WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 04:21 PM BST

PDB ID	:	1FAT
Title	:	PHYTOHEMAGGLUTININ-L
Authors	:	Hamelryck, T.; Loris, R.
Deposited on	:	1996-06-12
Resolution	:	2.80 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 following versions of software and data (see references (i)) were used in the production of this report:

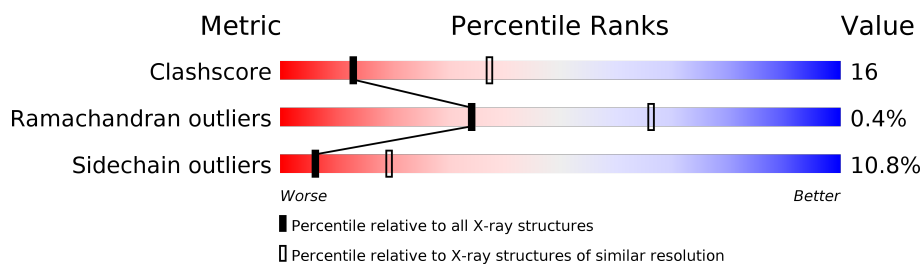|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.80 Å.

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

Metric	Percentile Ranks	Value
Clashscore		16
Ramachandran outliers		0.4%
Sidechain outliers		10.8%

Worse   *Better*

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

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	252	61% 25% 5% 8%
1	B	252	62% 25% 5% 8%
1	C	252	62% 25% 5% 8%
1	D	252	60% 27% 5% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7248 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 PHYTOHEMAGGLUTININ-L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	0	0	0
			1793	1135	301	357			
1	B	233	Total	C	N	O	0	0	0
			1797	1137	302	358			
1	C	232	Total	C	N	O	0	0	0
			1793	1135	301	357			
1	D	231	Total	C	N	O	0	0	0
			1785	1131	299	355			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	GLY	conflict	UNP P05087
B	235	GLU	GLY	conflict	UNP P05087
C	235	GLU	GLY	conflict	UNP P05087
D	235	GLU	GLY	conflict	UNP P05087

- 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
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0

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

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

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

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

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

- Molecule 5 is water.

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

3 Residue-property plots ⓘ

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.
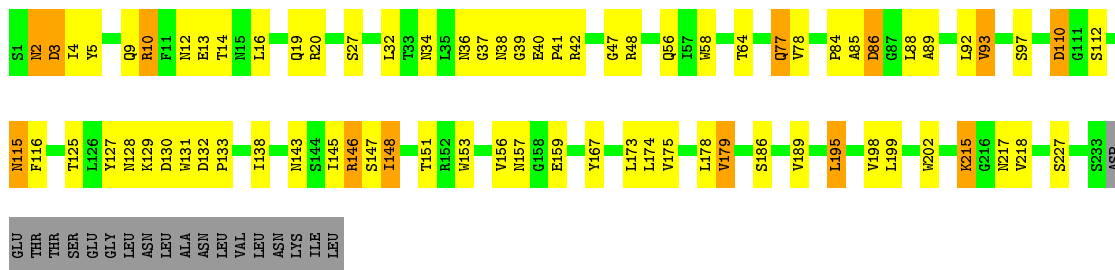
- Molecule 1: PHYTOHEMAGGLUTININ-L

Chain A:

