



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:50 am GMT

PDB ID : 4KDM  
Title : Crystal structure of the hemagglutinin of ferret-transmissible H5N1 virus  
Authors : Lu, X.; Shi, Y.; Zhang, W.; Zhang, Y.; Qi, J.; Gao, G.F.  
Deposited on : 2013-04-25  
Resolution : 2.50 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

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (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

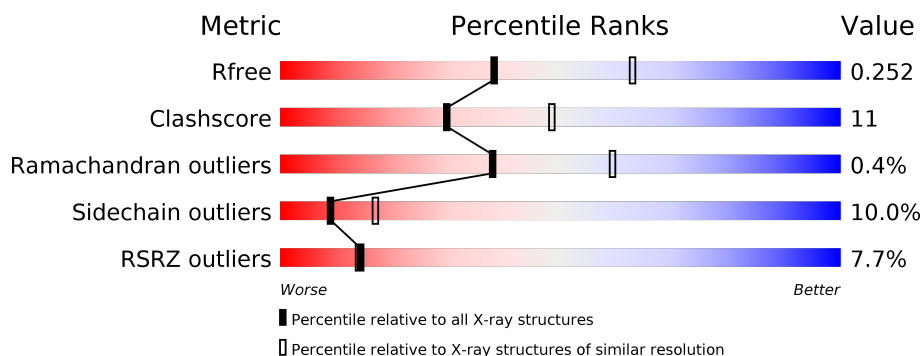
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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  $\geq 3$ , 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	322	<div> <div>0%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>5%</div> </div> </div>
1	C	322	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>6%</div> </div> </div>
1	E	322	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>29%</div> <div>5%</div> </div> </div>
2	B	175	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>•</div> </div> </div>
2	D	175	<div> <div>20%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>•</div> </div> </div>
2	F	175	<div> <div>26%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12221 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	C	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			
1	E	322	Total	C	N	O	S	0	0	0
			2559	1621	440	483	15			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	EXPRESSION TAG	UNP Q6DQ33
A	158	ASP	ASN	engineered mutation	UNP Q6DQ33
A	224	LYS	ASN	engineered mutation	UNP Q6DQ33
A	226	LEU	GLN	engineered mutation	UNP Q6DQ33
A	319	ILE	THR	engineered mutation	UNP Q6DQ33
C	4	GLN	-	EXPRESSION TAG	UNP Q6DQ33
C	158	ASP	ASN	engineered mutation	UNP Q6DQ33
C	224	LYS	ASN	engineered mutation	UNP Q6DQ33
C	226	LEU	GLN	engineered mutation	UNP Q6DQ33
C	319	ILE	THR	engineered mutation	UNP Q6DQ33
E	4	GLN	-	EXPRESSION TAG	UNP Q6DQ33
E	158	ASP	ASN	engineered mutation	UNP Q6DQ33
E	224	LYS	ASN	engineered mutation	UNP Q6DQ33
E	226	LEU	GLN	engineered mutation	UNP Q6DQ33
E	319	ILE	THR	engineered mutation	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

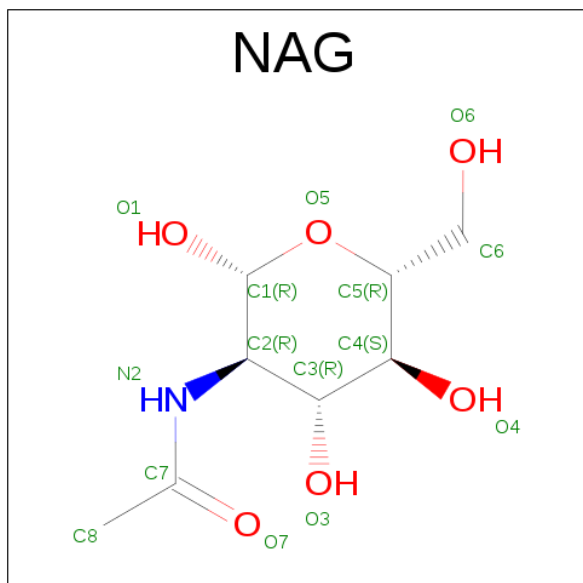
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

- 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	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		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

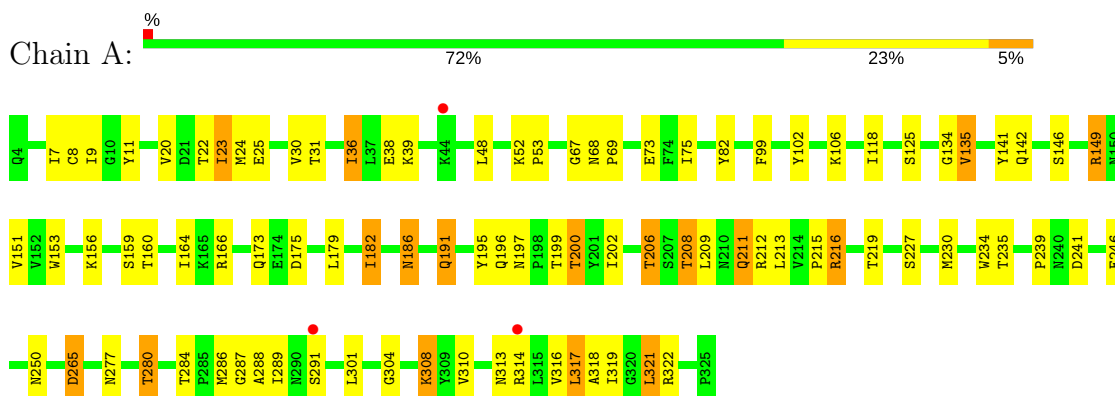
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total 53	O 53	0	0
5	B	13	Total 13	O 13	0	0
5	C	42	Total 42	O 42	0	0
5	D	17	Total 17	O 17	0	0
5	E	33	Total 33	O 33	0	0
5	F	12	Total 12	O 12	0	0

