



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 12:26 AM EDT

PDB ID : 3FVC
Title : Crystal structure of a trimeric variant of the Epstein-Barr virus glycoprotein B
Authors : Backovic, M.
Deposited on : unknown
Resolution : 3.20 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

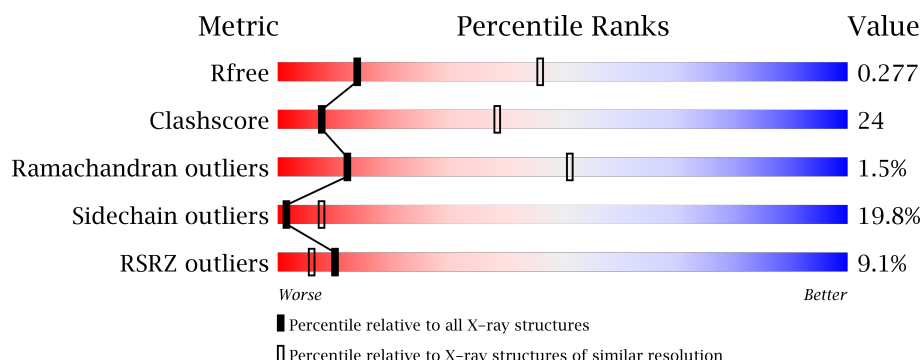
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	663	

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
2	NAG	A	687	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4552 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 Glycoprotein GP110.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	4501	2833	775	872	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	HIS	TRP	ENGINEERED	UNP P03188
A	113	ARG	TYR	ENGINEERED	UNP P03188
A	193	ARG	TRP	ENGINEERED	UNP P03188
A	194	VAL	LEU	ENGINEERED	UNP P03188
A	195	GLU	ILE	ENGINEERED	UNP P03188
A	196	ALA	TRP	ENGINEERED	UNP P03188

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (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		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

Chain A:

8% 44% 32% 8% 16%

GLN THR PRO GLU GLN PRO ALA PRO ALA THR VAL GLN PRO THR ALA THR VAL GLN PRO THR ALA THR ARG ARG Q42 Q43 T44 T45 F46 P47 P48 R49 F43 V50 C51 E52 E53 S54 S55 S56 E57 D58 L59 F60 R61 F62 G63 S64 D65 D66 Q67 Q68 P69 S70 GLY THR ARG ARG H76 H77 H78 E79 G80 L81 L82

