



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:06 PM GMT

PDB ID : 4NRK
Title : Structure of hemagglutinin with F95Y mutation of influenza virus B/Lee/40 complex with LSTc
Authors : Ni, F.; Mbawuike, I.N.; Kondrashkina, E.; Wang, Q.
Deposited on : 2013-11-26
Resolution : 2.63 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

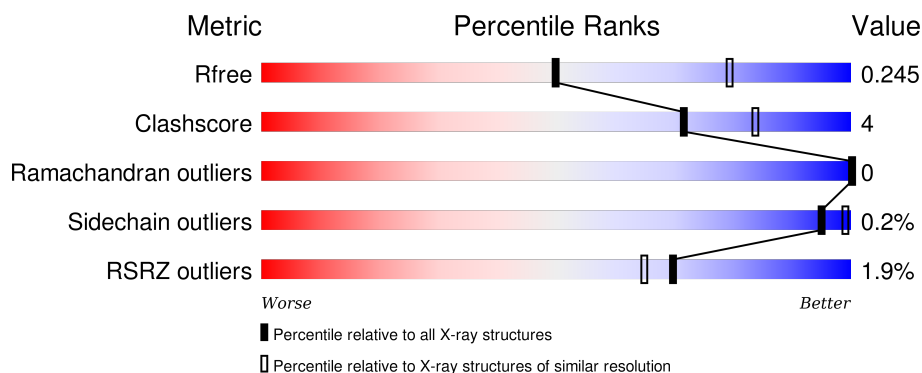
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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	346	<div> <div>2%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	C	346	<div> <div>2%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	E	346	<div> <div>%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
2	B	182	<div> <div>5%</div> <div>85%</div> <div>7%</div> <div>8%</div> </div>
2	D	182	<div> <div>84%</div> <div>9%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	182	

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	401	-	-	-	X
3	NAG	C	409	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2591	1625	459	491	16			
1	C	341	Total	C	N	O	S	0	0	0
			2596	1628	460	492	16			
1	E	340	Total	C	N	O	S	0	0	0
			2591	1625	459	491	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ARG	LYS	CONFLICT	UNP P03460
A	76	ILE	THR	CONFLICT	UNP P03460
A	90	VAL	ALA	CONFLICT	UNP P03460
A	95	TYR	PHE	ENGINEERED MUTATION	UNP P03460
A	147	THR	ALA	CONFLICT	UNP P03460
A	167	ILE	THR	CONFLICT	UNP P03460
C	38	ARG	LYS	CONFLICT	UNP P03460
C	76	ILE	THR	CONFLICT	UNP P03460
C	90	VAL	ALA	CONFLICT	UNP P03460
C	95	TYR	PHE	ENGINEERED MUTATION	UNP P03460
C	147	THR	ALA	CONFLICT	UNP P03460
C	167	ILE	THR	CONFLICT	UNP P03460
E	38	ARG	LYS	CONFLICT	UNP P03460
E	76	ILE	THR	CONFLICT	UNP P03460
E	90	VAL	ALA	CONFLICT	UNP P03460
E	95	TYR	PHE	ENGINEERED MUTATION	UNP P03460
E	147	THR	ALA	CONFLICT	UNP P03460
E	167	ILE	THR	CONFLICT	UNP P03460

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	168	Total	C	N	O	S	0	0	0
			1275	797	218	254	6			
2	D	168	Total	C	N	O	S	0	0	0
			1275	797	218	254	6			
2	F	168	Total	C	N	O	S	0	0	0
			1275	797	218	254	6			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	54	SER	TYR	CONFLICT	UNP P03460
B	177	GLY	-	EXPRESSION TAG	UNP P03460
B	178	ALA	-	EXPRESSION TAG	UNP P03460
B	179	LEU	-	EXPRESSION TAG	UNP P03460
B	180	VAL	-	EXPRESSION TAG	UNP P03460
B	181	PRO	-	EXPRESSION TAG	UNP P03460
B	182	ARG	-	EXPRESSION TAG	UNP P03460
D	54	SER	TYR	CONFLICT	UNP P03460
D	177	GLY	-	EXPRESSION TAG	UNP P03460
D	178	ALA	-	EXPRESSION TAG	UNP P03460
D	179	LEU	-	EXPRESSION TAG	UNP P03460
D	180	VAL	-	EXPRESSION TAG	UNP P03460
D	181	PRO	-	EXPRESSION TAG	UNP P03460
D	182	ARG	-	EXPRESSION TAG	UNP P03460
F	54	SER	TYR	CONFLICT	UNP P03460
F	177	GLY	-	EXPRESSION TAG	UNP P03460
F	178	ALA	-	EXPRESSION TAG	UNP P03460
F	179	LEU	-	EXPRESSION TAG	UNP P03460
F	180	VAL	-	EXPRESSION TAG	UNP P03460
F	181	PRO	-	EXPRESSION TAG	UNP P03460
F	182	ARG	-	EXPRESSION TAG	UNP P03460