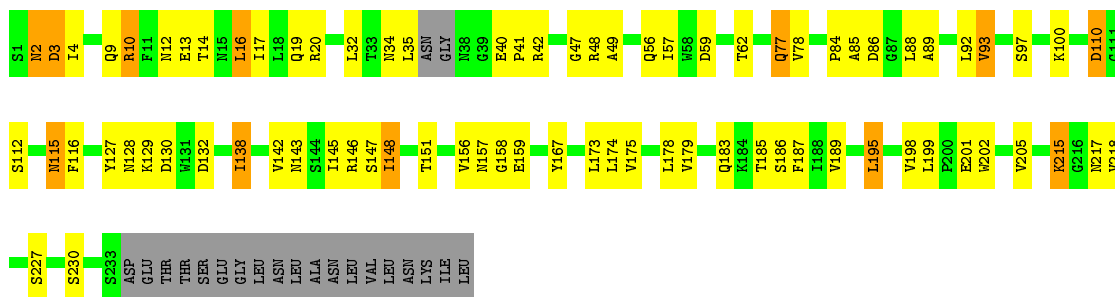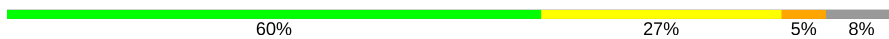- Molecule 1: PHYTOHEMAGGLUTININ-L

Chain B:

- Molecule 1: PHYTOHEMAGGLUTININ-L

Chain C:

- Molecule 1: PHYTOHEMAGGLUTININ-L

Chain D:

60%   27%   5%   8%

S1 N2 D3 I4 Q9 R10 F11 N12 E13 T14 N15 L16 I17 L18 Q19 R20 L32 T33 N34 L35 ASN GLY N38 G39 E40 P41 R42 G47 R48 A49 Q56 I57 W58 D59 T62 Q77 V78 P84 A85 D86 G87 L88 A89 L92 V93 S97 K100 D110 G111

S112 N115 F116 Y127 N128 K129 D130 W131 D132 I138 V142 N143 S144 I145 R146 S147 I148 T151 V156 N157 G158 E159 Y167 L173 L174 V175 L178 V179 Q183 K184 T185 S186 F187 I188 V189 L195 V198 L199 P200 E201 W202 V205 K215 G216 N217 V218

S227 S230 S233 ASP GLU THR THR SER GLU GLY LEU ASN LEU ALA ASN LEU VAL LEU ASN LYS ILE LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.30Å 121.20Å 90.80Å 90.00° 93.70° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 14.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.0 (10.00-2.80) 88.4 (14.96-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.19 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.200 , 0.230 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 44.5	EDS
L-test for twinning[2]	$<|L|>=0.50$, $<L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7248	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 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: CA, MN, NAG

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	0.85	0/1833	0.96	3/2499 (0.1%)
1	B	0.89	1/1838 (0.1%)	0.99	4/2507 (0.2%)
1	C	0.80	0/1833	0.97	2/2499 (0.1%)
1	D	0.80	0/1825	0.97	4/2488 (0.2%)
All	All	0.83	1/7329 (0.0%)	0.97	13/9993 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	LYS	CE-NZ	-5.69	1.34	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	B	215	LYS	CD-CE-NZ	-6.90	95.83	111.70
1	B	146	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	D	146	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	C	146	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	A	138	ILE	N-CA-C	-5.45	96.28	111.00
1	A	146	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	C	138	ILE	N-CA-C	-5.27	96.76	111.00
1	D	138	ILE	N-CA-C	-5.26	96.80	111.00
1	B	146	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	16	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	146	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	D	215	LYS	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1793	0	1724	60	0
1	B	1797	0	1728	53	0
1	C	1793	0	1724	60	0
1	D	1785	0	1718	61	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	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	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
All	All	7248	0	6946	227	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 16.

