Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 11:28 pm GMT

PDB ID	:	6THP
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:

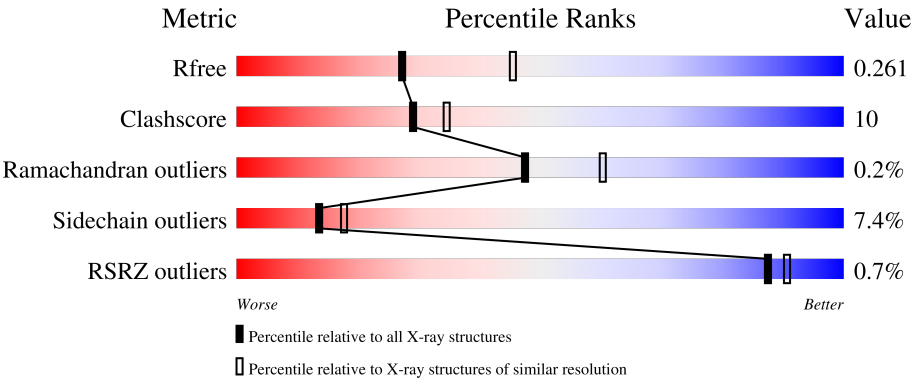
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	80% 19% .
1	B	696	% 74% 22% .

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

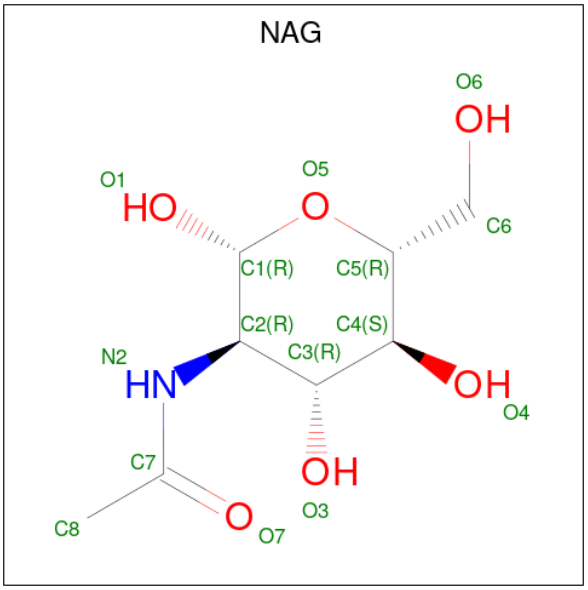
There are 5 unique types of molecules in this entry. The entry contains 11710 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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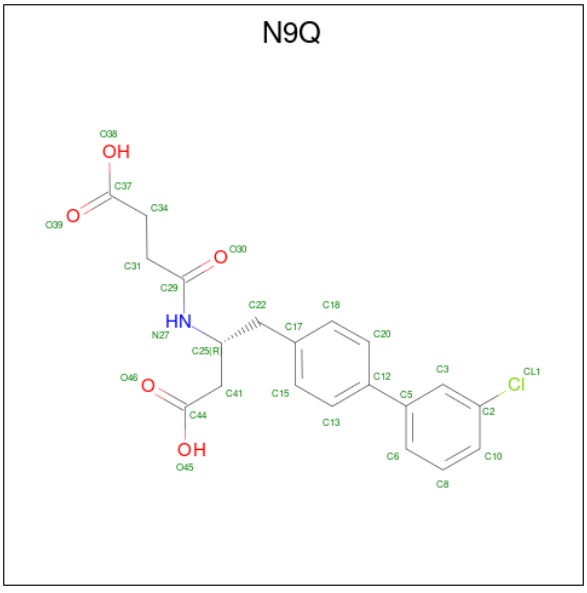
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is ZINC ION (three-letter code: 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 (three-letter code: N9Q) (formula: $C_{20}H_{20}ClNO_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