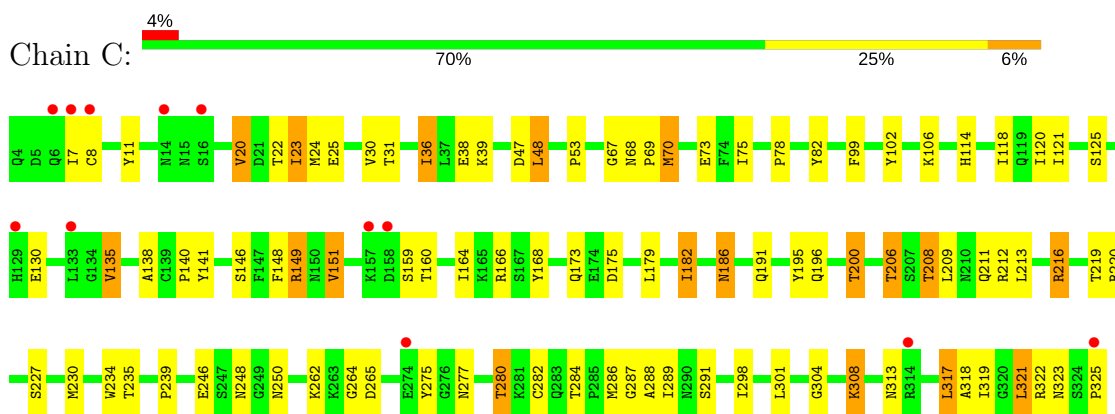
### 3 Residue-property plots

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.

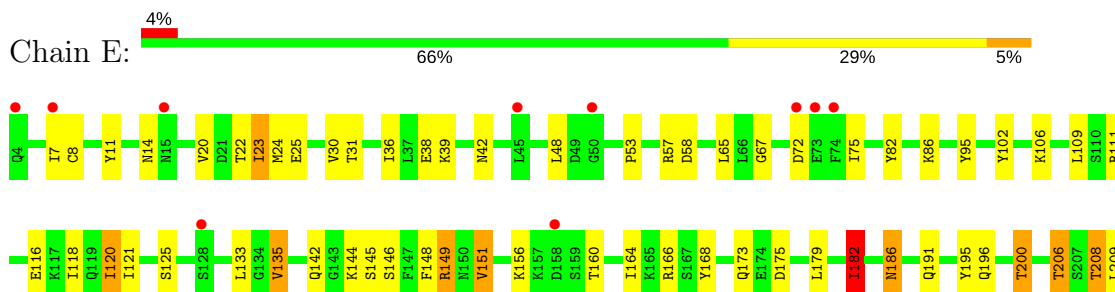
#### • Molecule 1: Hemagglutinin



#### • Molecule 1: Hemagglutinin

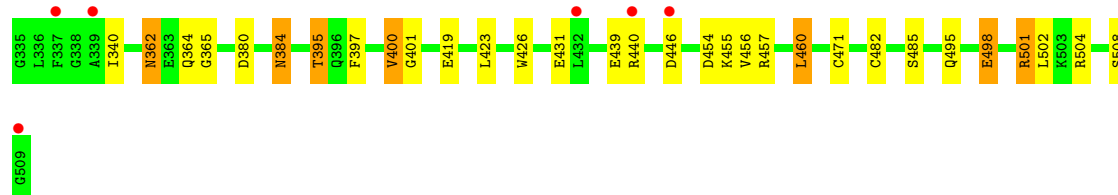
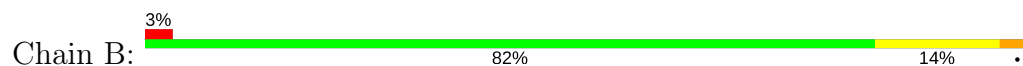


#### • Molecule 1: Hemagglutinin

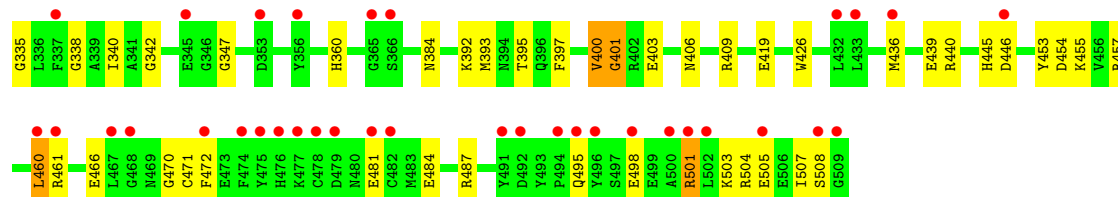
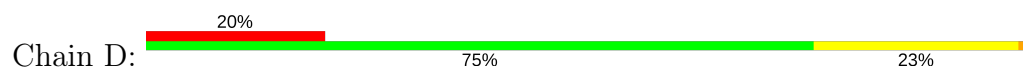