All (227) 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:C:19:GLN:NE2	1:C:48:ARG:HE	1.76	0.84
1:A:19:GLN:NE2	1:A:48:ARG:HE	1.82	0.78
1:B:78:VAL:H	1:B:157:ASN:HD21	1.34	0.76
1:D:19:GLN:NE2	1:D:48:ARG:HE	1.86	0.72
1:D:78:VAL:H	1:D:157:ASN:HD21	1.36	0.72
1:C:77:GLN:HA	1:C:157:ASN:HD21	1.56	0.70
1:D:34:ASN:HD22	1:D:42:ARG:HE	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASN:HD22	1:B:42:ARG:HE	1.40	0.69
1:A:78:VAL:H	1:A:157:ASN:HD21	1.37	0.68
1:A:77:GLN:HA	1:A:157:ASN:HD21	1.57	0.68
1:B:12:ASN:OD1	1:B:14:THR:HG23	1.93	0.68
1:C:19:GLN:HE22	1:C:48:ARG:HE	1.40	0.68
1:D:32:LEU:O	1:D:47:GLY:HA3	1.93	0.68
1:D:10:ARG:NH2	2:D:253:NAG:O7	2.27	0.67
1:C:78:VAL:H	1:C:157:ASN:HD21	1.43	0.66
1:A:19:GLN:HE22	1:A:48:ARG:HE	1.42	0.65
1:A:34:ASN:HD22	1:A:42:ARG:HE	1.45	0.65
1:A:195:LEU:HG	1:A:199:LEU:HD12	1.78	0.65
1:D:77:GLN:HA	1:D:157:ASN:HD21	1.61	0.65
1:D:78:VAL:H	1:D:157:ASN:ND2	1.95	0.64
1:C:77:GLN:HA	1:C:157:ASN:ND2	2.12	0.64
1:C:12:ASN:OD1	1:C:14:THR:HG23	1.98	0.64
1:A:77:GLN:HA	1:A:157:ASN:ND2	2.12	0.64
1:A:88:LEU:HD23	1:A:89:ALA:N	2.13	0.64
1:C:32:LEU:O	1:C:47:GLY:HA3	1.97	0.64
1:D:12:ASN:OD1	1:D:14:THR:HG23	1.98	0.64
1:B:19:GLN:NE2	1:B:48:ARG:HE	1.96	0.64
1:A:10:ARG:NH2	2:A:253:NAG:O7	2.31	0.63
1:A:12:ASN:OD1	1:A:14:THR:HG23	1.99	0.62
1:B:85:ALA:CB	1:B:217:ASN:HB3	2.30	0.62
1:C:195:LEU:HG	1:C:199:LEU:HD12	1.82	0.62
1:C:88:LEU:HD23	1:C:89:ALA:N	2.14	0.62
1:D:77:GLN:HA	1:D:157:ASN:ND2	2.14	0.62
1:D:195:LEU:HG	1:D:199:LEU:HD12	1.81	0.62
1:A:174:LEU:HD12	1:A:175:VAL:N	2.15	0.61
1:A:128:ASN:H	1:A:132:ASP:HB2	1.65	0.61
1:C:174:LEU:HD12	1:C:175:VAL:N	2.16	0.61
1:C:92:LEU:HD12	1:C:92:LEU:N	2.16	0.60
1:C:34:ASN:HD22	1:C:42:ARG:HE	1.46	0.60
1:A:78:VAL:H	1:A:157:ASN:ND2	1.99	0.60
1:D:85:ALA:CB	1:D:217:ASN:HB3	2.32	0.59
1:C:128:ASN:H	1:C:132:ASP:HB2	1.66	0.59
1:A:85:ALA:CB	1:A:217:ASN:HB3	2.31	0.59
1:B:195:LEU:HG	1:B:199:LEU:HD12	1.84	0.59
1:B:174:LEU:HD12	1:B:175:VAL:N	2.18	0.58
1:B:32:LEU:O	1:B:47:GLY:HA3	2.03	0.58
1:B:77:GLN:HA	1:B:157:ASN:HD21	1.68	0.58
1:B:78:VAL:H	1:B:157:ASN:ND2	1.98	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:VAL:HG21	1:D:84:PRO:HG3	1.85	0.57
1:B:77:GLN:HA	1:B:157:ASN:ND2	2.19	0.57
1:C:78:VAL:H	1:C:157:ASN:ND2	2.01	0.57
1:C:78:VAL:HG21	1:C:84:PRO:HG3	1.84	0.57
1:C:88:LEU:C	1:C:88:LEU:HD23	2.25	0.57
1:A:32:LEU:O	1:A:47:GLY:HA3	2.06	0.56
1:D:19:GLN:HE22	1:D:48:ARG:HE	1.50	0.56
1:C:85:ALA:CB	1:C:217:ASN:HB3	2.36	0.56
1:D:88:LEU:HD23	1:D:89:ALA:N	2.21	0.56
1:C:36:ASN:OD1	1:C:38:ASN:N	2.38	0.56
