Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 12:31 PM EDT

PDB ID	:	2EIG
Title	:	Lotus tetragonolobus seed lectin (Isoform)
Authors	:	Moreno, F.B.M.B.; Vicoti, M.M.; Abrego, J.R.B.; de Oliveira, T.M.; Bezerra, G.A.; Cavada, B.S.; Filgueira de Azevedo Jr., W.
Deposited on	:	2007-03-13
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

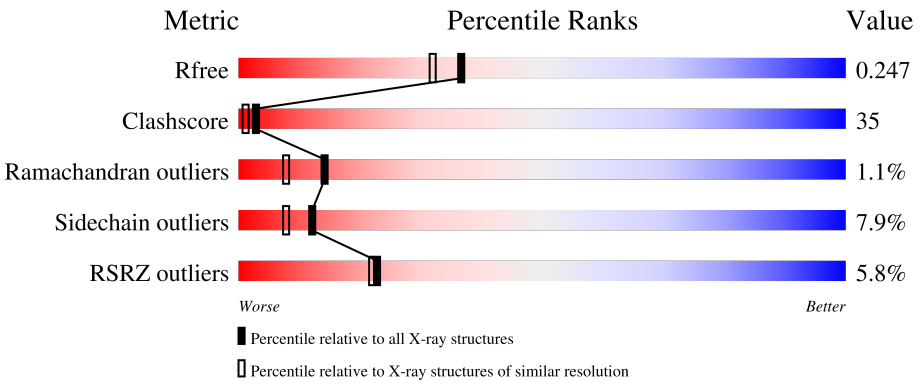
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	5% 61% 28% 9% • •
1	B	234	5% 64% 27% 6% • •
1	C	234	5% 60% 32% • • •
1	D	234	9% 50% 38% 6% • •

2 Entry composition (i)

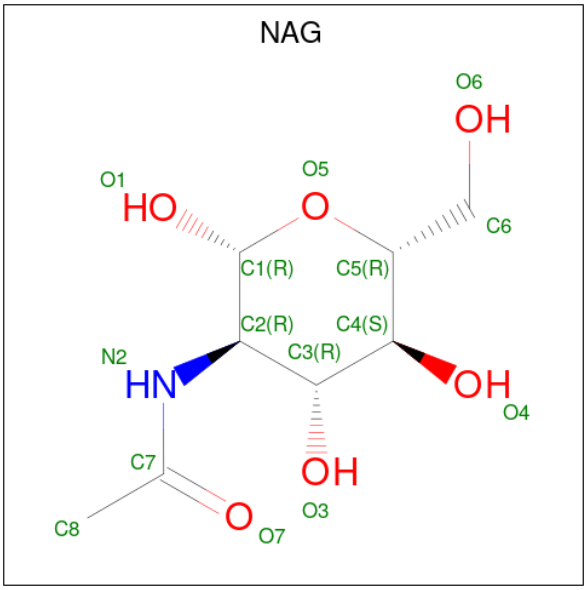
There are 5 unique types of molecules in this entry. The entry contains 7876 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1807	1151	301	352	3	0	0	0
1	B	230	1807	1151	301	352	3	0	0	0
1	C	230	1807	1151	301	352	3	0	0	0
1	D	230	1807	1151	301	352	3	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	14	8	1	5	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	1	1	1	0	0
			Total	Mn		
3	B	1	1	1	0	0
			Total	Mn		
3	C	1	1	1	0	0
			Total	Mn		
3	D	1	1	1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
			Total	Ca		
4	B	1	1	1	0	0
			Total	Ca		
4	C	1	1	1	0	0
			Total	Ca		
4	D	1	1	1	0	0

- Molecule 5 is water.

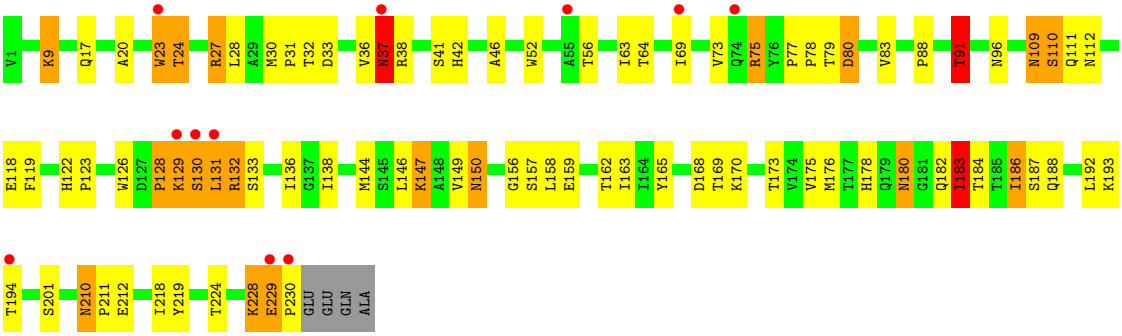
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	149	149	149	0	0
			Total	O		
5	B	181	181	181	0	0
			Total	O		
5	C	139	139	139	0	0
			Total	O		
5	D	129	129	129	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

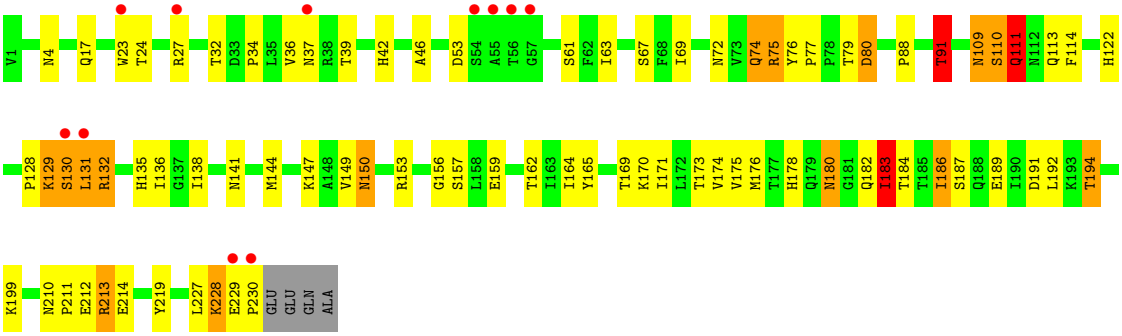
- Molecule 1: lectin

Chain A:



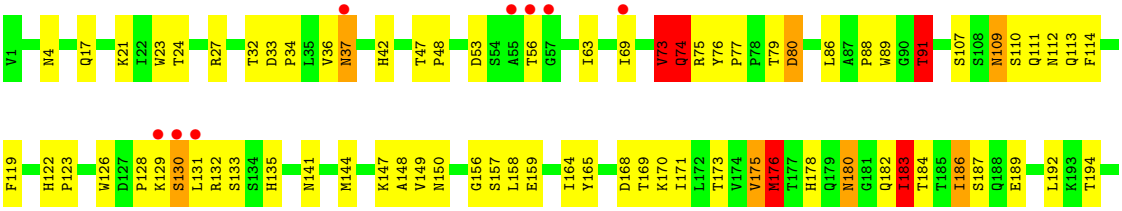
- Molecule 1: lectin

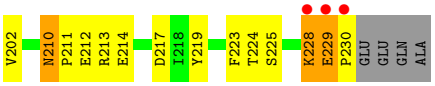
Chain B:



- Molecule 1: lectin

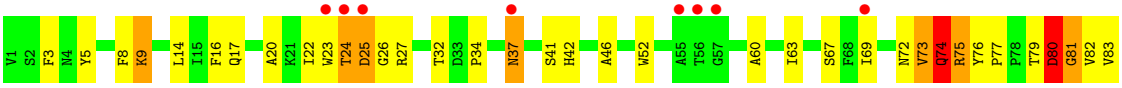
Chain C:

