



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:16 PM UTC

PDB ID : 5F4P / pdb_00005f4p
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

<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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

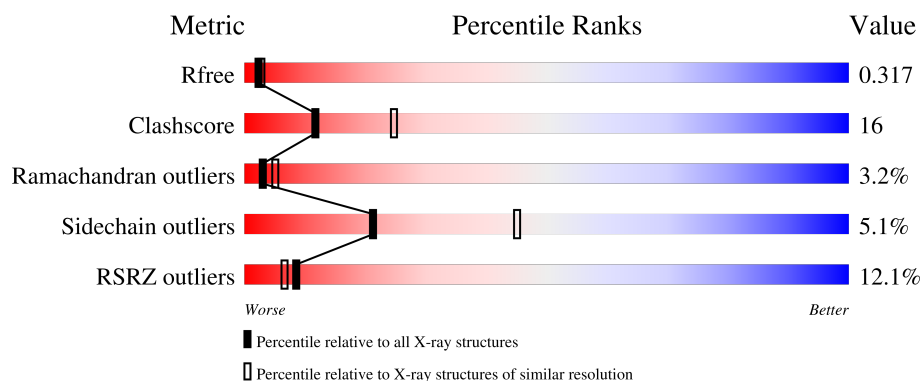
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	350	11% 64% 26% 5% .
1	D	350	13% 62% 29% ...

2 Entry composition [i](#)

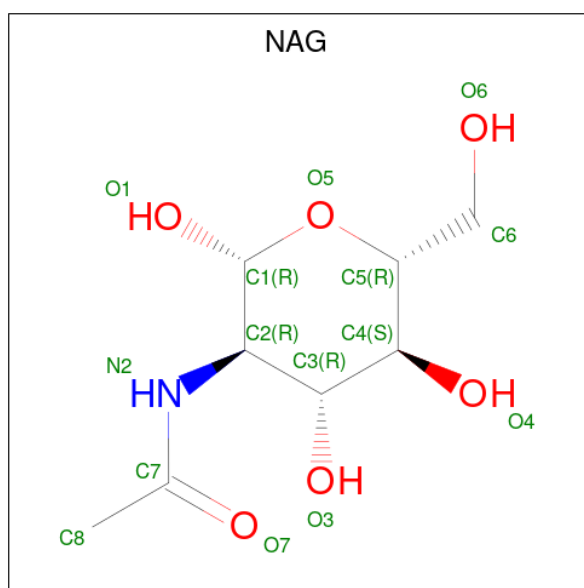
There are 4 unique types of molecules in this entry. The entry contains 5497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



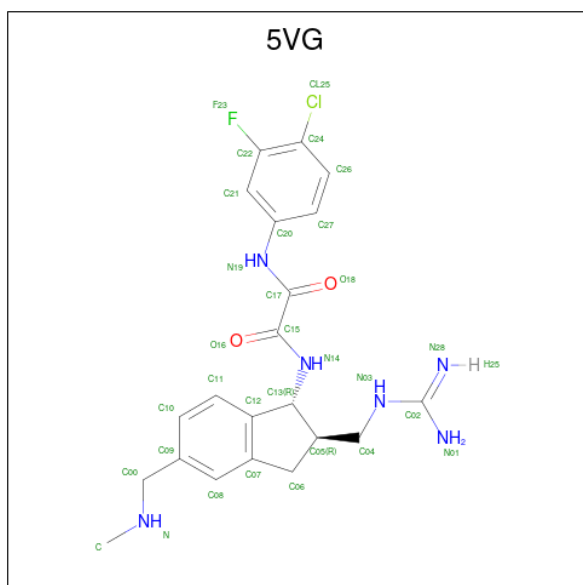
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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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 (CCD ID: 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		

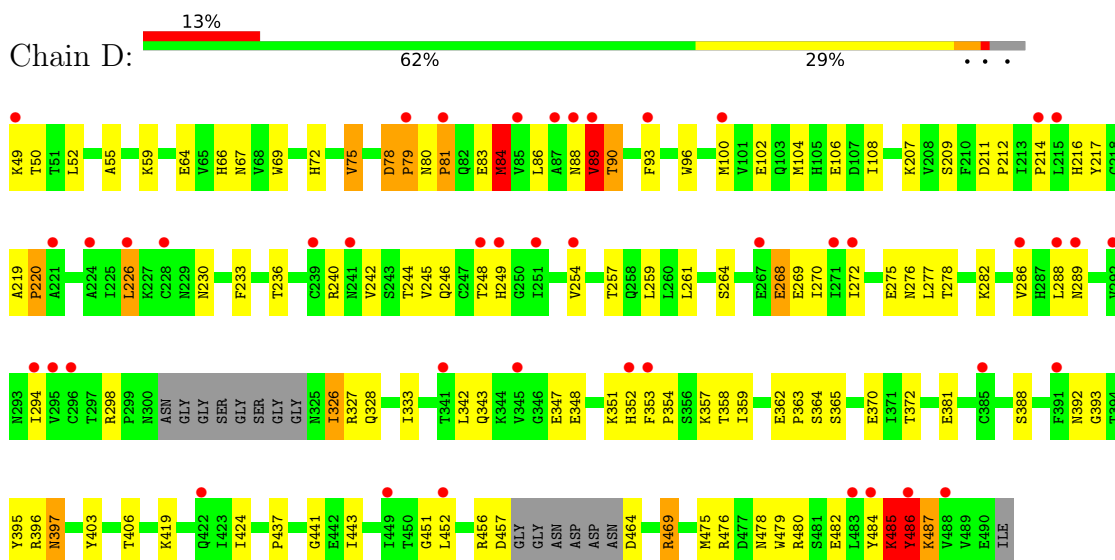
- Molecule 4 is water.