Y181 R265 R347 N348 R349 T350 K351 R354 R355 V356 V357 V358 R359 R360 R361 Q366 I369 T370 Y371 F372 F373 T374 S375 S376 G377 L378 L379 F380 P381 A382 V383 P384 L385 T386 P387 R388 S389 L390 A391 T392 S393 A394 V395 V396 V397 V398 V399 V400 V401 V402 V403 V404 V405 V406 V407 V408 V409 V410 V411 V412 V413 V414 V415 V416 V417 V418 V419 V420 V421 V422 V423 V424 V425 V426 V427 V428 V429 V430 V431 V432 V433 V434 V435 V436 V437 V438 V439 V440 V441 V442 V443 V444 V445 V446 V447 V448 V449 V450 V451 V452 V453 V454 V455 V456 V457 V458 V459 V460 V461 V462 V463 V464 V465 V466 V467 V468 V469 V470 V471 V472 V473 V474 V475 V476 V477 V478 V479 V480 V481 V482 V483 V484 V485 V486 V487 V488 V489 V490 V491 V492 V493 V494 V495 V496 V497 V498 V499 V500 V501 V502 V503 V504 V505 V506 V507 V508 V509 V510 V511 V512 V513 V514 V515 V516 V517 V518 V519 V520 V521 V522 V523 V524 V525 V526 V527 V528 V529 V530 V531 V532 V533 V534 V535 V536 V537 V538 V539 V540 V541 V542 V543 V544 V545 V546 V547 V548 V549 V550 V551 V552 V553 V554 V555 V556 V557 V558 V559 V560 V561 V562 V563 V564 V565 V566 V567 V568 V569 V570 V571 V572 V573 V574 V575 V576 V577 V578 V579 V580 V581 V582 V583 V584 V585 V586 V587 V588 V589 V590 V591 V592 V593 V594 V595 V596 V597 V598 V599 V600 V601 V602 V603 V604 V605 V606 V607 V608 V609 V610 V611 V612 V613 V614 V615 V616 V617 V618 V619 V620 V621 V622 V623 V624 V625 V626 V627 V628 V629 V630 V631 V632 V633 V634 V635 V636 V637 V638 V639 V640 V641 V642 V643 V644 V645 V646 V647 V648 V649 V650 V651 V652 V653 V654 V655 V656 V657 V658 V659 V660 V661 V662 V663 V664 V665 V666 V667 V668 V669 V670 V671 V672 V673 V674 V675 V676 V677 V678 V679 V680 V681 V682 V683 V684 V685 V686 V687 V688 V689 V690 V691 V692 V693 V694 V695 V696 V697 V698 V699 V700 V701 V702 V703 V704 V705 V706 V707 V708 V709 V710 V711 V712 V713 V714 V715 V716 V717 V718 V719 V720 V721 V722 V723 V724 V725 V726 V727 V728 V729 V730 V731 V732 V733 V734 V735 V736 V737 V738 V739 V740 V741 V742 V743 V744 V745 V746 V747 V748 V749 V750 V751 V752 V753 V754 V755 V756 V757 V758 V759 V760 V761 V762 V763 V764 V765 V766 V767 V768 V769 V770 V771 V772 V773 V774 V775 V776 V777 V778 V779 V780 V781 V782 V783 V784 V785 V786 V787 V788 V789 V790 V791 V792 V793 V794 V795 V796 V797 V798 V799 V800 V801 V802 V803 V804 V805 V806 V807 V808 V809 V810 V811 V812 V813 V814 V815 V816 V817 V818 V819 V820 V821 V822 V823 V824 V825 V826 V827 V828 V829 V830 V831 V832 V833 V834 V835 V836 V837 V838 V839 V840 V841 V842 V843 V844 V845 V846 V847 V848 V849 V850 V851 V852 V853 V854 V855 V856 V857 V858 V859 V860 V861 V862 V863 V864 V865 V866 V867 V868 V869 V870 V871 V872 V873 V874 V875 V876 V877 V878 V879 V880 V881 V882 V883 V884 V885 V886 V887 V888 V889 V890 V891 V892 V893 V894 V895 V896 V897 V898 V899 V900 V901 V902 V903 V904 V905 V906 V907 V908 V909 V910 V911 V912 V913 V914 V915 V916 V917 V918 V919 V920 V921 V922 V923 V924 V925 V926 V927 V928 V929 V930 V931 V932 V933 V934 V935 V936 V937 V938 V939 V940 V941 V942 V943 V944 V945 V946 V947 V948 V949 V950 V951 V952 V953 V954 V955 V956 V957 V958 V959 V960 V961 V962 V963 V964 V965 V966 V967 V968 V969 V970 V971 V972 V973 V974 V975 V976 V977 V978 V979 V980 V981 V982 V983 V984 V985 V986 V987 V988 V989 V990 V991 V992 V993 V994 V995 V996 V997 V998 V999 V1000

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.80Å 106.80Å 210.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.61 – 3.20 26.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (26.61-3.20) 98.4 (26.61-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.17Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.283 0.238 , 0.277	Depositor DCC
R_{free} test set	2153 reflections (10.19%)	DCC
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	4552	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.79	0/4590	0.85	2/6209 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	187	LEU	CB-CG-CD1	-5.88	101.01	111.00
1	A	82	LEU	CA-CB-CG	-5.02	103.76	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4501	0	4362	217	0
2	A	42	0	39	2	0
3	A	9	0	0	0	0
All	All	4552	0	4401	217	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 24.

