



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2016 – 04:31 PM EDT

PDB ID : 5F4P
Title : HIV-1 gp120 complex with BNM-III-170
Authors : Liang, S.; Hendrickson, W.A.
Deposited on : 2015-12-03
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

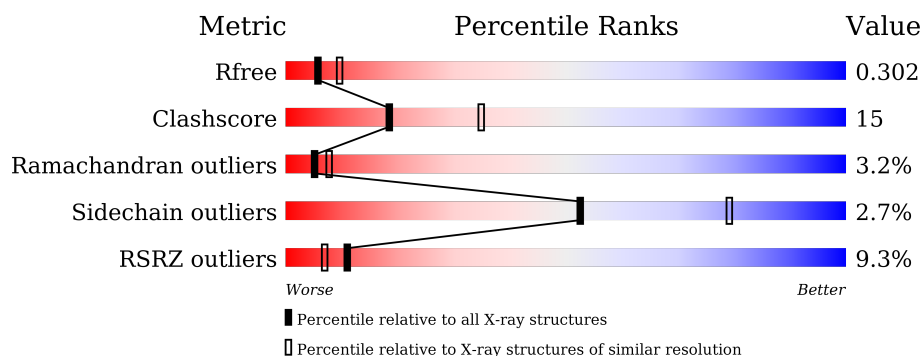
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	350	<div> <div>9%</div> <div>66%</div> <div>27%</div> <div>• •</div> </div>
1	D	350	<div> <div>9%</div> <div>63%</div> <div>28%</div> <div>• • •</div> </div>

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	507	-	-	-	X
2	NAG	D	503	-	-	-	X
2	NAG	D	506	-	-	-	X
3	5VG	A	501	-	-	-	X
3	5VG	D	507	-	-	-	X

2 Entry composition [i](#)

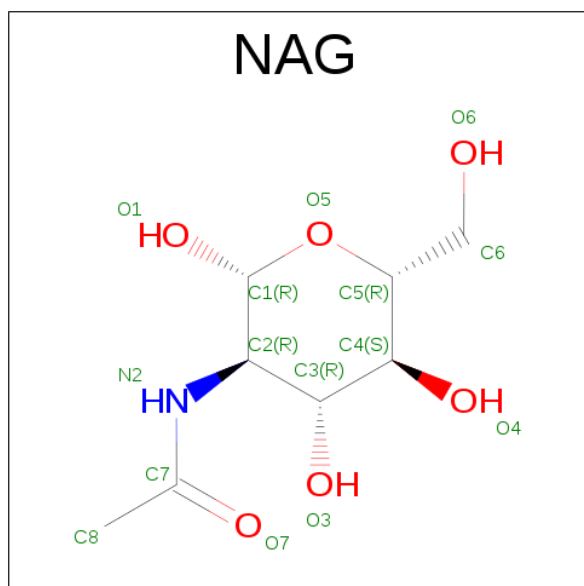
There are 4 unique types of molecules in this entry. The entry contains 5497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENVELOPE GLYCOPROTEIN GP120 of HIV-1 clade C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	A	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			

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



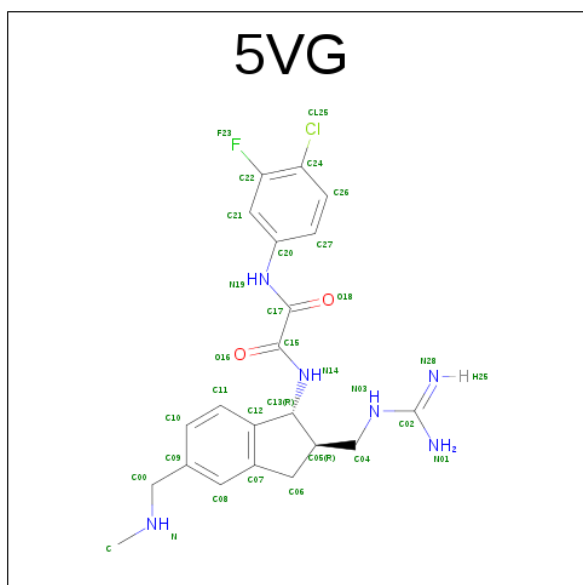
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	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	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 {N}'-[(1 {R},2 {R})-2-(carbamimidamidomethyl)-5-(methylaminomethyl)-2,3-dihydro-1 {H}-inden-1-yl]- {N}-(4-chloranyl-3-fluoranyl-phenyl)ethanediamide (three-letter code: 5VG) (formula: C₂₁H₂₄ClFN₆O₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	Cl	F	N	O	0	0
			31	21	1	1	6	2		
3	A	1	Total	C	Cl	F	N	O	0	0
			31	21	1	1	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	6	Total 6	O 6	0	0
4	A	7	Total 7	O 7	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	67.38Å 127.52Å 192.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.24 – 2.60 48.24 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.24-2.60) 99.2 (48.24-2.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.274 , 0.310 0.270 , 0.302	Depositor DCC
R_{free} test set	2410 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.772	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 26022 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5497	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 3.87% 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: NAG, 5VG

