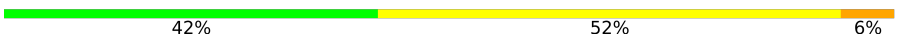
Chain A:

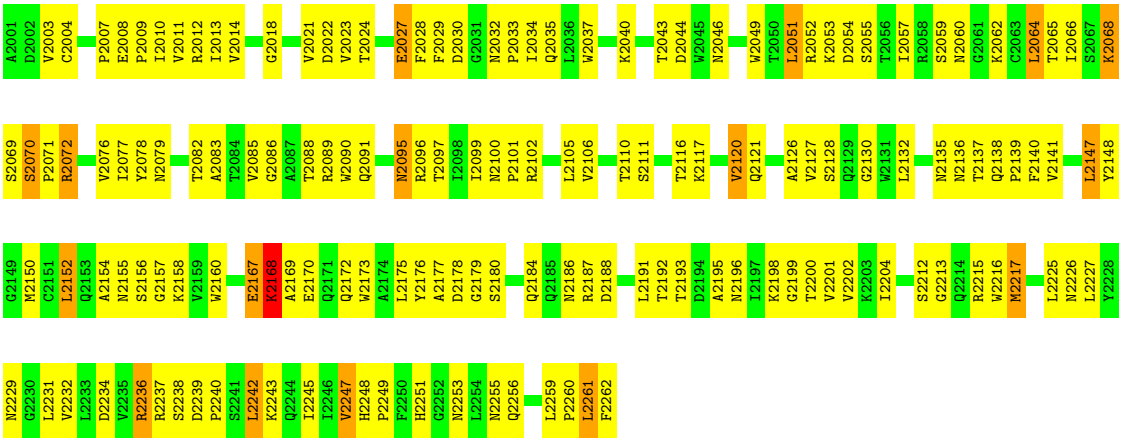
• Molecule 1: Agglutinin

Chain C:

• Molecule 2: Agglutinin

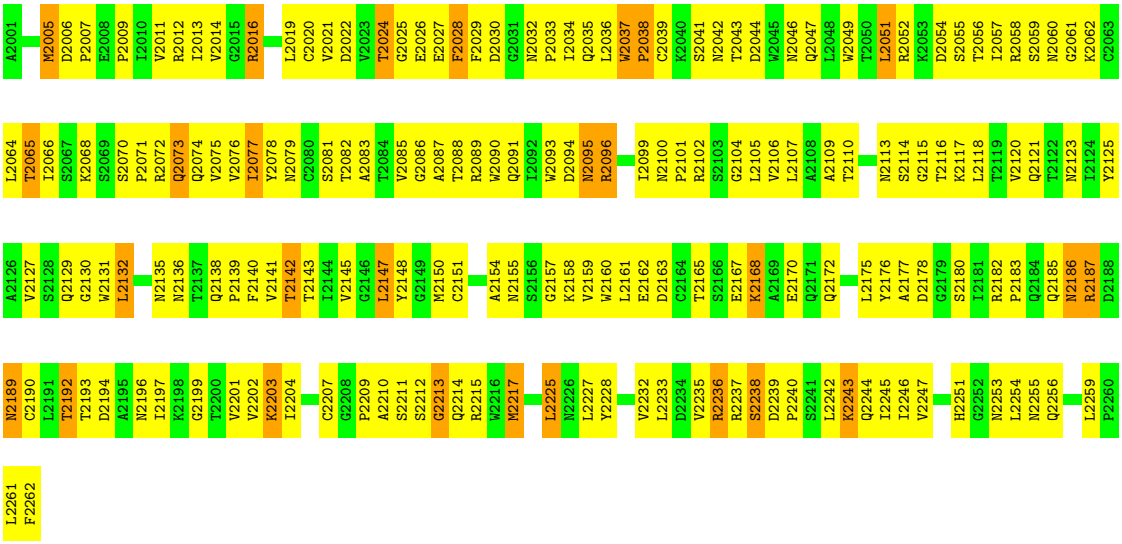
Chain B:





- Molecule 2: Agglutinin

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	97.63Å 97.63Å 207.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.11 – 2.63	Depositor
% Data completeness (in resolution range)	99.6 (26.11-2.63)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å^2)	61.0	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: GAL, SO4

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	0/2083	0.68	0/2836
1	C	0.43	0/2091	0.63	0/2847
2	B	0.44	0/2089	0.75	1/2850 (0.0%)
2	D	0.36	0/2089	0.71	0/2850
All	All	0.42	0/8352	0.69	1/11383 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2064	LEU	N-CA-C	-5.09	97.25	111.00

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	2038	0	1998	110	0
1	C	2045	0	2006	122	0
2	B	2044	0	2015	149	0
2	D	2044	0	2015	212	0
3	A	12	0	11	2	0
3	B	60	0	55	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	12	0	11	0	0
3	D	48	0	45	2	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	131	0	0	5	0
5	B	117	0	0	10	0
5	C	82	0	0	1	0
5	D	76	0	0	5	0
All	All	8759	0	8156	573	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 35.

