Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 07:47 PM EDT

PDB ID	:	1TI8
Title	:	H7 Haemagglutinin
Authors	:	Russell, R.J.; Gamblin, S.J.; Haire, L.F.; Stevens, D.J.; Xaio, B.; Ha, Y.; Skehel, J.J.
Deposited on	:	2004-06-02
Resolution	:	3.00 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:

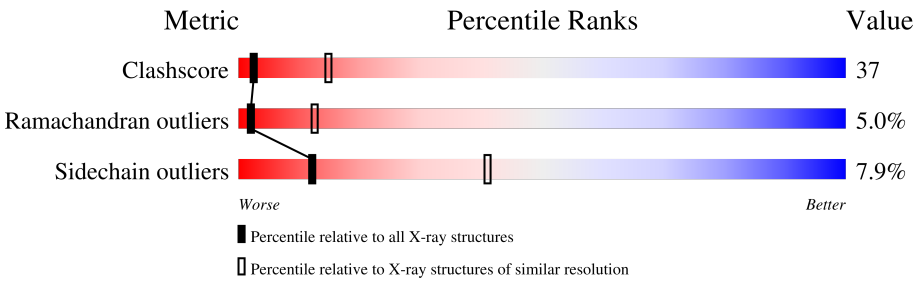
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	51% 41% 7% •
2	B	172	45% 44% 8% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	341	X	-	-	-
4	MAN	A	343	X	-	-	-
4	MAN	A	344	X	-	-	-
5	NAG	B	339	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3978 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 hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2401	1487	432	466	16	0	0	0

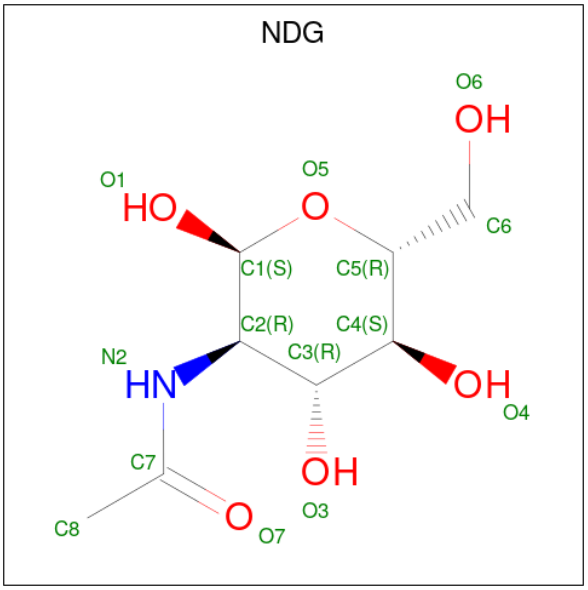
- Molecule 2 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	166	1346	831	234	274	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

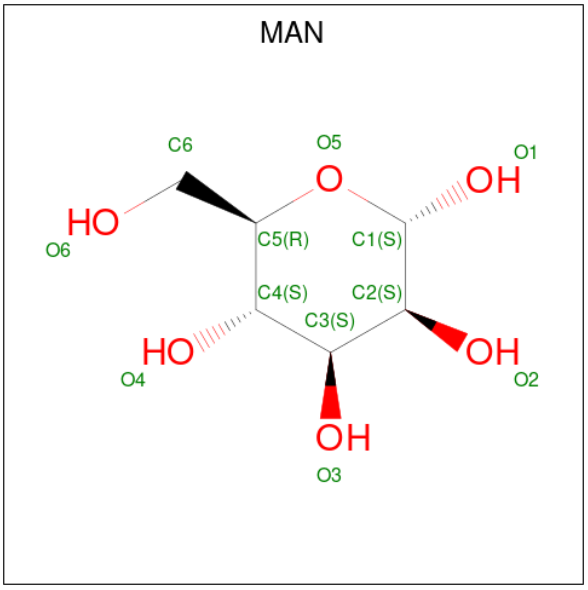
Chain	Residue	Modelled	Actual	Comment	Reference
B	111	THR	ALA	conflict	UNP Q701T7