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	0.34	0/2682	0.55	0/3640
1	D	0.29	0/2682	0.55	0/3640
All	All	0.32	0/5364	0.55	0/7280

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	4
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLU	Peptide
1	A	484	TYR	Peptide
1	A	485	LYS	Peptide
1	D	353	PHE	Peptide
1	D	484	TYR	Peptide
1	D	485	LYS	Peptide
1	D	486	TYR	Peptide

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	2627	0	2548	81	0
1	D	2627	0	2548	83	0
2	A	84	0	78	7	0
2	D	84	0	78	6	0
3	A	31	0	0	1	0
3	D	31	0	0	1	0
4	A	7	0	0	0	0
4	D	6	0	0	2	0
All	All	5497	0	5252	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:D:90:THR:HG23	1:D:240:ARG:HD2	1.39	1.02
1:A:276:ASN:HD22	2:A:504:NAG:H82	1.30	0.95
1:A:268:GLU:HG3	1:A:269:GLU:H	1.37	0.91
1:D:100:MET:SD	1:D:485:LYS:NZ	2.45	0.90
1:D:485:LYS:HE3	1:D:487:LYS:HA	1.56	0.86
1:D:268:GLU:O	1:D:289:ASN:ND2	2.09	0.86
1:D:364:SER:HA	1:D:469:ARG:HG2	1.64	0.78
1:A:340:ASN:OD1	1:A:344:LYS:NZ	2.17	0.78
1:D:276:ASN:ND2	1:D:278:THR:OG1	2.23	0.72
1:D:84:MET:HG2	1:D:244:THR:HB	1.72	0.72
1:D:83:GLU:HG2	1:D:245:VAL:HG12	1.71	0.71
1:A:268:GLU:CG	1:A:269:GLU:H	1.99	0.71
1:A:89:VAL:HG21	1:A:242:VAL:HB	1.73	0.69
1:A:229:ASN:HB2	1:A:241:ASN:O	1.92	0.69
1:A:334:ASN:HB3	1:A:337:LYS:HE2	1.73	0.68
1:A:485:LYS:NZ	1:A:487:LYS:HA	2.07	0.68
1:D:457:ASP:OD1	1:D:469:ARG:NH2	2.28	0.67
1:D:358:THR:HG23	1:D:396:ARG:HG3	1.75	0.66
1:D:298:ARG:NH1	1:D:326:ILE:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:O	1:A:487:LYS:NZ	2.21	0.66
1:A:98:ASN:HD21	1:A:485:LYS:HE3	1.62	0.65
1:A:485:LYS:HZ1	1:A:487:LYS:HA	1.60	0.65
1:A:276:ASN:OD1	1:A:278:THR:N	2.30	0.65
1:A:207:LYS:NZ	1:A:437:PRO:O	2.27	0.63
1:D:464:ASP:N	4:D:603:HOH:O	2.31	0.63
1:A:98:ASN:ND2	1:A:485:LYS:HE3	2.14	0.63
1:D:381:GLU:HG3	1:D:443:ILE:HD13	1.79	0.62
2:A:504:NAG:H83	2:A:504:NAG:H3	1.82	0.62
1:A:231:LYS:HB2	1:A:268:GLU:CD	2.20	0.61
1:A:289:ASN:HD21	2:A:505:NAG:H83	1.66	0.61
1:D:476:ARG:O	1:D:480:ARG:HG3	2.01	0.61
1:A:347:GLU:HG3	1:A:395:TYR:OH	2.01	0.60
1:D:89:VAL:HG21	1:D:240:ARG:O	2.02	0.60
1:D:49:LYS:HD2	1:D:50:THR:N	2.17	0.60
1:A:381:GLU:HG3	1:A:443:ILE:HD13	1.84	0.59
1:D:269:GLU:OE2	2:D:504:NAG:O6	2.20	0.59
1:D:89:VAL:HG23	1:D:240:ARG:HE	1.66	0.59
1:D:78:ASP:C	1:D:80:ASN:H	2.05	0.58
1:A:363:PRO:HG3	1:A:388:SER:HA	1.86	0.58