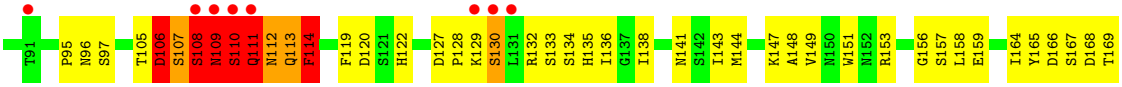


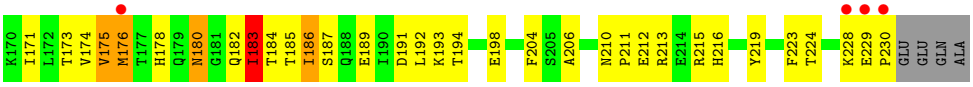


- Molecule 1: lectin

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.89Å 65.83Å 102.54Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	34.46 – 2.00 34.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.46-2.00) 99.4 (34.45-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.251 0.187 , 0.247	Depositor DCC
R_{free} test set	3128 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l 0.016 for -k,-h,-l 0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7876	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, NAG, CA

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	0.94	1/1857 (0.1%)	0.99	6/2540 (0.2%)
1	B	1.06	2/1857 (0.1%)	1.04	8/2540 (0.3%)
1	C	0.93	1/1857 (0.1%)	1.00	7/2540 (0.3%)
1	D	0.87	0/1857	1.05	9/2540 (0.4%)
All	All	0.95	4/7428 (0.1%)	1.02	30/10160 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	2
1	D	0	9
All	All	1	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	THR	CA-CB	8.52	1.75	1.53
1	B	132	ARG	CD-NE	-7.63	1.33	1.46
1	C	91	THR	CA-CB	6.60	1.70	1.53
1	B	91	THR	CB-CG2	6.39	1.73	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	SER	N-CA-C	-8.41	88.30	111.00
1	C	176	MET	CB-CG-SD	-8.02	88.34	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	SER	CB-CA-C	6.76	122.95	110.10
1	C	183	ILE	CB-CA-C	-6.67	98.25	111.60
1	D	111	GLN	C-N-CA	6.66	138.35	121.70
1	C	73	VAL	N-CA-C	-6.61	93.15	111.00
1	D	183	ILE	CB-CA-C	-6.56	98.49	111.60
1	D	114	PHE	N-CA-C	6.47	128.47	111.00
1	B	131	LEU	N-CA-C	-6.45	93.58	111.00
1	B	183	ILE	CB-CA-C	-6.43	98.73	111.60
1	A	130	SER	N-CA-C	-6.14	94.42	111.00
1	B	111	GLN	N-CA-C	-5.98	94.85	111.00
1	C	183	ILE	CG1-CB-CG2	5.96	124.52	111.40
1	D	109	ASN	N-CA-C	5.96	127.08	111.00
1	C	109	ASN	C-N-CA	5.81	136.22	121.70
1	C	130	SER	N-CA-C	-5.70	95.62	111.00
1	A	183	ILE	CB-CA-C	-5.58	100.44	111.60
1	B	213	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	74	GLN	N-CA-C	-5.44	96.31	111.00
1	D	108	SER	C-N-CA	5.38	135.14	121.70
1	A	109	ASN	C-N-CA	5.36	135.10	121.70
1	A	119	PHE	N-CA-C	-5.36	96.54	111.00
1	B	132	ARG	CG-CD-NE	-5.27	100.74	111.80
1	D	80	ASP	CA-C-N	5.24	126.67	116.20
1	A	147	LYS	CD-CE-NZ	5.23	123.73	111.70
1	C	74	GLN	N-CA-C	-5.13	97.15	111.00
1	A	109	ASN	N-CA-C	-5.08	97.28	111.00
1	D	130	SER	N-CA-C	-5.05	97.37	111.00
1	B	130	SER	N-CA-CB	-5.04	102.95	110.50
1	D	106	ASP	C-N-CA	5.02	134.25	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	110	SER	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	VAL	Peptide
1	B	109	ASN	Peptide
1	B	110	SER	Peptide
1	D	106	ASP	Peptide
1	D	108	SER	Peptide