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

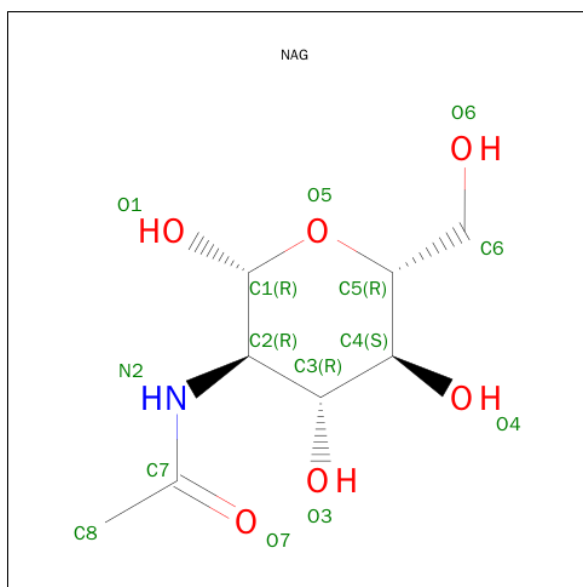
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			45	25	2	18		
5	C	3	Total	C	N	O	0	0
			45	25	2	18		
5	E	3	Total	C	N	O	0	0
			45	25	2	18		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	3	Total	C	N	O	0	0
			39	22	2	15		

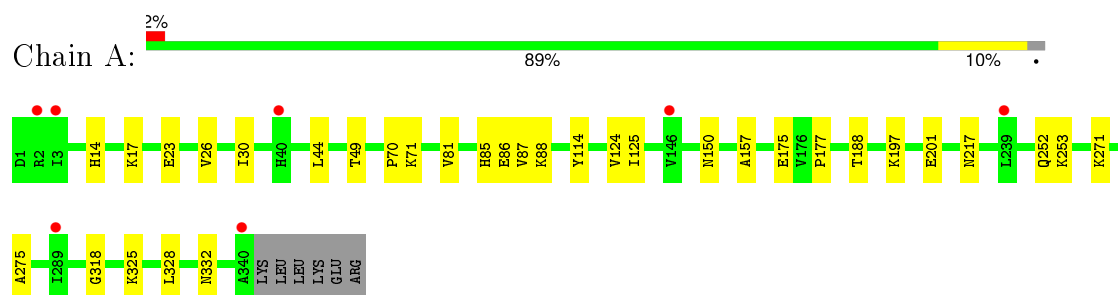
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	88	Total	O	0	0
			88	88		
7	B	21	Total	O	0	0
			21	21		
7	C	72	Total	O	0	0
			72	72		
7	D	34	Total	O	0	0
			34	34		
7	E	104	Total	O	0	0
			104	104		
7	F	31	Total	O	0	0
			31	31		

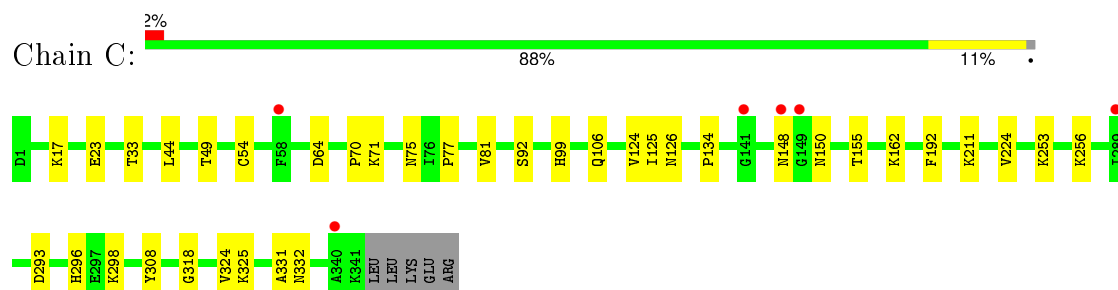
3 Residue-property plots [i](#)

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.

