



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:00 PM GMT

PDB ID : 4K64
Title : Structure of an avian influenza H5 hemagglutinin from the influenza virus complexed with human receptor analog LSTc
Authors : Zhang, W.; Shi, Y.; Lu, X.; Shu, Y.; Qi, J.; Gao, G.F.
Deposited on : 2013-04-15
Resolution : 2.60 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

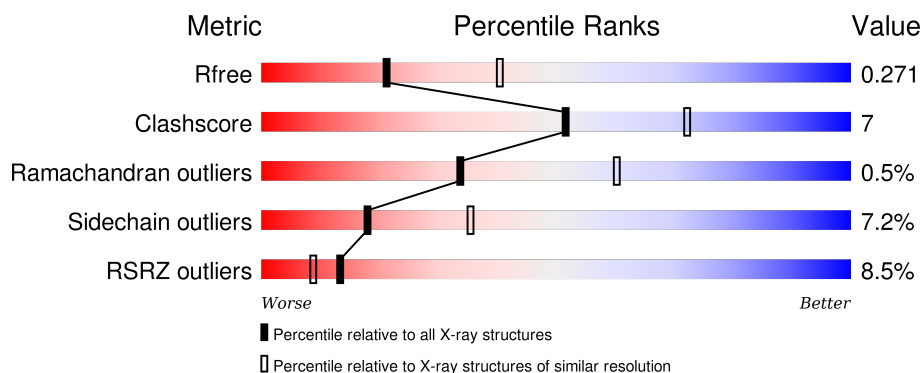
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	321	<div> <div></div> <div>79%20%•</div> </div>
1	C	321	<div> <div></div> <div>79%20%•</div> </div>
1	E	321	<div> <div>9%</div> <div>75%23%•</div> </div>
1	G	321	<div> <div>10%</div> <div>74%24%•</div> </div>
2	B	164	<div> <div>2%</div> <div>84%15%•</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	164	
2	F	164	
2	H	164	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	601	-	-	-	X
3	NAG	E	601	-	-	-	X
3	NAG	G	601	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15829 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	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	C	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	E	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	G	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	EXPRESSION TAG	UNP A8HWY8
C	4	GLN	-	EXPRESSION TAG	UNP A8HWY8
E	4	GLN	-	EXPRESSION TAG	UNP A8HWY8
G	4	GLN	-	EXPRESSION TAG	UNP A8HWY8

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	D	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	F	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	H	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	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		
3	G	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
			32	17	1	14		
4	C	2	Total	C	N	O	0	0
			32	17	1	14		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total	O	0	0
			86	86		
5	B	25	Total	O	0	0
			25	25		
5	C	81	Total	O	0	0
			81	81		

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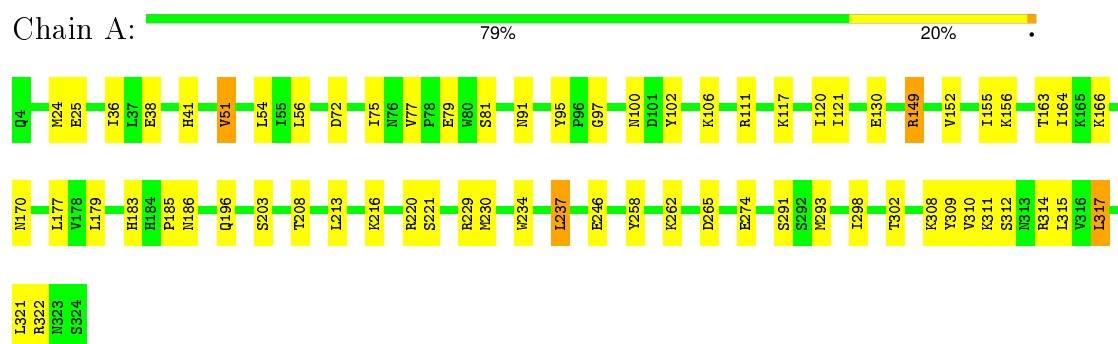
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	20	Total 20	O 20	0	0
5	E	8	Total 8	O 8	0	0
5	F	2	Total 2	O 2	0	0
5	G	9	Total 9	O 9	0	0
5	H	2	Total 2	O 2	0	0

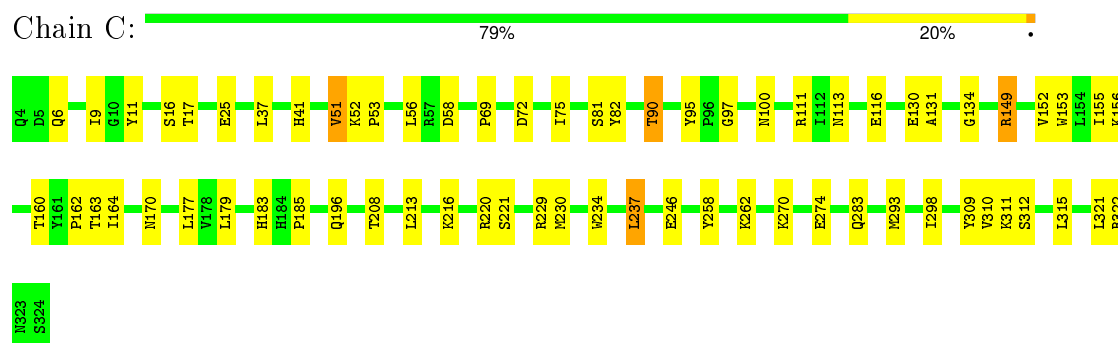
3 Residue-property plots [i](#)

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.

