



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 04:06 PM EST

PDB ID : 4XKD  
Title : Crystal structure of hemagglutinin from Taiwan (2013) H6N1 influenza virus  
Authors : Tzarum, N.; Zhu, X.; Wilson, I.A.  
Deposited on : 2015-01-11  
Resolution : 2.48 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

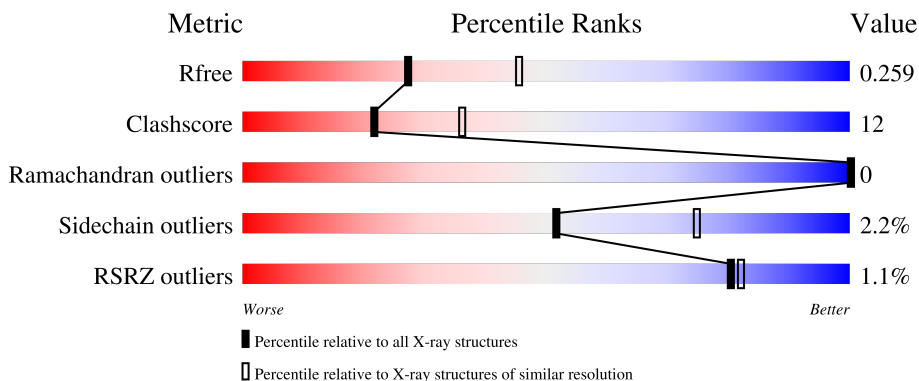
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	333	 77% 20% ..
1	C	333	 75% 21% ..
1	E	333	 69% 27% ..
2	B	180	 77% 18% ..
2	D	180	 2% 81% 16% ..

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Mol	Chain	Length	Quality of chain
2	F	180	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '77%', a yellow segment labeled '19%', and a very small grey segment at the end. A small black dot is visible at the far right end of the bar.</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12228 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
			Total	C	N	O	S			
1	A	330	Total 2600	C 1648	N 443	O 496	S 13	0	0	0
1	C	326	Total 2569	C 1629	N 437	O 490	S 13	0	0	0
1	E	325	Total 2565	C 1627	N 437	O 488	S 13	0	0	0

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	Total 1385	C 862	N 243	O 273	S 7	0	0	0
2	D	173	Total 1393	C 868	N 244	O 274	S 7	0	0	0
2	F	172	Total 1385	C 862	N 243	O 273	S 7	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

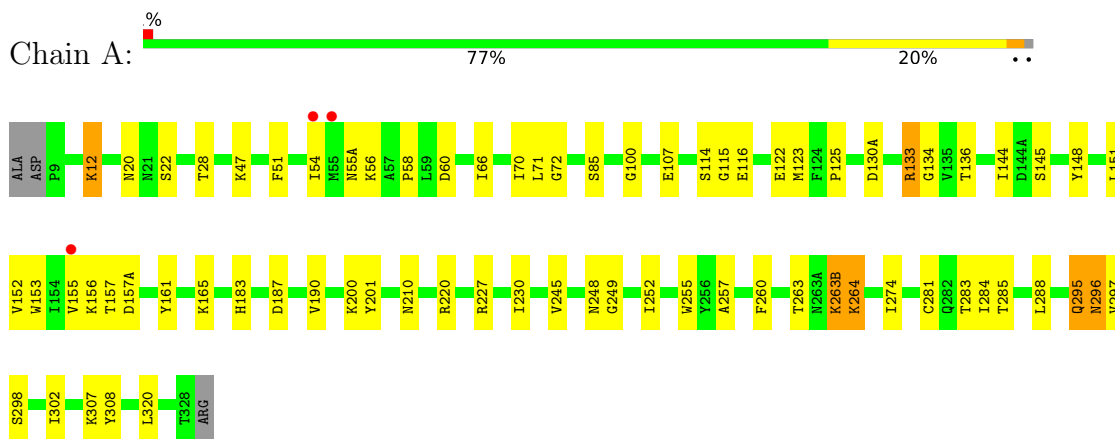
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	42	42	42	0	0
4	B	41	41	41	0	0
4	C	63	63	63	0	0
4	D	17	17	17	0	0
4	E	51	51	51	0	0
4	F	33	33	33	0	0

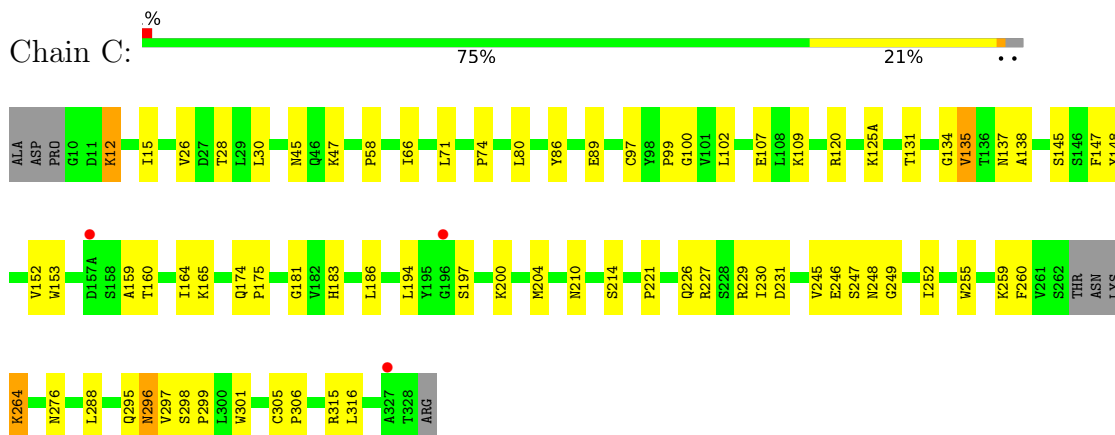
### 3 Residue-property plots [i](#)

