



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2026 – 02:08 PM EDT

PDB ID : 11TN / pdb_000011tn
Title : Candida glabrata Glycogen Debranching Enzyme (GDE) in complex with Miglustat
Authors : Mishra, N.; Paz, A.
Deposited on : 2026-03-12
Resolution : 3.24 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

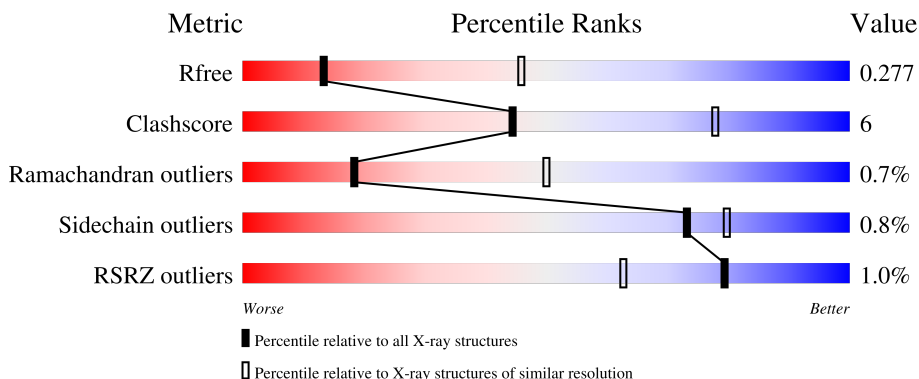
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	1524	
1	B	1524	

2 Entry composition [i](#)

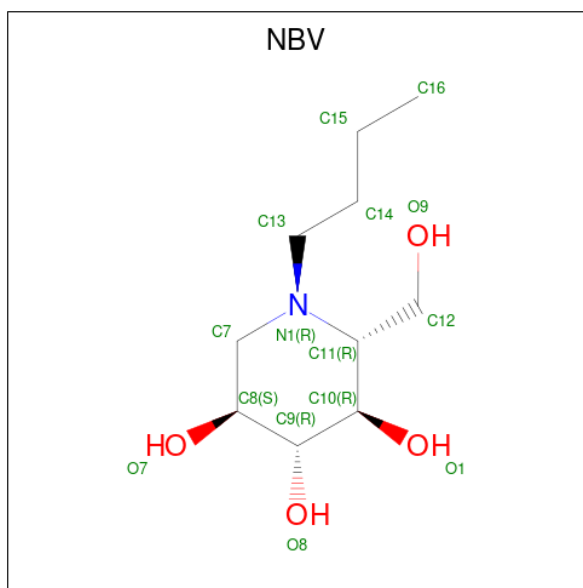
There are 2 unique types of molecules in this entry. The entry contains 23473 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen debranching enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1524	Total	C	N	O	S	0	0	0
			12264	7821	2061	2330	52			
1	B	1388	Total	C	N	O	S	0	0	0
			11179	7131	1884	2114	50			

- Molecule 2 is (2R,3R,4R,5S)-1-BUTYL-2-(HYDROXYMETHYL)PIPERIDINE-3,4,5-TRIOL (CCD ID: NBV) (formula: $C_{10}H_{21}NO_4$) (labeled as "Ligand of Interest" by depositor).