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Mol	Chain	Res	Type	Group
1	D	109	ASN	Peptide
1	D	110	SER	Peptide
1	D	111	GLN	Peptide
1	D	113	GLN	Peptide
1	D	228	LYS	Peptide
1	D	73	VAL	Peptide
1	D	80	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1807	0	1748	139	0
1	B	1807	0	1749	135	0
1	C	1807	0	1749	134	0
1	D	1807	0	1749	163	0
2	A	14	0	13	0	0
2	B	14	0	13	2	0
2	C	14	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	149	0	0	13	0
5	B	181	0	0	19	0
5	C	139	0	0	4	0
5	D	129	0	0	15	0
All	All	7876	0	7034	502	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 (502) 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:91:THR:CB	1:A:91:THR:CA	1.75	1.64
1:B:4:ASN:HD21	2:B:3001:NAG:C1	1.30	1.41
1:C:173:THR:HB	5:C:2131:HOH:O	1.31	1.27
1:B:91:THR:HB	5:B:3167:HOH:O	1.39	1.19
1:B:169:THR:HG23	1:C:147:LYS:HZ2	1.09	1.18
1:D:110:SER:HB3	1:D:111:GLN:HB2	1.18	1.15
1:D:75:ARG:HD2	5:D:1517:HOH:O	1.43	1.13
1:A:132:ARG:HH21	1:A:132:ARG:HG3	1.12	1.12
1:C:79:THR:HG23	1:C:212:GLU:HB3	1.16	1.12
1:B:79:THR:HG23	1:B:212:GLU:HB3	1.15	1.11
1:D:111:GLN:N	1:D:112:ASN:HB2	1.66	1.11
1:A:79:THR:HG23	1:A:212:GLU:HB3	1.13	1.11
1:B:175:VAL:HG11	1:C:63:ILE:HD12	1.19	1.08
1:B:169:THR:HG23	1:C:147:LYS:NZ	1.66	1.08
1:A:147:LYS:HE2	1:A:186:ILE:HG12	1.17	1.07
1:B:4:ASN:ND2	2:B:3001:NAG:C1	2.16	1.07
1:D:111:GLN:H	1:D:112:ASN:HB2	0.92	1.07
1:D:136:ILE:HD13	1:D:176:MET:SD	1.95	1.07
1:B:128:PRO:HB2	1:B:132:ARG:HD2	1.35	1.06
1:A:136:ILE:HD13	1:A:176:MET:HE3	1.06	1.04
1:A:175:VAL:HG11	1:D:63:ILE:HD12	1.39	1.03
1:A:79:THR:CG2	1:A:212:GLU:HB3	1.88	1.03
1:D:96:ASN:O	1:D:107:SER:HB2	1.59	1.02
1:C:147:LYS:HE2	1:C:186:ILE:HG12	1.39	1.02
1:C:79:THR:CG2	1:C:212:GLU:HB3	1.89	1.02
1:B:176:MET:HB3	5:B:3165:HOH:O	0.84	1.01
1:D:110:SER:CB	1:D:111:GLN:HB2	1.91	1.01
1:A:37:ASN:ND2	5:A:1238:HOH:O	1.93	1.00
1:B:136:ILE:HD13	1:B:176:MET:SD	2.02	0.99
1:B:175:VAL:HG23	1:B:183:ILE:CG2	1.93	0.99
1:B:79:THR:CG2	1:B:212:GLU:HB3	1.93	0.99
1:C:88:PRO:O	1:C:91:THR:HG22	1.63	0.99
1:C:79:THR:HG23	1:C:212:GLU:CB	1.91	0.99
1:B:147:LYS:HB3	1:B:186:ILE:HD11	1.43	0.99
1:B:63:ILE:HD12	1:C:175:VAL:HG11	1.41	0.98
1:B:147:LYS:HE2	1:B:187:SER:O	1.63	0.97
1:B:79:THR:HG23	1:B:212:GLU:CB	1.94	0.97
1:C:175:VAL:HG23	1:C:183:ILE:CG2	1.95	0.97
1:A:63:ILE:HD12	1:D:175:VAL:HG11	1.44	0.96
1:B:164:ILE:HD13	1:C:175:VAL:HG12	1.48	0.95
1:B:147:LYS:NZ	1:C:169:THR:HG23	1.82	0.95
1:D:175:VAL:HG22	1:D:183:ILE:CG2	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:PRO:HG2	1:B:212:GLU:HG3	1.47	0.93
1:C:175:VAL:HG23	1:C:183:ILE:HG22	1.51	0.93
1:C:147:LYS:NZ	1:C:187:SER:H	1.67	0.93
1:B:91:THR:CG2	5:B:3167:HOH:O	2.16	0.92
1:A:147:LYS:HB3	1:A:186:ILE:HD11	1.52	0.91
1:A:136:ILE:HD13	1:A:176:MET:CE	1.98	0.91
1:A:63:ILE:CD1	1:D:175:VAL:HG11	2.02	0.90
1:D:110:SER:HB3	1:D:111:GLN:CB	2.01	0.89
1:A:147:LYS:HE3	1:D:168:ASP:OD2	1.73	0.88
1:D:128:PRO:C	1:D:130:SER:H	1.76	0.88
1:D:113:GLN:O	5:D:1524:HOH:O	1.91	0.87
1:C:37:ASN:ND2	1:C:210:ASN:OD1	2.07	0.87
1:B:175:VAL:HG23	1:B:183:ILE:HG21	1.55	0.87
1:A:79:THR:HG23	1:A:212:GLU:CB	2.03	0.86
1:A:136:ILE:CD1	1:A:176:MET:HE3	1.99	0.86
1:D:173:THR:HG23	1:D:187:SER:OG	1.75	0.86
1:D:79:THR:HG22	1:D:122:HIS:HB2	1.56	0.86
1:D:111:GLN:H	1:D:112:ASN:CB	1.85	0.86
1:C:147:LYS:HZ1	1:C:187:SER:H	1.20	0.86
1:B:109:ASN:OD1	1:B:110:SER:HA	1.76	0.85
1:B:129:LYS:O	1:B:129:LYS:HG2	1.73	0.85
1:B:171:ILE:HD12	1:C:171:ILE:HD13	1.60	0.84
1:C:77:PRO:HG2	1:C:212:GLU:HG3	1.59	0.83
1:D:79:THR:HG23	1:D:212:GLU:HB3	1.60	0.83
1:C:79:THR:CG2	1:C:212:GLU:CB	2.55	0.83
1:C:228:LYS:HE3	1:C:228:LYS:H	1.44	0.82
1:A:132:ARG:HG3	1:A:132:ARG:NH2	1.92	0.82
1:A:159:GLU:OE2	1:A:178:HIS:HD2	1.61	0.82
1:D:147:LYS:HE3	1:D:186:ILE:CG1	2.09	0.82
1:D:175:VAL:HG22	1:D:183:ILE:HG22	1.60	0.82
1:D:24:THR:HG22	1:D:25:ASP:H	1.46	0.81
1:D:96:ASN:O	1:D:107:SER:CB	2.28	0.81
1:C:36:VAL:O	1:C:37:ASN:HB2	1.78	0.81
1:A:147:LYS:CE	1:A:186:ILE:HG12	2.07	0.81
1:D:32:THR:HG21	5:D:1492:HOH:O	1.79	0.81
1:D:147:LYS:HE3	1:D:186:ILE:HG12	1.62	0.80
1:A:138:ILE:HD12	1:A:186:ILE:HD13	1.63	0.80
1:A:183:ILE:HG13	1:D:224:THR:HG22	1.63	0.80
1:B:136:ILE:HG21	1:B:176:MET:SD	2.22	0.80
1:A:175:VAL:HG23	1:A:183:ILE:CG2	2.13	0.79
1:B:175:VAL:CG2	1:B:183:ILE:CG2	2.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PRO:O	1:A:91:THR:HG22	1.82	0.79
1:A:175:VAL:HG11	1:D:63:ILE:CD1	2.12	0.79
1:A:77:PRO:HG2	1:A:212:GLU:HG3	1.64	0.79
1:D:174:VAL:HG12	1:D:176:MET:HE2	1.65	0.79
1:D:77:PRO:HG2	1:D:212:GLU:HG3	1.63	0.78
1:A:23:TRP:HD1	1:A:27:ARG:HG2	1.49	0.78
1:B:130:SER:HB3	5:B:3174:HOH:O	1.82	0.78
1:B:164:ILE:CD1	1:C:175:VAL:HG12	2.13	0.78
1:D:175:VAL:CG2	1:D:183:ILE:HG21	2.14	0.78
1:B:147:LYS:CE	1:B:187:SER:O	2.32	0.78
1:A:147:LYS:HE2	1:A:186:ILE:CG1	2.09	0.77
1:C:228:LYS:H	1:C:228:LYS:CE	1.98	0.77
1:B:175:VAL:CG2	1:B:183:ILE:HG21	2.14	0.77
1:A:63:ILE:HD12	1:D:175:VAL:CG1	2.15	0.76
1:D:72:ASN:HD21	1:D:153:ARG:HH12	1.33	0.76
1:D:174:VAL:HG12	1:D:176:MET:CE	2.15	0.76
1:D:79:THR:HG22	1:D:122:HIS:CB	2.16	0.76
1:A:79:THR:CG2	1:A:212:GLU:CB	2.63	0.75
1:D:130:SER:HB3	5:D:1469:HOH:O	1.85	0.75
1:B:132:ARG:HD3	1:B:135:HIS:HB3	1.69	0.75
1:D:149:VAL:HG21	1:D:184:THR:CG2	2.17	0.75
1:B:79:THR:CG2	1:B:212:GLU:CB	2.60	0.74
1:A:132:ARG:HH21	1:A:132:ARG:CG	1.97	0.74
1:B:72:ASN:HD21	1:B:153:ARG:HH12	1.33	0.74
1:A:149:VAL:HG11	1:A:184:THR:CG2	2.17	0.74
1:A:175:VAL:CG2	1:A:183:ILE:HG21	2.18	0.74
1:B:147:LYS:HD2	1:C:168:ASP:OD2	1.88	0.73
1:C:147:LYS:HE2	1:C:186:ILE:CG1	2.16	0.73
1:A:175:VAL:CG1	1:D:63:ILE:HD12	2.16	0.73
1:D:136:ILE:HG21	1:D:176:MET:SD	2.28	0.73
1:B:228:LYS:HD3	1:B:230:PRO:HD2	1.71	0.73
1:C:27:ARG:HE	1:C:217:ASP:CB	2.02	0.73