1:D:298:ARG:HD3	1:D:443:ILE:HD12	1.86	0.57
1:A:86:LEU:HD12	1:A:87:ALA:H	1.69	0.57
1:A:264:SER:N	1:A:482:GLU:OE2	2.38	0.57
1:A:86:LEU:HG	1:A:89:VAL:HG12	1.86	0.57
1:D:275:GLU:OE1	1:D:282:LYS:NZ	2.35	0.57
1:D:343:GLN:HG2	1:D:403:TYR:HB3	1.86	0.57
1:D:485:LYS:HD2	1:D:486:TYR:HB2	1.87	0.56
1:A:276:ASN:OD1	1:A:276:ASN:C	2.44	0.55
1:A:456:ARG:NH1	1:A:466:GLU:OE2	2.39	0.55
1:A:83:GLU:OE2	1:A:227:LYS:NZ	2.35	0.55
1:A:476:ARG:HA	1:A:479:TRP:CD1	2.41	0.55
1:D:216:HIS:ND1	1:D:248:THR:O	2.38	0.55
1:D:217:TYR:O	1:D:248:THR:HG23	2.06	0.54
1:D:84:MET:CG	1:D:244:THR:HB	2.38	0.54
1:A:286:VAL:HB	1:A:452:LEU:HB2	1.90	0.53
2:D:503:NAG:H83	2:D:503:NAG:H3	1.90	0.53
1:A:226:LEU:HA	1:A:244:THR:HA	1.91	0.53
1:D:298:ARG:HH12	1:D:326:ILE:HA	1.74	0.53
1:A:93:PHE:CE2	1:A:239:CYS:HB3	2.44	0.52
1:D:254:VAL:HG11	1:D:261:LEU:HB2	1.89	0.52
1:A:105:HIS:CD2	1:A:476:ARG:HH21	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:GLU:O	1:D:469:ARG:HG3	2.10	0.52
1:A:361:PHE:O	1:A:392:ASN:HA	2.09	0.52
1:D:392:ASN:HD21	2:D:506:NAG:C1	2.22	0.52
1:D:90:THR:CG2	1:D:240:ARG:HD2	2.24	0.52
1:A:298:ARG:NH1	1:A:441:GLY:O	2.42	0.52
1:D:351:LYS:HB3	1:D:352:HIS:ND1	2.25	0.52
1:A:231:LYS:HB2	1:A:268:GLU:OE2	2.09	0.51
1:D:476:ARG:HH21	1:D:480:ARG:NH2	2.09	0.51
1:D:64:GLU:OE1	1:D:67:ASN:ND2	2.43	0.51
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.75	0.51
1:A:51:THR:HA	1:A:103:GLN:NE2	2.26	0.51
1:D:289:ASN:HD21	2:D:504:NAG:H83	1.76	0.51
1:D:359:ILE:HB	1:D:395:TYR:HB3	1.91	0.51
1:A:268:GLU:CG	1:A:269:GLU:N	2.71	0.51
1:A:104:MET:O	1:A:108:ILE:HG12	2.12	0.50
1:D:93:PHE:CE1	1:D:487:LYS:HE2	2.46	0.49
1:A:485:LYS:HD2	1:A:486:TYR:HB2	1.93	0.49
1:D:392:ASN:OD1	1:D:406:THR:OG1	2.29	0.49
1:D:86:LEU:CD2	1:D:88:ASN:H	2.24	0.49
1:D:240:ARG:O	1:D:242:VAL:N	2.44	0.49
1:A:474:ASP:OD1	1:A:476:ARG:HG2	2.12	0.49
1:A:214:PRO:HG3	1:A:252:LYS:HE2	1.95	0.49
1:A:268:GLU:O	2:A:505:NAG:H83	2.13	0.48
1:D:104:MET:O	1:D:108:ILE:HG12	2.13	0.48
1:A:254:VAL:HG11	1:A:261:LEU:HB2	1.95	0.48
1:D:476:ARG:HA	1:D:479:TRP:CD1	2.48	0.48
1:A:50:THR:HG22	1:A:488:VAL:HG21	1.95	0.48
1:D:66:HIS:CD2	1:D:212:PRO:HA	2.48	0.48
1:A:344:LYS:HD2	1:A:344:LYS:N	2.29	0.47
1:D:248:THR:HG21	1:D:486:TYR:CE2	2.49	0.47
1:D:278:THR:O	1:D:456:ARG:NH2	2.48	0.47
1:A:89:VAL:HG22	1:A:90:THR:N	2.29	0.47
1:A:408:ARG:HG2	1:A:409:SER:N	2.29	0.47