1:A:36:ASN:OD1	1:A:38:ASN:HB2	2.05	0.55
1:C:19:GLN:HE21	1:C:48:ARG:HB2	1.70	0.55
1:C:35:LEU:HD13	1:C:39:GLY:HA2	1.89	0.55
1:C:174:LEU:HD12	1:C:175:VAL:H	1.70	0.54
1:A:19:GLN:HE21	1:A:48:ARG:HB2	1.73	0.54
1:A:9:GLN:H	1:B:2:ASN:ND2	2.06	0.54
1:D:128:ASN:H	1:D:132:ASP:HB2	1.73	0.54
1:B:92:LEU:HD12	1:B:92:LEU:N	2.23	0.54
1:B:128:ASN:H	1:B:132:ASP:HB2	1.72	0.53
1:C:93:VAL:HG13	1:C:97:SER:CB	2.38	0.53
1:B:93:VAL:HG13	1:B:97:SER:CB	2.39	0.53
1:B:88:LEU:HD23	1:B:89:ALA:N	2.23	0.53
1:D:78:VAL:N	1:D:157:ASN:HD21	2.06	0.53
1:A:2:ASN:ND2	1:B:9:GLN:H	2.07	0.53
1:B:19:GLN:HE22	1:B:48:ARG:HE	1.58	0.52
1:A:78:VAL:HG21	1:A:84:PRO:HG3	1.91	0.52
1:B:127:TYR:HE2	1:B:129:LYS:HD2	1.75	0.52
1:D:19:GLN:HE22	1:D:48:ARG:HH21	1.58	0.52
1:C:110:ASP:HB2	1:C:116:PHE:CE1	2.45	0.51
1:C:9:GLN:H	1:D:2:ASN:ND2	2.08	0.51
1:D:34:ASN:O	1:D:35:LEU:HD23	2.10	0.51
1:B:34:ASN:HD22	1:B:42:ARG:NE	2.07	0.51
1:D:174:LEU:HD12	1:D:175:VAL:N	2.26	0.51
1:D:19:GLN:HE21	1:D:48:ARG:HB2	1.74	0.51
1:A:93:VAL:HG13	1:A:97:SER:CB	2.41	0.50
1:A:92:LEU:HD12	1:A:92:LEU:N	2.26	0.50
1:B:110:ASP:HB3	1:B:112:SER:H	1.75	0.50
1:B:38:ASN:N	1:B:38:ASN:HD22	2.09	0.50
1:D:88:LEU:C	1:D:88:LEU:HD23	2.32	0.50
1:B:36:ASN:OD1	1:B:40:GLU:HB2	2.11	0.50
1:D:35:LEU:HA	1:D:40:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:ASP:OD1	1:D:3:ASP:N	2.44	0.50
1:A:174:LEU:HD12	1:A:175:VAL:H	1.74	0.50
1:B:78:VAL:N	1:B:157:ASN:HD21	2.06	0.50
1:C:4:ILE:CG2	1:C:230:SER:HB3	2.42	0.50
1:D:92:LEU:N	1:D:92:LEU:HD12	2.27	0.50
1:B:110:ASP:HB2	1:B:116:PHE:CE1	2.47	0.50
1:A:78:VAL:HG13	1:A:218:VAL:O	2.12	0.50
1:C:46:LEU:HD23	1:C:47:GLY:N	2.27	0.50
1:B:85:ALA:HB2	1:B:217:ASN:HB3	1.93	0.49
1:D:110:ASP:HB2	1:D:116:PHE:CE1	2.47	0.49
1:D:127:TYR:HE2	1:D:129:LYS:HD2	1.77	0.49
1:A:78:VAL:N	1:A:157:ASN:HD21	2.07	0.49
1:D:178:LEU:C	1:D:178:LEU:HD23	2.33	0.49
1:D:4:ILE:CG2	1:D:230:SER:HB3	2.43	0.49
1:B:174:LEU:HD12	1:B:175:VAL:H	1.77	0.48
1:B:78:VAL:HG21	1:B:84:PRO:HG3	1.95	0.48
1:A:131:TRP:HB2	1:A:146:ARG:HG3	1.95	0.48
1:D:156:VAL:HG12	1:D:159:GLU:HG2	1.95	0.48
1:D:178:LEU:HD23	1:D:179:VAL:N	2.29	0.48
1:C:19:GLN:HE22	1:C:48:ARG:HH21	1.62	0.48
1:B:178:LEU:HD23	1:B:179:VAL:N	2.28	0.48
1:B:167:TYR:CZ	1:B:195:LEU:HD22	2.48	0.47
1:C:145:ILE:HG13	1:C:145:ILE:O	2.12	0.47
1:D:10:ARG:HG3	1:D:10:ARG:O	2.13	0.47
1:C:127:TYR:HE2	1:C:129:LYS:HD2	1.78	0.47
1:C:157:ASN:HD22	1:C:158:GLY:N	2.11	0.47
1:C:167:TYR:CZ	1:C:195:LEU:HD22	2.49	0.47
1:D:142:VAL:O	1:D:143:ASN:HB2	2.15	0.47
1:B:3:ASP:OD1	1:B:3:ASP:N	2.47	0.47
