



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:50 am GMT

PDB ID : 4WST
Title : The crystal structure of hemagglutinin from A/Taiwan/1/2013 influenza virus
Authors : Yang, H.; Carney, P.J.; Chang, J.; Villanueva, J.M.; Stevens, J.
Deposited on : 2014-10-28
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

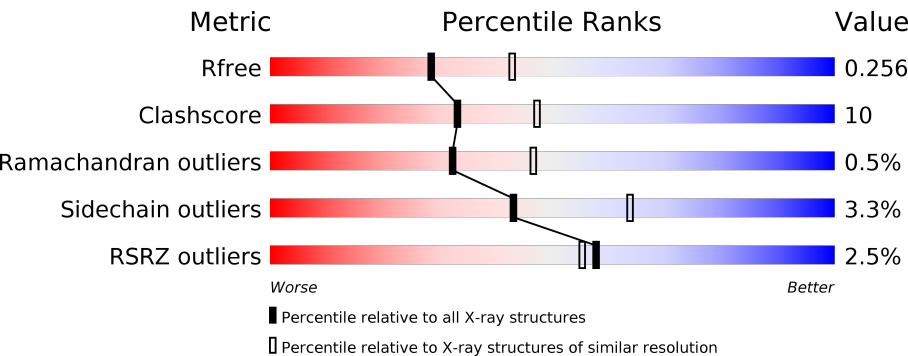
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

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 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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. 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 $\leq 5\%$. 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	334	<div><div>0%</div><div>83%13%..</div></div>
1	C	334	<div><div>0%</div><div>82%14%..</div></div>
1	E	334	<div><div>2%</div><div>82%14%..</div></div>
1	G	334	<div><div>2%</div><div>84%13%..</div></div>
1	I	334	<div><div>2%</div><div>84%12%..</div></div>
1	K	334	<div><div>2%</div><div>83%14%..</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	

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
3	NAG	A	401	X	-	-	-
3	NAG	C	401	X	-	-	-
3	NAG	E	401	X	-	-	-
3	NAG	G	401	X	-	-	-
3	NAG	I	401	X	-	-	-
3	NAG	K	401	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24510 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.

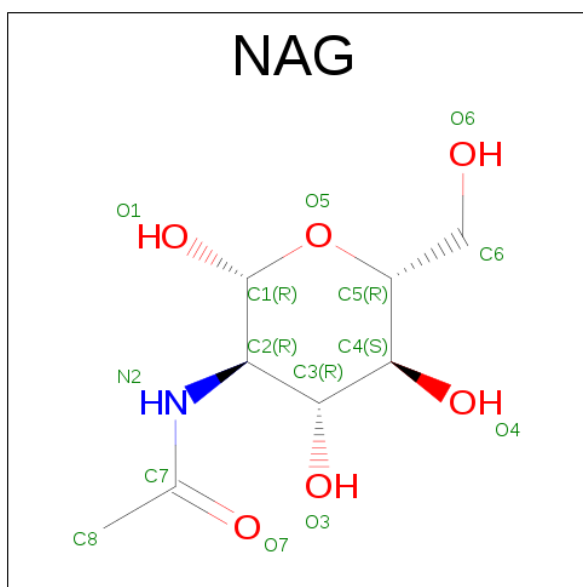
- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2566	1626	437	490	13			
1	C	325	Total	C	N	O	S	0	0	0
			2566	1626	437	490	13			
1	E	325	Total	C	N	O	S	0	0	0
			2566	1626	437	490	13			
1	G	325	Total	C	N	O	S	0	0	0
			2566	1626	437	490	13			
1	I	325	Total	C	N	O	S	0	0	0
			2566	1626	437	490	13			
1	K	325	Total	C	N	O	S	0	0	0
			2566	1626	437	490	13			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	168	Total	C	N	O	S	0	0	0
			1353	845	234	267	7			
2	D	168	Total	C	N	O	S	0	0	0
			1353	845	234	267	7			
2	F	168	Total	C	N	O	S	0	0	0
			1353	845	234	267	7			
2	H	168	Total	C	N	O	S	0	0	0
			1353	845	234	267	7			
2	J	168	Total	C	N	O	S	0	0	0
			1353	845	234	267	7			
2	L	168	Total	C	N	O	S	0	0	0
			1353	845	234	267	7			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		

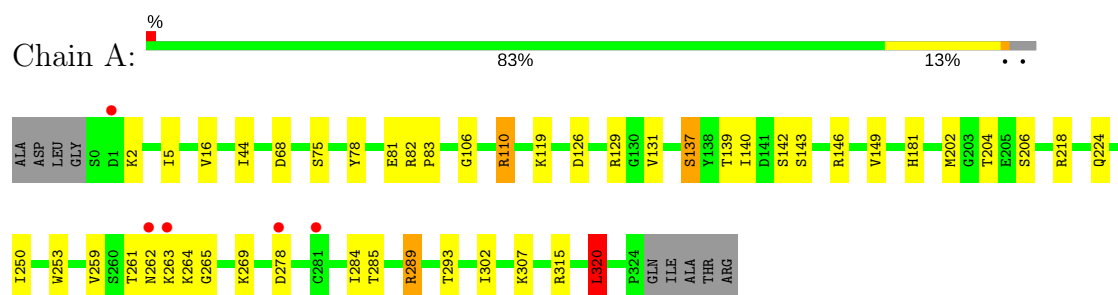
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	33	Total	O	0	0
			33	33		
4	C	91	Total	O	0	0
			91	91		
4	D	43	Total	O	0	0
			43	43		
4	E	94	Total	O	0	0
			94	94		
4	F	46	Total	O	0	0
			46	46		
4	G	99	Total	O	0	0
			99	99		
4	H	36	Total	O	0	0
			36	36		
4	I	65	Total	O	0	0
			65	65		
4	J	28	Total	O	0	0
			28	28		
4	K	66	Total	O	0	0
			66	66		
4	L	38	Total	O	0	0
			38	38		

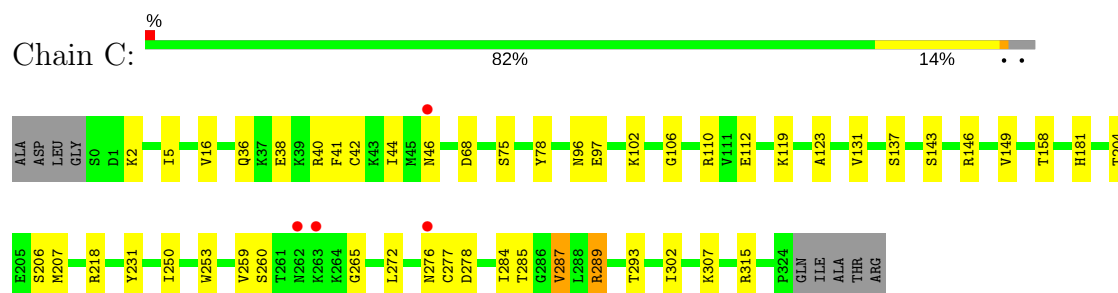
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

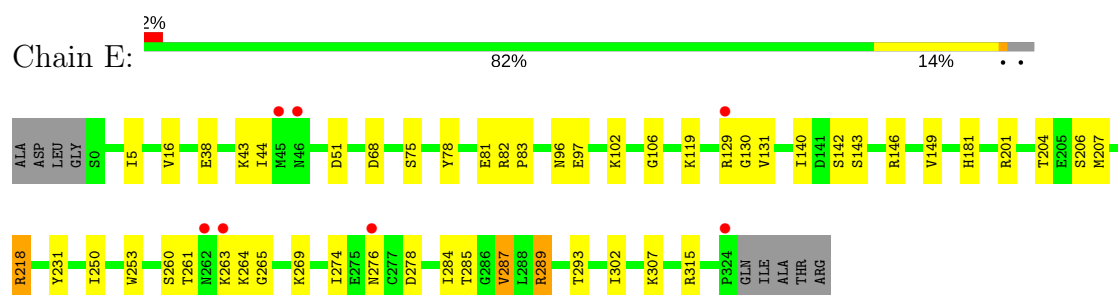
- Molecule 1: Hemagglutinin HA1 chain



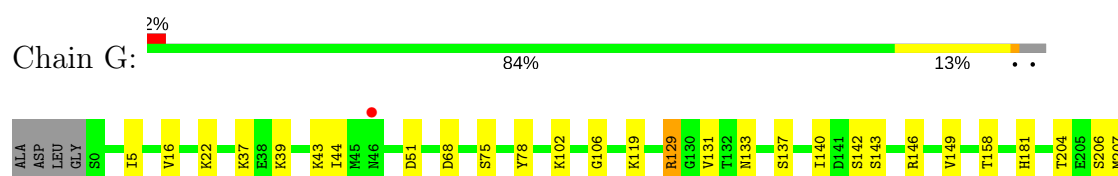
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

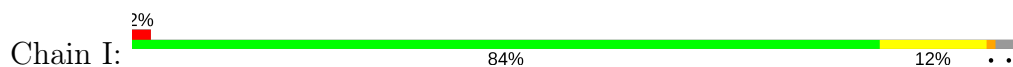


- Molecule 1: Hemagglutinin HA1 chain

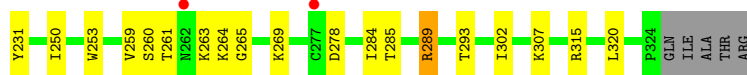
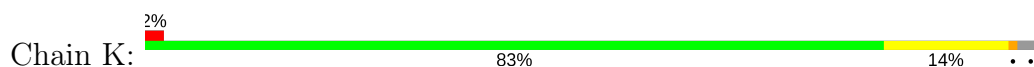




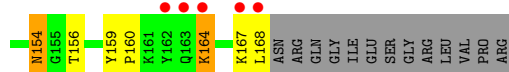
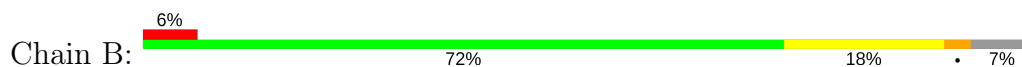
• Molecule 1: Hemagglutinin HA1 chain



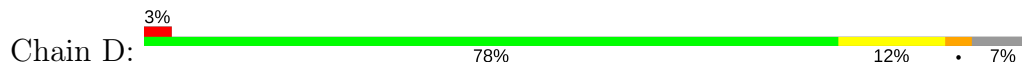
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 2: Hemagglutinin HA2 chain