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

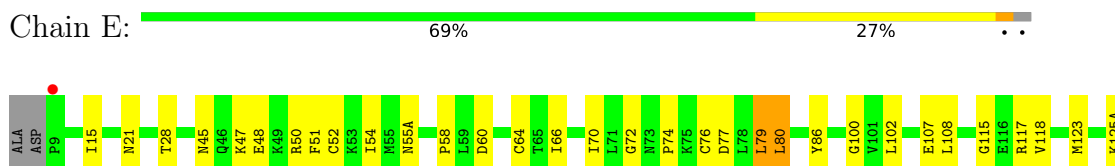
- Molecule 1: Hemagglutinin HA1 chain

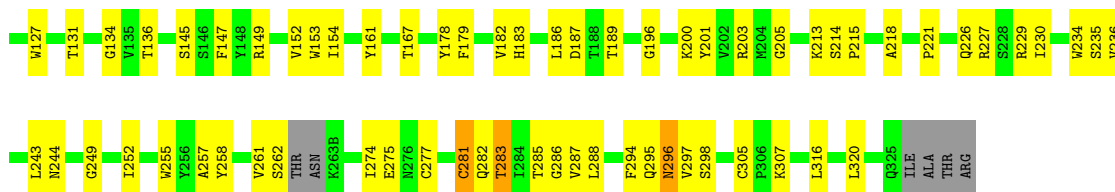


- Molecule 1: Hemagglutinin HA1 chain

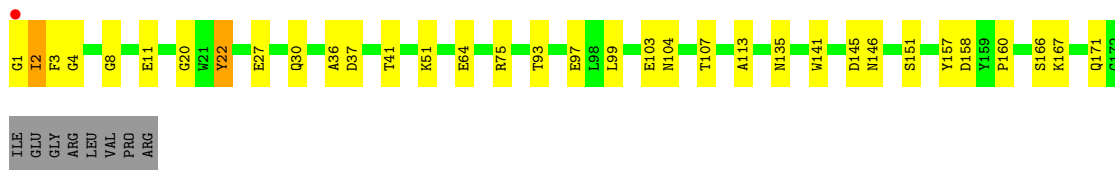
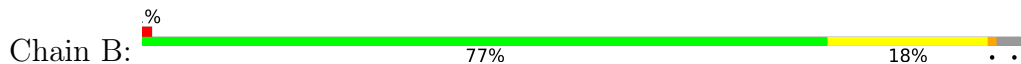


- Molecule 1: Hemagglutinin HA1 chain

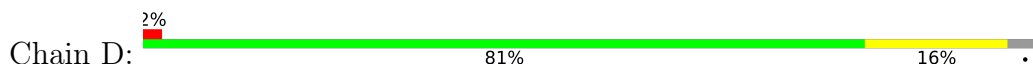




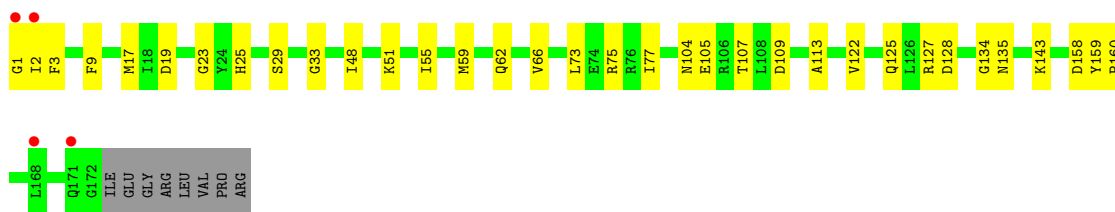
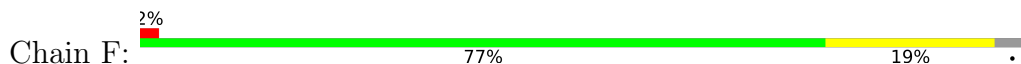
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.45Å 98.96Å 132.86Å 90.00° 126.12° 90.00°	Depositor
Resolution (Å)	49.48 – 2.48 49.48 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.48-2.48) 91.9 (49.48-2.48)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.48Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.207 , 0.257 0.210 , 0.259	Depositor DCC
$R_{free}$ test set	3354 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtrriage
Anisotropy	0.521	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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	0.56	2/2662 (0.1%)	0.66	1/3622 (0.0%)
1	C	0.61	2/2629 (0.1%)	0.74	5/3576 (0.1%)
1	E	0.58	0/2626	0.65	0/3570
2	B	0.58	0/1413	0.69	1/1902 (0.1%)
2	D	0.57	0/1421	0.68	1/1913 (0.1%)
2	F	0.58	0/1413	0.68	1/1902 (0.1%)
All	All	0.58	4/12164 (0.0%)	0.68	9/16485 (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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	135	VAL	CB-CG1	-7.68	1.36	1.52
1	A	12	LYS	CD-CE	5.50	1.65	1.51
1	C	12	LYS	CD-CE	5.27	1.64	1.51
1	A	12	LYS	CG-CD	5.02	1.69	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	SER	N-CA-CB	-11.87	92.70	110.50
1	A	12	LYS	CD-CE-NZ	8.16	130.48	111.70
2	B	1	GLY	N-CA-C	-8.13	92.77	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLY	N-CA-C	-7.98	93.14	113.10
1	C	12	LYS	CD-CE-NZ	7.51	128.98	111.70
2	F	1	GLY	N-CA-C	-6.76	96.20	113.10
1	C	316	LEU	CA-CB-CG	5.98	129.06	115.30
1	C	109	LYS	CD-CE-NZ	5.98	125.45	111.70
1	C	197	SER	N-CA-C	5.94	127.04	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	134	GLY	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	2600	0	2548	65	0
1	C	2569	0	2516	57	0
1	E	2565	0	2515	92	0
2	B	1385	0	1298	33	0
2	D	1393	0	1307	32	0
2	F	1385	0	1296	31	0
3	A	28	0	26	0	0
3	D	14	0	13	1	0
3	E	28	0	26	0	0
3	F	14	0	13	0	0
4	A	42	0	0	1	0
4	B	41	0	0	0	0
4	C	63	0	0	0	0
4	D	17	0	0	2	0
4	E	51	0	0	1	0
4	F	33	0	0	3	0
All	All	12228	0	11558	279	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 12.

