



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:38 PM EDT

PDB ID : 3TGR / pdb_00003tgr
Title : Crystal structure of unliganded HIV-1 clade C strain C1086 gp120 core
Authors : Kwon, Y.D.; Kwong, P.D.
Deposited on : 2011-08-17
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

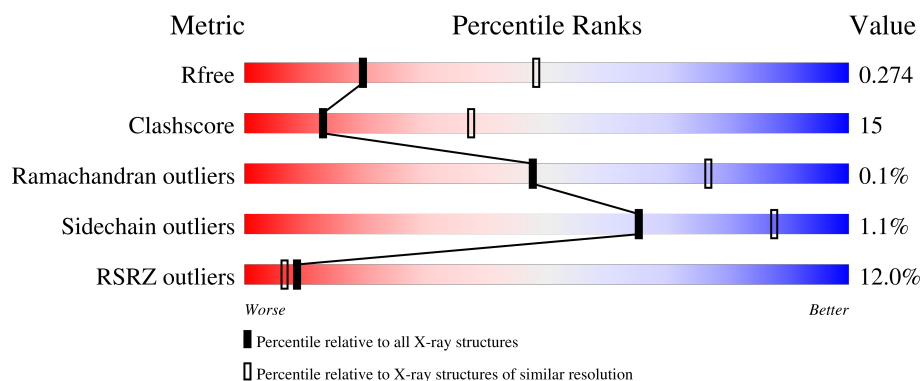
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	358	11% 68% 28% .
1	B	358	13% 67% 28% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5713 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 HIV-1 clade C1086 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2714	1697	475	522	20			
1	B	346	Total	C	N	O	S	0	0	0
			2714	1697	475	522	20			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

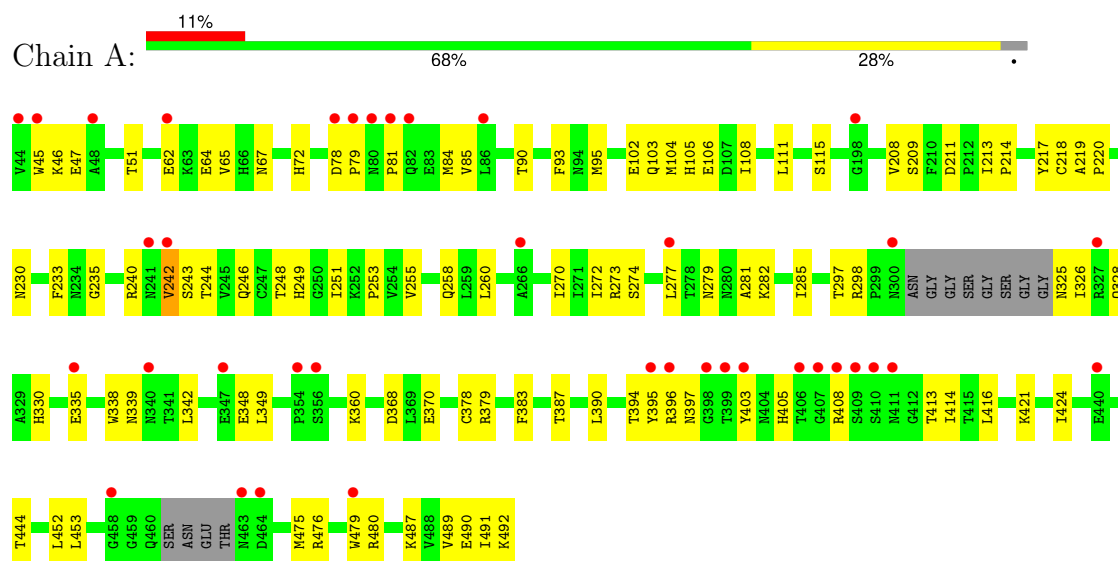
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	34	Total	O	0	0
			34	34		