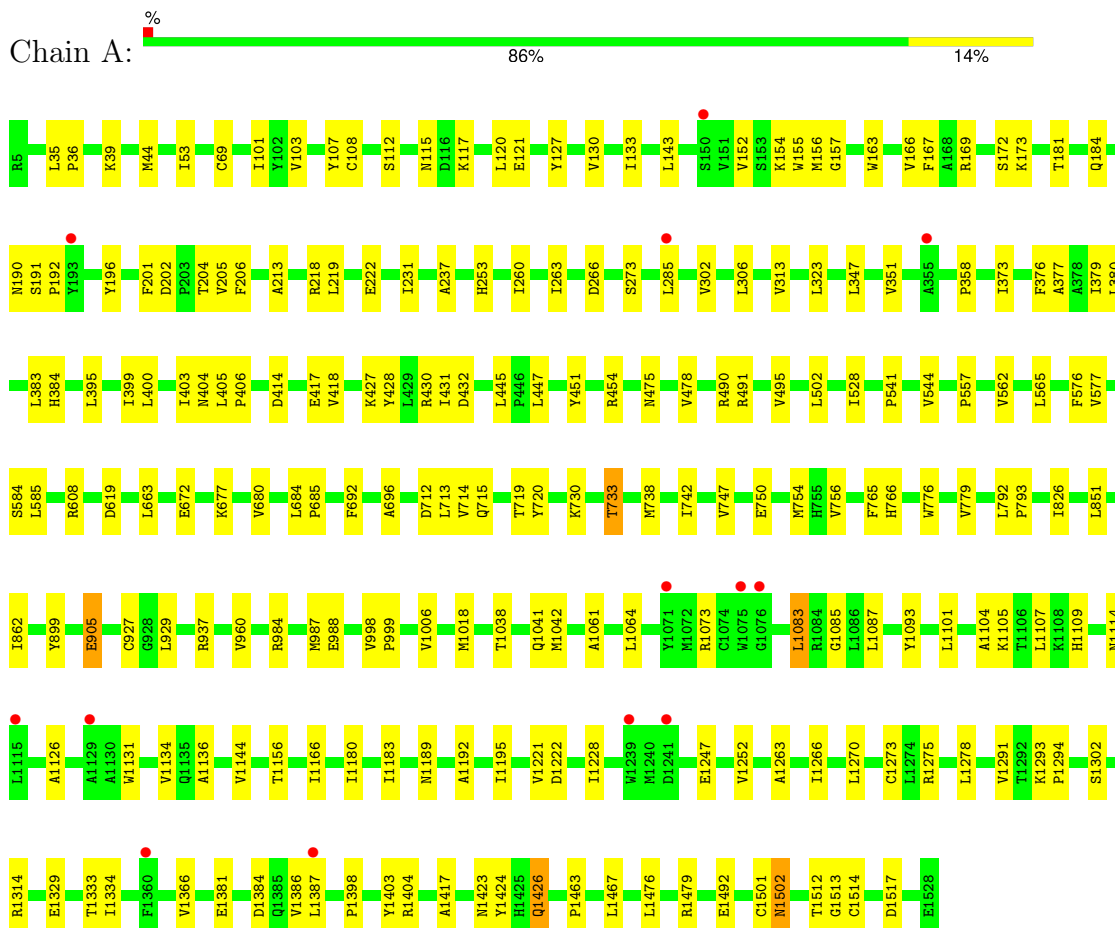


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		

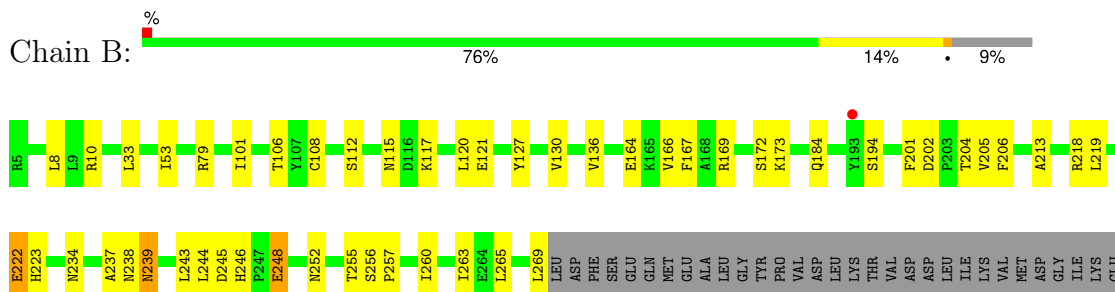
3 Residue-property plots

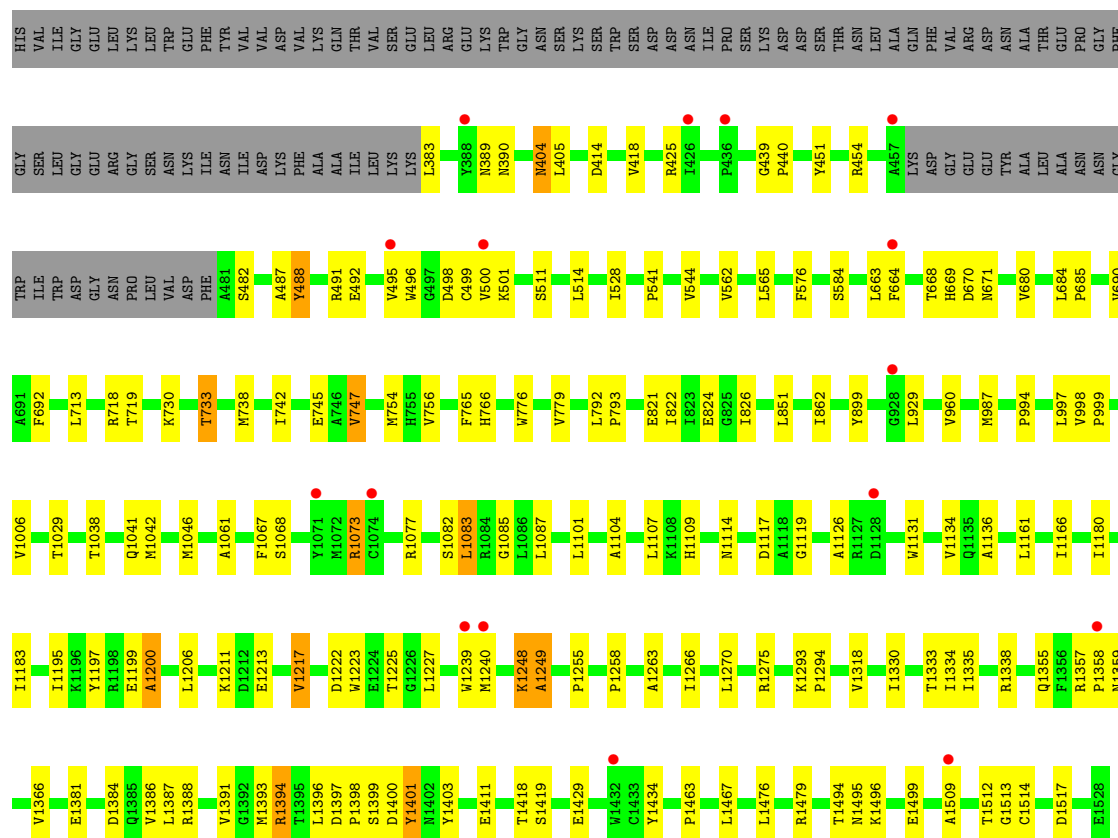
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Glycogen debranching enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	159.08Å 199.27Å 254.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.11 – 3.24 127.11 – 3.24	Depositor EDS
% Data completeness (in resolution range)	56.7 (127.11-3.24) 56.7 (127.11-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.105)	Depositor
R, R_{free}	0.235 , 0.274 0.241 , 0.277	Depositor DCC
R_{free} test set	1857 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 94.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	23473	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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: NBV

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	0.46	0/12574	0.86	1/17049 (0.0%)
1	B	0.46	0/11463	0.87	1/15542 (0.0%)
All	All	0.46	0/24037	0.87	2/32591 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	1222	ASP	CA-CB-CG	5.17	117.77	112.60

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	12264	0	11948	135	0
1	B	11179	0	10899	141	0
2	A	15	0	21	4	0
2	B	15	0	21	0	0
All	All	23473	0	22889	277	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 6.