1:A:231:LYS:C	1:A:233:PHE:H	2.18	0.47
1:D:93:PHE:HE1	1:D:487:LYS:HE2	1.80	0.47
1:D:478:ASN:O	1:D:481:SER:OG	2.29	0.47
1:A:464:ASP:OD1	1:A:465:THR:OG1	2.32	0.46
1:D:441:GLY:O	4:D:601:HOH:O	2.21	0.46
1:A:485:LYS:CG	1:A:486:TYR:H	2.29	0.46
1:D:286:VAL:HB	1:D:452:LEU:HB2	1.97	0.46
1:A:327:ARG:NH1	1:A:438:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LYS:HG3	1:A:486:TYR:H	1.81	0.46
1:D:249:HIS:CD2	1:D:486:TYR:OH	2.69	0.46
1:D:268:GLU:O	2:D:504:NAG:H83	2.16	0.46
1:D:79:PRO:C	1:D:81:PRO:HD3	2.36	0.46
1:A:228:CYS:C	1:A:229:ASN:HD22	2.19	0.46
1:A:51:THR:HA	1:A:103:GLN:HE22	1.80	0.45
1:A:64:GLU:OE2	1:A:66:HIS:ND1	2.45	0.45
1:A:50:THR:O	1:A:103:GLN:NE2	2.49	0.45
1:D:78:ASP:HA	1:D:79:PRO:HD2	1.73	0.45
1:A:279:ASN:HB3	1:A:282:LYS:HG3	1.99	0.45
1:A:85:VAL:HA	1:A:243:SER:HA	1.98	0.45
1:D:86:LEU:HD22	1:D:89:VAL:HG13	1.98	0.45
1:D:89:VAL:HG23	1:D:90:THR:H	1.82	0.45
2:A:504:NAG:H3	2:A:504:NAG:C8	2.46	0.45
1:A:85:VAL:HG13	1:A:243:SER:OG	2.17	0.45
1:D:364:SER:OG	1:D:372:THR:HA	2.17	0.45
1:A:410:SER:O	1:A:413:THR:HG22	2.17	0.44
1:D:64:GLU:HA	1:D:209:SER:HB3	1.99	0.44
1:D:272:ILE:HG12	1:D:348:GLU:HG2	1.98	0.44
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.84	0.44
1:D:357:LYS:HB3	1:D:464:ASP:O	2.17	0.44
1:D:327:ARG:HG2	1:D:327:ARG:HH11	1.82	0.44
1:A:276:ASN:ND2	2:A:504:NAG:H82	2.14	0.44
1:A:227:LYS:HA	1:A:486:TYR:HA	2.00	0.43
1:A:485:LYS:HD2	1:A:486:TYR:N	2.33	0.43
1:D:276:ASN:OD1	1:D:277:LEU:N	2.50	0.43
1:D:207:LYS:NZ	1:D:437:PRO:O	2.34	0.43
1:A:259:LEU:HB2	1:A:374:HIS:CE1	2.53	0.43
1:A:66:HIS:CD2	1:A:212:PRO:HA	2.54	0.43
1:A:392:ASN:HD21	2:A:507:NAG:C1	2.32	0.43
1:D:90:THR:HA	1:D:240:ARG:HG2	2.00	0.43
1:A:249:HIS:CE1	1:A:482:GLU:HG3	2.54	0.42
1:D:102:GLU:O	1:D:106:GLU:HG2	2.19	0.42
1:D:96:TRP:HD1	1:D:236:THR:HG23	1.85	0.42
1:D:264:SER:N	1:D:482:GLU:OE2	2.52	0.42
1:A:344:LYS:HA	1:A:347:GLU:HB2	2.01	0.42
1:A:485:LYS:CG	1:A:486:TYR:N	2.82	0.42
1:A:66:HIS:CD2	1:A:111:LEU:HD21	2.54	0.42
1:D:370:GLU:HG2	3:D:507:5VG:N19	2.33	0.42
1:D:69:TRP:HA	1:D:72:HIS:CD2	2.54	0.42
1:D:288:LEU:HG	1:D:451:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:GLU:OE2	1:D:66:HIS:ND1	2.52	0.42
1:D:230:ASN:HB3	1:D:233:PHE:HB2	2.02	0.42
1:D:393:GLY:HA3	1:D:403:TYR:CE1	2.55	0.42
1:A:93:PHE:HE2	1:A:239:CYS:HB3	1.84	0.42
1:A:257:THR:O	1:A:259:LEU:N	2.49	0.42
1:D:226:LEU:HD23	1:D:244:THR:OG1	2.21	0.41
