



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:04 PM GMT

PDB ID : 4KDN
Title : Crystal structure of the hemagglutinin of ferret-transmissible H5N1 virus in complex with avian receptor analog LSTa
Authors : Lu, X.; Shi, Y.; Zhang, W.; Zhang, Y.; Qi, J.; Gao, G.F.
Deposited on : 2013-04-25
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
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

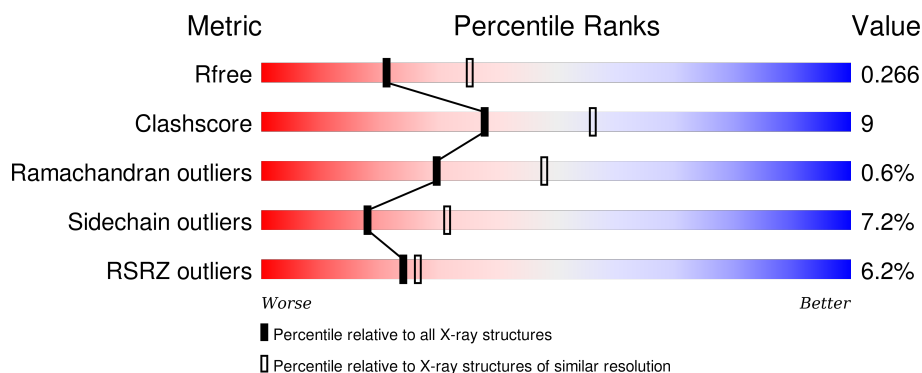
1 Overall quality at a glance

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}	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (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 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	322	<div> <div></div> <div>74% 21% 5%</div> </div>
1	C	322	<div> <div></div> <div>72% 23% 5%</div> </div>
1	E	322	<div> <div>3%</div> <div>74% 22% 5%</div> </div>
2	B	175	<div> <div>9%</div> <div>85% 13% .</div> </div>
2	D	175	<div> <div>18%</div> <div>79% 19% .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	175	

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
5	SIA	C	604	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12269 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.

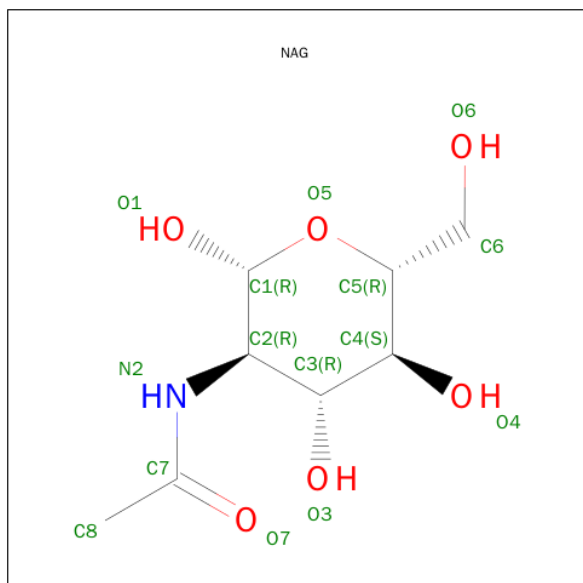
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

Continued on next page...

Continued from previous page...

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: $C_8H_{15}NO_6$).

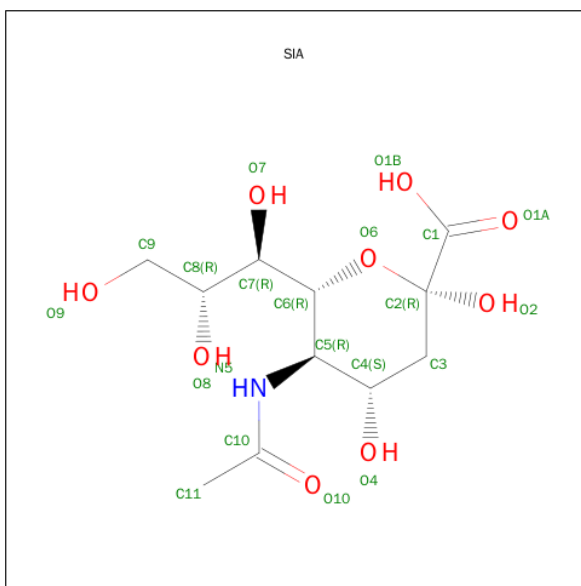


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

- 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 SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	11	1	9		
5	C	1	Total	C	N	O	0	0
			21	11	1	9		

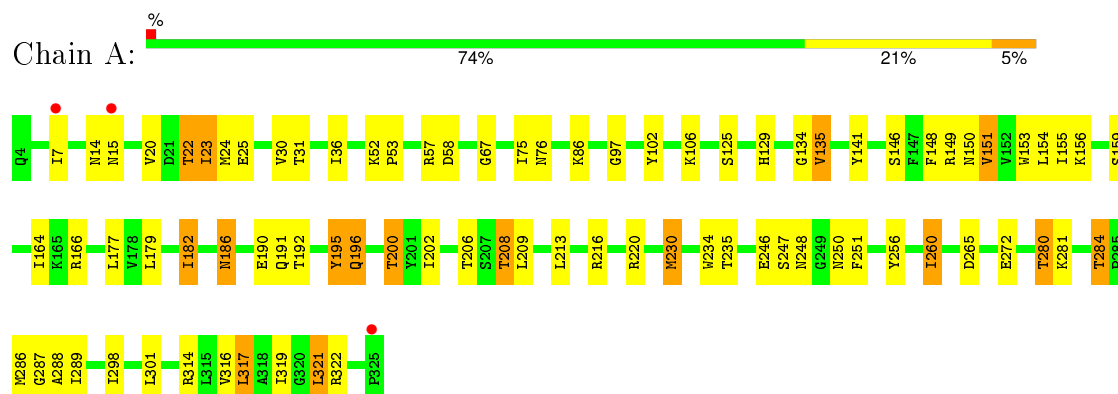
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	66	Total	O	0	0
			66	66		
6	B	20	Total	O	0	0
			20	20		
6	C	37	Total	O	0	0
			37	37		
6	D	13	Total	O	0	0
			13	13		
6	E	30	Total	O	0	0
			30	30		
6	F	10	Total	O	0	0
			10	10		

