



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:45 PM GMT

PDB ID : 1V2I
Title : Structure of the hemagglutinin-neuraminidase from human parainfluenza virus type III
Authors : Lawrence, M.C.; Borg, N.A.; Streltsov, V.A.; Pilling, P.A.; Epa, V.C.; Varghese, J.N.; McKimm-Breschkin, J.L.; Colman, P.M.
Deposited on : 2003-10-16
Resolution : 2.20 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

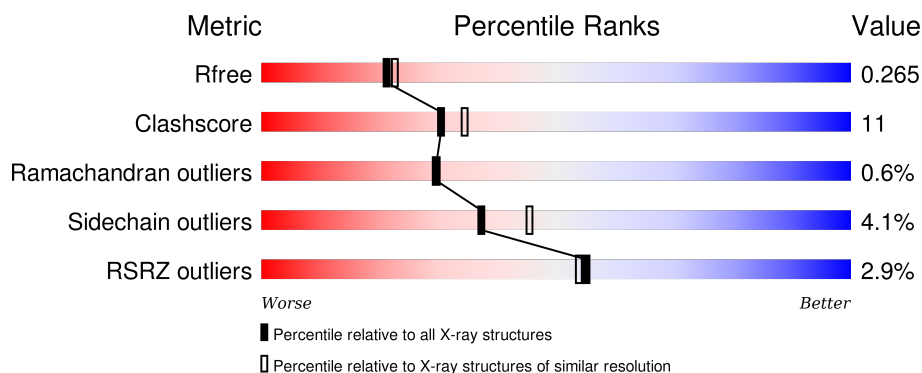
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

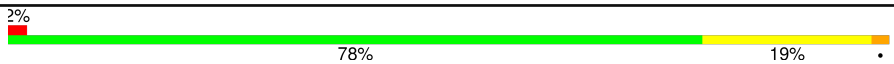
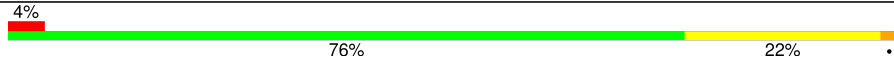
The reported resolution of this entry is 2.20 Å.

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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	431	 2% 78% 19% •
1	B	431	 4% 76% 22% •

2 Entry composition [i](#)

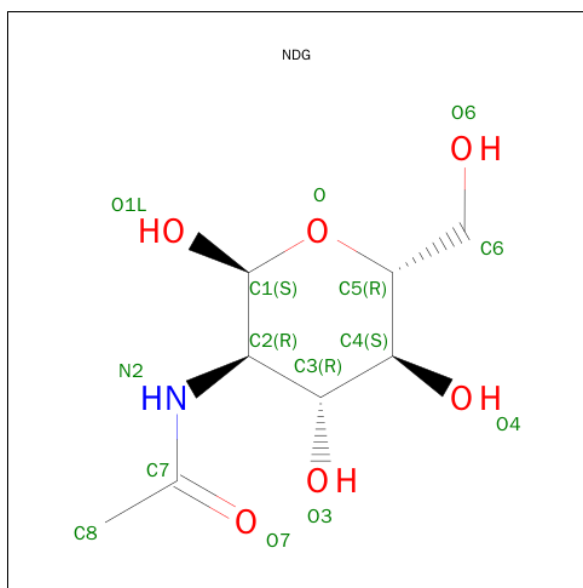
There are 8 unique types of molecules in this entry. The entry contains 7301 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-neuraminidase glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	1	0
			3382	2142	581	639	20			
1	B	431	Total	C	N	O	S	0	0	0
			3376	2138	579	639	20			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

- 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		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		