All (573) 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)
2:D:2033:PRO:HA	2:D:2076:VAL:HG12	1.40	1.02
1:C:1246:ILE:H	1:C:1246:ILE:HD12	1.29	0.97
2:D:2159:VAL:HG22	2:D:2203:LYS:HA	1.48	0.94
2:D:2072:ARG:HG2	2:D:2121:GLN:HE22	1.32	0.93
2:D:2225:LEU:HB2	2:D:2232:VAL:HG12	1.51	0.92
1:C:1047:ASN:ND2	1:C:1049:VAL:HG22	1.89	0.87
2:D:2127:VAL:HB	2:D:2210:ALA:HB1	1.59	0.85
2:D:2190:CYS:O	2:D:2192:THR:HG22	1.75	0.84
1:C:1125:ARG:HH11	1:C:1128:GLN:HG2	1.43	0.82
2:B:2086:GLY:CA	2:B:2102:ARG:HG3	2.10	0.82
2:B:2062:LYS:HB3	2:B:2077:ILE:HG13	1.62	0.81
2:D:2070:SER:O	2:D:2073:GLN:HB2	1.79	0.81
1:C:1233:ARG:HD2	1:C:1237:SER:OG	1.80	0.81
1:C:1182:TYR:HA	2:D:2259:LEU:HD11	1.62	0.80
2:D:2145:VAL:HG21	2:D:2261:LEU:HD12	1.63	0.79
2:D:2138:GLN:HE21	2:D:2139:PRO:HD2	1.47	0.78
2:B:2078:TYR:HD2	2:B:2083:ALA:HB2	1.46	0.78
1:C:1075:ASP:HB3	1:C:1078:ASN:HD21	1.47	0.77
2:B:2033:PRO:HA	2:B:2076:VAL:HG12	1.66	0.77
2:D:2150:MET:HE1	2:D:2240:PRO:HG3	1.64	0.77
2:D:2072:ARG:CG	2:D:2121:GLN:HE22	1.98	0.77
1:A:1156:CYS:HG	1:C:1156:CYS:HG	0.77	0.76
2:B:2176:TYR:OH	2:B:2187:ARG:HD3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1185:GLY:HA3	2:D:2259:LEU:HD22	1.68	0.76
1:C:1228:PRO:HB2	1:C:1240:ASN:HB3	1.67	0.76
2:D:2024:THR:HA	2:D:2035:GLN:HE21	1.50	0.76
2:D:2148:TYR:HB2	2:D:2150:MET:HE2	1.68	0.75
2:B:2070:SER:HB3	2:B:2071:PRO:CD	2.16	0.75
2:D:2034:ILE:HG12	2:D:2076:VAL:HA	1.68	0.75
2:B:2070:SER:HB3	2:B:2071:PRO:HD3	1.67	0.74
2:D:2086:GLY:HA3	2:D:2102:ARG:HG3	1.68	0.74
2:B:2079:ASN:ND2	3:B:5005:GAL:H5	2.03	0.74
2:D:2024:THR:HG22	2:D:2035:GLN:HB3	1.69	0.74
2:D:2138:GLN:NE2	2:D:2139:PRO:HD2	2.03	0.74
2:D:2079:ASN:HB3	2:D:2082:THR:OG1	1.89	0.73
2:B:2068:LYS:HD3	2:B:2068:LYS:H	1.54	0.73
2:B:2139:PRO:HG2	2:B:2187:ARG:NH1	2.03	0.73
1:C:1062:LEU:HB3	1:C:1147:ILE:CD1	2.18	0.72
2:D:2037:TRP:HA	2:D:2037:TRP:CE3	2.24	0.72
2:D:2130:GLY:HA2	2:D:2215:ARG:HH21	1.53	0.72
2:B:2078:TYR:CD2	2:B:2083:ALA:HB2	2.24	0.72
2:D:2012:ARG:HH22	2:D:2041:SER:HA	1.54	0.72
1:C:1047:ASN:HD21	1:C:1049:VAL:HG22	1.53	0.72
2:D:2032:ASN:OD1	2:D:2033:PRO:HD2	1.90	0.71
1:A:1063:SER:HA	1:A:1068:LEU:O	1.91	0.71
2:B:2259:LEU:HD12	2:B:2260:PRO:HD2	1.71	0.71
1:C:1246:ILE:H	1:C:1246:ILE:CD1	2.04	0.71
1:C:1085:ARG:HG2	1:C:1085:ARG:HH11	1.57	0.70
1:C:1081:VAL:CG1	1:C:1171:ILE:HG12	2.22	0.69
1:A:1018:VAL:HG11	1:A:1192:ARG:HG2	1.73	0.69
1:A:1143:LEU:O	1:A:1147:ILE:HG13	1.92	0.69
2:D:2037:TRP:HA	2:D:2037:TRP:HE3	1.56	0.69
2:D:2078:TYR:CD1	2:D:2083:ALA:HB2	2.26	0.69
1:C:1047:ASN:HB2	1:C:1256:TYR:CD1	2.27	0.69
2:D:2066:ILE:HG13	2:D:2066:ILE:O	1.91	0.69
1:A:1132:LEU:HB3	1:A:1134:GLU:HG2	1.75	0.69
2:B:2030:ASP:HB3	2:B:2078:TYR:CE1	2.28	0.69
2:D:2022:ASP:HB2	2:D:2037:TRP:HB2	1.74	0.69
2:B:2202:VAL:O	5:B:7376:HOH:O	2.11	0.69
2:B:2068:LYS:HD3	2:B:2068:LYS:N	2.08	0.69
2:D:2183:PRO:HD2	2:D:2189:ASN:O	1.93	0.68
2:B:2089:ARG:NH1	2:B:2102:ARG:HH21	1.91	0.68
2:D:2161:LEU:HD22	2:D:2235:VAL:HG11	1.74	0.68
2:D:2212:SER:HB3	2:D:2228:TYR:CB	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:VAL:O	1:A:1207:GLU:HG3	1.94	0.68
2:D:2099:ILE:O	2:D:2101:PRO:HD3	1.93	0.68
2:D:2239:ASP:HB3	2:D:2242:LEU:HG	1.75	0.68
1:C:1086:ALA:HB1	1:C:1151:TYR:HA	1.76	0.68
2:D:2068:LYS:HB3	2:D:2073:GLN:HG2	1.75	0.68
1:A:1093:PHE:O	1:A:1095:PRO:HD3	1.94	0.68
1:A:1099:GLU:HG3	5:A:7100:HOH:O	1.94	0.68
2:D:2014:VAL:HG22	2:D:2020:CYS:SG	2.33	0.67
2:D:2022:ASP:CB	2:D:2037:TRP:HB2	2.25	0.67
2:B:2095:ASN:ND2	3:B:5002:GAL:O2	2.27	0.67
2:D:2157:GLY:O	2:D:2203:LYS:HB2	1.95	0.67
1:A:1064:ASN:HB2	1:A:1144:GLU:OE2	1.95	0.67
1:A:1064:ASN:HB2	1:A:1144:GLU:CD	2.16	0.66
1:A:1193:TYR:O	1:A:1195:ARG:HG3	1.95	0.66
2:B:2086:GLY:HA3	2:B:2102:ARG:HG3	1.76	0.66
1:C:1012:THR:HA	1:C:1063:SER:O	1.96	0.66
1:C:1075:ASP:HB3	1:C:1078:ASN:ND2	2.10	0.66
2:D:2192:THR:HB	2:D:2214:GLN:HG3	1.76	0.66
1:C:1095:PRO:HG2	1:C:1101:ALA:HA	1.77	0.66
1:A:1119:PHE:HB2	1:A:1125:ARG:HG2	1.77	0.66
1:C:1040:HIS:HD2	1:C:1244:VAL:HG11	1.60	0.66
1:A:1052:PRO:HG2	1:A:1055:GLN:CG	2.25	0.65
2:D:2072:ARG:HG2	2:D:2121:GLN:NE2	2.08	0.65
2:D:2162:GLU:HG3	2:D:2163:ASP:H	1.62	0.65
2:D:2044:ASP:C	2:D:2046:ASN:H	1.99	0.65
2:D:2086:GLY:CA	2:D:2102:ARG:HG3	2.27	0.65
2:D:2196:ASN:O	2:D:2197:ILE:HD13	1.98	0.64
2:B:2237:ARG:HD2	2:B:2242:LEU:HD21	1.78	0.64
2:B:2105:LEU:HB3	2:B:2120:VAL:HG13	1.78	0.64
1:A:1200:ASP:HB2	1:A:1201:PRO:HD2	1.79	0.64
2:B:2236:ARG:HG3	2:B:2242:LEU:HD23	1.78	0.63
2:D:2078:TYR:HE1	2:D:2082:THR:HG1	1.46	0.63
1:C:1060:VAL:HG12	1:C:1062:LEU:HD13	1.80	0.63
1:A:1150:LEU:HD12	1:A:1163:LEU:CD2	2.29	0.63
2:D:2026:GLU:HG2	2:D:2046:ASN:HB2	1.80	0.63
2:D:2207:CYS:HB2	5:D:7255:HOH:O	1.97	0.63
1:A:1097:ASN:OD1	1:A:1099:GLU:HB2	1.99	0.63
1:A:1138:LEU:CD1	1:A:1199:PRO:HG3	2.29	0.63
2:B:2079:ASN:HB3	2:B:2082:THR:HB	1.79	0.62
1:A:1090:ALA:O	1:A:1114:SER:HA	1.98	0.62
1:C:1204:ILE:O	1:C:1207:GLU:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2106:VAL:HG13	2:D:2123:ASN:HB2	1.81	0.62
2:B:2099:ILE:O	2:B:2101:PRO:HD3	2.00	0.62
2:D:2068:LYS:HB3	2:D:2073:GLN:CG	2.29	0.62
1:C:1060:VAL:HG12	1:C:1062:LEU:CD1	2.30	0.62
2:D:2159:VAL:HG13	2:D:2204:ILE:HG23	1.82	0.62
1:A:1052:PRO:HG2	1:A:1055:GLN:HG2	1.82	0.62
1:A:1234:ARG:NH1	2:B:2261:LEU:HD23	2.15	0.62
2:D:2236:ARG:HG2	2:D:2246:ILE:CG2	2.31	0.61
1:C:1119:PHE:HB2	1:C:1125:ARG:HG2	1.82	0.61
2:D:2032:ASN:HD22	2:D:2077:ILE:HD11	1.65	0.61
2:B:2160:TRP:HA	2:B:2245:ILE:CD1	2.31	0.61
1:C:1203:VAL:O	1:C:1207:GLU:HG2	2.01	0.61
1:A:1087:GLY:HA2	5:A:7154:HOH:O	2.01	0.61
1:A:1060:VAL:HG23	1:A:1060:VAL:O	2.00	0.61
1:A:1098:GLN:NE2	1:C:1098:GLN:HB2	2.16	0.61
2:D:2095:ASN:OD1	3:D:5502:GAL:O2	2.18	0.60
1:A:1010:ASN:HB2	5:A:7172:HOH:O	2.02	0.60
2:D:2150:MET:CE	2:D:2240:PRO:HG3	2.32	0.60
2:D:2064:LEU:HD23	2:D:2090:TRP:CE2	2.36	0.60
2:B:2240:PRO:HA	5:B:7042:HOH:O	2.02	0.60
1:C:1097:ASN:OD1	1:C:1099:GLU:HG2	2.02	0.59
3:B:5004:GAL:H62	5:B:7186:HOH:O	2.01	0.59
1:C:1051:LEU:HD12	1:C:1052:PRO:HD2	1.83	0.59
2:D:2140:PHE:HZ	2:D:2262:PHE:CD2	2.20	0.59
2:D:2160:TRP:CD1	2:D:2243:LYS:HG3	2.38	0.59
3:B:5005:GAL:H61	3:B:5006:GAL:H5	1.85	0.59
2:D:2052:ARG:HB3	2:D:2054:ASP:OD2	2.02	0.59
2:B:2028:PHE:CE2	2:B:2060:ASN:HB3	2.38	0.58
2:B:2111:SER:HB3	2:B:2116:THR:OG1	2.03	0.58
2:D:2024:THR:HA	2:D:2035:GLN:NE2	2.18	0.58
2:D:2068:LYS:O	2:D:2073:GLN:HG2	2.03	0.58
2:B:2040:LYS:HE3	2:B:2044:ASP:OD1	2.03	0.58
1:A:1062:LEU:O	1:A:1069:SER:HA	2.04	0.58
1:C:1196:ARG:O	1:C:1196:ARG:HG3	2.04	0.58
2:D:2235:VAL:HG22	2:D:2255:ASN:HB2	1.86	0.58
2:D:2025:GLY:H	2:D:2035:GLN:NE2	2.02	0.58
1:A:1045:LEU:HD21	1:A:1253:LEU:HD13	1.86	0.57
2:B:2184:GLN:HA	2:B:2184:GLN:OE1	2.04	0.57