1:D:175:VAL:CG2	1:D:183:ILE:CG2	2.67	0.73
1:D:122:HIS:HD2	5:D:1414:HOH:O	1.70	0.73
1:C:74:GLN:H	1:C:76:TYR:H	1.37	0.72
1:B:72:ASN:HD22	1:B:153:ARG:HH22	1.37	0.72
1:B:109:ASN:OD1	1:B:111:GLN:HB2	1.88	0.72
1:B:147:LYS:HZ3	1:C:169:THR:HG23	1.53	0.72
1:B:175:VAL:HG23	1:B:183:ILE:HG22	1.72	0.71
1:D:147:LYS:HE2	1:D:187:SER:O	1.90	0.71
1:C:27:ARG:HE	1:C:217:ASP:HB3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:THR:HG22	1:D:122:HIS:CG	2.26	0.71
1:D:176:MET:HE3	1:D:184:THR:O	1.90	0.71
1:A:175:VAL:CG2	1:A:183:ILE:CG2	2.69	0.70
1:A:147:LYS:HD3	1:A:187:SER:O	1.90	0.70
1:B:191:ASP:O	1:B:194:THR:HG23	1.92	0.70
1:C:147:LYS:CE	1:C:186:ILE:HG12	2.19	0.70
1:A:91:THR:CA	1:A:91:THR:HB	2.12	0.70
1:B:169:THR:CG2	1:C:147:LYS:NZ	2.52	0.70
1:C:175:VAL:CG2	1:C:183:ILE:CG2	2.69	0.70
1:A:175:VAL:HG21	1:D:63:ILE:CG2	2.22	0.70
1:A:175:VAL:HG23	1:A:183:ILE:HG21	1.74	0.69
1:B:72:ASN:ND2	1:B:153:ARG:HH22	1.90	0.69
1:B:79:THR:HG22	1:B:122:HIS:CG	2.27	0.69
1:A:129:LYS:C	1:A:130:SER:O	2.24	0.69
1:D:17:GLN:HB2	1:D:42:HIS:HB2	1.75	0.69
1:D:32:THR:CG2	5:D:1492:HOH:O	2.37	0.68
1:B:128:PRO:CB	1:B:132:ARG:HD2	2.20	0.68
1:D:159:GLU:OE2	1:D:178:HIS:HD2	1.75	0.68
1:A:149:VAL:HG11	1:A:184:THR:HG22	1.75	0.68
1:B:129:LYS:O	1:B:129:LYS:CG	2.40	0.68
1:C:69:ILE:HG13	1:C:158:LEU:HA	1.73	0.68
1:B:178:HIS:HE1	1:B:184:THR:OG1	1.77	0.68
1:C:69:ILE:HG12	1:C:157:SER:C	2.14	0.68
1:B:36:VAL:HG22	1:B:39:THR:HG22	1.76	0.68
1:B:183:ILE:HG13	1:C:224:THR:HG22	1.76	0.67
1:D:178:HIS:HE1	1:D:184:THR:OG1	1.76	0.67
1:B:128:PRO:C	1:B:130:SER:H	1.96	0.67
1:A:132:ARG:HG2	1:A:150:ASN:HB2	1.77	0.67
1:D:79:THR:CG2	1:D:212:GLU:HB3	2.23	0.67
1:B:130:SER:HB2	1:B:132:ARG:HG3	1.76	0.67
1:C:178:HIS:HE1	1:C:184:THR:OG1	1.78	0.66
1:D:113:GLN:HA	1:D:141:ASN:ND2	2.11	0.66
1:C:228:LYS:H	1:C:228:LYS:CD	2.08	0.66
1:D:75:ARG:CD	5:D:1517:HOH:O	2.17	0.66
1:C:113:GLN:HA	1:C:141:ASN:ND2	2.10	0.66
1:C:109:ASN:HD21	1:C:111:GLN:HB2	1.61	0.66
1:B:46:ALA:HB1	5:B:3118:HOH:O	1.97	0.65
1:A:69:ILE:HD13	1:A:156:GLY:O	1.97	0.65
1:D:175:VAL:HG23	1:D:185:THR:HG22	1.79	0.65
1:A:168:ASP:O	1:C:170:LYS:NZ	2.30	0.65
1:C:107:SER:O	1:D:110:SER:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:CE	1:D:168:ASP:OD2	2.44	0.64
1:D:149:VAL:HG21	1:D:184:THR:HG22	1.78	0.64
1:A:175:VAL:HG23	1:A:183:ILE:HG22	1.78	0.64
1:A:36:VAL:O	1:A:37:ASN:HB3	1.97	0.64
1:B:228:LYS:HG2	5:B:3172:HOH:O	1.96	0.64
1:A:37:ASN:HB2	1:A:210:ASN:OD1	1.97	0.64
1:A:78:PRO:O	1:A:79:THR:HG22	1.99	0.63
1:B:175:VAL:CG1	1:C:63:ILE:HD12	2.12	0.63
1:C:147:LYS:HZ1	1:C:187:SER:N	1.92	0.63
1:B:17:GLN:HB2	1:B:42:HIS:HB2	1.79	0.63
1:B:175:VAL:HG11	1:C:63:ILE:CD1	2.12	0.63
1:D:198:GLU:HG2	5:D:1452:HOH:O	1.97	0.63
1:A:123:PRO:HG3	1:A:133:SER:HA	1.80	0.63
1:B:229:GLU:HB3	5:B:3071:HOH:O	1.99	0.63
1:A:23:TRP:HB2	5:A:1145:HOH:O	1.97	0.62
1:A:194:THR:HG21	1:B:147:LYS:HA	1.81	0.62
1:B:169:THR:HG23	1:C:147:LYS:HZ3	1.64	0.62
1:C:79:THR:HG23	1:C:212:GLU:CG	2.29	0.62
1:B:138:ILE:HD12	1:B:186:ILE:HD13	1.82	0.62
1:D:175:VAL:HG23	1:D:185:THR:CG2	2.30	0.61
1:B:91:THR:CB	5:B:3167:HOH:O	2.12	0.61
1:D:20:ALA:HB2	1:D:41:SER:HB3	1.82	0.61
1:A:175:VAL:HG12	1:D:164:ILE:CD1	2.29	0.61
1:A:37:ASN:CG	1:A:38:ARG:H	2.03	0.61
1:A:178:HIS:HE1	1:A:184:THR:OG1	1.83	0.61
1:D:113:GLN:HA	1:D:141:ASN:HD22	1.65	0.61
1:A:112:ASN:O	1:B:144:MET:HE1	2.00	0.61
1:C:34:PRO:O	1:C:213:ARG:HD3	2.01	0.60
1:A:188:GLN:HE22	1:B:189:GLU:HG2	1.65	0.60
1:B:150:ASN:ND2	5:B:3122:HOH:O	2.33	0.60
1:A:147:LYS:NZ	1:D:169:THR:HG23	2.17	0.60
1:D:147:LYS:HE3	1:D:186:ILE:HG13	1.82	0.60
1:C:147:LYS:C	1:C:186:ILE:HD11	2.22	0.59
1:C:21:LYS:HB2	1:C:32:THR:HB	1.84	0.59
1:B:32:THR:CG2	5:B:3102:HOH:O	2.50	0.59
1:B:159:GLU:OE2	1:B:178:HIS:HD2	1.85	0.59
1:D:96:ASN:HB2	1:D:107:SER:HB3	1.84	0.59
1:B:79:THR:HB	1:B:80:ASP:HA	1.84	0.59
1:A:149:VAL:CG1	1:A:184:THR:CG2	2.80	0.59
1:C:175:VAL:HG23	1:C:183:ILE:HG21	1.82	0.59
1:B:129:LYS:HA	5:B:3065:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:VAL:CG2	1:D:184:THR:CG2	2.80	0.58
1:A:69:ILE:HG13	1:A:219:TYR:HE1	1.67	0.58
1:A:46:ALA:HB1	5:A:1165:HOH:O	2.02	0.58
1:B:147:LYS:NZ	1:B:187:SER:H	2.02	0.58
1:D:147:LYS:C	1:D:186:ILE:HD11	2.24	0.58
1:D:147:LYS:HZ1	1:D:187:SER:H	1.50	0.58
1:A:69:ILE:CG1	1:A:158:LEU:HA	2.34	0.58
1:D:46:ALA:HB3	5:D:1530:HOH:O	2.03	0.58
1:B:79:THR:HG22	1:B:122:HIS:HB2	1.85	0.57
1:C:173:THR:HG23	1:C:187:SER:OG	2.02	0.57
1:D:69:ILE:HD13	1:D:156:GLY:O	2.05	0.57
1:A:69:ILE:HG12	1:A:158:LEU:HA	1.85	0.57
1:B:147:LYS:HZ1	1:B:187:SER:H	1.52	0.57
1:D:27:ARG:NH2	1:D:215:ARG:NH2	2.53	0.57
1:D:109:ASN:OD1	1:D:111:GLN:HB3	2.03	0.57
1:D:74:GLN:NE2	5:D:1495:HOH:O	2.32	0.57
1:A:69:ILE:HB	1:A:219:TYR:OH	2.05	0.57
1:A:180:ASN:HD21	1:A:182:GLN:HB2	1.69	0.57
1:D:194:THR:HG22	5:D:1449:HOH:O	2.05	0.57
1:B:147:LYS:HZ1	1:C:169:THR:HG23	1.66	0.57
1:A:78:PRO:O	1:A:79:THR:CG2	2.53	0.56
1:A:170:LYS:HG2	5:A:1237:HOH:O	2.05	0.56
1:B:164:ILE:HD13	1:C:175:VAL:CG1	2.31	0.56
1:D:165:TYR:CZ	1:D:192:LEU:HG	2.39	0.56
1:D:128:PRO:C	1:D:130:SER:N	2.51	0.56
1:C:109:ASN:O	1:C:112:ASN:ND2	2.39	0.56
1:A:75:ARG:H	1:A:75:ARG:HD2	1.71	0.56
1:B:171:ILE:HD12	1:C:171:ILE:CD1	2.34	0.56
1:D:69:ILE:CG2	1:D:156:GLY:HA2	2.35	0.56
1:A:126:TRP:HB2	1:A:144:MET:HG3	1.88	0.56
1:B:164:ILE:CD1	1:C:175:VAL:CG1	2.83	0.56
1:D:129:LYS:HB2	5:D:1460:HOH:O	2.04	0.56
1:A:23:TRP:CD1	1:A:27:ARG:HG2	2.37	0.55
1:C:147:LYS:O	1:C:186:ILE:HD11	2.06	0.55
1:C:178:HIS:CE1	1:C:184:THR:OG1	2.59	0.55
1:A:91:THR:CA	1:A:91:THR:CG2	2.79	0.55
1:D:79:THR:HB	1:D:80:ASP:HA	1.89	0.55
1:C:79:THR:CG2	1:C:212:GLU:HG2	2.36	0.55
1:A:147:LYS:HZ2	1:D:169:THR:HG23	1.71	0.55
1:A:175:VAL:HG21	1:D:63:ILE:HG21	1.89	0.55