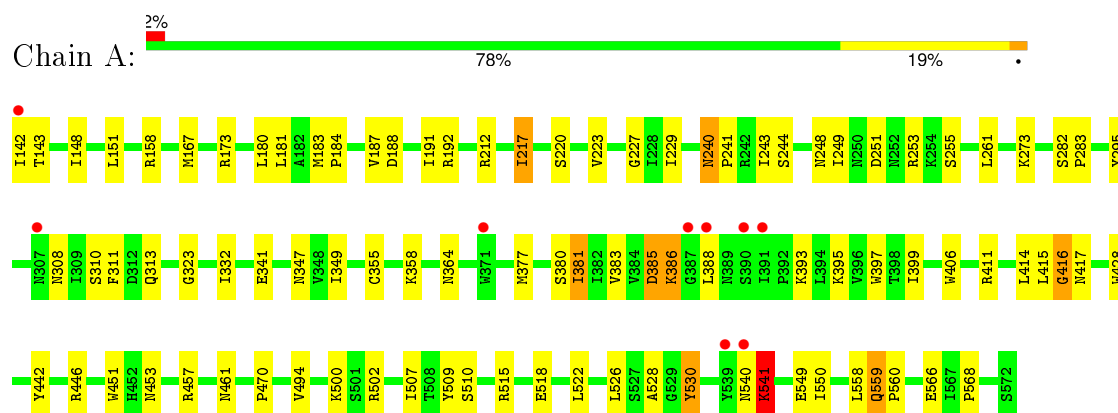
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	172	Total	O	0	0
			172	172		
8	B	200	Total	O	0	0
			200	200		

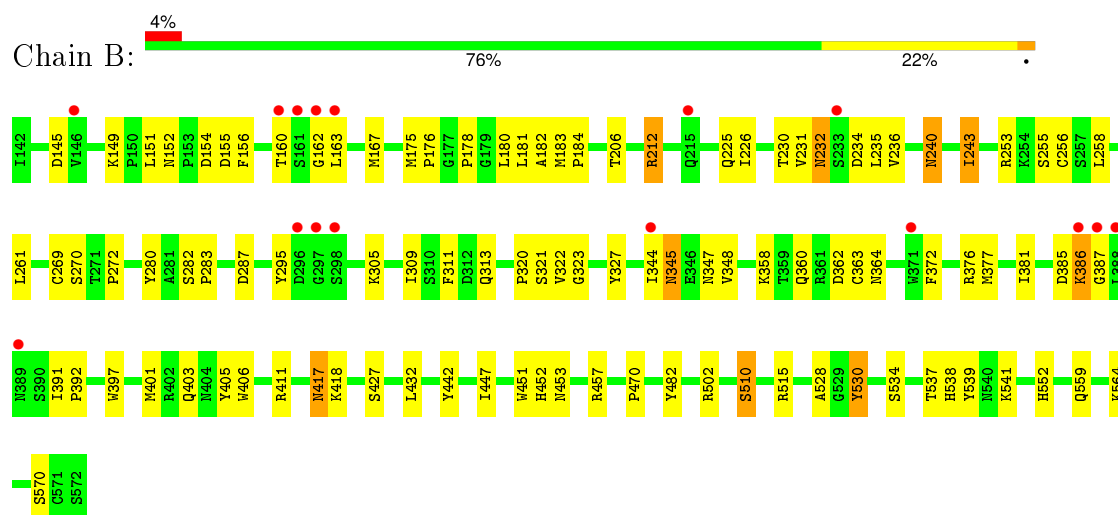
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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-neuraminidase glycoprotein



- Molecule 1: hemagglutinin-neuraminidase glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.50 Å 93.78 Å 105.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.30 – 2.20 18.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.5 (18.30-2.20) 94.4 (18.30-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.21 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.259 0.192 , 0.265	Depositor DCC
R_{free} test set	4018 reflections (9.99%)	DCC
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 40251 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7301	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: BMA, NAG, PO4, NDG, CA, MAN

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	0.52	0/3468	0.81	2/4730 (0.0%)
1	B	0.52	0/3457	0.82	0/4715
All	All	0.52	0/6925	0.81	2/9445 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	LYS	N-CA-C	-6.52	93.39	111.00
1	A	509	TYR	N-CA-C	-5.00	97.50	111.00

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	3382	0	3349	67	0
1	B	3376	0	3345	88	0
2	A	14	0	13	0	0
3	A	61	0	52	2	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	B	56	0	50	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	172	0	0	4	0
8	B	200	0	0	6	0
All	All	7301	0	6835	152	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 11.