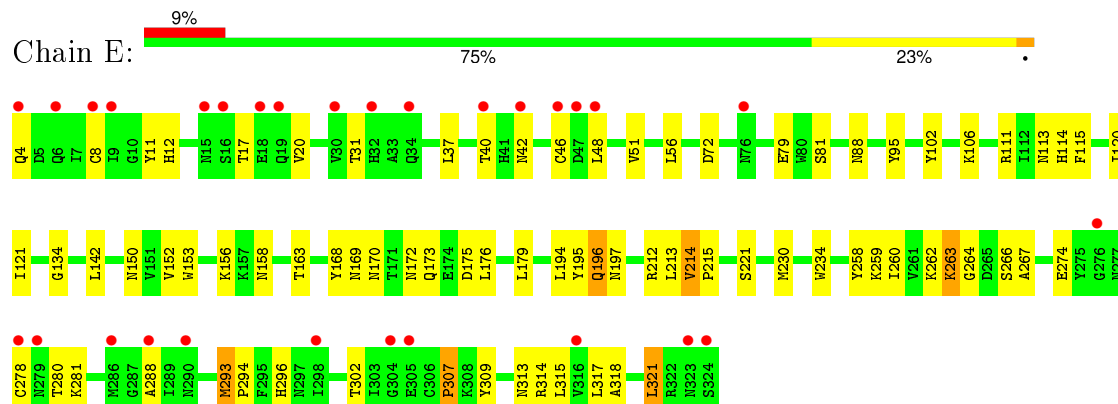
• Molecule 1: Hemagglutinin



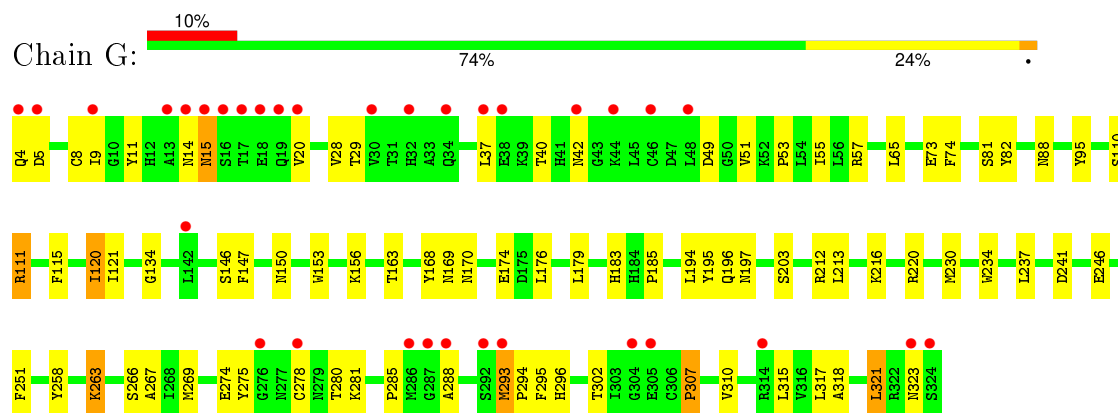
• Molecule 1: Hemagglutinin



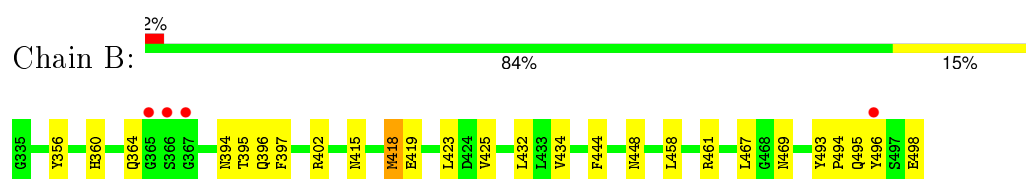
• Molecule 1: Hemagglutinin



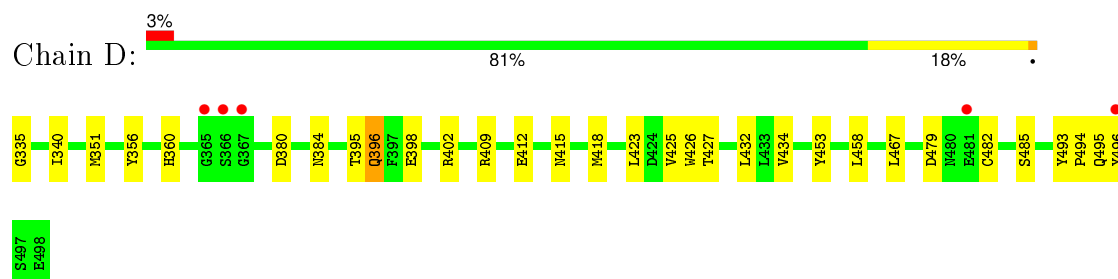
- Molecule 1: Hemagglutinin



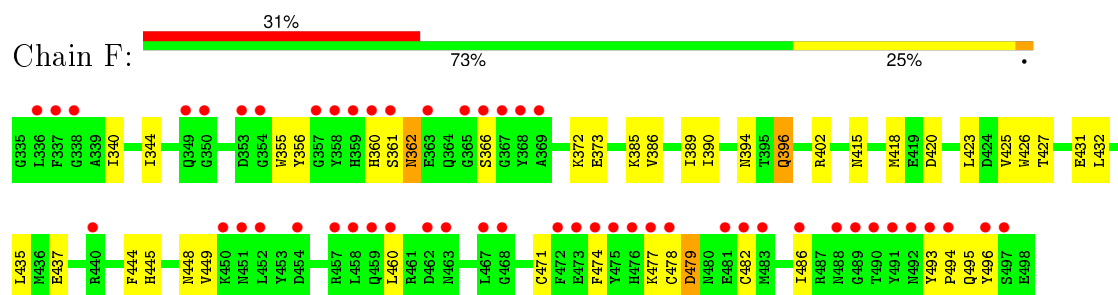
- Molecule 2: Hemagglutinin



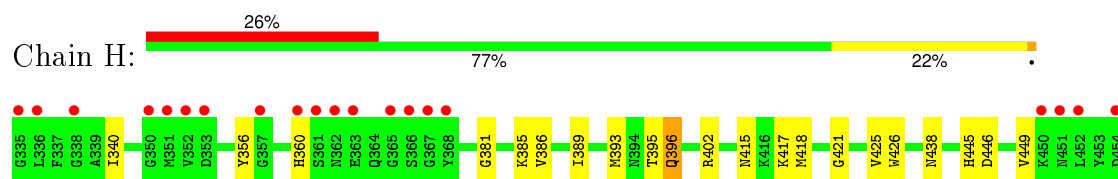
- Molecule 2: Hemagglutinin

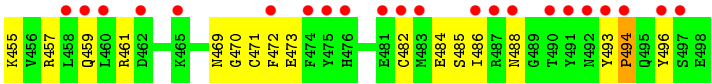


- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin





4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	70.34Å 70.34Å 491.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.04 – 2.60 36.04 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.5 (36.04-2.60) 92.5 (36.04-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.221 , 0.280 0.211 , 0.271	Depositor DCC
R_{free} test set	3864 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.7	EDS
Estimated twinning fraction	0.391 for -h,-k,l 0.437 for -h,-k,l 0.093 for h,-h-k,-l 0.087 for -k,-h,-l	Xtriage
Reported twinning fraction	0.391 for -h,-k,l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 77142 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15829	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, 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	0.25	0/2603	0.44	0/3537
1	C	0.26	0/2603	0.43	0/3537
1	E	0.22	0/2603	0.41	0/3537
1	G	0.24	0/2603	0.46	2/3537 (0.1%)
2	B	0.25	0/1355	0.43	0/1823
2	D	0.24	0/1355	0.41	0/1823
2	F	0.24	0/1355	0.43	1/1823 (0.1%)
2	H	0.22	0/1355	0.39	0/1823
All	All	0.24	0/15832	0.43	3/21440 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	212	ARG	NE-CZ-NH1	7.95	124.28	120.30
2	F	460	LEU	CB-CA-C	7.41	124.29	110.20
1	G	212	ARG	NE-CZ-NH2	-5.97	117.32	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2541	0	2478	34	0
1	C	2541	0	2478	38	0
1	E	2541	0	2477	43	0
1	G	2541	0	2478	49	0
2	B	1328	0	1231	13	0
2	D	1328	0	1231	16	0
2	F	1328	0	1231	22	0
2	H	1328	0	1231	25	0
3	A	14	0	13	0	0
3	C	14	0	13	0	0
3	E	14	0	13	0	0
3	G	14	0	13	0	0
4	A	32	0	27	0	0
4	C	32	0	27	0	0
5	A	86	0	0	4	0
5	B	25	0	0	1	0
5	C	81	0	0	6	0
5	D	20	0	0	2	0
5	E	8	0	0	0	0
5	F	2	0	0	0	0
5	G	9	0	0	3	0
5	H	2	0	0	0	0
All	All	15829	0	14941	208	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 7.