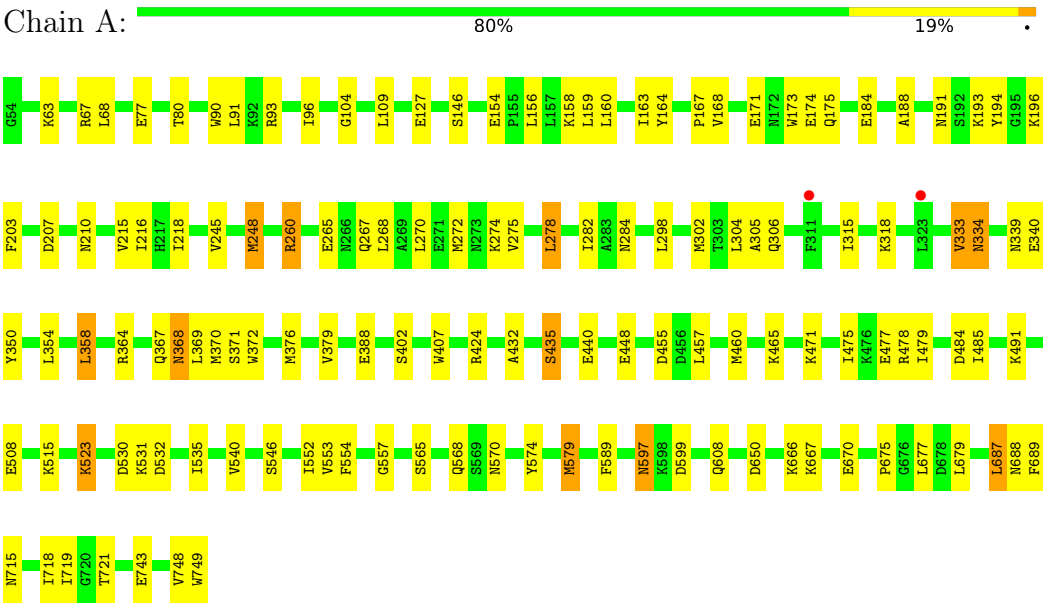
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	218	Total O 218 218	0	0
5	B	134	Total O 134 134	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

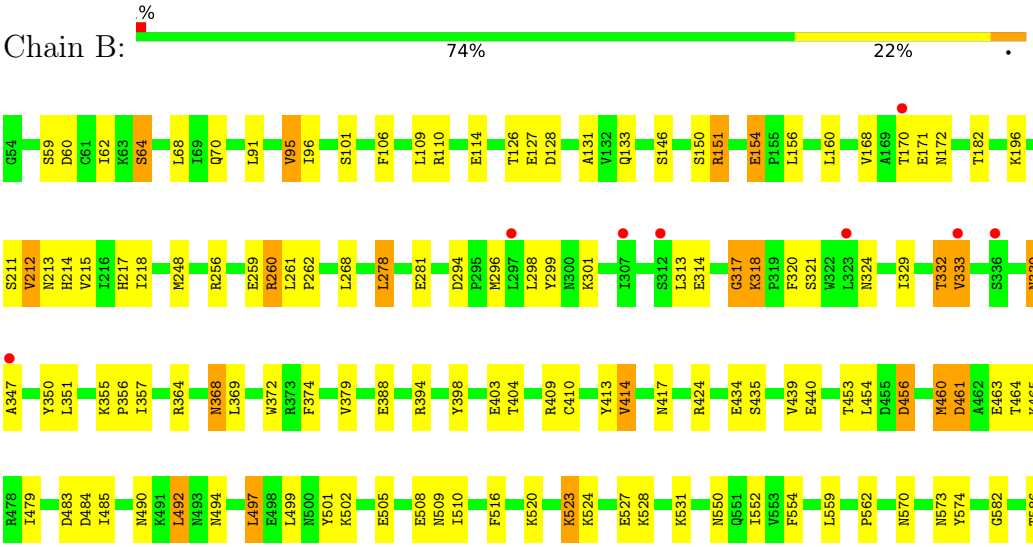
• Molecule 1: Neprilysin

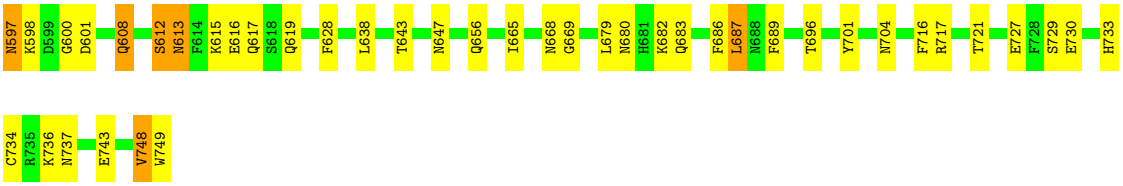
Chain A:



• Molecule 1: Neprilysin

Chain B:




N597
K598
D599
G600
D601
Q608
S612
N613
F614
K615
E616
Q617
S618
Q619
F628
L638
T643
N647
Q656
I665
N668
G669
L679
N680
H681
K682
Q683
F686
L687
N688
F689
T696
Y701
N704
F716
R717
T721
E727
F728
S729
E730
H733
C734
R735
K736
N737
E743
V748
W749