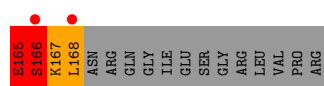


• Molecule 2: Hemagglutinin HA2 chain

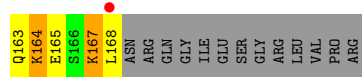


• Molecule 2: Hemagglutinin HA2 chain

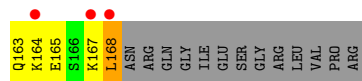
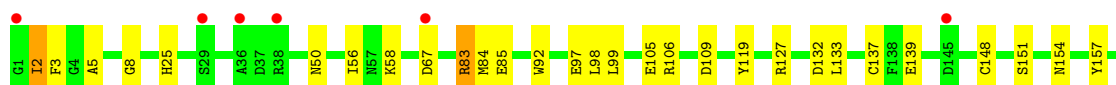




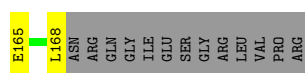
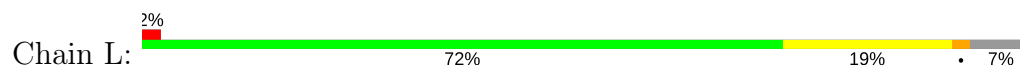
● Molecule 2: Hemagglutinin HA2 chain



● Molecule 2: Hemagglutinin HA2 chain



● Molecule 2: Hemagglutinin HA2 chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.63Å 100.61Å 175.48Å 90.00° 99.66° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 48.30 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.40) 96.6 (48.30-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.222 , 0.253 0.226 , 0.256	Depositor DCC
R_{free} test set	7372 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24510	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.40 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1515e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.77	0/2627	0.83	3/3574 (0.1%)
1	C	0.75	0/2627	0.77	2/3574 (0.1%)
1	E	0.75	0/2627	0.78	2/3574 (0.1%)
1	G	0.74	0/2627	0.79	2/3574 (0.1%)
1	I	0.69	1/2627 (0.0%)	0.76	3/3574 (0.1%)
1	K	0.69	0/2627	0.77	1/3574 (0.0%)
2	B	0.80	0/1381	0.91	3/1860 (0.2%)
2	D	0.81	0/1381	0.90	3/1860 (0.2%)
2	F	0.86	0/1381	1.07	11/1860 (0.6%)
2	H	0.77	0/1381	0.91	4/1860 (0.2%)
2	J	0.79	1/1381 (0.1%)	0.90	5/1860 (0.3%)
2	L	0.80	0/1381	0.90	3/1860 (0.2%)
All	All	0.76	2/24048 (0.0%)	0.84	42/32604 (0.1%)

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
2	F	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	150	TRP	CB-CG	-5.88	1.39	1.50
2	J	67	ASP	CB-CG	5.65	1.63	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	106	ARG	NE-CZ-NH2	-9.53	115.53	120.30
2	J	106	ARG	NE-CZ-NH2	-9.19	115.70	120.30
2	F	127	ARG	CB-CG-CD	9.16	135.41	111.60
2	L	106	ARG	NE-CZ-NH2	-9.12	115.74	120.30
2	H	106	ARG	NE-CZ-NH2	-9.03	115.78	120.30
2	D	106	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	F	165	GLU	N-CA-C	8.43	133.75	111.00
2	B	106	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	G	129	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	H	83	ARG	NE-CZ-NH2	-7.15	116.72	120.30
2	F	83	ARG	NE-CZ-NH2	-7.05	116.77	120.30
2	F	145	ASP	N-CA-CB	-6.83	98.30	110.60
2	L	168	LEU	CB-CG-CD1	6.80	122.57	111.00
2	J	83	ARG	NE-CZ-NH2	-6.68	116.96	120.30
2	F	133	LEU	CA-CB-CG	6.58	130.43	115.30
1	I	208	ASN	CB-CA-C	-6.19	98.02	110.40
2	D	83	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	F	142	HIS	N-CA-CB	-5.98	99.84	110.60
2	F	145	ASP	CB-CG-OD1	-5.96	112.94	118.30
2	L	83	ARG	NE-CZ-NH2	-5.91	117.35	120.30
2	B	83	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	261	THR	O-C-N	5.57	131.60	122.70
2	F	139	GLU	N-CA-CB	5.53	120.55	110.60
2	J	168	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	218	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	H	156	THR	CB-CA-C	-5.39	97.04	111.60
1	G	102	LYS	CD-CE-NZ	5.29	123.88	111.70
2	F	163	GLN	N-CA-CB	5.27	120.08	110.60
2	H	67	ASP	CB-CA-C	-5.25	99.89	110.40
1	E	102	LYS	CD-CE-NZ	5.23	123.73	111.70
2	F	164	LYS	N-CA-CB	-5.23	101.19	110.60
1	I	218	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	D	106	ARG	CG-CD-NE	-5.18	100.93	111.80
2	J	106	ARG	CG-CD-NE	-5.17	100.95	111.80
2	J	83	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	E	218	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	320	LEU	CA-CB-CG	5.12	127.07	115.30
1	C	102	LYS	CD-CE-NZ	5.11	123.45	111.70
1	I	102	LYS	CD-CE-NZ	5.09	123.42	111.70
1	K	102	LYS	CD-CE-NZ	5.07	123.36	111.70
2	B	106	ARG	CG-CD-NE	-5.01	101.27	111.80
1	C	218	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	164	LYS	Peptide
2	F	166	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2566	0	2514	28	0
1	C	2566	0	2514	29	0
1	E	2566	0	2514	33	0
1	G	2566	0	2514	26	0
1	I	2566	0	2514	24	0
1	K	2566	0	2514	26	1
2	B	1353	0	1268	33	1
2	D	1353	0	1268	33	0
2	F	1353	0	1267	83	0
2	H	1353	0	1268	75	0
2	J	1353	0	1268	34	0
2	L	1353	0	1268	72	0
3	A	42	0	39	1	0
3	C	42	0	39	1	0
3	E	42	0	39	0	0
3	G	42	0	39	0	0
3	I	42	0	39	1	0
3	K	42	0	39	0	0
4	A	105	0	0	3	0
4	B	33	0	0	2	0
4	C	91	0	0	8	0
4	D	43	0	0	2	0
4	E	94	0	0	3	0
4	F	46	0	0	2	0
4	G	99	0	0	6	0
4	H	36	0	0	3	0
4	I	65	0	0	6	0
4	J	28	0	0	2	0
4	K	66	0	0	1	0
4	L	38	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	24510	0	22925	457	1

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 10.