All (152) 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:B:417:ASN:H	1:B:417:ASN:HD22	1.15	0.92
1:B:510:SER:HB2	1:B:515:ARG:HA	1.57	0.87
1:B:417:ASN:ND2	1:B:417:ASN:H	1.77	0.81
1:A:142:ILE:HG13	1:A:143:THR:HG23	1.62	0.79
1:A:347:ASN:HD22	1:A:364:ASN:HD21	1.27	0.79
1:A:248:ASN:HB3	1:A:251:ASP:OD2	1.86	0.76
1:B:417:ASN:N	1:B:417:ASN:HD22	1.81	0.76
1:B:403:GLN:HE21	1:B:447:ILE:H	1.31	0.76
1:A:446:ARG:HH11	1:A:446:ARG:HB3	1.52	0.74
1:A:183:MET:HE2	1:B:181:LEU:H	1.52	0.74
1:A:358:LYS:HD2	1:A:470:PRO:HG2	1.72	0.71
1:B:175:MET:HE2	1:B:564:LYS:HB2	1.70	0.70
1:B:360:GLN:HE21	1:B:364:ASN:ND2	1.89	0.70
1:A:241:PRO:HG2	8:B:5308:HOH:O	1.91	0.70
1:A:386:LYS:N	1:A:386:LYS:HD3	2.07	0.69
1:A:310:SER:OG	1:A:395:LYS:HG2	1.93	0.69
1:B:182:ALA:H	1:B:225:GLN:HE22	1.41	0.69
1:B:360:GLN:HE21	1:B:364:ASN:HD21	1.39	0.69
1:A:446:ARG:NH1	1:A:446:ARG:HB3	2.06	0.68
1:A:217:ILE:H	1:A:217:ILE:HD13	1.60	0.67
1:B:231:VAL:CG1	1:B:235:LEU:HA	2.26	0.66
1:B:427:SER:HB3	8:B:5235:HOH:O	1.95	0.66
1:A:541:LYS:HA	1:A:541:LYS:HE3	1.79	0.65
1:B:231:VAL:HG13	1:B:235:LEU:HA	1.78	0.65
1:B:184:PRO:HD3	1:B:559:GLN:OE1	1.97	0.64
1:B:175:MET:HE2	1:B:564:LYS:CB	2.26	0.64
1:A:261:LEU:HB2	1:A:332:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HG23	1:A:143:THR:H	1.62	0.63
1:B:212:ARG:O	1:B:212:ARG:HG3	2.01	0.61
1:B:231:VAL:HG11	1:B:235:LEU:HD23	1.81	0.61
1:A:212:ARG:HG2	1:A:212:ARG:HH11	1.66	0.61
1:B:451:TRP:CH2	1:B:453:ASN:HB2	2.36	0.61
1:B:149:LYS:HE3	8:B:5353:HOH:O	2.03	0.59
1:B:403:GLN:NE2	1:B:447:ILE:H	1.99	0.59
1:A:243:ILE:HD12	1:A:244:SER:H	1.68	0.59
1:A:323:GLY:HA3	1:A:411:ARG:HB3	1.85	0.59
1:A:349:ILE:HG13	8:A:5289:HOH:O	2.05	0.56
1:A:451:TRP:CZ2	3:A:3512:NAG:H5	2.40	0.56
1:B:552:HIS:HE1	8:B:5384:HOH:O	1.88	0.55
1:B:226:ILE:HB	1:B:243:ILE:HD13	1.88	0.55
1:A:180:LEU:HD23	1:B:182:ALA:HA	1.89	0.55
1:B:243:ILE:HD12	1:B:243:ILE:N	2.22	0.55
1:A:173:ARG:NH2	8:A:5329:HOH:O	2.38	0.55
1:B:386:LYS:CG	1:B:387:GLY:N	2.69	0.55
1:A:151:LEU:C	1:A:151:LEU:HD23	2.28	0.55
1:B:386:LYS:HG2	1:B:387:GLY:N	2.21	0.54
1:A:142:ILE:HG23	1:A:143:THR:N	2.22	0.54
1:B:451:TRP:CZ2	1:B:453:ASN:HB2	2.43	0.54
1:A:515:ARG:HD2	1:A:518:GLU:OE1	2.07	0.53
1:A:428:TRP:CD2	1:A:470:PRO:HA	2.44	0.53
1:A:167:MET:HG2	1:A:568:PRO:O	2.10	0.52
1:A:510:SER:HB2	1:A:515:ARG:HA	1.91	0.52
1:B:167:MET:HG2	1:B:570:SER:HB2	1.91	0.52
1:B:226:ILE:HB	1:B:243:ILE:CD1	2.39	0.52
1:B:162:GLY:C	1:B:163:LEU:HD22	2.30	0.52
1:B:323:GLY:HA3	1:B:411:ARG:HB3	1.92	0.51
1:B:152:ASN:ND2	1:B:155:ASP:OD2	2.43	0.51
1:B:175:MET:CE	1:B:564:LYS:HB2	2.40	0.50
1:A:386:LYS:N	1:A:386:LYS:CD	2.72	0.50
1:B:358:LYS:HA	1:B:362:ASP:OD2	2.11	0.50
1:A:148:ILE:HD13	1:A:229:ILE:HG22	1.94	0.50
1:B:348:VAL:HG12	1:B:401:MET:HB3	1.94	0.50
1:A:530:TYR:C	1:A:530:TYR:CD2	2.85	0.50
1:B:417:ASN:ND2	1:B:417:ASN:N	2.46	0.49
1:B:386:LYS:CG	1:B:387:GLY:H	2.24	0.49
1:A:451:TRP:CH2	1:A:453:ASN:HB2	2.47	0.49
1:B:372:PHE:HA	8:B:5267:HOH:O	2.11	0.49
1:B:377:MET:HG3	1:B:406:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ASP:O	1:B:392:PRO:HA	2.13	0.49
1:B:232:ASN:ND2	1:B:236:VAL:H	2.10	0.49
1:B:386:LYS:HB2	1:B:392:PRO:HB3	1.95	0.49
1:B:311:PHE:HB3	1:B:313:GLN:O	2.13	0.48
1:A:192:ARG:HG3	1:A:192:ARG:HH11	1.77	0.48
1:A:347:ASN:ND2	1:A:364:ASN:HD21	2.02	0.48
1:B:502:ARG:HB3	1:B:528:ALA:O	2.14	0.48
1:B:432:LEU:HD23	1:B:452:HIS:CD2	2.49	0.48
1:B:397:TRP:CD2	1:B:442:TYR:HB3	2.49	0.47
1:B:377:MET:HG3	1:B:406:TRP:CE2	2.49	0.47
1:B:269:CYS:HA	1:B:320:PRO:HG2	1.96	0.47