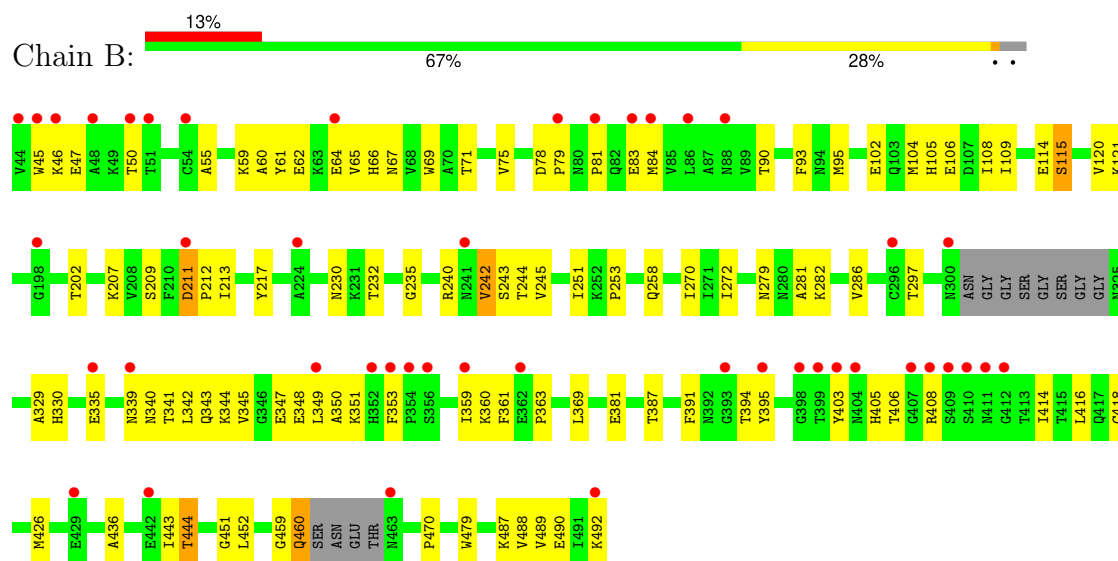
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 ($RSRZ > 2$). 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: HIV-1 clade C1086 gp120



• Molecule 1: HIV-1 clade C1086 gp120



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	67.86Å 127.51Å 193.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.29 – 2.80 45.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (45.29-2.80) 92.8 (45.29-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.07 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.223 , 0.282 0.222 , 0.274	Depositor DCC
R_{free} test set	1170 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5713	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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	0.25	0/2771	0.70	2/3758 (0.1%)
1	B	0.26	0/2771	0.71	2/3758 (0.1%)
All	All	0.25	0/5542	0.70	4/7516 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ASP	CA-C-N	6.43	126.45	119.89
1	A	211	ASP	C-N-CA	6.43	126.45	119.89
1	B	211	ASP	CA-C-N	5.17	126.30	119.84
1	B	211	ASP	C-N-CA	5.17	126.30	119.84

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	2714	0	2626	78	0
1	B	2714	0	2629	86	0
2	A	112	0	104	4	0
2	B	84	0	78	1	0
3	A	55	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	0	0	1	0
All	All	5713	0	5437	166	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 15.