4 Data and refinement statistics (i)

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 58.12 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.94-2.54) 99.8 (58.12-2.54)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.00%)	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)	0.34 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.54	0/5713	0.64	0/7727
1	B	0.57	0/5713	0.65	0/7727
All	All	0.56	0/11426	0.65	0/15454

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5595	0	5446	95	0
1	B	5595	0	5446	123	0
2	A	56	0	52	0	0
2	B	56	0	52	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	0	1	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	214	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 (214) 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: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: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:67:ARG:HH22	1:A:688:ASN:HD21	1.40	0.69
1:A:597:ASN:HD22	1:A:597:ASN:C	1.94	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: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
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:A:457:LEU:HD12	1:A:460:MET:HE1	1.80	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:597:ASN:C	1:B:597:ASN:HD22	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:597:ASN:C	1:B:597:ASN:ND2	2.67	0.48
1:B:643:THR:HB	1:B:647:ASN:HD21	1.79	0.48
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
1:B:461:ASP:OD2	1:B:461:ASP:C	2.53	0.47
1:A:367:GLN:HA	1:A:370:MET:HE2	1.97	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:151:ARG:O	1:B:154:GLU:HB3	2.17	0.45
1:B:460:MET:HE1	1:B:464:THR:HB	1.98	0.44
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
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: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: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:460:MET:HE2	1:B:465:LYS:HG2	1.99	0.43
1:A:457:LEU:HD12	1:A:460:MET:CE	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:460:MET:HB3	1:A:460:MET:HE2	1.87	0.43
1:B:68:LEU:HD22	1:B:687:LEU:HD13	2.00	0.43
1:A:202:LEU:HD13	1:A:202:LEU:C	2.40	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:508:GLU:OE1	1:A:508:GLU:N	2.50	0.43
1:A:196:LYS:C	1:A:197:LYS:HD3	2.38	0.42
1:B:439:VAL:HG21	1:B:559:LEU:HD22	2.01	0.42
1:A:579:MET:HE2	4:A:806:N9Q:C3	2.48	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:613:ASN:OD1	1:B:613:ASN:N	2.52	0.42
1:B:60:ASP:O	1:B:64:SER:HB2	2.19	0.42
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:B:460:MET:HE2	1:B:465:LYS:CG	2.49	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:A:460:MET:HE3	1:A:465:LYS:HG2	2.02	0.41
1:A:597:ASN:ND2	1:A:597:ASN:C	2.66	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:586:THR:O	1:B:587:HIS:C	2.58	0.41
1:B:727:GLU:OE1	1:B:727:GLU:N	2.34	0.41
1:B:460:MET:HE2	1:B:460:MET:HB3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	694/696 (100%)	668 (96%)	26 (4%)	0	100	100
1	B	694/696 (100%)	635 (92%)	56 (8%)	3 (0%)	34	46
All	All	1388/1392 (100%)	1303 (94%)	82 (6%)	3 (0%)	47	60

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	605/605 (100%)	569 (94%)	36 (6%)	19	25
1	B	605/605 (100%)	552 (91%)	53 (9%)	10	12
All	All	1210/1210 (100%)	1121 (93%)	89 (7%)	13	18

All (89) 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	175	GLN
1	A	197	LYS
1	A	215	VAL
1	A	248	MET
1	A	260	ARG
1	A	270	LEU
1	A	274	LYS
1	A	278	LEU
1	A	298	LEU
1	A	333	VAL
1	A	334	ASN
1	A	340	GLU
1	A	358	LEU
1	A	368	ASN
1	A	371	SER
1	A	379	VAL
1	A	402	SER
1	A	435	SER
1	A	448	GLU
1	A	455	ASP
1	A	523	LYS

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Mol	Chain	Res	Type
1	A	546	SER
1	A	579	MET
1	A	597	ASN
1	A	608	GLN
1	A	667	LYS
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	106	PHE
1	B	126	THR
1	B	127	GLU
1	B	146	SER
1	B	150	SER
1	B	151	ARG
1	B	154	GLU
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	260	ARG
1	B	278	LEU
1	B	332	THR
1	B	333	VAL
1	B	339	ASN
1	B	364	ARG
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	453	THR
1	B	456	ASP

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Mol	Chain	Res	Type
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	597	ASN
1	B	608	GLN
1	B	612	SER
1	B	613	ASN
1	B	668	ASN
1	B	687	LEU
1	B	730	GLU
1	B	748	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	213	ASN
1	A	257	GLN
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	656	GLN
1	A	668	ASN
1	A	688	ASN