- Molecule 3 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



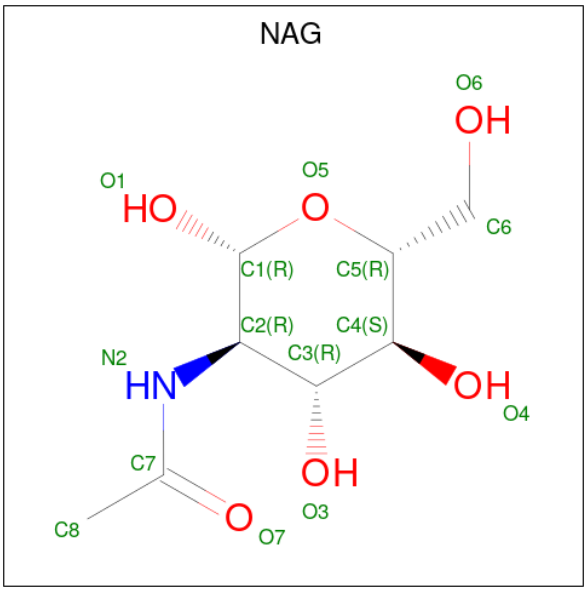
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			12	6	6			
4	A	1	Total	C	O		0	0
			12	6	6			
4	A	1	Total	C	O		0	0
			12	6	6			
4	A	1	Total	C	O		0	0
			12	6	6			
4	A	1	Total	C	O		0	0
			12	6	6			

- Molecule 5 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		
5	A	1	15	8	1	6	0	0
			Total	C	N	O		
5	B	1	15	8	1	6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	94	94	94	0	0
			Total	O		
6	B	32	32	32	0	0

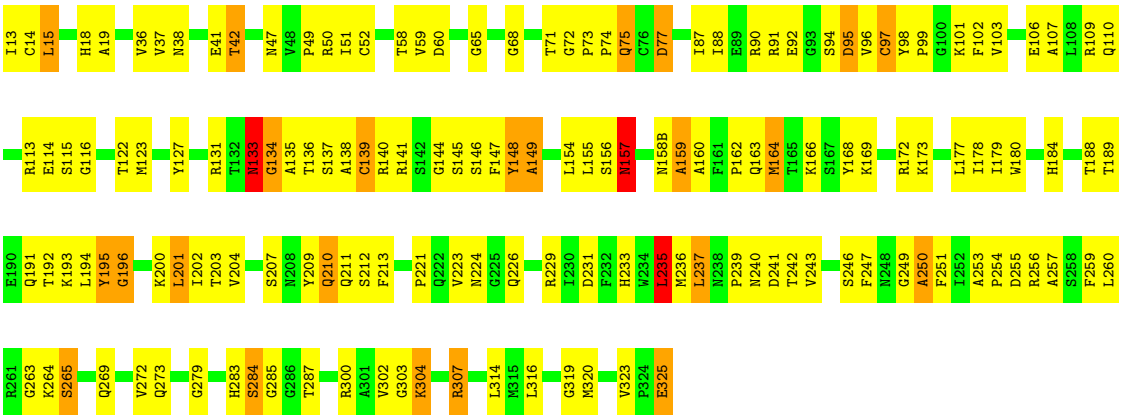
3 Residue-property plots (i)

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: hemagglutinin

Chain A: 51% 41% 7% •



• Molecule 2: hemagglutinin

Chain B: 45% 44% 8% • •

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	118.20Å 118.20Å 298.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3978	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

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: MAN, NDG, 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	0.43	0/2447	0.70	1/3306 (0.0%)
2	B	0.39	0/1370	0.62	2/1847 (0.1%)
All	All	0.42	0/3817	0.67	3/5153 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	10	ILE	N-CA-C	-6.33	93.90	111.00
1	A	235	LEU	CA-CB-CG	5.86	128.78	115.30
2	B	70	PHE	N-CA-C	-5.23	96.87	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	2401	0	2345	183	0
2	B	1346	0	1248	117	0
3	A	15	0	12	3	0
4	A	60	0	60	6	0
5	A	15	0	15	2	0
5	B	15	0	15	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	94	0	0	5	0
6	B	32	0	0	2	0
All	All	3978	0	3695	281	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 37.