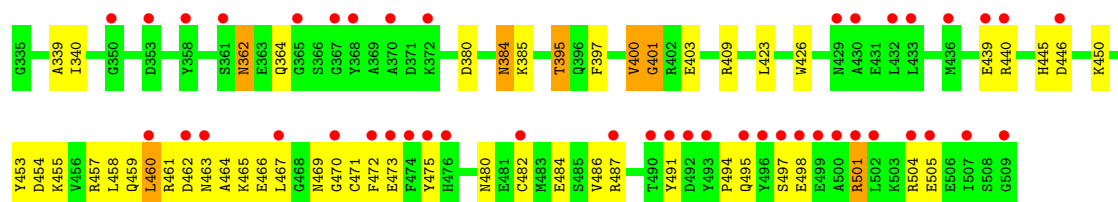
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.76Å 243.85Å 71.61Å 90.00° 110.01° 90.00°	Depositor
Resolution (Å)	35.07 – 2.50 35.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (35.07-2.50) 99.5 (35.61-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.215 , 0.251 0.213 , 0.252	Depositor DCC
$R_{free}$ test set	3718 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12221	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	0.30	0/2621	0.55	0/3558
1	C	0.29	0/2621	0.53	0/3558
1	E	0.29	0/2621	0.55	1/3558 (0.0%)
2	B	0.37	0/1443	0.51	1/1939 (0.1%)
2	D	0.37	0/1443	0.48	1/1939 (0.1%)
2	F	0.36	0/1443	0.50	0/1939
All	All	0.32	0/12192	0.53	3/16491 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	460	LEU	CB-CA-C	7.13	123.75	110.20
1	E	182	ILE	CB-CA-C	-5.44	100.72	111.60
2	D	460	LEU	CB-CA-C	5.20	120.09	110.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2559	0	2513	61	0
1	C	2559	0	2513	60	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2559	0	2513	69	1
2	B	1416	0	1319	23	0
2	D	1416	0	1319	33	0
2	F	1416	0	1319	42	0
3	A	14	0	13	0	0
3	C	14	0	13	0	0
3	E	14	0	13	0	0
4	A	28	0	25	1	0
4	C	28	0	25	0	0
4	E	28	0	25	0	0
5	A	53	0	0	8	0
5	B	13	0	0	2	0
5	C	42	0	0	4	0
5	D	17	0	0	6	0
5	E	33	0	0	6	0
5	F	12	0	0	2	0
All	All	12221	0	11610	253	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 11.