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Mol	Chain	Res	Type
1	B	70	GLN
1	B	213	ASN
1	B	217	HIS
1	B	257	GLN
1	B	316	ASN
1	B	339	ASN
1	B	368	ASN
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	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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
4	N9Q	A	806	3	28,28,28	1.41	4 (14%)	36,37,37	1.28	4 (11%)
2	NAG	B	803	1	14,14,15	0.69	0	17,19,21	1.64	4 (23%)
2	NAG	B	804	1	14,14,15	0.52	0	17,19,21	1.46	2 (11%)
2	NAG	B	802	1	14,14,15	0.55	0	17,19,21	1.38	1 (5%)
2	NAG	A	801	1	14,14,15	0.54	0	17,19,21	2.35	6 (35%)
2	NAG	B	801	1	14,14,15	0.38	0	17,19,21	2.14	4 (23%)
4	N9Q	B	806	3	28,28,28	1.42	4 (14%)	36,37,37	1.32	4 (11%)
2	NAG	A	802	1	14,14,15	0.52	0	17,19,21	1.50	3 (17%)
2	NAG	A	804	1	14,14,15	0.65	0	17,19,21	2.09	3 (17%)
2	NAG	A	803	1	14,14,15	0.49	0	17,19,21	1.32	3 (17%)

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
4	N9Q	A	806	3	-	5/21/21/21	0/2/2/2
2	NAG	B	803	1	-	2/6/23/26	0/1/1/1
2	NAG	B	804	1	-	2/6/23/26	0/1/1/1
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	801	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
4	N9Q	B	806	3	-	5/21/21/21	0/2/2/2
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
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	806	N9Q	O39-C37	3.79	1.34	1.22
4	B	806	N9Q	O39-C37	3.42	1.33	1.22
4	B	806	N9Q	O46-C44	3.40	1.33	1.22
4	A	806	N9Q	O46-C44	2.99	1.32	1.22
4	A	806	N9Q	O38-C37	-2.80	1.21	1.30
4	A	806	N9Q	O45-C44	-2.73	1.21	1.30
4	B	806	N9Q	O38-C37	-2.49	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	806	N9Q	O45-C44	-2.17	1.23	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	NAG	C1-O5-C5	5.95	120.25	112.19
2	B	801	NAG	C1-O5-C5	5.76	120.00	112.19
2	A	804	NAG	C4-C3-C2	5.33	118.82	111.02
2	B	802	NAG	C1-O5-C5	4.78	118.67	112.19
2	B	801	NAG	C4-C3-C2	-4.52	104.40	111.02
2	A	804	NAG	C1-O5-C5	4.45	118.23	112.19
2	B	803	NAG	C1-O5-C5	4.00	117.62	112.19
2	A	802	NAG	C1-O5-C5	3.97	117.57	112.19
4	A	806	N9Q	C17-C22-C25	-3.95	104.81	113.78
2	A	801	NAG	O5-C1-C2	3.85	117.37	111.29
2	B	804	NAG	C2-N2-C7	3.49	127.87	122.90
2	B	804	NAG	C1-O5-C5	3.44	116.85	112.19
2	A	801	NAG	C3-C4-C5	3.34	116.20	110.24
4	B	806	N9Q	C17-C22-C25	-3.29	106.32	113.78
2	A	803	NAG	C1-O5-C5	3.22	116.56	112.19
2	A	804	NAG	C3-C4-C5	3.18	115.91	110.24
2	A	801	NAG	O5-C5-C6	2.97	111.86	107.20
4	A	806	N9Q	O45-C44-C41	2.93	123.46	114.07
2	B	801	NAG	O5-C5-C6	2.90	111.75	107.20
2	A	801	NAG	C4-C3-C2	2.72	115.00	111.02
2	B	803	NAG	O5-C5-C6	2.63	111.33	107.20
2	B	803	NAG	O5-C1-C2	-2.62	107.15	111.29
4	B	806	N9Q	O38-C37-C34	2.52	122.11	114.03
4	A	806	N9Q	O46-C44-C41	-2.52	114.73	122.80
2	A	802	NAG	C1-C2-N2	-2.47	106.27	110.49
2	A	801	NAG	C2-N2-C7	-2.42	119.46	122.90
4	B	806	N9Q	O39-C37-C34	-2.41	115.33	123.08
2	A	802	NAG	C4-C3-C2	2.35	114.46	111.02
4	B	806	N9Q	O45-C44-C41	2.30	121.43	114.07
2	A	803	NAG	O5-C1-C2	-2.21	107.79	111.29
4	A	806	N9Q	O38-C37-C34	2.12	120.83	114.03
2	A	803	NAG	C3-C4-C5	-2.10	106.49	110.24
2	B	803	NAG	C3-C4-C5	-2.08	106.54	110.24
2	B	801	NAG	C2-N2-C7	-2.00	120.05	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	801	NAG	C1

All (22) 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
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	801	NAG	O5-C5-C6-O6
2	A	804	NAG	O5-C5-C6-O6

There are no ring outliers.