All (217) 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:A:623:GLN:HG3	1:A:625:PHE:CE1	1.71	1.25
1:A:660:ILE:C	1:A:660:ILE:HD12	1.67	1.12
1:A:533:GLN:NE2	1:A:533:GLN:HA	1.64	1.08
1:A:361:ARG:HH11	1:A:361:ARG:HG2	0.98	1.08
1:A:533:GLN:HE21	1:A:533:GLN:CA	1.69	1.06
1:A:554:ARG:HB2	1:A:571:GLN:HE21	1.24	0.99
1:A:361:ARG:HG2	1:A:361:ARG:NH1	1.76	0.96
1:A:533:GLN:HE21	1:A:533:GLN:HA	0.80	0.96
1:A:538:LEU:HA	1:A:557:VAL:HG12	1.47	0.93
1:A:592:SER:OG	1:A:607:ASP:HA	1.72	0.90
1:A:238:GLY:O	1:A:239:LYS:HB2	1.73	0.87
1:A:259:ILE:HD11	1:A:274:ARG:NE	1.90	0.85
1:A:323:THR:O	1:A:323:THR:HG23	1.76	0.85
1:A:602:ILE:HD12	1:A:619:ILE:HD12	1.58	0.85
1:A:623:GLN:CG	1:A:625:PHE:CE1	2.58	0.84
1:A:81:LEU:HD12	1:A:383:LEU:HD11	1.59	0.84
1:A:361:ARG:HH11	1:A:361:ARG:CG	1.87	0.83
1:A:632:LEU:H	1:A:632:LEU:HD23	1.42	0.83
1:A:554:ARG:HB2	1:A:571:GLN:NE2	1.94	0.83
1:A:259:ILE:HD11	1:A:274:ARG:CZ	2.09	0.82
1:A:660:ILE:O	1:A:660:ILE:HD12	1.79	0.82
1:A:542:MET:HB2	1:A:608:TYR:HB3	1.63	0.81
1:A:47:PRO:O	1:A:49:ARG:HG3	1.81	0.80
1:A:605:TYR:CD2	1:A:610:HIS:HA	2.17	0.80
1:A:106:ILE:HD11	1:A:187:LEU:HD11	1.62	0.80
1:A:184:GLN:OE1	1:A:184:GLN:HA	1.81	0.78
1:A:672:ALA:HB1	1:A:675:ARG:NH1	1.99	0.77
1:A:374:THR:HG22	1:A:376:GLY:H	1.49	0.76
1:A:237:ASP:N	1:A:237:ASP:OD1	2.17	0.76
1:A:184:GLN:CA	1:A:184:GLN:OE1	2.34	0.75
1:A:232:MET:HE1	1:A:244:PHE:HE2	1.51	0.74
1:A:330:THR:HG21	1:A:372:PHE:HD2	1.50	0.74
1:A:71:PHE:HD2	1:A:71:PHE:C	1.91	0.74
1:A:188:TYR:CE2	1:A:201:ARG:HD2	2.24	0.72
1:A:334:ILE:HB	1:A:370:THR:HB	1.70	0.72
1:A:71:PHE:C	1:A:71:PHE:CD2	2.62	0.72
1:A:574:THR:O	1:A:575:ASP:HB2	1.89	0.71
1:A:232:MET:HE2	1:A:244:PHE:CD2	2.25	0.71
1:A:160:ASP:OD1	1:A:202:THR:HB	1.92	0.70
1:A:295:CYS:SG	1:A:296:PRO:HD2	2.32	0.70
1:A:168:LEU:CD2	1:A:183:SER:HB3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ILE:HD13	1:A:383:LEU:HB3	1.75	0.69
1:A:192:GLY:HA3	1:A:199:ARG:HD3	1.75	0.69
1:A:623:GLN:HG3	1:A:625:PHE:HE1	1.51	0.68
1:A:672:ALA:HB1	1:A:675:ARG:HH11	1.57	0.68
1:A:554:ARG:CB	1:A:571:GLN:HE21	2.05	0.68
1:A:81:LEU:HG	1:A:385:LEU:HD11	1.75	0.68
1:A:61:ARG:HG3	1:A:62:PHE:N	2.09	0.67
1:A:605:TYR:CE2	1:A:610:HIS:HB2	2.29	0.67
1:A:330:THR:HG21	1:A:372:PHE:CD2	2.28	0.67
1:A:323:THR:O	1:A:323:THR:CG2	2.43	0.66
1:A:647:ASP:N	1:A:647:ASP:OD2	2.24	0.66
1:A:101:LYS:HD3	1:A:145:VAL:HG22	1.77	0.66
1:A:632:LEU:CD2	1:A:632:LEU:H	2.08	0.66