All (208) 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:479:ASP:OD2	5:D:513:HOH:O	1.93	0.87
1:E:172:ASN:HD22	1:E:259:LYS:HD3	1.45	0.82
1:C:116:GLU:OE2	5:C:755:HOH:O	1.98	0.81
1:A:166:LYS:NZ	5:A:737:HOH:O	2.11	0.81
1:A:149:ARG:NH2	5:A:714:HOH:O	2.15	0.79
1:G:241:ASP:OD1	5:G:704:HOH:O	1.98	0.79
1:C:311:LYS:HE3	2:D:423:LEU:HD23	1.68	0.75
1:G:156:LYS:HD2	1:G:196:GLN:HG2	1.69	0.75
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.68	0.74
1:E:4:GLN:NE2	2:F:474:PHE:O	2.21	0.73
2:H:469:ASN:ND2	2:H:471:CYS:SG	2.64	0.71
1:C:131:ALA:O	5:C:706:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:VAL:HG21	1:G:318:ALA:HB2	1.73	0.69
1:A:309:TYR:HE2	2:B:423:LEU:HD21	1.57	0.69
2:H:455:LYS:O	2:H:459:GLN:NE2	2.26	0.69
1:C:69:PRO:O	5:C:728:HOH:O	2.11	0.69
1:C:156:LYS:HD2	1:C:196:GLN:HG2	1.75	0.68
1:E:51:VAL:HG23	1:E:81:SER:HB3	1.75	0.68
1:A:91:ASN:ND2	5:A:750:HOH:O	2.28	0.67
1:G:321:LEU:HB3	2:H:445:HIS:HD2	1.60	0.67
1:E:120:ILE:HG13	1:E:121:ILE:HG13	1.77	0.67
1:A:310:VAL:HG12	1:A:312:SER:H	1.60	0.67
1:G:51:VAL:HG13	1:G:81:SER:HB3	1.77	0.66
1:C:309:TYR:HE2	2:D:423:LEU:HD21	1.60	0.66
1:G:197:ASN:ND2	5:G:708:HOH:O	2.19	0.65
1:G:317:LEU:HD23	2:H:386:VAL:HG22	1.78	0.65
1:G:150:ASN:ND2	1:G:258:TYR:OH	2.30	0.64
1:C:149:ARG:NH2	5:C:710:HOH:O	2.32	0.63
1:C:310:VAL:HG12	1:C:312:SER:H	1.64	0.63
1:A:311:LYS:HE3	2:B:423:LEU:HD23	1.81	0.62
1:C:52:LYS:HG2	1:C:53:PRO:HD2	1.81	0.62
1:G:296:HIS:HD2	1:G:307:PRO:HB2	1.65	0.61
2:F:493:TYR:O	2:F:495:GLN:N	2.34	0.61
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.83	0.60
1:C:270:LYS:NZ	5:C:723:HOH:O	2.23	0.60
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.86	0.58
1:C:9:ILE:HD13	2:D:453:TYR:HA	1.85	0.58
1:C:41:HIS:HB3	1:C:298:ILE:HD13	1.85	0.58
2:D:396:GLN:HG3	2:D:426:TRP:CD2	2.39	0.58
1:G:55:ILE:HD12	1:G:275:TYR:HB2	1.86	0.57
1:E:120:ILE:HB	1:E:168:TYR:CZ	2.38	0.57
1:G:111:ARG:O	1:G:263:LYS:NZ	2.36	0.57
1:E:111:ARG:O	1:E:263:LYS:NZ	2.37	0.57
1:C:310:VAL:HG13	2:D:427:THR:HA	1.87	0.57
2:D:380:ASP:O	2:D:384:ASN:ND2	2.37	0.57
1:G:169:ASN:OD1	1:G:170:ASN:N	2.38	0.57
1:A:41:HIS:HB3	1:A:298:ILE:HD13	1.87	0.57
1:G:15:ASN:OD1	1:G:15:ASN:N	2.37	0.57
1:E:296:HIS:HD2	1:E:307:PRO:HB2	1.70	0.57
1:A:95:TYR:CD2	1:A:230:MET:HG2	2.40	0.56
1:E:317:LEU:HD23	2:F:386:VAL:HG22	1.88	0.56
1:C:25:GLU:OE2	1:C:322:ARG:NH2	2.39	0.56
2:F:444:PHE:O	2:F:448:ASN:ND2	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:396:GLN:HG3	2:F:426:TRP:CD2	2.41	0.55
1:E:169:ASN:OD1	1:E:170:ASN:N	2.38	0.55
1:G:321:LEU:HB3	2:H:445:HIS:CD2	2.41	0.55
1:E:266:SER:OG	1:E:267:ALA:N	2.40	0.55
1:A:120:ILE:HG13	1:A:121:ILE:HG13	1.89	0.55
2:F:479:ASP:OD2	2:F:479:ASP:N	2.36	0.55
1:A:164:ILE:O	1:A:246:GLU:HA	2.07	0.54
1:E:195:TYR:O	1:E:197:ASN:N	2.39	0.54
1:A:309:TYR:HD2	2:B:423:LEU:HD11	1.71	0.54
2:F:402:ARG:NH1	2:F:415:ASN:OD1	2.40	0.54
1:G:280:THR:OG1	1:G:281:LYS:N	2.40	0.54
1:C:309:TYR:HD2	2:D:423:LEU:HD11	1.73	0.54
1:G:174:GLU:OE1	1:G:174:GLU:N	2.40	0.53
1:A:54:LEU:HD22	1:A:77:VAL:HG11	1.90	0.53
2:D:493:TYR:O	2:D:495:GLN:N	2.42	0.53
2:F:361:SER:HA	2:F:366:SER:HA	1.91	0.53
2:B:444:PHE:O	2:B:448:ASN:ND2	2.42	0.52
1:C:58:ASP:HB3	1:C:90:THR:HG23	1.91	0.52
1:E:150:ASN:ND2	1:E:258:TYR:OH	2.42	0.52
1:G:37:LEU:HB2	1:G:315:LEU:HB2	1.90	0.52
2:B:498:GLU:OE1	5:B:508:HOH:O	2.19	0.52
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.92	0.52
1:C:309:TYR:CD2	2:D:423:LEU:HD11	2.45	0.52
1:E:280:THR:OG1	1:E:281:LYS:N	2.43	0.52