All (277) 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:A:152:VAL:HG11	1:A:155:TRP:CE3	2.05	0.91
1:A:1038:THR:HG21	1:A:1512:THR:HG21	1.60	0.84
1:B:1038:THR:HG21	1:B:1512:THR:HG21	1.61	0.81
1:A:1424:TYR:OH	2:A:1601:NBV:H161	1.86	0.75
1:B:1400:ASP:O	1:B:1401:TYR:HB3	1.88	0.74
1:B:244:LEU:HD13	1:B:514:LEU:HB2	1.69	0.73
1:A:152:VAL:CG1	1:A:155:TRP:CE3	2.71	0.73
1:B:1240:MET:HE2	1:B:1359:ASN:HD21	1.53	0.72
1:B:1082:SER:HB3	1:B:1509:ALA:O	1.90	0.71
1:B:668:THR:HG22	1:B:671:ASN:OD1	1.90	0.70
1:A:1134:VAL:HG11	1:A:1273:CYS:SG	2.35	0.66
1:B:718:ARG:O	1:B:719:THR:OG1	2.09	0.66
1:A:1278:LEU:HD21	1:A:1302:SER:HA	1.75	0.66
1:A:417:GLU:OE1	1:A:490:ARG:NE	2.28	0.65
1:A:152:VAL:HG11	1:A:155:TRP:CZ3	2.31	0.65
1:B:33:LEU:HD21	1:B:747:VAL:HG13	1.81	0.63
1:B:692:PHE:HB3	1:B:765:PHE:CE2	2.34	0.63
1:B:383:LEU:O	1:B:383:LEU:HD12	2.00	0.62
1:B:1333:THR:C	1:B:1335:ILE:H	2.09	0.61
1:B:738:MET:HE1	1:B:862:ILE:HG21	1.83	0.61
1:A:692:PHE:HB3	1:A:765:PHE:CE2	2.35	0.61
1:B:487:ALA:O	1:B:488:TYR:HB2	1.99	0.61
1:B:1029:THR:HG21	1:B:1479:ARG:HH22	1.65	0.61
1:B:167:PHE:CG	1:B:219:LEU:HD21	2.36	0.60
1:A:167:PHE:CG	1:A:219:LEU:HD21	2.37	0.60
1:A:173:LYS:HA	1:A:733:THR:HG23	1.85	0.59
1:B:684:LEU:HB3	1:B:685:PRO:HD3	1.83	0.59
1:B:718:ARG:O	1:B:821:GLU:O	2.21	0.59
1:A:351:VAL:HG23	1:A:403:ILE:HD11	1.85	0.59
1:B:1199:GLU:HG2	1:B:1206:LEU:CD2	2.33	0.58
1:B:1107:LEU:HD22	1:B:1183:ILE:HG23	1.85	0.58
1:A:684:LEU:HB3	1:A:685:PRO:HD3	1.84	0.57
1:A:383:LEU:HD12	1:A:384:HIS:HB2	1.87	0.57
1:B:173:LYS:HA	1:B:733:THR:HG23	1.86	0.56
1:A:738:MET:HE1	1:A:862:ILE:HG21	1.88	0.56
1:B:1400:ASP:O	1:B:1401:TYR:CB	2.54	0.56
1:B:1495:ASN:O	1:B:1499:GLU:HB2	2.06	0.56
1:A:205:VAL:HG13	1:A:206:PHE:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:PHE:HB3	1:A:765:PHE:CD2	2.41	0.55
1:A:1107:LEU:HD22	1:A:1183:ILE:HG23	1.87	0.55
1:B:1197:TYR:CE1	1:B:1217:VAL:HG21	2.40	0.55
1:B:730:LYS:O	1:B:733:THR:OG1	2.24	0.55
1:A:101:ILE:N	1:A:101:ILE:HD12	2.21	0.55
1:A:730:LYS:O	1:A:733:THR:OG1	2.24	0.55
1:A:1083:LEU:HD22	1:A:1136:ALA:HB1	1.89	0.55
1:B:218:ARG:O	1:B:222:GLU:HG2	2.06	0.55
1:A:899:TYR:CG	1:A:1041:GLN:HG2	2.42	0.54