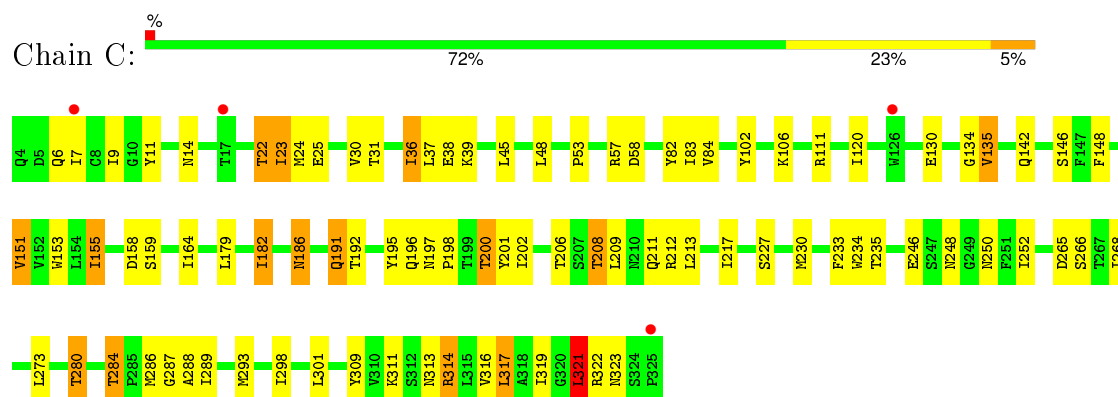
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

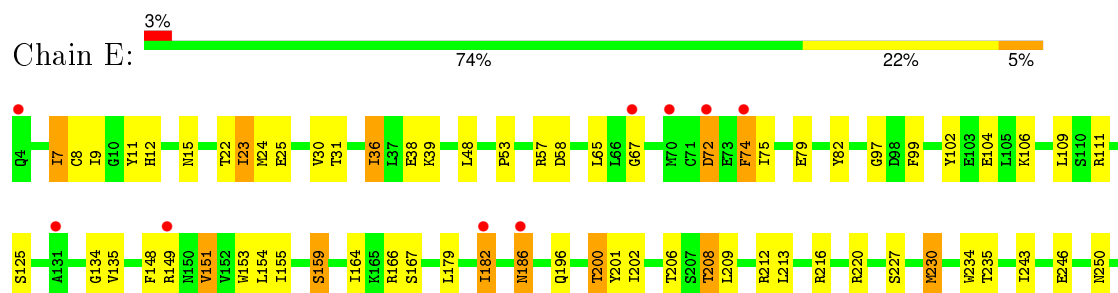
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

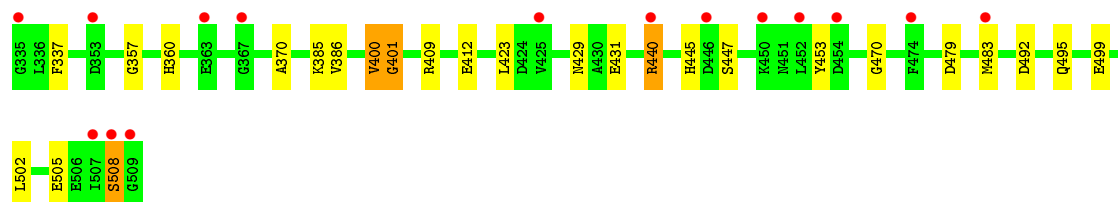
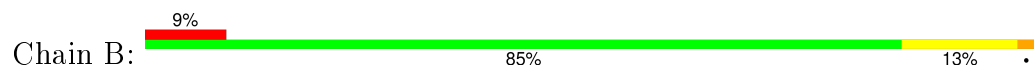


• Molecule 1: Hemagglutinin

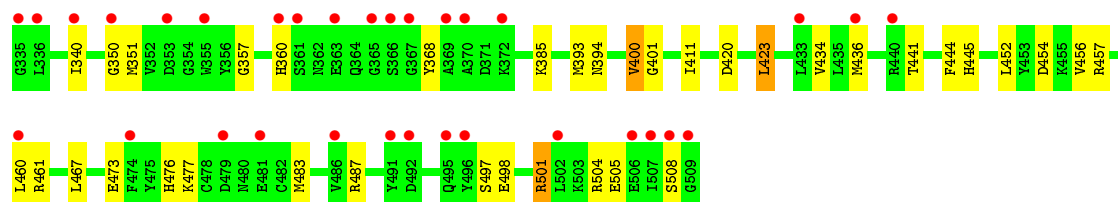
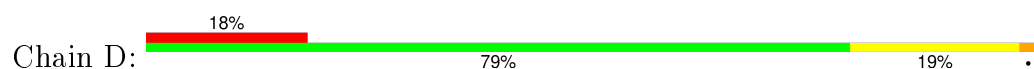