1:D:3:PHE:CD1	1:D:5:TYR:HE2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ASN:CG	1:D:111:GLN:HB3	2.27	0.55
1:A:180:ASN:ND2	1:A:182:GLN:H	2.05	0.55
1:C:109:ASN:C	1:D:110:SER:H	2.10	0.55
1:B:129:LYS:C	1:B:130:SER:O	2.37	0.55
1:D:95:PRO:O	1:D:106:ASP:HB2	2.07	0.55
1:C:53:ASP:OD2	1:C:56:THR:HG23	2.07	0.54
1:C:109:ASN:ND2	1:C:111:GLN:HB2	2.21	0.54
1:B:61:SER:O	1:C:183:ILE:HD11	2.07	0.54
1:D:81:GLY:CA	1:D:216:HIS:NE2	2.71	0.54
1:A:146:LEU:HD21	5:B:3063:HOH:O	2.07	0.54
1:A:147:LYS:NZ	1:D:168:ASP:HB3	2.22	0.54
1:D:24:THR:HG22	1:D:25:ASP:N	2.20	0.54
1:C:147:LYS:NZ	1:C:187:SER:N	2.48	0.54
1:A:228:LYS:HD3	1:A:228:LYS:N	2.22	0.54
1:A:112:ASN:O	1:B:144:MET:CE	2.55	0.54
1:A:128:PRO:C	1:A:130:SER:H	2.08	0.54
1:A:69:ILE:HG21	1:A:156:GLY:HA2	1.89	0.53
1:B:162:THR:HB	1:B:175:VAL:CG1	2.38	0.53
1:D:73:VAL:O	1:D:76:TYR:HB2	2.09	0.53
1:A:126:TRP:HB2	1:A:144:MET:CG	2.38	0.53
1:A:144:MET:HE3	5:A:1114:HOH:O	2.08	0.53
1:B:36:VAL:HG22	1:B:39:THR:CG2	2.39	0.53
1:C:176:MET:HE1	1:C:176:MET:N	2.22	0.53
1:D:72:ASN:HD22	1:D:153:ARG:HH22	1.57	0.53
1:B:175:VAL:HG12	1:C:164:ILE:CD1	2.39	0.53
1:B:191:ASP:O	1:B:194:THR:CG2	2.56	0.53
1:C:132:ARG:HD2	1:C:135:HIS:HB3	1.90	0.53
1:C:189:GLU:OE2	5:C:2132:HOH:O	2.18	0.53
1:B:169:THR:HG22	1:D:189:GLU:OE2	2.07	0.53
1:B:69:ILE:CG2	1:B:156:GLY:HA2	2.39	0.52
1:C:86:LEU:HG	1:C:202:VAL:HG12	1.92	0.52
1:D:119:PHE:HE2	1:D:176:MET:HG2	1.73	0.52
1:A:150:ASN:ND2	5:A:1140:HOH:O	2.35	0.52
1:B:34:PRO:O	1:B:213:ARG:HD3	2.10	0.52
1:A:20:ALA:HB2	1:A:41:SER:HB3	1.91	0.52
1:A:136:ILE:HG21	1:A:176:MET:HE1	1.90	0.52
1:C:36:VAL:O	1:C:37:ASN:CB	2.53	0.52
1:B:63:ILE:HD12	1:C:175:VAL:CG1	2.27	0.52
1:C:164:ILE:HB	5:C:2131:HOH:O	2.09	0.52
1:B:79:THR:O	1:B:214:GLU:HG2	2.11	0.51
1:C:79:THR:HG23	1:C:212:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASN:HD22	1:B:211:PRO:HA	1.75	0.51
1:C:75:ARG:HD3	1:C:75:ARG:N	2.25	0.51
1:A:109:ASN:ND2	5:A:1207:HOH:O	2.44	0.51
1:B:114:PHE:H	1:B:141:ASN:ND2	2.09	0.51
1:A:147:LYS:NZ	1:D:166:ASP:OD2	2.43	0.51
1:B:178:HIS:CE1	1:B:184:THR:OG1	2.61	0.51
1:C:129:LYS:C	1:C:130:SER:O	2.43	0.51
1:D:81:GLY:HA2	1:D:216:HIS:NE2	2.26	0.51
1:A:69:ILE:HG12	1:A:157:SER:C	2.30	0.51
1:A:147:LYS:HZ2	1:D:168:ASP:HB3	1.75	0.51
1:D:14:LEU:HD12	5:D:1455:HOH:O	2.09	0.51
1:C:112:ASN:O	1:D:144:MET:HE1	2.10	0.51
1:A:17:GLN:HB2	1:A:42:HIS:HB2	1.92	0.51
1:C:114:PHE:H	1:C:141:ASN:HD22	1.58	0.51
1:C:119:PHE:HE2	1:C:176:MET:SD	2.33	0.51
5:A:1159:HOH:O	1:D:182:GLN:HG2	2.10	0.50
1:B:199:LYS:HD2	5:B:3130:HOH:O	2.11	0.50
1:D:180:ASN:ND2	1:D:182:GLN:H	2.09	0.50
1:D:180:ASN:C	1:D:180:ASN:HD22	2.14	0.50
1:B:32:THR:HG22	5:B:3102:HOH:O	2.11	0.50
1:C:228:LYS:CD	1:C:228:LYS:N	2.74	0.50
1:D:72:ASN:ND2	1:D:153:ARG:HH12	2.05	0.50
1:A:133:SER:HB2	5:A:1201:HOH:O	2.12	0.50
1:B:149:VAL:HG11	1:B:184:THR:CG2	2.42	0.50
1:B:175:VAL:HG12	1:C:164:ILE:HD13	1.94	0.50
1:A:63:ILE:CD1	1:D:175:VAL:CG1	2.82	0.50
5:A:1148:HOH:O	1:D:171:ILE:CD1	2.60	0.50
1:B:67:SER:HA	1:B:159:GLU:O	2.12	0.50
1:B:79:THR:HG23	1:B:212:GLU:CG	2.41	0.50
1:D:229:GLU:HA	1:D:230:PRO:C	2.32	0.49
1:D:75:ARG:HD2	1:D:75:ARG:H	1.77	0.49
1:D:127:ASP:O	1:D:129:LYS:N	2.45	0.49
1:D:210:ASN:HD22	1:D:211:PRO:HA	1.77	0.49
1:A:69:ILE:HG12	1:A:157:SER:O	2.13	0.49
1:D:97:SER:HA	1:D:105:THR:O	2.13	0.49
1:B:183:ILE:HG13	1:C:224:THR:CG2	2.42	0.49
1:D:210:ASN:HD22	1:D:213:ARG:NH2	2.11	0.49
1:B:147:LYS:CE	1:C:169:THR:HG23	2.42	0.49
1:B:32:THR:HG21	5:B:3102:HOH:O	2.13	0.49
1:B:91:THR:HG22	5:B:3167:HOH:O	1.97	0.49
1:B:72:ASN:HD21	1:B:153:ARG:NH1	2.08	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:HG22	1:B:122:HIS:CB	2.43	0.48
1:C:112:ASN:O	1:D:144:MET:CE	2.61	0.48
1:D:16:PHE:CZ	1:D:22:ILE:HD11	2.47	0.48
1:C:17:GLN:HB2	1:C:42:HIS:HB2	1.94	0.48
1:C:130:SER:HB2	1:C:132:ARG:HG3	1.94	0.48
1:C:21:LYS:NZ	1:C:32:THR:HG21	2.28	0.48
1:C:149:VAL:HG11	1:C:184:THR:CG2	2.44	0.48
1:A:52:TRP:CD2	1:A:193:LYS:HG3	2.48	0.48
1:A:128:PRO:C	1:A:130:SER:N	2.67	0.48
1:A:79:THR:HG22	1:A:122:HIS:HB2	1.96	0.48
1:C:165:TYR:CZ	1:C:192:LEU:HG	2.49	0.48
1:D:175:VAL:HG21	1:D:183:ILE:HG21	1.94	0.47
1:D:79:THR:HB	1:D:80:ASP:CG	2.34	0.47
1:C:148:ALA:HA	1:C:186:ILE:HD12	1.96	0.47
1:A:132:ARG:NH2	1:A:132:ARG:CG	2.64	0.47
1:A:229:GLU:N	1:A:230:PRO:HD3	2.29	0.47
1:C:123:PRO:HG3	1:C:133:SER:HA	1.95	0.47
1:D:46:ALA:CB	5:D:1530:HOH:O	2.62	0.47
1:B:69:ILE:HG12	1:B:157:SER:C	2.35	0.47
1:D:74:GLN:HG3	1:D:75:ARG:HD2	1.97	0.47
1:D:128:PRO:O	1:D:130:SER:N	2.48	0.47
1:B:69:ILE:HB	1:B:219:TYR:OH	2.15	0.47
1:C:147:LYS:CE	1:C:186:ILE:CG1	2.86	0.47
1:C:175:VAL:CG2	1:C:183:ILE:HG21	2.39	0.47
1:A:109:ASN:OD1	1:A:111:GLN:HB2	2.14	0.47
1:B:69:ILE:HG23	1:B:156:GLY:C	2.35	0.47
1:C:69:ILE:HD13	1:C:156:GLY:O	2.14	0.47
1:C:69:ILE:HB	1:C:219:TYR:OH	2.15	0.47
1:C:79:THR:CG2	1:C:212:GLU:CG	2.90	0.47
1:B:147:LYS:CE	1:C:169:THR:CG2	2.93	0.47
1:D:210:ASN:ND2	1:D:213:ARG:HH22	2.13	0.47
1:A:79:THR:HG21	1:A:212:GLU:CB	2.45	0.47
1:C:132:ARG:HD3	1:C:150:ASN:HB3	1.96	0.47
1:A:175:VAL:HG12	1:D:164:ILE:HD13	1.96	0.46
1:B:53:ASP:HB2	1:B:227:LEU:HD21	1.97	0.46
1:B:138:ILE:HD11	1:B:174:VAL:HG23	1.98	0.46
1:D:74:GLN:H	1:D:74:GLN:HG2	1.08	0.46
1:D:127:ASP:O	1:D:128:PRO:C	2.51	0.46
1:A:91:THR:CB	1:A:91:THR:C	2.76	0.46
1:C:147:LYS:NZ	1:C:187:SER:O	2.45	0.46
1:A:149:VAL:CG1	1:A:184:THR:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLU:N	1:B:230:PRO:CD	2.78	0.46
1:B:75:ARG:HD2	1:B:76:TYR:CE2	2.51	0.46
1:A:56:THR:HG21	1:A:230:PRO:C	2.36	0.46
1:A:159:GLU:OE2	1:A:178:HIS:CD2	2.53	0.46
1:A:162:THR:HB	1:A:175:VAL:CG1	2.46	0.46
1:C:73:VAL:O	1:C:76:TYR:HB2	2.16	0.46
1:D:143:ILE:HD12	1:D:143:ILE:HA	1.79	0.46