All (253) 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:206:THR:HG22	1:E:208:THR:H	1.37	0.89
4:A:602:NAG:O3	5:A:753:HOH:O	1.88	0.89
1:E:58:ASP:OD1	5:E:726:HOH:O	1.90	0.88
1:E:38:GLU:OE1	5:E:725:HOH:O	1.92	0.87
1:C:138:ALA:O	5:C:705:HOH:O	1.94	0.84
2:D:461:ARG:NH2	2:F:466:GLU:O	2.10	0.84
1:A:206:THR:HG22	1:A:208:THR:H	1.42	0.83
1:A:284:THR:HG22	1:A:286:MET:H	1.44	0.82
1:A:182:ILE:HD11	1:A:213:LEU:HD13	1.63	0.81
1:E:318:ALA:O	5:E:730:HOH:O	1.98	0.81
1:A:38:GLU:OE1	5:A:727:HOH:O	1.98	0.80
1:A:199:THR:OG1	5:A:752:HOH:O	1.99	0.80
1:E:57:ARG:NH1	1:E:72:ASP:OD1	2.15	0.79
1:C:206:THR:HG22	1:C:208:THR:H	1.48	0.78
1:E:67:GLY:HA3	1:E:149:ARG:HG2	1.66	0.77
1:C:135:VAL:HG22	1:C:146:SER:HA	1.67	0.77
1:E:284:THR:HG22	1:E:286:MET:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:OE1	5:C:734:HOH:O	2.03	0.76
2:B:419:GLU:O	5:B:608:HOH:O	2.04	0.75
1:C:186:ASN:N	1:C:186:ASN:OD1	2.20	0.74
1:C:284:THR:HG22	1:C:286:MET:H	1.50	0.74
1:E:280:THR:HG21	1:E:288:ALA:HB1	1.69	0.74
2:F:403:GLU:OE2	5:F:604:HOH:O	2.05	0.74
1:E:186:ASN:OD1	1:E:186:ASN:N	2.21	0.74
1:A:22:THR:HG22	1:A:24:MET:H	1.53	0.73
1:A:135:VAL:HG22	1:A:146:SER:HA	1.70	0.73
1:A:186:ASN:OD1	1:A:186:ASN:N	2.19	0.72
1:C:280:THR:HG21	1:C:288:ALA:HB1	1.72	0.72
2:D:347:GLY:O	5:D:607:HOH:O	2.08	0.71
1:E:25:GLU:OE2	1:E:322:ARG:NH2	2.22	0.70
2:D:453:TYR:HE1	2:D:470:GLY:HA2	1.56	0.70
1:E:22:THR:HG22	1:E:24:MET:H	1.58	0.69
1:C:130:GLU:O	5:C:703:HOH:O	2.11	0.69
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.75	0.69
1:A:125:SER:OG	1:A:166:ARG:NH2	2.26	0.68
2:F:484:GLU:HG2	2:F:487:ARG:HH12	1.58	0.67
1:A:265:ASP:OD2	2:D:409:ARG:NH2	2.27	0.67
1:C:25:GLU:OE2	1:C:322:ARG:NH2	2.28	0.67
2:F:494:PRO:HA	2:F:497:SER:HB3	1.75	0.67
1:C:182:ILE:HD11	1:C:213:LEU:HD13	1.77	0.66
1:A:301:LEU:HA	2:B:400:VAL:HG22	1.77	0.66
1:C:216:ARG:O	1:C:220:ARG:NH2	2.30	0.65
1:C:22:THR:HG22	1:C:24:MET:H	1.61	0.65
2:B:362:ASN:OD1	2:B:364:GLN:NE2	2.30	0.65
1:A:25:GLU:OE2	1:A:322:ARG:NH2	2.29	0.64
1:C:284:THR:HB	1:C:287:GLY:O	1.97	0.64
1:E:39:LYS:NZ	1:E:313:ASN:O	2.27	0.64
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.79	0.64
2:D:453:TYR:CE1	2:D:470:GLY:HA2	2.32	0.64
2:F:466:GLU:HG2	2:F:472:PHE:HE2	1.63	0.63
1:E:8:CYS:HA	2:F:471:CYS:HA	1.79	0.62
1:A:212:ARG:NH1	5:A:732:HOH:O	2.14	0.62
1:C:39:LYS:NZ	1:C:313:ASN:O	2.22	0.62
1:A:289:ILE:HG22	1:A:291:SER:HB3	1.81	0.62
1:A:39:LYS:NZ	1:A:313:ASN:O	2.21	0.61
2:B:508:SER:OG	2:F:501:ARG:NE	2.28	0.61
1:E:145:SER:OG	5:E:732:HOH:O	2.16	0.61
2:D:440:ARG:NH1	2:F:439:GLU:OE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:GLY:HA3	1:C:149:ARG:HB2	1.81	0.60
2:B:431:GLU:OE1	5:B:605:HOH:O	2.17	0.60
2:D:393:MET:O	5:D:617:HOH:O	2.17	0.60
1:C:120:ILE:HG23	1:C:121:ILE:HG13	1.84	0.60
1:C:289:ILE:HG22	1:C:291:SER:HB3	1.83	0.59
2:D:360:HIS:HD2	2:D:487:ARG:HH21	1.50	0.59
1:A:280:THR:HG21	1:A:288:ALA:HB1	1.84	0.59
1:A:20:VAL:HG11	1:A:318:ALA:HB2	1.82	0.59
1:E:125:SER:OG	1:E:166:ARG:NH2	2.35	0.59
2:F:364:GLN:HE22	2:F:480:ASN:H	1.50	0.59
1:A:191:GLN:OE1	1:A:250:ASN:ND2	2.34	0.59
1:A:314:ARG:HG3	1:A:316:VAL:HG23	1.85	0.59
1:A:31:THR:HB	1:A:321:LEU:H	1.68	0.58
1:C:23:ILE:HG22	1:C:24:MET:HG3	1.86	0.58
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.86	0.57
1:A:206:THR:HG21	5:A:708:HOH:O	2.03	0.57
2:D:335:GLY:N	5:D:601:HOH:O	2.38	0.57
2:D:466:GLU:HG2	2:D:472:PHE:HE2	1.68	0.57
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.87	0.56
1:C:22:THR:HG23	2:D:439:GLU:HB2	1.86	0.56
1:E:23:ILE:HG22	1:E:24:MET:HG3	1.86	0.56
1:A:36:ILE:HG12	1:A:317:LEU:HD22	1.88	0.56
1:A:11:TYR:CZ	2:B:340:ILE:HG23	2.41	0.56
1:A:284:THR:HB	1:A:287:GLY:O	2.06	0.56
2:B:440:ARG:HH21	2:F:440:ARG:HH21	1.54	0.56
1:E:182:ILE:CD1	1:E:213:LEU:HD13	2.36	0.55