1:D:55:ALA:HA	1:D:75:VAL:O	2.20	0.41
1:A:353:PHE:HA	1:A:354:PRO:HD2	1.91	0.41
1:A:364:SER:OG	1:A:372:THR:HA	2.20	0.41
1:A:298:ARG:HH11	1:A:443:ILE:HG13	1.86	0.41
1:A:89:VAL:CG2	1:A:90:THR:N	2.83	0.41
1:D:363:PRO:HG3	1:D:388:SER:HA	2.03	0.41
1:D:276:ASN:HD22	2:D:503:NAG:H82	1.85	0.41
1:A:359:ILE:HB	1:A:395:TYR:HB3	2.02	0.41
1:D:294:ILE:HD12	1:D:333:ILE:HD11	2.03	0.41
1:A:370:GLU:HG2	3:A:501:5VG:N19	2.35	0.41
1:D:475:MET:O	1:D:478:ASN:HB2	2.20	0.41
1:D:214:PRO:HG2	1:A:61:TYR:CE2	2.56	0.41
1:D:342:LEU:HA	1:D:342:LEU:HD23	1.84	0.41
1:A:331:CYS:O	1:A:415:THR:HA	2.21	0.40
1:D:257:THR:O	1:D:259:LEU:N	2.50	0.40
1:D:485:LYS:HD2	1:D:486:TYR:N	2.36	0.40
1:A:110:SER:O	1:A:114:GLU:HG3	2.20	0.40
1:D:219:ALA:HA	1:D:220:PRO:HD3	1.81	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	329/350 (94%)	294 (89%)	26 (8%)	9 (3%)	6 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	329/350 (94%)	292 (89%)	25 (8%)	12 (4%)	4	6
All	All	658/700 (94%)	586 (89%)	51 (8%)	21 (3%)	5	8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	485	LYS
1	A	81	PRO
1	A	354	PRO
1	A	365	SER
1	A	485	LYS
1	D	79	PRO
1	A	83	GLU
1	A	90	THR
1	A	486	TYR
1	D	84	MET
1	D	226	LEU
1	D	486	TYR
1	D	81	PRO
1	D	365	SER
1	D	487	LYS
1	A	79	PRO
1	D	89	VAL
1	D	270	ILE
1	A	220	PRO
1	D	354	PRO
1	D	220	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/305 (97%)	289 (97%)	8 (3%)	52	79
1	D	297/305 (97%)	289 (97%)	8 (3%)	52	79
All	All	594/610 (97%)	578 (97%)	16 (3%)	52	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	88	ASN
1	D	90	THR
1	D	249	HIS
1	D	328	GLN
1	D	347	GLU
1	D	352	HIS
1	D	397	ASN
1	D	469	ARG
1	A	78	ASP
1	A	89	VAL
1	A	102	GLU
1	A	229	ASN
1	A	231	LYS
1	A	240	ARG
1	A	276	ASN
1	A	485	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	234	ASN
1	D	249	HIS
1	D	289	ASN
1	A	98	ASN
1	A	229	ASN
1	A	234	ASN
1	A	249	HIS
1	A	289	ASN
1	A	293	ASN
1	A	392	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	5VG	A	501	-	30,33,33	2.13	11 (36%)	36,46,46	2.02	6 (16%)
2	NAG	A	502	-	14,14,15	0.41	0	15,19,21	0.32	0
2	NAG	A	503	-	14,14,15	0.42	0	15,19,21	0.38	0
2	NAG	A	504	-	14,14,15	0.27	0	15,19,21	1.52	1 (6%)
2	NAG	A	505	-	14,14,15	0.38	0	15,19,21	0.51	0
2	NAG	A	506	-	14,14,15	0.29	0	15,19,21	0.36	0
2	NAG	A	507	-	14,14,15	0.27	0	15,19,21	0.61	0
2	NAG	D	501	-	14,14,15	0.31	0	15,19,21	0.27	0