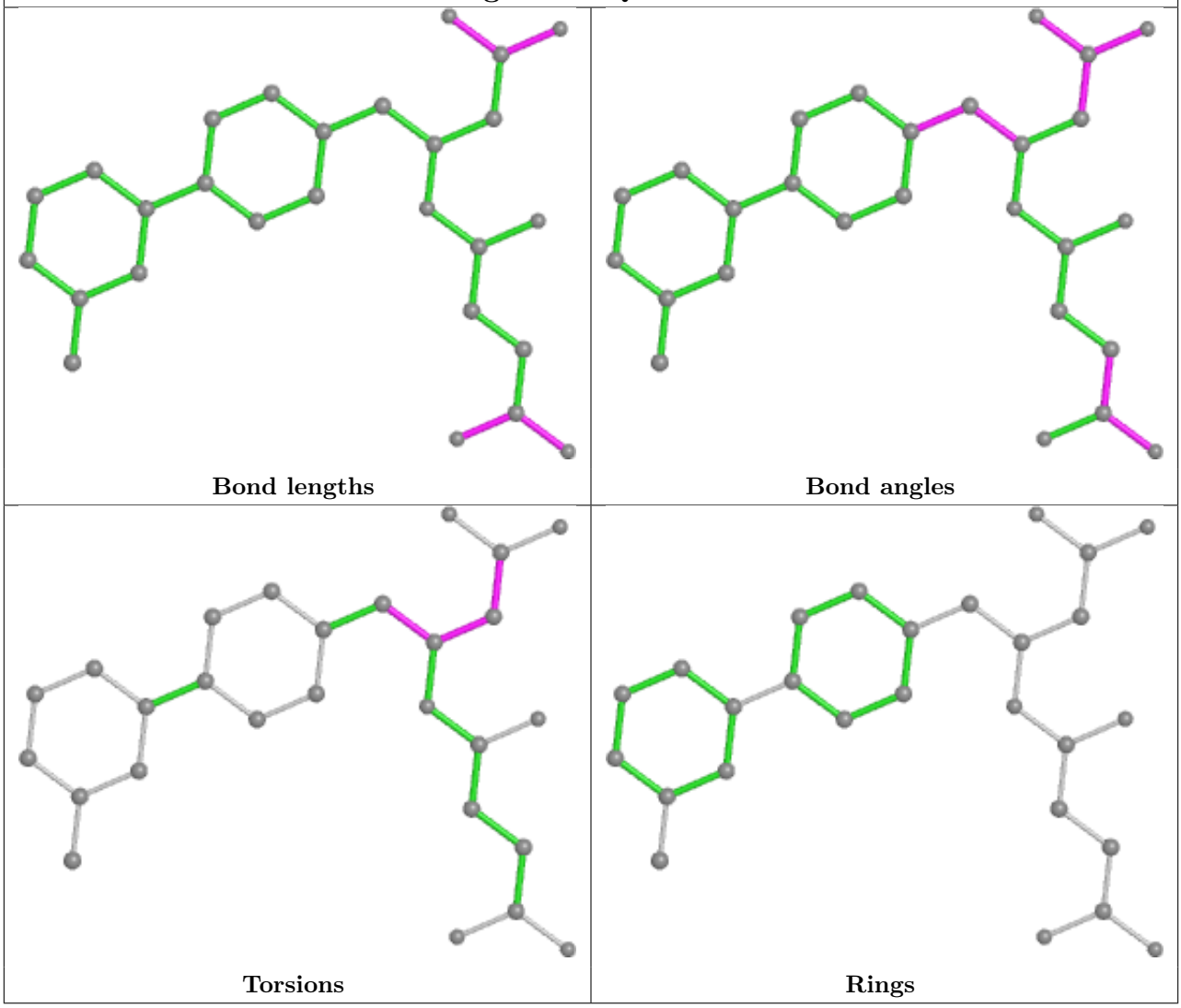
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	806	N9Q	1	0