2:H:340:ILE:N	2:H:446:ASP:OD2	2.37	0.52
1:E:321:LEU:HB3	2:F:445:HIS:CD2	2.45	0.51
1:E:293:MET:HG3	1:E:294:PRO:HD2	1.92	0.51
1:C:164:ILE:O	1:C:246:GLU:HA	2.09	0.51
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.91	0.51
1:E:12:HIS:N	2:F:355:TRP:O	2.43	0.51
1:C:113:ASN:HB2	1:C:262:LYS:HG2	1.92	0.51
2:D:402:ARG:NH1	2:D:415:ASN:OD1	2.44	0.50
1:G:14:ASN:OD1	1:G:323:ASN:ND2	2.44	0.50
1:A:177:LEU:HB3	1:A:258:TYR:HB2	1.93	0.50
2:B:418:MET:HG3	2:B:419:GLU:N	2.25	0.50
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.92	0.50
1:C:315:LEU:HD22	2:D:434:VAL:HG21	1.93	0.50
1:G:179:LEU:HD23	1:G:234:TRP:HB3	1.93	0.50
1:G:14:ASN:O	1:G:323:ASN:ND2	2.41	0.50
1:G:120:ILE:HG12	1:G:121:ILE:HG13	1.94	0.50
1:C:177:LEU:HB3	1:C:258:TYR:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:TYR:CE2	1:A:106:LYS:HD2	2.48	0.49
1:C:95:TYR:CD2	1:C:230:MET:HG2	2.48	0.49
1:G:317:LEU:HD21	2:H:389:ILE:HD12	1.94	0.49
2:H:402:ARG:NH1	2:H:415:ASN:OD1	2.46	0.49
1:G:280:THR:HG21	1:G:288:ALA:HB1	1.94	0.49
1:C:37:LEU:HB2	1:C:315:LEU:HB2	1.94	0.48
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.95	0.48
1:A:51:VAL:HG22	1:A:81:SER:HB3	1.96	0.48
2:B:493:TYR:O	2:B:495:GLN:N	2.47	0.48
1:C:216:LYS:O	1:C:220:ARG:NH2	2.46	0.48
1:C:160:THR:HG22	1:C:162:PRO:HD3	1.95	0.48
1:C:170:ASN:HB2	1:C:237:LEU:HD13	1.96	0.48
2:H:396:GLN:HG3	2:H:426:TRP:CD2	2.49	0.48
1:A:309:TYR:CD2	2:B:423:LEU:HD11	2.48	0.48
1:E:294:PRO:HB3	2:F:390:ILE:HG23	1.96	0.48
1:A:25:GLU:OE2	1:A:322:ARG:NH2	2.46	0.48
1:G:110:SER:HB2	1:G:111:ARG:HE	1.78	0.48
2:H:484:GLU:OE1	2:H:488:ASN:ND2	2.47	0.48
1:E:46:CYS:HB2	1:E:280:THR:HG22	1.95	0.47
1:E:309:TYR:HE2	2:F:423:LEU:HD21	1.79	0.47
1:C:6:GLN:NE2	5:C:746:HOH:O	2.39	0.47
1:G:14:ASN:H	1:G:323:ASN:HD21	1.62	0.47
1:E:317:LEU:HD21	2:F:389:ILE:HD12	1.97	0.47
1:A:183:HIS:O	1:A:185:PRO:HD3	2.14	0.47
1:G:11:TYR:CZ	2:H:340:ILE:HG23	2.50	0.47
1:E:175:ASP:HB2	1:E:260:ILE:HD12	1.96	0.47
1:E:95:TYR:CD2	1:E:230:MET:HG2	2.50	0.47
1:G:4:GLN:HG2	1:G:5:ASP:H	1.80	0.46
1:G:120:ILE:HB	1:G:168:TYR:CZ	2.50	0.46
1:A:117:LYS:NZ	5:A:735:HOH:O	2.23	0.46
1:C:51:VAL:HG22	1:C:81:SER:HB3	1.97	0.46
1:E:113:ASN:ND2	1:E:264:GLY:HA3	2.31	0.46
2:H:482:CYS:HA	2:H:485:SER:HB3	1.98	0.46
1:G:203:SER:OG	1:G:246:GLU:HB3	2.15	0.46
1:G:146:SER:OG	1:G:147:PHE:N	2.48	0.46
1:E:102:TYR:CE2	1:E:106:LYS:HD2	2.50	0.46
2:B:396:GLN:HB3	2:B:397:PHE:H	1.58	0.46
1:G:293:MET:HG3	1:G:294:PRO:HD2	1.98	0.46
2:B:419:GLU:O	2:B:423:LEU:HB2	2.15	0.45
1:E:296:HIS:CD2	1:E:307:PRO:HB2	2.49	0.45
1:A:97:GLY:HA3	1:A:230:MET:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ASN:HD21	1:E:288:ALA:HB3	1.81	0.45
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.97	0.45
1:A:216:LYS:O	1:A:220:ARG:NH2	2.49	0.45
2:H:482:CYS:O	2:H:486:ILE:HG13	2.17	0.45
2:D:409:ARG:NH1	2:D:412:GLU:OE2	2.50	0.45
2:F:385:LYS:HD3	2:F:437:GLU:HB3	1.97	0.45
1:G:195:TYR:O	1:G:197:ASN:N	2.45	0.45
1:A:72:ASP:HA	1:A:75:ILE:HG13	1.98	0.45
1:E:48:LEU:O	1:E:51:VAL:HG22	2.17	0.45
1:G:57:ARG:NH1	1:G:73:GLU:OE2	2.50	0.45
2:H:417:LYS:HB3	2:H:417:LYS:HE2	1.58	0.45
1:G:294:PRO:HG2	1:G:295:PHE:HD2	1.81	0.45
2:B:469:ASN:OD1	2:B:469:ASN:N	2.50	0.45
1:E:11:TYR:CZ	2:F:340:ILE:HG23	2.52	0.44
1:A:79:GLU:OE2	1:A:262:LYS:NZ	2.50	0.44
1:A:97:GLY:HA2	1:A:229:ARG:HD2	2.00	0.44
2:F:445:HIS:O	2:F:449:VAL:HG23	2.17	0.44
1:A:203:SER:OG	1:A:246:GLU:HB3	2.17	0.44
2:D:482:CYS:O	2:D:485:SER:OG	2.27	0.44
1:E:31:THR:OG1	1:E:321:LEU:N	2.46	0.43