All (281) 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:116:GLY:HA2	1:A:265:SER:HB3	1.45	0.95
1:A:302:VAL:HG11	2:B:65:LEU:HB3	1.48	0.93
2:B:150:ALA:HA	2:B:153:ARG:HE	1.34	0.92
1:A:269:GLN:HE22	2:B:68:ASN:ND2	1.70	0.89
2:B:15:GLU:HB3	6:B:346:HOH:O	1.73	0.87
1:A:207:SER:HB3	1:A:241:ASP:OD2	1.75	0.87
3:A:340:NDG:C1	5:B:339:NAG:O4	2.25	0.84
1:A:75:GLN:H	1:A:75:GLN:NE2	1.75	0.84
1:A:237:LEU:HG	1:A:243:VAL:HG23	1.58	0.83
1:A:13:ILE:HD11	2:B:24:PHE:HB3	1.60	0.82
2:B:121:ARG:HG2	2:B:125:GLN:NE2	1.96	0.80
1:A:304:LYS:HD2	2:B:62:GLN:HB2	1.64	0.78
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.46	0.78
1:A:131:ARG:HE	1:A:133:ASN:ND2	1.82	0.78
4:A:341:MAN:O2	4:A:345:MAN:H1	1.82	0.77
1:A:237:LEU:HG	1:A:243:VAL:CG2	2.15	0.76
1:A:109:ARG:O	1:A:113:ARG:HG3	1.86	0.76
1:A:283:HIS:CD2	1:A:285:GLY:H	2.04	0.76
1:A:13:ILE:HD13	2:B:26:HIS:HB3	1.68	0.75
2:B:158:ASP:OD2	2:B:161:ARG:HG3	1.87	0.75
1:A:131:ARG:HH21	1:A:133:ASN:HD22	1.34	0.75
2:B:3:PHE:HB2	2:B:112:ASP:HB3	1.67	0.74
1:A:42:THR:HB	1:A:314:LEU:O	1.88	0.74
4:A:343:MAN:O3	4:A:344:MAN:H1	1.87	0.74
4:A:341:MAN:O4	4:A:343:MAN:H5	1.88	0.74
1:A:122:THR:HA	1:A:256:ARG:HG2	1.70	0.73
1:A:123:MET:CE	1:A:257:ALA:HB2	2.18	0.73
1:A:68:GLY:N	1:A:95:ASP:HB3	2.04	0.72
2:B:26:HIS:HB2	2:B:149:MET:CE	2.20	0.71
1:A:72:GLY:HA3	1:A:149:ALA:HB3	1.73	0.71
2:B:24:PHE:CD1	2:B:153:ARG:HG2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:HD12	1:A:202:ILE:N	2.06	0.70
1:A:316:LEU:HD22	2:B:55:LEU:HD12	1.74	0.70
1:A:192:THR:HA	1:A:196:GLY:O	1.92	0.69
1:A:155:LEU:HD11	1:A:194:LEU:HD22	1.74	0.69
1:A:164:MET:HE2	1:A:247:PHE:CZ	2.26	0.69
1:A:123:MET:HE3	1:A:257:ALA:HB2	1.75	0.69
1:A:178:ILE:HD11	1:A:237:LEU:HD12	1.75	0.68
1:A:237:LEU:CD2	1:A:241:ASP:HB3	2.24	0.67
4:A:342:MAN:O2	4:A:343:MAN:H1	1.94	0.67
2:B:28:ASN:ND2	2:B:145:ASP:HA	2.10	0.67
1:A:179:ILE:O	1:A:254:PRO:HB3	1.95	0.67
1:A:116:GLY:CA	1:A:265:SER:HB3	2.22	0.67
2:B:82:ASN:ND2	2:B:85:ARG:NH1	2.43	0.66
1:A:237:LEU:HD22	1:A:241:ASP:HB3	1.78	0.65
1:A:241:ASP:OD1	1:A:242:THR:N	2.29	0.65
1:A:269:GLN:NE2	2:B:68:ASN:ND2	2.43	0.65
1:A:156:SER:HB2	1:A:195:TYR:HA	1.78	0.64
2:B:67:ASP:OD2	2:B:85:ARG:NH2	2.25	0.64
1:A:98:TYR:HD1	1:A:136:THR:HG21	1.62	0.64
1:A:269:GLN:HE22	2:B:68:ASN:HD22	1.43	0.64
2:B:26:HIS:CD2	2:B:149:MET:HG3	2.33	0.64
1:A:50:ARG:HA	1:A:272:VAL:CG1	2.28	0.64
2:B:68:ASN:ND2	2:B:70:PHE:O	2.31	0.64
1:A:75:GLN:H	1:A:75:GLN:HE21	1.43	0.63