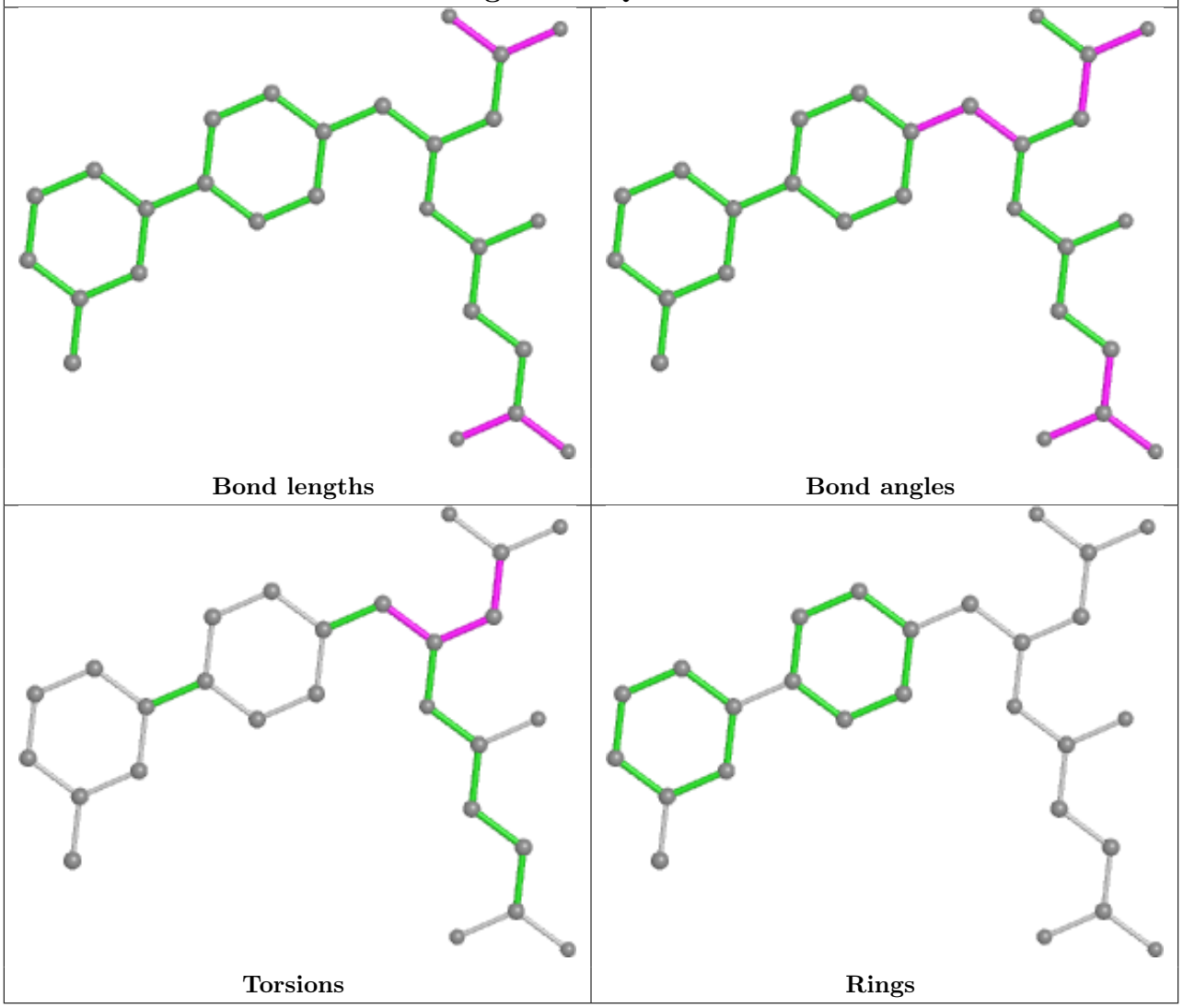
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand N9Q A 806



Ligand N9Q B 806



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, 95^{th} 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%)	-0.01	2 (0%) 94 96	23, 39, 59, 65	0
1	B	696/696 (100%)	0.07	8 (1%) 80 85	23, 41, 60, 67	0
All	All	1392/1392 (100%)	0.03	10 (0%) 87 90	23, 40, 59, 67	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	333	VAL	4.5
1	B	347	ALA	3.8
1	B	323	LEU	3.6
1	B	307	ILE	3.4
1	B	297	LEU	3.0
1	B	170	THR	2.9
1	B	312	SER	2.4
1	B	336	SER	2.3
1	A	323	LEU	2.3
1	A	311	PHE	2.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