All (279) 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:E:305:CYS:O	2:F:62:GLN:NE2	1.61	1.33
1:E:64:CYS:CB	1:E:76:CYS:SG	2.17	1.31
2:F:2:ILE:HG21	2:F:109:ASP:CG	1.69	1.13
1:A:157:THR:HG22	1:A:157(A):ASP:H	1.17	1.09
1:E:64:CYS:SG	1:E:76:CYS:SG	1.18	1.09
1:E:77:ASP:HA	1:E:80:LEU:CD1	1.82	1.08
2:D:69:GLU:OE1	4:D:301:HOH:O	1.75	1.03
1:A:114:SER:O	1:A:263:THR:HG22	1.64	0.97
2:F:2:ILE:CG2	2:F:109:ASP:OD1	2.15	0.94
1:A:157:THR:HG22	1:A:157(A):ASP:N	1.79	0.93
1:C:12:LYS:NZ	2:D:25:HIS:HE1	1.70	0.88
2:F:2:ILE:HG22	2:F:109:ASP:OD1	1.73	0.88
1:A:157:THR:CG2	1:A:157(A):ASP:H	1.88	0.86
1:E:77:ASP:HA	1:E:80:LEU:HD13	1.55	0.86
2:F:2:ILE:CG2	2:F:109:ASP:CG	2.43	0.85
1:A:210:ASN:HD21	1:C:229:ARG:HG3	1.40	0.85
1:E:50:ARG:NH2	1:E:277:CYS:SG	2.50	0.84
1:E:64:CYS:HB3	1:E:76:CYS:SG	2.16	0.84
1:E:77:ASP:HA	1:E:80:LEU:HD12	1.60	0.81
1:A:295:GLN:NE2	1:A:298:SER:H	1.80	0.80
2:F:17:MET:SD	2:F:23:GLY:HA3	2.22	0.79
1:E:125(A):LYS:CG	1:E:131:THR:HG21	2.15	0.77
1:E:52:CYS:HG	1:E:277:CYS:HG	0.77	0.76
1:A:263:THR:OG1	1:A:263(B):LYS:HG3	1.86	0.76
1:E:47:LYS:HD3	1:E:297:VAL:HG13	1.67	0.75
1:A:288:LEU:HD11	1:A:295:GLN:HG3	1.70	0.74
1:C:125(A):LYS:HG2	1:C:131:THR:CG2	2.18	0.74
2:B:30:GLN:NE2	2:B:145:ASP:HB2	2.03	0.73
1:C:12:LYS:HZ1	2:D:25:HIS:HE1	1.36	0.73
2:F:25:HIS:NE2	4:F:303:HOH:O	2.22	0.73
2:B:51:LYS:HZ1	2:B:107:THR:HG22	1.54	0.72
2:B:51:LYS:NZ	2:B:107:THR:CG2	2.53	0.71
2:B:51:LYS:NZ	2:B:107:THR:HG22	2.05	0.71
1:C:288:LEU:HD11	1:C:297:VAL:HG21	1.72	0.71
1:A:295:GLN:NE2	1:A:308:TYR:HD1	1.89	0.71
3:D:201:NAG:O3	3:D:201:NAG:H83	1.91	0.71
1:C:125(A):LYS:HG2	1:C:131:THR:HG23	1.73	0.71
1:E:283:THR:HG22	1:E:285:THR:H	1.57	0.69
2:D:97:GLU:OE1	4:D:302:HOH:O	2.11	0.69
2:D:167:LYS:HA	2:D:170:ARG:HE	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ASP:CA	1:E:80:LEU:HD13	2.24	0.67
1:E:77:ASP:OD1	1:E:80:LEU:HD11	1.94	0.67
1:C:135:VAL:HG12	1:C:145:SER:HB3	1.76	0.66
2:F:128:ASP:OD1	2:F:159:TYR:OH	2.12	0.66
2:F:2:ILE:HG21	2:F:109:ASP:OD1	1.83	0.65
2:B:30:GLN:NE2	2:B:146:ASN:H	1.95	0.65
1:C:12:LYS:NZ	2:D:25:HIS:CE1	2.59	0.65
1:E:186:LEU:HD22	1:E:227:ARG:HB2	1.78	0.65
1:A:187:ASP:HB3	1:A:190:VAL:H	1.61	0.65
1:E:77:ASP:OD1	1:E:80:LEU:CD1	2.46	0.64
1:A:130(A):ASP:HB3	1:A:155:VAL:O	1.98	0.64
2:D:133:LEU:HD11	2:D:139:GLU:HB2	1.78	0.64
1:A:295:GLN:HE22	1:A:308:TYR:HD1	1.46	0.64
1:C:28:THR:HG23	2:D:105:GLU:HB2	1.80	0.63
1:E:131:THR:HG23	1:E:152:VAL:HG11	1.80	0.63
2:B:11:GLU:HG3	2:B:135:ASN:OD1	1.99	0.63
1:E:47:LYS:HD3	1:E:297:VAL:CG1	2.29	0.63
1:E:123:MET:HE2	1:E:257:ALA:HB2	1.81	0.63
1:E:125(A):LYS:HG2	1:E:131:THR:HG21	1.81	0.62
2:B:103:GLU:O	2:B:107:THR:HG23	1.99	0.62
2:B:75:ARG:N	1:E:107:GLU:OE2	2.28	0.62
1:C:295:GLN:HG2	1:C:306:PRO:HG2	1.80	0.61
1:E:187:ASP:HB3	1:E:189:THR:H	1.65	0.61
1:E:125(A):LYS:CD	1:E:131:THR:HG21	2.30	0.61
1:E:50:ARG:CZ	1:E:277:CYS:SG	2.88	0.61
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.81	0.60
2:F:2:ILE:HG21	2:F:109:ASP:OD2	2.00	0.60
1:E:45:ASN:HA	1:E:296:ASN:HD21	1.66	0.60
1:E:201:TYR:HD1	1:E:203:ARG:HG3	1.67	0.60
2:B:51:LYS:HZ2	2:B:107:THR:CG2	2.15	0.60
1:A:47:LYS:HD3	1:A:297:VAL:HG13	1.85	0.59
1:E:54:ILE:HD11	1:E:282:GLN:HB2	1.83	0.59
1:E:125(A):LYS:HD3	1:E:131:THR:CG2	2.32	0.59