All (166) 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:272:ILE:CD1	1:B:349:LEU:HD23	1.73	1.19
1:B:272:ILE:HD13	1:B:349:LEU:CD2	1.86	1.04
1:B:272:ILE:HD13	1:B:349:LEU:HD23	1.01	0.99
1:B:335:GLU:OE1	1:B:408:ARG:HD2	1.70	0.90
1:A:105:HIS:HD1	1:A:479:TRP:HZ3	1.22	0.87
1:B:395:TYR:HD2	1:B:403:TYR:HA	1.42	0.84
1:B:350:ALA:HB2	1:B:359:ILE:HD11	1.60	0.81
1:A:64:GLU:HG2	1:A:209:SER:HB3	1.63	0.81
1:A:335:GLU:HG2	1:A:414:ILE:HG13	1.62	0.81
1:B:105:HIS:HD1	1:B:479:TRP:HZ3	1.32	0.78
1:A:90:THR:HG22	1:A:240:ARG:HA	1.67	0.76
1:A:342:LEU:HB2	1:A:403:TYR:HE1	1.53	0.74
1:A:395:TYR:HD2	1:A:403:TYR:HA	1.51	0.74
1:B:242:VAL:HG12	1:B:243:SER:H	1.52	0.74
1:A:270:ILE:H	2:A:789:NAG:H61	1.53	0.73
1:A:242:VAL:HG12	1:A:243:SER:H	1.55	0.71
1:A:325:ASN:HB3	1:A:328:GLN:HB2	1.71	0.71
1:B:105:HIS:HA	1:B:479:TRP:CZ3	2.27	0.70
1:B:335:GLU:CD	1:B:408:ARG:HD2	2.17	0.69
1:B:459:GLY:O	1:B:460:GLN:C	2.35	0.69
1:A:105:HIS:ND1	1:A:479:TRP:HZ3	1.92	0.68
1:A:102:GLU:O	1:A:106:GLU:HG2	1.94	0.67
1:A:104:MET:O	1:A:108:ILE:HG12	1.95	0.67
1:A:405:HIS:HB3	1:A:408:ARG:NH2	2.10	0.66
2:A:762:NAG:H62	2:A:948:NAG:H82	1.79	0.65
1:B:297:THR:HG22	1:B:444:THR:HB	1.78	0.64
1:B:339:ASN:HA	1:B:403:TYR:CZ	2.33	0.64
1:A:342:LEU:HB2	1:A:403:TYR:CE1	2.33	0.64
1:B:120:VAL:HG22	1:B:202:THR:HG22	1.80	0.63
1:A:395:TYR:CD2	1:A:403:TYR:HA	2.32	0.62
1:B:105:HIS:ND1	1:B:479:TRP:HZ3	1.96	0.62
1:B:279:ASN:HD22	1:B:282:LYS:HG2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ASN:ND2	1:B:282:LYS:HG2	2.15	0.61
1:A:339:ASN:HA	1:A:403:TYR:CZ	2.36	0.61
1:B:84:MET:HB2	1:B:244:THR:HB	1.84	0.60
1:B:342:LEU:HB2	1:B:403:TYR:HE1	1.66	0.60
1:A:78:ASP:N	1:A:79:PRO:HA	2.16	0.60
1:A:279:ASN:HD22	1:A:282:LYS:HG2	1.66	0.60
1:B:345:VAL:O	1:B:349:LEU:HG	2.01	0.60
1:B:104:MET:O	1:B:108:ILE:HG12	2.02	0.59
1:B:286:VAL:HB	1:B:452:LEU:HB2	1.85	0.59
1:B:46:LYS:O	1:B:489:VAL:HG23	2.04	0.57
1:A:272:ILE:HD13	1:A:349:LEU:HD23	1.87	0.57
1:B:272:ILE:CD1	1:B:349:LEU:CD2	2.61	0.57
1:B:395:TYR:CD2	1:B:403:TYR:HA	2.31	0.57
1:A:78:ASP:HB2	1:A:81:PRO:HD3	1.87	0.56
1:B:90:THR:HG22	1:B:240:ARG:HA	1.86	0.56
1:A:84:MET:HB2	1:A:244:THR:HB	1.87	0.56
1:A:298:ARG:HG2	1:A:328:GLN:O	2.06	0.56
1:B:121:LYS:HE3	1:B:426:MET:HE1	1.88	0.55
1:B:47:GLU:HG2	1:B:487:LYS:HE3	1.88	0.55
1:A:490:GLU:HG2	1:A:492:LYS:HB2	1.88	0.55
1:A:279:ASN:HD21	1:A:281:ALA:HB3	1.72	0.55
1:B:78:ASP:N	1:B:79:PRO:HA	2.22	0.55
1:B:335:GLU:HG2	1:B:414:ILE:HG13	1.88	0.55
1:B:341:THR:O	1:B:345:VAL:HG23	2.07	0.55
1:B:102:GLU:O	1:B:106:GLU:HG2	2.07	0.54