3:B:5002:GAL:H61	5:B:7121:HOH:O	2.04	0.57
1:A:1200:ASP:OD2	1:A:1234:ARG:HG2	2.04	0.57
1:A:1234:ARG:HH11	2:B:2261:LEU:HD23	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2035:GLN:HA	2:D:2116:THR:O	2.04	0.57
2:D:2054:ASP:O	2:D:2055:SER:HB2	2.03	0.57
2:B:2245:ILE:N	2:B:2245:ILE:HD12	2.20	0.57
2:B:2068:LYS:H	2:B:2068:LYS:CD	2.11	0.57
2:D:2027:GLU:HG2	2:D:2029:PHE:HD2	1.67	0.57
2:B:2148:TYR:HB2	2:B:2150:MET:HG3	1.85	0.57
2:D:2251:HIS:CE1	2:D:2253:ASN:HB2	2.40	0.57
1:C:1180:PHE:CD2	1:C:1206:LEU:HG	2.39	0.56
2:B:2184:GLN:HE22	2:B:2187:ARG:HH21	1.52	0.56
1:A:1161:PRO:O	1:A:1165:ARG:HG3	2.05	0.56
1:C:1062:LEU:HB3	1:C:1147:ILE:HD13	1.87	0.56
2:B:2064:LEU:HD23	2:B:2090:TRP:CE2	2.40	0.56
2:D:2106:VAL:CG1	2:D:2123:ASN:HB2	2.35	0.56
1:A:1222:GLN:HE22	2:B:2091:GLN:HA	1.71	0.56
1:A:1024:PHE:O	1:A:1028:VAL:HG23	2.06	0.56
2:B:2193:THR:HG23	2:B:2193:THR:O	2.06	0.56
2:D:2019:LEU:HD12	2:D:2038:PRO:HA	1.88	0.56
1:A:1086:ALA:HB3	5:A:7330:HOH:O	2.06	0.56
2:B:2154:ALA:HB2	2:B:2173:TRP:CH2	2.41	0.56
1:C:1065:HIS:C	1:C:1067:GLU:H	2.08	0.56
2:D:2011:VAL:HA	2:D:2135:ASN:OD1	2.05	0.56
1:A:1075:ASP:OD1	1:A:1077:THR:HB	2.05	0.56
2:B:2132:LEU:HB2	2:B:2177:ALA:HB1	1.87	0.55
1:C:1213:LEU:CD1	1:C:1229:ILE:HG21	2.36	0.55
2:D:2162:GLU:HG3	2:D:2163:ASP:N	2.20	0.55
1:C:1167:PHE:O	1:C:1171:ILE:HG13	2.06	0.55
1:C:1228:PRO:HB3	1:C:1242:TYR:CD2	2.40	0.55
2:D:2107:LEU:HD11	2:D:2118:LEU:HD13	1.87	0.55
2:D:2154:ALA:HA	2:D:2158:LYS:O	2.07	0.55
1:A:1200:ASP:HB2	1:A:1201:PRO:CD	2.37	0.55
2:B:2079:ASN:HD22	3:B:5005:GAL:H5	1.70	0.55
2:B:2105:LEU:CB	2:B:2120:VAL:HG13	2.37	0.55
1:C:1085:ARG:HG2	1:C:1085:ARG:NH1	2.19	0.55
2:B:2052:ARG:HD3	5:B:7128:HOH:O	2.05	0.55
2:D:2125:TYR:HA	2:D:2215:ARG:NH1	2.22	0.55
2:B:2132:LEU:HD22	2:B:2177:ALA:HA	1.88	0.55
2:B:2136:ASN:HA	5:B:7053:HOH:O	2.07	0.55
2:B:2152:LEU:HD21	2:B:2245:ILE:HG12	1.88	0.55
1:A:1091:TYR:HA	1:A:1115:PHE:O	2.06	0.55
2:D:2012:ARG:NH2	2:D:2041:SER:HA	2.21	0.55
1:C:1062:LEU:HB3	1:C:1147:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2013:ILE:N	2:D:2013:ILE:HD12	2.22	0.55
1:A:1213:LEU:HD22	1:A:1247:LEU:HD13	1.89	0.54
2:D:2176:TYR:CD1	2:D:2182:ARG:HD3	2.42	0.54
2:B:2186:ASN:OD1	2:B:2188:ASP:HB2	2.06	0.54
1:A:1138:LEU:HD12	1:A:1199:PRO:HG3	1.88	0.54
1:C:1200:ASP:HB2	1:C:1201:PRO:HD2	1.89	0.54
1:A:1221:ASN:O	1:A:1222:GLN:HG3	2.08	0.54
1:A:1086:ALA:HB1	1:A:1151:TYR:HA	1.89	0.54
1:C:1101:ALA:O	1:C:1105:THR:HG23	2.07	0.54
2:B:2051:LEU:N	2:B:2051:LEU:CD1	2.70	0.54
2:B:2079:ASN:ND2	3:B:5005:GAL:C5	2.71	0.54
1:C:1215:THR:HG22	1:C:1216:ALA:N	2.22	0.54
2:D:2095:ASN:O	2:D:2096:ARG:HB2	2.08	0.54
2:D:2072:ARG:HA	2:D:2121:GLN:OE1	2.08	0.54
2:B:2155:ASN:HD21	2:B:2170:GLU:HG2	1.71	0.54
2:D:2132:LEU:HB2	2:D:2177:ALA:HB1	1.89	0.54
2:D:2044:ASP:C	2:D:2046:ASN:N	2.62	0.53
1:A:1051:LEU:HD12	1:A:1052:PRO:HD2	1.91	0.53
1:A:1176:GLU:OE2	1:A:1207:GLU:HB3	2.09	0.53
1:C:1095:PRO:HG3	1:C:1104:ILE:HD13	1.91	0.53
1:C:1117:PHE:HB3	1:C:1119:PHE:CE1	2.44	0.53
2:B:2155:ASN:HB2	2:B:2160:TRP:CZ3	2.44	0.53
2:B:2239:ASP:HB3	2:B:2242:LEU:HD22	1.89	0.53
1:C:1085:ARG:NH1	1:C:1087:GLY:O	2.42	0.53
2:B:2049:TRP:HE3	2:B:2057:ILE:O	1.91	0.53
2:D:2127:VAL:HB	2:D:2210:ALA:CB	2.36	0.53
1:A:1048:ARG:HH22	1:A:1100:ASP:CG	2.12	0.53
1:A:1248:ILE:N	1:A:1249:PRO:HD2	2.22	0.53
2:B:2009:PRO:HG2	2:B:2051:LEU:HD22	1.91	0.53
2:D:2247:VAL:HG23	2:D:2247:VAL:O	2.08	0.53
1:A:1039:ARG:CZ	1:A:1260:PRO:HG3	2.39	0.53
2:D:2147:LEU:O	2:D:2150:MET:HB2	2.09	0.53
2:D:2212:SER:HB3	2:D:2228:TYR:HB2	1.91	0.53
1:A:1010:ASN:ND2	3:A:5001:GAL:O3	2.42	0.52
1:A:1176:GLU:OE1	1:A:1179:ARG:HD2	2.09	0.52
2:D:2042:ASN:C	2:D:2044:ASP:H	2.13	0.52
1:A:1232:GLN:HG2	1:A:1238:LYS:HG2	1.89	0.52
2:D:2155:ASN:HB2	2:D:2160:TRP:CH2	2.44	0.52
2:D:2155:ASN:HB2	2:D:2160:TRP:HH2	1.75	0.52
2:D:2159:VAL:CG2	2:D:2203:LYS:HA	2.32	0.52
2:B:2070:SER:HA	5:B:7181:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1192:ARG:HG3	1:C:1193:TYR:CD1	2.44	0.52
2:D:2006:ASP:OD2	2:D:2006:ASP:N	2.43	0.52
2:D:2028:PHE:N	2:D:2028:PHE:CD2	2.78	0.52
2:D:2125:TYR:HD1	2:D:2215:ARG:HH12	1.58	0.52
2:D:2165:THR:HB	2:D:2168:LYS:HB2	1.90	0.52
1:A:1046:PRO:HD2	1:A:1076:VAL:HG12	1.91	0.52
1:C:1127:GLU:OE1	1:C:1133:ARG:HD3	2.09	0.52
2:D:2135:ASN:ND2	3:D:5503:GAL:O2	2.42	0.52
2:B:2030:ASP:HB3	2:B:2078:TYR:CD1	2.45	0.52
2:D:2019:LEU:HB2	2:D:2036:LEU:HG	1.92	0.51
1:A:1004:LYS:HD2	1:A:1004:LYS:N	2.25	0.51
1:C:1213:LEU:HD11	1:C:1229:ILE:HG21	1.91	0.51
1:A:1200:ASP:OD2	1:A:1202:SER:OG	2.28	0.51
2:D:2049:TRP:CE3	2:D:2057:ILE:HG22	2.46	0.51
2:B:2029:PHE:O	2:B:2029:PHE:CD1	2.63	0.51
1:A:1047:ASN:O	1:A:1051:LEU:HB2	2.11	0.51
2:B:2155:ASN:O	2:B:2156:SER:HB3	2.11	0.51
2:B:2072:ARG:HB3	5:B:7165:HOH:O	2.09	0.51
2:D:2052:ARG:HD3	2:D:2058:ARG:HD3	1.93	0.51
1:C:1113:ASN:C	1:C:1113:ASN:HD22	2.14	0.51
1:C:1161:PRO:O	1:C:1164:ALA:HB3	2.11	0.51
1:A:1048:ARG:NH2	1:A:1100:ASP:OD1	2.44	0.51
2:B:2157:GLY:HA2	2:B:2204:ILE:HB	1.93	0.51
1:C:1033:THR:HG23	1:C:1033:THR:O	2.10	0.51
2:D:2033:PRO:CA	2:D:2076:VAL:HG12	2.29	0.51
2:D:2193:THR:O	2:D:2193:THR:HG23	2.11	0.51
1:A:1095:PRO:HG2	1:A:1101:ALA:HA	1.92	0.50
2:B:2065:THR:OG1	2:B:2088:THR:HG22	2.11	0.50
2:D:2022:ASP:HB3	2:D:2035:GLN:HG3	1.93	0.50
1:C:1219:GLU:HG3	1:C:1219:GLU:O	2.12	0.50
2:B:2013:ILE:O	2:B:2021:VAL:HG23	2.11	0.50
1:C:1200:ASP:HB2	1:C:1201:PRO:CD	2.42	0.50
1:C:1226:ALA:HA	2:D:2009:PRO:HB3	1.94	0.50
2:D:2032:ASN:HB3	2:D:2077:ILE:HD11	1.93	0.50
2:D:2180:SER:HA	2:D:2214:GLN:O	2.12	0.50
1:C:1006:TYR:HB3	1:C:1007:PRO:HD2	1.93	0.50
1:C:1201:PRO:HB3	1:C:1232:GLN:OE1	2.12	0.50
2:D:2079:ASN:OD1	2:D:2081:SER:HB2	2.12	0.50
2:B:2022:ASP:OD1	2:B:2037:TRP:CB	2.60	0.50
1:C:1234:ARG:NH2	2:D:2261:LEU:HB3	2.27	0.50
2:D:2212:SER:HB3	2:D:2228:TYR:CG	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2024:THR:HA	2:B:2035:GLN:NE2	2.27	0.50
2:B:2069:SER:O	2:B:2071:PRO:HD2	2.12	0.50
2:D:2240:PRO:O	2:D:2243:LYS:HD2	2.12	0.50
2:B:2022:ASP:OD2	2:B:2023:VAL:N	2.45	0.49
2:D:2034:ILE:O	2:D:2118:LEU:HG	2.11	0.49
1:A:1043:PRO:HD2	1:A:1252:ALA:O	2.12	0.49
1:A:1085:ARG:NH1	1:A:1087:GLY:O	2.45	0.49
2:D:2237:ARG:NE	2:D:2237:ARG:HA	2.28	0.49
1:A:1226:ALA:HB2	2:B:2007:PRO:CB	2.43	0.49
2:B:2085:VAL:HG23	2:B:2086:GLY:N	2.27	0.49
1:C:1125:ARG:NH1	1:C:1128:GLN:HG2	2.19	0.49
2:D:2199:GLY:HA2	2:D:2246:ILE:HD12	1.94	0.49
2:D:2209:PRO:HG2	2:D:2214:GLN:HE22	1.76	0.49
2:B:2095:ASN:OD1	2:B:2095:ASN:N	2.45	0.49
2:B:2217:MET:HB2	2:B:2227:LEU:HD21	1.92	0.49
2:B:2003:VAL:HG12	2:B:2004:CYS:N	2.27	0.49
1:C:1018:VAL:HG23	1:C:1019:GLU:N	2.27	0.49
1:C:1185:GLY:HA3	2:D:2259:LEU:CD2	2.38	0.49
2:B:2196:ASN:HD22	2:B:2229:ASN:HD22	1.60	0.49
