



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:27 PM UTC

PDB ID : 6THP / pdb_00006thp
Title : Neprilysin in complex with the inhibitor (R)-4-(1-carboxy-3-(3'-chlorobiphenyl-4-yl)propan-2-ylamino)-4-oxobutanoic acid
Authors : Schiering, N.; Wiesmann, C.
Deposited on : 2019-11-21
Resolution : 2.54 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

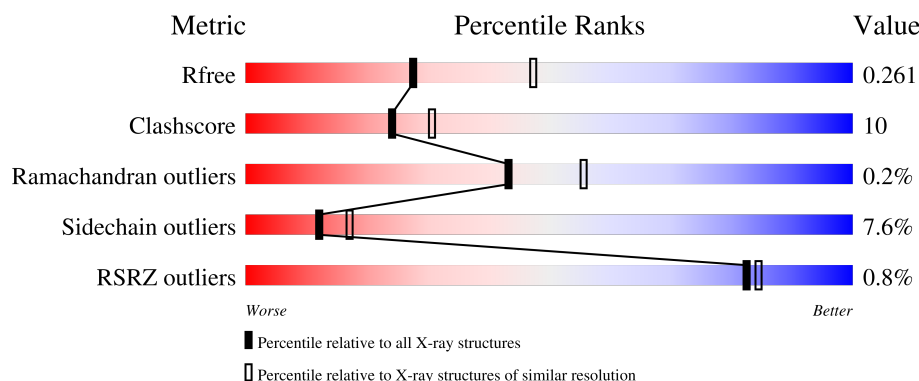
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	696	 79% 19% .
1	B	696	 72% 23% .

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	B	801	X	-	-	-

2 Entry composition [i](#)

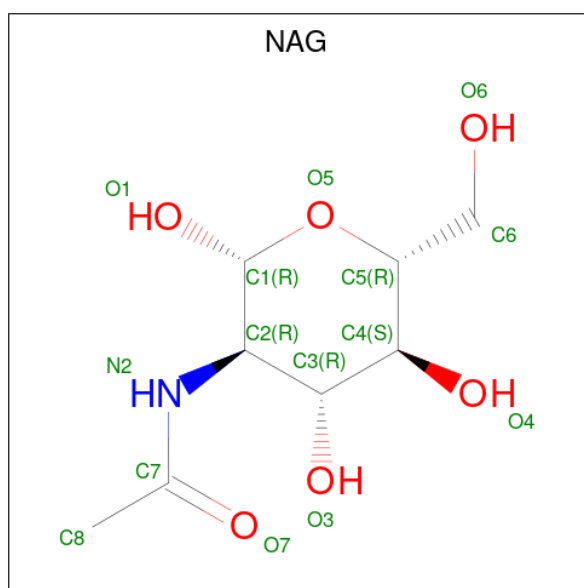
There are 5 unique types of molecules in this entry. The entry contains 11710 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Neprilysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	0	0
			5595	3538	957	1074	26			
1	B	696	Total	C	N	O	S	0	0	0
			5595	3538	957	1074	26			

- 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...

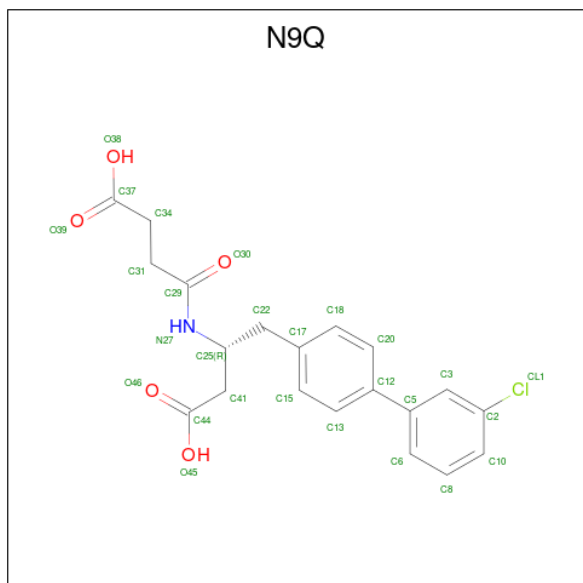
Continued from previous page...

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is 4-[(2 {R})-1-[4-(3-chlorophenyl)phenyl]-4-oxidanyl-4-oxidanylidene-butan-2-yl]amino]-4-oxidanylidene-butanoic acid (CCD ID: N9Q) (formula: C₂₀H₂₀ClNO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 20	Cl 1	N 1	O 5	0	0
4	B	1	Total 27	C 20	Cl 1	N 1	O 5	0	0

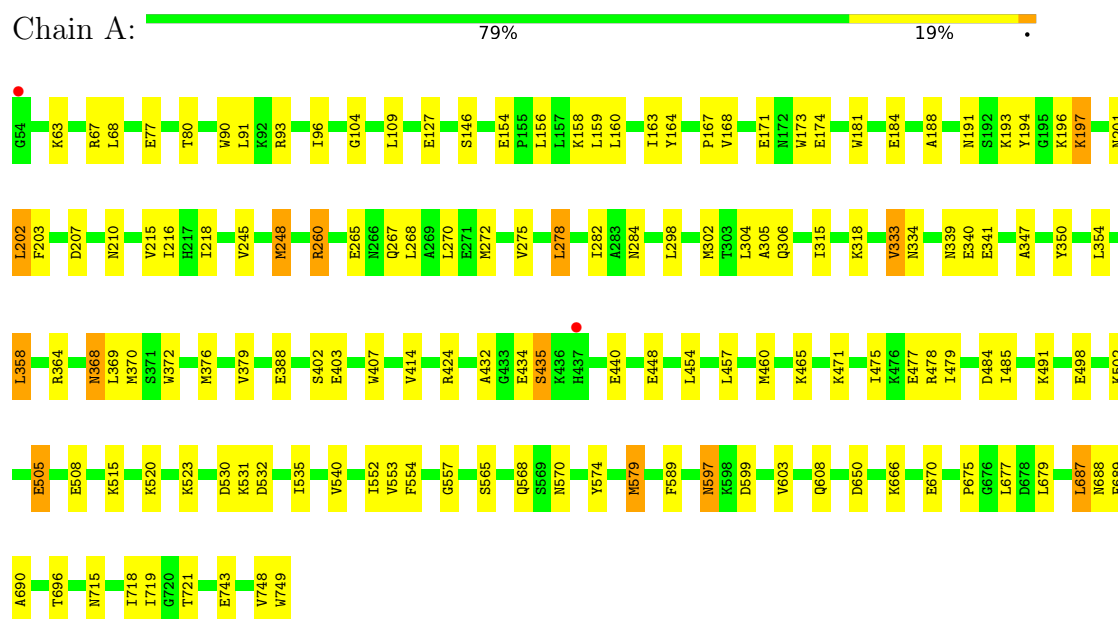
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	218	Total 218	O 218	0	0
5	B	134	Total 134	O 134	0	0