1:B:451:GLY:C	1:B:452:LEU:HD12	2.32	0.54
1:B:64:GLU:HG2	1:B:209:SER:HB3	1.90	0.54
1:B:212:PRO:HB3	1:B:253:PRO:HD2	1.89	0.54
1:A:379:ARG:NH1	3:A:494:HOH:O	2.40	0.53
1:B:62:GLU:HG3	1:B:64:GLU:H	1.73	0.53
1:A:258:GLN:OE1	1:A:387:THR:HG21	2.09	0.53
1:A:255:VAL:HG13	1:A:475:MET:SD	2.49	0.53
1:A:51:THR:HA	1:A:103:GLN:HE22	1.74	0.52
1:A:270:ILE:HB	1:A:348:GLU:HG3	1.90	0.52
1:A:45:TRP:HB2	1:A:489:VAL:HG21	1.92	0.52
1:B:105:HIS:HA	1:B:479:TRP:HZ3	1.74	0.52
1:B:67:ASN:ND2	1:B:213:ILE:HD11	2.24	0.51
1:A:213:ILE:HG23	1:A:214:PRO:HD2	1.92	0.51
1:A:335:GLU:HG3	1:A:413:THR:HA	1.92	0.51
1:B:207:LYS:HE2	1:B:436:ALA:HB3	1.92	0.51
1:B:45:TRP:HB2	1:B:489:VAL:HG21	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ILE:O	1:B:253:PRO:HD3	2.12	0.50
1:A:47:GLU:HG2	1:A:487:LYS:HE3	1.94	0.50
1:A:360:LYS:HG2	1:A:394:THR:HG22	1.95	0.49
1:A:396:ARG:O	1:A:397:ASN:HB2	2.12	0.49
1:B:342:LEU:HB2	1:B:403:TYR:CE1	2.45	0.49
1:B:78:ASP:HB2	1:B:81:PRO:HD3	1.95	0.49
1:B:279:ASN:HD21	1:B:281:ALA:HB3	1.78	0.49
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.79	0.48
1:A:217:TYR:O	1:A:248:THR:HG23	2.13	0.48
1:A:335:GLU:HG2	1:A:414:ILE:CG1	2.39	0.48
1:A:208:VAL:HG22	1:A:209:SER:N	2.28	0.48
1:A:270:ILE:H	2:A:789:NAG:C6	2.25	0.48
1:A:279:ASN:ND2	1:A:282:LYS:HG2	2.29	0.48
1:B:64:GLU:OE1	1:B:211:ASP:HB3	2.14	0.48
1:A:62:GLU:HG3	1:A:64:GLU:H	1.79	0.47
1:A:405:HIS:C	1:A:408:ARG:HH22	2.22	0.47
1:A:335:GLU:OE2	1:A:408:ARG:HB3	2.15	0.47
1:B:104:MET:HE1	1:B:251:ILE:HG21	1.96	0.47
1:B:349:LEU:O	1:B:353:PHE:HD2	1.98	0.47
1:A:249:HIS:O	1:A:251:ILE:HG13	2.15	0.47
1:A:378:CYS:HB3	1:A:383:PHE:CE2	2.49	0.47
1:B:330:HIS:HA	1:B:416:LEU:O	2.14	0.47
1:B:105:HIS:O	1:B:109:ILE:HG13	2.15	0.46
1:B:230:ASN:C	1:B:232:THR:H	2.23	0.46
1:B:104:MET:HE1	1:B:251:ILE:CG2	2.45	0.46
1:A:46:LYS:O	1:A:489:VAL:HG23	2.15	0.46
1:B:347:GLU:O	1:B:351:LYS:HG3	2.16	0.46
2:A:948:NAG:H81	3:A:518:HOH:O	2.15	0.46
1:B:340:ASN:O	1:B:344:LYS:HG3	2.15	0.46
1:A:273:ARG:HB2	1:A:285:ILE:HB	1.97	0.45
1:B:50:THR:HG22	1:B:488:VAL:HG11	1.98	0.45
1:A:67:ASN:CG	1:A:213:ILE:HD11	2.41	0.45
1:A:330:HIS:HA	1:A:416:LEU:O	2.16	0.45
1:B:65:VAL:HG21	1:B:115:SER:HB3	1.98	0.45
1:B:104:MET:HA	1:B:217:TYR:OH	2.16	0.45
1:B:363:PRO:HG2	2:B:892:NAG:H81	1.97	0.45
1:B:79:PRO:HD2	3:B:35:HOH:O	2.17	0.45
1:B:242:VAL:HG12	1:B:243:SER:N	2.27	0.45
1:A:368:ASP:HB3	1:A:370:GLU:OE1	2.16	0.45
1:B:105:HIS:ND1	1:B:479:TRP:CZ3	2.72	0.45
1:B:258:GLN:CD	1:B:470:PRO:HB2	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ALA:HB3	1:B:418:CYS:HB2	1.99	0.45