1:C:1255:VAL:HG13	1:C:1257:ARG:HD3	1.94	0.49
2:D:2078:TYR:CG	2:D:2083:ALA:HB2	2.47	0.49
2:D:2064:LEU:HD23	2:D:2090:TRP:NE1	2.26	0.49
2:D:2085:VAL:HG12	2:D:2089:ARG:HD3	1.94	0.49
1:A:1181:GLN:OE1	1:A:1252:ALA:HB2	2.13	0.49
2:D:2062:LYS:HD2	2:D:2078:TYR:C	2.32	0.49
2:D:2235:VAL:HG23	2:D:2238:SER:HA	1.94	0.49
1:A:1075:ASP:HB3	1:A:1078:ASN:OD1	2.13	0.49
1:A:1101:ALA:O	1:A:1105:THR:HG23	2.13	0.49
1:A:1123:TYR:CD2	1:A:1133:ARG:NH1	2.81	0.49
2:B:2160:TRP:HA	2:B:2245:ILE:HD13	1.95	0.49
2:B:2200:THR:HB	2:B:2247:VAL:CG2	2.43	0.49
2:D:2236:ARG:HG2	2:D:2246:ILE:HG23	1.93	0.49
1:C:1039:ARG:O	1:C:1040:HIS:HB2	2.13	0.49
1:C:1078:ASN:HD22	1:C:1078:ASN:N	2.11	0.49
1:C:1190:ARG:HG3	1:C:1190:ARG:HH11	1.77	0.48
2:D:2036:LEU:HD13	2:D:2118:LEU:HD21	1.95	0.48
2:D:2123:ASN:HA	2:D:2129:GLN:HE22	1.78	0.48
1:A:1228:PRO:HB2	1:A:1240:ASN:OD1	2.13	0.48
2:B:2054:ASP:O	2:B:2055:SER:HB2	2.12	0.48
2:B:2059:SER:O	2:B:2060:ASN:HB3	2.13	0.48
2:B:2065:THR:HG22	2:B:2066:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2142:THR:OG1	2:D:2143:THR:N	2.46	0.48
2:D:2176:TYR:OH	2:D:2187:ARG:HD3	2.13	0.48
2:B:2011:VAL:HA	2:B:2135:ASN:OD1	2.13	0.48
2:D:2044:ASP:HB3	2:D:2046:ASN:HB3	1.94	0.48
2:B:2012:ARG:HD2	2:B:2137:THR:CG2	2.43	0.48
1:C:1091:TYR:N	1:C:1091:TYR:CD1	2.80	0.48
2:D:2217:MET:HE3	5:D:7275:HOH:O	2.12	0.48
2:D:2254:LEU:HD23	5:D:7316:HOH:O	2.13	0.48
2:B:2251:HIS:CE1	2:B:2253:ASN:HB2	2.48	0.48
1:C:1183:ILE:HG12	1:C:1203:VAL:HG13	1.96	0.48
2:D:2062:LYS:HE2	2:D:2079:ASN:HA	1.95	0.48
1:C:1223:GLY:O	1:C:1243:ASP:HA	2.14	0.48
1:A:1112:GLN:NE2	1:C:1160:ILE:HB	2.28	0.48
2:B:2158:LYS:HD2	5:B:7376:HOH:O	2.13	0.48
2:D:2013:ILE:HB	2:D:2021:VAL:HG22	1.95	0.48
2:D:2038:PRO:O	2:D:2047:GLN:NE2	2.47	0.48
1:A:1141:GLY:HA3	1:A:1196:ARG:NH2	2.29	0.48
1:A:1185:GLY:HA3	2:B:2259:LEU:HD22	1.94	0.48
2:B:2169:ALA:HA	2:B:2172:GLN:HG2	1.95	0.48
2:B:2086:GLY:HA2	2:B:2102:ARG:HG3	1.94	0.47
2:D:2025:GLY:H	2:D:2035:GLN:HE21	1.60	0.47
2:B:2029:PHE:O	2:B:2030:ASP:C	2.52	0.47
2:D:2160:TRP:HA	2:D:2245:ILE:HD13	1.96	0.47
1:A:1138:LEU:HD11	1:A:1199:PRO:HG3	1.95	0.47
2:B:2213:GLY:HA2	2:B:2226:ASN:HD21	1.79	0.47
1:C:1037:ASP:O	1:C:1044:VAL:HB	2.15	0.47
1:C:1099:GLU:CD	1:C:1099:GLU:H	2.16	0.47
2:D:2049:TRP:HE3	2:D:2057:ILE:HG22	1.78	0.47
2:B:2160:TRP:HB2	2:B:2243:LYS:HA	1.95	0.47
1:C:1034:THR:HG22	1:C:1035:GLY:N	2.30	0.47
2:D:2116:THR:CG2	2:D:2117:LYS:N	2.78	0.47
2:B:2096:ARG:O	2:B:2130:GLY:HA2	2.14	0.47
2:D:2005:MET:O	2:D:2005:MET:SD	2.73	0.47
2:B:2008:GLU:OE2	2:B:2053:LYS:HG2	2.13	0.47
2:B:2099:ILE:HG13	2:B:2106:VAL:HG12	1.97	0.47
2:B:2141:VAL:HG22	2:B:2184:GLN:HE22	1.79	0.47
1:C:1040:HIS:CD2	1:C:1244:VAL:HG11	2.45	0.47
2:D:2125:TYR:HD1	2:D:2215:ARG:NH1	2.13	0.47
1:A:1060:VAL:HG22	1:A:1072:LEU:HB2	1.97	0.47
1:A:1188:ARG:O	1:A:1192:ARG:HB2	2.13	0.47
1:C:1249:PRO:HG2	1:C:1250:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2236:ARG:HG3	2:D:2244:GLN:OE1	2.15	0.47
1:C:1035:GLY:O	1:C:1036:ALA:HB3	2.14	0.46
1:A:1040:HIS:HD2	1:A:1244:VAL:HG11	1.80	0.46
2:D:2236:ARG:HG2	2:D:2246:ILE:HG21	1.97	0.46
1:A:1090:ALA:HB3	1:A:1114:SER:HB3	1.96	0.46
1:A:1242:TYR:CE1	2:B:2136:ASN:HB2	2.50	0.46
1:C:1053:ILE:HG23	1:C:1054:SER:N	2.31	0.46
2:D:2012:ARG:HH22	2:D:2042:ASN:H	1.64	0.46
2:D:2202:VAL:HG13	2:D:2245:ILE:O	2.15	0.46
1:A:1053:ILE:HG23	1:A:1054:SER:N	2.30	0.46
2:B:2032:ASN:OD1	2:B:2033:PRO:HD2	2.15	0.46
2:B:2095:ASN:O	2:B:2096:ARG:HB2	2.15	0.46
2:B:2196:ASN:HB3	2:B:2229:ASN:HB3	1.97	0.46
2:B:2198:LYS:HG2	2:B:2199:GLY:N	2.31	0.46
1:C:1242:TYR:CE1	2:D:2136:ASN:HB2	2.51	0.46
2:D:2157:GLY:HA2	2:D:2204:ILE:HG12	1.98	0.46
2:D:2182:ARG:HG2	2:D:2189:ASN:O	2.15	0.46
1:A:1074:LEU:CD2	1:A:1081:VAL:HG22	2.45	0.46
1:C:1180:PHE:CD1	1:C:1180:PHE:N	2.84	0.46
2:D:2019:LEU:HB3	2:D:2036:LEU:O	2.15	0.46
2:B:2079:ASN:HB3	2:B:2082:THR:CB	2.45	0.46
2:D:2168:LYS:HE2	2:D:2170:GLU:OE1	2.15	0.46
1:A:1231:LEU:O	1:A:1238:LYS:HA	2.17	0.45
2:B:2010:ILE:N	2:B:2010:ILE:HD12	2.31	0.45
1:C:1221:ASN:ND2	2:D:2007:PRO:O	2.49	0.45
2:D:2196:ASN:C	2:D:2197:ILE:HD13	2.36	0.45
1:C:1065:HIS:C	1:C:1067:GLU:N	2.70	0.45
1:A:1060:VAL:CG2	1:A:1072:LEU:HB2	2.47	0.45
2:B:2012:ARG:HD2	2:B:2137:THR:HG21	1.98	0.45
2:B:2110:THR:HG22	2:B:2121:GLN:NE2	2.32	0.45
1:C:1022:THR:O	1:C:1026:ARG:HG3	2.17	0.45
2:D:2016:ARG:N	2:D:2178:ASP:HB3	2.31	0.45
2:B:2198:LYS:HG3	2:B:2249:PRO:HD3	1.99	0.45
2:D:2125:TYR:HB3	2:D:2227:LEU:HB2	1.97	0.45
2:D:2062:LYS:CD	2:D:2079:ASN:HA	2.46	0.45
1:A:1140:THR:HG23	1:A:1191:ILE:HG12	1.99	0.45
2:B:2089:ARG:HH12	2:B:2102:ARG:HH21	1.64	0.45
2:B:2237:ARG:C	2:B:2239:ASP:N	2.68	0.45
1:C:1078:ASN:O	1:C:1179:ARG:NH2	2.44	0.45
1:C:1202:SER:OG	1:C:1203:VAL:N	2.50	0.45
2:D:2148:TYR:CD1	2:D:2150:MET:HE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:PRO:CG	1:A:1104:ILE:HD13	2.47	0.45
2:B:2237:ARG:NH2	5:B:7192:HOH:O	2.50	0.45
2:D:2093:TRP:HB3	2:D:2095:ASN:HD21	1.82	0.45
2:D:2251:HIS:CE1	2:D:2256:GLN:HG3	2.52	0.45
2:B:2126:ALA:HA	2:B:2212:SER:HA	1.99	0.45
2:D:2036:LEU:HD22	2:D:2109:ALA:HB1	1.99	0.45
2:D:2107:LEU:HG	2:D:2131:TRP:CZ2	2.52	0.45
2:B:2023:VAL:HB	2:B:2046:ASN:HB2	1.98	0.44
2:D:2021:VAL:HG23	2:D:2021:VAL:O	2.16	0.44
2:D:2064:LEU:HB3	2:D:2090:TRP:NE1	2.33	0.44
2:D:2066:ILE:O	2:D:2066:ILE:CG1	2.64	0.44
2:D:2095:ASN:H	2:D:2095:ASN:ND2	2.15	0.44
1:A:1073:ALA:C	1:A:1074:LEU:HD23	2.38	0.44
1:C:1034:THR:C	1:C:1036:ALA:H	2.20	0.44
2:D:2217:MET:HA	5:D:7329:HOH:O	2.17	0.44
1:A:1009:ILE:N	1:A:1009:ILE:HD12	2.32	0.44
1:C:1040:HIS:HA	2:D:2094:ASP:OD1	2.17	0.44
1:A:1180:PHE:CD1	1:A:1183:ILE:HD12	2.53	0.44
1:C:1180:PHE:CE2	1:C:1206:LEU:HG	2.53	0.44
2:D:2028:PHE:N	2:D:2028:PHE:HD2	2.16	0.44
2:D:2032:ASN:ND2	2:D:2077:ILE:HD11	2.32	0.44
1:A:1119:PHE:HB2	1:A:1125:ARG:CG	2.44	0.44
2:B:2013:ILE:HB	2:B:2021:VAL:CG2	2.47	0.44
1:C:1034:THR:HG22	1:C:1035:GLY:H	1.83	0.44
2:D:2093:TRP:HB3	2:D:2095:ASN:ND2	2.32	0.44
2:D:2202:VAL:HG23	2:D:2203:LYS:N	2.32	0.44
1:A:1033:THR:O	1:A:1034:THR:C	2.55	0.44
1:A:1079:ALA:O	1:A:1175:SER:OG	2.33	0.44
2:D:2062:LYS:HE3	5:D:7379:HOH:O	2.16	0.44
2:D:2161:LEU:CD2	2:D:2235:VAL:HG11	2.45	0.44
1:A:1181:GLN:OE1	1:A:1251:ILE:C	2.56	0.44
2:B:2176:TYR:HB2	2:B:2180:SER:OG	2.18	0.44
1:C:1116:THR:HG22	1:C:1117:PHE:O	2.18	0.44
1:C:1179:ARG:NH1	5:C:7332:HOH:O	2.50	0.44
1:A:1123:TYR:CD1	1:A:1133:ARG:HD3	2.53	0.43
2:D:2211:SER:C	2:D:2213:GLY:H	2.21	0.43
1:A:1246:ILE:H	1:A:1246:ILE:HG13	1.49	0.43
1:C:1172:GLN:HA	1:C:1176:GLU:CG	2.48	0.43
1:C:1176:GLU:OE2	1:C:1207:GLU:CB	2.66	0.43
2:D:2051:LEU:N	2:D:2051:LEU:HD23	2.33	0.43
2:D:2065:THR:HA	2:D:2087:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2161:LEU:HD12	2:D:2161:LEU:HA	1.86	0.43