1:A:374:THR:CG2	1:A:376:GLY:H	2.09	0.65
1:A:383:LEU:HD13	1:A:383:LEU:O	1.97	0.65
1:A:601:GLU:HB3	1:A:615:GLU:HA	1.79	0.65
1:A:660:ILE:CD1	1:A:660:ILE:C	2.48	0.64
1:A:348:ASN:HD22	1:A:348:ASN:C	2.00	0.64
1:A:593:GLN:O	1:A:594:TYR:HD2	1.80	0.64
1:A:232:MET:HE1	1:A:244:PHE:CE2	2.32	0.63
1:A:168:LEU:HD23	1:A:183:SER:HB3	1.78	0.63
1:A:46:PHE:CD2	1:A:46:PHE:N	2.68	0.62
1:A:112:HIS:HB2	1:A:195:GLU:OE2	2.00	0.61
1:A:128:ASP:O	1:A:132:THR:HG23	2.00	0.61
1:A:559:PHE:HE2	1:A:561:PHE:CE2	2.18	0.61
1:A:232:MET:CE	1:A:244:PHE:CE2	2.83	0.61
1:A:509:ILE:HG13	1:A:510:TYR:N	2.15	0.61
1:A:168:LEU:HD12	1:A:208:ILE:HD12	1.82	0.61
1:A:124:LYS:O	1:A:281:THR:HA	2.00	0.61
1:A:81:LEU:HD12	1:A:383:LEU:CD1	2.31	0.61
1:A:626:ILE:HD12	1:A:626:ILE:H	1.66	0.61
1:A:448:LYS:HD2	1:A:449:SER:H	1.66	0.60
1:A:101:LYS:HD3	1:A:145:VAL:CG2	2.32	0.60
1:A:273:ARG:CZ	1:A:288:LEU:HD23	2.31	0.60
1:A:374:THR:HG22	1:A:376:GLY:N	2.15	0.60
1:A:671:ILE:HA	1:A:674:LEU:HD22	1.83	0.59
1:A:138:ILE:O	1:A:139:TYR:HB2	2.02	0.59
1:A:168:LEU:HD12	1:A:208:ILE:CD1	2.33	0.59
1:A:50:VAL:HG13	1:A:50:VAL:O	2.02	0.58
1:A:325:SER:OG	1:A:462:GLN:HG3	2.03	0.58
1:A:48:PHE:HZ	1:A:599:GLY:H	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:MET:CB	1:A:608:TYR:HB3	2.34	0.58
1:A:67:GLN:O	1:A:69:PRO:HD3	2.04	0.58
1:A:348:ASN:C	1:A:348:ASN:ND2	2.57	0.58
1:A:626:ILE:N	1:A:626:ILE:HD12	2.19	0.57
1:A:559:PHE:HE2	1:A:561:PHE:CZ	2.22	0.57
1:A:645:SER:O	1:A:649:GLN:HG2	2.04	0.57
1:A:486:GLU:O	1:A:490:GLN:HG2	2.05	0.57
1:A:605:TYR:CE2	1:A:610:HIS:HA	2.39	0.56
1:A:658:GLU:HG3	1:A:662:ARG:HD3	1.86	0.56
1:A:660:ILE:HD12	1:A:661:PHE:N	2.18	0.56
1:A:259:ILE:CD1	1:A:274:ARG:CZ	2.82	0.55
1:A:313:LYS:O	1:A:331:THR:CG2	2.55	0.55
1:A:672:ALA:CB	1:A:675:ARG:HH11	2.19	0.55
1:A:57:GLY:O	1:A:58:ASP:OD1	2.26	0.54
1:A:354:LYS:HD3	1:A:354:LYS:N	2.23	0.53
1:A:46:PHE:HD2	1:A:46:PHE:H	1.56	0.53
1:A:560:SER:OG	1:A:561:PHE:N	2.42	0.53
1:A:80:GLY:HA2	1:A:385:LEU:HD12	1.89	0.53
1:A:188:TYR:CD2	1:A:201:ARG:HB3	2.44	0.53
1:A:656:ASP:O	1:A:657:LEU:C	2.43	0.53
1:A:99:TYR:C	1:A:100:THR:HG22	2.28	0.52
1:A:678:LEU:O	1:A:679:ASP:C	2.47	0.52
1:A:331:THR:O	1:A:332:VAL:HB	2.10	0.52
1:A:347:VAL:HG12	1:A:348:ASN:N	2.25	0.52
1:A:348:ASN:HD22	1:A:349:LYS:N	2.08	0.52
1:A:600:ASN:C	1:A:601:GLU:HG3	2.30	0.52
1:A:533:GLN:NE2	1:A:533:GLN:CA	2.44	0.52
1:A:623:GLN:HG3	1:A:625:PHE:CZ	2.36	0.51
1:A:380:LEU:N	1:A:380:LEU:HD12	2.26	0.51