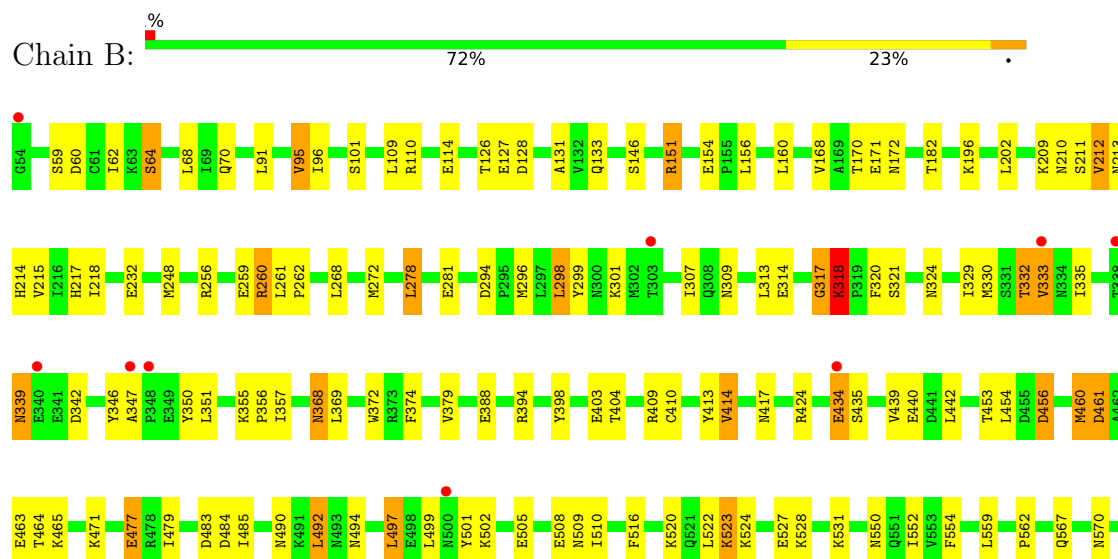
3 Residue-property plots

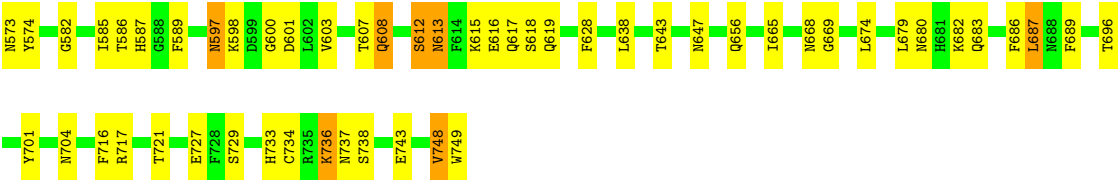
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Neprilysin



• Molecule 1: Neprilysin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.79Å 109.39Å 248.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.94 – 2.54 65.94 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.94-2.54) 99.8 (65.94-2.54)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, R_{free}	0.205 , 0.264 0.206 , 0.261	Depositor DCC
R_{free} test set	2732 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.1	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	0.93	EDS
Total number of atoms	11710	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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, N9Q, ZN

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	0.66	0/5713	0.92	0/7727
1	B	0.67	0/5713	0.94	4/7727 (0.1%)
All	All	0.67	0/11426	0.93	4/15454 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	738	SER	N-CA-C	-6.58	101.84	110.53
1	B	434	GLU	N-CA-C	-5.61	105.17	111.28
1	B	674	LEU	CA-C-N	5.05	124.81	119.76
1	B	674	LEU	C-N-CA	5.05	124.81	119.76

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	5595	0	5446	100	0
1	B	5595	0	5446	127	0
2	A	56	0	52	0	0
2	B	56	0	52	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	27	0	0	2	0
4	B	27	0	0	0	0
5	A	218	0	0	6	0
5	B	134	0	0	4	0
All	All	11710	0	10996	223	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 10.