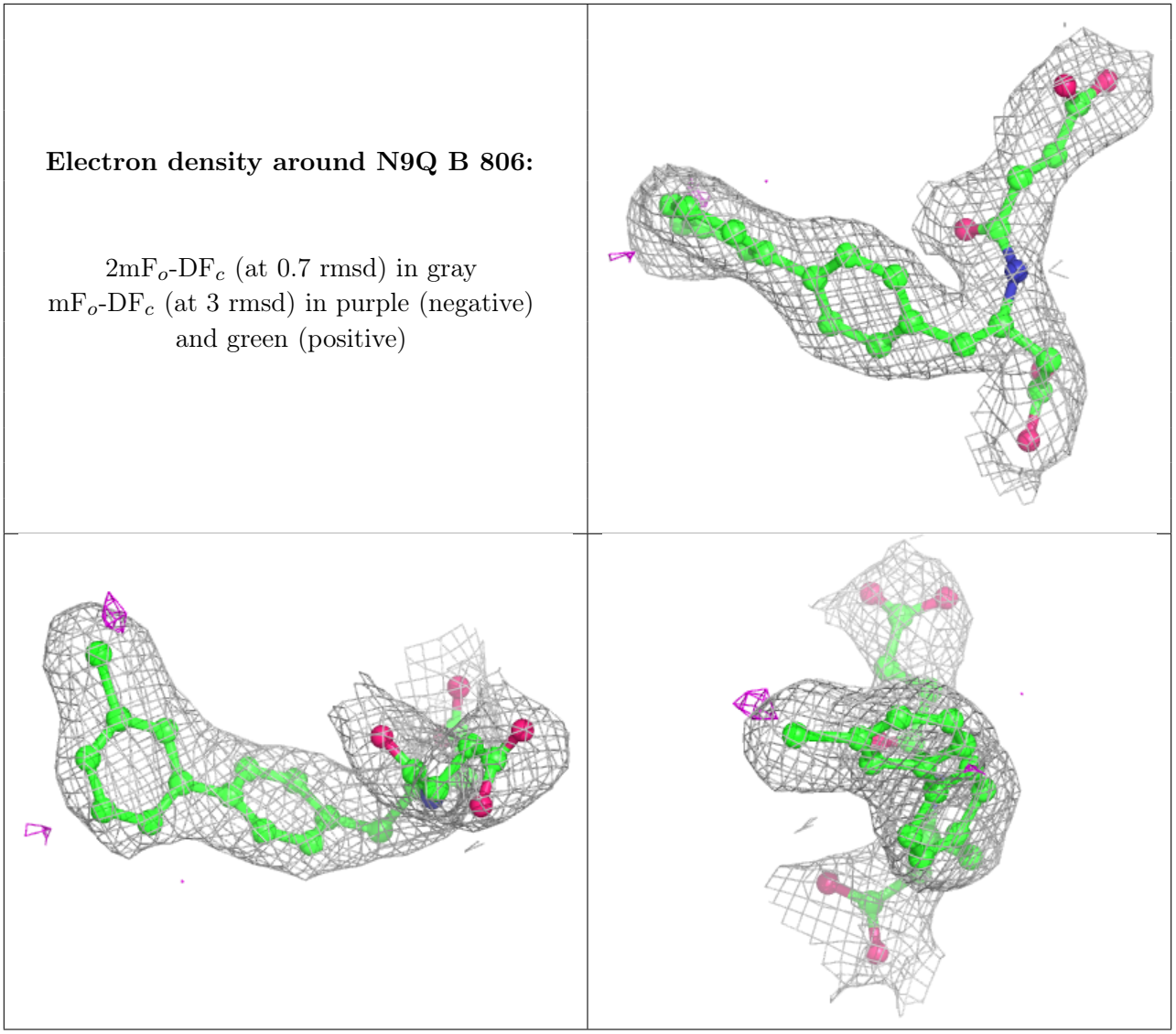
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	804	14/15	0.80	0.23	56,60,61,62	0
2	NAG	A	804	14/15	0.82	0.16	53,55,56,57	0
2	NAG	B	803	14/15	0.86	0.18	44,46,48,48	0
2	NAG	A	802	14/15	0.87	0.18	56,57,58,58	0
2	NAG	B	801	14/15	0.87	0.18	53,56,58,60	0
2	NAG	A	801	14/15	0.90	0.16	45,49,53,55	0
2	NAG	B	802	14/15	0.90	0.14	57,61,66,66	0
2	NAG	A	803	14/15	0.95	0.16	31,33,36,36	0
4	N9Q	B	806	27/27	0.97	0.15	20,23,39,42	0
4	N9Q	A	806	27/27	0.98	0.14	19,23,39,42	0
3	ZN	B	805	1/1	0.99	0.11	31,31,31,31	0
3	ZN	A	805	1/1	1.00	0.14	25,25,25,25	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.