1:A:227:ARG:HH21	1:E:244:ASN:HD21	1.50	0.58
1:C:221:PRO:O	1:C:229:ARG:NH2	2.36	0.58
1:A:123:MET:HE2	1:A:257:ALA:HB2	1.85	0.58
2:D:28:ASN:OD1	2:D:30:GLN:HB2	2.04	0.57
1:A:152:VAL:HG23	1:A:255:TRP:HB2	1.86	0.57
1:A:144:ILE:HG22	1:A:145:SER:H	1.70	0.57
2:D:17:MET:CE	2:D:23:GLY:HA3	2.35	0.57
1:E:28:THR:HG22	2:F:104:ASN:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:PRO:HG2	1:E:274:ILE:HD13	1.87	0.56
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.88	0.56
2:B:30:GLN:HE21	2:B:145:ASP:HB2	1.71	0.56
1:C:159:ALA:HB1	1:C:160:THR:HG22	1.88	0.56
2:F:19:ASP:OD1	4:F:301:HOH:O	2.18	0.56
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.86	0.56
1:E:45:ASN:HA	1:E:296:ASN:ND2	2.21	0.56
1:A:200:LYS:NZ	1:A:248:ASN:O	2.34	0.56
1:E:283:THR:HB	1:E:286:GLY:O	2.05	0.56
1:A:66:ILE:O	1:A:70:ILE:HG13	2.06	0.56
1:E:283:THR:HG23	1:E:298:SER:HB3	1.88	0.56
2:B:167:LYS:O	2:B:171:GLN:HG2	2.06	0.55
2:D:25:HIS:HD2	2:D:33:GLY:O	1.89	0.55
1:A:12:LYS:HG2	2:B:27:GLU:HB2	1.88	0.55
1:A:151:LEU:O	4:A:502:HOH:O	2.18	0.55
1:E:201:TYR:CD1	1:E:203:ARG:HG3	2.41	0.55
1:E:183:HIS:HB2	1:E:252:ILE:HD11	1.89	0.55
1:E:125(A):LYS:CD	1:E:131:THR:CG2	2.84	0.55
1:E:288:LEU:HD21	1:E:297:VAL:HG21	1.88	0.55
2:B:51:LYS:HZ1	2:B:107:THR:CG2	2.18	0.54
1:C:28:THR:HG22	1:C:30:LEU:H	1.71	0.54
1:A:107:GLU:OE2	2:D:75:ARG:N	2.33	0.54
1:C:74:PRO:HG3	1:C:147:PHE:O	2.08	0.54
1:A:288:LEU:CD1	1:A:295:GLN:HG3	2.39	0.53
1:C:28:THR:HG22	1:C:30:LEU:N	2.24	0.53
2:B:93:THR:O	2:B:97:GLU:HG3	2.10	0.52
2:D:145:ASP:HB3	2:D:148:CYS:H	1.74	0.52
1:A:157:THR:CG2	1:A:157(A):ASP:N	2.50	0.52
1:E:125(A):LYS:HD3	1:E:131:THR:HG21	1.92	0.52
1:A:133:ARG:CD	1:A:155:VAL:HG11	2.40	0.52
1:E:21:ASN:OD1	4:E:501:HOH:O	2.18	0.52
1:A:227:ARG:NH2	1:E:244:ASN:HD21	2.08	0.52
1:A:295:GLN:HE21	1:A:297:VAL:N	2.08	0.52
1:E:52:CYS:HG	1:E:277:CYS:CB	2.22	0.52
2:B:151:SER:OG	2:B:157:TYR:HA	2.10	0.52
1:C:15:ILE:HD11	2:D:122:VAL:HG21	1.92	0.52
2:F:105:GLU:OE1	4:F:302:HOH:O	2.19	0.51
1:C:125(A):LYS:HB3	1:C:131:THR:HG21	1.92	0.51
1:A:12:LYS:HG2	2:B:27:GLU:CB	2.40	0.51
1:C:80:LEU:HD11	1:C:120:ARG:CZ	2.41	0.51
2:F:158:ASP:OD1	2:F:160:PRO:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:THR:HG22	1:E:131:THR:O	2.10	0.50
1:A:156:LYS:HG2	1:A:157:THR:O	2.12	0.50
1:A:116:GLU:HB3	1:A:263:THR:HB	1.91	0.50
1:C:47:LYS:HD3	1:C:297:VAL:HG13	1.93	0.50
1:A:201:TYR:CD2	1:A:248:ASN:HB2	2.47	0.50
2:B:30:GLN:HE21	2:B:146:ASN:H	1.58	0.49
1:E:125(A):LYS:HE2	1:E:131:THR:HG22	1.94	0.49
2:B:51:LYS:HZ2	2:B:107:THR:HG23	1.77	0.49
1:C:137:ASN:OD1	1:C:137:ASN:N	2.44	0.49
1:E:127:TRP:CD1	1:E:154:ILE:HD11	2.46	0.49
1:A:12:LYS:HE2	2:B:27:GLU:OE1	2.13	0.49
1:E:283:THR:CG2	1:E:285:THR:H	2.25	0.49
2:F:19:ASP:OD1	2:F:19:ASP:N	2.46	0.48
1:A:133:ARG:NH1	1:A:155:VAL:HG21	2.29	0.48
2:D:171:GLN:OE1	2:D:171:GLN:HA	2.12	0.48
2:D:167:LYS:O	2:D:170:ARG:HG2	2.14	0.48
1:A:130(A):ASP:N	1:A:155:VAL:O	2.46	0.47
2:B:141:TRP:HB2	2:B:166:SER:HB2	1.96	0.47
1:A:187:ASP:CB	1:A:190:VAL:H	2.26	0.47
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.49	0.47
1:C:174:GLN:OE1	1:C:259:LYS:HD3	2.15	0.47
2:B:51:LYS:NZ	2:B:107:THR:HG23	2.29	0.47
1:C:125(A):LYS:CG	1:C:131:THR:HG21	2.44	0.47
1:E:316:LEU:HD11	2:F:55:ILE:HD12	1.95	0.47