1:A:137:SER:O	1:A:140:ARG:HG3	1.98	0.63
2:B:82:ASN:ND2	2:B:85:ARG:HH12	1.96	0.63
2:B:88:MET:CE	2:B:88:MET:HA	2.29	0.63
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.33	0.63
2:B:59:THR:C	2:B:61:GLN:H	2.01	0.62
1:A:73:PRO:HB2	1:A:75:GLN:HE22	1.65	0.62
1:A:15:LEU:O	1:A:15:LEU:HD22	1.99	0.61
1:A:158(B):ASN:HA	1:A:192:THR:O	2.01	0.61
1:A:96:VAL:HG12	1:A:97:CYS:N	2.14	0.61
3:A:340:NDG:O4	4:A:341:MAN:O1	2.18	0.61
2:B:82:ASN:ND2	5:B:339:NAG:H1	2.15	0.61
1:A:180:TRP:HZ3	1:A:235:LEU:HD13	1.65	0.61
1:A:180:TRP:CZ3	1:A:235:LEU:HD13	2.35	0.60
2:B:82:ASN:ND2	5:B:339:NAG:C1	2.65	0.60
2:B:105:GLN:NE2	6:B:341:HOH:O	2.35	0.60
2:B:118:LEU:O	2:B:121:ARG:HB3	2.00	0.60
2:B:25:ARG:HH21	2:B:34:THR:HG21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:HG3	1:A:157:ASN:HA	1.83	0.60
2:B:159:HIS:CD2	2:B:160:SER:H	2.20	0.60
1:A:237:LEU:CG	1:A:243:VAL:HG23	2.31	0.60
1:A:162:PRO:HG2	1:A:164:MET:HG3	1.85	0.59
2:B:127:ARG:HG3	2:B:159:HIS:ND1	2.16	0.59
1:A:136:THR:HG23	1:A:139:CYS:H	1.67	0.59
2:B:119:TYR:OH	2:B:132:GLU:HG3	2.02	0.59
1:A:123:MET:HG3	1:A:254:PRO:O	2.02	0.58
1:A:316:LEU:HD22	2:B:55:LEU:CD1	2.33	0.58
2:B:2:LEU:HG	2:B:109:ASP:OD2	2.03	0.58
2:B:148:CYS:O	2:B:151:SER:HB3	2.03	0.58
1:A:191:GLN:NE2	1:A:200:LYS:HG3	2.19	0.58
2:B:150:ALA:HB2	2:B:153:ARG:NH2	2.20	0.57
1:A:302:VAL:HG11	2:B:65:LEU:CB	2.27	0.57
1:A:68:GLY:O	1:A:73:PRO:HD2	2.04	0.56
1:A:269:GLN:O	1:A:284:SER:HA	2.05	0.56
1:A:319:GLY:HA2	2:B:21:TRP:CH2	2.40	0.56
1:A:210:GLN:HG3	1:A:210:GLN:O	2.04	0.56
1:A:106:GLU:HG3	1:A:110:GLN:NE2	2.20	0.56
1:A:169:LYS:HE3	1:A:240:ASN:O	2.06	0.56
1:A:255:ASP:OD1	1:A:256:ARG:HG3	2.06	0.56
2:B:26:HIS:HB2	2:B:149:MET:SD	2.45	0.56
2:B:82:ASN:CG	5:B:339:NAG:C1	2.74	0.56
1:A:131:ARG:CZ	1:A:155:LEU:HD23	2.35	0.56
1:A:203:THR:HG22	1:A:212:SER:HB2	1.86	0.56
1:A:123:MET:HE1	1:A:257:ALA:HB2	1.88	0.56
1:A:179:ILE:HG22	1:A:180:TRP:N	2.21	0.56
1:A:307:ARG:H	1:A:307:ARG:HD3	1.71	0.56
2:B:150:ALA:HA	2:B:153:ARG:NE	2.14	0.56
1:A:51:ILE:HD13	1:A:88:ILE:HD13	1.88	0.56
2:B:127:ARG:HG3	2:B:159:HIS:CE1	2.41	0.55
2:B:164:GLU:C	2:B:166:ALA:H	2.10	0.55
1:A:99:PRO:HB3	1:A:223:VAL:HB	1.88	0.55
2:B:28:ASN:HB2	2:B:144:CYS:O	2.06	0.55
1:A:97:CYS:HB2	1:A:148:TYR:CZ	2.42	0.54
1:A:38:ASN:ND2	5:A:349:NAG:C1	2.71	0.54
2:B:141:PHE:O	2:B:142:HIS:HB3	2.06	0.54
2:B:18:ILE:HD13	2:B:18:ILE:H	1.71	0.54
1:A:71:THR:HB	1:A:148:TYR:CD2	2.42	0.54
1:A:107:ALA:HB2	6:A:429:HOH:O	2.06	0.54