All (457) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:ARG:HD3	2:H:159:TYR:CE1	1.30	1.66
2:L:127:ARG:HD3	2:L:159:TYR:CE1	1.31	1.64
2:H:127:ARG:CD	2:H:159:TYR:CE1	2.21	1.24
2:L:127:ARG:CD	2:L:159:TYR:CE1	2.23	1.20
1:C:277:CYS:SG	4:C:519:HOH:O	2.00	1.17
2:L:127:ARG:HG2	2:L:128:ASP:N	1.50	1.15
2:F:127:ARG:HG2	2:F:128:ASP:N	1.61	1.12
2:F:164:LYS:HG2	2:F:165:GLU:H	1.05	1.11
1:E:129:ARG:HG3	1:E:130:GLY:H	1.09	1.11
2:F:165:GLU:O	4:F:232:HOH:O	1.69	1.09
2:H:127:ARG:HD3	2:H:159:TYR:CD1	1.86	1.09
2:F:127:ARG:CD	2:F:159:TYR:CE1	2.36	1.09
2:L:127:ARG:CZ	2:L:129:ASN:CG	2.24	1.06
2:L:127:ARG:HD3	2:L:159:TYR:CD1	1.89	1.06
2:H:127:ARG:HG2	2:H:128:ASP:N	1.47	1.06
2:F:127:ARG:HD2	2:F:159:TYR:CE1	1.90	1.05
2:H:127:ARG:NE	2:H:129:ASN:HB2	1.76	1.00
2:F:127:ARG:CG	2:F:159:TYR:HE1	1.74	1.00
2:H:127:ARG:CZ	2:H:129:ASN:CG	2.30	1.00
2:H:168:LEU:HD12	4:H:203:HOH:O	1.60	1.00
2:F:127:ARG:CZ	2:F:129:ASN:HA	1.92	0.99
1:I:110:ARG:HD3	4:I:546:HOH:O	1.63	0.98
2:L:127:ARG:CG	2:L:128:ASP:N	2.27	0.98
2:F:164:LYS:HG2	2:F:165:GLU:N	1.72	0.98
2:H:127:ARG:CG	2:H:128:ASP:N	2.24	0.96
2:L:127:ARG:HD3	2:L:159:TYR:HE1	1.22	0.96
2:D:167:LYS:HG3	2:D:168:LEU:N	1.78	0.95
2:L:127:ARG:NE	2:L:129:ASN:HB2	1.82	0.95
2:H:168:LEU:O	4:H:203:HOH:O	1.84	0.94
1:E:129:ARG:CG	1:E:130:GLY:H	1.81	0.93
2:F:127:ARG:CG	2:F:128:ASP:N	2.32	0.91
2:L:164:LYS:HG3	2:L:165:GLU:H	1.36	0.91
2:H:127:ARG:CZ	2:H:129:ASN:HB2	2.01	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:ARG:HD3	2:H:159:TYR:HE1	1.23	0.89
2:F:127:ARG:NH2	2:F:166:SER:OG	2.06	0.89
2:H:167:LYS:HG3	2:H:168:LEU:N	1.87	0.89
1:C:204:THR:HG22	1:C:206:SER:H	1.39	0.88
2:F:32:SER:O	1:G:276:ASN:ND2	2.07	0.88
1:E:204:THR:HG22	1:E:206:SER:H	1.38	0.87
1:I:204:THR:HG22	1:I:206:SER:H	1.40	0.87
1:K:204:THR:HG22	1:K:206:SER:H	1.38	0.87
2:F:127:ARG:HE	2:F:128:ASP:C	1.76	0.87
2:H:127:ARG:CZ	2:H:129:ASN:CB	2.53	0.86
2:H:127:ARG:CG	2:H:159:TYR:HE1	1.88	0.86
1:E:129:ARG:HG3	1:E:130:GLY:N	1.89	0.86
2:F:127:ARG:CD	2:F:159:TYR:HE1	1.83	0.86
1:A:204:THR:HG22	1:A:206:SER:H	1.39	0.85
1:G:204:THR:HG22	1:G:206:SER:H	1.41	0.85
1:I:2:LYS:NZ	4:I:507:HOH:O	2.09	0.84
2:F:142:HIS:CE1	2:F:162:TYR:CD1	2.65	0.83
2:F:127:ARG:NE	2:F:129:ASN:N	2.27	0.82
1:G:278:ASP:O	1:G:289:ARG:NH2	2.12	0.82
2:L:127:ARG:CZ	2:L:129:ASN:HB2	2.10	0.82
2:L:127:ARG:CZ	2:L:129:ASN:CB	2.57	0.82
1:C:278:ASP:O	1:C:289:ARG:NH2	2.13	0.82
2:L:127:ARG:CG	2:L:159:TYR:HE1	1.92	0.82
2:L:131:ASN:O	4:L:231:HOH:O	1.98	0.81
2:F:127:ARG:CG	2:F:159:TYR:CE1	2.63	0.81
1:A:278:ASP:O	1:A:289:ARG:NH2	2.15	0.80
1:E:278:ASP:O	1:E:289:ARG:NH2	2.13	0.80
1:K:278:ASP:O	1:K:289:ARG:NH2	2.15	0.79
2:D:167:LYS:HD3	2:D:168:LEU:HD13	1.65	0.78
2:D:167:LYS:HG3	2:D:168:LEU:H	1.45	0.78
1:I:278:ASP:O	1:I:289:ARG:NH2	2.15	0.78
2:F:147:GLU:HG3	2:F:147:GLU:O	1.83	0.77
2:L:127:ARG:NH2	2:L:157:TYR:HE2	1.83	0.76
2:F:142:HIS:CE1	2:F:162:TYR:CE1	2.73	0.76
1:C:40:ARG:HD2	4:C:519:HOH:O	1.86	0.75
2:H:127:ARG:CG	2:H:128:ASP:H	2.00	0.75
2:F:164:LYS:HE2	2:F:165:GLU:HB3	1.69	0.75
1:I:110:ARG:NH1	4:I:546:HOH:O	2.07	0.74
2:F:127:ARG:HD3	2:F:129:ASN:OD1	1.87	0.74
2:H:127:ARG:NE	2:H:129:ASN:CB	2.51	0.74
2:F:127:ARG:NE	2:F:128:ASP:OD1	2.21	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:ARG:NE	2:F:128:ASP:C	2.40	0.74
2:D:164:LYS:O	2:D:167:LYS:HG2	1.88	0.73
1:E:129:ARG:CG	1:E:130:GLY:N	2.45	0.73
1:A:320:LEU:HD23	2:B:111:HIS:HB3	1.70	0.73
2:B:164:LYS:O	2:B:168:LEU:HD12	1.89	0.73
2:L:127:ARG:NH2	2:L:157:TYR:CE2	2.56	0.73
2:F:127:ARG:NH2	2:F:129:ASN:HA	2.03	0.73
1:K:110:ARG:HB3	1:K:259:VAL:CG1	2.19	0.72
1:E:293:THR:HG21	2:F:56:ILE:HG12	1.71	0.72
2:H:127:ARG:NH1	2:H:129:ASN:CG	2.43	0.72
1:G:37:LYS:NZ	4:G:530:HOH:O	2.21	0.72
1:I:38:GLU:HB2	1:I:287:VAL:HG13	1.71	0.72
2:H:167:LYS:HG3	2:H:168:LEU:H	1.52	0.72
2:H:127:ARG:CD	2:H:159:TYR:HE1	1.82	0.71
1:I:110:ARG:HB3	1:I:259:VAL:CG1	2.21	0.71
1:E:38:GLU:HB2	1:E:287:VAL:HG13	1.72	0.71
2:L:127:ARG:NE	2:L:129:ASN:CB	2.53	0.71
2:F:147:GLU:OE2	4:F:208:HOH:O	2.09	0.71
4:G:505:HOH:O	2:H:25:HIS:NE2	2.23	0.71
2:L:127:ARG:NH1	2:L:129:ASN:CG	2.43	0.70
1:C:110:ARG:HB3	1:C:259:VAL:CG1	2.21	0.70
2:F:133:LEU:HD11	2:F:139:GLU:HG2	1.71	0.70
2:F:142:HIS:HB2	2:F:165:GLU:HG3	1.72	0.70
2:D:164:LYS:HG3	4:D:213:HOH:O	1.92	0.70
2:H:127:ARG:NH2	2:H:157:TYR:HE2	1.90	0.70
2:L:127:ARG:CG	2:L:128:ASP:H	2.03	0.70
2:L:132:ASP:O	2:L:137:CYS:O	2.10	0.70
1:A:110:ARG:HB3	1:A:259:VAL:CG1	2.22	0.70
2:D:132:ASP:O	2:D:137:CYS:O	2.10	0.69
2:D:167:LYS:CD	2:D:168:LEU:HD13	2.23	0.69
2:B:132:ASP:O	2:B:137:CYS:O	2.11	0.69
2:F:132:ASP:O	2:F:133:LEU:HB2	1.91	0.69
2:H:159:TYR:CZ	2:H:163:GLN:OE1	2.44	0.69
2:F:133:LEU:HD11	2:F:139:GLU:CG	2.22	0.69
1:C:38:GLU:HB2	1:C:287:VAL:HG13	1.74	0.69
2:F:132:ASP:O	2:F:137:CYS:O	2.09	0.69
1:K:78:TYR:CD1	1:K:302:ILE:HD11	2.28	0.69
2:J:132:ASP:O	2:J:137:CYS:O	2.10	0.69
1:A:2:LYS:NZ	4:A:507:HOH:O	2.09	0.68
2:F:127:ARG:HG2	2:F:129:ASN:N	2.08	0.68
2:F:127:ARG:CD	2:F:128:ASP:OD1	2.42	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ASN:C	2:B:154:ASN:HD22	1.97	0.68
2:H:127:ARG:NH2	2:H:157:TYR:CE2	2.62	0.68
2:F:127:ARG:CZ	2:F:129:ASN:CA	2.70	0.67
2:H:132:ASP:O	2:H:137:CYS:O	2.11	0.67
2:H:164:LYS:O	2:H:167:LYS:HG2	1.95	0.67
1:G:5:ILE:HD11	2:H:122:VAL:HG21	1.76	0.67
2:L:164:LYS:HE3	2:L:165:GLU:HG3	1.76	0.67
2:H:127:ARG:CD	2:H:159:TYR:CD1	2.63	0.67
1:I:78:TYR:CD1	1:I:302:ILE:HD11	2.30	0.66
2:L:127:ARG:CD	2:L:159:TYR:CD1	2.66	0.66
2:F:126:LEU:O	2:F:129:ASN:HB2	1.95	0.66
1:K:293:THR:HG21	2:L:56:ILE:HG12	1.77	0.66
1:A:293:THR:HG21	2:B:56:ILE:HG12	1.78	0.65
2:F:127:ARG:NH2	2:F:166:SER:CB	2.59	0.65
1:C:204:THR:HG21	4:C:549:HOH:O	1.95	0.65
1:G:293:THR:HG21	2:H:56:ILE:HG12	1.76	0.65
2:F:127:ARG:HG2	2:F:128:ASP:CA	2.26	0.65
1:I:237:PRO:O	4:I:563:HOH:O	2.13	0.65
2:L:164:LYS:HG3	2:L:165:GLU:N	2.08	0.65
1:E:201:ARG:NH1	4:E:568:HOH:O	2.22	0.64
2:H:127:ARG:HE	2:H:129:ASN:HB2	1.60	0.64
1:K:43:LYS:HE3	1:K:46:ASN:HA	1.80	0.64
1:A:78:TYR:CD1	1:A:302:ILE:HD11	2.33	0.64
1:E:5:ILE:HD11	2:F:122:VAL:HG21	1.79	0.63
2:F:142:HIS:HE1	2:F:162:TYR:CE1	2.15	0.63
2:J:163:GLN:HG2	2:J:164:LYS:HD2	1.80	0.63
2:F:127:ARG:HG2	2:F:129:ASN:H	1.64	0.63
1:E:96:ASN:OD1	1:E:97:GLU:HG2	1.99	0.63
2:F:127:ARG:HD2	2:F:159:TYR:CZ	2.33	0.63
1:G:68:ASP:OD2	1:G:146:ARG:NH1	2.31	0.63
2:L:164:LYS:CG	2:L:165:GLU:H	2.09	0.62
1:A:68:ASP:OD2	1:A:146:ARG:NH1	2.32	0.62
1:C:68:ASP:OD2	1:C:146:ARG:NH1	2.32	0.62
1:E:78:TYR:CD1	1:E:302:ILE:HD11	2.35	0.62
2:L:127:ARG:CD	2:L:159:TYR:HE1	1.83	0.62
1:E:68:ASP:OD2	1:E:146:ARG:NH1	2.33	0.61
1:K:96:ASN:OD1	1:K:97:GLU:HG2	1.99	0.61