1:D:148:ALA:HA	1:D:186:ILE:HD12	1.98	0.46
1:A:36:VAL:O	1:A:37:ASN:CB	2.63	0.46
1:A:175:VAL:HG12	1:D:164:ILE:HD11	1.98	0.46
1:B:147:LYS:HE2	1:C:169:THR:CG2	2.46	0.46
1:B:113:GLN:HA	1:B:141:ASN:ND2	2.31	0.46
1:A:23:TRP:HZ3	5:A:1236:HOH:O	1.98	0.46
1:B:165:TYR:CZ	1:B:192:LEU:HG	2.51	0.46
1:B:69:ILE:HG13	1:B:219:TYR:HE1	1.81	0.45
1:D:69:ILE:HG12	1:D:157:SER:C	2.37	0.45
1:D:96:ASN:CB	1:D:107:SER:HB3	2.45	0.45
1:D:178:HIS:CE1	1:D:184:THR:OG1	2.63	0.45
1:A:149:VAL:HG13	1:A:184:THR:HG21	1.98	0.45
1:D:83:VAL:O	1:D:204:PHE:HA	2.16	0.45
1:B:173:THR:HG23	1:B:187:SER:OG	2.16	0.45
1:C:228:LYS:N	1:C:228:LYS:HD3	2.31	0.45
1:B:79:THR:CG2	1:B:122:HIS:CG	2.99	0.45
1:C:74:GLN:HB3	1:C:75:ARG:H	1.42	0.45
1:D:180:ASN:ND2	1:D:180:ASN:C	2.69	0.45
1:A:91:THR:CB	1:A:91:THR:HA	2.19	0.45
1:A:32:THR:HG23	1:A:33:ASP:N	2.31	0.45
1:C:180:ASN:ND2	1:C:182:GLN:H	2.14	0.45
1:A:169:THR:HG23	1:D:147:LYS:HZ3	1.82	0.45
1:B:131:LEU:HD12	5:B:3054:HOH:O	2.16	0.45
1:B:180:ASN:ND2	1:B:182:GLN:H	2.15	0.45
1:A:9:LYS:HG3	5:A:1144:HOH:O	2.17	0.45
1:A:224:THR:HG22	1:D:183:ILE:HG13	1.99	0.45
1:C:228:LYS:HE3	1:C:228:LYS:N	2.22	0.44
1:B:114:PHE:H	1:B:141:ASN:HD22	1.65	0.44
1:D:106:ASP:O	1:D:112:ASN:ND2	2.49	0.44
1:A:91:THR:HG21	1:A:201:SER:OG	2.18	0.44
1:A:178:HIS:CE1	1:A:184:THR:OG1	2.67	0.44
1:B:183:ILE:CG1	1:C:224:THR:HG22	2.45	0.44
1:C:126:TRP:HB2	1:C:144:MET:HG2	1.98	0.44
1:D:82:VAL:HG23	1:D:206:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:ARG:HD2	1:D:135:HIS:HB3	1.99	0.44
1:C:79:THR:HG21	1:C:212:GLU:CB	2.43	0.44
5:C:2138:HOH:O	1:D:194:THR:HG22	2.18	0.44
1:C:229:GLU:N	1:C:230:PRO:CD	2.80	0.44
1:D:3:PHE:CD1	1:D:5:TYR:CE2	3.05	0.44
5:A:1176:HOH:O	1:B:129:LYS:HE2	2.18	0.44
1:B:37:ASN:HB3	1:B:210:ASN:HB2	2.00	0.43
1:C:79:THR:O	1:C:214:GLU:HG2	2.18	0.43
1:A:69:ILE:CG2	1:A:156:GLY:HA2	2.48	0.43
1:A:210:ASN:HD22	1:A:211:PRO:HA	1.83	0.43
1:B:149:VAL:HG11	1:B:184:THR:HG22	2.00	0.43
1:A:28:LEU:HB3	1:A:218:ILE:HB	2.01	0.43
1:B:27:ARG:HE	1:B:219:TYR:HE2	1.65	0.43
1:D:60:ALA:O	1:D:167:SER:HB3	2.18	0.43
1:D:191:ASP:O	1:D:194:THR:OG1	2.31	0.43
1:B:88:PRO:O	1:B:91:THR:HB	2.19	0.43
1:C:210:ASN:HD22	1:C:211:PRO:HA	1.83	0.43
1:C:194:THR:HG21	1:D:147:LYS:HG3	2.01	0.43
1:A:23:TRP:CG	1:A:24:THR:N	2.87	0.43
1:A:79:THR:HB	1:A:80:ASP:HA	2.00	0.43
1:C:114:PHE:H	1:C:141:ASN:ND2	2.17	0.43
1:D:79:THR:CG2	1:D:122:HIS:CG	3.00	0.43
1:D:136:ILE:HG13	1:D:151:TRP:HB2	1.99	0.43
1:C:192:LEU:HD23	1:C:192:LEU:HA	1.68	0.43
1:D:180:ASN:HD21	1:D:182:GLN:HB2	1.84	0.43
1:B:169:THR:CG2	1:C:147:LYS:HZ3	2.25	0.43
1:D:34:PRO:O	1:D:213:ARG:HD3	2.18	0.43
1:A:63:ILE:HB	1:D:175:VAL:HG21	2.00	0.43
1:D:37:ASN:HB2	1:D:210:ASN:HB2	2.01	0.43
1:B:79:THR:CG2	1:B:212:GLU:HG2	2.49	0.42
1:C:69:ILE:HG12	1:C:157:SER:O	2.19	0.42
1:C:149:VAL:HG11	1:C:184:THR:HG22	2.01	0.42
1:D:69:ILE:HG13	1:D:219:TYR:HE1	1.84	0.42
1:D:3:PHE:CZ	1:D:223:PHE:HB3	2.54	0.42
1:D:122:HIS:HE1	5:D:1528:HOH:O	2.03	0.42
1:A:173:THR:HG23	1:A:187:SER:HB2	2.00	0.42
1:C:79:THR:HB	1:C:80:ASP:HA	2.00	0.42
1:B:130:SER:CB	1:B:132:ARG:NH2	2.83	0.42
1:B:169:THR:HG21	1:C:187:SER:HB2	2.02	0.42
1:C:69:ILE:CG1	1:C:158:LEU:HA	2.48	0.42
1:C:159:GLU:OE2	1:C:178:HIS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:LYS:HE3	1:D:9:LYS:HB3	1.79	0.42
1:D:129:LYS:C	1:D:130:SER:O	2.58	0.42
1:C:48:PRO:HG3	1:C:89:TRP:CE2	2.54	0.42
1:D:52:TRP:CD2	1:D:193:LYS:HG3	2.54	0.42
1:D:138:ILE:HG13	1:D:186:ILE:HD13	2.02	0.42
1:D:8:PHE:HB3	1:D:22:ILE:HD12	2.02	0.42
1:C:176:MET:HB2	1:C:176:MET:HE2	1.08	0.42
1:C:128:PRO:C	1:C:130:SER:H	2.19	0.41
1:A:64:THR:HG22	1:A:163:ILE:HB	2.03	0.41
1:A:183:ILE:CG1	1:D:224:THR:HG22	2.40	0.41
1:B:75:ARG:HD2	1:B:76:TYR:CD2	2.55	0.41
1:A:131:LEU:HA	1:A:131:LEU:HD22	1.69	0.41
1:A:162:THR:HB	1:A:175:VAL:HG13	2.02	0.41
1:A:146:LEU:O	1:B:194:THR:HG21	2.21	0.41
1:B:74:GLN:O	1:B:75:ARG:HG3	2.20	0.41
1:C:21:LYS:HD2	1:C:32:THR:HG21	2.02	0.41
1:A:109:ASN:CG	1:A:111:GLN:H	2.24	0.41
1:B:23:TRP:CG	1:B:24:THR:N	2.88	0.41
1:B:91:THR:HG23	5:B:3050:HOH:O	2.20	0.41
1:A:30:MET:HA	1:A:31:PRO:HA	1.88	0.41
1:A:229:GLU:N	1:A:230:PRO:CD	2.83	0.41
1:C:119:PHE:CE2	1:C:176:MET:SD	3.13	0.41
1:C:4:ASN:HD21	2:C:2001:NAG:C1	2.33	0.41
1:C:32:THR:HG23	1:C:33:ASP:N	2.36	0.41
1:D:72:ASN:ND2	1:D:153:ARG:HH22	2.19	0.41
1:A:9:LYS:HE3	1:A:9:LYS:HB3	1.96	0.41
1:A:83:VAL:HG12	1:A:118:GLU:HA	2.02	0.41
1:A:147:LYS:HE3	1:D:168:ASP:CG	2.41	0.41
5:B:3133:HOH:O	1:C:173:THR:HG21	2.20	0.41
1:C:223:PHE:CE2	1:C:225:SER:HB3	2.56	0.41
1:D:120:ASP:O	1:D:134:SER:HA	2.20	0.41
1:A:136:ILE:HG21	1:A:176:MET:CE	2.51	0.41
1:B:69:ILE:HG21	1:B:156:GLY:HA2	2.02	0.40
1:D:69:ILE:HG21	1:D:156:GLY:HA2	2.02	0.40
1:D:69:ILE:CG1	1:D:219:TYR:HE1	2.34	0.40
1:D:147:LYS:NZ	1:D:187:SER:H	2.19	0.40
1:A:228:LYS:N	1:A:228:LYS:CD	2.84	0.40
1:D:79:THR:HG22	1:D:122:HIS:CD2	2.55	0.40
1:D:173:THR:HG23	1:D:187:SER:HG	1.83	0.40
1:A:165:TYR:CZ	1:A:192:LEU:HG	2.55	0.40
1:A:228:LYS:HD3	1:A:228:LYS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ASP:HB3	1:B:194:THR:CG2	2.52	0.40
1:C:147:LYS:HB3	1:C:186:ILE:HD11	2.04	0.40
1:A:37:ASN:CG	1:A:38:ARG:N	2.72	0.40
1:A:169:THR:HG23	1:D:147:LYS:NZ	2.36	0.40
1:D:8:PHE:O	1:D:26:GLY:HA2	2.20	0.40
1:D:67:SER:HB2	1:D:158:LEU:HD11	2.02	0.40
1:C:79:THR:HG22	1:C:122:HIS:CG	2.56	0.40
1:C:107:SER:HA	1:D:110:SER:OG	2.21	0.40
1:C:229:GLU:N	1:C:230:PRO:HD2	2.36	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	228/234 (97%)	211 (92%)	14 (6%)	3 (1%)	12 6
1	B	228/234 (97%)	212 (93%)	16 (7%)	0	100 100
1	C	228/234 (97%)	215 (94%)	12 (5%)	1 (0%)	34 30
1	D	228/234 (97%)	210 (92%)	12 (5%)	6 (3%)	5 2
All	All	912/936 (97%)	848 (93%)	54 (6%)	10 (1%)	14 8