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

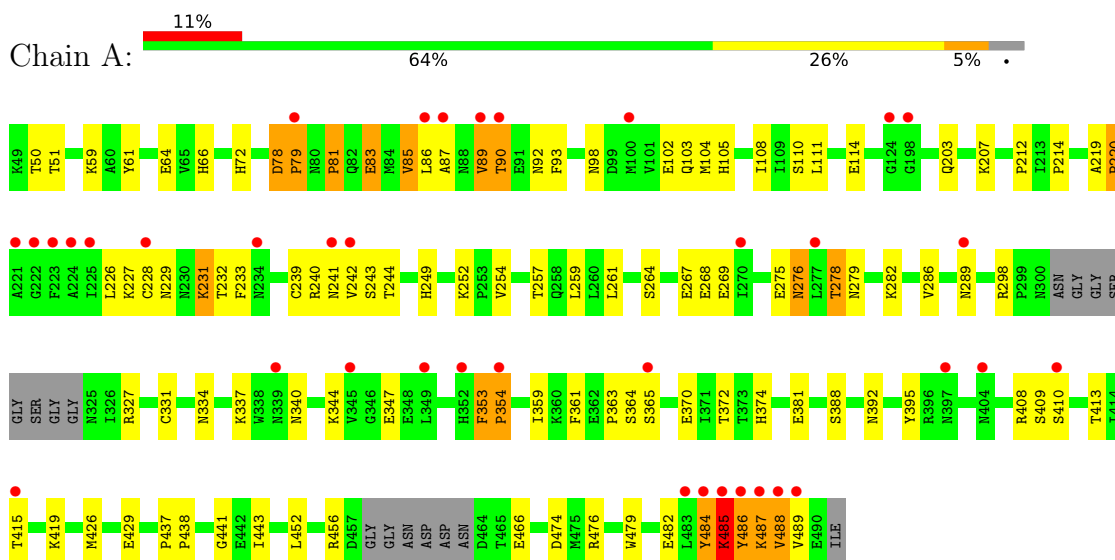
3 Residue-property plots

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: ENVELOPE GLYCOPROTEIN GP120 of HIV-1 clade C



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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 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.24-2.60) 99.6 (48.24-2.60)	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 1.8.4_1496	Depositor
R, R_{free}	0.274 , 0.310 0.278 , 0.317	Depositor DCC
R_{free} test set	1264 reflections (2.34%)	wwPDB-VP
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 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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: 5VG, 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	0.42	0/2682	0.87	5/3640 (0.1%)
1	D	0.38	0/2682	0.86	7/3640 (0.2%)
All	All	0.40	0/5364	0.87	12/7280 (0.2%)

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.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78	ASP	CA-C-N	7.33	129.00	119.84
1	D	78	ASP	C-N-CA	7.33	129.00	119.84
1	D	89	VAL	N-CA-C	6.77	123.42	109.34
1	A	353	PHE	CA-C-N	6.16	127.54	119.84
1	A	353	PHE	C-N-CA	6.16	127.54	119.84
1	A	78	ASP	CA-C-N	-6.06	112.26	119.84
1	A	78	ASP	C-N-CA	-6.06	112.26	119.84
1	D	486	TYR	N-CA-C	-5.90	98.23	110.80
1	A	484	TYR	N-CA-C	-5.28	106.34	112.89
1	D	246	GLN	N-CA-C	-5.14	107.56	113.88
1	D	211	ASP	CA-C-N	5.08	126.19	119.84
1	D	211	ASP	C-N-CA	5.08	126.19	119.84

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	84	0
1	D	2627	0	2548	85	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	1	0
4	D	6	0	0	2	0
All	All	5497	0	5252	171	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 16.