1:C:78:TYR:CD1	1:C:302:ILE:HD11	2.34	0.61
2:F:142:HIS:CE1	2:F:143:LYS:O	2.54	0.61
1:C:96:ASN:OD1	1:C:97:GLU:HG2	2.00	0.61
2:H:132:ASP:O	2:H:133:LEU:HB2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:ARG:NH2	2:H:129:ASN:CB	2.64	0.61
1:K:261:THR:OG1	1:K:263:LYS:HG3	2.00	0.61
1:A:149:VAL:HG23	1:A:253:TRP:HB2	1.83	0.61
2:L:133:LEU:HG	4:L:231:HOH:O	2.01	0.61
2:F:127:ARG:CG	2:F:128:ASP:H	2.13	0.60
1:K:149:VAL:HG23	1:K:253:TRP:HB2	1.82	0.60
2:L:127:ARG:HE	2:L:129:ASN:HB2	1.61	0.60
2:D:132:ASP:O	2:D:133:LEU:HB2	2.01	0.60
1:E:149:VAL:HG23	1:E:253:TRP:HB2	1.83	0.60
1:I:68:ASP:OD2	1:I:146:ARG:NH1	2.34	0.60
1:G:149:VAL:HG23	1:G:253:TRP:HB2	1.84	0.60
2:F:127:ARG:NH1	2:F:165:GLU:OE2	2.33	0.60
1:C:293:THR:HG21	2:D:56:ILE:HG12	1.84	0.60
2:J:132:ASP:O	2:J:133:LEU:HB2	2.01	0.59
1:C:5:ILE:HD11	2:D:122:VAL:HG21	1.84	0.59
1:K:68:ASP:OD2	1:K:146:ARG:NH1	2.35	0.59
2:F:162:TYR:O	2:F:165:GLU:OE1	2.20	0.59
2:H:127:ARG:NH2	2:H:129:ASN:HB2	2.16	0.59
1:I:149:VAL:HG23	1:I:253:TRP:HB2	1.84	0.59
1:C:149:VAL:HG23	1:C:253:TRP:HB2	1.84	0.59
2:F:127:ARG:CG	2:F:128:ASP:OD1	2.51	0.59
2:L:127:ARG:NH2	2:L:129:ASN:CB	2.65	0.59
2:B:154:ASN:ND2	2:B:156:THR:OG1	2.34	0.59
1:G:78:TYR:CD1	1:G:302:ILE:HD11	2.38	0.59
2:L:132:ASP:O	2:L:133:LEU:HB2	2.03	0.59
1:G:146:ARG:NH2	4:G:565:HOH:O	2.33	0.58
2:J:164:LYS:HE3	2:J:167:LYS:HG3	1.85	0.58
2:H:127:ARG:HG2	2:H:128:ASP:CA	2.32	0.58
2:F:162:TYR:O	2:F:165:GLU:CD	2.42	0.58
1:E:263:LYS:HG3	1:E:264:LYS:O	2.04	0.58
2:B:132:ASP:O	2:B:133:LEU:HB2	2.03	0.58
2:F:127:ARG:HG3	2:F:128:ASP:OD1	2.04	0.57
1:I:38:GLU:HB2	1:I:287:VAL:CG1	2.35	0.57
2:L:151:SER:OG	2:L:157:TYR:HA	2.04	0.57
1:A:263:LYS:CG	1:A:264:LYS:H	2.18	0.57
2:L:127:ARG:NH2	2:L:157:TYR:OH	2.37	0.57
1:K:43:LYS:HG3	1:K:47:LYS:C	2.24	0.56
1:C:5:ILE:HG13	2:D:119:TYR:HA	1.88	0.56
2:D:164:LYS:O	2:D:167:LYS:CG	2.53	0.56
1:G:22:LYS:HE2	2:J:50:ASN:HD21	1.70	0.56
3:A:400:NAG:O4	4:A:529:HOH:O	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:127:ARG:CD	2:F:129:ASN:OD1	2.49	0.56
2:H:127:ARG:CG	2:H:159:TYR:CE1	2.72	0.56
2:H:167:LYS:CG	2:H:168:LEU:N	2.65	0.56
1:K:261:THR:OG1	1:K:263:LYS:CG	2.53	0.56
2:F:127:ARG:HD3	2:F:159:TYR:CE1	2.38	0.56
2:H:127:ARG:NH2	2:H:157:TYR:OH	2.39	0.56
2:L:127:ARG:NH2	2:L:129:ASN:HB2	2.21	0.56
4:I:507:HOH:O	2:J:25:HIS:NE2	2.33	0.56
2:F:127:ARG:NH2	2:F:165:GLU:OE2	2.38	0.56
2:L:164:LYS:HG3	2:L:165:GLU:HG3	1.89	0.55
1:C:38:GLU:HB2	1:C:287:VAL:CG1	2.37	0.55
2:D:164:LYS:O	2:D:167:LYS:HB3	2.06	0.55
2:H:126:LEU:O	2:H:127:ARG:NE	2.33	0.55
1:A:5:ILE:HG13	2:B:119:TYR:HA	1.89	0.55
1:C:36:GLN:O	4:C:551:HOH:O	2.18	0.55
2:D:167:LYS:CG	2:D:168:LEU:N	2.60	0.55
1:I:293:THR:HG21	2:J:56:ILE:HG12	1.89	0.55
2:L:127:ARG:HG2	2:L:128:ASP:CA	2.33	0.55
2:F:127:ARG:NH2	2:F:166:SER:HB2	2.20	0.54
2:J:154:ASN:HB3	4:J:223:HOH:O	2.06	0.54
2:D:164:LYS:O	2:D:167:LYS:CB	2.56	0.54
2:H:164:LYS:O	2:H:167:LYS:CG	2.55	0.54
1:E:38:GLU:HB2	1:E:287:VAL:CG1	2.35	0.54
2:J:151:SER:OG	2:J:157:TYR:HA	2.07	0.54
3:C:400:NAG:O4	4:C:572:HOH:O	2.19	0.54
2:F:151:SER:OG	2:F:157:TYR:HA	2.08	0.54
2:F:127:ARG:HD3	2:F:129:ASN:CG	2.28	0.53
2:B:125:GLN:O	4:B:205:HOH:O	2.18	0.53
1:C:42:CYS:SG	4:C:519:HOH:O	2.56	0.53
2:J:164:LYS:CE	2:J:167:LYS:HG3	2.38	0.53
2:L:127:ARG:CZ	2:L:129:ASN:ND2	2.71	0.53
2:H:127:ARG:HG3	2:H:159:TYR:HE1	1.70	0.53
2:F:167:LYS:HG3	2:F:168:LEU:N	2.24	0.52
1:A:263:LYS:HG2	1:A:264:LYS:H	1.74	0.52
1:C:110:ARG:NH2	1:C:112:GLU:OE2	2.42	0.52
2:D:167:LYS:CG	2:D:168:LEU:H	2.19	0.52
2:L:127:ARG:HG2	2:L:129:ASN:H	1.75	0.52
1:G:129:ARG:O	4:G:581:HOH:O	2.19	0.52
2:H:127:ARG:HG2	2:H:129:ASN:H	1.74	0.52
2:L:127:ARG:NH1	2:L:129:ASN:OD1	2.43	0.52
2:L:164:LYS:HE3	2:L:165:GLU:CG	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:ASP:O	2:D:133:LEU:CB	2.58	0.52
2:F:127:ARG:NH2	2:F:128:ASP:O	2.42	0.52
2:L:127:ARG:HG3	2:L:159:TYR:HE1	1.74	0.52
2:J:164:LYS:HE3	2:J:164:LYS:HA	1.91	0.51
1:K:5:ILE:HG13	2:L:119:TYR:HA	1.92	0.51
1:E:261:THR:CG2	1:E:263:LYS:HG2	2.40	0.51
2:J:165:GLU:OE1	4:J:216:HOH:O	2.19	0.51
2:L:106:ARG:NH2	4:L:222:HOH:O	2.43	0.51
2:J:132:ASP:O	2:J:133:LEU:CB	2.58	0.51
2:H:98:LEU:HD21	2:J:99:LEU:HD13	1.92	0.51
2:H:159:TYR:CE2	2:H:163:GLN:OE1	2.63	0.50
4:K:506:HOH:O	2:L:25:HIS:NE2	2.34	0.50
2:H:167:LYS:CG	2:H:168:LEU:H	2.22	0.50
2:L:126:LEU:O	2:L:127:ARG:NE	2.34	0.50
1:A:320:LEU:HD23	2:B:111:HIS:CB	2.41	0.50
1:G:297:VAL:O	4:G:585:HOH:O	2.20	0.50
1:I:5:ILE:HG13	2:J:119:TYR:HA	1.92	0.50
2:B:132:ASP:O	2:B:133:LEU:CB	2.59	0.50
2:F:127:ARG:HG2	2:F:128:ASP:C	2.32	0.50
1:I:126:ASP:OD2	1:I:129:ARG:NH1	2.45	0.50
2:F:127:ARG:NE	2:F:129:ASN:CA	2.75	0.49
2:H:132:ASP:O	2:H:133:LEU:CB	2.59	0.49
2:L:127:ARG:CG	2:L:159:TYR:CE1	2.76	0.49
2:L:132:ASP:O	2:L:133:LEU:CB	2.60	0.49
2:H:164:LYS:O	2:H:167:LYS:HB3	2.13	0.49
1:G:106:GLY:O	1:G:265:GLY:HA3	2.12	0.49
2:H:127:ARG:HD2	2:H:129:ASN:OD1	2.13	0.49
2:L:127:ARG:HD2	2:L:129:ASN:OD1	2.13	0.49
2:F:128:ASP:O	2:F:141:TRP:CE3	2.66	0.49
2:B:2:ILE:HG21	2:B:109:ASP:CG	2.33	0.49
1:E:261:THR:HG21	1:E:263:LYS:HG2	1.93	0.49
2:H:127:ARG:NH1	2:H:129:ASN:OD1	2.45	0.49
2:F:158:ASP:OD2	2:F:160:PRO:HD2	2.13	0.49
2:F:160:PRO:HA	2:F:163:GLN:HG3	1.94	0.48
2:H:105:GLU:OE2	4:H:204:HOH:O	2.20	0.48
2:L:164:LYS:CG	2:L:165:GLU:N	2.74	0.48
2:D:99:LEU:HD13	2:L:98:LEU:HD21	1.95	0.48
1:K:106:GLY:O	1:K:265:GLY:HA3	2.13	0.48
1:G:39:LYS:HE2	4:G:530:HOH:O	2.12	0.48
1:E:106:GLY:O	1:E:265:GLY:HA3	2.13	0.48
2:F:132:ASP:O	2:F:133:LEU:CB	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLY:O	1:A:265:GLY:HA3	2.13	0.48
2:F:164:LYS:CG	2:F:165:GLU:H	1.98	0.48
1:I:106:GLY:O	1:I:265:GLY:HA3	2.13	0.48
2:H:161:LYS:HE2	2:H:162:TYR:CZ	2.49	0.47
1:K:54:ASP:N	1:K:54:ASP:OD1	2.38	0.47
2:B:133:LEU:HD11	2:B:139:GLU:HG3	1.95	0.47
2:D:2:ILE:HG21	2:D:109:ASP:CG	2.34	0.47
2:F:164:LYS:O	2:F:167:LYS:HB3	2.13	0.47
2:J:2:ILE:HG21	2:J:109:ASP:CG	2.34	0.47
2:B:82:LYS:NZ	4:B:217:HOH:O	2.45	0.47
2:L:148:CYS:O	2:L:151:SER:HB3	2.15	0.47
1:C:96:ASN:HB2	4:C:511:HOH:O	2.13	0.47
1:E:181:HIS:HB2	1:E:250:ILE:HD11	1.97	0.47
1:A:5:ILE:HD11	2:B:122:VAL:HG21	1.96	0.47
2:D:133:LEU:HD11	2:D:139:GLU:HG3	1.97	0.47
2:H:156:THR:HG22	2:H:156:THR:O	2.13	0.47
1:C:106:GLY:O	1:C:265:GLY:HA3	2.15	0.47
2:F:129:ASN:HD22	2:F:157:TYR:HE2	1.61	0.47
2:H:127:ARG:CD	2:H:129:ASN:H	2.28	0.47
2:L:127:ARG:NH1	2:L:129:ASN:ND2	2.63	0.47
2:L:127:ARG:NH2	2:L:129:ASN:CG	2.67	0.47
2:F:147:GLU:CG	2:F:147:GLU:O	2.57	0.47
1:I:284:ILE:HG23	1:I:285:THR:HG23	1.97	0.47
2:L:127:ARG:CZ	2:L:129:ASN:OD1	2.63	0.47
2:L:2:ILE:HG21	2:L:109:ASP:CG	2.35	0.47
1:C:119:LYS:HE2	1:C:253:TRP:CZ2	2.50	0.46