1:A:47:GLU:HG2	1:A:487:LYS:CE	2.47	0.45
1:B:342:LEU:CB	1:B:403:TYR:HE1	2.30	0.44
1:A:297:THR:HG22	1:A:444:THR:HB	1.99	0.44
1:A:65:VAL:HG21	1:A:115:SER:HB3	1.99	0.44
1:A:67:ASN:ND2	1:A:213:ILE:HD11	2.31	0.44
1:B:93:PHE:CE1	1:B:487:LYS:HB3	2.52	0.44
1:B:343:GLN:HB2	1:B:403:TYR:CD1	2.53	0.44
1:A:421:LYS:HB3	1:A:421:LYS:HE2	1.78	0.44
1:B:381:GLU:HG3	1:B:443:ILE:HD13	1.99	0.44
1:B:490:GLU:HG2	1:B:492:LYS:HB2	1.98	0.44
1:B:360:LYS:HG2	1:B:394:THR:HG22	2.00	0.44
1:B:405:HIS:CG	1:B:406:THR:H	2.36	0.43
1:B:272:ILE:HD11	1:B:349:LEU:HD23	1.85	0.43
1:A:72:HIS:ND1	1:A:72:HIS:C	2.76	0.43
1:B:348:GLU:OE2	1:B:348:GLU:HA	2.18	0.43
1:B:369:LEU:HD23	1:B:369:LEU:HA	1.87	0.43
1:B:391:PHE:CE1	1:B:470:PRO:HB3	2.53	0.43
1:A:208:VAL:HG22	1:A:209:SER:H	1.83	0.43
1:B:65:VAL:HB	1:B:115:SER:OG	2.18	0.43
1:A:104:MET:HA	1:A:217:TYR:OH	2.18	0.43
1:A:476:ARG:O	1:A:480:ARG:HG3	2.19	0.43
1:B:95:MET:SD	1:B:235:GLY:HA3	2.59	0.43
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.53	0.43
1:A:230:ASN:HB3	1:A:233:PHE:HB2	2.01	0.43
1:A:452:LEU:HD12	1:A:452:LEU:N	2.34	0.42
1:A:490:GLU:C	1:A:492:LYS:H	2.27	0.42
1:A:105:HIS:HA	1:A:479:TRP:CZ3	2.53	0.42
1:A:260:LEU:HD21	1:A:453:LEU:HD21	2.01	0.42
1:A:491:ILE:HG22	1:A:491:ILE:O	2.18	0.42
1:A:403:TYR:C	1:A:403:TYR:CD2	2.97	0.42
1:B:66:HIS:CE1	1:B:212:PRO:HA	2.55	0.42
1:A:242:VAL:HG12	1:A:243:SER:N	2.27	0.42
1:B:335:GLU:OE2	1:B:408:ARG:HB3	2.19	0.41
1:A:95:MET:SD	1:A:235:GLY:HA3	2.60	0.41
1:A:111:LEU:HD12	1:A:111:LEU:O	2.21	0.41
1:A:218:CYS:HA	1:A:246:GLN:O	2.20	0.41
1:B:258:GLN:OE1	1:B:387:THR:HG21	2.20	0.41
1:A:338:TRP:CZ2	1:A:390:LEU:HG	2.56	0.41
1:B:45:TRP:HB2	1:B:489:VAL:CG2	2.50	0.41
1:A:65:VAL:HB	1:A:115:SER:OG	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASP:HB3	3:A:513:HOH:O	2.20	0.41
1:A:108:ILE:HD12	1:A:253:PRO:HB3	2.03	0.41
1:A:274:SER:HB3	1:A:277:LEU:HD23	2.02	0.41
1:B:60:ALA:HA	1:B:71:THR:HG21	2.02	0.41
1:B:69:TRP:HD1	1:B:114:GLU:OE1	2.02	0.41
1:B:55:ALA:HA	1:B:75:VAL:O	2.21	0.41
1:B:59:LYS:HB3	1:B:61:TYR:CE1	2.56	0.41
1:B:270:ILE:HB	1:B:348:GLU:HG3	2.03	0.41
1:B:359:ILE:HG22	1:B:361:PHE:CE2	2.56	0.40
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.90	0.40
1:B:83:GLU:HG2	1:B:245:VAL:CG1	2.52	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	340/358 (95%)	315 (93%)	25 (7%)	0	100	100
1	B	340/358 (95%)	318 (94%)	21 (6%)	1 (0%)	36	66
All	All	680/716 (95%)	633 (93%)	46 (7%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	SER