1:A:178:ILE:HD12	1:A:243:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:VAL:HG21	1:A:233:HIS:CE1	2.43	0.54
1:A:209:TYR:O	1:A:210:GLN:HB3	2.06	0.53
1:A:209:TYR:CZ	1:A:211:GLN:HG2	2.43	0.53
2:B:111:THR:O	2:B:112:ASP:C	2.46	0.53
1:A:38:ASN:ND2	5:A:349:NAG:O5	2.41	0.53
1:A:147:PHE:O	1:A:148:TYR:O	2.25	0.53
1:A:164:MET:CE	1:A:166:LYS:HE2	2.39	0.53
2:B:55:LEU:CD2	2:B:99:LEU:HD21	2.38	0.53
1:A:177:LEU:HD13	1:A:236:MET:HE1	1.90	0.53
1:A:15:LEU:HD13	1:A:15:LEU:H	1.74	0.53
1:A:98:TYR:CD1	1:A:136:THR:HG21	2.43	0.53
1:A:325:GLU:HG2	2:B:12:ASN:ND2	2.24	0.52
1:A:41:GLU:HG3	1:A:42:THR:N	2.24	0.52
1:A:68:GLY:H	1:A:95:ASP:HB3	1.72	0.52
2:B:119:TYR:HE1	2:B:136:GLY:HA2	1.74	0.52
2:B:150:ALA:HB2	2:B:153:ARG:HH21	1.75	0.52
2:B:27:GLN:HA	2:B:32:GLU:HG2	1.91	0.52
2:B:82:ASN:ND2	5:B:339:NAG:C5	2.72	0.52
1:A:98:TYR:CE1	1:A:226:GLN:HG3	2.44	0.52
2:B:19:ASP:OD1	2:B:36:ALA:HB3	2.09	0.52
2:B:82:ASN:CG	5:B:339:NAG:H1	2.30	0.52
1:A:144:GLY:O	1:A:145:SER:HB3	2.10	0.51
1:A:319:GLY:HA2	2:B:21:TRP:HH2	1.75	0.51
1:A:195:TYR:CZ	1:A:250:ALA:HA	2.45	0.51
2:B:59:THR:C	2:B:61:GLN:N	2.63	0.51
1:A:65:GLY:O	1:A:68:GLY:N	2.43	0.51
1:A:96:VAL:CG1	1:A:97:CYS:N	2.74	0.51
2:B:51:LYS:NZ	2:B:106:HIS:ND1	2.52	0.51
1:A:19:ALA:HB2	6:A:423:HOH:O	2.11	0.51
1:A:49:PRO:O	1:A:272:VAL:HG11	2.11	0.51
2:B:82:ASN:ND2	5:B:339:NAG:O5	2.44	0.51
1:A:49:PRO:O	1:A:272:VAL:CG1	2.59	0.50
2:B:17:LEU:O	2:B:17:LEU:HG	2.12	0.50
2:B:88:MET:HA	2:B:88:MET:HE3	1.91	0.50
1:A:115:SER:HB2	1:A:260:LEU:HD22	1.93	0.50
2:B:59:THR:O	2:B:61:GLN:N	2.45	0.50
1:A:123:MET:HE2	1:A:168:TYR:CD1	2.46	0.50
2:B:55:LEU:HD22	2:B:99:LEU:HD21	1.94	0.50
2:B:82:ASN:ND2	5:B:339:NAG:H5	2.27	0.50
2:B:123:LYS:HA	2:B:138:PHE:CE2	2.47	0.50
2:B:133:ASP:CG	2:B:134:GLY:N	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:HA	2:B:26:HIS:HA	1.93	0.49
2:B:43:SER:O	2:B:47:GLN:HG3	2.13	0.49
1:A:15:LEU:HD13	2:B:136:GLY:O	2.13	0.49
1:A:249:GLY:O	1:A:251:PHE:N	2.46	0.49
1:A:307:ARG:H	1:A:307:ARG:CD	2.25	0.49
1:A:320:MET:HA	2:B:111:THR:HG21	1.95	0.49
1:A:323:VAL:CG1	2:B:12:ASN:HA	2.43	0.49
1:A:49:PRO:C	1:A:272:VAL:HG11	2.33	0.48
2:B:160:SER:HA	2:B:163:ARG:HB2	1.95	0.48
1:A:131:ARG:NH2	1:A:133:ASN:HD22	2.04	0.48
1:A:323:VAL:HG11	2:B:12:ASN:HA	1.94	0.48
1:A:15:LEU:HD21	2:B:119:TYR:HD1	1.78	0.48
1:A:135:ALA:HB1	1:A:146:SER:HA	1.95	0.48
1:A:279:GLY:HA3	1:A:287:THR:HG21	1.96	0.48
1:A:58:THR:HG22	1:A:59:VAL:N	2.29	0.47