1:A:361:ARG:NH1	1:A:361:ARG:CG	2.54	0.51
1:A:144:ALA:CB	2:A:1:NAG:H82	2.41	0.51
1:A:55:SER:O	1:A:56:HIS:C	2.48	0.51
1:A:465:TYR:CD1	1:A:465:TYR:C	2.84	0.51
1:A:380:LEU:N	1:A:380:LEU:CD1	2.74	0.51
1:A:334:ILE:HG22	1:A:372:PHE:CZ	2.46	0.51
1:A:554:ARG:NH1	1:A:572:LEU:O	2.43	0.50
1:A:232:MET:HE2	1:A:244:PHE:HD2	1.73	0.50
1:A:593:GLN:NE2	1:A:595:TYR:OH	2.43	0.50
1:A:152:LEU:N	1:A:152:LEU:HD23	2.27	0.50
1:A:247:ARG:HB2	1:A:250:SER:OG	2.11	0.50
1:A:672:ALA:HA	1:A:675:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:MET:HB2	1:A:608:TYR:CB	2.40	0.50
1:A:559:PHE:CE2	1:A:561:PHE:CE2	3.00	0.50
1:A:237:ASP:OD1	1:A:240:ASN:HB2	2.11	0.49
1:A:215:SER:HB2	1:A:222:PHE:HB3	1.94	0.49
1:A:249:ASP:OD1	1:A:249:ASP:N	2.44	0.49
1:A:478:ASP:OD1	1:A:478:ASP:N	2.43	0.49
1:A:295:CYS:SG	1:A:296:PRO:CD	3.00	0.49
1:A:531:VAL:HG12	1:A:561:PHE:CE1	2.47	0.49
1:A:80:GLY:HA3	1:A:382:TRP:CH2	2.48	0.49
1:A:351:MET:SD	1:A:383:LEU:HD12	2.53	0.49
1:A:71:PHE:CZ	1:A:477:GLY:HA2	2.48	0.48
1:A:617:ASP:OD1	1:A:617:ASP:N	2.47	0.48
1:A:529:VAL:O	1:A:529:VAL:HG13	2.14	0.48
1:A:144:ALA:HB3	2:A:1:NAG:H82	1.95	0.48
1:A:450:LEU:H	1:A:450:LEU:HD12	1.79	0.48
1:A:656:ASP:O	1:A:660:ILE:HG23	2.12	0.48
1:A:343:ILE:O	1:A:344:GLU:C	2.52	0.47
1:A:605:TYR:CZ	1:A:610:HIS:HB2	2.49	0.47
1:A:505:VAL:O	1:A:509:ILE:HG23	2.14	0.47
1:A:129:SER:HA	1:A:132:THR:HG23	1.96	0.47
1:A:232:MET:CE	1:A:244:PHE:CD2	2.97	0.47
1:A:372:PHE:HB2	1:A:380:LEU:HB2	1.95	0.47
1:A:379:LEU:HB2	1:A:450:LEU:HD23	1.96	0.47
1:A:505:VAL:O	1:A:509:ILE:CG2	2.63	0.47
1:A:60:PHE:CD1	1:A:60:PHE:N	2.81	0.47
1:A:575:ASP:O	1:A:576:ASN:HB2	2.14	0.47
1:A:238:GLY:O	1:A:239:LYS:CB	2.49	0.47
1:A:497:LEU:HA	1:A:497:LEU:HD23	1.77	0.47
1:A:232:MET:HE2	1:A:244:PHE:CE2	2.48	0.47
1:A:181:TYR:O	1:A:207:LEU:HD23	2.16	0.46
1:A:259:ILE:HG21	1:A:259:ILE:HD12	1.71	0.46
1:A:328:THR:OG1	1:A:330:THR:HG23	2.16	0.46
1:A:232:MET:HE3	1:A:246:GLU:HG3	1.97	0.46
1:A:448:LYS:HD2	1:A:449:SER:N	2.32	0.45
1:A:313:LYS:O	1:A:331:THR:HG22	2.15	0.45
1:A:657:LEU:HA	1:A:657:LEU:HD22	1.64	0.45
1:A:108:ILE:HG23	1:A:108:ILE:O	2.17	0.45
1:A:138:ILE:HD13	1:A:138:ILE:HG21	1.66	0.45
1:A:143:ASN:HB2	1:A:158:ASP:HB2	1.98	0.45
1:A:318:VAL:HG11	1:A:470:ARG:HH12	1.82	0.45
1:A:510:TYR:HD2	1:A:514:VAL:HG11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.72	0.44
1:A:259:ILE:HD11	1:A:274:ARG:CD	2.46	0.44
1:A:141:CYS:O	1:A:166:VAL:HG22	2.17	0.44