All (171) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:72:HIS:NE2	4:A:601:HOH:O	2.29	0.66
1:A:231:LYS:HB2	1:A:268:GLU:CD	2.20	0.66
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:276:ASN:OD1	1:A:278:THR:N	2.30	0.65
1:D:78:ASP:C	1:D:80:ASN:H	2.05	0.63
1:D:464:ASP:N	4:D:603:HOH:O	2.31	0.63
1:A:207:LYS:NZ	1:A:437:PRO:O	2.27	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:H3	2:A:504:NAG:H83	1.82	0.62
1:D:476:ARG:O	1:D:480:ARG:HG3	2.01	0.61
1:A:289:ASN:HD21	2:A:505:NAG:H83	1.66	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:A:276:ASN:OD1	1:A:276:ASN:C	2.44	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:485:LYS:HZ3	1:A:487:LYS:HA	1.72	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:D:298:ARG:HH12	1:D:326:ILE:HA	1.74	0.53
1:A:226:LEU:HA	1:A:244:THR:HA	1.91	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:485:LYS:HZ1	1:A:487:LYS:HA	1.73	0.52
1:D:362:GLU:O	1:D:469:ARG:HG3	2.10	0.52
1:A:105:HIS:CD2	1:A:476:ARG:HH21	2.28	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:D:351:LYS:HB3	1:D:352:HIS:ND1	2.25	0.52
1:A:298:ARG:NH1	1:A:441:GLY:O	2.42	0.52
1:A:231:LYS:C	1:A:233:PHE:H	2.18	0.52
1:D:64:GLU:OE1	1:D:67:ASN:ND2	2.43	0.51
1:D:476:ARG:HH21	1:D:480:ARG:NH2	2.09	0.51
1:A:231:LYS:HB2	1:A:268:GLU:OE2	2.09	0.51
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.75	0.51
1:D:289:ASN:HD21	2:D:504:NAG:H83	1.76	0.51
1:A:51:THR:HA	1:A:103:GLN:NE2	2.26	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:D:79:PRO:C	1:D:81:PRO:HD3	2.36	0.50
1:A:104:MET:O	1:A:108:ILE:HG12	2.12	0.50
1:A:228:CYS:C	1:A:229:ASN:HD22	2.19	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:86:LEU:CD2	1:D:88:ASN:H	2.24	0.49
1:D:392:ASN:OD1	1:D:406:THR:OG1	2.29	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:D:104:MET:O	1:D:108:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLU:O	2:A:505:NAG:H83	2.13	0.48
1:D:476:ARG:HA	1:D:479:TRP:CD1	2.48	0.48
1:A:254:VAL:HG11	1:A:261:LEU:HB2	1.95	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: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:344:LYS:N	1:A:344:LYS:HD2	2.29	0.47
1:A:89:VAL:HG22	1:A:90:THR:N	2.29	0.47
1:D:93:PHE:HE1	1:D:487:LYS:HE2	1.80	0.47
1:A:408:ARG:HG2	1:A:409:SER:N	2.29	0.47
1:D:441:GLY:O	4:D:601:HOH:O	2.21	0.46
1:D:286:VAL:HB	1:D:452:LEU:HB2	1.97	0.46
1:A:485:LYS:CG	1:A:486:TYR:H	2.29	0.46
1:D:249:HIS:CD2	1:D:486:TYR:OH	2.69	0.46
1:A:327:ARG:NH1	1:A:438:PRO:HD2	2.31	0.46
1:A:485:LYS:HG3	1:A:486:TYR:H	1.81	0.46
1:D:268:GLU:O	2:D:504:NAG:H83	2.16	0.46
1:D:78:ASP:C	1:D:80:ASN:N	2.73	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: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
1:A:85:VAL:HA	1:A:243:SER:HA	1.98	0.45
1:A:279:ASN:HB3	1:A:282:LYS:HG3	1.99	0.45
2:A:504:NAG:H3	2:A:504:NAG:C8	2.46	0.45
1:D:52:LEU:HD21	1:D:100:MET:HE3	1.97	0.45
1:D:364:SER:OG	1:D:372:THR:HA	2.17	0.45
1:A:85:VAL:HG13	1:A:243:SER:OG	2.17	0.45
1:D:64:GLU:HA	1:D:209:SER:HB3	1.99	0.44
1:A:410:SER:O	1:A:413:THR:HG22	2.17	0.44
1:D:272:ILE:HG12	1:D:348:GLU:HG2	1.98	0.44
1:D:357:LYS:HB3	1:D:464:ASP:O	2.17	0.44
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.84	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:207:LYS:NZ	1:D:437:PRO:O	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ASN:OD1	1:D:277:LEU:N	2.50	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:D:90:THR:HA	1:D:240:ARG:HG2	2.00	0.43
1:A:392:ASN:HD21	2:A:507:NAG:C1	2.32	0.43
1:D:96:TRP:HD1	1:D:236:THR:HG23	1.85	0.42
1:D:102:GLU:O	1:D:106:GLU:HG2	2.19	0.42
1:D:264:SER:N	1:D:482:GLU:OE2	2.52	0.42
1:A:249:HIS:CE1	1:A:482:GLU:HG3	2.54	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:D:69:TRP:HA	1:D:72:HIS:CD2	2.54	0.42
1:D:370:GLU:HG2	3:D:507:5VG:N19	2.33	0.42
1:A:66:HIS:CD2	1:A:111:LEU:HD21	2.54	0.42
1:D:64:GLU:OE2	1:D:66:HIS:ND1	2.52	0.42
1:D:288:LEU:HG	1:D:451:GLY:HA2	2.01	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:55:ALA:HA	1:D:75:VAL:O	2.20	0.41
1:D:226:LEU:HD23	1:D:244:THR:OG1	2.21	0.41
1:D:276:ASN:HD22	2:D:503:NAG:H82	1.85	0.41
1:D:363:PRO:HG3	1:D:388:SER:HA	2.03	0.41
1:A:89:VAL:CG2	1:A:90:THR:N	2.83	0.41
1:A:298:ARG:HH11	1:A:443:ILE:HG13	1.86	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:D:294:ILE:HD12	1:D:333:ILE:HD11	2.03	0.41
1:A:359:ILE:HB	1:A:395:TYR:HB3	2.02	0.41
1:D:475:MET:O	1:D:478:ASN:HB2	2.20	0.41
1:A:370:GLU:HG2	3:A:501:5VG:N19	2.35	0.41
1:D:214:PRO:HG2	1:A:61:TYR:CE2	2.56	0.41
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.84	0.41
1:A:79:PRO:C	1:A:81:PRO:HD3	2.45	0.41
1:D:397:ASN:OD1	1:D:397:ASN:C	2.64	0.41
1:A:426:MET:HE3	1:A:429:GLU:HB2	2.03	0.41
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:331:CYS:O	1:A:415:THR:HA	2.21	0.40
1:A:110:SER:O	1:A:114:GLU:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	4	7
1	D	329/350 (94%)	292 (89%)	25 (8%)	12 (4%)	2	4
All	All	658/700 (94%)	586 (89%)	51 (8%)	21 (3%)	3	5