1:E:206:THR:HB	1:E:209:LEU:HB3	1.88	0.55
1:A:23:ILE:HG22	1:A:24:MET:HG3	1.89	0.55
2:F:362:ASN:H	2:F:362:ASN:HD22	1.55	0.55
1:E:284:THR:HB	1:E:287:GLY:O	2.06	0.55
2:F:501:ARG:HD3	2:F:505:GLU:HG3	1.88	0.55
1:A:164:ILE:O	1:A:246:GLU:HA	2.07	0.55
1:E:120:ILE:HD13	1:E:257:ALA:HB3	1.89	0.54
1:E:289:ILE:HD11	1:E:298:ILE:HG13	1.89	0.54
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.90	0.54
1:E:289:ILE:HG22	1:E:291:SER:HB3	1.89	0.54
1:C:301:LEU:HA	2:D:400:VAL:HG22	1.89	0.54
1:E:116:GLU:HB3	1:E:259:LYS:HB2	1.90	0.54
2:F:466:GLU:HG2	2:F:472:PHE:CE2	2.41	0.54
1:C:304:GLY:HA2	2:D:397:PHE:CD1	2.43	0.53
1:A:22:THR:HG23	2:B:439:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:THR:HG21	1:C:250:ASN:OD1	2.08	0.53
1:E:11:TYR:CZ	2:F:340:ILE:HG23	2.44	0.53
1:A:200:THR:HG21	1:A:250:ASN:OD1	2.09	0.53
1:A:73:GLU:OE2	1:A:141:TYR:OH	2.24	0.53
1:C:200:THR:HA	1:C:248:ASN:HD22	1.74	0.53
1:E:182:ILE:HD11	1:E:213:LEU:HD13	1.91	0.53
2:D:466:GLU:HG2	2:D:472:PHE:CE2	2.44	0.52
2:D:454:ASP:OD1	2:D:457:ARG:NH1	2.42	0.52
2:B:362:ASN:ND2	2:B:365:GLY:O	2.43	0.52
1:A:197:ASN:ND2	5:A:712:HOH:O	1.92	0.52
1:E:148:PHE:HB2	1:E:151:VAL:HG12	1.92	0.52
1:E:182:ILE:HD11	1:E:233:PHE:CE1	2.45	0.52
2:D:403:GLU:OE2	5:D:612:HOH:O	2.18	0.52
1:A:102:TYR:CE2	1:A:106:LYS:HD2	2.45	0.51
1:C:102:TYR:CZ	1:C:106:LYS:HD2	2.46	0.51
1:C:280:THR:HB	1:C:282:CYS:H	1.75	0.51
2:B:362:ASN:HD22	2:B:362:ASN:H	1.59	0.51
2:F:482:CYS:O	2:F:486:VAL:HG23	2.11	0.51
1:E:320:GLY:O	2:F:445:HIS:NE2	2.44	0.51
1:E:301:LEU:HA	2:F:400:VAL:HG22	1.93	0.51
1:E:135:VAL:HG22	1:E:146:SER:HA	1.92	0.50
1:E:200:THR:HG21	1:E:250:ASN:OD1	2.10	0.50
1:A:52:LYS:HG2	1:A:53:PRO:HD2	1.93	0.50
1:E:53:PRO:HB3	1:E:82:TYR:CE2	2.47	0.50
1:E:133:LEU:N	5:E:714:HOH:O	2.44	0.50
2:F:463:ASN:ND2	2:F:491:TYR:OH	2.26	0.50
1:E:164:ILE:O	1:E:246:GLU:HA	2.12	0.50
1:E:156:LYS:NZ	1:E:196:GLN:OE1	2.42	0.49
1:A:206:THR:HB	1:A:209:LEU:HB3	1.93	0.49
1:A:212:ARG:HB2	1:C:216:ARG:HG2	1.93	0.49
1:E:216:ARG:O	1:E:220:ARG:NH2	2.45	0.49
1:C:125:SER:CB	1:C:166:ARG:HH22	2.25	0.49
2:B:508:SER:HG	2:F:501:ARG:HE	1.58	0.49
2:F:453:TYR:CE1	2:F:470:GLY:HA2	2.47	0.49
1:A:159:SER:O	1:A:196:GLN:HG3	2.12	0.49
1:C:206:THR:HB	1:C:209:LEU:HB3	1.94	0.49
1:C:164:ILE:O	1:C:246:GLU:HA	2.12	0.49
2:F:364:GLN:HE22	2:F:480:ASN:N	2.09	0.49
2:D:481:GLU:O	2:D:484:GLU:HB3	2.13	0.49
2:F:339:ALA:HB2	2:F:450:LYS:HB2	1.94	0.48
2:B:454:ASP:OD1	2:B:457:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:380:ASP:O	2:F:384:ASN:HB2	2.14	0.48
2:F:454:ASP:OD1	2:F:457:ARG:NH1	2.45	0.48
2:B:482:CYS:O	2:B:485:SER:OG	2.21	0.48
1:C:125:SER:HB2	1:C:166:ARG:HH22	1.79	0.48
1:E:211:GLN:OE1	1:E:213:LEU:HD11	2.14	0.48
1:C:308:LYS:HD2	2:D:426:TRP:CE2	2.49	0.48
2:F:465:LYS:HB2	2:F:475:TYR:CZ	2.48	0.48
1:E:14:ASN:O	1:E:323:ASN:ND2	2.42	0.48
2:D:505:GLU:HA	2:D:508:SER:HB3	1.95	0.47
1:C:323:ASN:O	1:C:325:PRO:HD3	2.15	0.47
2:D:501:ARG:HD3	2:D:505:GLU:HG3	1.97	0.47
1:A:200:THR:HG22	1:A:215:PRO:HG3	1.97	0.47
1:C:102:TYR:CE2	1:C:106:LYS:HD2	2.50	0.47
1:C:53:PRO:HB3	1:C:82:TYR:CE2	2.50	0.47
1:E:111:ARG:HH11	1:E:266:SER:HB3	1.79	0.47
1:E:120:ILE:HG13	1:E:168:TYR:CE1	2.50	0.47
1:E:321:LEU:HB3	2:F:445:HIS:CD2	2.50	0.47
1:C:70:MET:SD	1:C:140:PRO:HD2	2.55	0.47
2:D:503:LYS:O	2:D:507:ILE:HG12	2.15	0.47
2:F:462:ASP:O	2:F:504:ARG:NH1	2.48	0.47
1:A:99:PHE:HB3	1:A:102:TYR:HB2	1.97	0.46
1:C:73:GLU:OE2	1:C:141:TYR:OH	2.19	0.46
2:F:460:LEU:HD13	2:F:464:ALA:HB3	1.98	0.46
1:A:211:GLN:NE2	5:A:725:HOH:O	2.37	0.46
1:A:308:LYS:HD2	2:B:426:TRP:CE2	2.51	0.46
1:E:296:HIS:CD2	1:E:307:PRO:HG2	2.51	0.46
1:A:211:GLN:OE1	1:A:213:LEU:HD11	2.14	0.46
1:E:57:ARG:O	1:E:86:LYS:HG3	2.14	0.46
2:F:362:ASN:OD1	2:F:364:GLN:NE2	2.48	0.46
1:C:99:PHE:HB3	1:C:102:TYR:HB2	1.98	0.46