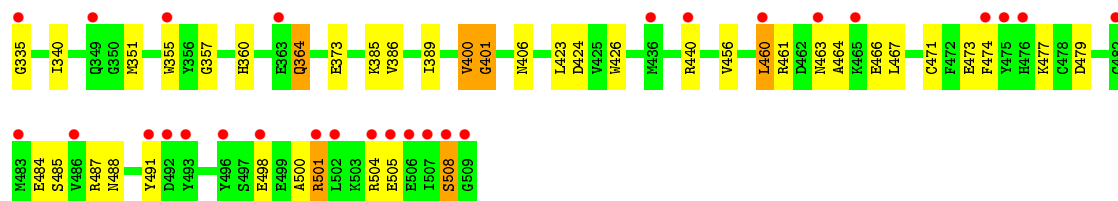
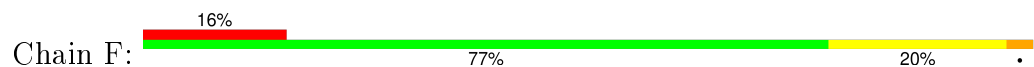
● Molecule 2: Hemagglutinin



● 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, α , β , γ	66.68Å 245.16Å 68.56Å 90.00° 113.75° 90.00°	Depositor
Resolution (Å)	35.37 – 2.48 35.37 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.1 (35.37-2.48) 97.1 (35.37-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.223 , 0.259 0.230 , 0.266	Depositor DCC
R_{free} test set	3468 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.9	EDS
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 68647 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12269	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SIA, 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	0.34	0/2621	0.58	1/3558 (0.0%)
1	C	0.31	0/2621	0.58	2/3558 (0.1%)
1	E	0.29	0/2621	0.54	0/3558
2	B	0.30	0/1443	0.47	0/1939
2	D	0.29	0/1443	0.47	0/1939
2	F	0.30	0/1443	0.49	1/1939 (0.1%)
All	All	0.31	0/12192	0.54	4/16491 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	ASP	N-CA-C	-5.55	96.01	111.00
2	F	460	LEU	CB-CA-C	5.45	120.56	110.20
1	A	195	TYR	N-CA-C	-5.33	96.62	111.00
1	C	321	LEU	CA-CB-CG	5.04	126.90	115.30

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	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2559	0	2513	55	0
1	E	2559	0	2513	62	0
2	B	1416	0	1319	20	0
2	D	1416	0	1319	28	0
2	F	1416	0	1319	30	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	21	0	17	3	0
5	C	21	0	17	1	0
6	A	66	0	0	11	0
6	B	20	0	0	4	0
6	C	37	0	0	4	0
6	D	13	0	0	2	0
6	E	30	0	0	6	0
6	F	10	0	0	4	0
All	All	12269	0	11644	218	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 9.