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

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Mol	Chain	Res	Type
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%)	280 (94%)	17 (6%)	18	40
1	D	297/305 (97%)	284 (96%)	13 (4%)	25	50
All	All	594/610 (97%)	564 (95%)	30 (5%)	21	45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	59	LYS
1	D	75	VAL
1	D	84	MET
1	D	90	THR
1	D	268	GLU
1	D	326	ILE
1	D	328	GLN
1	D	347	GLU
1	D	397	ASN
1	D	419	LYS
1	D	424	ILE
1	D	469	ARG
1	D	485	LYS
1	A	59	LYS
1	A	78	ASP
1	A	85	VAL
1	A	89	VAL
1	A	102	GLU
1	A	203	GLN

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Mol	Chain	Res	Type
1	A	231	LYS
1	A	232	THR
1	A	240	ARG
1	A	267	GLU
1	A	276	ASN
1	A	278	THR
1	A	419	LYS
1	A	485	LYS
1	A	487	LYS
1	A	488	VAL
1	A	489	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	72	HIS
1	D	92	ASN
1	D	234	ASN
1	D	249	HIS
1	D	289	ASN
1	A	98	ASN
1	A	234	ASN
1	A	249	HIS
1	A	289	ASN
1	A	293	ASN
1	A	425	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 oligosaccharides 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
2	NAG	D	503	-	14,14,15	0.39	0	17,19,21	1.50	2 (11%)
2	NAG	D	504	-	14,14,15	0.40	0	17,19,21	0.73	0
2	NAG	A	503	-	14,14,15	0.41	0	17,19,21	0.49	0
2	NAG	A	502	-	14,14,15	0.43	0	17,19,21	0.40	0
3	5VG	D	507	-	33,33,33	2.46	11 (33%)	39,46,46	1.34	4 (10%)
2	NAG	A	505	-	14,14,15	0.41	0	17,19,21	0.56	0
2	NAG	D	501	-	14,14,15	0.32	0	17,19,21	0.38	0
2	NAG	D	502	-	14,14,15	0.26	0	17,19,21	0.43	0
2	NAG	A	507	-	14,14,15	0.30	0	17,19,21	0.75	0
2	NAG	A	506	-	14,14,15	0.28	0	17,19,21	0.46	0
2	NAG	A	504	-	14,14,15	0.30	0	17,19,21	1.52	1 (5%)
2	NAG	D	506	-	14,14,15	0.36	0	17,19,21	0.59	0
3	5VG	A	501	-	33,33,33	2.48	12 (36%)	39,46,46	1.22	4 (10%)
2	NAG	D	505	-	14,14,15	0.13	0	17,19,21	0.50	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	D	503	-	-	5/6/23/26	0/1/1/1
2	NAG	D	504	-	-	4/6/23/26	0/1/1/1
2	NAG	A	503	-	-	0/6/23/26	0/1/1/1
2	NAG	A	502	-	-	1/6/23/26	0/1/1/1
3	5VG	D	507	-	-	5/20/32/32	0/3/3/3
2	NAG	A	505	-	-	3/6/23/26	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	A	507	-	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	506	-	-	2/6/23/26	0/1/1/1
2	NAG	A	504	-	-	5/6/23/26	0/1/1/1
2	NAG	D	506	-	-	4/6/23/26	0/1/1/1
3	5VG	A	501	-	-	2/20/32/32	0/3/3/3
2	NAG	D	505	-	-	2/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	507	5VG	C02-N03	7.30	1.47	1.33
3	A	501	5VG	C02-N03	7.26	1.47	1.33
3	A	501	5VG	C17-N19	5.00	1.46	1.35
3	A	501	5VG	C15-N14	4.96	1.44	1.34
3	D	507	5VG	C17-N19	4.88	1.45	1.35
3	D	507	5VG	C15-N14	4.87	1.44	1.34
3	D	507	5VG	C05-C13	-4.14	1.49	1.54
3	A	501	5VG	C05-C13	-4.06	1.49	1.54
3	A	501	5VG	C11-C10	3.99	1.45	1.38
3	D	507	5VG	C11-C10	3.92	1.45	1.38
3	D	507	5VG	C08-C09	3.34	1.45	1.39
3	A	501	5VG	C08-C09	3.24	1.44	1.39
3	D	507	5VG	C27-C26	2.58	1.43	1.38
3	A	501	5VG	C06-C05	-2.51	1.49	1.54
3	A	501	5VG	C27-C26	2.51	1.42	1.38
3	A	501	5VG	C07-C12	2.51	1.43	1.39
3	D	507	5VG	C06-C05	-2.47	1.49	1.54
3	A	501	5VG	C00-N	-2.47	1.43	1.46
3	D	507	5VG	C07-C12	2.41	1.43	1.39
3	D	507	5VG	C00-N	-2.38	1.43	1.46
3	A	501	5VG	C24-C22	2.33	1.42	1.38
3	D	507	5VG	C24-C22	2.28	1.41	1.38
3	A	501	5VG	C21-C22	2.01	1.41	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	504	NAG	C2-N2-C7	5.58	130.37	122.90
2	D	503	NAG	C2-N2-C7	4.84	129.39	122.90
3	D	507	5VG	C15-C17-N19	4.25	119.43	112.25
3	A	501	5VG	C15-C17-N19	3.44	118.05	112.25
2	D	503	NAG	C1-C2-N2	3.04	115.22	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	507	5VG	C20-N19-C17	-2.94	122.24	127.45
3	A	501	5VG	C17-C15-N14	2.80	120.43	113.73
3	D	507	5VG	C17-C15-N14	2.48	119.68	113.73
3	A	501	5VG	C06-C07-C12	-2.11	108.03	110.95
3	D	507	5VG	C12-C13-N14	-2.11	108.59	114.77
3	A	501	5VG	C20-N19-C17	-2.04	123.84	127.45