2:H:461:ARG:HG3	2:H:493:TYR:CE2	2.52	0.43
1:G:65:LEU:O	1:G:150:ASN:ND2	2.39	0.43
1:E:79:GLU:HG3	1:E:114:HIS:HB2	1.99	0.43
1:E:313:ASN:N	1:E:313:ASN:OD1	2.50	0.43
1:G:95:TYR:CD2	1:G:230:MET:HG2	2.53	0.43
1:G:216:LYS:O	1:G:220:ARG:NH2	2.51	0.43
1:E:321:LEU:HB3	2:F:445:HIS:HD2	1.83	0.43
2:D:335:GLY:HA3	5:D:502:HOH:O	2.18	0.43
1:A:308:LYS:HD3	1:A:308:LYS:HA	1.85	0.43
1:A:36:ILE:HD13	1:A:317:LEU:HD22	1.99	0.43
1:E:37:LEU:HB2	1:E:315:LEU:HB2	1.99	0.43
1:A:315:LEU:HD22	2:B:434:VAL:HG21	2.01	0.43
1:G:42:ASN:HD21	1:G:288:ALA:HB3	1.83	0.43
1:C:183:HIS:O	1:C:185:PRO:HD3	2.18	0.43
1:C:97:GLY:HA3	1:C:230:MET:O	2.19	0.43
1:G:295:PHE:HE1	2:H:393:MET:HE2	1.83	0.43
1:G:183:HIS:O	1:G:185:PRO:HD3	2.19	0.43
1:G:251:PHE:N	5:G:701:HOH:O	2.52	0.42
1:C:97:GLY:HA2	1:C:229:ARG:HD2	2.00	0.42
1:C:82:TYR:CZ	1:C:283:GLN:HG2	2.54	0.42
1:C:11:TYR:CZ	2:D:340:ILE:HG23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ASP:HA	1:C:75:ILE:HG13	2.01	0.42
1:G:317:LEU:HD12	2:H:438:ASN:OD1	2.20	0.42
2:H:457:ARG:HA	2:H:472:PHE:HE2	1.85	0.42
1:E:172:ASN:ND2	1:E:259:LYS:HD3	2.25	0.42
1:A:121:ILE:HG23	1:A:166:LYS:HE2	2.02	0.42
1:A:130:GLU:HB2	1:A:155:ILE:HG13	2.02	0.42
1:A:38:GLU:OE1	1:A:291:SER:OG	2.31	0.42
2:F:482:CYS:O	2:F:486:ILE:HG13	2.20	0.42
1:A:170:ASN:HB2	1:A:237:LEU:HD13	2.02	0.42
1:G:8:CYS:HA	2:H:471:CYS:HA	2.01	0.42
1:E:280:THR:HG21	1:E:288:ALA:HB1	2.01	0.42
2:B:402:ARG:NH1	2:B:415:ASN:OD1	2.53	0.42
2:H:445:HIS:O	2:H:449:VAL:HG23	2.20	0.42
1:G:269:MET:HE2	1:G:285:PRO:HD3	2.01	0.42
1:C:315:LEU:HA	1:C:315:LEU:HD23	1.91	0.41
1:G:9:ILE:N	2:H:470:GLY:O	2.51	0.41
1:C:130:GLU:HB2	1:C:155:ILE:HG13	2.02	0.41
2:H:457:ARG:HA	2:H:472:PHE:CE2	2.55	0.41
1:E:20:VAL:HG21	1:E:318:ALA:HB2	2.02	0.41
2:H:493:TYR:HB3	2:H:494:PRO:HD3	2.01	0.41
1:E:8:CYS:HA	2:F:471:CYS:HA	2.01	0.41
2:H:381:GLY:O	2:H:385:LYS:N	2.49	0.41
1:G:53:PRO:HG3	1:G:82:TYR:CZ	2.56	0.41
2:F:477:LYS:HD3	2:F:477:LYS:HA	1.85	0.41
2:H:421:GLY:O	2:H:425:VAL:HG13	2.20	0.41
1:E:114:HIS:HB3	1:E:262:LYS:HB3	2.03	0.40
1:E:173:GLN:H	1:E:173:GLN:HG2	1.77	0.40
2:F:362:ASN:ND2	2:F:478:CYS:O	2.54	0.40
1:G:266:SER:OG	1:G:267:ALA:N	2.54	0.40
1:G:57:ARG:H	1:G:74:PHE:HZ	1.68	0.40
1:E:214:VAL:HA	1:E:215:PRO:HD3	1.89	0.40
2:F:431:GLU:O	2:F:435:LEU:HG	2.22	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	319/321 (99%)	307 (96%)	12 (4%)	0	100	100
1	C	319/321 (99%)	308 (97%)	11 (3%)	0	100	100
1	E	319/321 (99%)	291 (91%)	26 (8%)	2 (1%)	30	56
1	G	319/321 (99%)	298 (93%)	20 (6%)	1 (0%)	46	72
2	B	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	30	56
2	D	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	16	33
2	F	162/164 (99%)	145 (90%)	15 (9%)	2 (1%)	16	33
2	H	162/164 (99%)	142 (88%)	18 (11%)	2 (1%)	16	33
All	All	1924/1940 (99%)	1794 (93%)	120 (6%)	10 (0%)	34	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	396	GLN
2	F	494	PRO
2	H	396	GLN
1	E	307	PRO
2	F	396	GLN
2	B	494	PRO
2	D	494	PRO
1	G	307	PRO
1	E	196	GLN
2	H	494	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	288/288 (100%)	268 (93%)	20 (7%)	19	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	288/288 (100%)	271 (94%)	17 (6%)	24	47
1	E	288/288 (100%)	265 (92%)	23 (8%)	15	29
1	G	288/288 (100%)	267 (93%)	21 (7%)	17	35
2	B	140/140 (100%)	128 (91%)	12 (9%)	13	25
2	D	140/140 (100%)	129 (92%)	11 (8%)	15	30
2	F	140/140 (100%)	126 (90%)	14 (10%)	9	18
2	H	140/140 (100%)	134 (96%)	6 (4%)	35	64
All	All	1712/1712 (100%)	1588 (93%)	124 (7%)	18	35