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	305/312 (98%)	301 (99%)	4 (1%)	61	86
1	B	305/312 (98%)	302 (99%)	3 (1%)	68	88
All	All	610/624 (98%)	603 (99%)	7 (1%)	65	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	A	242	VAL
1	A	326	ILE
1	A	424	ILE
1	B	242	VAL
1	B	444	THR
1	B	460	GLN

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

Mol	Chain	Res	Type
1	A	92	ASN
1	A	229	ASN
1	A	279	ASN
1	A	293	ASN
1	B	203	GLN
1	B	216	HIS
1	B	279	ASN
1	B	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	B	886	1	14,14,15	0.26	0	17,19,21	0.55	0
2	NAG	A	734	1	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	A	948	1	14,14,15	0.27	0	17,19,21	0.69	0
2	NAG	A	789	1	14,14,15	0.26	0	17,19,21	0.97	1 (5%)
2	NAG	B	776	1	14,14,15	0.24	0	17,19,21	0.58	0
2	NAG	B	789	1	14,14,15	0.27	0	17,19,21	0.87	1 (5%)
2	NAG	A	886	1	14,14,15	0.25	0	17,19,21	0.60	0
2	NAG	A	776	1	14,14,15	0.32	0	17,19,21	0.58	0
2	NAG	A	892	1	14,14,15	0.28	0	17,19,21	0.52	0
2	NAG	B	762	1	14,14,15	0.28	0	17,19,21	0.63	0
2	NAG	A	839	1	14,14,15	0.31	0	17,19,21	0.96	0
2	NAG	B	734	1	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	B	892	1	14,14,15	0.25	0	17,19,21	0.62	0
2	NAG	A	762	1	14,14,15	0.30	0	17,19,21	0.47	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
2	NAG	B	886	1	-	2/6/23/26	0/1/1/1
2	NAG	A	734	1	-	0/6/23/26	0/1/1/1
2	NAG	A	948	1	-	0/6/23/26	0/1/1/1
2	NAG	A	789	1	-	4/6/23/26	0/1/1/1
2	NAG	B	776	1	-	5/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	789	1	-	3/6/23/26	0/1/1/1
2	NAG	A	886	1	-	2/6/23/26	0/1/1/1
2	NAG	A	776	1	-	0/6/23/26	0/1/1/1
2	NAG	A	892	1	-	2/6/23/26	0/1/1/1
2	NAG	B	762	1	-	2/6/23/26	0/1/1/1
2	NAG	A	839	1	-	3/6/23/26	0/1/1/1
2	NAG	B	734	1	-	2/6/23/26	0/1/1/1
2	NAG	B	892	1	-	4/6/23/26	0/1/1/1
2	NAG	A	762	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	789	NAG	O5-C1-C2	-2.52	107.39	111.29
2	B	789	NAG	O5-C1-C2	-2.26	107.79	111.29