1:C:296:ASN:HD22	1:C:296:ASN:C	2.17	0.47
1:A:165:LYS:HA	1:A:245:VAL:O	2.15	0.47
2:D:128:ASP:HB2	2:D:170:ARG:NH1	2.30	0.47
2:F:125:GLN:O	2:F:127:ARG:HG3	2.15	0.47
1:E:296:ASN:H	1:E:296:ASN:HD22	1.63	0.46
2:B:158:ASP:OD1	2:B:160:PRO:HD2	2.16	0.46
2:F:3:PHE:CE1	2:F:113:ALA:HB2	2.50	0.46
1:C:152:VAL:HG23	1:C:255:TRP:HB2	1.98	0.46
1:A:264:LYS:O	1:A:302:ILE:HD11	2.16	0.46
1:A:283:THR:HB	1:A:298:SER:HB3	1.98	0.46
1:E:51:PHE:HB3	1:E:86:TYR:OH	2.16	0.46
1:E:52:CYS:SG	1:E:287:VAL:HG21	2.56	0.46
1:C:66:ILE:HG13	1:C:89:GLU:OE2	2.15	0.46
1:C:135:VAL:CG1	1:C:145:SER:HB3	2.41	0.46
2:D:145:ASP:N	2:D:148:CYS:HB3	2.30	0.46
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.51	0.46
1:E:100:GLY:HA3	1:E:230:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125(A):LYS:HD3	1:E:131:THR:HG22	1.98	0.46
1:C:107:GLU:OE2	2:F:75:ARG:N	2.37	0.46
2:F:29:SER:OG	2:F:143:LYS:HE2	2.16	0.46
1:A:58:PRO:HG2	1:A:274:ILE:HD13	1.98	0.46
1:E:66:ILE:O	1:E:70:ILE:HG13	2.16	0.46
1:E:77:ASP:O	1:E:80:LEU:HB2	2.16	0.46
1:A:60:ASP:HB2	1:A:274:ILE:HD12	1.97	0.45
1:E:50:ARG:NH1	1:E:275:GLU:OE1	2.46	0.45
1:E:74:PRO:HG3	1:E:147:PHE:O	2.16	0.45
1:E:294:PHE:CZ	2:F:59:MET:HG3	2.52	0.45
1:E:294:PHE:HZ	2:F:59:MET:HG3	1.80	0.45
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.51	0.45
1:C:45:ASN:HA	1:C:296:ASN:ND2	2.32	0.45
1:C:97:CYS:HB2	1:C:138:ALA:O	2.16	0.45
2:D:129:ASN:HA	2:D:166:SER:OG	2.17	0.45
1:C:99:PRO:HG3	1:C:226:GLN:HB2	1.98	0.45
2:D:128:ASP:HB2	2:D:170:ARG:HH12	1.81	0.45
2:D:17:MET:SD	2:D:23:GLY:HA3	2.57	0.45
1:A:201:TYR:CE2	1:A:248:ASN:HB2	2.52	0.45
1:C:164:ILE:HG12	1:C:247:SER:O	2.17	0.45
1:C:210:ASN:OD1	1:E:229:ARG:HG3	2.16	0.45
1:E:125(A):LYS:HB3	1:E:131:THR:HG21	1.98	0.45
2:D:170:ARG:O	2:D:173:ILE:HG22	2.17	0.45
1:A:47:LYS:HD3	1:A:297:VAL:CG1	2.45	0.45
1:C:200:LYS:HA	1:C:248:ASN:HD21	1.81	0.45
1:E:115:GLY:HA2	1:E:262:SER:HA	1.99	0.45
1:E:125(A):LYS:CB	1:E:131:THR:HG21	2.46	0.45
1:A:20:ASN:OD1	1:A:22:SER:HB3	2.18	0.44
2:B:3:PHE:CE2	2:B:113:ALA:HB2	2.52	0.44
2:B:20:GLY:HA3	2:B:36:ALA:HB1	1.99	0.44
2:F:66:VAL:HG23	2:F:66:VAL:O	2.17	0.44
2:B:20:GLY:HA3	2:B:36:ALA:CB	2.47	0.44
2:B:22:TYR:H	2:B:41:THR:HG22	1.81	0.44
1:C:175:PRO:HD2	1:C:260:PHE:O	2.16	0.44
2:D:25:HIS:CD2	2:D:33:GLY:O	2.70	0.44
1:E:108:LEU:HB2	1:E:234:TRP:NE1	2.32	0.44
1:A:72:GLY:O	1:A:148:TYR:HA	2.18	0.44
1:A:296:ASN:C	1:A:296:ASN:HD22	2.21	0.44
1:A:133:ARG:HD3	1:A:155:VAL:HG11	2.00	0.44
1:E:136:THR:O	1:E:145:SER:HA	2.18	0.44
1:C:107:GLU:HG2	2:F:73:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLY:O	1:E:149:ARG:HG2	2.17	0.43
2:F:9:PHE:O	2:F:135:ASN:HA	2.18	0.43
2:B:99:LEU:HD13	2:D:98:LEU:HD21	1.99	0.43
1:A:295:GLN:HG2	1:A:297:VAL:H	1.84	0.43
1:E:70:ILE:HD13	1:E:179:PHE:CZ	2.53	0.43
1:E:186:LEU:HA	1:E:218:ALA:O	2.18	0.43
1:A:307:LYS:HB2	1:A:307:LYS:HE2	1.68	0.43
1:C:165:LYS:HG2	1:C:246:GLU:HG3	2.01	0.43
1:E:152:VAL:HG23	1:E:255:TRP:HB2	2.01	0.43
1:E:283:THR:HG22	1:E:285:THR:N	2.28	0.43
2:F:77:ILE:H	2:F:77:ILE:HG13	1.67	0.43
1:A:51:PHE:HB2	1:A:274:ILE:HG12	2.00	0.43
1:C:12:LYS:HZ2	2:D:25:HIS:CE1	2.36	0.43
1:E:15:ILE:HD11	2:F:122:VAL:HG21	1.99	0.43
1:E:196:GLY:H	1:E:200:LYS:HZ1	1.66	0.43
1:C:200:LYS:HD2	1:C:249:GLY:HA3	2.01	0.43