All (223) 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:260:ARG:HB2	1:B:260:ARG:HH11	1.19	1.02
1:B:151:ARG:HG2	1:B:151:ARG:HH11	1.25	0.99
1:B:339:ASN:HB2	5:B:1005:HOH:O	1.63	0.98
1:B:260:ARG:HB2	1:B:260:ARG:NH1	1.80	0.94
1:A:579:MET:HE2	4:A:806:N9Q:C3	2.06	0.86
1:B:388:GLU:HG2	5:B:936:HOH:O	1.81	0.81
1:B:168:VAL:H	1:B:368:ASN:HD21	1.28	0.80
1:A:597:ASN:ND2	1:A:599:ASP:H	1.80	0.79
1:A:484:ASP:OD1	1:A:491:LYS:NZ	2.14	0.77
1:A:334:ASN:HB2	5:A:1075:HOH:O	1.84	0.76
1:A:570:ASN:O	1:A:574:TYR:HD2	1.68	0.76
1:A:597:ASN:C	1:A:597:ASN:HD22	1.94	0.74
1:A:597:ASN:HD22	1:A:599:ASP:H	1.35	0.74
1:B:202:LEU:HD23	1:B:218:ILE:CD1	2.18	0.74
1:B:151:ARG:HH11	1:B:151:ARG:CG	2.01	0.73
1:A:202:LEU:HD21	1:A:216:ILE:CG2	2.20	0.71
1:B:456:ASP:OD2	1:B:456:ASP:N	2.23	0.71
1:B:717:ARG:O	1:B:721:THR:HG23	1.90	0.70
1:A:460:MET:HE3	1:A:465:LYS:HG2	1.73	0.70
1:A:67:ARG:HH22	1:A:688:ASN:HD21	1.40	0.69
1:B:260:ARG:HH11	1:B:260:ARG:CB	2.01	0.69
1:A:690:ALA:HA	1:A:718:ILE:HD12	1.76	0.68
1:A:354:LEU:HG	1:A:358:LEU:HD22	1.72	0.68
1:B:410:CYS:O	1:B:414:VAL:HG13	1.93	0.67
1:B:597:ASN:C	1:B:597:ASN:HD22	2.02	0.66
1:B:211:SER:HB3	1:B:600:GLY:O	1.95	0.66
1:B:314:GLU:OE1	1:B:317:GLY:HA2	1.96	0.65
1:B:502:LYS:HB2	1:B:505:GLU:HB2	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:H	1:A:368:ASN:HD21	1.45	0.65
1:A:67:ARG:HH22	1:A:688:ASN:ND2	1.94	0.65
1:A:432:ALA:HB3	1:A:435:SER:OG	1.97	0.64
1:B:589:PHE:HB3	1:B:749:TRP:CZ2	2.33	0.64
1:A:202:LEU:HD21	1:A:216:ILE:HG23	1.79	0.63
1:B:608:GLN:O	1:B:612:SER:HB2	1.98	0.63
1:A:535:ILE:HG12	1:A:553:VAL:HG21	1.81	0.62
1:B:333:VAL:HG11	1:B:523:LYS:HB3	1.80	0.62
1:B:259:GLU:HB2	1:B:261:LEU:HG	1.79	0.62
1:B:736:LYS:HE2	1:B:743:GLU:HG2	1.80	0.62
1:A:278:LEU:HD22	1:A:282:ILE:HD11	1.82	0.61
1:A:63:LYS:HG2	1:B:70:GLN:HE21	1.66	0.60
1:B:110:ARG:O	1:B:114:GLU:HG3	2.00	0.60
1:B:298:LEU:HD13	1:B:346:TYR:CD1	2.35	0.60
1:A:245:VAL:HG22	1:A:248:MET:HE3	1.84	0.59
1:A:305:ALA:HB2	1:A:339:ASN:HB3	1.85	0.58
1:B:347:ALA:O	1:B:351:LEU:HG	2.03	0.58
1:B:679:LEU:HB3	1:B:683:GLN:HB2	1.85	0.57
1:A:457:LEU:HD12	1:A:460:MET:HE2	1.86	0.57
1:B:151:ARG:HG2	1:B:151:ARG:NH1	2.05	0.57
1:A:372:TRP:O	1:A:376:MET:HB2	2.04	0.57
1:A:67:ARG:HH12	1:A:688:ASN:ND2	2.03	0.57
1:B:477:GLU:HG3	1:B:479:ILE:HD11	1.88	0.56
1:A:193:LYS:HE2	1:A:515:LYS:NZ	2.19	0.56
1:B:301:LYS:HD2	1:B:342:ASP:HB3	1.86	0.56
1:A:191:ASN:ND2	1:A:197:LYS:HD2	2.20	0.56
1:A:202:LEU:CD2	1:A:216:ILE:HG23	2.34	0.56
1:A:202:LEU:HD23	1:A:218:ILE:HD11	1.87	0.56
1:B:737:ASN:HD21	1:B:743:GLU:HG3	1.71	0.55
1:A:388:GLU:HG2	5:A:1071:HOH:O	2.06	0.55
1:B:202:LEU:HD23	1:B:218:ILE:HD13	1.85	0.55
1:A:388:GLU:CG	5:A:1071:HOH:O	2.54	0.55
1:B:586:THR:O	1:B:589:PHE:N	2.30	0.55
1:A:197:LYS:HD3	1:A:197:LYS:N	2.21	0.55
1:B:680:ASN:OD1	1:B:683:GLN:HG3	2.07	0.54
1:A:284:ASN:HB3	5:A:986:HOH:O	2.07	0.54
1:B:196:LYS:HE3	1:B:374:PHE:HA	1.90	0.54
1:B:321:SER:CB	1:B:324:ASN:HB3	2.38	0.54
1:A:347:ALA:HB1	1:A:350:TYR:HB3	1.90	0.54
1:B:321:SER:HB3	1:B:324:ASN:HB3	1.88	0.54
1:A:715:ASN:O	1:A:719:ILE:HG12	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LEU:O	1:B:320:PHE:N	2.40	0.53
1:B:171:GLU:HG2	5:B:981:HOH:O	2.08	0.53
1:B:597:ASN:C	1:B:597:ASN:ND2	2.67	0.53
1:B:424:ARG:HD2	1:B:485:ILE:O	2.08	0.53
1:A:333:VAL:HG11	1:A:523:LYS:HB3	1.91	0.53
1:A:159:LEU:HD11	1:A:194:TYR:OH	2.09	0.53
1:B:347:ALA:HB1	1:B:350:TYR:HB3	1.90	0.53
1:B:460:MET:HE1	1:B:465:LYS:N	2.25	0.52
1:A:245:VAL:HA	1:A:248:MET:HG3	1.92	0.52
1:B:214:HIS:ND1	1:B:524:LYS:O	2.36	0.52
1:B:461:ASP:C	1:B:461:ASP:OD2	2.53	0.52
1:A:67:ARG:HH12	1:A:688:ASN:HD22	1.57	0.51
1:B:329:ILE:O	1:B:332:THR:OG1	2.22	0.51
1:A:96:ILE:HD11	1:A:696:THR:HG23	1.92	0.51
1:B:202:LEU:HD23	1:B:218:ILE:HD11	1.89	0.51
1:B:680:ASN:OD1	1:B:682:LYS:HB2	2.09	0.51
1:B:461:ASP:OD2	1:B:463:GLU:HG2	2.10	0.51
1:A:68:LEU:HD22	1:A:687:LEU:HD13	1.92	0.50
1:A:675:PRO:HB2	1:B:62:ILE:HD11	1.93	0.50
1:A:315:ILE:O	1:A:318:LYS:HB2	2.09	0.50
1:B:552:ILE:HD12	1:B:554:PHE:HE2	1.76	0.50
1:A:154:GLU:HG3	1:A:158:LYS:HE3	1.93	0.50
1:A:477:GLU:HG3	1:A:479:ILE:HD11	1.93	0.50
1:B:131:ALA:CB	1:B:492:LEU:HD13	2.41	0.50
1:B:552:ILE:HD12	1:B:554:PHE:CE2	2.45	0.50
1:A:407:TRP:HZ2	1:B:95:VAL:HG11	1.76	0.50
1:A:407:TRP:CZ2	1:B:95:VAL:HG11	2.47	0.49
1:A:202:LEU:CD2	1:A:216:ILE:CG2	2.88	0.49
1:B:299:TYR:OH	1:B:301:LYS:HE2	2.12	0.49
1:A:202:LEU:HD21	1:A:216:ILE:HG21	1.94	0.49
1:A:552:ILE:HD12	1:A:554:PHE:HE2	1.78	0.49
1:B:748:VAL:HG13	5:B:995:HOH:O	2.13	0.49
1:B:355:LYS:HB3	1:B:356:PRO:CD	2.42	0.49
1:A:90:TRP:CZ2	1:A:104:GLY:HA2	2.48	0.49
1:A:302:MET:HG2	1:A:306:GLN:HE21	1.78	0.48
1:B:101:SER:HB3	1:B:398:TYR:HB3	1.94	0.48
1:A:196:LYS:C	1:A:197:LYS:HD3	2.38	0.48
1:B:643:THR:HB	1:B:647:ASN:HD21	1.79	0.48
1:A:202:LEU:HD13	1:A:202:LEU:C	2.40	0.47
1:A:202:LEU:HD23	1:A:218:ILE:CD1	2.44	0.47
1:B:471:LYS:HE2	1:B:550:ASN:ND2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LEU:HD13	1:B:346:TYR:HD1	1.79	0.47
1:B:524:LYS:HA	1:B:527:GLU:HG3	1.97	0.47
1:A:666:LYS:HE2	5:A:1108:HOH:O	2.15	0.47