2:L:127:ARG:NE	2:L:129:ASN:CG	2.67	0.46
2:F:133:LEU:HD11	2:F:139:GLU:HG3	1.97	0.46
1:I:181:HIS:HB2	1:I:250:ILE:HD11	1.97	0.46
2:J:163:GLN:CG	2:J:164:LYS:HD2	2.44	0.46
1:K:5:ILE:HD11	2:L:122:VAL:HG21	1.97	0.46
2:L:151:SER:OG	2:L:156:THR:O	2.30	0.46
2:B:147:GLU:O	2:B:147:GLU:OE1	2.34	0.46
2:D:121:LYS:HD3	2:D:121:LYS:HA	1.60	0.46
1:G:16:VAL:HG12	1:G:315:ARG:HG2	1.98	0.46
1:K:181:HIS:HB2	1:K:250:ILE:HD11	1.97	0.46
1:A:119:LYS:HE2	1:A:253:TRP:CZ2	2.51	0.46
2:B:99:LEU:HD13	2:J:98:LEU:HD21	1.96	0.46
1:A:320:LEU:HD23	2:B:111:HIS:CG	2.51	0.46
2:J:133:LEU:HD11	2:J:139:GLU:HG3	1.96	0.46
2:J:2:ILE:CG2	2:J:109:ASP:OD1	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:LYS:HE2	1:G:276:ASN:OD1	2.15	0.46
2:L:127:ARG:HG3	2:L:128:ASP:OD1	2.16	0.46
1:A:181:HIS:HB2	1:A:250:ILE:HD11	1.98	0.46
2:H:2:ILE:HG21	2:H:109:ASP:CG	2.36	0.46
2:F:165:GLU:CD	2:F:166:SER:N	2.70	0.46
2:J:148:CYS:O	2:J:151:SER:HB3	2.15	0.46
2:L:127:ARG:CG	2:L:128:ASP:OD1	2.64	0.46
2:H:133:LEU:HD11	2:H:139:GLU:HG3	1.97	0.45
1:A:264:LYS:NZ	2:B:64:GLU:HB3	2.31	0.45
2:H:127:ARG:HG3	2:H:128:ASP:OD1	2.17	0.45
2:H:127:ARG:CZ	2:H:129:ASN:ND2	2.78	0.45
1:K:119:LYS:HE2	1:K:253:TRP:CZ2	2.52	0.45
1:E:43:LYS:HE2	1:E:276:ASN:OD1	2.16	0.45
2:F:165:GLU:C	2:F:167:LYS:HG2	2.36	0.45
2:F:166:SER:O	2:F:168:LEU:N	2.50	0.45
1:K:16:VAL:HG12	1:K:315:ARG:HG2	1.99	0.45
2:L:133:LEU:HD11	2:L:139:GLU:HG3	1.97	0.45
1:G:181:HIS:HB2	1:G:250:ILE:HD11	1.98	0.45
1:A:284:ILE:HG23	1:A:285:THR:HG23	1.98	0.45
2:F:148:CYS:O	2:F:151:SER:HB3	2.16	0.45
1:K:284:ILE:HG23	1:K:285:THR:HG23	1.99	0.45
2:D:98:LEU:HD21	2:F:99:LEU:HD13	1.99	0.45
2:F:165:GLU:HA	2:F:167:LYS:HE2	1.99	0.45
1:E:51:ASP:HB2	1:E:274:ILE:HD12	1.98	0.45
2:H:127:ARG:NH1	2:H:129:ASN:ND2	2.65	0.45
2:B:60:ASN:CG	2:B:60:ASN:O	2.54	0.45
2:D:2:ILE:CG2	2:D:109:ASP:OD1	2.65	0.45
2:B:2:ILE:CG2	2:B:109:ASP:OD1	2.64	0.44
1:E:96:ASN:HD22	1:E:231:TYR:HE1	1.65	0.44
2:D:168:LEU:O	4:D:225:HOH:O	2.21	0.44
1:E:5:ILE:HG13	2:F:119:TYR:HA	1.99	0.44
1:G:140:ILE:HG22	1:G:142:SER:H	1.82	0.44
1:E:119:LYS:HE2	1:E:253:TRP:CZ2	2.52	0.44
1:I:16:VAL:HG12	1:I:315:ARG:HG2	1.99	0.44
2:J:5:ALA:O	2:J:8:GLY:CA	2.65	0.44
2:L:127:ARG:CD	2:L:129:ASN:H	2.30	0.44
1:C:181:HIS:HB2	1:C:250:ILE:HD11	1.98	0.44
2:F:127:ARG:CB	2:F:159:TYR:CE1	3.01	0.44
2:H:127:ARG:CG	2:H:128:ASP:OD1	2.66	0.44
2:J:167:LYS:CB	2:J:168:LEU:HD12	2.48	0.44
2:B:85:GLU:OE2	2:J:83:ARG:NH2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:159:TYR:HB3	2:L:160:PRO:HD3	1.98	0.44
2:L:2:ILE:CG2	2:L:109:ASP:OD1	2.65	0.44
2:H:164:LYS:O	2:H:167:LYS:CB	2.66	0.44
2:H:164:LYS:HB2	2:H:165:GLU:H	1.67	0.44
1:K:140:ILE:HG22	1:K:142:SER:H	1.83	0.44
2:F:98:LEU:HD21	2:L:99:LEU:HD13	1.98	0.43
2:H:1:GLY:O	2:H:2:ILE:HG22	2.18	0.43
1:G:119:LYS:HE2	1:G:253:TRP:CZ2	2.52	0.43
2:H:2:ILE:CG2	2:H:109:ASP:OD1	2.66	0.43
2:H:83:ARG:NH2	2:J:85:GLU:OE2	2.52	0.43
2:H:127:ARG:NE	2:H:159:TYR:CD1	2.86	0.43
1:I:109:GLU:HB3	1:I:261:THR:HG22	1.99	0.43
2:J:5:ALA:O	2:J:8:GLY:HA3	2.18	0.43
2:D:106:ARG:HH22	2:L:105:GLU:CD	2.22	0.43
1:A:140:ILE:HG22	1:A:142:SER:H	1.84	0.43
2:B:5:ALA:O	2:B:8:GLY:CA	2.66	0.43
2:D:167:LYS:CG	2:D:168:LEU:HD13	2.49	0.43
2:F:97:GLU:HB3	2:L:58:LYS:HE3	1.99	0.43
1:G:131:VAL:CG2	1:G:143:SER:HA	2.49	0.43
2:L:5:ALA:O	2:L:8:GLY:CA	2.67	0.43
2:F:164:LYS:C	2:F:165:GLU:OE1	2.57	0.43
1:I:119:LYS:HE2	1:I:253:TRP:CZ2	2.53	0.43
1:E:16:VAL:HG12	1:E:315:ARG:HG2	2.01	0.43
1:I:131:VAL:CG2	1:I:143:SER:HA	2.48	0.43
1:I:307:LYS:HE2	2:J:92:TRP:CD2	2.54	0.43
2:F:105:GLU:CD	2:L:106:ARG:HH22	2.23	0.43
1:C:131:VAL:CG2	1:C:143:SER:HA	2.49	0.42
2:B:1:GLY:O	2:B:2:ILE:HG22	2.19	0.42
2:B:5:ALA:O	2:B:8:GLY:HA3	2.18	0.42
2:F:159:TYR:HB3	2:F:160:PRO:HD3	2.00	0.42
1:A:131:VAL:CG2	1:A:143:SER:HA	2.49	0.42
2:D:2:ILE:HG23	2:D:3:PHE:N	2.34	0.42
1:G:5:ILE:HG13	2:H:119:TYR:HA	2.00	0.42
2:D:5:ALA:O	2:D:8:GLY:CA	2.68	0.42
1:G:5:ILE:HD13	2:H:24:TYR:CD1	2.55	0.42
2:J:2:ILE:HG23	2:J:3:PHE:N	2.33	0.42
2:L:5:ALA:O	2:L:8:GLY:HA3	2.20	0.42
1:E:131:VAL:CG2	1:E:143:SER:HA	2.49	0.42
2:B:98:LEU:HD21	2:H:99:LEU:HD13	2.01	0.42
2:L:2:ILE:HG23	2:L:3:PHE:N	2.33	0.42
1:C:284:ILE:HG23	1:C:285:THR:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:TYR:HB3	2:H:160:PRO:HD3	2.02	0.42
2:H:97:GLU:HB3	2:J:58:LYS:HE3	2.02	0.42
1:C:204:THR:HB	1:C:207:MET:HG3	2.02	0.42
2:D:1:GLY:O	2:D:2:ILE:HG22	2.20	0.42
2:H:5:ALA:O	2:H:8:GLY:CA	2.67	0.42
2:B:105:GLU:CD	2:H:106:ARG:HH22	2.23	0.42
2:F:5:ALA:O	2:F:8:GLY:HA3	2.20	0.42
1:G:284:ILE:HG23	1:G:285:THR:HG23	2.01	0.42
2:H:164:LYS:N	2:H:164:LYS:HD3	2.34	0.42
1:A:224:GLN:NE2	4:A:553:HOH:O	2.50	0.41
1:A:81:GLU:O	1:A:269:LYS:HA	2.20	0.41
1:E:81:GLU:O	1:E:269:LYS:HA	2.20	0.41
2:L:1:GLY:O	2:L:2:ILE:HG22	2.19	0.41
1:A:126:ASP:OD2	1:A:129:ARG:NH1	2.52	0.41
1:E:218:ARG:NE	4:E:513:HOH:O	2.50	0.41
1:I:204:THR:HB	1:I:207:MET:HG3	2.01	0.41
2:H:84:MET:HB2	2:J:84:MET:SD	2.60	0.41
1:K:131:VAL:CG2	1:K:143:SER:HA	2.51	0.41
1:A:137:SER:HB3	1:A:139:THR:H	1.85	0.41
2:F:127:ARG:CD	2:F:129:ASN:N	2.83	0.41
1:G:51:ASP:HB2	1:G:274:ILE:HD12	2.01	0.41
2:D:161:LYS:HE2	2:D:162:TYR:CZ	2.55	0.41
2:H:5:ALA:O	2:H:8:GLY:HA3	2.20	0.41
1:K:81:GLU:O	1:K:269:LYS:HA	2.21	0.41
1:K:96:ASN:HD22	1:K:231:TYR:HE1	1.69	0.41
2:D:159:TYR:HB3	2:D:160:PRO:HD3	2.03	0.41
4:E:566:HOH:O	2:F:25:HIS:NE2	2.19	0.41
1:C:123:ALA:O	4:C:538:HOH:O	2.22	0.41
1:E:284:ILE:HG23	1:E:285:THR:HG23	2.02	0.41
2:D:5:ALA:O	2:D:8:GLY:HA3	2.21	0.41
2:L:127:ARG:NE	2:L:159:TYR:CD1	2.88	0.41
1:A:82:ARG:HA	1:A:83:PRO:HD3	1.91	0.41
2:D:2:ILE:HG23	2:D:3:PHE:CD2	2.56	0.41
1:E:140:ILE:HG22	1:E:142:SER:H	1.85	0.41
2:H:131:ASN:OD1	2:J:127:ARG:NH1	2.54	0.41
1:C:41:PHE:CE1	1:C:272:LEU:HB2	2.56	0.41
1:E:82:ARG:HA	1:E:83:PRO:HD3	1.89	0.41
2:F:5:ALA:O	2:F:8:GLY:CA	2.69	0.41
1:K:43:LYS:HG3	1:K:47:LYS:O	2.21	0.41
2:B:127:ARG:HD2	2:B:159:TYR:CD1	2.55	0.40
2:B:58:LYS:HE3	2:J:97:GLU:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:204:THR:HB	1:K:207:MET:HG3	2.03	0.40
2:L:127:ARG:NH2	2:L:129:ASN:ND2	2.69	0.40
2:B:106:ARG:HH22	2:J:105:GLU:CD	2.25	0.40
2:B:2:ILE:HG21	2:B:109:ASP:OD1	2.21	0.40
1:C:16:VAL:HG12	1:C:315:ARG:HG2	2.03	0.40
1:C:96:ASN:HD22	1:C:231:TYR:HE1	1.67	0.40
2:H:167:LYS:HG3	2:H:168:LEU:HG	2.03	0.40
2:J:151:SER:HG	2:J:157:TYR:HA	1.86	0.40
1:E:204:THR:HB	1:E:207:MET:HG3	2.03	0.40
1:A:16:VAL:HG12	1:A:315:ARG:HG2	2.03	0.40
2:B:159:TYR:HB3	2:B:160:PRO:HD3	2.03	0.40
2:B:2:ILE:HG23	2:B:3:PHE:N	2.36	0.40
1:G:204:THR:HB	1:G:207:MET:HG3	2.03	0.40
3:I:401:NAG:H82	4:I:558:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:THR:OG1	1:K:139:THR:O[4_546]	2.00	0.20