2:B:2033:PRO:HB2	2:B:2117:LYS:HD2	2.00	0.43
2:B:2147:LEU:HD22	2:B:2148:TYR:CD2	2.54	0.43
1:C:1176:GLU:OE1	1:C:1179:ARG:HD2	2.19	0.43
2:D:2105:LEU:HB3	2:D:2120:VAL:HB	2.00	0.43
2:D:2154:ALA:HB2	2:D:2159:VAL:HG12	2.00	0.43
2:B:2135:ASN:ND2	3:B:5004:GAL:O2	2.52	0.43
2:B:2140:PHE:HZ	2:B:2262:PHE:CD2	2.35	0.43
1:C:1206:LEU:HD12	1:C:1206:LEU:HA	1.66	0.43
2:D:2042:ASN:O	2:D:2044:ASP:N	2.52	0.43
2:D:2235:VAL:HG23	2:D:2235:VAL:O	2.18	0.43
1:A:1155:THR:HA	1:C:1156:CYS:SG	2.58	0.43
1:C:1085:ARG:NH1	1:C:1085:ARG:CG	2.82	0.43
2:D:2062:LYS:HD2	2:D:2078:TYR:O	2.18	0.43
2:D:2116:THR:HG22	2:D:2117:LYS:N	2.33	0.43
2:D:2157:GLY:HA2	2:D:2204:ILE:CG1	2.49	0.43
2:B:2192:THR:HG22	2:B:2193:THR:N	2.34	0.43
1:C:1045:LEU:HD21	1:C:1253:LEU:HD13	1.99	0.43
1:C:1255:VAL:O	1:C:1257:ARG:HG2	2.18	0.43
2:D:2049:TRP:CD2	2:D:2059:SER:HB2	2.53	0.43
1:A:1138:LEU:N	1:A:1197:SER:O	2.35	0.43
2:D:2065:THR:O	2:D:2075:VAL:HA	2.18	0.43
2:B:2095:ASN:OD1	3:B:5002:GAL:O2	2.37	0.43
2:B:2191:LEU:HD12	2:B:2191:LEU:HA	1.79	0.43
1:C:1104:ILE:C	1:C:1106:HIS:H	2.22	0.43
2:D:2143:THR:HG22	2:D:2172:GLN:OE1	2.19	0.43
2:B:2027:GLU:HB3	2:B:2029:PHE:CD2	2.53	0.43
2:D:2140:PHE:CZ	2:D:2262:PHE:CD2	3.05	0.43
2:D:2027:GLU:HG2	2:D:2029:PHE:CD2	2.52	0.43
1:C:1107:LEU:HD12	1:C:1107:LEU:HA	1.88	0.42
2:D:2012:ARG:NH2	2:D:2042:ASN:H	2.16	0.42
2:D:2232:VAL:O	2:D:2247:VAL:HA	2.19	0.42
1:A:1219:GLU:O	2:B:2007:PRO:HG3	2.19	0.42
2:B:2034:ILE:HG12	2:B:2076:VAL:HA	2.01	0.42
1:C:1242:TYR:CD1	2:D:2136:ASN:HB2	2.54	0.42
2:D:2016:ARG:HA	2:D:2178:ASP:HB3	2.01	0.42
1:A:1042:ILE:HA	1:A:1043:PRO:HD3	1.91	0.42
1:A:1244:VAL:HG13	1:A:1245:SER:N	2.33	0.42
2:D:2159:VAL:HG23	2:D:2159:VAL:O	2.19	0.42
1:A:1033:THR:C	1:A:1035:GLY:N	2.72	0.42
2:B:2138:GLN:OE1	2:B:2139:PRO:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1047:ASN:HD21	1:C:1049:VAL:CG2	2.29	0.42
1:C:1092:PHE:CE2	1:C:1107:LEU:HB3	2.54	0.42
2:D:2005:MET:O	2:D:2007:PRO:HD3	2.19	0.42
2:B:2008:GLU:HG2	2:B:2052:ARG:HA	2.00	0.42
2:B:2179:GLY:O	2:B:2216:TRP:N	2.46	0.42
2:B:2248:HIS:ND1	2:B:2249:PRO:HD2	2.34	0.42
1:C:1204:ILE:HG22	1:C:1208:ASN:ND2	2.35	0.42
1:C:1256:TYR:C	1:C:1256:TYR:CD2	2.93	0.42
2:D:2072:ARG:O	2:D:2073:GLN:O	2.38	0.42
2:D:2054:ASP:O	2:D:2089:ARG:HG2	2.19	0.42
2:B:2062:LYS:HB3	2:B:2077:ILE:CG1	2.43	0.42
1:C:1065:HIS:O	1:C:1067:GLU:N	2.52	0.42
2:D:2019:LEU:HD12	2:D:2038:PRO:CA	2.49	0.42
2:D:2123:ASN:HA	2:D:2129:GLN:NE2	2.34	0.42
1:A:1039:ARG:O	1:A:1040:HIS:HB2	2.19	0.42
2:B:2167:GLU:HG3	2:B:2168:LYS:N	2.34	0.42
1:C:1113:ASN:C	1:C:1113:ASN:ND2	2.73	0.42
2:D:2099:ILE:HD11	2:D:2104:GLY:HA2	2.02	0.42
2:D:2151:CYS:O	2:D:2161:LEU:HD12	2.19	0.42
2:D:2251:HIS:HE1	2:D:2253:ASN:HB2	1.82	0.42
1:A:1056:ARG:HG2	1:A:1056:ARG:HH11	1.84	0.42
2:B:2225:LEU:HD12	2:B:2231:LEU:O	2.19	0.42
1:C:1064:ASN:HB2	1:C:1144:GLU:CD	2.40	0.42
1:C:1119:PHE:HB2	1:C:1125:ARG:CG	2.48	0.42
1:C:1133:ARG:O	1:C:1199:PRO:HD2	2.20	0.42
1:C:1171:ILE:O	1:C:1175:SER:HB2	2.20	0.42
2:D:2113:ASN:O	2:D:2115:GLY:N	2.53	0.42
1:A:1195:ARG:HH11	1:A:1195:ARG:HG2	1.83	0.41
2:B:2028:PHE:O	2:B:2062:LYS:NZ	2.53	0.41
2:D:2059:SER:O	2:D:2060:ASN:HB3	2.19	0.41
2:B:2195:ALA:HB3	2:B:2200:THR:CG2	2.50	0.41
1:C:1029:ARG:HH22	1:C:1181:GLN:HA	1.85	0.41
2:D:2056:THR:OG1	2:D:2058:ARG:HD2	2.20	0.41
1:A:1033:THR:O	1:A:1035:GLY:N	2.53	0.41
1:A:1226:ALA:HB2	2:B:2007:PRO:HB2	2.03	0.41
2:B:2014:VAL:HG12	2:B:2018:GLY:HA2	2.03	0.41
2:B:2195:ALA:HB3	2:B:2200:THR:HG21	2.01	0.41
2:B:2248:HIS:CE1	2:B:2249:PRO:HD2	2.55	0.41
1:C:1228:PRO:HB3	1:C:1242:TYR:CE2	2.54	0.41
2:B:2132:LEU:CB	2:B:2177:ALA:HB1	2.49	0.41
1:C:1117:PHE:CG	1:C:1119:PHE:CZ	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1128:GLN:HG3	1:C:1129:LEU:N	2.35	0.41
2:D:2165:THR:O	2:D:2165:THR:HG22	2.20	0.41
1:A:1010:ASN:ND2	3:A:5001:GAL:O2	2.51	0.41
1:A:1011:PHE:HB2	1:A:1024:PHE:CD1	2.55	0.41
1:C:1092:PHE:HE2	1:C:1107:LEU:HB3	1.84	0.41
1:C:1137:GLU:O	1:C:1142:PRO:HB3	2.21	0.41
2:B:2147:LEU:HG	2:B:2255:ASN:HA	2.03	0.41
1:C:1123:TYR:O	1:C:1127:GLU:HG3	2.21	0.41
2:D:2032:ASN:O	2:D:2076:VAL:HB	2.21	0.41
2:B:2097:THR:OG1	2:B:2215:ARG:NH2	2.41	0.41
1:C:1141:GLY:O	1:C:1144:GLU:HB3	2.21	0.41
2:D:2070:SER:OG	2:D:2071:PRO:HD2	2.20	0.41
1:A:1107:LEU:HD23	1:A:1107:LEU:HA	1.83	0.41
2:B:2152:LEU:HD23	2:B:2152:LEU:HA	1.79	0.41
2:B:2232:VAL:HG22	2:B:2248:HIS:O	2.21	0.41
2:D:2013:ILE:HB	2:D:2021:VAL:CG2	2.50	0.41
2:D:2064:LEU:O	2:D:2088:THR:HA	2.20	0.41
2:D:2201:VAL:HG21	2:D:2244:GLN:NE2	2.35	0.41
1:A:1117:PHE:CG	1:A:1119:PHE:CZ	3.09	0.41
1:A:1222:GLN:NE2	5:A:7398:HOH:O	2.54	0.41
2:B:2127:VAL:HG13	2:B:2178:ASP:HB2	2.03	0.41
2:B:2155:ASN:HB2	2:B:2160:TRP:CH2	2.56	0.41
2:B:2237:ARG:HB2	2:B:2242:LEU:CD2	2.51	0.41
2:B:2237:ARG:O	2:B:2239:ASP:N	2.54	0.41
1:C:1072:LEU:HD23	1:C:1072:LEU:HA	1.88	0.41
2:D:2180:SER:OG	2:D:2182:ARG:HD2	2.20	0.41
2:D:2236:ARG:HG3	2:D:2244:GLN:HG3	2.02	0.41
1:A:1215:THR:O	1:A:1216:ALA:C	2.59	0.41
2:B:2234:ASP:OD1	2:B:2256:GLN:NE2	2.50	0.41
1:C:1053:ILE:CG2	1:C:1054:SER:N	2.84	0.41
2:D:2233:LEU:HD23	2:D:2233:LEU:HA	1.85	0.41
2:D:2245:ILE:HD12	2:D:2245:ILE:N	2.35	0.41
1:A:1021:TYR:O	1:A:1024:PHE:HB3	2.21	0.40
1:A:1060:VAL:O	1:A:1060:VAL:CG2	2.67	0.40
1:A:1185:GLY:HA3	2:B:2259:LEU:CD2	2.51	0.40
2:B:2089:ARG:NH1	2:B:2102:ARG:NH2	2.65	0.40
2:D:2099:ILE:HG12	2:D:2100:ASN:N	2.35	0.40
1:A:1074:LEU:HA	1:A:1080:TYR:O	2.21	0.40
2:B:2175:LEU:N	2:B:2175:LEU:CD1	2.84	0.40
1:C:1176:GLU:OE2	1:C:1207:GLU:HB2	2.21	0.40
1:C:1243:ASP:O	1:C:1246:ILE:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:THR:CG2	1:A:1191:ILE:HG12	2.52	0.40
2:B:2071:PRO:O	2:B:2072:ARG:HB2	2.22	0.40
1:C:1223:GLY:HA3	1:C:1244:VAL:HG12	2.02	0.40
2:D:2030:ASP:OD2	2:D:2062:LYS:NZ	2.51	0.40
1:A:1038:VAL:O	1:A:1039:ARG:HG3	2.21	0.40
2:B:2022:ASP:OD2	2:B:2022:ASP:C	2.60	0.40
2:D:2012:ARG:C	2:D:2013:ILE:HD12	2.42	0.40
2:D:2022:ASP:HB3	2:D:2035:GLN:CG	2.52	0.40
1:A:1022:THR:O	1:A:1026:ARG:HG3	2.21	0.40
1:A:1230:GLN:CD	1:A:1238:LYS:HD3	2.41	0.40
2:B:2090:TRP:CZ3	2:B:2100:ASN:HB2	2.57	0.40
2:B:2184:GLN:NE2	2:B:2187:ARG:HH21	2.19	0.40
2:B:2248:HIS:CG	2:B:2249:PRO:HD2	2.56	0.40
1:C:1092:PHE:CD1	1:C:1092:PHE:N	2.90	0.40
1:C:1222:GLN:HE22	2:D:2091:GLN:HA	1.87	0.40
2:D:2095:ASN:ND2	2:D:2095:ASN:N	2.68	0.40
2:D:2161:LEU:HD22	2:D:2235:VAL:CG1	2.46	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	257/262 (98%)	243 (95%)	13 (5%)	1 (0%)	34 48
1	C	258/262 (98%)	229 (89%)	25 (10%)	4 (2%)	9 13
2	B	260/262 (99%)	225 (86%)	29 (11%)	6 (2%)	6 8
2	D	260/262 (99%)	199 (76%)	42 (16%)	19 (7%)	1 0
All	All	1035/1048 (99%)	896 (87%)	109 (10%)	30 (3%)	4 6