1:A:66:ILE:CG1	1:A:488:LYS:HA	2.47	0.44
1:A:63:SER:O	1:A:64:SER:C	2.56	0.44
1:A:71:PHE:CE1	1:A:480:ALA:HB2	2.53	0.44
1:A:313:LYS:O	1:A:331:THR:HG23	2.18	0.44
1:A:574:THR:O	1:A:575:ASP:CB	2.62	0.44
1:A:129:SER:O	1:A:130:TYR:C	2.55	0.44
1:A:62:PHE:O	1:A:63:SER:C	2.55	0.44
1:A:518:ARG:HB3	1:A:518:ARG:HE	1.66	0.43
1:A:509:ILE:O	1:A:509:ILE:HD12	2.18	0.43
1:A:257:TYR:CD2	1:A:274:ARG:HD3	2.53	0.43
1:A:306:THR:HG22	1:A:319:THR:HB	2.00	0.43
1:A:498:THR:HG22	1:A:505:VAL:HG11	2.01	0.43
1:A:554:ARG:HA	1:A:555:PRO:HD3	1.91	0.43
1:A:604:VAL:O	1:A:605:TYR:HD2	2.01	0.43
1:A:193:ARG:H	1:A:193:ARG:HG2	1.69	0.43
1:A:650:ARG:C	1:A:652:SER:H	2.21	0.43
1:A:140:GLN:HA	1:A:166:VAL:O	2.19	0.43
1:A:605:TYR:CE2	1:A:610:HIS:CB	2.98	0.43
1:A:184:GLN:N	1:A:205:ASN:OD1	2.40	0.43
1:A:494:LEU:O	1:A:498:THR:HG23	2.19	0.43
1:A:49:ARG:HD3	1:A:513:ALA:HB1	1.99	0.42
1:A:259:ILE:HD13	1:A:259:ILE:HG23	1.76	0.42
1:A:283:THR:HG22	1:A:284:LEU:N	2.33	0.42
1:A:303:PHE:HB3	1:A:306:THR:CG2	2.49	0.42
1:A:576:ASN:HD21	1:A:598:SER:HA	1.83	0.42
1:A:265:ARG:HB2	1:A:265:ARG:HE	1.31	0.42
1:A:217:SER:HA	1:A:219:PHE:N	2.35	0.42
1:A:58:ASP:O	1:A:525:VAL:N	2.52	0.42
1:A:104:THR:HB	1:A:203:THR:HG23	2.02	0.42
1:A:347:VAL:CG1	1:A:348:ASN:N	2.81	0.41
1:A:539:ARG:HD3	1:A:556:LEU:CB	2.49	0.41
1:A:576:ASN:HD21	1:A:598:SER:CA	2.33	0.41
1:A:602:ILE:HG22	1:A:603:HIS:N	2.36	0.41
1:A:71:PHE:HZ	1:A:476:LEU:O	2.03	0.41
1:A:358:VAL:O	1:A:358:VAL:HG13	2.20	0.41
1:A:295:CYS:HA	1:A:296:PRO:HD3	1.69	0.41
1:A:366:GLN:OE1	1:A:384:PRO:HD3	2.20	0.41
1:A:85:PHE:O	1:A:378:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ASP:N	1:A:360:ASP:OD2	2.53	0.41
1:A:461:ILE:C	1:A:463:PHE:N	2.74	0.41
1:A:650:ARG:O	1:A:652:SER:N	2.54	0.41
1:A:201:ARG:HD3	1:A:201:ARG:HH11	1.68	0.40
1:A:324:SER:HB2	1:A:459:VAL:HG23	2.02	0.40
1:A:150:ASP:C	1:A:152:LEU:H	2.24	0.40
1:A:221:PHE:C	1:A:221:PHE:CD2	2.95	0.40
1:A:299:HIS:CG	1:A:346:GLN:HE22	2.40	0.40
1:A:355:TYR:CD1	1:A:355:TYR:C	2.92	0.40
1:A:85:PHE:CD1	1:A:299:HIS:HA	2.56	0.40
1:A:66:ILE:HG12	1:A:488:LYS:HA	2.04	0.40
1:A:63:SER:O	1:A:65:ASP:N	2.55	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	547/663 (82%)	479 (88%)	60 (11%)	8 (2%)	12	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	VAL
1	A	341	LYS
1	A	651	ALA
1	A	48	PHE
1	A	534	ALA
1	A	503	THR
1	A	358	VAL
1	A	57	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	500/585 (86%)	401 (80%)	99 (20%)	1 8