5.3 Torsion angles

5.3.1 Protein backbone

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	323/334 (97%)	314 (97%)	9 (3%)	0	100	100
1	C	323/334 (97%)	314 (97%)	9 (3%)	0	100	100
1	E	323/334 (97%)	315 (98%)	8 (2%)	0	100	100
1	G	323/334 (97%)	315 (98%)	8 (2%)	0	100	100
1	I	323/334 (97%)	314 (97%)	9 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	323/334 (97%)	315 (98%)	8 (2%)	0	100	100
2	B	166/181 (92%)	157 (95%)	8 (5%)	1 (1%)	28	41
2	D	166/181 (92%)	155 (93%)	7 (4%)	4 (2%)	7	7
2	F	166/181 (92%)	154 (93%)	8 (5%)	4 (2%)	7	7
2	H	166/181 (92%)	156 (94%)	7 (4%)	3 (2%)	10	12
2	J	166/181 (92%)	157 (95%)	8 (5%)	1 (1%)	28	41
2	L	166/181 (92%)	157 (95%)	7 (4%)	2 (1%)	15	21
All	All	2934/3090 (95%)	2823 (96%)	96 (3%)	15 (0%)	32	46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2	ILE
2	D	2	ILE
2	F	2	ILE
2	F	164	LYS
2	F	165	GLU
2	F	167	LYS
2	H	2	ILE
2	H	164	LYS
2	J	2	ILE
2	L	2	ILE
2	L	164	LYS
2	D	165	GLU
2	D	167	LYS
2	H	167	LYS
2	D	164	LYS

5.3.2 Protein sidechains ⓘ

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	286/292 (98%)	277 (97%)	9 (3%)	45	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	286/292 (98%)	275 (96%)	11 (4%)	38	58
1	E	286/292 (98%)	280 (98%)	6 (2%)	59	78
1	G	286/292 (98%)	277 (97%)	9 (3%)	45	66
1	I	286/292 (98%)	279 (98%)	7 (2%)	54	74
1	K	286/292 (98%)	276 (96%)	10 (4%)	41	61
2	B	143/154 (93%)	136 (95%)	7 (5%)	29	46
2	D	143/154 (93%)	141 (99%)	2 (1%)	71	86
2	F	143/154 (93%)	130 (91%)	13 (9%)	11	16
2	H	143/154 (93%)	138 (96%)	5 (4%)	41	61
2	J	143/154 (93%)	143 (100%)	0	100	100
2	L	143/154 (93%)	138 (96%)	5 (4%)	41	61
All	All	2574/2676 (96%)	2490 (97%)	84 (3%)	43	64

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	75	SER
1	A	110	ARG
1	A	137	SER
1	A	202	MET
1	A	262	ASN
1	A	289	ARG
1	A	307	LYS
1	A	320	LEU
2	B	39	GLU
2	B	110	LEU
2	B	147	GLU
2	B	151	SER
2	B	154	ASN
2	B	164	LYS
2	B	167	LYS
1	C	2	LYS
1	C	44	ILE
1	C	46	ASN
1	C	75	SER
1	C	137	SER
1	C	158	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	260	SER
1	C	276	ASN
1	C	287	VAL
1	C	289	ARG
1	C	307	LYS
2	D	121	LYS
2	D	151	SER
1	E	44	ILE
1	E	75	SER
1	E	260	SER
1	E	287	VAL
1	E	289	ARG
1	E	307	LYS
2	F	2	ILE
2	F	29	SER
2	F	30	GLN
2	F	127	ARG
2	F	139	GLU
2	F	141	TRP
2	F	142	HIS
2	F	145	ASP
2	F	163	GLN
2	F	164	LYS
2	F	165	GLU
2	F	166	SER
2	F	168	LEU
1	G	44	ILE
1	G	75	SER
1	G	133	ASN
1	G	137	SER
1	G	158	THR
1	G	260	SER
1	G	269	LYS
1	G	289	ARG
1	G	307	LYS
2	H	29	SER
2	H	67	ASP
2	H	127	ARG
2	H	143	LYS
2	H	151	SER
1	I	44	ILE
1	I	75	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	208	ASN
1	I	260	SER
1	I	261	THR
1	I	269	LYS
1	I	289	ARG
1	K	44	ILE
1	K	54	ASP
1	K	75	SER
1	K	156	SER
1	K	158	THR
1	K	260	SER
1	K	264	LYS
1	K	289	ARG
1	K	307	LYS
1	K	320	LEU
2	L	67	ASP
2	L	82	LYS
2	L	121	LYS
2	L	127	ARG
2	L	143	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	262	ASN
2	B	154	ASN
1	C	46	ASN
2	F	142	HIS
1	G	133	ASN
1	G	224	GLN
2	J	50	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues 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	NAG	A	400	1	14,14,15	0.55	0	15,19,21	1.14	1 (6%)
3	NAG	A	401	1	14,14,15	1.14	2 (14%)	15,19,21	1.92	6 (40%)
3	NAG	A	402	1	14,14,15	0.52	0	15,19,21	2.40	4 (26%)
3	NAG	C	400	1	14,14,15	0.58	0	15,19,21	1.76	1 (6%)
3	NAG	C	401	1	14,14,15	1.10	1 (7%)	15,19,21	1.81	6 (40%)
3	NAG	C	402	1	14,14,15	0.79	1 (7%)	15,19,21	2.00	4 (26%)
3	NAG	E	400	1	14,14,15	0.49	0	15,19,21	1.76	3 (20%)
3	NAG	E	401	1	14,14,15	0.83	1 (7%)	15,19,21	1.49	4 (26%)
3	NAG	E	402	1	14,14,15	0.93	1 (7%)	15,19,21	1.93	4 (26%)
3	NAG	G	400	1	14,14,15	0.50	0	15,19,21	1.86	3 (20%)
3	NAG	G	401	1	14,14,15	1.09	1 (7%)	15,19,21	1.46	3 (20%)
3	NAG	G	402	1	14,14,15	0.81	1 (7%)	15,19,21	2.02	5 (33%)
3	NAG	I	400	1	14,14,15	0.54	0	15,19,21	1.04	0
3	NAG	I	401	1	14,14,15	1.04	1 (7%)	15,19,21	1.73	1 (6%)
3	NAG	I	402	1	14,14,15	0.43	0	15,19,21	1.70	4 (26%)
3	NAG	K	400	1	14,14,15	0.80	0	15,19,21	2.04	4 (26%)
3	NAG	K	401	1	14,14,15	1.01	2 (14%)	15,19,21	1.97	4 (26%)
3	NAG	K	402	1	14,14,15	0.48	0	15,19,21	2.15	3 (20%)