1:B:210:ASN:ND2	1:B:213:ASN:HB2	2.30	0.47
1:A:589:PHE:HB3	1:A:749:TRP:CZ2	2.50	0.46
1:A:278:LEU:HD22	1:A:282:ILE:CD1	2.44	0.46
1:A:267:GLN:HA	1:A:267:GLN:NE2	2.31	0.46
1:B:272:MET:HE2	1:B:272:MET:HA	1.97	0.46
1:B:321:SER:OG	1:B:324:ASN:HB3	2.15	0.46
1:B:679:LEU:HA	1:B:683:GLN:OE1	2.15	0.46
1:B:570:ASN:O	1:B:574:TYR:HD2	1.98	0.46
1:B:628:PHE:HB2	1:B:638:LEU:HD12	1.97	0.46
1:A:184:GLU:O	1:A:188:ALA:HB2	2.15	0.46
1:B:278:LEU:HD13	1:B:369:LEU:CD2	2.46	0.46
1:B:471:LYS:HG3	1:B:598:LYS:HA	1.97	0.46
1:B:586:THR:O	1:B:587:HIS:C	2.58	0.46
1:A:478:ARG:HH22	1:A:532:ASP:HA	1.81	0.46
1:B:248:MET:HG2	1:B:372:TRP:CE2	2.51	0.46
1:B:314:GLU:HG2	1:B:318:LYS:H	1.80	0.46
1:A:193:LYS:HE2	1:A:515:LYS:HZ3	1.81	0.46
1:A:540:VAL:O	1:A:557:GLY:HA3	2.16	0.46
1:A:597:ASN:ND2	1:A:597:ASN:C	2.66	0.45
1:B:281:GLU:OE2	1:B:357:ILE:HG12	2.15	0.45
1:B:520:LYS:O	1:B:524:LYS:HG3	2.17	0.45
1:A:181:TRP:HZ2	1:A:370:MET:HE1	1.80	0.45
1:B:613:ASN:O	1:B:616:GLU:HB2	2.15	0.45
1:B:613:ASN:HA	1:B:616:GLU:HG3	1.98	0.45
1:B:665:ILE:O	1:B:669:GLY:N	2.47	0.45
1:A:260:ARG:HH11	1:A:260:ARG:HB2	1.82	0.45
1:B:294:ASP:OD1	1:B:296:MET:HB2	2.17	0.45
1:B:597:ASN:ND2	1:B:601:ASP:H	2.15	0.45
1:B:643:THR:HB	1:B:647:ASN:ND2	2.32	0.45
1:B:217:HIS:HD2	1:B:346:TYR:CE2	2.35	0.45
1:A:272:MET:O	1:A:275:VAL:HB	2.17	0.45
1:B:209:LYS:HE2	1:B:299:TYR:CE1	2.52	0.45
1:A:579:MET:HE2	4:A:806:N9Q:C2	2.47	0.45
1:B:151:ARG:O	1:B:154:GLU:HB3	2.17	0.45
1:A:457:LEU:HD12	1:A:460:MET:CE	2.46	0.45
1:B:460:MET:CE	1:B:464:THR:HB	2.47	0.44
1:B:494:ASN:O	1:B:497:LEU:HB2	2.17	0.44
1:B:686:PHE:O	1:B:689:PHE:HB3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HD11	1:B:562:PRO:HD2	1.98	0.44
1:B:128:ASP:O	1:B:133:GLN:NE2	2.46	0.44
1:B:404:THR:HG23	1:B:409:ARG:CG	2.47	0.44
1:A:67:ARG:NH2	1:A:688:ASN:HD21	2.12	0.44
1:A:478:ARG:C	1:A:479:ILE:HG13	2.42	0.44
1:A:502:LYS:CB	1:A:505:GLU:HG3	2.48	0.44
1:A:650:ASP:HB3	1:A:721:THR:HG21	1.99	0.44
1:B:701:TYR:O	1:B:704:ASN:HB3	2.17	0.44
1:B:330:MET:HE3	1:B:335:ILE:HB	1.99	0.44
1:A:471:LYS:O	1:A:475:ILE:HG13	2.18	0.44
1:A:579:MET:SD	1:A:689:PHE:HE2	2.40	0.44
1:B:278:LEU:HD13	1:B:369:LEU:HD23	2.00	0.44
1:B:502:LYS:H	1:B:509:ASN:HD21	1.64	0.44
1:B:607:THR:O	1:B:608:GLN:C	2.61	0.43
1:A:677:LEU:HD22	1:A:679:LEU:HD12	2.00	0.43
1:B:615:LYS:O	1:B:619:GLN:HB2	2.17	0.43
1:A:424:ARG:HD2	1:A:485:ILE:O	2.18	0.43
1:A:354:LEU:HG	1:A:358:LEU:CD2	2.46	0.43
1:B:210:ASN:HD21	1:B:213:ASN:ND2	2.16	0.43
1:B:748:VAL:HG22	1:B:749:TRP:CD1	2.53	0.43
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.86	0.43
1:A:207:ASP:HB3	1:A:210:ASN:O	2.18	0.43
1:B:499:LEU:HD13	1:B:501:TYR:OH	2.18	0.43
1:A:265:GLU:HA	1:A:268:LEU:HD12	2.00	0.43
1:A:167:PRO:HG3	1:A:173:TRP:CE2	2.54	0.43
1:A:388:GLU:HG3	5:A:1071:HOH:O	2.17	0.43
1:A:565:SER:HB3	1:A:568:GLN:HG2	2.00	0.43
1:B:68:LEU:HD22	1:B:687:LEU:HD13	2.00	0.43
1:A:535:ILE:CG1	1:A:553:VAL:HG21	2.49	0.43
1:B:210:ASN:OD1	1:B:212:VAL:HG23	2.18	0.43
1:A:454:LEU:HD22	1:A:460:MET:HE1	2.01	0.43
1:A:508:GLU:OE1	1:A:508:GLU:N	2.50	0.43
1:B:439:VAL:HG21	1:B:559:LEU:HD22	2.01	0.42
1:B:268:LEU:HD23	1:B:268:LEU:HA	1.66	0.42
1:A:278:LEU:HD13	1:A:369:LEU:HD22	2.00	0.42
1:B:60:ASP:CG	1:B:567:GLN:HB3	2.44	0.42
1:A:579:MET:HE1	1:A:650:ASP:HA	2.00	0.42
1:B:460:MET:HE2	1:B:460:MET:HB3	1.65	0.42
1:B:613:ASN:OD1	1:B:613:ASN:N	2.52	0.42
1:B:522:LEU:C	1:B:524:LYS:H	2.28	0.42
1:B:60:ASP:O	1:B:64:SER:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:CD2	1:B:218:ILE:HD13	2.47	0.42
1:B:217:HIS:CD2	1:B:346:TYR:HE2	2.38	0.42
1:A:77:GLU:HB3	1:A:80:THR:OG1	2.20	0.41
1:B:256:ARG:NH1	1:B:262:PRO:O	2.52	0.41
1:B:321:SER:OG	1:B:324:ASN:CB	2.68	0.41
1:A:304:LEU:HD12	1:A:341:GLU:HB3	2.02	0.41
1:B:96:ILE:HD11	1:B:696:THR:HG23	2.01	0.41
1:B:307:ILE:C	1:B:309:ASN:H	2.27	0.41
1:A:93:ARG:HE	1:A:93:ARG:HB2	1.75	0.41
1:B:202:LEU:HD12	1:B:329:ILE:HD13	2.02	0.41
1:B:454:LEU:O	1:B:465:LYS:HD3	2.20	0.41
1:A:174:GLU:OE2	1:A:364:ARG:HD2	2.20	0.41
1:B:727:GLU:OE1	1:B:727:GLU:N	2.34	0.41
1:B:638:LEU:HD11	1:B:716:PHE:CD1	2.56	0.41
1:B:729:SER:HB3	1:B:734:CYS:HB2	2.01	0.41
1:B:570:ASN:HA	1:B:573:ASN:HB2	2.02	0.41
1:A:163:ILE:O	1:A:164:TYR:HB2	2.21	0.41
1:B:413:TYR:CZ	1:B:417:ASN:ND2	2.89	0.41
1:B:440:GLU:HG3	1:B:479:ILE:HD13	2.02	0.41
1:B:729:SER:O	1:B:733:HIS:N	2.54	0.41
1:A:440:GLU:HG3	1:A:479:ILE:CD1	2.51	0.41
1:A:202:LEU:HD13	1:A:203:PHE:N	2.36	0.40
1:A:530:ASP:OD1	1:A:531:LYS:N	2.54	0.40
1:B:516:PHE:O	1:B:520:LYS:HB2	2.21	0.40
1:B:582:GLY:HA2	1:B:656:GLN:HE21	1.86	0.40
1:A:193:LYS:HE2	1:A:515:LYS:HZ2	1.84	0.40
1:A:197:LYS:HG3	1:A:201:ASN:OD1	2.21	0.40
1:B:461:ASP:O	1:B:465:LYS:HG3	2.22	0.40
1:B:613:ASN:O	1:B:617:GLN:HG2	2.21	0.40
1:A:159:LEU:HD11	1:A:194:TYR:CZ	2.57	0.40
1:A:334:ASN:C	1:A:334:ASN:HD22	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	694/696 (100%)	668 (96%)	26 (4%)	0	100	100
1	B	694/696 (100%)	635 (92%)	56 (8%)	3 (0%)	30	39
All	All	1388/1392 (100%)	1303 (94%)	82 (6%)	3 (0%)	43	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	LYS
1	B	317	GLY
1	B	523	LYS