1:E:167:THR:HA	1:E:243:LEU:O	2.18	0.43
1:C:125(A):LYS:CG	1:C:131:THR:CG2	2.92	0.43
1:E:79:LEU:O	1:E:80:LEU:HD12	2.19	0.43
1:E:221:PRO:O	1:E:229:ARG:NH2	2.36	0.43
1:C:204:MET:HG2	1:C:245:VAL:HG22	2.01	0.42
2:F:51:LYS:HZ2	2:F:107:THR:HG1	1.60	0.42
1:C:100:GLY:HA3	1:C:230:ILE:O	2.19	0.42
1:A:130(A):ASP:CB	1:A:155:VAL:O	2.66	0.42
1:C:264:LYS:HE3	2:D:64:GLU:OE1	2.20	0.42
1:E:200:LYS:O	1:E:215:PRO:HD2	2.19	0.42
1:A:28:THR:HG22	2:B:104:ASN:HB3	2.01	0.42
1:A:201:TYR:H	1:A:248:ASN:HB3	1.84	0.42
1:C:58:PRO:HB3	1:C:86:TYR:CZ	2.55	0.42
1:E:134:GLY:HA3	1:E:153:TRP:HB3	2.02	0.42
1:C:12:LYS:HG2	2:D:27:GLU:HB3	2.02	0.42
1:E:125(A):LYS:HE2	1:E:131:THR:CG2	2.49	0.42
2:F:48:ILE:CD1	2:F:107:THR:HG23	2.49	0.42
1:C:200:LYS:O	1:C:214:SER:HB2	2.20	0.42
1:E:48:GLU:HB2	1:E:287:VAL:HB	2.01	0.42
1:E:117:ARG:HB3	1:E:261:VAL:HG13	2.02	0.42
1:A:284:ILE:HG23	1:A:285:THR:HG23	2.02	0.42
1:A:71:LEU:O	1:A:148:TYR:HB3	2.20	0.42
1:C:298:SER:HA	1:C:299:PRO:HD2	1.88	0.42
1:E:60:ASP:HB2	1:E:274:ILE:HD12	2.02	0.42
1:A:220:ARG:HG3	1:E:205:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:HIS:HA	2:F:33:GLY:O	2.20	0.42
1:A:295:GLN:NE2	1:A:308:TYR:CD1	2.79	0.42
2:B:4:GLY:O	2:B:8:GLY:HA3	2.20	0.41
1:C:12:LYS:CE	2:D:25:HIS:CE1	3.03	0.41
1:E:28:THR:HB	2:F:105:GLU:HB2	2.00	0.41
1:E:226:GLN:O	1:E:229:ARG:NH2	2.52	0.41
1:A:115:GLY:HA3	1:A:260:PHE:CZ	2.56	0.41
1:C:12:LYS:HE2	2:D:27:GLU:OE1	2.20	0.41
1:C:183:HIS:HB2	1:C:252:ILE:HD11	2.02	0.41
1:C:26:VAL:HG12	1:C:315:ARG:HG2	2.03	0.41
1:E:77:ASP:OD2	1:E:149:ARG:NH2	2.51	0.41
2:B:51:LYS:NZ	2:B:103:GLU:OE2	2.50	0.41
1:E:182:VAL:HG21	1:E:213:LYS:HB3	2.03	0.41
1:E:235:SER:OG	1:E:236:VAL:N	2.54	0.41
1:E:281:CYS:SG	1:E:288:LEU:HB2	2.60	0.41
2:D:156:THR:O	2:D:156:THR:HG22	2.21	0.41
1:A:54:ILE:HA	1:A:54:ILE:HD13	1.78	0.41
1:A:100:GLY:HA3	1:A:230:ILE:O	2.21	0.41
1:C:12:LYS:HE3	2:D:25:HIS:CE1	2.56	0.41
1:C:45:ASN:HA	1:C:296:ASN:HD21	1.86	0.41
1:A:156:LYS:HG2	1:A:157:THR:N	2.37	0.41
1:A:56:LYS:HB3	1:A:85:SER:HB3	2.03	0.40
2:B:37:ASP:O	2:B:41:THR:HG23	2.20	0.40
1:C:71:LEU:O	1:C:148:TYR:HB3	2.21	0.40
1:C:186:LEU:HD13	1:C:227:ARG:HB2	2.03	0.40
1:C:301:TRP:CD1	1:C:305:CYS:SG	3.15	0.40
1:A:122:GLU:OE1	1:A:125:PRO:HA	2.21	0.40
2:B:2:ILE:HG23	2:B:3:PHE:N	2.36	0.40
1:E:123:MET:HE1	1:E:178:TYR:HB2	2.03	0.40
1:E:196:GLY:H	1:E:200:LYS:NZ	2.19	0.40
2:B:2:ILE:O	2:B:2:ILE:HG12	2.21	0.40
2:D:58:LYS:HA	2:D:58:LYS:HD3	1.70	0.40
1:E:118:VAL:HB	1:E:258:TYR:CD1	2.57	0.40
1:C:181:GLY:HA2	1:C:231:ASP:O	2.21	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	328/333 (98%)	319 (97%)	9 (3%)	0	100	100
1	C	322/333 (97%)	316 (98%)	6 (2%)	0	100	100
1	E	321/333 (96%)	307 (96%)	14 (4%)	0	100	100
2	B	170/180 (94%)	169 (99%)	1 (1%)	0	100	100
2	D	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
2	F	170/180 (94%)	163 (96%)	7 (4%)	0	100	100
All	All	1482/1539 (96%)	1443 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	289/291 (99%)	280 (97%)	9 (3%)	40	64
1	C	285/291 (98%)	280 (98%)	5 (2%)	59	80
1	E	285/291 (98%)	274 (96%)	11 (4%)	32	55
2	B	146/153 (95%)	143 (98%)	3 (2%)	53	76
2	D	147/153 (96%)	147 (100%)	0	100	100
2	F	146/153 (95%)	146 (100%)	0	100	100
All	All	1298/1332 (97%)	1270 (98%)	28 (2%)	52	75