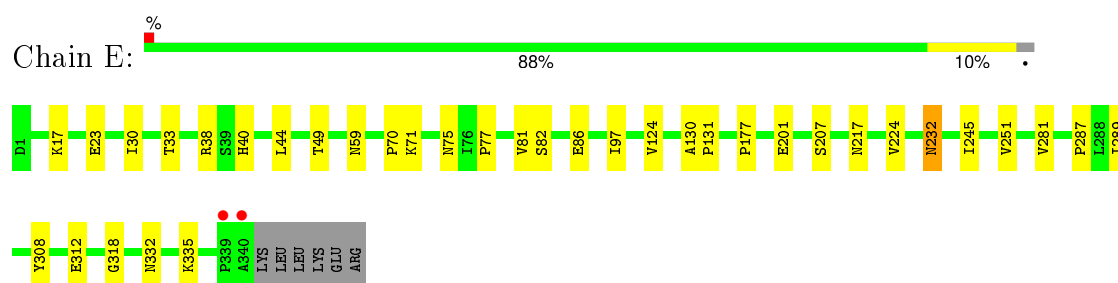
- Molecule 1: Hemagglutinin HA1 chain



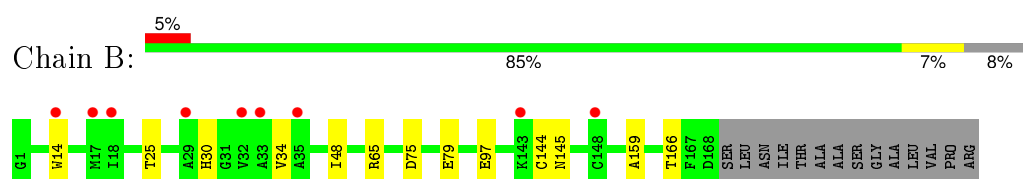
- Molecule 1: Hemagglutinin HA1 chain



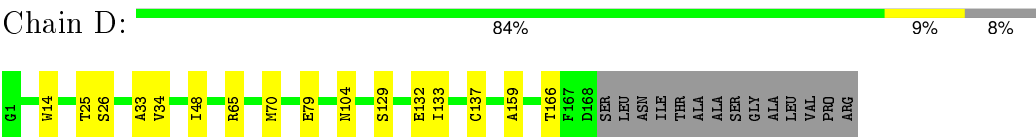
- Molecule 1: Hemagglutinin HA1 chain



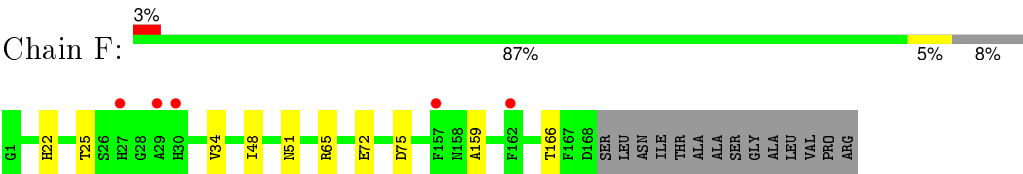
- Molecule 2: Hemagglutinin HA2 chain



● Molecule 2: Hemagglutinin HA2 chain



● Molecule 2: Hemagglutinin HA2 chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.61Å 128.30Å 211.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.87 – 2.63 45.87 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.87-2.63) 100.0 (45.87-2.63)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1452)	Depositor
R, R_{free}	0.207 , 0.245 0.207 , 0.245	Depositor DCC
R_{free} test set	3437 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 68512 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12547	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, BMA, 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	0.22	0/2650	0.42	0/3603
1	C	0.22	0/2655	0.43	0/3610
1	E	0.22	0/2650	0.42	0/3603
2	B	0.21	0/1294	0.35	0/1744
2	D	0.21	0/1294	0.37	0/1744
2	F	0.21	0/1294	0.36	0/1744
All	All	0.22	0/11837	0.40	0/16048

There are no bond length outliers.

There are no bond angle outliers.

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	2591	0	2584	24	0
1	C	2596	0	2586	28	0
1	E	2591	0	2583	24	0
2	B	1275	0	1246	10	0
2	D	1275	0	1246	14	0
2	F	1275	0	1246	7	0
3	A	112	0	100	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	84	0	75	1	0
3	E	140	0	125	2	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
5	A	45	0	38	1	0
5	C	45	0	38	1	0
5	E	45	0	38	1	0
6	C	39	0	34	1	0
7	A	88	0	0	8	0
7	B	21	0	0	2	0
7	C	72	0	0	9	0
7	D	34	0	0	4	0
7	E	104	0	0	9	0
7	F	31	0	0	2	0
All	All	12547	0	12017	103	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 4.