1:A:164:MET:HE1	1:A:166:LYS:HE2	1.96	0.47
2:B:100:VAL:O	2:B:104:ASN:ND2	2.46	0.47
2:B:128:GLU:CD	2:B:128:GLU:H	2.18	0.47
1:A:164:MET:HE2	1:A:164:MET:HB3	1.78	0.47
3:A:340:NDG:C1	5:B:339:NAG:HO4	2.27	0.47
1:A:156:SER:OG	1:A:159:ALA:HB3	2.14	0.47
1:A:37:VAL:O	1:A:38:ASN:HB2	2.15	0.47
1:A:147:PHE:CG	1:A:148:TYR:N	2.84	0.46
1:A:160:ALA:HA	1:A:196:GLY:CA	2.44	0.46
1:A:316:LEU:CD2	2:B:55:LEU:HD12	2.45	0.46
1:A:41:GLU:CG	1:A:42:THR:N	2.78	0.46
1:A:15:LEU:HD13	1:A:15:LEU:N	2.30	0.46
1:A:41:GLU:CG	1:A:42:THR:H	2.28	0.46
1:A:207:SER:CB	1:A:241:ASP:OD2	2.57	0.46
2:B:104:ASN:O	2:B:105:GLN:C	2.54	0.46
1:A:103:VAL:HG21	1:A:233:HIS:HE1	1.81	0.46
1:A:253:ALA:HB1	6:A:430:HOH:O	2.15	0.46
1:A:131:ARG:NE	1:A:133:ASN:ND2	2.60	0.46
5:B:339:NAG:HO1	5:B:339:NAG:C7	2.30	0.45
1:A:13:ILE:HB	2:B:149:MET:SD	2.56	0.45
2:B:123:LYS:HA	2:B:138:PHE:HE2	1.79	0.45
1:A:184:HIS:N	1:A:229:ARG:O	2.40	0.45
1:A:172:ARG:HD3	1:A:259:PHE:CZ	2.52	0.45
1:A:203:THR:OG1	1:A:246:SER:HB2	2.16	0.45
1:A:13:ILE:HD12	1:A:14:CYS:H	1.82	0.45
2:B:114:GLU:O	2:B:117:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLN:HB3	6:A:386:HOH:O	2.16	0.45
4:A:341:MAN:O2	4:A:345:MAN:C1	2.58	0.45
1:A:116:GLY:HA3	1:A:263:GLY:O	2.17	0.45
1:A:320:MET:CA	2:B:111:THR:HG21	2.48	0.44
2:B:19:ASP:HB3	2:B:36:ALA:HB2	1.99	0.44
1:A:41:GLU:HG3	1:A:42:THR:H	1.81	0.44
1:A:60:ASP:OD2	1:A:90:ARG:NH2	2.38	0.44
1:A:50:ARG:HA	1:A:272:VAL:HG11	1.99	0.44
2:B:121:ARG:HG2	2:B:125:GLN:HE21	1.80	0.44
1:A:164:MET:HE2	1:A:247:PHE:HZ	1.79	0.44
2:B:126:LEU:HD12	2:B:138:PHE:CD2	2.52	0.44
1:A:36:VAL:HG23	1:A:38:ASN:H	1.83	0.44
2:B:56:ILE:HG22	2:B:56:ILE:O	2.18	0.44
1:A:74:PRO:HA	1:A:77:ASP:OD1	2.18	0.44
1:A:133:ASN:HB2	1:A:134:GLY:H	1.63	0.44
2:B:164:GLU:O	2:B:166:ALA:N	2.45	0.44
1:A:74:PRO:HD2	1:A:97:CYS:SG	2.58	0.44
1:A:87:ILE:HG22	1:A:88:ILE:N	2.33	0.44
1:A:191:GLN:C	1:A:193:LYS:H	2.20	0.44
2:B:21:TRP:CD1	2:B:41:THR:HG23	2.53	0.43
1:A:50:ARG:HA	1:A:272:VAL:HG12	1.98	0.43
1:A:97:CYS:HB2	1:A:148:TYR:CE1	2.53	0.43
1:A:145:SER:HB3	6:A:395:HOH:O	2.18	0.43
2:B:107:THR:O	2:B:110:LEU:HB3	2.19	0.43
1:A:127:TYR:CZ	1:A:154:LEU:HD21	2.54	0.43
2:B:22:TYR:HE2	2:B:115:MET:HB2	1.84	0.43
1:A:51:ILE:CD1	1:A:88:ILE:HD13	2.49	0.43
2:B:159:HIS:CG	2:B:160:SER:N	2.87	0.43
1:A:249:GLY:C	1:A:251:PHE:N	2.72	0.43
2:B:158:ASP:O	2:B:159:HIS:C	2.57	0.43
1:A:90:ARG:HB3	1:A:92:GLU:CD	2.39	0.43
1:A:325:GLU:HG2	2:B:12:ASN:HD21	1.83	0.43
2:B:133:ASP:CG	2:B:134:GLY:H	2.22	0.43