1:A:1333:THR:HG23	1:A:1334:ILE:HG23	1.88	0.54
1:B:692:PHE:HB3	1:B:765:PHE:CD2	2.42	0.54
1:B:562:VAL:HG11	1:B:663:LEU:HD13	1.89	0.54
1:A:285:LEU:HD23	1:A:285:LEU:H	1.73	0.54
1:B:112:SER:HB3	1:B:120:LEU:HD21	1.89	0.54
1:B:899:TYR:CG	1:B:1041:GLN:HG2	2.43	0.54
1:B:1199:GLU:O	1:B:1200:ALA:HB3	2.07	0.54
1:A:103:VAL:HG13	1:A:557:PRO:HB3	1.90	0.54
1:B:1083:LEU:HD22	1:B:1136:ALA:HB1	1.90	0.54
1:A:562:VAL:HG11	1:A:663:LEU:HD13	1.89	0.54
1:B:1199:GLU:HG2	1:B:1206:LEU:HD23	1.89	0.53
1:B:1255:PRO:HG2	1:B:1258:PRO:HG3	1.91	0.53
1:A:1134:VAL:CG1	1:A:1273:CYS:SG	2.96	0.53
1:A:347:LEU:HD12	1:A:347:LEU:C	2.34	0.53
1:A:172:SER:O	1:A:733:THR:CG2	2.56	0.53
1:B:172:SER:O	1:B:733:THR:CG2	2.55	0.53
1:A:69:CYS:SG	1:A:107:TYR:HB3	2.48	0.53
1:A:1404:ARG:HG3	1:A:1417:ALA:HB1	1.90	0.52
1:A:405:LEU:N	1:A:406:PRO:HD2	2.24	0.52
1:B:202:ASP:CG	1:B:204:THR:HG22	2.35	0.52
1:B:1318:VAL:HG22	1:B:1330:ILE:HD12	1.92	0.52
1:A:108:CYS:HB3	1:A:127:TYR:CD2	2.45	0.52
1:A:202:ASP:CG	1:A:204:THR:HG22	2.35	0.51
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.45	0.51
1:B:1248:LYS:O	1:B:1249:ALA:HB3	2.09	0.51
1:A:192:PRO:HG2	1:A:713:LEU:HD12	1.93	0.51
1:A:475:ASN:HB3	1:A:478:VAL:HG12	1.92	0.51
1:A:112:SER:HB2	1:A:120:LEU:HD21	1.92	0.51
1:A:619:ASP:OD1	1:A:937:ARG:HD2	2.10	0.51
1:A:451:TYR:CZ	1:A:491:ARG:HD3	2.46	0.51
1:B:234:ASN:O	1:B:501:LYS:HB2	2.10	0.51
1:B:256:SER:N	1:B:257:PRO:HD3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:ASN:HA	1:A:1291:VAL:HG13	1.93	0.51
1:A:1192:ALA:CB	1:A:1291:VAL:CG1	2.88	0.51
1:A:213:ALA:HA	1:A:528:ILE:HG23	1.93	0.50
1:B:389:ASN:OD1	1:B:454:ARG:NH1	2.41	0.50
1:B:1333:THR:C	1:B:1335:ILE:N	2.70	0.50
1:B:1388:ARG:HG3	1:B:1393:MET:HE1	1.92	0.50
1:B:1046:MET:HG3	1:B:1073:ARG:HD2	1.93	0.50
1:A:1247:GLU:HG3	1:A:1252:VAL:HG21	1.93	0.50
1:B:205:VAL:HG23	1:B:206:PHE:CD2	2.46	0.50
1:B:1330:ILE:HG22	1:B:1330:ILE:O	2.10	0.50
1:A:152:VAL:HG12	1:A:720:TYR:OH	2.12	0.49
1:A:347:LEU:HD11	1:A:399:ILE:HD12	1.93	0.49
1:B:389:ASN:CG	1:B:454:ARG:HH12	2.19	0.49
1:A:998:VAL:HB	1:A:999:PRO:HD3	1.93	0.49
1:B:8:LEU:HD21	1:B:10:ARG:HG3	1.93	0.49
1:B:1042:MET:HG3	1:B:1509:ALA:HB2	1.93	0.49