All (103) 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:224:VAL:O	7:E:587:HOH:O	1.83	0.97
1:A:175:GLU:OE1	7:A:524:HOH:O	1.92	0.87
1:E:86:GLU:OE2	7:E:528:HOH:O	1.93	0.86
2:D:79:GLU:OE1	7:D:322:HOH:O	1.97	0.81
3:A:401:NAG:O7	7:A:563:HOH:O	2.00	0.80
1:C:148:ASN:O	7:C:559:HOH:O	2.01	0.79
1:C:54:CYS:SG	7:C:555:HOH:O	2.43	0.77
1:E:335:LYS:O	7:E:555:HOH:O	2.03	0.76
1:C:256:LYS:NZ	7:C:564:HOH:O	2.20	0.75
1:C:293:ASP:O	7:C:570:HOH:O	2.03	0.74
2:D:129:SER:OG	7:D:330:HOH:O	2.06	0.74
5:E:414:NAG:O7	7:E:594:HOH:O	2.09	0.70
1:A:271:LYS:NZ	7:A:576:HOH:O	2.24	0.70
2:D:159:ALA:HB3	2:D:166:THR:HG22	1.73	0.69
2:B:65:ARG:O	7:B:303:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:406:NAG:H83	3:E:406:NAG:H3	1.75	0.68
2:D:132:GLU:OE2	7:D:333:HOH:O	2.14	0.66
2:B:79:GLU:OE2	7:B:315:HOH:O	2.12	0.65
1:C:331:ALA:H	2:D:104:ASN:HD21	1.42	0.64
1:C:324:VAL:O	7:C:558:HOH:O	2.13	0.64
1:A:150:ASN:ND2	7:A:584:HOH:O	2.29	0.64
2:B:159:ALA:HB3	2:B:166:THR:HG22	1.82	0.62
2:D:65:ARG:NH1	7:D:326:HOH:O	2.14	0.61
1:C:331:ALA:H	2:D:104:ASN:ND2	1.98	0.61
2:F:25:THR:HG22	2:F:34:VAL:HG22	1.82	0.60
1:E:33:THR:HG22	1:E:308:TYR:HB2	1.84	0.59
2:D:14:TRP:CE2	2:D:25:THR:HG21	2.37	0.59
2:F:51:ASN:ND2	7:F:322:HOH:O	2.36	0.59
5:C:413:NAG:H83	5:C:413:NAG:H3	1.84	0.59
1:C:17:LYS:HG2	1:C:23:GLU:HG2	1.88	0.56
2:F:159:ALA:HB3	2:F:166:THR:HG22	1.88	0.56
2:F:65:ARG:O	7:F:305:HOH:O	2.18	0.55
3:E:406:NAG:O7	7:E:558:HOH:O	2.18	0.55
1:E:30:ILE:HG13	1:E:332:ASN:HB2	1.89	0.54
2:D:25:THR:HG22	2:D:34:VAL:HG22	1.88	0.54
1:A:332:ASN:HA	2:B:48:ILE:HD13	1.90	0.54
1:E:49:THR:HG23	1:E:81:VAL:HG12	1.89	0.54
1:A:30:ILE:HG13	1:A:332:ASN:HB2	1.91	0.53
3:C:410:NAG:H83	3:C:410:NAG:H3	1.91	0.53
5:A:412:NAG:H3	5:A:412:NAG:H83	1.91	0.53
1:C:134:PRO:HB2	1:C:162:LYS:HG3	1.90	0.53
1:E:232:ASN:HD22	1:E:232:ASN:N	2.06	0.52
1:A:197:LYS:NZ	1:A:201:GLU:OE2	2.38	0.52
1:C:192:PHE:O	7:C:512:HOH:O	2.18	0.51
1:E:17:LYS:HG2	1:E:23:GLU:HG2	1.92	0.51
1:C:332:ASN:HA	2:D:48:ILE:HD13	1.91	0.51
1:A:85:HIS:N	7:A:539:HOH:O	2.45	0.49
1:E:201:GLU:HG3	1:E:207:SER:HB3	1.95	0.49
1:E:332:ASN:HA	2:F:48:ILE:HD13	1.94	0.49
2:D:26:SER:HB3	2:D:33:ALA:HB3	1.95	0.49
1:A:49:THR:HG23	1:A:81:VAL:HG12	1.95	0.48
1:A:271:LYS:O	7:A:503:HOH:O	2.18	0.48
1:E:86:GLU:OE1	7:E:518:HOH:O	2.20	0.48
1:C:124:VAL:HG13	1:C:125:ILE:HG12	1.97	0.47
1:C:49:THR:HG23	1:C:81:VAL:HG12	1.95	0.47
1:A:17:LYS:HG2	1:A:23:GLU:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:HG13	1:A:125:ILE:HG12	1.96	0.47
1:E:75:ASN:O	1:E:77:PRO:HD3	2.15	0.47
1:C:211:LYS:HG2	1:C:224:VAL:HG22	1.97	0.46