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	507	5VG	C09-C00-N-C
3	D	507	5VG	N03-C04-C05-C13
3	A	501	5VG	C09-C00-N-C
3	A	501	5VG	N03-C04-C05-C13
2	D	506	NAG	O5-C5-C6-O6
2	A	507	NAG	O5-C5-C6-O6
2	D	505	NAG	O5-C5-C6-O6
2	D	506	NAG	C4-C5-C6-O6
2	A	504	NAG	O5-C5-C6-O6
2	D	505	NAG	C4-C5-C6-O6
2	A	507	NAG	C4-C5-C6-O6
2	A	506	NAG	O5-C5-C6-O6
2	D	503	NAG	C8-C7-N2-C2
2	D	503	NAG	O7-C7-N2-C2
2	D	504	NAG	C8-C7-N2-C2
2	D	504	NAG	O7-C7-N2-C2
2	D	506	NAG	C8-C7-N2-C2
2	D	506	NAG	O7-C7-N2-C2
2	A	504	NAG	C8-C7-N2-C2
2	A	504	NAG	O7-C7-N2-C2
2	A	505	NAG	C8-C7-N2-C2
2	A	505	NAG	O7-C7-N2-C2
2	A	507	NAG	C8-C7-N2-C2
2	A	507	NAG	O7-C7-N2-C2
2	A	506	NAG	C4-C5-C6-O6
2	A	504	NAG	C4-C5-C6-O6
2	D	504	NAG	O5-C5-C6-O6
2	D	503	NAG	C3-C2-N2-C7
2	A	504	NAG	C3-C2-N2-C7
2	A	505	NAG	O5-C5-C6-O6
2	D	504	NAG	C4-C5-C6-O6

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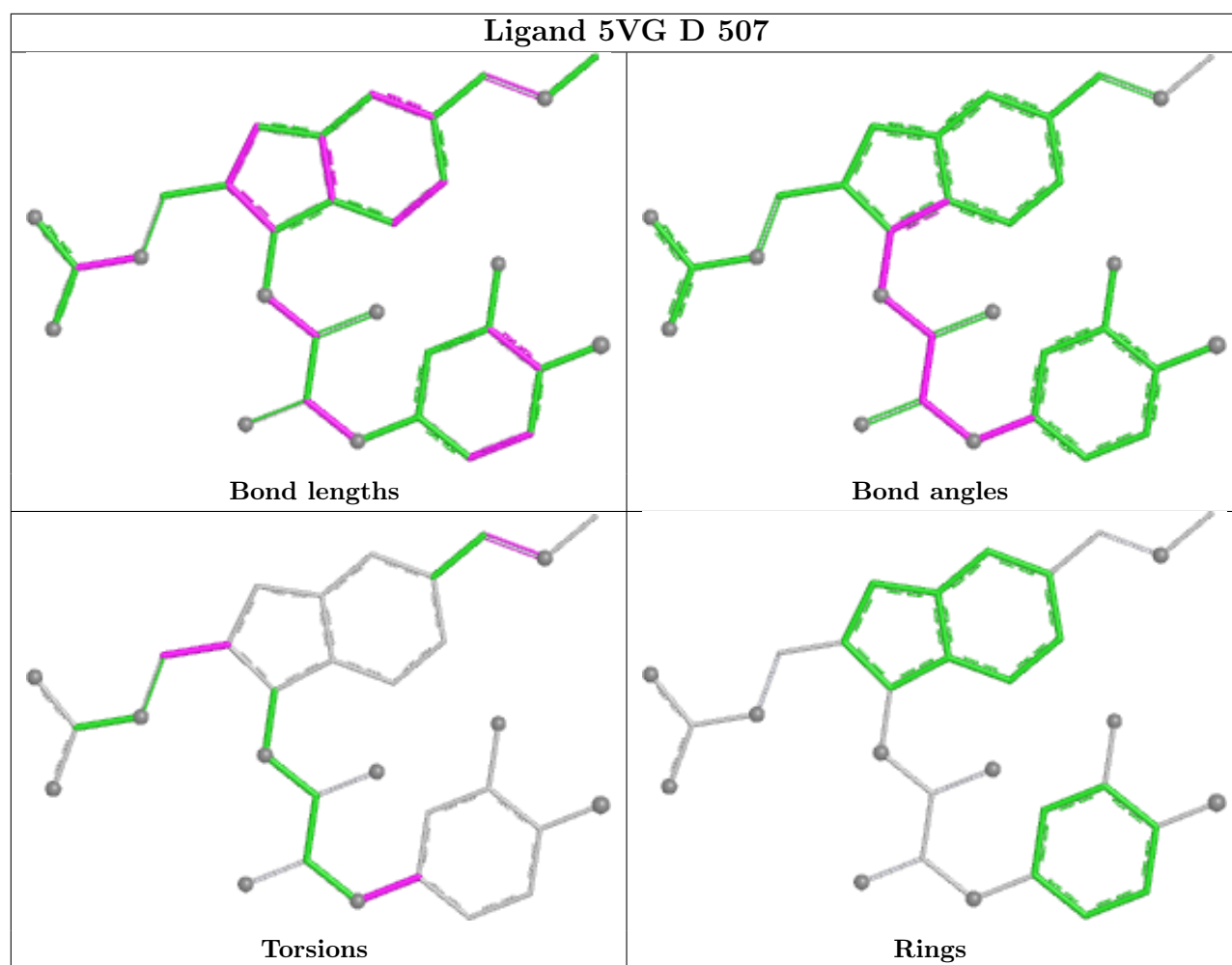
Mol	Chain	Res	Type	Atoms
2	D	503	NAG	C1-C2-N2-C7
2	A	502	NAG	C1-C2-N2-C7
3	D	507	5VG	C27-C20-N19-C17
3	D	507	5VG	C21-C20-N19-C17
3	D	507	5VG	N03-C04-C05-C06
2	D	503	NAG	O5-C5-C6-O6