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	NAG	A	400	1	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	C	400	1	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	402	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	400	1	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	402	1	-	0/6/23/26	0/1/1/1
3	NAG	G	400	1	-	0/6/23/26	0/1/1/1
3	NAG	G	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	G	402	1	-	0/6/23/26	0/1/1/1
3	NAG	I	400	1	-	0/6/23/26	0/1/1/1
3	NAG	I	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	I	402	1	-	0/6/23/26	0/1/1/1
3	NAG	K	400	1	-	0/6/23/26	0/1/1/1
3	NAG	K	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	K	402	1	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	401	NAG	C1-C2	2.07	1.55	1.52
3	E	401	NAG	C3-C2	2.13	1.57	1.52
3	A	401	NAG	C3-C2	2.17	1.57	1.52
3	I	401	NAG	C3-C2	2.36	1.57	1.52
3	K	401	NAG	C3-C2	2.43	1.57	1.52
3	C	402	NAG	C1-C2	2.50	1.55	1.52
3	G	402	NAG	C1-C2	2.54	1.56	1.52
3	E	402	NAG	C1-C2	2.76	1.56	1.52
3	C	401	NAG	C1-C2	2.82	1.56	1.52
3	A	401	NAG	C1-C2	2.90	1.56	1.52
3	G	401	NAG	C1-C2	3.02	1.56	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAG	O5-C1-C2	-5.54	103.77	111.47
3	K	401	NAG	O5-C1-C2	-4.64	105.02	111.47
3	K	400	NAG	O5-C1-C2	-4.58	105.10	111.47
3	C	402	NAG	O5-C1-C2	-3.49	106.61	111.47
3	E	400	NAG	O5-C1-C2	-3.43	106.70	111.47
3	G	400	NAG	C2-N2-C7	-2.82	118.83	122.94
3	K	400	NAG	C4-C3-C2	-2.76	106.98	111.02
3	A	401	NAG	O5-C1-C2	-2.72	107.68	111.47
3	K	402	NAG	C6-C5-C4	-2.69	106.70	113.00
3	C	401	NAG	O7-C7-C8	-2.57	117.38	122.06
3	E	402	NAG	C3-C4-C5	-2.56	105.71	110.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	C3-C4-C5	-2.54	105.75	110.22
3	A	401	NAG	O7-C7-C8	-2.48	117.54	122.06
3	E	401	NAG	O3-C3-C4	-2.38	105.17	110.36
3	G	402	NAG	O5-C1-C2	-2.36	108.19	111.47
3	K	401	NAG	O7-C7-C8	-2.29	117.88	122.06
3	C	401	NAG	O6-C6-C5	-2.29	103.64	111.34
3	E	402	NAG	O7-C7-C8	-2.29	117.89	122.06
3	G	400	NAG	C3-C4-C5	-2.26	106.23	110.22
3	E	400	NAG	O7-C7-C8	-2.23	118.00	122.06
3	C	402	NAG	O7-C7-C8	-2.22	118.02	122.06
3	I	402	NAG	O5-C1-C2	-2.22	108.39	111.47
3	E	401	NAG	O5-C1-C2	-2.18	108.43	111.47
3	I	402	NAG	O3-C3-C4	-2.18	105.61	110.36
3	G	401	NAG	O7-C7-C8	-2.17	118.10	122.06
3	C	401	NAG	O5-C1-C2	-2.15	108.49	111.47
3	K	400	NAG	O7-C7-C8	-2.14	118.15	122.06
3	I	402	NAG	C6-C5-C4	-2.14	107.98	113.00
3	C	401	NAG	C3-C4-C5	-2.07	106.57	110.22
3	G	402	NAG	C6-C5-C4	-2.04	108.22	113.00
3	K	402	NAG	O5-C1-C2	-2.04	108.63	111.47
3	G	402	NAG	O7-C7-C8	-2.03	118.36	122.06
3	E	401	NAG	C1-C2-N2	-2.02	107.05	110.49
3	G	401	NAG	C2-N2-C7	2.14	126.06	122.94
3	K	401	NAG	C1-O5-C5	2.27	115.29	112.17
3	C	402	NAG	C1-C2-N2	2.28	114.39	110.49
3	G	402	NAG	C1-C2-N2	2.40	114.59	110.49
3	A	401	NAG	C4-C3-C2	2.56	114.76	111.02
3	A	401	NAG	C1-O5-C5	2.59	115.74	112.17
3	E	401	NAG	O3-C3-C2	2.66	115.10	109.39
3	E	402	NAG	C1-C2-N2	2.71	115.12	110.49
3	G	401	NAG	O3-C3-C2	2.75	115.27	109.39
3	C	401	NAG	C4-C3-C2	2.85	115.19	111.02
3	A	402	NAG	O4-C4-C5	2.92	116.65	109.28
3	C	401	NAG	C2-N2-C7	3.33	127.80	122.94
3	A	401	NAG	C2-N2-C7	3.46	127.99	122.94
3	A	400	NAG	C1-O5-C5	3.46	116.94	112.17
3	K	401	NAG	C4-C3-C2	3.57	116.25	111.02
3	K	400	NAG	O3-C3-C2	3.91	117.77	109.39
3	A	402	NAG	C1-O5-C5	3.96	117.62	112.17
3	A	402	NAG	C1-C2-N2	3.97	117.27	110.49
3	E	400	NAG	C1-O5-C5	4.51	118.38	112.17
3	E	402	NAG	C1-O5-C5	4.95	118.99	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	402	NAG	C1-O5-C5	4.99	119.04	112.17
3	I	401	NAG	C4-C3-C2	5.16	118.59	111.02
3	C	402	NAG	C1-O5-C5	5.26	119.41	112.17
3	C	400	NAG	C1-O5-C5	5.42	119.64	112.17
3	G	400	NAG	C1-O5-C5	5.67	119.98	112.17
3	G	402	NAG	C1-O5-C5	5.71	120.04	112.17
3	K	402	NAG	C1-O5-C5	6.85	121.60	112.17

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	401	NAG	C1
3	I	401	NAG	C1
3	C	401	NAG	C1
3	E	401	NAG	C1
3	A	401	NAG	C1
3	K	401	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	NAG	1	0
3	C	400	NAG	1	0
3	I	401	NAG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 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	NAG	A	400	1	14,14,15	0.55	0	15,19,21	1.14	1 (6%)
3	NAG	A	401	1	14,14,15	1.14	2 (14%)	15,19,21	1.92	6 (40%)
3	NAG	A	402	1	14,14,15	0.52	0	15,19,21	2.40	4 (26%)
3	NAG	C	400	1	14,14,15	0.58	0	15,19,21	1.76	1 (6%)
3	NAG	C	401	1	14,14,15	1.10	1 (7%)	15,19,21	1.81	6 (40%)
3	NAG	C	402	1	14,14,15	0.79	1 (7%)	15,19,21	2.00	4 (26%)
3	NAG	E	400	1	14,14,15	0.49	0	15,19,21	1.76	3 (20%)
3	NAG	E	401	1	14,14,15	0.83	1 (7%)	15,19,21	1.49	4 (26%)
3	NAG	E	402	1	14,14,15	0.93	1 (7%)	15,19,21	1.93	4 (26%)
3	NAG	G	400	1	14,14,15	0.50	0	15,19,21	1.86	3 (20%)
3	NAG	G	401	1	14,14,15	1.09	1 (7%)	15,19,21	1.46	3 (20%)
3	NAG	G	402	1	14,14,15	0.81	1 (7%)	15,19,21	2.02	5 (33%)
3	NAG	I	400	1	14,14,15	0.54	0	15,19,21	1.04	0
3	NAG	I	401	1	14,14,15	1.04	1 (7%)	15,19,21	1.73	1 (6%)
3	NAG	I	402	1	14,14,15	0.43	0	15,19,21	1.70	4 (26%)
3	NAG	K	400	1	14,14,15	0.80	0	15,19,21	2.04	4 (26%)
3	NAG	K	401	1	14,14,15	1.01	2 (14%)	15,19,21	1.97	4 (26%)
3	NAG	K	402	1	14,14,15	0.48	0	15,19,21	2.15	3 (20%)