1:C:157:ASN:ND2	1:C:158:GLY:N	2.62	0.47
1:C:156:VAL:HG12	1:C:159:GLU:HG2	1.97	0.47
1:D:167:TYR:CZ	1:D:195:LEU:HD22	2.50	0.47
1:C:127:TYR:CE2	1:C:129:LYS:HD2	2.50	0.47
1:D:115:ASN:HD21	1:D:143:ASN:HD21	1.62	0.47
1:A:115:ASN:ND2	1:A:117:HIS:H	2.13	0.47
1:A:36:ASN:O	1:A:38:ASN:N	2.48	0.47
1:A:167:TYR:CZ	1:A:195:LEU:HD22	2.50	0.47
1:D:34:ASN:HD22	1:D:42:ARG:NE	2.11	0.47
1:C:19:GLN:HE22	1:C:48:ARG:NE	2.10	0.46
1:B:127:TYR:CE2	1:B:129:LYS:HD2	2.50	0.46
1:B:4:ILE:HG13	1:B:5:TYR:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:VAL:HG13	1:C:218:VAL:O	2.15	0.46
1:B:19:GLN:HE21	1:B:48:ARG:HB2	1.80	0.46
1:A:3:ASP:N	1:A:3:ASP:OD1	2.46	0.46
1:B:156:VAL:HG12	1:B:159:GLU:HG2	1.97	0.45
1:C:146:ARG:HH11	1:C:146:ARG:HD3	1.63	0.45
1:C:70:THR:HA	1:C:227:SER:O	2.16	0.45
1:B:93:VAL:CG1	1:B:97:SER:HB3	2.46	0.45
1:C:10:ARG:O	1:C:10:ARG:HG3	2.15	0.45
1:A:127:TYR:HE2	1:A:129:LYS:HD2	1.81	0.45
1:A:41:PRO:HB2	1:A:218:VAL:HB	1.99	0.45
1:C:163:VAL:HG12	1:C:164:LEU:N	2.31	0.45
1:C:12:ASN:O	1:C:16:LEU:HD22	2.16	0.45
1:A:34:ASN:HD22	1:A:42:ARG:NE	2.14	0.45
1:A:4:ILE:CG2	1:A:230:SER:HB3	2.46	0.45
1:B:56:GLN:HB2	1:B:202:TRP:CH2	2.52	0.45
1:C:178:LEU:HD23	1:C:178:LEU:C	2.37	0.45
1:A:156:VAL:HG12	1:A:159:GLU:HG2	1.99	0.45
1:B:145:ILE:O	1:B:145:ILE:HG13	2.17	0.45
1:A:110:ASP:HB2	1:A:116:PHE:CE1	2.52	0.44
1:D:93:VAL:HG13	1:D:97:SER:CB	2.47	0.44
1:A:56:GLN:HB2	1:A:202:TRP:CH2	2.52	0.44
1:D:195:LEU:HA	1:D:195:LEU:HD12	1.76	0.44
1:D:127:TYR:CE2	1:D:129:LYS:HD2	2.53	0.44
1:B:84:PRO:HB2	1:B:125:THR:HB	1.99	0.44
1:A:127:TYR:CE2	1:A:129:LYS:HD2	2.53	0.44
1:D:187:PHE:N	1:D:187:PHE:CD1	2.85	0.44
1:B:151:THR:CG2	1:B:189:VAL:HG22	2.48	0.44
1:A:93:VAL:O	1:A:203:VAL:HB	2.18	0.43
1:B:138:ILE:HG13	1:B:153:TRP:HB2	1.99	0.43
1:A:10:ARG:O	1:A:10:ARG:HG3	2.15	0.43
1:B:127:TYR:HD1	1:B:133:PRO:O	2.01	0.43
1:B:37:GLY:C	1:B:39:GLY:H	2.22	0.43
1:B:88:LEU:HD23	1:B:88:LEU:C	2.39	0.43
1:C:34:ASN:HD22	1:C:42:ARG:NE	2.14	0.43
1:C:115:ASN:HD21	1:C:143:ASN:HD21	1.65	0.43
1:A:85:ALA:HB2	1:A:217:ASN:HB3	1.99	0.43
1:D:57:ILE:HD12	1:D:57:ILE:HA	1.85	0.43
1:B:41:PRO:HB2	1:B:218:VAL:HB	2.00	0.43
1:C:178:LEU:HD23	1:C:179:VAL:N	2.34	0.43
1:C:195:LEU:HD12	1:C:195:LEU:HA	1.80	0.43
1:C:9:GLN:H	1:D:2:ASN:HD21	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:O	1:A:143:ASN:HB2	2.19	0.43
1:C:78:VAL:N	1:C:157:ASN:HD21	2.11	0.42
1:D:145:ILE:HG13	1:D:145:ILE:O	2.19	0.42
1:D:110:ASP:HB3	1:D:112:SER:H	1.83	0.42
1:A:110:ASP:HB3	1:A:112:SER:H	1.83	0.42
1:A:84:PRO:HB2	1:A:125:THR:HB	2.01	0.42