1:A:383:VAL:HG12	1:A:385:ASP:OD1	2.15	0.47
1:B:255:SER:O	1:B:320:PRO:HB2	2.15	0.47
1:A:184:PRO:HG3	1:A:191:ILE:HG13	1.97	0.47
1:A:526:LEU:HD11	1:A:550:ILE:HG23	1.97	0.47
1:B:261:LEU:HG	1:B:327:TYR:CE1	2.50	0.47
1:B:538:HIS:O	1:B:539:TYR:HB2	2.15	0.47
1:B:537:THR:HA	1:B:541:LYS:O	2.15	0.47
1:B:232:ASN:HD21	1:B:236:VAL:HB	1.79	0.46
1:B:321:SER:O	1:B:322:VAL:HB	2.15	0.46
1:A:377:MET:HG3	1:A:406:TRP:CZ2	2.51	0.46
1:B:151:LEU:HD11	1:B:156:PHE:CD2	2.51	0.46
1:A:283:PRO:HB3	1:A:341:GLU:CD	2.35	0.45
1:A:381:ILE:CD1	1:A:399:ILE:HD11	2.47	0.45
1:B:151:LEU:C	1:B:151:LEU:HD23	2.38	0.45
1:A:393:LYS:HG2	8:A:5265:HOH:O	2.16	0.45
1:A:515:ARG:CD	1:A:518:GLU:OE1	2.64	0.45
1:A:223:VAL:HG21	1:B:178:PRO:HB3	1.99	0.45
1:A:181:LEU:H	1:B:183:MET:CE	2.29	0.45
1:B:391:ILE:HG23	1:B:392:PRO:HD2	1.98	0.45
1:A:397:TRP:CD2	1:A:442:TYR:HB3	2.52	0.45
1:B:175:MET:HG3	1:B:564:LYS:O	2.17	0.44
1:A:428:TRP:CG	1:A:470:PRO:HA	2.52	0.44
1:A:415:LEU:O	1:A:416:GLY:C	2.55	0.44
3:A:3511:NAG:O6	3:A:3512:NAG:H82	2.18	0.44
1:A:451:TRP:CZ2	1:A:453:ASN:HB2	2.53	0.44
1:B:280:TYR:CD1	1:B:372:PHE:HD2	2.36	0.44
1:B:482:TYR:CD1	1:B:534:SER:HA	2.52	0.44
1:B:154:ASP:OD1	1:B:418:LYS:NZ	2.50	0.44
1:A:502:ARG:HB3	1:A:528:ALA:O	2.17	0.44
1:B:145:ASP:OD1	1:B:230:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLY:HA2	8:A:5260:HOH:O	2.17	0.44
1:B:256:CYS:O	1:B:322:VAL:HA	2.18	0.44
1:B:391:ILE:N	1:B:391:ILE:HD12	2.32	0.43
1:A:227:GLY:HA3	1:A:240:ASN:O	2.18	0.43
1:B:348:VAL:HG22	1:B:364:ASN:HD22	1.82	0.43
1:B:182:ALA:H	1:B:225:GLN:NE2	2.14	0.43
1:B:167:MET:CG	1:B:570:SER:HB2	2.48	0.43
1:B:530:TYR:CD2	1:B:530:TYR:C	2.92	0.43
1:B:405:TYR:O	1:B:406:TRP:C	2.57	0.43
1:B:376:ARG:HB3	1:B:401:MET:HE2	2.01	0.43
1:B:381:ILE:HA	1:B:381:ILE:HD13	1.88	0.43
1:A:217:ILE:HG12	1:A:217:ILE:O	2.18	0.43
1:B:287:ASP:OD1	1:B:305:LYS:HD2	2.19	0.42
1:A:273:LYS:HA	1:A:273:LYS:HD3	1.76	0.42
1:B:344:ILE:HG22	1:B:345:ASN:N	2.34	0.42
1:A:549:GLU:OE2	1:A:560:PRO:HG3	2.20	0.42
1:A:251:ASP:OD2	1:A:253:ARG:NH1	2.51	0.42
1:B:391:ILE:HG23	1:B:392:PRO:CD	2.49	0.42
1:A:220:SER:O	1:A:249:ILE:HA	2.20	0.42
1:B:282:SER:HA	1:B:283:PRO:HD3	1.95	0.42
1:B:287:ASP:CG	1:B:305:LYS:HD2	2.40	0.42
1:A:192:ARG:HG3	1:A:192:ARG:NH1	2.35	0.42
1:A:355:CYS:HB3	1:A:358:LYS:HG3	2.01	0.42
1:A:243:ILE:HD12	1:B:240:ASN:ND2	2.34	0.41
1:A:282:SER:HA	1:A:283:PRO:HD3	1.91	0.41
1:A:559:GLN:HA	1:A:560:PRO:HD3	1.75	0.41
5:B:3511:NAG:H61	5:B:3512:NAG:C8	2.50	0.41
1:A:311:PHE:HB3	1:A:313:GLN:O	2.20	0.41
1:B:253:ARG:HG3	8:B:5314:HOH:O	2.19	0.41
1:A:541:LYS:HE2	1:A:566:GLU:OE1	2.19	0.41
1:A:212:ARG:HG2	1:A:212:ARG:NH1	2.34	0.41
1:B:163:LEU:HD22	1:B:163:LEU:N	2.36	0.41
1:B:347:ASN:HA	1:B:364:ASN:HD21	1.86	0.41
1:B:176:PRO:O	1:B:236:VAL:HG11	2.20	0.41
1:B:344:ILE:CG2	1:B:345:ASN:N	2.84	0.41
1:A:187:VAL:O	1:A:188:ASP:HB2	2.21	0.41
1:B:270:SER:OG	1:B:272:PRO:HD3	2.20	0.41
1:A:446:ARG:CB	1:A:446:ARG:HH11	2.29	0.41
1:B:309:ILE:HB	1:B:311:PHE:CE1	2.56	0.41
1:B:206:THR:HB	1:B:258:LEU:HD11	2.03	0.41
1:A:494:VAL:HG22	1:A:507:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:CYS:SG	1:B:470:PRO:HG3	2.61	0.40
1:A:243:ILE:CD1	1:A:244:SER:H	2.34	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	430/431 (100%)	394 (92%)	33 (8%)	3 (1%)	26	25
1	B	429/431 (100%)	396 (92%)	31 (7%)	2 (0%)	34	35
All	All	859/862 (100%)	790 (92%)	64 (8%)	5 (1%)	30	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	386	LYS
1	B	234	ASP
1	A	416	GLY
1	A	522	LEU
1	A	540	ASN