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	110	SER
1	C	37	ASN
1	D	112	ASN
1	D	114	PHE
1	D	110	SER

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Mol	Chain	Res	Type
1	D	107	SER
1	D	108	SER
1	A	128	PRO
1	D	81	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	206/209 (99%)	186 (90%)	20 (10%)	8 4
1	B	206/209 (99%)	193 (94%)	13 (6%)	18 13
1	C	206/209 (99%)	189 (92%)	17 (8%)	11 7
1	D	206/209 (99%)	191 (93%)	15 (7%)	14 9
All	All	824/836 (99%)	759 (92%)	65 (8%)	12 8

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	23	TRP
1	A	24	THR
1	A	27	ARG
1	A	37	ASN
1	A	75	ARG
1	A	80	ASP
1	A	91	THR
1	A	96	ASN
1	A	110	SER
1	A	129	LYS
1	A	131	LEU
1	A	132	ARG
1	A	150	ASN
1	A	180	ASN
1	A	183	ILE
1	A	186	ILE

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Mol	Chain	Res	Type
1	A	210	ASN
1	A	228	LYS
1	A	229	GLU
1	B	74	GLN
1	B	75	ARG
1	B	80	ASP
1	B	91	THR
1	B	111	GLN
1	B	129	LYS
1	B	150	ASN
1	B	170	LYS
1	B	180	ASN
1	B	183	ILE
1	B	186	ILE
1	B	194	THR
1	B	228	LYS
1	C	23	TRP
1	C	24	THR
1	C	47	THR
1	C	73	VAL
1	C	74	GLN
1	C	80	ASP
1	C	91	THR
1	C	110	SER
1	C	131	LEU
1	C	175	VAL
1	C	176	MET
1	C	180	ASN
1	C	183	ILE
1	C	186	ILE
1	C	210	ASN
1	C	228	LYS
1	C	229	GLU
1	D	9	LYS
1	D	23	TRP
1	D	24	THR
1	D	25	ASP
1	D	37	ASN
1	D	74	GLN
1	D	75	ARG
1	D	110	SER
1	D	114	PHE