1:E:287:PRO:HG2	1:E:289:ILE:HD11	1.97	0.46
1:A:87:VAL:HG12	1:A:88:LYS:HG3	1.97	0.46
1:E:217:ASN:ND2	1:E:251:VAL:O	2.49	0.46
1:C:64:ASP:OD2	1:C:92:SER:OG	2.23	0.46
1:A:124:VAL:HG22	1:A:177:PRO:HD2	1.98	0.45
1:A:44:LEU:HD11	1:A:318:GLY:HA3	1.99	0.45
1:A:14:HIS:HB2	1:A:26:VAL:HG23	1.99	0.45
1:C:126:ASN:N	7:C:517:HOH:O	2.49	0.45
1:E:38:ARG:HG3	7:E:604:HOH:O	2.17	0.45
1:C:296:HIS:CE1	1:C:298:LYS:HB2	2.52	0.45
1:E:97:ILE:HG12	1:E:245:ILE:HD11	1.99	0.44
1:A:188:THR:OG1	1:A:252:GLN:NE2	2.51	0.44
1:A:325:LYS:HB2	1:A:325:LYS:HE3	1.71	0.44
1:C:150:ASN:N	6:C:403:NAG:O6	2.50	0.44
1:E:38:ARG:N	7:E:604:HOH:O	2.24	0.44
1:C:325:LYS:HE3	1:C:325:LYS:HB2	1.74	0.44
2:D:133:ILE:HD12	2:D:137:CYS:HB2	2.00	0.43
1:C:75:ASN:O	1:C:77:PRO:HD3	2.18	0.43
1:E:312:GLU:OE1	7:E:593:HOH:O	2.21	0.43
1:C:44:LEU:HD11	1:C:318:GLY:HA3	2.00	0.43
1:C:70:PRO:O	1:C:71:LYS:HB2	2.18	0.43
1:C:33:THR:HG22	1:C:308:TYR:HB2	2.00	0.43
1:E:124:VAL:HG22	1:E:177:PRO:HD2	2.01	0.42
2:B:30:HIS:NE2	2:B:144:CYS:O	2.52	0.42
1:A:217:ASN:HD22	2:F:72:GLU:HB3	1.83	0.42
1:A:157:ALA:HA	7:A:513:HOH:O	2.19	0.42
1:A:114:TYR:CG	1:A:275:ALA:HB1	2.54	0.42
2:B:25:THR:HG22	2:B:34:VAL:HG22	2.01	0.42
1:E:40:HIS:ND1	1:E:289:ILE:HB	2.34	0.42
1:C:106:GLN:HB3	2:D:70:MET:CE	2.49	0.42
1:E:130:ALA:HA	1:E:131:PRO:HD3	1.96	0.42
1:E:44:LEU:HD11	1:E:318:GLY:HA3	2.02	0.42
1:C:99:HIS:ND1	7:C:532:HOH:O	2.06	0.42
2:B:30:HIS:CD2	2:B:145:ASN:HA	2.55	0.41
2:B:75:ASP:OD2	1:C:253:LYS:HE3	2.20	0.41
1:C:155:THR:O	7:C:551:HOH:O	2.22	0.41
1:A:253:LYS:HE3	2:F:75:ASP:OD2	2.21	0.41
1:A:328:LEU:HD21	2:B:97:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:TRP:CE2	2:B:25:THR:HG21	2.56	0.41
1:A:70:PRO:O	1:A:71:LYS:HB2	2.20	0.41
1:A:86:GLU:N	7:A:539:HOH:O	2.22	0.40
1:C:106:GLN:O	2:D:70:MET:HE2	2.21	0.40
1:E:70:PRO:O	1:E:71:LYS:HB2	2.21	0.40
1:E:82:SER:HB2	1:E:281:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/346 (98%)	325 (96%)	13 (4%)	0	100	100
1	C	339/346 (98%)	327 (96%)	12 (4%)	0	100	100
1	E	338/346 (98%)	325 (96%)	13 (4%)	0	100	100
2	B	166/182 (91%)	164 (99%)	2 (1%)	0	100	100
2	D	166/182 (91%)	164 (99%)	2 (1%)	0	100	100
2	F	166/182 (91%)	164 (99%)	2 (1%)	0	100	100
All	All	1513/1584 (96%)	1469 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/298 (98%)	292 (100%)	0	100	100
1	C	292/298 (98%)	292 (100%)	0	100	100
1	E	292/298 (98%)	290 (99%)	2 (1%)	88	96
2	B	135/145 (93%)	135 (100%)	0	100	100
2	D	135/145 (93%)	135 (100%)	0	100	100
2	F	135/145 (93%)	134 (99%)	1 (1%)	88	96
All	All	1281/1329 (96%)	1278 (100%)	3 (0%)	95	99