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	391/390 (100%)	371 (95%)	20 (5%)	29	34
1	B	390/390 (100%)	378 (97%)	12 (3%)	47	59
All	All	781/780 (100%)	749 (96%)	32 (4%)	37	45

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	217	ILE
1	A	240	ASN
1	A	255	SER
1	A	295	TYR
1	A	308	ASN
1	A	380	SER
1	A	381	ILE
1	A	385	ASP
1	A	386	LYS
1	A	388	LEU
1	A	414	LEU
1	A	417	ASN
1	A	457	ARG
1	A	461	ASN
1	A	500	LYS
1	A	530	TYR
1	A	541	LYS
1	A	558	LEU
1	A	559	GLN
1	B	160	THR
1	B	180	LEU
1	B	212	ARG
1	B	232	ASN
1	B	240	ASN
1	B	243	ILE
1	B	295	TYR
1	B	345	ASN
1	B	417	ASN
1	B	457	ARG
1	B	510	SER
1	B	530	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	250	ASN
1	A	262	ASN
1	A	347	ASN
1	A	461	ASN
1	A	504	ASN
1	A	540	ASN
1	B	225	GLN
1	B	232	ASN
1	B	240	ASN
1	B	313	GLN
1	B	345	ASN
1	B	347	ASN
1	B	364	ASN
1	B	403	GLN
1	B	417	ASN
1	B	504	ASN
1	B	552	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 ⓘ