2	NAG	D	502	-	14,14,15	0.27	0	15,19,21	0.31	0
2	NAG	D	503	-	14,14,15	0.36	0	15,19,21	1.36	1 (6%)
2	NAG	D	504	-	14,14,15	0.36	0	15,19,21	0.60	0
2	NAG	D	505	-	14,14,15	0.13	0	15,19,21	0.41	0
2	NAG	D	506	-	14,14,15	0.35	0	15,19,21	0.51	0
3	5VG	D	507	-	30,33,33	2.10	10 (33%)	36,46,46	2.10	6 (16%)

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	5VG	A	501	-	-	0/17/32/32	0/3/3/3
2	NAG	A	502	-	-	0/6/23/26	0/1/1/1
2	NAG	A	503	-	-	0/6/23/26	0/1/1/1
2	NAG	A	504	-	-	0/6/23/26	0/1/1/1
2	NAG	A	505	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	506	-	-	0/6/23/26	0/1/1/1
2	NAG	A	507	-	-	0/6/23/26	0/1/1/1
2	NAG	D	501	-	-	0/6/23/26	0/1/1/1
2	NAG	D	502	-	-	0/6/23/26	0/1/1/1
2	NAG	D	503	-	-	0/6/23/26	0/1/1/1
2	NAG	D	504	-	-	0/6/23/26	0/1/1/1
2	NAG	D	505	-	-	0/6/23/26	0/1/1/1
2	NAG	D	506	-	-	0/6/23/26	0/1/1/1
3	5VG	D	507	-	-	0/17/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	507	5VG	C05-C13	-3.83	1.49	1.54
3	A	501	5VG	C05-C13	-3.76	1.49	1.54
3	A	501	5VG	C-N	-2.95	1.41	1.47
3	D	507	5VG	C-N	-2.88	1.41	1.47
3	A	501	5VG	C06-C05	-2.81	1.49	1.53
3	D	507	5VG	C06-C05	-2.76	1.49	1.53
3	A	501	5VG	C21-C22	2.02	1.41	1.37
3	D	507	5VG	C07-C12	2.05	1.43	1.39
3	A	501	5VG	C27-C26	2.06	1.42	1.38
3	D	507	5VG	C27-C26	2.12	1.43	1.38
3	A	501	5VG	C07-C12	2.12	1.43	1.39
3	D	507	5VG	C24-C22	2.22	1.41	1.38
3	A	501	5VG	C24-C22	2.26	1.42	1.38
3	A	501	5VG	C08-C09	3.09	1.44	1.39
3	D	507	5VG	C08-C09	3.18	1.45	1.39
3	D	507	5VG	C10-C11	3.21	1.45	1.38
3	A	501	5VG	C10-C11	3.27	1.45	1.38
3	D	507	5VG	C17-N19	4.72	1.45	1.35
3	A	501	5VG	C17-N19	4.83	1.46	1.35
3	D	507	5VG	C15-N14	4.88	1.44	1.34
3	A	501	5VG	C15-N14	4.97	1.44	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	507	5VG	C12-C13-N14	-4.11	108.59	114.40
3	D	507	5VG	C20-N19-C17	-3.01	122.24	127.60
3	A	501	5VG	C12-C13-N14	-2.89	110.32	114.40
3	A	501	5VG	C06-C07-C12	-2.57	108.03	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	5VG	C07-C12-C13	-2.56	108.42	110.37
3	D	507	5VG	C06-C07-C12	-2.38	108.24	110.96
3	D	507	5VG	C07-C12-C13	-2.29	108.62	110.37
3	A	501	5VG	C20-N19-C17	-2.11	123.84	127.60
2	D	503	NAG	C2-N2-C7	4.83	129.39	123.11
3	A	501	5VG	C15-C17-N19	5.13	118.05	112.06
2	A	504	NAG	C2-N2-C7	5.59	130.37	123.11
3	D	507	5VG	C15-C17-N19	6.31	119.43	112.06
3	D	507	5VG	C17-C15-N14	7.11	119.68	113.22