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2070	SER
2	B	2167	GLU
2	B	2168	LYS
2	D	2024	THR
2	D	2073	GLN
2	D	2114	SER
2	B	2072	ARG
1	C	1066	ALA
2	D	2038	PRO
2	D	2043	THR
2	D	2168	LYS
2	D	2236	ARG
2	D	2243	LYS
2	B	2128	SER
1	C	1194	ASN
2	D	2110	THR
2	D	2167	GLU
2	D	2186	ASN
2	D	2194	ASP
1	A	1107	LEU
1	C	1078	ASN
1	C	1192	ARG
2	D	2016	ARG
2	D	2238	SER
2	D	2185	GLN
2	D	2187	ARG
2	B	2238	SER
2	D	2096	ARG
2	D	2061	GLY
2	D	2213	GLY

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	221/224 (99%)	211 (96%)	10 (4%)	27 42
1	C	222/224 (99%)	205 (92%)	17 (8%)	13 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	230/230 (100%)	215 (94%)	15 (6%)	17 26
2	D	230/230 (100%)	210 (91%)	20 (9%)	10 14
All	All	903/908 (99%)	841 (93%)	62 (7%)	15 23

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1048	ARG
1	A	1059	LEU
1	A	1084	CYS
1	A	1085	ARG
1	A	1091	TYR
1	A	1116	THR
1	A	1150	LEU
1	A	1163	LEU
1	A	1192	ARG
1	A	1197	SER
2	B	2027	GLU
2	B	2043	THR
2	B	2051	LEU
2	B	2068	LYS
2	B	2095	ASN
2	B	2120	VAL
2	B	2147	LEU
2	B	2152	LEU
2	B	2168	LYS
2	B	2201	VAL
2	B	2217	MET
2	B	2236	ARG
2	B	2242	LEU
2	B	2247	VAL
2	B	2261	LEU
1	C	1038	VAL
1	C	1049	VAL
1	C	1055	GLN
1	C	1062	LEU
1	C	1068	LEU
1	C	1078	ASN
1	C	1081	VAL
1	C	1091	TYR
1	C	1096	ASP