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Mol	Chain	Res	Type
1	D	133	SER
1	D	175	VAL
1	D	176	MET
1	D	180	ASN
1	D	183	ILE
1	D	186	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	58	ASN
1	A	96	ASN
1	A	141	ASN
1	A	178	HIS
1	A	180	ASN
1	A	188	GLN
1	A	210	ASN
1	B	4	ASN
1	B	17	GLN
1	B	58	ASN
1	B	72	ASN
1	B	74	GLN
1	B	141	ASN
1	B	178	HIS
1	B	180	ASN
1	B	210	ASN
1	C	17	GLN
1	C	37	ASN
1	C	58	ASN
1	C	141	ASN
1	C	178	HIS
1	C	180	ASN
1	C	210	ASN
1	D	17	GLN
1	D	58	ASN
1	D	72	ASN
1	D	122	HIS
1	D	141	ASN
1	D	178	HIS
1	D	180	ASN
1	D	210	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	3001	-	14,14,15	0.52	0	17,19,21	0.85	0
2	NAG	C	2001	-	14,14,15	0.59	0	17,19,21	1.15	1 (5%)
2	NAG	A	1001	1	14,14,15	0.77	0	17,19,21	1.49	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
2	NAG	B	3001	-	-	1/6/23/26	0/1/1/1
2	NAG	C	2001	-	-	4/6/23/26	0/1/1/1
2	NAG	A	1001	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	NAG	C4-C3-C2	3.95	116.80	111.02
2	A	1001	NAG	C1-O5-C5	2.66	115.76	112.19
2	A	1001	NAG	C1-C2-N2	-2.20	106.96	110.43
2	C	2001	NAG	O5-C5-C6	2.15	111.84	107.66

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001	NAG	C8-C7-N2-C2
2	C	2001	NAG	O7-C7-N2-C2
2	C	2001	NAG	C4-C5-C6-O6
2	C	2001	NAG	O5-C5-C6-O6
2	A	1001	NAG	O5-C5-C6-O6
2	A	1001	NAG	C4-C5-C6-O6
2	B	3001	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3001	NAG	2	0
2	C	2001	NAG	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	230/234 (98%)	0.12	11 (4%)	30	29	12, 20, 34, 44	0
1	B	230/234 (98%)	0.00	11 (4%)	30	29	10, 16, 30, 49	0
1	C	230/234 (98%)	0.09	11 (4%)	30	29	13, 20, 35, 51	0
1	D	230/234 (98%)	0.32	20 (8%)	10	9	15, 24, 40, 54	0
All	All	920/936 (98%)	0.13	53 (5%)	23	22	10, 20, 36, 54	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	LEU	7.4
1	D	23	TRP	7.0
1	C	230	PRO	6.0
1	B	131	LEU	5.6
1	B	230	PRO	5.5
1	D	230	PRO	5.5
1	D	129	LYS	5.5
1	C	229	GLU	5.4
1	D	131	LEU	5.3
1	B	229	GLU	5.2
1	A	230	PRO	4.8
1	A	37	ASN	4.5
1	D	110	SER	4.5
1	A	23	TRP	4.4
1	C	131	LEU	4.0
1	D	56	THR	3.8
1	C	228	LYS	3.7
1	C	130	SER	3.7
1	A	129	LYS	3.5
1	C	55	ALA	3.4
1	D	25	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	55	ALA	3.2
1	B	55	ALA	3.1
1	D	229	GLU	3.1
1	D	130	SER	3.1
1	A	229	GLU	3.1
1	A	69	ILE	3.1
1	A	194	THR	3.0
1	D	69	ILE	3.0
1	B	54	SER	3.0
1	C	69	ILE	2.9
1	D	37	ASN	2.9
1	A	74	GLN	2.9
1	D	228	LYS	2.9
1	C	56	THR	2.9
1	A	55	ALA	2.8
1	D	108	SER	2.7
1	D	24	THR	2.7
1	B	37	ASN	2.6
1	C	129	LYS	2.6
1	B	57	GLY	2.5
1	C	57	GLY	2.4
1	C	37	ASN	2.4
1	B	27	ARG	2.4
1	B	130	SER	2.4
1	B	56	THR	2.3
1	A	130	SER	2.3
1	D	57	GLY	2.2
1	D	109	ASN	2.1
1	D	91	THR	2.1
1	D	111	GLN	2.0
1	B	23	TRP	2.0
1	D	176	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2001	14/15	0.63	0.18	58,64,66,67	0
2	NAG	B	3001	14/15	0.79	0.21	51,55,57,58	0
2	NAG	A	1001	14/15	0.85	0.24	44,52,54,55	0
3	MN	A	1101	1/1	0.99	0.04	18,18,18,18	0
4	CA	B	1202	1/1	0.99	0.09	14,14,14,14	0
3	MN	C	1301	1/1	1.00	0.06	20,20,20,20	0
3	MN	D	1401	1/1	1.00	0.05	20,20,20,20	0
4	CA	A	1102	1/1	1.00	0.05	19,19,19,19	0
3	MN	B	1201	1/1	1.00	0.06	17,17,17,17	0
4	CA	C	1302	1/1	1.00	0.05	18,18,18,18	0
4	CA	D	1402	1/1	1.00	0.06	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.