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	605/605 (100%)	569 (94%)	36 (6%)	17	26
1	B	605/605 (100%)	549 (91%)	56 (9%)	8	10
All	All	1210/1210 (100%)	1118 (92%)	92 (8%)	12	17

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	127	GLU
1	A	146	SER
1	A	156	LEU
1	A	160	LEU
1	A	171	GLU
1	A	197	LYS
1	A	202	LEU
1	A	215	VAL
1	A	248	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	260	ARG
1	A	270	LEU
1	A	278	LEU
1	A	298	LEU
1	A	333	VAL
1	A	340	GLU
1	A	358	LEU
1	A	368	ASN
1	A	379	VAL
1	A	402	SER
1	A	403	GLU
1	A	414	VAL
1	A	434	GLU
1	A	435	SER
1	A	448	GLU
1	A	498	GLU
1	A	505	GLU
1	A	520	LYS
1	A	579	MET
1	A	597	ASN
1	A	603	VAL
1	A	608	GLN
1	A	670	GLU
1	A	687	LEU
1	A	743	GLU
1	A	748	VAL
1	B	59	SER
1	B	64	SER
1	B	91	LEU
1	B	95	VAL
1	B	126	THR
1	B	127	GLU
1	B	146	SER
1	B	151	ARG
1	B	156	LEU
1	B	160	LEU
1	B	170	THR
1	B	172	ASN
1	B	182	THR
1	B	212	VAL
1	B	215	VAL
1	B	232	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	260	ARG
1	B	278	LEU
1	B	298	LEU
1	B	318	LYS
1	B	332	THR
1	B	333	VAL
1	B	339	ASN
1	B	368	ASN
1	B	379	VAL
1	B	394	ARG
1	B	403	GLU
1	B	414	VAL
1	B	434	GLU
1	B	435	SER
1	B	442	LEU
1	B	453	THR
1	B	456	ASP
1	B	460	MET
1	B	461	ASP
1	B	477	GLU
1	B	483	ASP
1	B	484	ASP
1	B	490	ASN
1	B	492	LEU
1	B	497	LEU
1	B	508	GLU
1	B	510	ILE
1	B	528	LYS
1	B	531	LYS
1	B	585	ILE
1	B	597	ASN
1	B	603	VAL
1	B	608	GLN
1	B	612	SER
1	B	613	ASN
1	B	618	SER
1	B	668	ASN
1	B	687	LEU
1	B	736	LYS
1	B	748	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	213	ASN
1	A	267	GLN
1	A	306	GLN
1	A	316	ASN
1	A	334	ASN
1	A	368	ASN
1	A	490	ASN
1	A	509	ASN
1	A	550	ASN
1	A	570	ASN
1	A	597	ASN
1	A	608	GLN
1	A	619	GLN
1	A	688	ASN
1	B	70	GLN
1	B	105	ASN
1	B	189	GLN
1	B	213	ASN
1	B	217	HIS
1	B	267	GLN
1	B	310	ASN
1	B	316	ASN
1	B	339	ASN
1	B	368	ASN
1	B	445	GLN
1	B	452	GLN
1	B	509	ASN
1	B	550	ASN
1	B	597	ASN
1	B	608	GLN
1	B	609	GLN
1	B	617	GLN
1	B	619	GLN
1	B	642	ASN
1	B	647	ASN
1	B	656	GLN
1	B	688	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	804	1	14,14,15	0.54	0	17,19,21	1.49	2 (11%)
2	NAG	B	801	1	14,14,15	0.38	0	17,19,21	2.11	4 (23%)
2	NAG	B	802	1	14,14,15	0.58	0	17,19,21	1.40	1 (5%)
2	NAG	B	803	1	14,14,15	0.71	0	17,19,21	1.59	3 (17%)
2	NAG	A	803	1	14,14,15	0.48	0	17,19,21	1.32	3 (17%)
2	NAG	A	802	1	14,14,15	0.53	0	17,19,21	1.54	3 (17%)
2	NAG	A	804	1	14,14,15	0.66	0	17,19,21	2.09	3 (17%)
4	N9Q	B	806	3	28,28,28	1.47	4 (14%)	36,37,37	1.34	5 (13%)
2	NAG	A	801	1	14,14,15	0.53	0	17,19,21	2.32	6 (35%)
4	N9Q	A	806	3	28,28,28	1.45	4 (14%)	36,37,37	1.31	4 (11%)