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Mol	Chain	Res	Type
1	C	1099	GLU
1	C	1107	LEU
1	C	1113	ASN
1	C	1128	GLN
1	C	1143	LEU
1	C	1206	LEU
1	C	1250	ILE
1	C	1256	TYR
2	D	2005	MET
2	D	2028	PHE
2	D	2037	TRP
2	D	2039	CYS
2	D	2051	LEU
2	D	2065	THR
2	D	2074	GLN
2	D	2077	ILE
2	D	2095	ASN
2	D	2132	LEU
2	D	2141	VAL
2	D	2142	THR
2	D	2147	LEU
2	D	2175	LEU
2	D	2186	ASN
2	D	2189	ASN
2	D	2192	THR
2	D	2203	LYS
2	D	2217	MET
2	D	2225	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1010	ASN
1	A	1023	ASN
1	A	1098	GLN
1	A	1112	GLN
1	A	1135	ASN
1	A	1222	GLN
1	A	1230	GLN
1	A	1232	GLN
2	B	2035	GLN
2	B	2155	ASN

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Mol	Chain	Res	Type
2	B	2196	ASN
2	B	2253	ASN
1	C	1023	ASN
1	C	1040	HIS
1	C	1047	ASN
1	C	1055	GLN
1	C	1078	ASN
1	C	1113	ASN
1	C	1128	GLN
1	C	1172	GLN
1	C	1221	ASN
2	D	2035	GLN
2	D	2060	ASN
2	D	2079	ASN
2	D	2113	ASN
2	D	2121	GLN
2	D	2135	ASN
2	D	2138	GLN
2	D	2186	ASN
2	D	2189	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
4	SO4	A	6001	-	4,4,4	0.21	0	6,6,6	0.20	0
4	SO4	A	6004	-	4,4,4	0.33	0	6,6,6	0.07	0
3	GAL	D	5502	-	12,12,12	2.29	4 (33%)	17,17,17	1.37	4 (23%)
3	GAL	B	5006	-	12,12,12	2.26	4 (33%)	17,17,17	1.46	3 (17%)
3	GAL	B	5004	-	12,12,12	2.17	4 (33%)	17,17,17	1.47	3 (17%)
4	SO4	D	6502	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	C	6501	-	4,4,4	0.28	0	6,6,6	0.04	0
4	SO4	C	6504	-	4,4,4	0.25	0	6,6,6	0.23	0
3	GAL	A	5001	-	12,12,12	2.07	3 (25%)	17,17,17	1.54	3 (17%)
3	GAL	B	5002	-	12,12,12	2.21	4 (33%)	17,17,17	1.44	3 (17%)
4	SO4	B	6003	-	4,4,4	0.25	0	6,6,6	0.11	0
4	SO4	D	6503	-	4,4,4	0.26	0	6,6,6	0.11	0
4	SO4	A	6005	-	4,4,4	0.36	0	6,6,6	0.09	0
3	GAL	D	5504	-	12,12,12	2.18	3 (25%)	17,17,17	1.46	3 (17%)
3	GAL	B	5003	-	12,12,12	2.06	3 (25%)	17,17,17	1.42	3 (17%)
3	GAL	B	5005	-	12,12,12	2.22	3 (25%)	17,17,17	1.57	4 (23%)
3	GAL	D	5505	-	12,12,12	2.25	4 (33%)	17,17,17	1.27	2 (11%)
3	GAL	C	5501	-	12,12,12	2.21	4 (33%)	17,17,17	1.49	3 (17%)
4	SO4	B	6006	-	4,4,4	0.30	0	6,6,6	0.09	0
4	SO4	B	6002	-	4,4,4	0.28	0	6,6,6	0.13	0
3	GAL	D	5503	-	12,12,12	2.33	4 (33%)	17,17,17	1.40	3 (17%)