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	51	VAL
1	A	56	LEU
1	A	100	ASN
1	A	111	ARG
1	A	149	ARG
1	A	152	VAL
1	A	163	THR
1	A	186	ASN
1	A	208	THR
1	A	213	LEU
1	A	221	SER
1	A	237	LEU
1	A	265	ASP
1	A	274	GLU
1	A	293	MET
1	A	302	THR
1	A	314	ARG
1	A	317	LEU
1	A	321	LEU
2	B	356	TYR
2	B	360	HIS
2	B	364	GLN
2	B	394	ASN
2	B	395	THR
2	B	418	MET
2	B	425	VAL
2	B	432	LEU

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Mol	Chain	Res	Type
2	B	458	LEU
2	B	461	ARG
2	B	467	LEU
2	B	496	TYR
1	C	16	SER
1	C	17	THR
1	C	51	VAL
1	C	56	LEU
1	C	90	THR
1	C	100	ASN
1	C	111	ARG
1	C	149	ARG
1	C	152	VAL
1	C	163	THR
1	C	208	THR
1	C	213	LEU
1	C	221	SER
1	C	237	LEU
1	C	274	GLU
1	C	293	MET
1	C	321	LEU
2	D	351	MET
2	D	356	TYR
2	D	360	HIS
2	D	395	THR
2	D	398	GLU
2	D	418	MET
2	D	425	VAL
2	D	432	LEU
2	D	458	LEU
2	D	467	LEU
2	D	496	TYR
1	E	17	THR
1	E	40	THR
1	E	56	LEU
1	E	72	ASP
1	E	88	ASN
1	E	115	PHE
1	E	142	LEU
1	E	152	VAL
1	E	158	ASN
1	E	163	THR