1:C:182:ILE:HD11	1:C:213:LEU:CD1	2.44	0.46
1:C:291:SER:HA	5:C:734:HOH:O	2.16	0.46
1:A:102:TYR:CZ	1:A:106:LYS:HD2	2.50	0.46
1:C:36:ILE:HG12	1:C:317:LEU:HD22	1.97	0.45
2:D:360:HIS:CD2	2:D:487:ARG:HH21	2.31	0.45
1:E:125:SER:C	1:E:166:ARG:HH22	2.20	0.45
1:C:120:ILE:HD11	1:C:168:TYR:CZ	2.50	0.45
1:A:23:ILE:HG23	2:F:385:LYS:HG3	1.98	0.45
1:E:120:ILE:HG23	1:E:121:ILE:HG13	1.99	0.45
1:E:280:THR:HB	1:E:282:CYS:H	1.82	0.45
2:F:454:ASP:O	2:F:458:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.52	0.45
2:B:498:GLU:O	2:B:502:LEU:HG	2.16	0.45
1:E:294:PRO:HG2	1:E:295:PHE:CD1	2.51	0.45
1:A:289:ILE:CG2	1:A:291:SER:HB3	2.46	0.45
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.16	0.45
1:E:31:THR:HB	1:E:321:LEU:H	1.82	0.45
2:F:457:ARG:HD2	2:F:466:GLU:OE2	2.17	0.45
1:C:24:MET:HE2	2:D:439:GLU:OE1	2.17	0.45
1:C:289:ILE:HD11	1:C:298:ILE:HG13	1.98	0.44
1:E:25:GLU:CD	1:E:322:ARG:HH22	2.17	0.44
1:A:11:TYR:HB2	1:A:321:LEU:HD11	2.00	0.44
1:A:182:ILE:HG23	1:A:202:ILE:HD12	1.99	0.44
1:A:216:ARG:HG2	1:E:212:ARG:HB2	1.99	0.44
1:A:304:GLY:HA2	2:B:397:PHE:CE1	2.53	0.44
1:E:65:LEU:HD11	1:E:109:LEU:HD11	1.98	0.44
1:E:102:TYR:CE2	1:E:106:LYS:HD2	2.52	0.44
1:E:308:LYS:HD2	2:F:426:TRP:CE2	2.53	0.44
1:A:8:CYS:HA	2:B:471:CYS:HA	2.00	0.44
1:C:67:GLY:CA	1:C:149:ARG:H	2.30	0.44
1:C:67:GLY:HA3	1:C:149:ARG:H	1.82	0.44
2:D:406:ASN:O	5:D:615:HOH:O	2.21	0.44
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.18	0.44
2:F:484:GLU:HG2	2:F:487:ARG:NH1	2.30	0.44
2:F:467:LEU:HD21	2:F:473:GLU:HB2	2.00	0.44
1:C:20:VAL:HG21	1:C:318:ALA:HB2	2.00	0.43
1:E:142:GLN:C	1:E:144:LYS:H	2.22	0.43
2:F:469:ASN:HB2	2:F:471:CYS:HB2	2.00	0.43
1:C:262:LYS:NZ	1:C:264:GLY:O	2.46	0.43
1:E:65:LEU:HD11	1:E:109:LEU:CD1	2.48	0.43
1:A:142:GLN:N	5:A:704:HOH:O	2.20	0.43
1:C:148:PHE:HB2	1:C:151:VAL:HG12	2.00	0.42
1:E:304:GLY:HA2	2:F:397:PHE:CD1	2.53	0.42
1:E:22:THR:HG23	2:F:439:GLU:HB2	1.99	0.42
1:A:67:GLY:HA3	1:A:149:ARG:HB2	2.02	0.42
1:C:78:PRO:O	1:C:114:HIS:HA	2.19	0.42
1:E:308:LYS:HD2	2:F:426:TRP:NE1	2.35	0.42
2:F:400:VAL:HA	2:F:401:GLY:HA3	1.68	0.42
1:C:11:TYR:CZ	2:D:340:ILE:HG23	2.54	0.42
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.92	0.42
1:A:25:GLU:CD	1:A:322:ARG:HH22	2.20	0.42
1:A:9:ILE:HD11	2:B:456:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:ARG:HH22	2:D:436:MET:HB3	1.84	0.42
1:C:68:ASN:HA	1:C:69:PRO:HD3	1.85	0.42
2:B:395:THR:O	2:B:395:THR:OG1	2.38	0.42
1:C:321:LEU:HB3	2:D:445:HIS:CD2	2.54	0.42
2:D:392:LYS:HD3	2:D:392:LYS:HA	1.91	0.42
1:E:206:THR:HG23	1:E:241:ASP:OD2	2.20	0.42
1:C:31:THR:HB	1:C:321:LEU:H	1.85	0.41
2:D:338:GLY:O	2:D:342:GLY:HA3	2.20	0.41
2:D:400:VAL:HA	2:D:401:GLY:HA3	1.70	0.41
2:F:395:THR:OG1	2:F:395:THR:O	2.38	0.41
1:A:134:GLY:HA3	1:A:153:TRP:HB3	2.01	0.41
1:A:206:THR:HG23	1:A:241:ASP:OD2	2.21	0.41
1:C:212:ARG:HB2	1:E:216:ARG:HG2	2.01	0.41
1:C:47:ASP:OD1	1:C:275:TYR:OH	2.34	0.41
1:E:314:ARG:HE	1:E:314:ARG:HB3	1.57	0.41
1:A:304:GLY:HA2	2:B:397:PHE:CD1	2.55	0.41
1:E:42:ASN:ND2	1:E:278:CYS:SG	2.94	0.41
2:D:419:GLU:OE2	5:D:613:HOH:O	2.22	0.41
1:E:212:ARG:NE	5:E:703:HOH:O	1.92	0.41
2:B:501:ARG:HG2	2:B:504:ARG:NH2	2.36	0.41
2:D:501:ARG:HG2	2:D:504:ARG:NH2	2.36	0.41
1:E:95:TYR:CE1	1:E:226:LEU:HD13	2.56	0.41
1:A:159:SER:C	1:A:196:GLN:HG3	2.42	0.41
1:E:182:ILE:HG12	1:E:231:GLU:HB3	2.03	0.40
1:C:159:SER:O	1:C:196:GLN:HG3	2.21	0.40
1:C:8:CYS:HA	2:D:471:CYS:HA	2.03	0.40
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.22	0.40
1:E:317:LEU:HA	1:E:317:LEU:HD12	1.83	0.40
1:A:68:ASN:HA	1:A:69:PRO:HD3	1.91	0.40
2:B:380:ASP:O	2:B:384:ASN:HB2	2.22	0.40
2:F:409:ARG:NH1	5:F:611:HOH:O	2.55	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)
1:C:141:TYR:O	1:E:144:LYS:NZ[1_655]	2.14	0.06