1:A:73:PRO:HB2	1:A:75:GLN:NE2	2.32	0.42
1:A:114:GLU:HA	1:A:265:SER:O	2.19	0.42
1:A:91:ARG:HA	2:B:70:PHE:CD1	2.54	0.42
1:A:131:ARG:HE	1:A:133:ASN:HD21	1.64	0.42
1:A:272:VAL:CG1	1:A:273:GLN:N	2.81	0.42
2:B:145:ASP:O	2:B:148:CYS:N	2.53	0.42
1:A:47:ASN:OD1	1:A:283:HIS:HE1	2.02	0.42
1:A:141:ARG:C	1:A:144:GLY:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLY:C	1:A:251:PHE:H	2.21	0.42
2:B:27:GLN:HG3	2:B:32:GLU:CG	2.49	0.42
2:B:99:LEU:HD12	2:B:103:GLU:HG2	2.01	0.42
1:A:223:VAL:O	1:A:224:ASN:C	2.57	0.42
1:A:138:ALA:HB2	1:A:226:GLN:HG2	2.02	0.42
1:A:201:LEU:O	1:A:247:PHE:HA	2.19	0.42
1:A:163:GLN:O	1:A:164:MET:O	2.38	0.42
2:B:18:ILE:HD13	2:B:18:ILE:N	2.35	0.42
1:A:131:ARG:NH1	1:A:155:LEU:HD23	2.35	0.41
2:B:70:PHE:N	2:B:70:PHE:CD2	2.86	0.41
1:A:235:LEU:C	1:A:235:LEU:CD2	2.89	0.41
2:B:55:LEU:HD21	2:B:99:LEU:HD11	2.02	0.41
2:B:88:MET:HA	2:B:88:MET:HE2	1.99	0.41
2:B:164:GLU:C	2:B:166:ALA:N	2.73	0.41
1:A:239:PRO:O	1:A:240:ASN:HB2	2.21	0.41
1:A:180:TRP:CE2	1:A:233:HIS:HB2	2.55	0.41
1:A:303:GLY:HA2	2:B:62:GLN:HG3	2.02	0.41
2:B:162:TYR:CD1	2:B:162:TYR:N	2.88	0.41
2:B:153:ARG:C	2:B:155:ASN:H	2.24	0.41
2:B:115:MET:HE3	2:B:115:MET:HA	2.02	0.41
1:A:65:GLY:HA3	1:A:95:ASP:OD1	2.20	0.41
1:A:101:LYS:HG2	1:A:231:ASP:OD1	2.21	0.41
1:A:160:ALA:HA	1:A:196:GLY:HA3	2.03	0.41
2:B:145:ASP:O	2:B:148:CYS:HB3	2.20	0.41
2:B:159:HIS:CD2	2:B:160:SER:N	2.89	0.41
1:A:173:LYS:O	1:A:239:PRO:CG	2.69	0.41
1:A:178:ILE:CD1	1:A:243:VAL:HG21	2.51	0.41
1:A:180:TRP:HB2	1:A:251:PHE:CE1	2.56	0.41
1:A:303:GLY:O	2:B:62:GLN:HA	2.20	0.41
1:A:202:ILE:N	1:A:202:ILE:CD1	2.76	0.40
1:A:264:LYS:O	1:A:265:SER:HB3	2.21	0.40
2:B:18:ILE:H	2:B:18:ILE:CD1	2.33	0.40
2:B:44:ALA:O	2:B:45:ILE:C	2.59	0.40
1:A:213:PHE:N	1:A:213:PHE:CD1	2.89	0.40
1:A:304:LYS:HD2	2:B:62:GLN:CB	2.44	0.40
1:A:106:GLU:HA	1:A:106:GLU:OE1	2.21	0.40
1:A:300:ARG:HE	2:B:67:ASP:HB2	1.86	0.40
1:A:75:GLN:H	1:A:75:GLN:CD	2.20	0.40
1:A:172:ARG:HD3	1:A:259:PHE:CE2	2.55	0.40
1:A:179:ILE:HG22	1:A:180:TRP:H	1.85	0.40
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:GLU:HB2	2:B:141:PHE:HE1	1.86	0.40
1:A:74:PRO:CD	1:A:97:CYS:SG	3.09	0.40
1:A:158(B):ASN:O	1:A:159:ALA:O	2.40	0.40
2:B:126:LEU:HD12	2:B:138:PHE:HD2	1.87	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	312/314 (99%)	260 (83%)	39 (12%)	13 (4%)	3 16
2	B	164/172 (95%)	129 (79%)	24 (15%)	11 (7%)	1 6
All	All	476/486 (98%)	389 (82%)	63 (13%)	24 (5%)	2 12