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Mol	Chain	Res	Type
1	E	176	LEU
1	E	194	LEU
1	E	212	ARG
1	E	213	LEU
1	E	214	VAL
1	E	221	SER
1	E	263	LYS
1	E	274	GLU
1	E	278	CYS
1	E	293	MET
1	E	302	THR
1	E	314	ARG
1	E	321	LEU
2	F	344	ILE
2	F	356	TYR
2	F	360	HIS
2	F	362	ASN
2	F	372	LYS
2	F	373	GLU
2	F	394	ASN
2	F	418	MET
2	F	420	ASP
2	F	425	VAL
2	F	427	THR
2	F	432	LEU
2	F	479	ASP
2	F	496	TYR
1	G	15	ASN
1	G	28	VAL
1	G	29	THR
1	G	40	THR
1	G	49	ASP
1	G	88	ASN
1	G	111	ARG
1	G	115	PHE
1	G	120	ILE
1	G	163	THR
1	G	176	LEU
1	G	194	LEU
1	G	213	LEU
1	G	237	LEU
1	G	263	LYS

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Mol	Chain	Res	Type
1	G	274	GLU
1	G	278	CYS
1	G	293	MET
1	G	302	THR
1	G	310	VAL
1	G	321	LEU
2	H	356	TYR
2	H	360	HIS
2	H	395	THR
2	H	418	MET
2	H	473	GLU
2	H	496	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	150	ASN
1	E	172	ASN
1	E	296	HIS
1	G	119	GLN

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 ⓘ

4 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	SIA	A	602	4	16,20,21	2.58	5 (31%)	18,28,31	2.29	3 (16%)
4	GAL	A	603	4	12,12,12	0.59	0	17,17,17	0.92	1 (5%)
4	SIA	C	602	4	16,20,21	2.59	4 (25%)	18,28,31	2.50	4 (22%)
4	GAL	C	603	4	12,12,12	0.64	0	17,17,17	1.43	4 (23%)

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	SIA	A	602	4	-	0/14/34/38	0/1/1/1
4	GAL	A	603	4	-	0/2/22/22	0/1/1/1
4	SIA	C	602	4	-	0/14/34/38	0/1/1/1
4	GAL	C	603	4	-	0/2/22/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	SIA	C7-C6	-7.25	1.43	1.52
4	C	602	SIA	C7-C6	-6.98	1.44	1.52
4	C	602	SIA	O7-C7	-2.42	1.37	1.43
4	A	602	SIA	O7-C7	-2.41	1.37	1.43
4	A	602	SIA	C5-N5	2.01	1.49	1.45
4	A	602	SIA	O6-C6	3.89	1.50	1.43
4	C	602	SIA	C10-N5	3.91	1.49	1.34
4	A	602	SIA	C10-N5	3.98	1.49	1.34
4	C	602	SIA	O6-C6	4.66	1.51	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	SIA	O6-C2-C3	-9.03	92.50	109.86
4	A	602	SIA	O6-C2-C3	-7.92	94.64	109.86
4	C	603	GAL	O5-C1-C2	-2.63	105.61	109.80
4	C	602	SIA	C8-C7-C6	-2.06	108.87	113.01
4	A	603	GAL	C3-C4-C5	2.15	113.95	110.20
4	C	603	GAL	C3-C4-C5	2.22	114.06	110.20
4	C	602	SIA	C11-C10-N5	2.28	120.46	116.11
4	A	602	SIA	C3-C4-C5	2.64	114.42	111.47
4	C	603	GAL	C4-C3-C2	2.80	116.03	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	GAL	O5-C5-C4	2.85	115.03	109.68
4	C	602	SIA	O9-C9-C8	2.96	117.53	111.10
4	A	602	SIA	O9-C9-C8	2.96	117.54	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

4 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	0.49	0	15,19,21	0.96	1 (6%)
3	NAG	C	601	1	14,14,15	0.45	0	15,19,21	1.02	1 (6%)
3	NAG	E	601	1	14,14,15	0.46	0	15,19,21	1.09	2 (13%)
3	NAG	G	601	1	14,14,15	0.50	0	15,19,21	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	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
3	NAG	G	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	NAG	C2-N2-C7	-2.01	120.46	123.04
3	A	601	NAG	C1-O5-C5	2.36	115.24	112.25
3	E	601	NAG	C1-O5-C5	2.57	115.51	112.25
3	C	601	NAG	C1-O5-C5	2.96	116.00	112.25

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 [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	321/321 (100%)	-0.33	0 100 100	16, 37, 59, 83	0
1	C	321/321 (100%)	-0.35	0 100 100	14, 37, 58, 86	0
1	E	321/321 (100%)	0.37	29 (9%) 12 8	33, 72, 130, 180	0
1	G	321/321 (100%)	0.41	33 (10%) 9 5	29, 74, 131, 228	0
2	B	164/164 (100%)	0.10	4 (2%) 62 56	21, 51, 82, 114	0
2	D	164/164 (100%)	0.08	5 (3%) 54 47	18, 52, 84, 118	0
2	F	164/164 (100%)	1.43	51 (31%) 1 0	41, 123, 172, 198	0
2	H	164/164 (100%)	1.47	42 (25%) 1 0	40, 122, 175, 234	0
All	All	1940/1940 (100%)	0.28	164 (8%) 13 9	14, 56, 146, 234	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	492	ASN	9.3
2	H	474	PHE	7.5
2	F	474	PHE	6.6
2	H	493	TYR	6.0
2	F	366	SER	5.9
2	H	357	GLY	5.8
2	F	486	ILE	5.8
2	F	493	TYR	5.7
2	H	475	TYR	5.5
2	H	353	ASP	5.5
2	F	357	GLY	5.5
2	H	486	ILE	5.5
2	F	472	PHE	5.3
2	H	492	ASN	5.2
2	H	462	ASP	5.2
2	H	366	SER	5.2