All (218) 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:D:504:ARG:NH2	6:D:611:HOH:O	1.94	0.99
1:C:192:THR:O	1:C:195:TYR:O	1.91	0.89
1:A:272:GLU:OE1	6:A:737:HOH:O	1.95	0.83
1:A:206:THR:O	6:A:706:HOH:O	1.96	0.82
2:B:412:GLU:OE1	6:B:617:HOH:O	1.97	0.81
1:E:206:THR:HG22	1:E:208:THR:H	1.46	0.81
1:A:206:THR:HG22	1:A:208:THR:H	1.46	0.79
1:E:79:GLU:OE2	6:E:729:HOH:O	2.00	0.77
1:E:104:GLU:O	6:E:708:HOH:O	2.02	0.76
2:D:393:MET:SD	6:F:603:HOH:O	2.44	0.75
1:A:284:THR:HG22	1:A:286:MET:H	1.51	0.74
1:E:284:THR:HG22	1:E:286:MET:H	1.52	0.74
1:E:256:TYR:O	6:E:707:HOH:O	2.04	0.74
2:F:406:ASN:O	6:F:609:HOH:O	2.07	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:VAL:HG22	1:C:146:SER:HA	1.71	0.72
2:B:447:SER:OG	6:B:608:HOH:O	2.07	0.71
1:A:25:GLU:OE2	1:A:322:ARG:NH2	2.21	0.70
1:A:76:ASN:OD1	6:A:738:HOH:O	2.08	0.70
1:C:284:THR:HG22	1:C:286:MET:H	1.57	0.69
1:A:22:THR:HG22	1:A:24:MET:H	1.56	0.68
1:E:209:LEU:O	6:E:703:HOH:O	2.10	0.67
1:E:280:THR:HG21	1:E:288:ALA:HB1	1.75	0.67
1:A:192:THR:O	1:A:195:TYR:O	2.12	0.67
1:E:182:ILE:HG23	1:E:202:ILE:HD12	1.76	0.67
1:A:280:THR:HG21	1:A:288:ALA:HB1	1.77	0.66
1:C:25:GLU:OE2	1:C:322:ARG:NH2	2.24	0.66
1:C:22:THR:HG22	1:C:24:MET:H	1.61	0.66
1:A:31:THR:HB	1:A:321:LEU:H	1.59	0.66
1:E:22:THR:HG22	1:E:24:MET:H	1.59	0.65
1:A:190:GLU:OE1	6:A:718:HOH:O	2.15	0.65
1:A:206:THR:HG21	6:A:743:HOH:O	1.95	0.65
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.78	0.65
1:C:186:ASN:N	1:C:186:ASN:OD1	2.31	0.64
1:C:289:ILE:HD11	1:C:298:ILE:HG13	1.80	0.64
1:C:206:THR:HG22	1:C:208:THR:H	1.63	0.63
1:E:212:ARG:NE	6:E:724:HOH:O	2.02	0.63
1:C:134:GLY:N	1:C:155:ILE:HD11	2.14	0.62
1:E:31:THR:HB	1:E:321:LEU:H	1.65	0.62
2:D:360:HIS:HD2	2:D:487:ARG:HH21	1.46	0.62
2:D:461:ARG:NH2	2:F:466:GLU:O	2.32	0.62
1:E:186:ASN:ND2	1:E:227:SER:HB2	2.15	0.62
1:E:317:LEU:HD21	2:F:389:ILE:HD12	1.81	0.61
1:C:31:THR:HB	1:C:321:LEU:H	1.66	0.61
5:A:604:SIA:O9	6:A:718:HOH:O	2.17	0.60
1:E:186:ASN:OD1	1:E:186:ASN:N	2.34	0.60
1:C:301:LEU:HA	2:D:400:VAL:HG22	1.84	0.60
1:E:39:LYS:NZ	1:E:313:ASN:O	2.27	0.60
1:A:52:LYS:HG2	1:A:53:PRO:HD2	1.83	0.60
1:E:25:GLU:OE2	1:E:322:ARG:NH2	2.35	0.60
1:A:182:ILE:HG23	1:A:202:ILE:HD12	1.84	0.59
1:C:200:THR:HA	1:C:248:ASN:HD21	1.67	0.59
1:C:212:ARG:NH1	6:C:721:HOH:O	2.08	0.59
1:E:301:LEU:HA	2:F:400:VAL:HG22	1.83	0.59
2:D:385:LYS:HG3	1:E:23:ILE:HD12	1.84	0.59
1:C:314:ARG:HG3	1:C:316:VAL:HG23	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HB	1:A:209:LEU:HB3	1.85	0.58
2:F:463:ASN:ND2	2:F:491:TYR:OH	2.21	0.58
1:A:148:PHE:HB2	1:A:151:VAL:HG12	1.84	0.58
1:A:281:LYS:NZ	6:A:739:HOH:O	2.31	0.58
1:A:135:VAL:HG22	1:A:146:SER:HA	1.84	0.58
1:C:309:TYR:O	6:C:703:HOH:O	2.17	0.58
1:E:284:THR:HB	1:E:287:GLY:O	2.03	0.58
1:A:301:LEU:HA	2:B:400:VAL:HG22	1.85	0.58
2:F:460:LEU:HD13	2:F:464:ALA:HB3	1.85	0.57
2:D:360:HIS:CD2	2:D:487:ARG:HH21	2.21	0.57
1:E:148:PHE:HB2	1:E:151:VAL:HG12	1.86	0.57
2:B:385:LYS:HG3	1:C:23:ILE:HD12	1.86	0.57
1:A:186:ASN:OD1	1:A:186:ASN:N	2.37	0.56
1:A:129:HIS:O	6:A:760:HOH:O	2.17	0.56
2:F:505:GLU:HA	2:F:508:SER:HB3	1.88	0.56
1:C:39:LYS:NZ	1:C:313:ASN:O	2.28	0.56
1:C:201:TYR:OH	1:C:246:GLU:OE1	2.22	0.56