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	TYR
1	A	157	ASN
1	A	159	ALA
1	A	164	MET
2	B	30	GLN
1	A	134	GLY
1	A	149	ALA
1	A	196	GLY
1	A	210	GLN
1	A	250	ALA
2	B	60	ASN
1	A	52	CYS
1	A	133	ASN
2	B	11	GLU

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Mol	Chain	Res	Type
2	B	71	THR
2	B	142	HIS
2	B	154	ASN
1	A	265	SER
2	B	123	LYS
2	B	159	HIS
2	B	165	GLU
2	B	155	ASN
1	A	221	PRO
2	B	45	ILE

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	265/265 (100%)	243 (92%)	22 (8%)	11	39
2	B	142/148 (96%)	132 (93%)	10 (7%)	15	47
All	All	407/413 (98%)	375 (92%)	32 (8%)	12	41

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	18	HIS
1	A	42	THR
1	A	75	GLN
1	A	77	ASP
1	A	94	SER
1	A	95	ASP
1	A	97	CYS
1	A	102	PHE
1	A	133	ASN
1	A	139	CYS
1	A	157	ASN
1	A	188	THR

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Mol	Chain	Res	Type
1	A	189	THR
1	A	195	TYR
1	A	201	LEU
1	A	235	LEU
1	A	237	LEU
1	A	284	SER
1	A	304	LYS
1	A	307	ARG
1	A	325	GLU
2	B	18	ILE
2	B	54	ARG
2	B	65	LEU
2	B	68	ASN
2	B	88	MET
2	B	109	ASP
2	B	112	ASP
2	B	128	GLU
2	B	131	GLU
2	B	159	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	38	ASN
1	A	75	GLN
1	A	110	GLN
1	A	133	ASN
1	A	199	ASN
1	A	283	HIS
2	B	28	ASN
2	B	53	ASN
2	B	68	ASN
2	B	82	ASN
2	B	95	ASN
2	B	125	GLN
2	B	159	HIS

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)

8 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	$\#\|Z\| > 2$
3	NDG	A	340	-	15,15,15	0.56	0	21,21,21	1.09	2 (9%)
4	MAN	A	343	-	12,12,12	0.36	0	17,17,17	0.35	0
4	MAN	A	341	-	12,12,12	0.29	0	17,17,17	0.52	0
5	NAG	B	339	-	15,15,15	0.52	0	21,21,21	0.68	0
4	MAN	A	344	-	12,12,12	0.44	0	17,17,17	0.37	0
4	MAN	A	342	-	12,12,12	0.35	0	17,17,17	0.36	0
5	NAG	A	349	-	15,15,15	0.42	0	21,21,21	0.58	0
4	MAN	A	345	-	12,12,12	0.34	0	17,17,17	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDG	A	340	-	-	4/6/26/26	0/1/1/1
4	MAN	A	341	-	1/1/5/5	0/2/22/22	0/1/1/1
4	MAN	A	343	-	1/1/5/5	2/2/22/22	0/1/1/1
5	NAG	B	339	-	-	5/6/26/26	0/1/1/1
4	MAN	A	344	-	1/1/5/5	0/2/22/22	0/1/1/1
4	MAN	A	342	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	349	-	-	5/6/26/26	0/1/1/1
4	MAN	A	345	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	340	NDG	C3-C4-C5	2.81	115.33	110.23
3	A	340	NDG	C4-C3-C2	2.44	113.96	110.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	341	MAN	C1
4	A	343	MAN	C1
4	A	344	MAN	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	340	NDG	C8-C7-N2-C2
3	A	340	NDG	O7-C7-N2-C2
4	A	343	MAN	C4-C5-C6-O6
4	A	343	MAN	O5-C5-C6-O6
4	A	345	MAN	O5-C5-C6-O6
5	B	339	NAG	O5-C5-C6-O6
4	A	345	MAN	C4-C5-C6-O6
5	A	349	NAG	C3-C2-N2-C7
3	A	340	NDG	C3-C2-N2-C7
5	B	339	NAG	C8-C7-N2-C2
5	B	339	NAG	C4-C5-C6-O6
5	B	339	NAG	C3-C2-N2-C7
5	A	349	NAG	C8-C7-N2-C2
5	B	339	NAG	O7-C7-N2-C2
5	A	349	NAG	C1-C2-N2-C7
5	A	349	NAG	O7-C7-N2-C2
5	A	349	NAG	C4-C5-C6-O6
3	A	340	NDG	C1-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	340	NDG	3	0
4	A	343	MAN	3	0
4	A	341	MAN	4	0
5	B	339	NAG	10	0
4	A	344	MAN	1	0
4	A	342	MAN	1	0
5	A	349	NAG	2	0
4	A	345	MAN	2	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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.