1:A:379:ILE:HG22	1:A:383:LEU:HD23	1.95	0.49
1:A:1221:VAL:HG22	1:A:1228:ILE:HG12	1.94	0.49
1:B:213:ALA:HA	1:B:528:ILE:HG23	1.95	0.49
1:B:414:ASP:O	1:B:418:VAL:HG23	2.12	0.49
1:B:754:MET:HE2	1:B:756:VAL:HG23	1.95	0.49
1:A:754:MET:HE2	1:A:756:VAL:HG23	1.94	0.49
1:B:562:VAL:HG12	1:B:584:SER:HB2	1.95	0.49
1:B:1068:SER:C	1:B:1073:ARG:HG3	2.37	0.49
1:A:184:GLN:HA	1:A:201:PHE:HA	1.95	0.49
1:A:1061:ALA:HB2	1:A:1073:ARG:CZ	2.43	0.49
1:A:1042:MET:SD	1:A:1064:LEU:CD1	3.01	0.48
1:B:1248:LYS:O	1:B:1249:ALA:CB	2.60	0.48
1:B:668:THR:HG23	1:B:670:ASP:H	1.78	0.48
1:A:562:VAL:HG12	1:A:584:SER:HB2	1.95	0.48
2:A:1601:NBV:H162	2:A:1601:NBV:H7C2	1.96	0.48
1:B:1411:GLU:CD	1:B:1418:THR:HB	2.38	0.48
1:A:414:ASP:O	1:A:418:VAL:HG23	2.13	0.48
1:A:428:TYR:HA	1:A:432:ASP:HB2	1.96	0.48
1:B:115:ASN:C	1:B:117:LYS:H	2.22	0.48
1:A:285:LEU:HD21	1:A:430:ARG:HD2	1.96	0.48
1:A:577:VAL:HG22	1:A:585:LEU:HD11	1.96	0.48
1:B:565:LEU:HD21	1:B:576:PHE:HB2	1.96	0.48
1:A:608:ARG:HH11	1:A:750:GLU:HG2	1.78	0.48
1:A:562:VAL:HA	1:A:584:SER:O	2.14	0.47
1:A:1247:GLU:CG	1:A:1252:VAL:HG21	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1275:ARG:NH2	1:B:1366:VAL:O	2.47	0.47
1:A:273:SER:HB3	1:A:447:LEU:HD22	1.95	0.47
1:B:1061:ALA:HB2	1:B:1073:ARG:CZ	2.44	0.47
1:A:1192:ALA:HB3	1:A:1291:VAL:CG1	2.44	0.47
1:A:1275:ARG:NH2	1:A:1366:VAL:O	2.47	0.47
1:B:1114:ASN:HB2	1:B:1126:ALA:HB2	1.96	0.47
1:B:1393:MET:HE2	1:B:1434:TYR:CD2	2.50	0.47
1:A:1293:LYS:HB3	1:A:1294:PRO:HD2	1.97	0.47
1:B:194:SER:OG	1:B:237:ALA:HB2	2.15	0.47
1:B:779:VAL:HG11	1:B:851:LEU:HD11	1.97	0.47
1:B:243:LEU:HD13	1:B:496:TRP:CE3	2.50	0.47
1:B:184:GLN:HA	1:B:201:PHE:HA	1.95	0.47
1:A:156:MET:HE3	1:A:163:TRP:CD2	2.50	0.47
1:B:562:VAL:HA	1:B:584:SER:O	2.15	0.47
1:B:1335:ILE:HD11	1:B:1338:ARG:HG2	1.96	0.47
1:A:565:LEU:HD21	1:A:576:PHE:HB2	1.97	0.47
1:A:1192:ALA:CB	1:A:1291:VAL:HG11	2.45	0.47
1:A:120:LEU:HD23	1:A:121:GLU:N	2.30	0.46
1:A:380:LEU:HD12	1:A:395:LEU:HD22	1.97	0.46
1:A:672:GLU:HB2	1:A:677:LYS:HE2	1.97	0.46
1:B:1293:LYS:HB3	1:B:1294:PRO:HD2	1.97	0.46
1:B:33:LEU:HD21	1:B:747:VAL:CG1	2.44	0.46
1:B:1355:GLN:NE2	1:B:1400:ASP:OD2	2.49	0.46