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55(A)	ASN
1	A	133	ARG
1	A	136	THR
1	A	263(B)	LYS
1	A	264	LYS
1	A	281	CYS
1	A	295	GLN
1	A	296	ASN
1	A	320	LEU
2	B	2	ILE
2	B	22	TYR
2	B	64	GLU
1	C	102	LEU
1	C	194	LEU
1	C	264	LYS
1	C	276	ASN
1	C	296	ASN
1	E	55(A)	ASN
1	E	79	LEU
1	E	80	LEU
1	E	102	LEU
1	E	214	SER
1	E	281	CYS
1	E	283	THR
1	E	295	GLN
1	E	296	ASN
1	E	307	LYS
1	E	320	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	295	GLN
1	A	296	ASN
2	B	30	GLN
2	B	57	ASN
1	C	276	ASN
1	C	296	ASN
2	D	25	HIS
1	E	46	GLN

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Mol	Chain	Res	Type
1	E	244	ASN
1	E	296	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 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	E	402	1	14,14,15	0.46	0	17,19,21	0.89	1 (5%)
3	NAG	F	201	2	14,14,15	0.54	0	17,19,21	1.14	1 (5%)
3	NAG	A	401	1	14,14,15	0.54	0	17,19,21	2.20	3 (17%)
3	NAG	D	201	2	14,14,15	0.53	0	17,19,21	1.88	5 (29%)
3	NAG	A	402	1	14,14,15	0.85	1 (7%)	17,19,21	1.94	6 (35%)
3	NAG	E	401	1	14,14,15	0.46	0	17,19,21	1.67	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	402	1	-	4/6/23/26	0/1/1/1
3	NAG	F	201	2	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	-	3/6/23/26	0/1/1/1
3	NAG	D	201	2	-	2/6/23/26	0/1/1/1
3	NAG	A	402	1	-	2/6/23/26	0/1/1/1
3	NAG	E	401	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAG	C2-N2	-2.02	1.42	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	C2-N2-C7	5.95	131.37	122.90
3	A	401	NAG	C1-C2-N2	5.50	119.88	110.49
3	A	402	NAG	C1-C2-N2	4.12	117.52	110.49
3	E	401	NAG	O5-C5-C6	-4.03	100.89	107.20
3	D	201	NAG	O5-C5-C6	-3.89	101.10	107.20
3	D	201	NAG	C1-C2-N2	3.74	116.87	110.49
3	A	402	NAG	C2-N2-C7	-3.68	117.67	122.90
3	E	401	NAG	C6-C5-C4	-3.16	105.61	113.00
3	A	402	NAG	O3-C3-C4	-2.93	103.58	110.35
3	A	402	NAG	O5-C5-C6	2.91	111.76	107.20
3	D	201	NAG	C6-C5-C4	-2.88	106.26	113.00
3	E	401	NAG	C1-O5-C5	2.85	116.05	112.19
3	E	402	NAG	C1-O5-C5	2.78	115.96	112.19
3	A	402	NAG	C1-O5-C5	2.73	115.89	112.19
3	F	201	NAG	C1-O5-C5	2.72	115.88	112.19
3	D	201	NAG	C1-O5-C5	2.62	115.74	112.19
3	A	401	NAG	O5-C5-C6	-2.30	103.60	107.20
3	D	201	NAG	C2-N2-C7	-2.27	119.67	122.90
3	A	402	NAG	C6-C5-C4	-2.13	108.01	113.00