1:C:3:ASP:N	1:C:3:ASP:OD1	2.50	0.42
1:D:100:LYS:HA	1:D:100:LYS:HD3	1.82	0.42
1:D:17:ILE:O	1:D:49:ALA:HA	2.20	0.42
1:D:41:PRO:HB2	1:D:218:VAL:HB	2.00	0.42
1:A:127:TYR:HD1	1:A:133:PRO:O	2.01	0.42
1:A:85:ALA:HA	1:A:86:ASP:HA	1.85	0.42
1:D:174:LEU:HD12	1:D:175:VAL:H	1.84	0.42
1:B:195:LEU:HD12	1:B:195:LEU:HA	1.81	0.42
1:C:93:VAL:HG13	1:C:97:SER:HB3	2.01	0.42
1:A:157:ASN:HD22	1:A:158:GLY:N	2.18	0.42
1:A:36:ASN:HD21	1:A:40:GLU:HB2	1.85	0.42
1:C:41:PRO:HB2	1:C:218:VAL:HB	2.02	0.42
1:C:93:VAL:CG1	1:C:97:SER:HB3	2.49	0.42
1:C:46:LEU:C	1:C:46:LEU:HD23	2.40	0.42
1:D:157:ASN:HD22	1:D:158:GLY:N	2.17	0.42
1:A:115:ASN:HD21	1:A:143:ASN:HD21	1.68	0.42
1:A:2:ASN:HD21	1:B:9:GLN:H	1.67	0.42
1:A:88:LEU:C	1:A:88:LEU:HD23	2.40	0.42
1:A:93:VAL:CG1	1:A:97:SER:HB3	2.50	0.42
1:B:58:TRP:HB2	1:B:64:THR:O	2.19	0.41
1:B:148:ILE:HA	1:B:148:ILE:HD13	1.80	0.41
1:B:178:LEU:C	1:B:178:LEU:HD23	2.40	0.41
1:C:2:ASN:ND2	1:D:9:GLN:H	2.17	0.41
1:C:56:GLN:HB2	1:C:202:TRP:CH2	2.55	0.41
1:B:131:TRP:HB2	1:B:146:ARG:HG3	2.02	0.41
1:D:59:ASP:HB3	1:D:62:THR:OG1	2.20	0.41
1:B:115:ASN:HD21	1:B:143:ASN:HD21	1.68	0.41
1:C:57:ILE:HD12	1:C:57:ILE:HA	1.94	0.41
1:D:148:ILE:HD13	1:D:148:ILE:HA	1.84	0.41
1:D:183:GLN:HB2	1:D:185:THR:HG23	2.02	0.41
1:A:178:LEU:HD23	1:A:179:VAL:N	2.36	0.41
1:A:46:LEU:HD23	1:A:47:GLY:N	2.36	0.41
1:C:56:GLN:HB2	1:C:202:TRP:CZ2	2.56	0.41
1:A:226:TRP:CD1	1:A:227:SER:N	2.88	0.41
1:A:70:THR:HA	1:A:227:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:THR:CG2	1:D:189:VAL:HG22	2.51	0.41
1:D:85:ALA:HB2	1:D:217:ASN:HB3	2.02	0.41
1:D:85:ALA:HB3	1:D:217:ASN:HB3	2.01	0.41
1:C:2:ASN:HD21	1:D:9:GLN:H	1.69	0.41
1:D:156:VAL:CG1	1:D:159:GLU:HG2	2.51	0.41
1:D:138:ILE:HB	1:D:151:THR:HG22	2.03	0.41
1:B:85:ALA:HA	1:B:86:ASP:HA	1.85	0.41
1:D:56:GLN:HB2	1:D:202:TRP:CH2	2.56	0.41
1:A:138:ILE:HG13	1:A:153:TRP:HB2	2.03	0.40
1:C:156:VAL:HG21	1:C:183:GLN:HG3	2.03	0.40
1:A:178:LEU:C	1:A:178:LEU:HD23	2.41	0.40
1:A:59:ASP:HB3	1:A:62:THR:OG1	2.21	0.40
1:C:110:ASP:HB3	1:C:112:SER:H	1.86	0.40
1:A:127:TYR:CD1	1:A:133:PRO:O	2.74	0.40
1:D:57:ILE:N	1:D:201:GLU:O	2.50	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	228/252 (90%)	216 (95%)	11 (5%)	1 (0%)	34	66
1	B	231/252 (92%)	221 (96%)	9 (4%)	1 (0%)	34	66
1	C	228/252 (90%)	215 (94%)	12 (5%)	1 (0%)	34	66
1	D	227/252 (90%)	217 (96%)	9 (4%)	1 (0%)	34	66
All	All	914/1008 (91%)	869 (95%)	41 (4%)	4 (0%)	34	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	LYS
1	B	215	LYS
1	C	215	LYS
1	D	215	LYS