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	804	1	-	2/6/23/26	0/1/1/1
2	NAG	B	801	1	1/1/5/7	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	802	1	-	3/6/23/26	0/1/1/1
2	NAG	B	803	1	-	2/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	804	1	-	2/6/23/26	0/1/1/1
4	N9Q	B	806	3	-	5/21/21/21	0/2/2/2
2	NAG	A	801	1	-	2/6/23/26	0/1/1/1
4	N9Q	A	806	3	-	5/21/21/21	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	806	N9Q	O39-C37	3.86	1.34	1.22
4	B	806	N9Q	O39-C37	3.48	1.33	1.22
4	B	806	N9Q	O46-C44	3.46	1.33	1.22
4	A	806	N9Q	O46-C44	3.04	1.32	1.22
4	A	806	N9Q	O38-C37	-2.87	1.21	1.30
4	A	806	N9Q	O45-C44	-2.80	1.21	1.30
4	B	806	N9Q	O38-C37	-2.55	1.22	1.30
4	B	806	N9Q	O45-C44	-2.23	1.23	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAG	C1-O5-C5	6.02	120.25	112.19
2	B	801	NAG	C1-O5-C5	5.83	120.00	112.19
2	A	804	NAG	C4-C3-C2	5.33	118.82	111.02
2	B	802	NAG	C1-O5-C5	4.84	118.67	112.19
2	B	801	NAG	C4-C3-C2	-4.52	104.40	111.02
2	A	804	NAG	C1-O5-C5	4.51	118.23	112.19
2	B	803	NAG	C1-O5-C5	4.05	117.62	112.19
4	A	806	N9Q	C17-C22-C25	-4.05	104.81	113.71
2	A	802	NAG	C1-O5-C5	4.02	117.57	112.19
2	A	801	NAG	O5-C1-C2	3.93	117.37	111.29
2	B	804	NAG	C2-N2-C7	3.71	127.87	122.90
2	B	804	NAG	C1-O5-C5	3.48	116.85	112.19
4	B	806	N9Q	C17-C22-C25	-3.36	106.32	113.71
2	A	801	NAG	C3-C4-C5	3.29	116.20	110.23
2	A	803	NAG	C1-O5-C5	3.26	116.56	112.19
2	A	804	NAG	C3-C4-C5	3.13	115.91	110.23
4	A	806	N9Q	O45-C44-C41	3.04	123.46	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAG	C4-C3-C2	2.72	115.00	111.02
2	B	803	NAG	O5-C1-C2	-2.68	107.15	111.29
2	A	802	NAG	C1-C2-N2	-2.64	106.27	110.43
4	A	806	N9Q	O46-C44-C41	-2.64	114.73	122.84
4	B	806	N9Q	O38-C37-C34	2.57	122.11	114.00
2	A	801	NAG	C2-N2-C7	-2.57	119.46	122.90
4	B	806	N9Q	O39-C37-C34	-2.45	115.33	123.09
4	B	806	N9Q	O45-C44-C41	2.39	121.43	114.00
2	A	802	NAG	C4-C3-C2	2.35	114.46	111.02
2	A	803	NAG	O5-C1-C2	-2.26	107.79	111.29
4	A	806	N9Q	O38-C37-C34	2.16	120.83	114.00
2	A	801	NAG	O5-C5-C6	2.15	111.86	107.66
2	B	801	NAG	C2-N2-C7	-2.12	120.05	122.90
2	B	801	NAG	O5-C5-C6	2.10	111.75	107.66
4	B	806	N9Q	O46-C44-C41	-2.07	116.49	122.84
2	A	803	NAG	C3-C4-C5	-2.07	106.49	110.23
2	B	803	NAG	C3-C4-C5	-2.04	106.54	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	801	NAG	C1

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	N9Q	C22-C25-C41-C44
4	A	806	N9Q	N27-C25-C41-C44
4	B	806	N9Q	C22-C25-C41-C44
4	B	806	N9Q	N27-C25-C41-C44
2	A	801	NAG	O5-C5-C6-O6
2	B	803	NAG	O5-C5-C6-O6
2	B	802	NAG	O5-C5-C6-O6
2	B	803	NAG	C4-C5-C6-O6
2	B	804	NAG	O5-C5-C6-O6
2	B	802	NAG	C4-C5-C6-O6
2	B	801	NAG	C4-C5-C6-O6
2	A	801	NAG	C4-C5-C6-O6
2	B	804	NAG	C4-C5-C6-O6
4	A	806	N9Q	C25-C41-C44-O45
4	A	806	N9Q	C25-C41-C44-O46
4	B	806	N9Q	C25-C41-C44-O46

Continued on next page...

Continued from previous page...

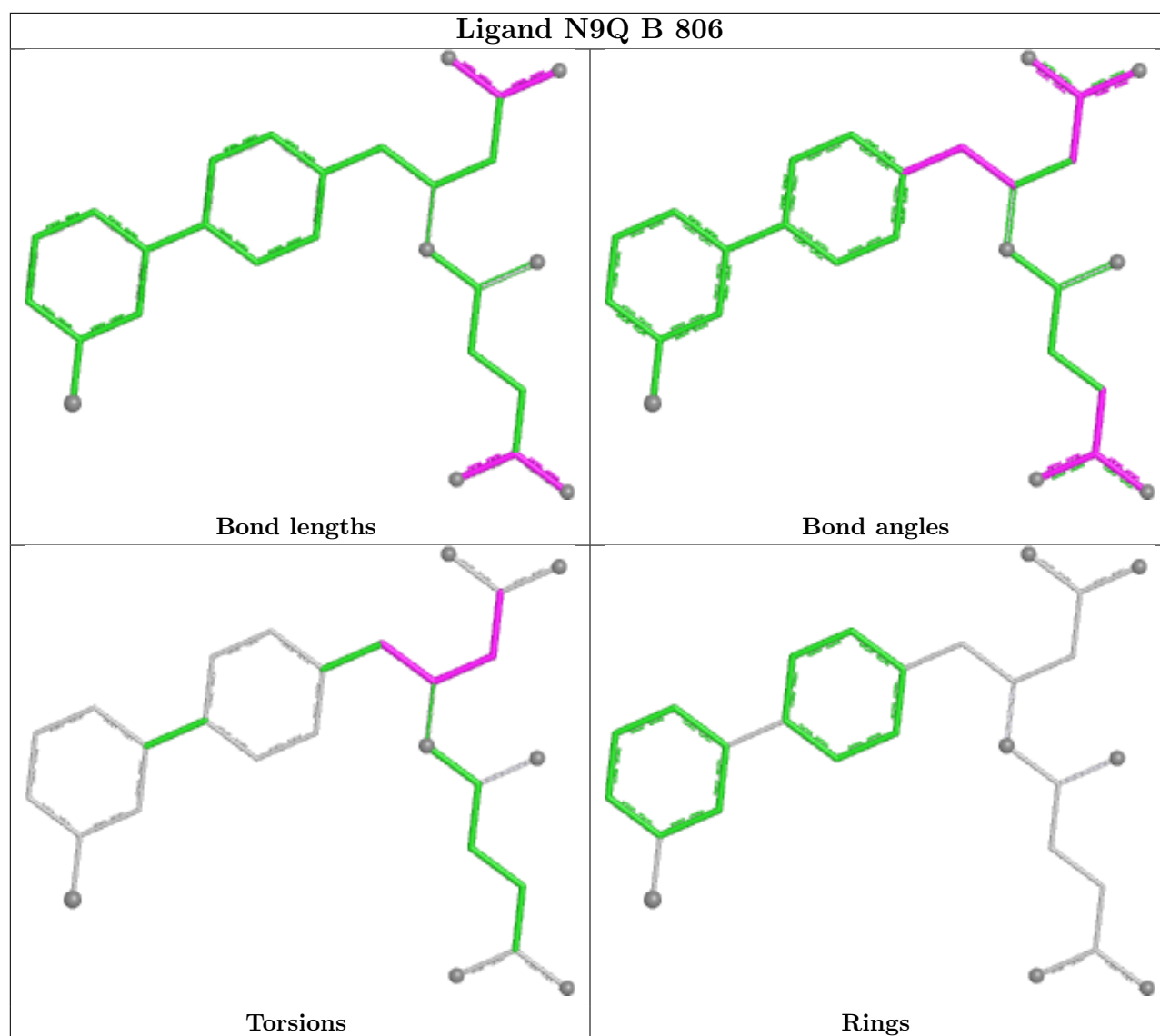
Mol	Chain	Res	Type	Atoms
2	A	804	NAG	C4-C5-C6-O6
4	B	806	N9Q	C25-C41-C44-O45
4	A	806	N9Q	C17-C22-C25-C41
4	B	806	N9Q	C17-C22-C25-C41
2	B	802	NAG	C1-C2-N2-C7
2	B	801	NAG	O5-C5-C6-O6
2	A	804	NAG	O5-C5-C6-O6