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	59	ASN
1	E	232	ASN
2	F	22	HIS

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

Mol	Chain	Res	Type
1	A	150	ASN
1	A	217	ASN
1	A	252	GLN
1	C	14	HIS
1	C	150	ASN
2	D	104	ASN
1	E	217	ASN
2	F	30	HIS

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 ⓘ

36 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	$\# Z > 2$
3	NAG	A	401	1,3	14,14,15	0.35	0	15,19,21	0.26	0
3	NAG	A	402	3	14,14,15	0.17	0	15,19,21	0.22	0
3	NAG	A	403	1,3	14,14,15	1.06	1 (7%)	15,19,21	2.26	2 (13%)
3	NAG	A	404	3	14,14,15	0.27	0	15,19,21	0.34	0
3	NAG	A	406	1,3	14,14,15	0.97	1 (7%)	15,19,21	1.50	1 (6%)
3	NAG	A	407	3	14,14,15	0.34	0	15,19,21	0.37	0
3	NAG	A	408	1,3	14,14,15	0.66	1 (7%)	15,19,21	0.98	1 (6%)
3	NAG	A	409	3	14,14,15	0.25	0	15,19,21	0.24	0
5	SIA	A	410	5	16,20,21	1.08	2 (12%)	18,28,31	1.41	5 (27%)
5	GAL	A	411	5	11,11,12	0.69	0	14,15,17	0.86	0
5	NAG	A	412	5	14,14,15	0.47	0	15,19,21	1.34	1 (6%)
3	NAG	C	401	1,3	14,14,15	1.40	1 (7%)	15,19,21	2.07	1 (6%)
3	NAG	C	402	3	14,14,15	0.52	0	15,19,21	1.07	1 (6%)
6	NAG	C	403	1,6	14,14,15	0.36	0	15,19,21	0.60	0
6	NAG	C	404	6	14,14,15	0.41	0	15,19,21	0.55	0
6	BMA	C	405	6	11,11,12	0.98	1 (9%)	14,15,17	1.11	1 (7%)
3	NAG	C	407	1,3	14,14,15	0.36	0	15,19,21	0.51	0
3	NAG	C	408	3	14,14,15	0.19	0	15,19,21	0.28	0
3	NAG	C	409	1,3	14,14,15	0.61	1 (7%)	15,19,21	0.46	0
3	NAG	C	410	3	14,14,15	0.33	0	15,19,21	1.31	1 (6%)
5	SIA	C	411	5	16,20,21	1.06	2 (12%)	18,28,31	1.62	4 (22%)
5	GAL	C	412	5	11,11,12	0.46	0	14,15,17	1.03	1 (7%)
5	NAG	C	413	5	14,14,15	0.39	0	15,19,21	1.31	1 (6%)
3	NAG	E	401	1,3	14,14,15	0.27	0	15,19,21	0.31	0
3	NAG	E	402	3	14,14,15	0.21	0	15,19,21	0.28	0
3	NAG	E	404	1,3	14,14,15	1.30	1 (7%)	15,19,21	2.01	1 (6%)
3	NAG	E	405	3	14,14,15	0.29	0	15,19,21	0.42	0
3	NAG	E	406	1,3	14,14,15	1.37	1 (7%)	15,19,21	1.53	3 (20%)
3	NAG	E	407	3	14,14,15	0.42	0	15,19,21	0.53	0
3	NAG	E	408	1,3	14,14,15	0.34	0	15,19,21	0.37	0
3	NAG	E	409	3	14,14,15	0.24	0	15,19,21	0.27	0
3	NAG	E	410	1,3	14,14,15	0.55	0	15,19,21	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	411	3	14,14,15	0.35	0	15,19,21	0.37	0
5	SIA	E	412	5	16,20,21	1.08	2 (12%)	18,28,31	1.59	4 (22%)
5	GAL	E	413	5	11,11,12	0.65	0	14,15,17	0.80	0
5	NAG	E	414	5	14,14,15	0.27	0	15,19,21	0.45	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	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	402	3	-	0/6/23/26	0/1/1/1
3	NAG	A	403	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	404	3	-	0/6/23/26	0/1/1/1
3	NAG	A	406	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	407	3	-	0/6/23/26	0/1/1/1
3	NAG	A	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	409	3	-	0/6/23/26	0/1/1/1
5	SIA	A	410	5	-	0/14/34/38	0/1/1/1
5	GAL	A	411	5	-	0/2/19/22	0/1/1/1
5	NAG	A	412	5	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	402	3	-	0/6/23/26	0/1/1/1
6	NAG	C	403	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	404	6	-	0/6/23/26	0/1/1/1
6	BMA	C	405	6	-	0/2/19/22	0/1/1/1
3	NAG	C	407	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	408	3	-	0/6/23/26	0/1/1/1
3	NAG	C	409	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	410	3	-	0/6/23/26	0/1/1/1
5	SIA	C	411	5	-	0/14/34/38	0/1/1/1
5	GAL	C	412	5	-	0/2/19/22	0/1/1/1
5	NAG	C	413	5	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	402	3	-	0/6/23/26	0/1/1/1
3	NAG	E	404	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	405	3	-	0/6/23/26	0/1/1/1
3	NAG	E	406	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	407	3	-	0/6/23/26	0/1/1/1
3	NAG	E	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	409	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	410	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	411	3	-	0/6/23/26	0/1/1/1
5	SIA	E	412	5	-	0/14/34/38	0/1/1/1
5	GAL	E	413	5	-	0/2/19/22	0/1/1/1
5	NAG	E	414	5	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	406	NAG	O5-C1	-4.66	1.35	1.43
5	E	412	SIA	C5-N5	-2.16	1.42	1.45
3	C	409	NAG	O5-C1	-2.15	1.40	1.43
5	A	410	SIA	C5-N5	-2.13	1.42	1.45
5	C	411	SIA	C5-N5	-2.10	1.42	1.45
5	E	412	SIA	C10-N5	2.08	1.42	1.34
5	C	411	SIA	C10-N5	2.09	1.42	1.34
5	A	410	SIA	C10-N5	2.11	1.42	1.34
3	A	408	NAG	O5-C1	2.17	1.47	1.43
6	C	405	BMA	C1-C2	2.40	1.57	1.52
3	A	406	NAG	O5-C1	3.54	1.49	1.43
3	A	403	NAG	O5-C1	3.79	1.50	1.43
3	E	404	NAG	O5-C1	4.78	1.51	1.43
3	C	401	NAG	O5-C1	5.15	1.52	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	411	SIA	C7-C6-C5	-3.92	108.38	114.32
5	E	412	SIA	C7-C6-C5	-3.42	109.14	114.32
6	C	405	BMA	O2-C2-C3	-3.21	103.67	110.12
5	C	411	SIA	O6-C2-C3	-3.11	103.87	109.86
5	E	412	SIA	C3-C4-C5	-2.83	108.32	111.47
5	A	410	SIA	O6-C2-C3	-2.77	104.52	109.86
5	E	412	SIA	O6-C2-C3	-2.55	104.95	109.86
5	A	410	SIA	C7-C6-C5	-2.52	110.51	114.32
5	C	411	SIA	C3-C4-C5	-2.47	108.72	111.47
5	A	410	SIA	C8-C7-C6	-2.20	108.58	113.01
3	E	406	NAG	C1-O5-C5	-2.15	109.51	112.25
5	A	410	SIA	C3-C4-C5	-2.11	109.13	111.47
5	E	412	SIA	C11-C10-N5	2.15	120.22	116.11
5	C	412	GAL	C1-O5-C5	2.15	114.98	112.25
5	C	411	SIA	C11-C10-N5	2.16	120.24	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	410	SIA	C11-C10-N5	2.27	120.46	116.11
3	E	406	NAG	C4-C3-C2	2.32	114.84	111.23
3	A	408	NAG	C1-O5-C5	3.49	116.68	112.25
3	C	402	NAG	C1-O5-C5	3.89	117.19	112.25
3	E	406	NAG	C2-N2-C7	4.29	128.56	123.04
5	A	412	NAG	C2-N2-C7	4.65	129.02	123.04
5	C	413	NAG	C2-N2-C7	4.68	129.05	123.04
3	C	410	NAG	C2-N2-C7	4.78	129.18	123.04
3	A	403	NAG	C2-N2-C7	4.97	129.43	123.04
3	A	406	NAG	C1-O5-C5	5.66	119.43	112.25
3	A	403	NAG	C1-O5-C5	6.77	120.83	112.25
3	E	404	NAG	C1-O5-C5	7.63	121.93	112.25
3	C	401	NAG	C1-O5-C5	7.81	122.16	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	1	0
5	A	412	NAG	1	0
6	C	403	NAG	1	0
3	C	410	NAG	1	0
5	C	413	NAG	1	0
3	E	406	NAG	2	0
5	E	414	NAG	1	0