9 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	3511	1,3	14,14,15	0.53	0	15,19,21	0.80	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	3512	3	14,14,15	0.55	0	15,19,21	0.81	1 (6%)
3	BMA	A	3513	3	11,11,12	0.50	0	14,15,17	0.83	0
3	MAN	A	3514	3	11,11,12	0.44	0	14,15,17	0.72	1 (7%)
3	MAN	A	3515	3	11,11,12	0.67	0	14,15,17	0.94	1 (7%)
5	NAG	B	3511	1,5	14,14,15	0.56	0	15,19,21	0.81	1 (6%)
5	NAG	B	3512	5	14,14,15	0.55	0	15,19,21	0.75	0
5	NAG	B	5231	1,5	14,14,15	0.70	0	15,19,21	1.07	1 (6%)
5	NAG	B	5232	5	14,14,15	0.55	0	15,19,21	1.04	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	3511	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3512	3	-	0/6/23/26	0/1/1/1
3	BMA	A	3513	3	-	0/2/19/22	0/1/1/1
3	MAN	A	3514	3	-	0/2/19/22	0/1/1/1
3	MAN	A	3515	3	-	0/2/19/22	0/1/1/1
5	NAG	B	3511	1,5	-	2/6/23/26	0/1/1/1
5	NAG	B	3512	5	-	0/6/23/26	0/1/1/1
5	NAG	B	5231	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	5232	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5232	NAG	C2-N2-C7	-2.97	119.23	123.04
5	B	3511	NAG	C2-N2-C7	-2.46	119.88	123.04
3	A	3512	NAG	C2-N2-C7	-2.33	120.04	123.04
3	A	3511	NAG	C2-N2-C7	-2.07	120.38	123.04
3	A	3514	MAN	C1-O5-C5	2.30	115.17	112.25
5	B	5231	NAG	C3-C4-C5	2.63	114.78	110.20
3	A	3515	MAN	C1-O5-C5	2.88	115.91	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	3511	NAG	O7-C7-N2-C2
5	B	3511	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3511	NAG	1	0
3	A	3512	NAG	2	0
5	B	3511	NAG	1	0
5	B	3512	NAG	1	0