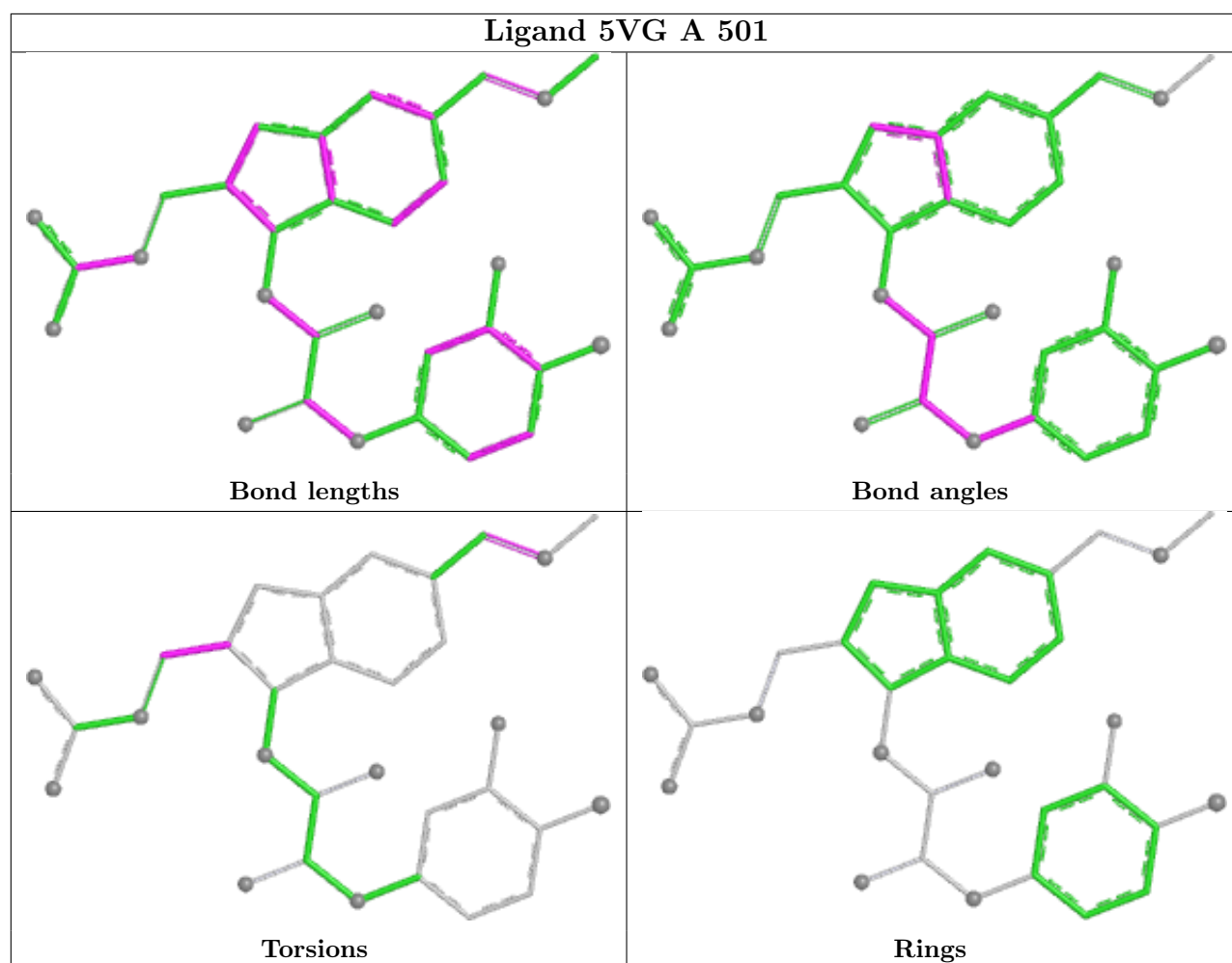
There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	503	NAG	2	0
2	D	504	NAG	3	0
3	D	507	5VG	1	0
2	A	505	NAG	2	0
2	A	507	NAG	1	0
2	A	504	NAG	4	0
2	D	506	NAG	1	0
3	A	501	5VG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	0.97	37 (11%) 10 8	38, 71, 106, 123	0
1	D	335/350 (95%)	1.06	44 (13%) 7 5	54, 81, 101, 125	0
All	All	670/700 (95%)	1.01	81 (12%) 8 6	38, 77, 103, 125	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	486	TYR	7.0
1	D	345	VAL	4.7
1	A	89	VAL	4.3
1	D	391	PHE	4.0
1	D	87	ALA	3.7
1	A	90	THR	3.5
1	A	485	LYS	3.4
1	D	483	LEU	3.4
1	A	79	PRO	3.4
1	A	277	LEU	3.3
1	A	349	LEU	3.3
1	A	87	ALA	3.3
1	A	198	GLY	3.2
1	D	292	VAL	3.2
1	A	354	PRO	3.2
1	A	345	VAL	3.2
1	A	234	ASN	3.1
1	D	81	PRO	3.1
1	D	294	ILE	3.1
1	D	272	ILE	3.1
1	D	254	VAL	3.0
1	D	449	ILE	3.0
1	A	289	ASN	2.9
1	A	124	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	224	ALA	2.9
1	D	93	PHE	2.9
1	D	452	LEU	2.9
1	D	488	VAL	2.8
1	A	489	VAL	2.8
1	D	100	MET	2.8
1	D	289	ASN	2.8
1	D	248	THR	2.8
1	A	270	ILE	2.7
1	A	397	ASN	2.7
1	A	404	ASN	2.7
1	A	100	MET	2.7
1	A	241	ASN	2.6
1	A	483	LEU	2.6
1	D	296	CYS	2.6
1	D	85	VAL	2.6
1	D	422	GLN	2.5
1	A	223	PHE	2.5
1	D	221	ALA	2.5
1	A	484	TYR	2.4
1	D	228	CYS	2.4
1	D	295	VAL	2.4
1	D	484	TYR	2.4
1	A	242	VAL	2.4
1	A	224	ALA	2.4
1	A	221	ALA	2.4
1	D	226	LEU	2.4
1	D	288	LEU	2.4
1	A	339	ASN	2.4
1	D	267	GLU	2.3
1	A	86	LEU	2.3
1	D	352	HIS	2.3
1	D	241	ASN	2.3
1	D	79	PRO	2.3
1	A	222	GLY	2.3
1	D	89	VAL	2.3
1	A	487	LYS	2.2
1	D	286	VAL	2.2
1	A	225	ILE	2.2
1	A	486	TYR	2.2
1	D	215	LEU	2.2
1	A	365	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	488	VAL	2.2
1	D	341	THR	2.1
1	D	249	HIS	2.1
1	A	415	THR	2.1
1	D	88	ASN	2.1
1	A	228	CYS	2.1
1	A	352	HIS	2.1
1	D	49	LYS	2.1
1	D	271	ILE	2.1
1	A	410	SER	2.0
1	D	251	ILE	2.0
1	D	239	CYS	2.0
1	D	385	CYS	2.0
1	D	353	PHE	2.0
1	D	214	PRO	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 oligosaccharides 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. 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.