1:C:182:ILE:HG23	1:C:202:ILE:HD12	1.87	0.56
1:E:206:THR:HB	1:E:209:LEU:HB3	1.87	0.56
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.88	0.56
1:C:211:GLN:OE1	1:C:213:LEU:HD11	2.06	0.56
1:C:182:ILE:HD11	1:C:233:PHE:CE1	2.40	0.55
1:C:182:ILE:CD1	1:C:213:LEU:HD13	2.36	0.55
2:F:401:GLY:HA3	6:F:601:HOH:O	2.06	0.55
1:C:280:THR:HG21	1:C:288:ALA:HB1	1.89	0.54
1:A:289:ILE:HD11	1:A:298:ILE:HG13	1.90	0.54
2:B:440:ARG:HH22	2:D:436:MET:HB3	1.72	0.54
1:C:11:TYR:CZ	2:D:340:ILE:HG23	2.42	0.54
2:F:484:GLU:O	2:F:488:ASN:N	2.30	0.54
1:E:12:HIS:HB2	2:F:355:TRP:HA	1.90	0.54
1:E:38:GLU:HB2	1:E:293:MET:HB2	1.90	0.53
1:E:9:ILE:HD11	2:F:456:VAL:HG21	1.90	0.53
1:E:317:LEU:HD23	2:F:386:VAL:HG22	1.90	0.53
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.89	0.52
5:C:604:SIA:O8	5:C:604:SIA:O6	2.20	0.52
1:E:200:THR:HG21	1:E:250:ASN:OD1	2.09	0.52
1:C:9:ILE:HD11	2:D:456:VAL:HG21	1.91	0.52
2:B:505:GLU:HA	2:B:508:SER:HB3	1.92	0.52
1:C:6:GLN:HG2	2:D:473:GLU:HA	1.91	0.51
1:A:57:ARG:HH21	1:A:86:LYS:NZ	2.07	0.51
2:D:394:ASN:ND2	2:F:424:ASP:OD1	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:602:NAG:O3	6:A:705:HOH:O	2.19	0.51
1:E:216:ARG:O	1:E:220:ARG:NH2	2.43	0.51
1:A:284:THR:HB	1:A:287:GLY:O	2.10	0.51
1:C:200:THR:HG21	1:C:250:ASN:OD1	2.10	0.50
1:E:74:PHE:HZ	1:E:149:ARG:HD3	1.75	0.50
1:A:314:ARG:HG2	1:A:316:VAL:HG23	1.92	0.50
1:E:72:ASP:C	1:E:74:PHE:H	2.14	0.50
1:E:53:PRO:HB3	1:E:82:TYR:CE2	2.46	0.50
1:E:102:TYR:CE2	1:E:106:LYS:HD2	2.47	0.50
1:E:31:THR:N	1:E:321:LEU:O	2.42	0.50
1:C:6:GLN:NE2	2:D:467:LEU:HD11	2.27	0.49
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.93	0.49
2:D:360:HIS:HB2	2:D:483:MET:SD	2.52	0.49
1:E:111:ARG:HH11	1:E:266:SER:HB3	1.77	0.49
1:A:150:ASN:HB3	1:A:256:TYR:HB2	1.94	0.49
2:F:467:LEU:HD21	2:F:473:GLU:HB2	1.94	0.49
1:C:37:LEU:HD23	1:C:39:LYS:HE2	1.93	0.49
1:E:74:PHE:CZ	1:E:149:ARG:HD3	2.47	0.49
1:C:321:LEU:HB3	2:D:445:HIS:CD2	2.48	0.49
1:A:200:THR:HG21	1:A:250:ASN:OD1	2.13	0.49
1:A:125:SER:OG	1:A:166:ARG:NH2	2.46	0.49
2:F:485:SER:HA	2:F:488:ASN:HB2	1.94	0.48
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.95	0.48
2:B:431:GLU:HA	6:B:609:HOH:O	2.13	0.48
1:E:25:GLU:CD	1:E:322:ARG:HH22	2.16	0.48
1:E:99:PHE:HB3	1:E:102:TYR:HB2	1.94	0.48
1:A:102:TYR:CE2	1:A:106:LYS:HD2	2.49	0.48
1:E:164:ILE:O	1:E:246:GLU:HA	2.13	0.48
1:E:125:SER:HB2	1:E:166:ARG:HH22	1.79	0.48
2:B:492:ASP:OD1	2:B:495:GLN:HB2	2.14	0.48
1:C:6:GLN:HE21	2:D:473:GLU:HG3	1.78	0.48
2:D:501:ARG:NE	2:D:505:GLU:OE2	2.47	0.48
1:C:148:PHE:HB2	1:C:151:VAL:HG12	1.96	0.48
2:D:454:ASP:OD1	2:D:457:ARG:NH1	2.46	0.47
2:D:350:GLY:HA3	2:D:368:TYR:CE1	2.49	0.47
1:C:164:ILE:O	1:C:246:GLU:HA	2.14	0.47
6:A:708:HOH:O	2:D:411:ILE:HG13	2.14	0.47
1:C:130:GLU:O	1:C:155:ILE:HD12	2.15	0.47
2:F:360:HIS:CD2	2:F:487:ARG:HH21	2.32	0.47
1:C:111:ARG:HH11	1:C:266:SER:HB3	1.80	0.47
1:E:125:SER:CB	1:E:166:ARG:HH22	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:HIS:HB2	2:B:483:MET:SD	2.55	0.47
1:E:36:ILE:HD13	1:E:36:ILE:HA	1.74	0.47
1:C:53:PRO:HB3	1:C:82:TYR:CE2	2.51	0.46
1:A:177:LEU:HB2	1:A:260:ILE:HD13	1.97	0.46
2:D:497:SER:O	2:D:501:ARG:HB2	2.15	0.46
1:A:14:ASN:ND2	6:A:730:HOH:O	2.16	0.46
1:C:142:GLN:N	6:C:710:HOH:O	2.46	0.46