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	46	PHE
1	A	49	ARG
1	A	51	CYS
1	A	59	LEU
1	A	60	PHE
1	A	64	SER
1	A	71	PHE
1	A	76	ASN
1	A	78	THR
1	A	84	VAL
1	A	86	LYS
1	A	87	ASP
1	A	88	ASN
1	A	96	VAL
1	A	99	TYR
1	A	100	THR
1	A	105	ASN
1	A	107	LEU
1	A	108	ILE
1	A	138	ILE
1	A	148	THR
1	A	153	THR
1	A	157	VAL
1	A	176	ASN
1	A	179	ARG
1	A	184	GLN
1	A	187	LEU
1	A	200	THR
1	A	203	THR

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Mol	Chain	Res	Type
1	A	207	LEU
1	A	223	VAL
1	A	229	THR
1	A	232	MET
1	A	241	LYS
1	A	242	GLU
1	A	243	THR
1	A	247	ARG
1	A	253	VAL
1	A	255	THR
1	A	258	LYS
1	A	267	THR
1	A	279	LYS
1	A	297	LEU
1	A	302	THR
1	A	304	ASP
1	A	309	THR
1	A	313	LYS
1	A	319	THR
1	A	323	THR
1	A	327	VAL
1	A	334	ILE
1	A	338	ASP
1	A	342	CYS
1	A	347	VAL
1	A	348	ASN
1	A	354	LYS
1	A	358	VAL
1	A	360	ASP
1	A	361	ARG
1	A	378	LEU
1	A	383	LEU
1	A	386	THR
1	A	448	LYS
1	A	450	LEU
1	A	472	ILE
1	A	475	MET
1	A	478	ASP
1	A	479	LEU
1	A	481	ARG
1	A	488	LYS
1	A	489	ARG