3	A	501	5VG	C17-C15-N14	7.93	120.43	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	5VG	1	0
2	A	504	NAG	4	0
2	A	505	NAG	2	0
2	A	507	NAG	1	0
2	D	503	NAG	2	0
2	D	504	NAG	3	0
2	D	506	NAG	1	0
3	D	507	5VG	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	335/350 (95%)	0.68	30 (8%) 12 8	38, 71, 106, 123	0
1	D	335/350 (95%)	0.74	32 (9%) 10 6	54, 81, 101, 125	0
All	All	670/700 (95%)	0.71	62 (9%) 11 7	38, 77, 103, 125	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	VAL	6.8
1	D	88	ASN	6.1
1	D	486	TYR	5.8
1	A	87	ALA	5.6
1	D	87	ALA	5.4
1	A	221	ALA	5.3
1	D	90	THR	5.1
1	D	239	CYS	4.8
1	D	89	VAL	4.3
1	A	223	PHE	4.3
1	D	223	PHE	4.2
1	D	86	LEU	4.1
1	A	88	ASN	4.1
1	D	85	VAL	4.1
1	A	489	VAL	4.1
1	A	84	MET	3.6
1	D	226	LEU	3.5
1	A	124	GLY	3.5
1	D	240	ARG	3.4
1	D	93	PHE	3.4
1	D	345	VAL	3.3
1	D	91	GLU	3.3
1	A	225	ILE	3.3
1	D	224	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	78	ASP	3.1
1	D	483	LEU	3.1
1	A	80	ASN	3.0
1	A	86	LEU	3.0
1	A	85	VAL	3.0
1	A	222	GLY	2.9
1	A	485	LYS	2.9
1	A	242	VAL	2.8
1	D	92	ASN	2.8
1	D	272	ILE	2.7
1	D	487	LYS	2.7
1	A	226	LEU	2.7
1	A	90	THR	2.6
1	D	484	TYR	2.5
1	D	248	THR	2.5
1	A	228	CYS	2.5
1	A	490	GLU	2.5
1	A	91	GLU	2.4
1	D	300	ASN	2.4
1	D	228	CYS	2.4
1	D	215	LEU	2.3
1	A	354	PRO	2.3
1	A	224	ALA	2.2
1	D	242	VAL	2.2
1	D	404	ASN	2.2
1	A	277	LEU	2.1
1	D	241	ASN	2.1
1	A	397	ASN	2.1
1	D	342	LEU	2.1
1	A	349	LEU	2.1
1	A	239	CYS	2.0
1	D	49	LYS	2.0
1	A	487	LYS	2.0
1	D	265	LEU	2.0
1	D	225	ILE	2.0
1	A	83	GLU	2.0
1	A	220	PRO	2.0
1	D	289	ASN	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 [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(Å ²)	Q<0.9
3	5VG	A	501	31/31	0.67	0.43	6.78	64,72,87,96	0
3	5VG	D	507	31/31	0.81	0.30	4.64	64,76,90,95	0
2	NAG	D	506	14/15	0.71	0.33	3.54	88,100,112,114	0
2	NAG	D	503	14/15	0.65	0.26	3.15	88,96,101,101	0
2	NAG	A	507	14/15	0.85	0.31	2.42	65,72,85,95	0
2	NAG	D	501	14/15	0.85	0.33	1.56	83,93,99,103	0
2	NAG	A	503	14/15	0.79	0.30	1.51	46,60,70,75	0
2	NAG	A	502	14/15	0.70	0.29	1.04	88,103,110,113	0
2	NAG	D	502	14/15	0.84	0.28	1.01	66,78,86,93	0
2	NAG	A	505	14/15	0.76	0.33	0.87	86,92,104,106	0
2	NAG	D	504	14/15	0.77	0.20	-1.14	88,94,100,109	0
2	NAG	A	506	14/15	0.83	0.28	-	71,81,88,89	0
2	NAG	A	504	14/15	0.73	0.44	-	85,92,102,110	0
2	NAG	D	505	14/15	0.81	0.25	-	69,88,94,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.