2:B:337:PHE:CE1	2:B:447:SER:HB2	2.51	0.46
2:B:357:GLY:HA3	2:B:370:ALA:HA	1.97	0.46
2:D:420:ASP:OD1	6:D:604:HOH:O	2.20	0.46
1:C:36:ILE:HA	1:C:36:ILE:HD13	1.68	0.46
1:A:67:GLY:O	1:A:149:ARG:HG3	2.16	0.46
1:C:186:ASN:ND2	1:C:227:SER:HB2	2.30	0.46
2:B:453:TYR:CE1	2:B:470:GLY:HA2	2.51	0.46
1:E:65:LEU:HD11	1:E:109:LEU:HD11	1.98	0.46
2:D:351:MET:SD	2:D:357:GLY:HA3	2.56	0.46
1:E:67:GLY:HA3	1:E:149:ARG:H	1.81	0.45
2:B:499:GLU:O	2:B:502:LEU:HB2	2.17	0.45
2:D:476:HIS:ND1	2:D:477:LYS:O	2.43	0.45
2:B:409:ARG:NE	6:B:610:HOH:O	2.50	0.45
1:E:308:LYS:HD2	2:F:426:TRP:CE2	2.51	0.45
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.98	0.45
2:F:351:MET:SD	2:F:357:GLY:HA3	2.57	0.45
2:F:364:GLN:HE22	2:F:479:ASP:HA	1.82	0.45
1:A:182:ILE:HG12	1:A:213:LEU:HD13	1.97	0.45
1:E:15:ASN:N	1:E:15:ASN:OD1	2.34	0.45
1:A:164:ILE:O	1:A:246:GLU:HA	2.16	0.45
2:B:400:VAL:HA	2:B:401:GLY:HA3	1.71	0.45
1:C:206:THR:HB	1:C:209:LEU:HB3	1.99	0.44
1:C:273:LEU:HD11	1:C:286:MET:C	2.38	0.44
1:A:317:LEU:HD23	2:B:386:VAL:HG22	1.99	0.44
1:C:200:THR:HA	1:C:248:ASN:ND2	2.30	0.44
2:F:400:VAL:HA	2:F:401:GLY:HA3	1.67	0.44
1:E:7:ILE:HB	2:F:474:PHE:CE1	2.52	0.44
1:A:23:ILE:HD12	2:F:385:LYS:HG3	1.99	0.44
2:F:335:GLY:O	6:F:604:HOH:O	2.21	0.44
2:F:500:ALA:O	2:F:504:ARG:N	2.50	0.44
2:B:479:ASP:OD1	2:B:479:ASP:N	2.44	0.44
1:C:102:TYR:CE2	1:C:106:LYS:HD2	2.53	0.44
1:A:97:GLY:HA3	1:A:230:MET:O	2.17	0.44
1:A:321:LEU:HB3	2:B:445:HIS:CD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:OG1	1:A:248:ASN:HB3	2.19	0.43
1:E:11:TYR:CZ	2:F:340:ILE:HG23	2.54	0.43
1:A:317:LEU:HA	1:A:317:LEU:HD12	1.84	0.43
1:C:45:LEU:HD13	1:C:84:VAL:HG21	2.01	0.43
2:D:441:THR:O	2:D:444:PHE:HB3	2.19	0.43
1:C:191:GLN:HG2	1:C:217:ILE:HD11	2.00	0.43
1:E:97:GLY:HA3	1:E:230:MET:O	2.19	0.42
1:A:247:SER:OG	1:A:251:PHE:HB2	2.19	0.42
1:E:201:TYR:OH	1:E:246:GLU:OE1	2.30	0.42
2:B:429:ASN:HD22	2:B:429:ASN:N	2.17	0.42
1:C:197:ASN:OD1	6:C:735:HOH:O	2.22	0.42
1:C:317:LEU:HD13	2:D:434:VAL:HG22	2.00	0.42
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.88	0.42
1:C:284:THR:HB	1:C:287:GLY:O	2.20	0.42
1:A:155:ILE:HG12	5:A:604:SIA:H111	2.02	0.41
1:E:167:SER:HA	1:E:243:ILE:O	2.19	0.41
1:C:14:ASN:OD1	1:C:323:ASN:ND2	2.53	0.41
1:C:83:ILE:HB	1:C:268:ILE:HG13	2.03	0.41
1:E:159:SER:O	1:E:196:GLN:HG3	2.20	0.41
1:A:134:GLY:HA2	5:A:604:SIA:H113	2.03	0.41
1:A:154:LEU:C	1:A:155:ILE:HD12	2.40	0.41
1:A:216:ARG:O	1:A:220:ARG:NH2	2.53	0.41
2:D:452:LEU:HD12	2:D:452:LEU:HA	1.85	0.41
2:B:508:SER:O	2:F:501:ARG:NH1	2.54	0.41
1:E:8:CYS:HA	2:F:471:CYS:HA	2.03	0.41
1:E:206:THR:HG22	1:E:208:THR:N	2.25	0.41
1:E:72:ASP:C	1:E:74:PHE:N	2.74	0.41
1:A:15:ASN:N	1:A:15:ASN:OD1	2.37	0.41
1:E:182:ILE:HG12	1:E:213:LEU:HD13	2.02	0.41
2:F:479:ASP:OD1	2:F:479:ASP:N	2.46	0.41
1:C:311:LYS:HB2	2:D:423:LEU:HD21	2.03	0.41
1:E:154:LEU:O	6:E:701:HOH:O	2.22	0.41
1:C:38:GLU:HB2	1:C:293:MET:HB2	2.03	0.41
1:E:12:HIS:N	2:F:355:TRP:O	2.47	0.40
1:E:266:SER:OG	1:E:267:THR:N	2.54	0.40
1:E:48:LEU:HA	1:E:48:LEU:HD23	1.93	0.40
1:C:134:GLY:HA3	1:C:153:TRP:HB3	2.03	0.40
1:A:150:ASN:HA	1:A:256:TYR:HD1	1.86	0.40
1:E:308:LYS:HD2	2:F:426:TRP:NE1	2.37	0.40
1:E:7:ILE:HA	1:E:7:ILE:HD13	1.85	0.40