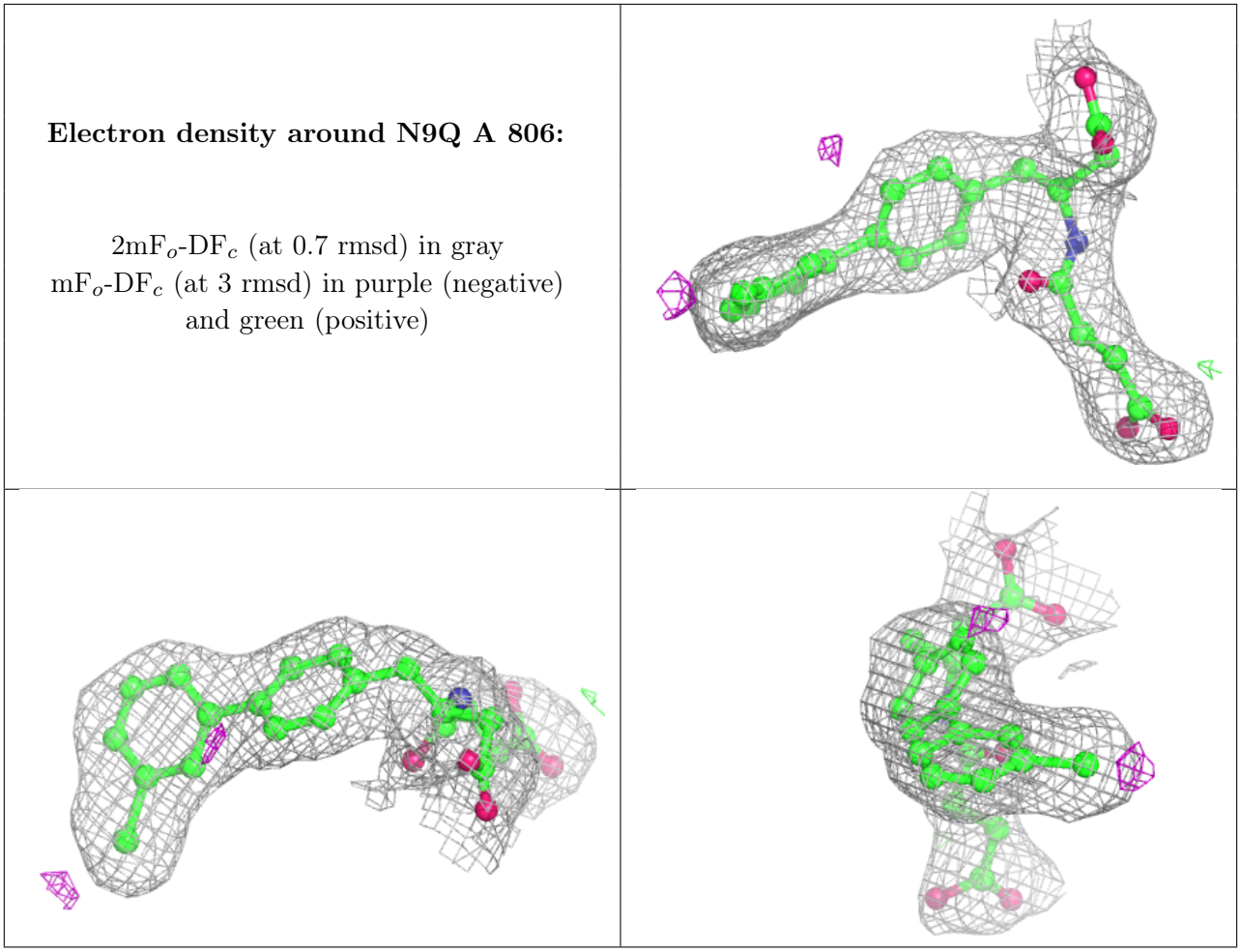
Electron density around N9Q B 806:

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



Electron density around N9Q A 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 (i)

There are no such residues in this entry.