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	NAG	A	400	1	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	C	400	1	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	402	1	-	0/6/23/26	0/1/1/1
3	NAG	E	400	1	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	402	1	-	0/6/23/26	0/1/1/1
3	NAG	G	400	1	-	0/6/23/26	0/1/1/1
3	NAG	G	401	1	1/1/5/7	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	402	1	-	0/6/23/26	0/1/1/1
3	NAG	I	400	1	-	0/6/23/26	0/1/1/1
3	NAG	I	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	I	402	1	-	0/6/23/26	0/1/1/1
3	NAG	K	400	1	-	0/6/23/26	0/1/1/1
3	NAG	K	401	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	K	402	1	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	401	NAG	C1-C2	2.07	1.55	1.52
3	E	401	NAG	C3-C2	2.13	1.57	1.52
3	A	401	NAG	C3-C2	2.17	1.57	1.52
3	I	401	NAG	C3-C2	2.36	1.57	1.52
3	K	401	NAG	C3-C2	2.43	1.57	1.52
3	C	402	NAG	C1-C2	2.50	1.55	1.52
3	G	402	NAG	C1-C2	2.54	1.56	1.52
3	E	402	NAG	C1-C2	2.76	1.56	1.52
3	C	401	NAG	C1-C2	2.82	1.56	1.52
3	A	401	NAG	C1-C2	2.90	1.56	1.52
3	G	401	NAG	C1-C2	3.02	1.56	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAG	O5-C1-C2	-5.54	103.77	111.47
3	K	401	NAG	O5-C1-C2	-4.64	105.02	111.47
3	K	400	NAG	O5-C1-C2	-4.58	105.10	111.47
3	C	402	NAG	O5-C1-C2	-3.49	106.61	111.47
3	E	400	NAG	O5-C1-C2	-3.43	106.70	111.47
3	G	400	NAG	C2-N2-C7	-2.82	118.83	122.94
3	K	400	NAG	C4-C3-C2	-2.76	106.98	111.02
3	A	401	NAG	O5-C1-C2	-2.72	107.68	111.47
3	K	402	NAG	C6-C5-C4	-2.69	106.70	113.00
3	C	401	NAG	O7-C7-C8	-2.57	117.38	122.06
3	E	402	NAG	C3-C4-C5	-2.56	105.71	110.22
3	A	401	NAG	C3-C4-C5	-2.54	105.75	110.22
3	A	401	NAG	O7-C7-C8	-2.48	117.54	122.06
3	E	401	NAG	O3-C3-C4	-2.38	105.17	110.36
3	G	402	NAG	O5-C1-C2	-2.36	108.19	111.47
3	K	401	NAG	O7-C7-C8	-2.29	117.88	122.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	NAG	O6-C6-C5	-2.29	103.64	111.34
3	E	402	NAG	O7-C7-C8	-2.29	117.89	122.06
3	G	400	NAG	C3-C4-C5	-2.26	106.23	110.22
3	E	400	NAG	O7-C7-C8	-2.23	118.00	122.06
3	C	402	NAG	O7-C7-C8	-2.22	118.02	122.06
3	I	402	NAG	O5-C1-C2	-2.22	108.39	111.47
3	E	401	NAG	O5-C1-C2	-2.18	108.43	111.47
3	I	402	NAG	O3-C3-C4	-2.18	105.61	110.36
3	G	401	NAG	O7-C7-C8	-2.17	118.10	122.06
3	C	401	NAG	O5-C1-C2	-2.15	108.49	111.47
3	K	400	NAG	O7-C7-C8	-2.14	118.15	122.06
3	I	402	NAG	C6-C5-C4	-2.14	107.98	113.00
3	C	401	NAG	C3-C4-C5	-2.07	106.57	110.22
3	G	402	NAG	C6-C5-C4	-2.04	108.22	113.00
3	K	402	NAG	O5-C1-C2	-2.04	108.63	111.47
3	G	402	NAG	O7-C7-C8	-2.03	118.36	122.06
3	E	401	NAG	C1-C2-N2	-2.02	107.05	110.49
3	G	401	NAG	C2-N2-C7	2.14	126.06	122.94
3	K	401	NAG	C1-O5-C5	2.27	115.29	112.17
3	C	402	NAG	C1-C2-N2	2.28	114.39	110.49
3	G	402	NAG	C1-C2-N2	2.40	114.59	110.49
3	A	401	NAG	C4-C3-C2	2.56	114.76	111.02
3	A	401	NAG	C1-O5-C5	2.59	115.74	112.17
3	E	401	NAG	O3-C3-C2	2.66	115.10	109.39
3	E	402	NAG	C1-C2-N2	2.71	115.12	110.49
3	G	401	NAG	O3-C3-C2	2.75	115.27	109.39
3	C	401	NAG	C4-C3-C2	2.85	115.19	111.02
3	A	402	NAG	O4-C4-C5	2.92	116.65	109.28
3	C	401	NAG	C2-N2-C7	3.33	127.80	122.94
3	A	401	NAG	C2-N2-C7	3.46	127.99	122.94
3	A	400	NAG	C1-O5-C5	3.46	116.94	112.17
3	K	401	NAG	C4-C3-C2	3.57	116.25	111.02
3	K	400	NAG	O3-C3-C2	3.91	117.77	109.39
3	A	402	NAG	C1-O5-C5	3.96	117.62	112.17
3	A	402	NAG	C1-C2-N2	3.97	117.27	110.49
3	E	400	NAG	C1-O5-C5	4.51	118.38	112.17
3	E	402	NAG	C1-O5-C5	4.95	118.99	112.17
3	I	402	NAG	C1-O5-C5	4.99	119.04	112.17
3	I	401	NAG	C4-C3-C2	5.16	118.59	111.02
3	C	402	NAG	C1-O5-C5	5.26	119.41	112.17
3	C	400	NAG	C1-O5-C5	5.42	119.64	112.17
3	G	400	NAG	C1-O5-C5	5.67	119.98	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	402	NAG	C1-O5-C5	5.71	120.04	112.17
3	K	402	NAG	C1-O5-C5	6.85	121.60	112.17

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	401	NAG	C1
3	I	401	NAG	C1
3	C	401	NAG	C1
3	E	401	NAG	C1
3	A	401	NAG	C1
3	K	401	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	NAG	1	0
3	C	400	NAG	1	0
3	I	401	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	325/334 (97%)	-0.28	5 (1%) 74 72	24, 37, 61, 128	0
1	C	325/334 (97%)	-0.33	4 (1%) 79 77	28, 40, 68, 119	0
1	E	325/334 (97%)	-0.35	7 (2%) 62 59	27, 39, 62, 110	0
1	G	325/334 (97%)	-0.28	6 (1%) 69 66	29, 43, 64, 115	0
1	I	325/334 (97%)	-0.17	7 (2%) 62 59	32, 49, 75, 128	0
1	K	325/334 (97%)	-0.15	6 (1%) 69 66	33, 49, 76, 123	0
2	B	168/181 (92%)	0.25	11 (6%) 20 18	26, 44, 83, 100	0
2	D	168/181 (92%)	0.11	5 (2%) 51 49	25, 41, 74, 99	0
2	F	168/181 (92%)	0.23	6 (3%) 43 42	26, 43, 98, 149	0
2	H	168/181 (92%)	0.10	5 (2%) 51 49	29, 47, 84, 116	0
2	J	168/181 (92%)	0.18	9 (5%) 26 25	27, 48, 74, 102	0
2	L	168/181 (92%)	0.08	3 (1%) 69 66	27, 45, 71, 102	0
All	All	2958/3090 (95%)	-0.12	74 (2%) 58 55	24, 44, 75, 149	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	LYS	6.6
1	A	262	ASN	6.4
1	E	263	LYS	5.5
2	B	1	GLY	5.3
2	H	1	GLY	5.2
1	G	263	LYS	5.1
2	D	1	GLY	4.9
2	J	29	SER	4.8
2	F	1	GLY	4.8
1	C	276	ASN	4.7
2	L	1	GLY	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	141	TRP	4.5
1	G	262	ASN	4.2
1	I	277	CYS	4.1
2	F	166	SER	4.0
2	J	38	ARG	4.0
2	J	1	GLY	3.8
1	E	324	PRO	3.8
1	I	262	ASN	3.7
2	H	168	LEU	3.6
2	D	168	LEU	3.6
2	J	164	LYS	3.5
2	L	127	ARG	3.4
2	B	18	ILE	3.3
2	B	164	LYS	3.3
1	E	45	MET	3.3
2	B	168	LEU	3.2
1	C	262	ASN	3.2
2	L	38	ARG	3.1
1	I	45	MET	3.1
2	F	127	ARG	3.1
2	B	35	ALA	3.1
1	K	46	ASN	3.0
2	J	167	LYS	3.0
2	F	29	SER	3.0
1	K	262	ASN	2.9
2	D	18	ILE	2.9
1	K	277	CYS	2.9
1	G	276	ASN	2.9
1	G	46	ASN	2.8
2	B	167	LYS	2.8
2	B	38	ARG	2.8
2	J	145	ASP	2.8
1	E	46	ASN	2.7
1	I	263	LYS	2.7
1	E	276	ASN	2.7
1	E	262	ASN	2.6
1	C	263	LYS	2.6
2	F	168	LEU	2.5
1	K	45	MET	2.5
1	C	46	ASN	2.5
1	A	1	ASP	2.5
1	A	278	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	159	TYR	2.4
1	K	139	THR	2.4
2	J	36	ALA	2.3
2	H	38	ARG	2.3
1	G	264	LYS	2.2
2	B	163	GLN	2.2
2	H	11	GLU	2.2
2	J	67	ASP	2.2
1	I	291	ASN	2.2
2	B	148	CYS	2.2
1	I	46	ASN	2.1
2	D	147	GLU	2.1
1	G	261	THR	2.1
2	D	164	LYS	2.1
1	A	281	CYS	2.1
2	B	36	ALA	2.1
1	K	140	ILE	2.1
2	J	168	LEU	2.1
1	E	129	ARG	2.1
2	B	162	TYR	2.1
1	I	276	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	E	402	14/15	0.82	0.31	-	75,85,96,97	0
3	NAG	C	402	14/15	0.88	0.24	-	72,80,87,89	0
3	NAG	G	401	14/15	0.71	0.20	-	80,98,105,107	0
3	NAG	A	402	14/15	0.92	0.22	-	56,67,72,72	0
3	NAG	I	401	14/15	0.68	0.19	-	83,90,98,100	0
3	NAG	K	402	14/15	0.87	0.24	-	72,84,95,100	0
3	NAG	I	402	14/15	0.83	0.25	-	84,96,100,107	0
3	NAG	E	400	14/15	0.84	0.23	-	88,104,110,113	0
3	NAG	G	400	14/15	0.85	0.18	-	79,96,111,114	0
3	NAG	A	400	14/15	0.85	0.14	-	89,100,106,108	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	400	14/15	0.86	0.17	-	96,107,116,118	0
3	NAG	C	401	14/15	0.68	0.22	-	74,105,115,116	0
3	NAG	E	401	14/15	0.76	0.18	-	83,94,101,106	0
3	NAG	I	400	14/15	0.81	0.24	-	103,112,116,116	0
3	NAG	K	400	14/15	0.79	0.24	-	101,108,125,125	0
3	NAG	A	401	14/15	0.75	0.15	-	78,88,94,94	0
3	NAG	G	402	14/15	0.86	0.32	-	82,89,95,97	0
3	NAG	K	401	14/15	0.72	0.22	-	75,89,93,95	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	E	402	14/15	0.82	0.31	-	75,85,96,97	0
3	NAG	C	402	14/15	0.88	0.24	-	72,80,87,89	0
3	NAG	G	401	14/15	0.71	0.20	-	80,98,105,107	0
3	NAG	A	402	14/15	0.92	0.22	-	56,67,72,72	0
3	NAG	I	401	14/15	0.68	0.19	-	83,90,98,100	0
3	NAG	K	402	14/15	0.87	0.24	-	72,84,95,100	0
3	NAG	I	402	14/15	0.83	0.25	-	84,96,100,107	0
3	NAG	E	400	14/15	0.84	0.23	-	88,104,110,113	0
3	NAG	G	400	14/15	0.85	0.18	-	79,96,111,114	0
3	NAG	A	400	14/15	0.85	0.14	-	89,100,106,108	0
3	NAG	C	400	14/15	0.86	0.17	-	96,107,116,118	0
3	NAG	C	401	14/15	0.68	0.22	-	74,105,115,116	0
3	NAG	E	401	14/15	0.76	0.18	-	83,94,101,106	0
3	NAG	I	400	14/15	0.81	0.24	-	103,112,116,116	0
3	NAG	K	400	14/15	0.79	0.24	-	101,108,125,125	0
3	NAG	A	401	14/15	0.75	0.15	-	78,88,94,94	0
3	NAG	G	402	14/15	0.86	0.32	-	82,89,95,97	0
3	NAG	K	401	14/15	0.72	0.22	-	75,89,93,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.