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Mol	Chain	Res	Type
1	A	509	ILE
1	A	510	TYR
1	A	533	GLN
1	A	550	MET
1	A	554	ARG
1	A	557	VAL
1	A	567	THR
1	A	569	GLU
1	A	574	THR
1	A	575	ASP
1	A	591	THR
1	A	601	GLU
1	A	614	ILE
1	A	617	ASP
1	A	625	PHE
1	A	632	LEU
1	A	637	ASP
1	A	643	LEU
1	A	647	ASP
1	A	648	GLU
1	A	650	ARG
1	A	652	SER
1	A	657	LEU
1	A	660	ILE
1	A	663	GLU
1	A	674	LEU
1	A	678	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	134	GLN
1	A	228	GLN
1	A	252	HIS
1	A	256	ASN
1	A	329	ASN
1	A	346	GLN
1	A	348	ASN
1	A	460	GLN
1	A	533	GLN
1	A	571	GLN

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Mol	Chain	Res	Type
1	A	576	ASN
1	A	593	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	1	1	14,14,15	0.86	0	15,19,21	2.50	5 (33%)
2	NAG	A	686	1	14,14,15	0.93	1 (7%)	15,19,21	1.41	2 (13%)
2	NAG	A	687	1	14,14,15	0.80	1 (7%)	15,19,21	1.37	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
2	NAG	A	1	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	686	1	-	0/6/23/26	0/1/1/1
2	NAG	A	687	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	687	NAG	C1-C2	2.09	1.55	1.52
2	A	686	NAG	C8-C7	2.28	1.55	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	O5-C1-C2	-4.33	105.44	111.47
2	A	686	NAG	C4-C3-C2	-3.30	106.18	111.02
2	A	1	NAG	C1-C2-N2	-2.43	106.33	110.49
2	A	687	NAG	O5-C1-C2	-2.30	108.27	111.47
2	A	1	NAG	O4-C4-C5	2.54	115.69	109.28
2	A	686	NAG	C1-C2-N2	2.82	115.30	110.49
2	A	1	NAG	C2-N2-C7	3.05	127.39	122.94
2	A	687	NAG	C1-O5-C5	4.04	117.73	112.17
2	A	1	NAG	C1-O5-C5	6.41	121.00	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	559/663 (84%)	0.47	51 (9%) 10 6	57, 77, 100, 108	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	552	TYR	5.6
1	A	551	CYS	5.2
1	A	550	MET	5.2
1	A	592	SER	4.6
1	A	591	THR	4.2
1	A	567	THR	4.0
1	A	332	VAL	3.9
1	A	43	GLN	3.6
1	A	68	CYS	3.4
1	A	553	SER	3.4
1	A	568	TYR	3.3
1	A	561	PHE	3.3
1	A	679	ASP	3.3
1	A	510	TYR	3.2
1	A	535	THR	3.2
1	A	331	THR	3.2
1	A	543	ARG	3.1
1	A	67	GLN	3.1
1	A	590	ALA	2.9
1	A	53	LEU	2.9
1	A	542	MET	2.8
1	A	70	SER	2.7
1	A	616	LEU	2.7
1	A	313	LYS	2.7
1	A	617	ASP	2.6
1	A	390	LEU	2.6
1	A	52	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	44	THR	2.5
1	A	526	SER	2.5
1	A	614	ILE	2.4
1	A	615	GLU	2.4
1	A	594	TYR	2.4
1	A	565	THR	2.4
1	A	569	GLU	2.4
1	A	269	PRO	2.4
1	A	618	GLY	2.4
1	A	65	ASP	2.4
1	A	534	ALA	2.4
1	A	609	HIS	2.4
1	A	613	THR	2.4
1	A	572	LEU	2.4
1	A	554	ARG	2.3
1	A	54	SER	2.2
1	A	267	THR	2.1
1	A	56	HIS	2.1
1	A	528	CYS	2.1
1	A	388	ARG	2.1
1	A	533	GLN	2.1
1	A	334	ILE	2.1
1	A	532	ASN	2.0
1	A	270	GLN	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](#)

There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
2	NAG	A	687	14/15	0.75	0.47	2.07	102,106,107,107	0
2	NAG	A	1	14/15	0.87	0.20	-1.63	68,69,70,71	0
2	NAG	A	686	14/15	0.71	0.41	-	99,102,104,104	0

6.5 Other polymers ⓘ

There are no such residues in this entry.