## 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	320/322 (99%)	297 (93%)	22 (7%)	1 (0%)	44	66
1	C	320/322 (99%)	301 (94%)	18 (6%)	1 (0%)	44	66
1	E	320/322 (99%)	299 (93%)	20 (6%)	1 (0%)	44	66
2	B	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	28	48
2	D	173/175 (99%)	165 (95%)	7 (4%)	1 (1%)	28	48
2	F	173/175 (99%)	166 (96%)	6 (4%)	1 (1%)	28	48
All	All	1479/1491 (99%)	1392 (94%)	81 (6%)	6 (0%)	38	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	C	277	ASN
1	E	277	ASN
2	B	401	GLY
2	D	401	GLY
2	F	401	GLY

### 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	290/290 (100%)	258 (89%)	32 (11%)	7	13
1	C	290/290 (100%)	257 (89%)	33 (11%)	7	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	290/290 (100%)	256 (88%)	34 (12%)	6	12
2	B	149/149 (100%)	138 (93%)	11 (7%)	16	30
2	D	149/149 (100%)	140 (94%)	9 (6%)	22	41
2	F	149/149 (100%)	136 (91%)	13 (9%)	12	23
All	All	1317/1317 (100%)	1185 (90%)	132 (10%)	9	17

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	23	ILE
1	A	30	VAL
1	A	36	ILE
1	A	48	LEU
1	A	75	ILE
1	A	118	ILE
1	A	135	VAL
1	A	149	ARG
1	A	151	VAL
1	A	160	THR
1	A	173	GLN
1	A	182	ILE
1	A	186	ASN
1	A	191	GLN
1	A	195	TYR
1	A	200	THR
1	A	206	THR
1	A	208	THR
1	A	211	GLN
1	A	216	ARG
1	A	219	THR
1	A	227	SER
1	A	230	MET
1	A	235	THR
1	A	265	ASP
1	A	280	THR
1	A	308	LYS
1	A	310	VAL
1	A	317	LEU
1	A	319	ILE
1	A	321	LEU

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Mol	Chain	Res	Type
2	B	362	ASN
2	B	384	ASN
2	B	395	THR
2	B	400	VAL
2	B	423	LEU
2	B	446	ASP
2	B	455	LYS
2	B	460	LEU
2	B	495	GLN
2	B	498	GLU
2	B	501	ARG
1	C	7	ILE
1	C	20	VAL
1	C	23	ILE
1	C	30	VAL
1	C	36	ILE
1	C	48	LEU
1	C	70	MET
1	C	75	ILE
1	C	118	ILE
1	C	135	VAL
1	C	149	ARG
1	C	151	VAL
1	C	160	THR
1	C	173	GLN
1	C	182	ILE
1	C	186	ASN
1	C	191	GLN
1	C	195	TYR
1	C	200	THR
1	C	206	THR
1	C	208	THR
1	C	211	GLN
1	C	216	ARG
1	C	219	THR
1	C	227	SER
1	C	230	MET
1	C	235	THR
1	C	265	ASP
1	C	280	THR
1	C	308	LYS
1	C	317	LEU

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Mol	Chain	Res	Type
1	C	319	ILE
1	C	321	LEU
2	D	384	ASN
2	D	395	THR
2	D	400	VAL
2	D	446	ASP
2	D	455	LYS
2	D	460	LEU
2	D	495	GLN
2	D	498	GLU
2	D	501	ARG
1	E	7	ILE
1	E	20	VAL
1	E	23	ILE
1	E	30	VAL
1	E	36	ILE
1	E	48	LEU
1	E	75	ILE
1	E	118	ILE
1	E	120	ILE
1	E	135	VAL
1	E	149	ARG
1	E	151	VAL
1	E	160	THR
1	E	173	GLN
1	E	182	ILE
1	E	186	ASN
1	E	191	GLN
1	E	195	TYR
1	E	200	THR
1	E	206	THR
1	E	208	THR
1	E	211	GLN
1	E	216	ARG
1	E	219	THR
1	E	227	SER
1	E	230	MET
1	E	235	THR
1	E	265	ASP
1	E	280	THR
1	E	308	LYS
1	E	310	VAL

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Mol	Chain	Res	Type
1	E	317	LEU
1	E	319	ILE
1	E	321	LEU
2	F	362	ASN
2	F	384	ASN
2	F	395	THR
2	F	400	VAL
2	F	423	LEU
2	F	446	ASP
2	F	455	LYS
2	F	459	GLN
2	F	460	LEU
2	F	461	ARG
2	F	495	GLN
2	F	498	GLU
2	F	501	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	364	GLN
1	C	248	ASN
2	D	360	HIS
2	F	364	GLN
2	F	429	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

6 carbohydrates 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
4	NAG	A	602	1,4	14,14,15	0.52	0	15,19,21	0.67	0
4	NAG	A	603	4	14,14,15	0.45	0	15,19,21	0.87	0
4	NAG	C	602	1,4	14,14,15	0.55	0	15,19,21	0.67	0
4	NAG	C	603	4	14,14,15	0.55	0	15,19,21	0.71	0
4	NAG	E	602	1,4	14,14,15	0.52	0	15,19,21	0.83	0
4	NAG	E	603	4	14,14,15	0.43	0	15,19,21	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	602	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	603	4	-	0/6/23/26	0/1/1/1
4	NAG	C	602	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	603	4	-	0/6/23/26	0/1/1/1
4	NAG	E	602	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	603	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	NAG	1	0

## 5.6 Ligand geometry ⓘ

3 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	601	1	14,14,15	0.47	0	15,19,21	0.74	0
3	NAG	C	601	1	14,14,15	0.50	0	15,19,21	0.83	0
3	NAG	E	601	1	14,14,15	0.42	0	15,19,21	1.41	2 (13%)