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	405	1	14,14,15	0.42	0	15,19,21	0.59	1 (6%)
4	NAG	B	201	2	14,14,15	0.73	1 (7%)	15,19,21	0.71	0
4	NAG	C	406	1	14,14,15	1.21	1 (7%)	15,19,21	0.93	2 (13%)
4	NAG	D	201	2	14,14,15	2.24	2 (14%)	15,19,21	3.05	1 (6%)
4	NAG	E	403	1	14,14,15	0.60	1 (7%)	15,19,21	0.49	0
4	NAG	F	201	2	14,14,15	0.33	0	15,19,21	0.87	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
4	NAG	A	405	1	-	0/6/23/26	0/1/1/1
4	NAG	B	201	2	-	0/6/23/26	0/1/1/1
4	NAG	C	406	1	-	0/6/23/26	0/1/1/1
4	NAG	D	201	2	-	0/6/23/26	0/1/1/1
4	NAG	E	403	1	-	0/6/23/26	0/1/1/1
4	NAG	F	201	2	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	406	NAG	O5-C1	-4.00	1.37	1.43
4	E	403	NAG	O5-C1	-2.01	1.40	1.43
4	B	201	NAG	O5-C1	2.62	1.48	1.43
4	D	201	NAG	C1-C2	4.11	1.58	1.52
4	D	201	NAG	O5-C1	7.27	1.55	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	406	NAG	C1-O5-C5	-2.49	109.09	112.25
4	A	405	NAG	C1-O5-C5	2.06	114.86	112.25
4	C	406	NAG	C3-C4-C5	2.23	114.08	110.20
4	F	201	NAG	C1-O5-C5	2.31	115.18	112.25
4	D	201	NAG	C1-O5-C5	11.56	126.92	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