There are no symmetry-related clashes.

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%)	300 (94%)	20 (6%)	0	100	100
1	C	320/322 (99%)	300 (94%)	19 (6%)	1 (0%)	46	66
1	E	320/322 (99%)	296 (92%)	22 (7%)	2 (1%)	30	48
2	B	173/175 (99%)	166 (96%)	5 (3%)	2 (1%)	16	27
2	D	173/175 (99%)	165 (95%)	6 (4%)	2 (1%)	16	27
2	F	173/175 (99%)	164 (95%)	7 (4%)	2 (1%)	16	27
All	All	1479/1491 (99%)	1391 (94%)	79 (5%)	9 (1%)	30	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	72	ASP
2	D	508	SER
1	E	74	PHE
2	F	508	SER
2	B	508	SER
2	B	401	GLY
2	D	401	GLY
2	F	401	GLY
1	C	198	PRO

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%)	263 (91%)	27 (9%)	11	19
1	C	290/290 (100%)	262 (90%)	28 (10%)	10	18
1	E	290/290 (100%)	267 (92%)	23 (8%)	15	27
2	B	149/149 (100%)	146 (98%)	3 (2%)	63	85
2	D	149/149 (100%)	144 (97%)	5 (3%)	44	70
2	F	149/149 (100%)	140 (94%)	9 (6%)	24	41
All	All	1317/1317 (100%)	1222 (93%)	95 (7%)	18	31

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	20	VAL
1	A	22	THR
1	A	23	ILE
1	A	30	VAL
1	A	36	ILE
1	A	58	ASP
1	A	75	ILE
1	A	135	VAL
1	A	141	TYR
1	A	151	VAL
1	A	159	SER
1	A	182	ILE
1	A	186	ASN
1	A	191	GLN
1	A	196	GLN
1	A	200	THR
1	A	208	THR
1	A	230	MET
1	A	235	THR
1	A	260	ILE
1	A	265	ASP
1	A	280	THR
1	A	284	THR
1	A	317	LEU
1	A	319	ILE
1	A	321	LEU
2	B	400	VAL
2	B	423	LEU
2	B	440	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	7	ILE
1	C	22	THR
1	C	23	ILE
1	C	30	VAL
1	C	36	ILE
1	C	57	ARG
1	C	58	ASP
1	C	120	ILE
1	C	135	VAL
1	C	151	VAL
1	C	155	ILE
1	C	159	SER
1	C	182	ILE
1	C	186	ASN
1	C	191	GLN
1	C	196	GLN
1	C	200	THR
1	C	208	THR
1	C	230	MET
1	C	235	THR
1	C	252	ILE
1	C	265	ASP
1	C	280	THR
1	C	284	THR
1	C	314	ARG
1	C	317	LEU
1	C	319	ILE
1	C	321	LEU
2	D	400	VAL
2	D	423	LEU
2	D	460	LEU
2	D	498	GLU
2	D	501	ARG
1	E	7	ILE
1	E	23	ILE
1	E	30	VAL
1	E	36	ILE
1	E	57	ARG
1	E	58	ASP
1	E	75	ILE
1	E	135	VAL
1	E	151	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	155	ILE
1	E	159	SER
1	E	182	ILE
1	E	186	ASN
1	E	200	THR
1	E	208	THR
1	E	230	MET
1	E	235	THR
1	E	265	ASP
1	E	280	THR
1	E	314	ARG
1	E	317	LEU
1	E	319	ILE
1	E	321	LEU
2	F	364	GLN
2	F	373	GLU
2	F	400	VAL
2	F	423	LEU
2	F	440	ARG
2	F	461	ARG
2	F	477	LYS
2	F	498	GLU
2	F	501	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
2	B	429	ASN
1	C	6	GLN
2	D	360	HIS
2	D	429	ASN
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	0.46	0	15,19,21	0.75	0
4	NAG	A	603	4	14,14,15	0.44	0	15,19,21	1.05	1 (6%)
4	NAG	C	602	1,4	14,14,15	0.56	0	15,19,21	0.69	0
4	NAG	C	603	4	14,14,15	0.56	0	15,19,21	0.60	0
4	NAG	E	602	1,4	14,14,15	0.58	0	15,19,21	1.28	2 (13%)
4	NAG	E	603	4	14,14,15	0.45	0	15,19,21	1.05	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.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAG	C2-N2-C7	-2.48	119.85	123.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	602	NAG	C3-C4-C5	2.19	114.01	110.20
4	E	602	NAG	C1-O5-C5	3.45	116.63	112.25

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 ⓘ

5 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	0.53	0	15,19,21	0.85	0
5	SIA	A	604	-	17,21,21	4.04	8 (47%)	19,31,31	1.55	3 (15%)
3	NAG	C	601	1	14,14,15	0.44	0	15,19,21	1.13	1 (6%)
5	SIA	C	604	-	17,21,21	4.01	9 (52%)	19,31,31	1.46	3 (15%)
3	NAG	E	601	1	14,14,15	0.54	0	15,19,21	0.83	1 (6%)

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
5	SIA	A	604	-	-	0/14/38/38	0/1/1/1
3	NAG	C	601	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
5	SIA	C	604	-	-	0/14/38/38	0/1/1/1
3	NAG	E	601	1	-	1/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	SIA	C7-C6	-9.83	1.40	1.52
5	C	604	SIA	C7-C6	-9.70	1.40	1.52
5	A	604	SIA	C3-C4	-8.15	1.40	1.53
5	C	604	SIA	C3-C4	-7.83	1.40	1.53
5	A	604	SIA	C3-C2	-5.86	1.44	1.51
5	C	604	SIA	C3-C2	-5.67	1.44	1.51
5	C	604	SIA	O2-C2	-2.79	1.37	1.40
5	A	604	SIA	O2-C2	-2.71	1.37	1.40
5	C	604	SIA	C6-C5	2.01	1.56	1.53
5	A	604	SIA	O4-C4	2.28	1.48	1.43
5	C	604	SIA	O4-C4	2.48	1.48	1.43
5	A	604	SIA	C10-N5	3.52	1.47	1.34
5	C	604	SIA	C10-N5	3.68	1.48	1.34
5	C	604	SIA	O6-C2	4.72	1.47	1.42
5	A	604	SIA	O6-C6	4.73	1.52	1.44
5	A	604	SIA	O6-C2	4.80	1.47	1.42
5	C	604	SIA	O6-C6	4.87	1.52	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	SIA	C8-C7-C6	-2.49	108.01	113.01
3	E	601	NAG	C1-O5-C5	2.13	114.96	112.25
5	C	604	SIA	O6-C6-C7	2.41	110.90	107.26
5	C	604	SIA	C11-C10-N5	2.49	120.87	116.11
5	A	604	SIA	O9-C9-C8	2.99	117.61	111.10
3	C	601	NAG	C1-O5-C5	3.10	116.18	112.25
5	C	604	SIA	O9-C9-C8	3.23	118.11	111.10
5	A	604	SIA	O6-C6-C7	3.38	112.38	107.26