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Mol	Chain	Res	Type	RSRZ
2	F	494	PRO	5.1
2	F	459	GLN	5.0
2	H	367	GLY	5.0
2	H	491	TYR	5.0
1	G	48	LEU	4.9
2	F	475	TYR	4.9
2	F	458	LEU	4.9
2	H	451	ASN	4.8
1	E	16	SER	4.7
2	H	488	ASN	4.7
2	F	353	ASP	4.6
2	H	476	HIS	4.6
2	H	465	LYS	4.5
1	G	323	ASN	4.4
2	H	458	LEU	4.4
2	F	367	GLY	4.3
2	H	360	HIS	4.3
2	H	350	GLY	4.3
1	E	323	ASN	4.2
1	G	5	ASP	4.2
1	E	48	LEU	4.2
2	H	472	PHE	4.1
2	F	497	SER	4.1
2	H	497	SER	4.1
1	G	46	CYS	4.0
1	G	15	ASN	3.9
2	H	490	THR	3.8
2	F	478	CYS	3.8
1	E	286	MET	3.7
2	H	481	GLU	3.7
2	F	457	ARG	3.6
2	B	365	GLY	3.6
2	H	336	LEU	3.5
2	F	360	HIS	3.5
2	F	481	GLU	3.5
1	E	276	GLY	3.5
1	G	278	CYS	3.5
2	F	365	GLY	3.5
2	F	482	CYS	3.4
2	F	354	GLY	3.4
2	H	487	ARG	3.4
2	H	454	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	338	GLY	3.4
2	F	488	ASN	3.4
2	F	350	GLY	3.3
2	B	367	GLY	3.3
1	E	76	ASN	3.3
1	E	46	CYS	3.3
2	F	483	MET	3.2
2	F	462	ASP	3.2
2	H	482	CYS	3.2
2	F	338	GLY	3.2
1	E	9	ILE	3.2
2	H	365	GLY	3.2
1	G	9	ILE	3.1
1	G	37	LEU	3.1
1	E	4	GLN	3.1
1	E	324	SER	3.1
2	H	335	GLY	3.1
2	F	490	THR	3.1
2	F	491	TYR	3.1
2	H	459	GLN	3.1
2	F	460	LEU	3.0
2	F	454	ASP	3.0
2	F	363	GLU	3.0
2	F	473	GLU	3.0
1	G	286	MET	3.0
1	E	15	ASN	3.0
2	H	361	SER	2.9
1	E	34	GLN	2.9
1	E	316	VAL	2.8
1	G	305	GLU	2.8
2	H	494	PRO	2.8
2	H	496	TYR	2.8
2	F	468	GLY	2.8
1	E	42	ASN	2.8
2	F	463	ASN	2.8
2	F	450	LYS	2.8
2	D	365	GLY	2.8
2	H	352	VAL	2.8
1	G	14	ASN	2.8
1	E	278	CYS	2.8
1	E	30	VAL	2.7
1	G	42	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	38	GLU	2.7
2	F	496	TYR	2.7
1	G	19	GLN	2.6
2	F	349	GLN	2.6
1	E	298	ILE	2.6
1	G	276	GLY	2.6
2	D	367	GLY	2.6
2	H	351	MET	2.6
1	E	18	GLU	2.6
2	F	337	PHE	2.5
2	F	368	TYR	2.5
1	G	32	HIS	2.5
1	G	16	SER	2.5
1	E	19	GLN	2.5
2	F	467	LEU	2.4
1	G	17	THR	2.4
2	D	496	TYR	2.4
1	G	44	LYS	2.4
1	E	40	THR	2.4
1	G	34	GLN	2.4
1	E	305	GLU	2.4
1	E	47	ASP	2.4
2	H	368	TYR	2.3
2	H	450	LYS	2.3
2	F	476	HIS	2.3
1	E	290	ASN	2.3
2	D	481	GLU	2.3
2	H	363	GLU	2.3
1	G	13	ALA	2.3
2	F	452	LEU	2.3
2	H	452	LEU	2.3
2	F	489	GLY	2.3
1	G	20	VAL	2.2
1	G	292	SER	2.2
1	G	314	ARG	2.2
1	G	18	GLU	2.2
1	E	32	HIS	2.2
2	F	361	SER	2.2
2	D	366	SER	2.2
2	F	369	ALA	2.2
1	G	293	MET	2.2
1	G	304	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	451	ASN	2.2
1	E	288	ALA	2.2
1	G	4	GLN	2.1
2	H	483	MET	2.2
1	G	324	SER	2.1
2	B	366	SER	2.1
1	E	8	CYS	2.1
2	F	477	LYS	2.1
1	E	6	GLN	2.1
2	F	440	ARG	2.1
1	G	287	GLY	2.1
2	H	362	ASN	2.1
2	F	336	LEU	2.1
2	F	359	HIS	2.1
1	E	304	GLY	2.1
1	G	288	ALA	2.1
1	G	142	LEU	2.0
1	G	30	VAL	2.0
2	F	358	TYR	2.0
2	H	460	LEU	2.0
1	E	279	ASN	2.0
2	B	496	TYR	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	SIA	C	602	20/21	0.95	0.13	-0.73	28,40,47,48	0
4	SIA	A	602	20/21	0.96	0.12	-0.89	26,39,46,50	0
4	GAL	C	603	12/12	0.82	0.23	-	52,69,82,83	0
4	GAL	A	603	12/12	0.81	0.22	-	52,71,84,95	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
3	NAG	G	601	14/15	0.74	0.42	5.01	90,110,118,125	0
3	NAG	E	601	14/15	0.80	0.37	4.09	97,116,124,129	0
3	NAG	C	601	14/15	0.91	0.24	2.59	35,56,71,83	0
3	NAG	A	601	14/15	0.92	0.22	1.78	34,62,74,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.