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	201/218 (92%)	178 (89%)	23 (11%)	5	18
1	B	201/218 (92%)	180 (90%)	21 (10%)	7	21
1	C	201/218 (92%)	178 (89%)	23 (11%)	5	18
1	D	200/218 (92%)	180 (90%)	20 (10%)	7	22
All	All	803/872 (92%)	716 (89%)	87 (11%)	6	19

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	ASP
1	A	10	ARG
1	A	13	GLU
1	A	16	LEU
1	A	20	ARG
1	A	27	SER
1	A	77	GLN
1	A	86	ASP
1	A	93	VAL
1	A	110	ASP
1	A	115	ASN
1	A	130	ASP
1	A	146	ARG
1	A	147	SER
1	A	148	ILE
1	A	173	LEU
1	A	174	LEU

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Mol	Chain	Res	Type
1	A	179	VAL
1	A	186	SER
1	A	195	LEU
1	A	198	VAL
1	A	227	SER
1	B	2	ASN
1	B	3	ASP
1	B	10	ARG
1	B	13	GLU
1	B	16	LEU
1	B	20	ARG
1	B	27	SER
1	B	77	GLN
1	B	86	ASP
1	B	93	VAL
1	B	110	ASP
1	B	115	ASN
1	B	130	ASP
1	B	147	SER
1	B	148	ILE
1	B	173	LEU
1	B	179	VAL
1	B	186	SER
1	B	195	LEU
1	B	198	VAL
1	B	227	SER
1	C	2	ASN
1	C	3	ASP
1	C	10	ARG
1	C	13	GLU
1	C	16	LEU
1	C	20	ARG
1	C	26	SER
1	C	27	SER
1	C	77	GLN
1	C	86	ASP
1	C	93	VAL
1	C	110	ASP
1	C	115	ASN
1	C	130	ASP
1	C	147	SER
1	C	148	ILE