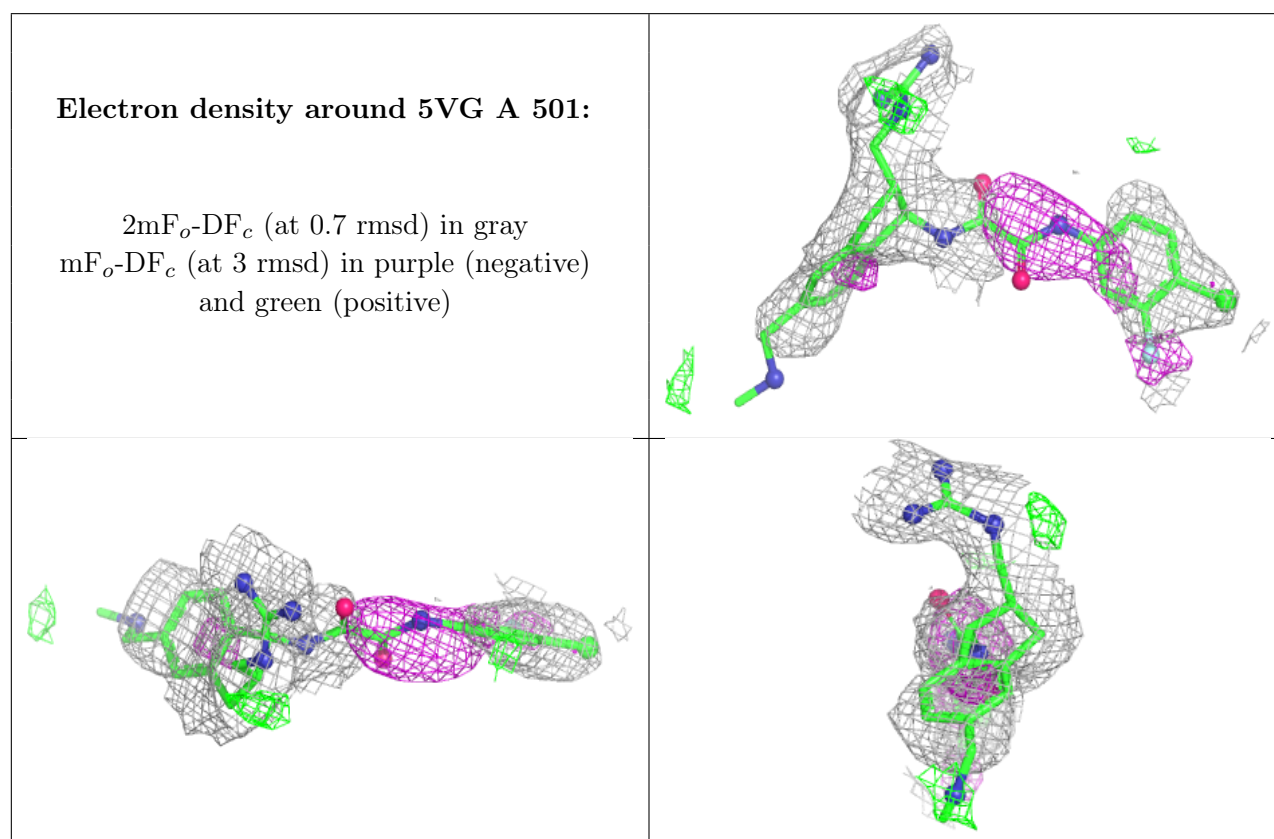
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	5VG	A	501	31/31	0.55	0.21	64,72,87,96	0
2	NAG	D	503	14/15	0.57	0.16	88,96,101,101	0
2	NAG	D	506	14/15	0.59	0.20	88,100,112,114	0
2	NAG	A	505	14/15	0.60	0.19	86,92,104,106	0
2	NAG	A	504	14/15	0.60	0.17	85,92,102,110	0
2	NAG	D	505	14/15	0.62	0.17	69,88,94,95	0
2	NAG	D	501	14/15	0.63	0.14	83,93,99,103	0
2	NAG	A	502	14/15	0.67	0.20	88,103,110,113	0