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	789	NAG	C8-C7-N2-C2
2	A	789	NAG	O7-C7-N2-C2
2	A	839	NAG	C3-C2-N2-C7
2	A	892	NAG	C8-C7-N2-C2
2	A	892	NAG	O7-C7-N2-C2
2	B	734	NAG	C8-C7-N2-C2
2	B	734	NAG	O7-C7-N2-C2
2	B	776	NAG	C8-C7-N2-C2
2	B	776	NAG	O7-C7-N2-C2
2	B	789	NAG	C8-C7-N2-C2
2	B	789	NAG	O7-C7-N2-C2
2	B	892	NAG	C8-C7-N2-C2
2	B	892	NAG	O7-C7-N2-C2
2	A	839	NAG	C8-C7-N2-C2
2	A	839	NAG	O7-C7-N2-C2
2	B	892	NAG	O5-C5-C6-O6
2	A	886	NAG	C8-C7-N2-C2
2	B	762	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	892	NAG	C4-C5-C6-O6
2	B	776	NAG	O5-C5-C6-O6
2	A	886	NAG	O7-C7-N2-C2
2	B	762	NAG	O7-C7-N2-C2
2	A	789	NAG	O5-C5-C6-O6
2	B	886	NAG	C8-C7-N2-C2
2	B	776	NAG	C4-C5-C6-O6
2	B	789	NAG	O5-C5-C6-O6
2	B	776	NAG	C3-C2-N2-C7
2	B	886	NAG	O7-C7-N2-C2
2	A	789	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	948	NAG	2	0
2	A	789	NAG	2	0
2	B	892	NAG	1	0
2	A	762	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	346/358 (96%)	0.63	38 (10%) 10 8	24, 59, 163, 225	0
1	B	346/358 (96%)	0.77	45 (13%) 7 6	38, 74, 158, 237	0
All	All	692/716 (96%)	0.70	83 (11%) 9 6	24, 68, 162, 237	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	TYR	8.2
1	A	463	ASN	6.2
1	A	410	SER	4.9
1	A	79	PRO	4.9
1	A	408	ARG	4.8
1	B	403	TYR	4.6
1	A	409	SER	4.6
1	B	463	ASN	4.6
1	A	464	ASP	4.4
1	B	335	GLU	4.1
1	A	335	GLU	3.9
1	A	44	VAL	3.8
1	A	399	THR	3.8
1	B	359	ILE	3.7
1	B	296	CYS	3.7
1	A	458	GLY	3.6
1	A	327	ARG	3.4
1	A	395	TYR	3.4
1	B	353	PHE	3.4
1	A	354	PRO	3.3
1	B	339	ASN	3.3
1	B	349	LEU	3.3
1	A	356	SER	3.3
1	B	395	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	411	ASN	3.2
1	B	356	SER	3.2
1	B	407	GLY	3.1
1	A	80	ASN	3.0
1	A	266	ALA	3.0
1	B	398	GLY	2.9
1	A	81	PRO	2.9
1	B	362	GLU	2.9
1	B	411	ASN	2.9
1	A	82	GLN	2.8
1	A	406	THR	2.8
1	B	300	ASN	2.8
1	B	224	ALA	2.7
1	A	277	LEU	2.7
1	B	442	GLU	2.7
1	A	407	GLY	2.6
1	B	241	ASN	2.6
1	B	410	SER	2.6
1	B	393	GLY	2.6
1	B	412	GLY	2.6
1	B	408	ARG	2.6
1	A	198	GLY	2.6
1	A	86	LEU	2.6
1	A	347	GLU	2.6
1	A	241	ASN	2.6
1	B	84	MET	2.5
1	B	399	THR	2.5
1	A	340	ASN	2.5
1	B	64	GLU	2.5
1	B	409	SER	2.5
1	B	492	LYS	2.4
1	B	354	PRO	2.4
1	B	86	LEU	2.4
1	B	44	VAL	2.4
1	B	50	THR	2.4
1	B	352	HIS	2.4
1	B	83	GLU	2.3
1	B	51	THR	2.3
1	B	429	GLU	2.3
1	B	48	ALA	2.2
1	A	479	TRP	2.2
1	B	404	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	45	TRP	2.2
1	B	54	CYS	2.2
1	A	398	GLY	2.2
1	B	46	LYS	2.1
1	B	198	GLY	2.1
1	A	396	ARG	2.1
1	A	440	GLU	2.1
1	B	88	ASN	2.1
1	B	79	PRO	2.1
1	A	78	ASP	2.1
1	A	48	ALA	2.1
1	A	242	VAL	2.1
1	A	300	ASN	2.1
1	B	81	PRO	2.1
1	B	211	ASP	2.1
1	A	45	TRP	2.1
1	A	62	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

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. 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	B-factors(Å ²)	Q<0.9
2	NAG	A	948	14/15	0.61	0.19	122,131,137,138	0
2	NAG	A	789	14/15	0.70	0.17	61,87,97,102	0
2	NAG	B	734	14/15	0.73	0.16	101,122,126,127	0
2	NAG	A	839	14/15	0.77	0.25	76,90,102,110	0
2	NAG	A	776	14/15	0.78	0.15	72,95,101,101	0
2	NAG	B	776	14/15	0.78	0.14	94,106,114,118	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	734	14/15	0.85	0.14	96,108,114,119	0
2	NAG	A	886	14/15	0.86	0.13	53,60,77,81	0
2	NAG	B	886	14/15	0.86	0.12	54,76,82,82	0
2	NAG	B	892	14/15	0.86	0.13	57,69,80,83	0
2	NAG	B	789	14/15	0.87	0.11	65,71,76,87	0
2	NAG	B	762	14/15	0.90	0.10	39,55,86,94	0
2	NAG	A	892	14/15	0.94	0.09	53,63,70,76	0
2	NAG	A	762	14/15	0.95	0.07	23,31,36,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.