1:B:120:LEU:HD23	1:B:121:GLU:N	2.30	0.46
1:A:417:GLU:OE1	1:A:490:ARG:NH2	2.48	0.46
1:A:1386:VAL:HG23	1:A:1387:LEU:HG	1.97	0.46
1:B:166:VAL:HG22	1:B:169:ARG:HH22	1.80	0.46
1:B:255:THR:C	1:B:257:PRO:HD3	2.41	0.46
1:B:680:VAL:HG11	1:B:826:ILE:HD13	1.98	0.46
1:B:1396:LEU:HD11	1:B:1400:ASP:OD2	2.16	0.46
1:A:376:PHE:CZ	1:A:380:LEU:HD21	2.51	0.45
1:A:395:LEU:C	1:A:395:LEU:HD23	2.41	0.45
1:A:1398:PRO:HA	1:A:1403:TYR:CG	2.51	0.45
1:B:269:LEU:HD12	1:B:269:LEU:C	2.41	0.45
1:B:1386:VAL:HG23	1:B:1387:LEU:HG	1.96	0.45
1:A:1463:PRO:HB3	1:A:1467:LEU:HD23	1.97	0.45
1:A:905:GLU:HG3	1:A:927:CYS:SG	2.56	0.45
1:A:1114:ASN:HB2	1:A:1126:ALA:HB2	1.98	0.45
1:A:1501:CYS:O	1:A:1502:ASN:CB	2.63	0.45
1:A:1109:HIS:O	1:A:1195:ILE:HG21	2.16	0.45
1:A:101:ILE:HG21	1:A:130:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ASP:HB3	1:A:715:GLN:HE21	1.81	0.45
1:B:488:TYR:HB3	1:B:499:CYS:HA	1.99	0.45
1:B:664:PHE:CE2	1:B:690:VAL:HG22	2.52	0.45
1:B:404:ASN:N	1:B:404:ASN:HD22	2.15	0.45
1:B:713:LEU:HD12	1:B:713:LEU:H	1.82	0.45
1:A:253:HIS:HB2	1:A:260:ILE:HG22	1.99	0.45
1:A:427:LYS:HA	1:A:431:ILE:HG22	1.99	0.45
1:A:1476:LEU:HA	1:A:1479:ARG:HD3	1.99	0.45
1:B:1398:PRO:HA	1:B:1403:TYR:CG	2.52	0.45
1:B:499:CYS:O	1:B:501:LYS:N	2.50	0.45
1:B:439:GLY:N	1:B:440:PRO:CD	2.80	0.45
1:B:1211:LYS:O	1:B:1213:GLU:N	2.48	0.45
1:B:1463:PRO:HB3	1:B:1467:LEU:HD23	1.99	0.45
1:B:244:LEU:HD22	1:B:511:SER:OG	2.17	0.44
1:B:1077:ARG:HD3	1:B:1239:TRP:CB	2.46	0.44
1:A:1314:ARG:NH1	1:A:1329:GLU:HG2	2.32	0.44
1:B:754:MET:HA	1:B:766:HIS:O	2.17	0.44
1:B:1109:HIS:O	1:B:1195:ILE:HG21	2.17	0.44
1:A:680:VAL:HG11	1:A:826:ILE:HD13	1.98	0.44
1:B:1131:TRP:HA	1:B:1134:VAL:HG22	2.00	0.44
1:B:488:TYR:HB3	1:B:498:ASP:O	2.18	0.44
1:B:405:LEU:HD12	1:B:405:LEU:N	2.33	0.44
1:A:302:VAL:O	1:A:306:LEU:HD23	2.18	0.44
1:A:323:LEU:HD11	1:A:377:ALA:HA	2.00	0.44
1:B:390:ASN:N	1:B:390:ASN:OD1	2.49	0.44
1:B:1199:GLU:O	1:B:1200:ALA:CB	2.66	0.43
1:A:779:VAL:HG11	1:A:851:LEU:HD11	1.99	0.43
1:B:1101:LEU:HD23	1:B:1180:ILE:HD11	2.00	0.43
1:A:400:LEU:HD23	1:A:403:ILE:HD12	2.00	0.43
1:B:53:ILE:HD12	1:B:53:ILE:N	2.33	0.43
1:A:263:ILE:O	1:A:454:ARG:NH2	2.51	0.43