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Mol	Chain	Res	Type
1	C	173	LEU
1	C	174	LEU
1	C	179	VAL
1	C	186	SER
1	C	195	LEU
1	C	198	VAL
1	C	227	SER
1	D	2	ASN
1	D	3	ASP
1	D	10	ARG
1	D	13	GLU
1	D	16	LEU
1	D	20	ARG
1	D	77	GLN
1	D	86	ASP
1	D	93	VAL
1	D	110	ASP
1	D	115	ASN
1	D	130	ASP
1	D	147	SER
1	D	148	ILE
1	D	173	LEU
1	D	186	SER
1	D	195	LEU
1	D	198	VAL
1	D	205	VAL
1	D	227	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	19	GLN
1	A	34	ASN
1	A	115	ASN
1	A	157	ASN
1	B	2	ASN
1	B	19	GLN
1	B	34	ASN
1	B	38	ASN
1	B	115	ASN
1	B	157	ASN

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Mol	Chain	Res	Type
1	C	2	ASN
1	C	19	GLN
1	C	34	ASN
1	C	115	ASN
1	C	157	ASN
1	D	2	ASN
1	D	19	GLN
1	D	34	ASN
1	D	115	ASN
1	D	157	ASN

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	C	253	1	14,14,15	0.43	0	17,19,21	0.74	0
2	NAG	D	253	1	14,14,15	0.68	0	17,19,21	0.85	0
2	NAG	A	253	1	14,14,15	0.46	0	17,19,21	0.78	0
2	NAG	B	253	1	14,14,15	0.56	0	17,19,21	0.92	0

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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	C	253	1	-	1/6/23/26	0/1/1/1
2	NAG	D	253	1	-	1/6/23/26	0/1/1/1
2	NAG	A	253	1	-	1/6/23/26	0/1/1/1
2	NAG	B	253	1	-	1/6/23/26	0/1/1/1

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
2	A	253	NAG	O5-C5-C6-O6
2	B	253	NAG	O5-C5-C6-O6
2	C	253	NAG	O5-C5-C6-O6
2	D	253	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	253	NAG	1	0
2	A	253	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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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