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	201	NAG	C8-C7-N2-C2

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
3	D	201	NAG	O7-C7-N2-C2
3	E	401	NAG	C8-C7-N2-C2
3	E	401	NAG	O7-C7-N2-C2
3	E	402	NAG	O5-C5-C6-O6
3	A	401	NAG	C8-C7-N2-C2
3	E	402	NAG	C8-C7-N2-C2
3	A	401	NAG	C1-C2-N2-C7
3	E	401	NAG	O5-C5-C6-O6
3	A	401	NAG	O7-C7-N2-C2
3	A	402	NAG	C8-C7-N2-C2
3	E	402	NAG	O7-C7-N2-C2
3	E	402	NAG	C4-C5-C6-O6
3	E	401	NAG	C4-C5-C6-O6
3	A	402	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	201	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	330/333 (99%)	-0.12	3 (0%) 84 86	27, 44, 62, 75	0
1	C	326/333 (97%)	-0.22	3 (0%) 84 86	26, 38, 57, 81	0
1	E	325/333 (97%)	-0.23	1 (0%) 94 94	27, 40, 54, 73	0
2	B	172/180 (95%)	-0.08	1 (0%) 89 90	25, 36, 54, 72	0
2	D	173/180 (96%)	0.02	4 (2%) 60 62	28, 38, 60, 77	0
2	F	172/180 (95%)	-0.09	4 (2%) 60 62	24, 37, 57, 82	0
All	All	1498/1539 (97%)	-0.14	16 (1%) 80 82	24, 39, 57, 82	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	GLY	5.4
2	D	1	GLY	5.3
2	F	1	GLY	4.9
2	D	173	ILE	4.7
1	E	9	PRO	4.2
1	C	196	GLY	4.0
2	F	171	GLN	3.2
1	A	155	VAL	3.1
1	A	54	ILE	2.6
2	F	168	LEU	2.4
2	F	2	ILE	2.3
1	C	157(A)	ASP	2.3
1	A	55	MET	2.1
2	D	2	ILE	2.1
2	D	164	LYS	2.1
1	C	327	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	D	201	14/15	0.63	0.32	66,78,85,88	0
3	NAG	F	201	14/15	0.65	0.27	61,70,80,86	0
3	NAG	E	401	14/15	0.76	0.39	87,98,105,109	0
3	NAG	A	401	14/15	0.78	0.17	68,81,85,87	0
3	NAG	E	402	14/15	0.83	0.16	57,73,83,85	0
3	NAG	A	402	14/15	0.87	0.13	65,70,77,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.