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	GAL	B	5005	-	-	0/2/22/22	0/1/1/1
3	GAL	D	5505	-	-	0/2/22/22	0/1/1/1
3	GAL	D	5502	-	-	0/2/22/22	0/1/1/1
3	GAL	C	5501	-	-	0/2/22/22	0/1/1/1
3	GAL	D	5504	-	-	0/2/22/22	0/1/1/1
3	GAL	A	5001	-	-	0/2/22/22	0/1/1/1
3	GAL	B	5002	-	-	0/2/22/22	0/1/1/1
3	GAL	B	5006	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	B	5004	-	-	0/2/22/22	0/1/1/1
3	GAL	B	5003	-	-	0/2/22/22	0/1/1/1
3	GAL	D	5503	-	-	0/2/22/22	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5502	GAL	C3-C2	-5.15	1.39	1.52
3	D	5503	GAL	C3-C2	-5.07	1.39	1.52
3	D	5505	GAL	C3-C2	-5.07	1.39	1.52
3	B	5003	GAL	C3-C2	-5.06	1.39	1.52
3	B	5005	GAL	C3-C2	-5.00	1.39	1.52
3	B	5006	GAL	C3-C2	-4.99	1.39	1.52
3	D	5504	GAL	C3-C2	-4.86	1.40	1.52
3	A	5001	GAL	C3-C2	-4.77	1.40	1.52
3	B	5002	GAL	C3-C2	-4.72	1.40	1.52
3	C	5501	GAL	C3-C2	-4.41	1.41	1.52
3	B	5004	GAL	C3-C2	-4.37	1.41	1.52
3	D	5503	GAL	C4-C3	3.77	1.61	1.52
3	D	5502	GAL	C4-C3	3.69	1.61	1.52
3	B	5006	GAL	C4-C3	3.67	1.61	1.52
3	C	5501	GAL	O3-C3	3.66	1.51	1.43
3	C	5501	GAL	C4-C3	3.63	1.61	1.52
3	D	5505	GAL	C4-C3	3.61	1.61	1.52
3	B	5005	GAL	C4-C3	3.57	1.61	1.52
3	B	5004	GAL	C4-C3	3.48	1.61	1.52
3	B	5002	GAL	C4-C3	3.48	1.61	1.52
3	D	5503	GAL	O3-C3	3.41	1.51	1.43
3	D	5504	GAL	O3-C3	3.34	1.50	1.43
3	B	5005	GAL	O3-C3	3.25	1.50	1.43
3	D	5504	GAL	C4-C3	3.22	1.60	1.52
3	B	5006	GAL	O3-C3	3.21	1.50	1.43
3	B	5004	GAL	O3-C3	3.13	1.50	1.43
3	B	5002	GAL	O3-C3	3.12	1.50	1.43
3	B	5003	GAL	C4-C3	3.04	1.60	1.52
3	D	5505	GAL	O3-C3	3.03	1.50	1.43
3	A	5001	GAL	C4-C3	3.02	1.60	1.52
3	A	5001	GAL	O3-C3	2.91	1.49	1.43
3	D	5502	GAL	O5-C1	2.68	1.49	1.42
3	B	5004	GAL	O5-C1	2.58	1.49	1.42
3	B	5003	GAL	O3-C3	2.55	1.49	1.43
3	D	5502	GAL	O3-C3	2.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5002	GAL	O5-C1	2.34	1.48	1.42
3	C	5501	GAL	O5-C1	2.17	1.48	1.42
3	D	5503	GAL	O5-C1	2.08	1.48	1.42
3	B	5006	GAL	O5-C1	2.06	1.48	1.42
3	D	5505	GAL	O5-C1	2.02	1.47	1.42

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	5001	GAL	O3-C3-C4	-3.64	101.94	110.35
3	B	5004	GAL	O3-C3-C4	-3.54	102.18	110.35
3	C	5501	GAL	O3-C3-C4	-3.46	102.36	110.35
3	B	5005	GAL	O3-C3-C4	-3.40	102.50	110.35
3	B	5003	GAL	O3-C3-C4	-3.30	102.73	110.35
3	D	5504	GAL	O3-C3-C4	-3.27	102.79	110.35
3	B	5002	GAL	O3-C3-C4	-3.24	102.87	110.35
3	B	5006	GAL	O3-C3-C4	-3.16	103.04	110.35
3	D	5502	GAL	O3-C3-C4	-3.13	103.12	110.35
3	B	5005	GAL	C4-C3-C2	3.12	116.26	110.82
3	D	5503	GAL	O3-C3-C4	-3.07	103.24	110.35
3	D	5505	GAL	O3-C3-C4	-2.98	103.47	110.35
3	B	5002	GAL	C4-C3-C2	2.87	115.84	110.82
3	B	5006	GAL	C4-C3-C2	2.83	115.77	110.82
3	C	5501	GAL	C4-C3-C2	2.82	115.75	110.82
3	A	5001	GAL	C4-C3-C2	2.81	115.73	110.82
3	B	5004	GAL	C4-C3-C2	2.70	115.53	110.82
3	D	5503	GAL	C4-C3-C2	2.67	115.48	110.82
3	C	5501	GAL	O3-C3-C2	2.60	116.35	110.35
3	B	5004	GAL	O3-C3-C2	2.59	116.33	110.35
3	D	5502	GAL	C4-C3-C2	2.53	115.25	110.82
3	B	5005	GAL	O3-C3-C2	2.53	116.19	110.35
3	A	5001	GAL	O3-C3-C2	2.49	116.12	110.35
3	D	5504	GAL	C4-C3-C2	2.48	115.15	110.82
3	D	5504	GAL	O3-C3-C2	2.46	116.03	110.35
3	B	5006	GAL	O3-C3-C2	2.36	115.81	110.35
3	B	5002	GAL	O3-C3-C2	2.33	115.73	110.35
3	B	5003	GAL	C4-C3-C2	2.30	114.84	110.82
3	D	5503	GAL	O3-C3-C2	2.27	115.59	110.35
3	D	5502	GAL	O3-C3-C2	2.15	115.32	110.35
3	D	5505	GAL	C4-C3-C2	2.12	114.53	110.82
3	D	5502	GAL	C1-C2-C3	-2.12	105.91	110.31
3	B	5003	GAL	O3-C3-C2	2.09	115.18	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5005	GAL	C1-C2-C3	-2.04	106.08	110.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5502	GAL	1	0
3	B	5006	GAL	1	0
3	B	5004	GAL	2	0
3	A	5001	GAL	2	0
3	B	5002	GAL	3	0
3	B	5005	GAL	4	0
3	D	5503	GAL	1	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.