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	SIA	3	0
5	C	604	SIA	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	322/322 (100%)	0.08	3 (0%) 85 88	25, 48, 75, 112	0
1	C	322/322 (100%)	0.11	4 (1%) 81 83	29, 56, 85, 146	0
1	E	322/322 (100%)	0.25	11 (3%) 49 53	28, 55, 92, 140	0
2	B	175/175 (100%)	0.59	15 (8%) 13 14	28, 62, 97, 143	0
2	D	175/175 (100%)	1.07	32 (18%) 2 2	28, 76, 120, 165	0
2	F	175/175 (100%)	0.95	28 (16%) 3 2	29, 79, 137, 198	0
All	All	1491/1491 (100%)	0.40	93 (6%) 24 26	25, 56, 107, 198	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	507	ILE	10.4
2	F	502	LEU	9.7
2	F	507	ILE	8.7
1	C	325	PRO	6.8
1	E	325	PRO	6.6
2	F	474	PHE	6.4
2	F	508	SER	6.1
2	B	509	GLY	5.9
2	F	475	TYR	5.8
2	B	508	SER	5.8
2	D	508	SER	5.6
2	D	460	LEU	5.3
1	E	4	GLN	4.5
2	F	483	MET	4.4
2	F	509	GLY	4.4
2	D	335	GLY	4.1
2	D	491	TYR	4.0
2	D	492	ASP	4.0
2	D	369	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	481	GLU	3.9
2	D	367	GLY	3.9
2	D	363	GLU	3.8
2	F	498	GLU	3.7
2	D	474	PHE	3.7
2	D	509	GLY	3.6
2	F	491	TYR	3.5
2	D	486	VAL	3.5
1	E	67	GLY	3.5
2	D	365	GLY	3.4
1	E	74	PHE	3.3
2	D	496	TYR	3.3
2	F	506	GLU	3.1
2	F	493	TYR	3.1
2	B	353	ASP	3.1
1	E	72	ASP	3.0
2	B	335	GLY	3.0
2	D	340	ILE	3.0
2	D	495	GLN	3.0
2	F	504	ARG	3.0
2	D	350	GLY	2.9
2	B	507	ILE	2.9
1	C	17	THR	2.9
2	D	366	SER	2.8
2	F	492	ASP	2.7
2	D	370	ALA	2.7
2	B	363	GLU	2.7
1	A	15	ASN	2.7
2	F	496	TYR	2.6
1	E	149	ARG	2.6
1	C	7	ILE	2.6
1	A	325	PRO	2.6
1	E	186	ASN	2.6
2	F	460	LEU	2.5
2	F	355	TRP	2.5
2	B	367	GLY	2.5
2	F	335	GLY	2.5
2	D	355	TRP	2.5
2	D	433	LEU	2.5
1	E	70	MET	2.5
1	E	131	ALA	2.4
2	F	349	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	476	HIS	2.4
2	F	363	GLU	2.4
2	D	436	MET	2.4
2	D	336	LEU	2.3
2	D	506	GLU	2.3
2	D	372	LYS	2.3
2	F	486	VAL	2.3
1	E	182	ILE	2.3
2	B	450	LYS	2.3
2	F	482	CYS	2.2
2	B	440	ARG	2.2
2	D	479	ASP	2.2
2	B	452	LEU	2.2
2	D	502	LEU	2.2
2	D	361	SER	2.2
2	B	483	MET	2.1
2	F	440	ARG	2.1
2	B	454	ASP	2.1
2	F	463	ASN	2.1
2	B	446	ASP	2.1
2	F	436	MET	2.1
2	D	360	HIS	2.1
2	D	440	ARG	2.1
1	A	7	ILE	2.1
2	B	474	PHE	2.1
1	E	323	ASN	2.0
2	F	501	ARG	2.0
2	D	353	ASP	2.0
2	F	465	LYS	2.0
1	C	126	TRP	2.0
2	F	505	GLU	2.0
2	B	425	VAL	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, 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
4	NAG	C	602	14/15	0.90	0.18	0.14	72,87,95,100	0
4	NAG	A	602	14/15	0.94	0.12	-1.14	38,50,60,62	0
4	NAG	E	603	14/15	0.82	0.25	-	86,100,106,111	0
4	NAG	C	603	14/15	0.85	0.37	-	111,116,120,121	0
4	NAG	A	603	14/15	0.89	0.13	-	58,72,76,82	0
4	NAG	E	602	14/15	0.93	0.15	-	57,73,84,90	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, 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
5	SIA	C	604	21/21	0.89	0.24	2.09	74,84,89,91	0
5	SIA	A	604	21/21	0.89	0.13	-0.88	57,69,80,83	0
3	NAG	C	601	14/15	0.87	0.14	-	110,114,120,120	0
3	NAG	A	601	14/15	0.90	0.25	-	78,86,90,92	0
3	NAG	E	601	14/15	0.81	0.31	-	100,107,113,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.