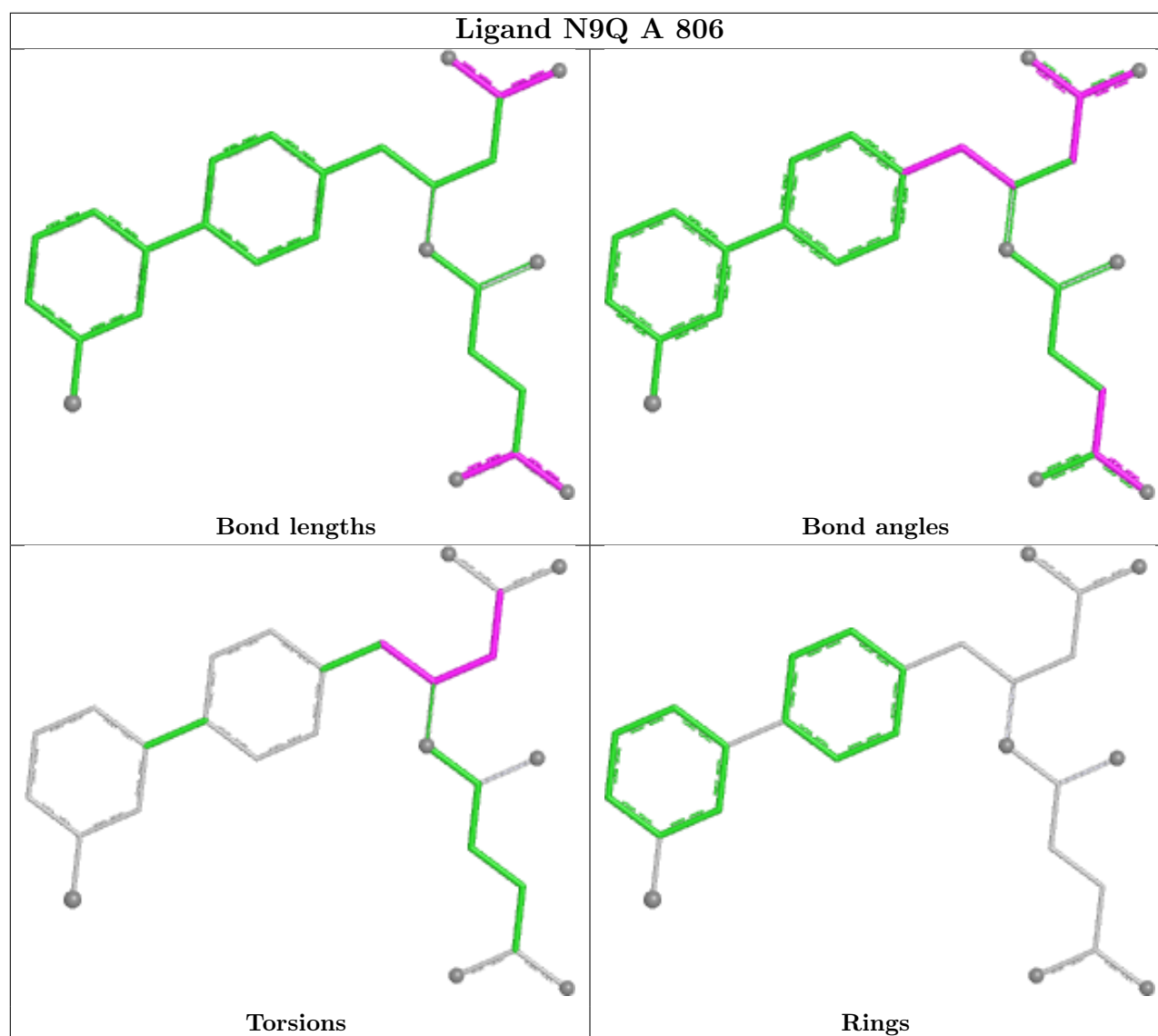
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	806	N9Q	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	696/696 (100%)	-0.04	2 (0%) 90 92	23, 39, 59, 65	0
1	B	696/696 (100%)	0.13	9 (1%) 75 75	23, 41, 60, 67	0
All	All	1392/1392 (100%)	0.05	11 (0%) 82 84	23, 40, 59, 67	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	GLY	2.7
1	A	437	HIS	2.6
1	B	338	THR	2.5
1	B	434	GLU	2.4
1	A	54	GLY	2.3
1	B	303	THR	2.2
1	B	333	VAL	2.1
1	B	500	ASN	2.1
1	B	347	ALA	2.1
1	B	348	PRO	2.1
1	B	340	GLU	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