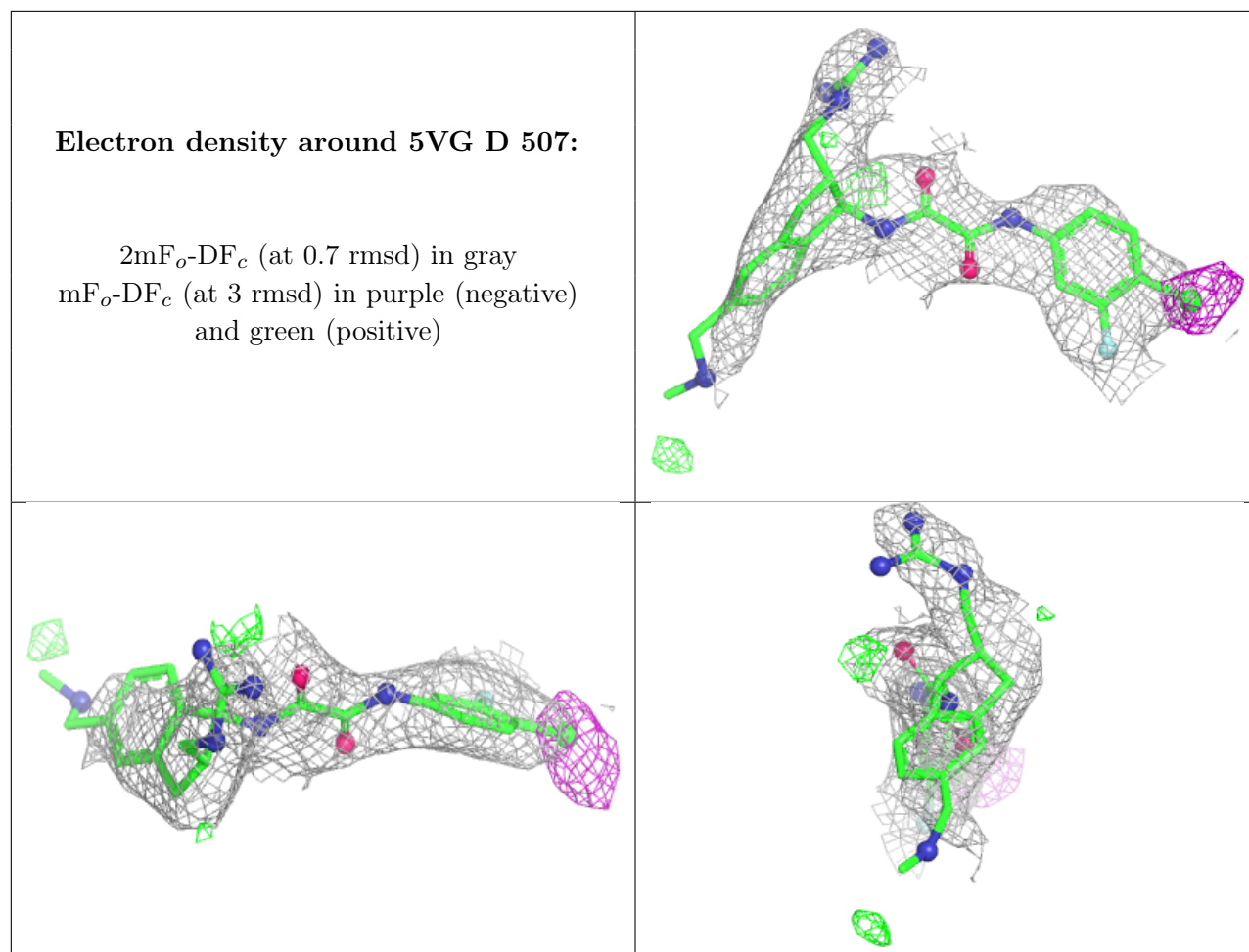
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	5VG	D	507	31/31	0.68	0.17	64,76,90,95	0
2	NAG	A	507	14/15	0.69	0.23	65,72,85,95	0
2	NAG	D	504	14/15	0.70	0.14	88,94,100,109	0
2	NAG	A	506	14/15	0.73	0.17	71,81,88,89	0
2	NAG	D	502	14/15	0.77	0.16	66,78,86,93	0
2	NAG	A	503	14/15	0.77	0.16	46,60,70,75	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers ⓘ

There are no such residues in this entry.