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	601	1	-	0/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	NAG	C4-C3-C2	-2.29	107.66	111.02
3	E	601	NAG	C1-O5-C5	4.15	117.88	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 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	322/322 (100%)	0.11	3 (0%) 84 85	20, 44, 72, 119	0
1	C	322/322 (100%)	0.21	12 (3%) 42 44	23, 51, 89, 121	0
1	E	322/322 (100%)	0.31	14 (4%) 36 38	30, 56, 97, 143	0
2	B	175/175 (100%)	0.47	6 (3%) 46 48	30, 57, 88, 140	0
2	D	175/175 (100%)	1.06	35 (20%) 1 1	25, 75, 123, 191	0
2	F	175/175 (100%)	1.28	45 (25%) 1 0	29, 84, 147, 196	0
All	All	1491/1491 (100%)	0.47	115 (7%) 14 14	20, 54, 115, 196	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	509	GLY	8.3
1	C	325	PRO	7.6
2	B	509	GLY	7.0
2	D	353	ASP	6.3
2	F	475	TYR	6.1
2	F	507	ILE	5.8
2	D	477	LYS	5.7
2	F	474	PHE	5.5
2	D	505	GLU	5.5
2	F	501	ARG	5.4
2	F	509	GLY	5.4
2	D	498	GLU	5.4
2	F	504	ARG	5.3
1	C	16	SER	5.3
2	F	487	ARG	4.9
2	F	460	LEU	4.7
2	F	350	GLY	4.7
2	F	492	ASP	4.4
1	E	15	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	73	GLU	4.0
2	F	472	PHE	3.9
1	C	7	ILE	3.9
2	D	481	GLU	3.9
2	D	491	TYR	3.9
2	D	474	PHE	3.8
2	F	490	THR	3.8
1	C	158	ASP	3.8
1	E	7	ILE	3.7
2	F	365	GLY	3.7
2	F	496	TYR	3.7
2	D	482	CYS	3.7
2	F	482	CYS	3.6
2	D	492	ASP	3.6
2	D	475	TYR	3.5
2	F	436	MET	3.5
1	E	291	SER	3.3
2	F	473	GLU	3.2
2	F	463	ASN	3.2
2	D	460	LEU	3.2
2	D	502	LEU	3.1
2	D	496	TYR	3.1
2	F	372	LYS	3.1
2	F	470	GLY	3.1
1	E	325	PRO	3.0
2	F	493	TYR	3.0
2	D	356	TYR	3.0
2	D	365	GLY	3.0
1	E	4	GLN	2.9
2	F	505	GLU	2.8
2	F	432	LEU	2.8
2	D	345	GLU	2.7
2	D	467	LEU	2.7
2	F	499	GLU	2.7
2	F	495	GLN	2.7
2	D	494	PRO	2.7
1	C	274	GLU	2.6
2	F	498	GLU	2.6
2	D	468	GLY	2.6
2	D	478	CYS	2.6
2	D	337	PHE	2.6
1	E	263	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	440	ARG	2.6
1	C	14	ASN	2.6
2	B	440	ARG	2.6
2	D	500	ALA	2.6
2	D	476	HIS	2.6
1	C	133	LEU	2.5
1	E	72	ASP	2.5
2	B	446	ASP	2.5
2	F	367	GLY	2.5
1	E	128	SER	2.5
1	A	314	ARG	2.5
1	A	291	SER	2.4
2	F	502	LEU	2.4
2	F	491	TYR	2.4
2	F	429	ASN	2.4
1	E	74	PHE	2.4
2	F	368	TYR	2.4
2	F	430	ALA	2.4
1	A	44	LYS	2.4
2	D	446	ASP	2.4
2	D	501	ARG	2.4
1	C	129	HIS	2.3
2	F	361	SER	2.3
1	C	157	LYS	2.3
1	E	50	GLY	2.3
2	D	366	SER	2.3
2	D	479	ASP	2.3
2	D	436	MET	2.3
2	F	476	HIS	2.3
2	D	433	LEU	2.3
1	E	45	LEU	2.2
2	D	508	SER	2.2
2	F	497	SER	2.2
1	C	314	ARG	2.2
1	C	6	GLN	2.2
2	B	339	ALA	2.2
2	F	433	LEU	2.2
2	D	432	LEU	2.2
2	F	462	ASP	2.2
2	D	461	ARG	2.1
2	D	472	PHE	2.1
2	F	467	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	158	ASP	2.1
2	F	446	ASP	2.1
1	E	324	SER	2.1
2	F	500	ALA	2.1
1	C	8	CYS	2.1
2	F	370	ALA	2.1
2	F	353	ASP	2.0
2	F	439	GLU	2.0
2	D	495	GLN	2.0
2	F	358	TYR	2.0
2	B	337	PHE	2.0
2	B	432	LEU	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](#)

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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	E	602	14/15	0.93	0.26	1.88	46,62,71,78	0
4	NAG	C	602	14/15	0.91	0.15	-0.28	47,71,85,85	0
4	NAG	A	602	14/15	0.95	0.10	-	28,43,53,55	0
4	NAG	A	603	14/15	0.81	0.21	-	52,56,66,72	0
4	NAG	E	603	14/15	0.73	0.51	-	73,89,97,99	0
4	NAG	C	603	14/15	0.88	0.36	-	80,89,92,96	0

## 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	C	601	14/15	0.83	0.20	-	79,85,90,90	0
3	NAG	A	601	14/15	0.83	0.24	-	78,82,87,87	0
3	NAG	E	601	14/15	0.80	0.33	-	85,92,96,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.