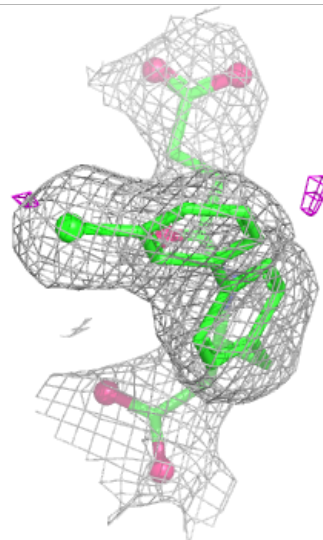
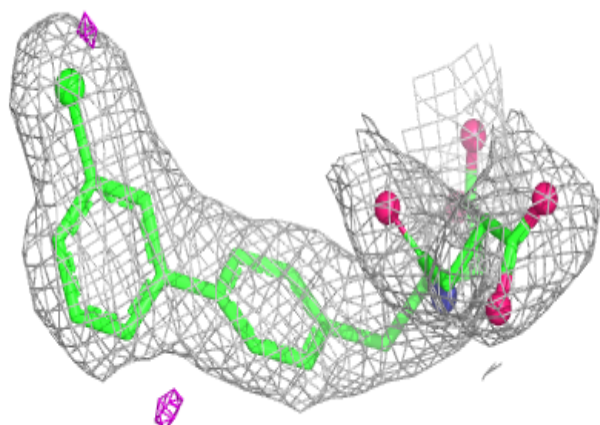
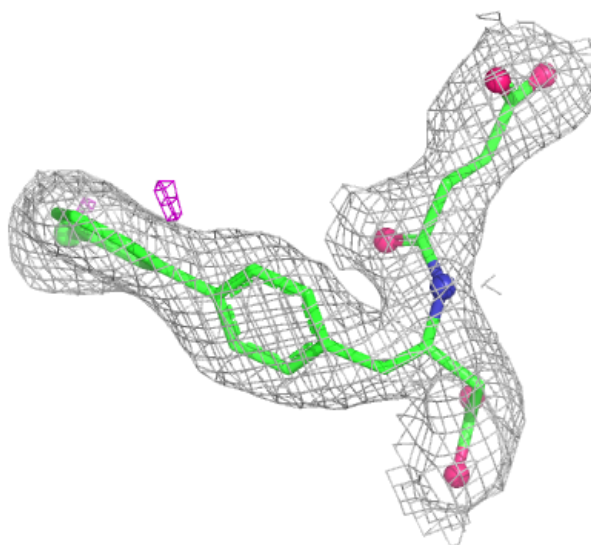
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

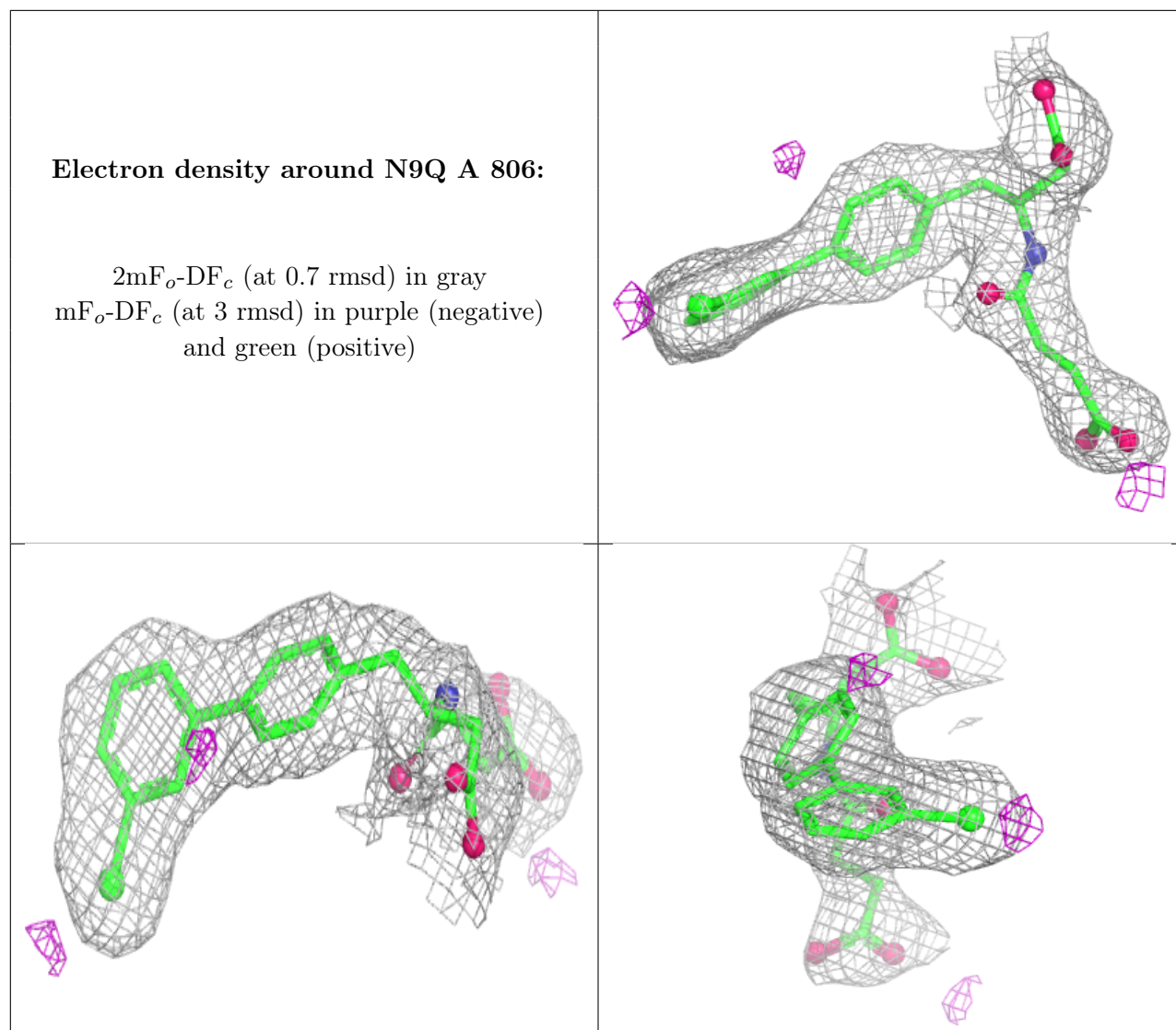
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	801	14/15	0.76	0.13	53,56,58,60	0
2	NAG	A	804	14/15	0.77	0.12	53,55,56,57	0
2	NAG	B	804	14/15	0.79	0.12	56,60,61,62	0
2	NAG	B	803	14/15	0.85	0.11	44,46,48,48	0
2	NAG	A	801	14/15	0.87	0.11	45,49,53,55	0
2	NAG	A	802	14/15	0.88	0.12	56,57,58,58	0
2	NAG	B	802	14/15	0.88	0.11	57,61,66,66	0
2	NAG	A	803	14/15	0.94	0.09	31,33,36,36	0
4	N9Q	B	806	27/27	0.96	0.07	20,23,39,42	0
4	N9Q	A	806	27/27	0.97	0.07	19,23,39,42	0
3	ZN	A	805	1/1	1.00	0.02	25,25,25,25	0
3	ZN	B	805	1/1	1.00	0.01	31,31,31,31	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.

Electron density around N9Q B 806:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.