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
7	PO4	A	2001	-	4,4,4	1.06	0	6,6,6	0.28	0
2	NDG	A	3081	1	14,14,15	0.71	0	15,19,21	0.69	0
4	NAG	A	5231	1	14,14,15	0.68	0	15,19,21	0.83	1 (6%)
7	PO4	B	2002	-	4,4,4	0.99	0	6,6,6	0.27	0
4	NAG	B	3081	1	14,14,15	0.61	0	15,19,21	0.99	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PO4	A	2001	-	-	0/0/0/0	0/0/0/0
2	NDG	A	3081	1	-	0/6/23/26	0/1/1/1
4	NAG	A	5231	1	-	0/6/23/26	0/1/1/1
7	PO4	B	2002	-	-	0/0/0/0	0/0/0/0
4	NAG	B	3081	1	-	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($^{\circ}$)	Ideal($^{\circ}$)
4	B	3081	NAG	C2-N2-C7	-2.39	119.97	123.04
4	A	5231	NAG	C2-N2-C7	-2.09	120.35	123.04
4	B	3081	NAG	C4-C3-C2	-2.03	108.07	111.23

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	431/431 (100%)	-0.26	9 (2%) 67 65	16, 29, 53, 85	0
1	B	431/431 (100%)	-0.17	16 (3%) 45 44	18, 31, 60, 99	1 (0%)
All	All	862/862 (100%)	-0.21	25 (2%) 55 54	16, 30, 56, 99	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	LEU	8.5
1	B	388	LEU	7.9
1	B	389	ASN	6.6
1	B	387	GLY	5.4
1	B	163	LEU	4.6
1	B	161	SER	3.8
1	B	160	THR	3.8
1	A	391	ILE	3.8
1	A	371	TRP	3.7
1	B	215	GLN	3.6
1	B	233	SER	3.5
1	B	371	TRP	3.5
1	A	387	GLY	3.4
1	A	390	SER	3.1
1	B	146	VAL	2.8
1	B	162	GLY	2.8
1	A	307	ASN	2.7
1	B	386	LYS	2.7
1	B	296	ASP	2.5
1	A	540	ASN	2.4
1	B	297	GLY	2.4
1	A	142	ILE	2.4
1	A	539	TYR	2.1
1	B	344	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	298	SER	2.1

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	A	3512	14/15	0.91	0.12	-	41,51,56,59	0
5	NAG	B	3512	14/15	0.82	0.17	-	60,63,67,68	0
5	NAG	B	5231	14/15	0.64	0.24	-	54,61,68,72	0
5	NAG	B	5232	14/15	0.80	0.44	-	83,87,88,89	0
5	NAG	B	3511	14/15	0.85	0.19	-	57,60,64,65	0
3	BMA	A	3513	11/12	0.87	0.11	-	48,52,57,67	0
3	MAN	A	3514	11/12	0.92	0.21	-	54,58,60,61	0
3	NAG	A	3511	14/15	0.94	0.11	-	45,50,54,57	0
3	MAN	A	3515	11/12	0.65	0.36	-	70,73,75,76	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
4	NAG	B	3081	14/15	0.90	0.20	1.93	49,52,60,65	0
2	NDG	A	3081	14/15	0.79	0.31	1.41	73,77,79,80	0
7	PO4	B	2002	5/5	0.98	0.11	0.98	28,30,40,43	0
7	PO4	A	2001	5/5	0.98	0.07	-1.13	35,41,42,44	0
6	CA	B	1002	1/1	0.99	0.05	-2.43	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	CA	A	1001	1/1	0.97	0.04	-2.50	27,27,27,27	0
4	NAG	A	5231	14/15	0.82	0.22	-	59,67,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.