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, 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	340/346 (98%)	-0.13	7 (2%) 67 61	22, 35, 57, 81	0
1	C	341/346 (98%)	0.02	6 (1%) 71 66	28, 44, 61, 75	0
1	E	340/346 (98%)	-0.27	2 (0%) 90 89	23, 36, 56, 75	0
2	B	168/182 (92%)	0.20	9 (5%) 29 23	24, 53, 82, 95	0
2	D	168/182 (92%)	-0.10	0 100 100	23, 45, 60, 73	0
2	F	168/182 (92%)	0.11	5 (2%) 54 47	20, 49, 69, 89	0
All	All	1525/1584 (96%)	-0.06	29 (1%) 70 65	20, 41, 66, 95	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	29	ALA	3.5
2	B	32	VAL	3.4
2	B	33	ALA	3.4
1	C	340	ALA	3.4
2	B	14	TRP	3.3
1	C	141	GLY	3.2
1	E	339	PRO	3.1
2	B	29	ALA	3.0
1	E	340	ALA	2.9
2	F	30	HIS	2.7
2	B	35	ALA	2.7
1	C	58	PHE	2.6
1	A	289	ILE	2.5
2	B	17	MET	2.3
2	B	148	CYS	2.3
1	A	340	ALA	2.3
1	A	146	VAL	2.3
1	A	2	ARG	2.3
1	C	148	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	3	ILE	2.1
2	B	143	LYS	2.1
2	F	157	PHE	2.1
2	F	27	HIS	2.1
2	B	18	ILE	2.1
2	F	162	PHE	2.1
1	C	149	GLY	2.0
1	A	239	LEU	2.0
1	C	289	ILE	2.0
1	A	40	HIS	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
3	NAG	C	401	14/15	0.90	0.28	4.50	54,63,72,79	0
3	NAG	C	409	14/15	0.94	0.24	2.77	42,59,74,75	0
3	NAG	A	401	14/15	0.90	0.31	1.96	50,64,79,84	0
3	NAG	A	406	14/15	0.91	0.24	1.58	53,62,74,74	0
3	NAG	E	401	14/15	0.90	0.26	1.17	53,64,76,81	0
3	NAG	E	410	14/15	0.90	0.18	0.77	47,57,67,75	0
3	NAG	C	407	14/15	0.94	0.24	0.67	48,57,70,85	0
3	NAG	A	408	14/15	0.89	0.20	0.42	55,74,85,88	0
3	NAG	E	404	14/15	0.94	0.16	0.26	41,48,55,58	0
5	SIA	A	410	20/21	0.94	0.16	0.05	28,35,44,47	0
6	NAG	C	403	14/15	0.84	0.22	0.03	53,61,65,77	0
5	SIA	C	411	20/21	0.89	0.22	-0.16	40,51,62,62	0
5	SIA	E	412	20/21	0.96	0.12	-1.34	28,35,39,42	0
3	NAG	E	406	14/15	0.71	0.28	-	44,66,79,80	0
3	NAG	A	409	14/15	0.79	0.24	-	60,90,96,96	0
5	NAG	A	412	14/15	0.71	0.30	-	68,88,98,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	402	14/15	0.78	0.43	-	87,93,100,102	0
3	NAG	A	404	14/15	0.84	0.34	-	63,77,90,91	0
5	GAL	A	411	11/12	0.92	0.15	-	35,51,72,78	0
3	NAG	A	407	14/15	0.77	0.43	-	80,88,97,103	0
6	BMA	C	405	11/12	0.82	0.17	-	55,62,74,75	0
3	NAG	E	408	14/15	0.92	0.22	-	45,58,74,80	0
3	NAG	E	405	14/15	0.87	0.16	-	52,65,76,77	0
3	NAG	C	402	14/15	0.84	0.33	-	76,80,89,95	0
5	GAL	C	412	11/12	0.85	0.22	-	53,77,91,91	0
3	NAG	C	408	14/15	0.80	0.32	-	65,84,96,99	0
3	NAG	E	411	14/15	0.76	0.31	-	76,82,86,86	0
5	GAL	E	413	11/12	0.95	0.22	-	35,51,74,79	0
3	NAG	E	402	14/15	0.82	0.35	-	79,85,92,97	0
3	NAG	A	403	14/15	0.87	0.20	-	53,67,72,77	0
3	NAG	C	410	14/15	0.81	0.25	-	69,80,90,93	0
5	NAG	E	414	14/15	0.77	0.37	-	79,91,95,100	0
6	NAG	C	404	14/15	0.88	0.26	-	42,60,74,75	0
3	NAG	E	407	14/15	0.74	0.35	-	64,79,86,87	0
3	NAG	E	409	14/15	0.88	0.33	-	74,91,95,99	0
5	NAG	C	413	14/15	0.59	0.52	-	89,115,121,121	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	E	403	14/15	0.66	0.32	-	59,86,91,92	0
4	NAG	C	406	14/15	0.65	0.42	-	80,96,104,104	0
4	NAG	A	405	14/15	0.88	0.26	-	72,81,90,91	0
4	NAG	D	201	14/15	0.80	0.32	-	69,82,92,96	0
4	NAG	B	201	14/15	0.69	0.38	-	115,124,131,132	0
4	NAG	F	201	14/15	0.85	0.28	-	74,85,91,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.