1:A:1492:GLU:OE2	2:A:1601:NBV:H163	2.19	0.43
1:B:238:ASN:O	1:B:239:ASN:HB3	2.18	0.43
1:B:1393:MET:HE2	1:B:1434:TYR:CE2	2.53	0.43
1:A:405:LEU:N	1:A:406:PRO:CD	2.82	0.43
1:A:166:VAL:HG22	1:A:169:ARG:HH22	1.82	0.43
1:A:754:MET:HA	1:A:766:HIS:O	2.18	0.43
1:A:36:PRO:HG2	1:A:44:MET:HE3	2.00	0.43
1:A:1105:LYS:NZ	1:A:1156:THR:OG1	2.50	0.43
1:B:668:THR:HG22	1:B:671:ASN:CG	2.43	0.43
1:B:718:ARG:NH1	1:B:822:ILE:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1131:TRP:CD1	1:B:1266:ILE:HG23	2.53	0.43
1:A:155:TRP:CH2	1:A:713:LEU:HD13	2.53	0.43
1:B:491:ARG:HH21	1:B:495:VAL:HG22	1.84	0.43
1:B:1394:ARG:HG3	1:B:1394:ARG:HH11	1.84	0.43
1:A:53:ILE:N	1:A:53:ILE:HD12	2.34	0.42
1:A:152:VAL:HG23	1:A:181:THR:OG1	2.18	0.42
1:A:313:VAL:HG13	1:A:404:ASN:HB3	2.01	0.42
1:A:1131:TRP:CD1	1:A:1266:ILE:HG23	2.53	0.42
1:B:260:ILE:HB	1:B:265:LEU:HB3	2.01	0.42
1:A:1101:LEU:HD23	1:A:1180:ILE:HD11	2.01	0.42
1:B:101:ILE:HG21	1:B:130:VAL:HG21	2.01	0.42
1:A:266:ASP:HB3	1:A:454:ARG:HH22	1.85	0.42
1:A:1424:TYR:CZ	2:A:1601:NBV:H161	2.55	0.42
1:B:1104:ALA:HB1	1:B:1183:ILE:HD13	2.02	0.42
1:A:115:ASN:C	1:A:117:LYS:H	2.28	0.42
1:B:792:LEU:HD12	1:B:793:PRO:HD2	2.02	0.42
1:A:1131:TRP:CH2	1:A:1270:LEU:HD13	2.55	0.42
1:B:1391:VAL:HG12	1:B:1494:THR:HG21	2.01	0.42
1:B:1240:MET:CE	1:B:1359:ASN:HD21	2.27	0.42
1:A:1083:LEU:HD12	1:A:1087:LEU:HD12	2.02	0.41
1:A:1104:ALA:HB1	1:A:1183:ILE:HD13	2.02	0.41
1:B:1263:ALA:HB3	1:B:1266:ILE:HD12	2.02	0.41
1:B:1476:LEU:HD12	1:B:1476:LEU:C	2.45	0.41
1:A:1263:ALA:HB3	1:A:1266:ILE:HD12	2.03	0.41
1:B:222:GLU:O	1:B:223:HIS:HB2	2.19	0.41
1:B:668:THR:OG1	1:B:669:HIS:N	2.53	0.41
1:B:960:VAL:HG13	1:B:987:MET:SD	2.61	0.41
1:B:1381:GLU:O	1:B:1384:ASP:HB3	2.20	0.41
1:A:35:LEU:HD22	1:A:133:ILE:HD13	2.03	0.41
1:A:451:TYR:CG	1:A:495:VAL:HG21	2.56	0.41
1:B:79:ARG:HH22	1:B:106:THR:HG21	1.85	0.41
1:A:541:PRO:O	1:A:544:VAL:HG22	2.21	0.41
1:B:994:PRO:HD2	1:B:997:LEU:HD12	2.02	0.41
1:B:1197:TYR:CE1	1:B:1217:VAL:CG2	3.04	0.41
1:A:1423:ASN:HA	1:A:1426:GLN:HG2	2.03	0.41
1:B:1083:LEU:HD12	1:B:1087:LEU:HD12	2.02	0.41
1:A:218:ARG:O	1:A:222:GLU:HB3	2.21	0.41
1:A:984:ARG:O	1:A:988:GLU:HG2	2.20	0.41
1:A:1403:TYR:O	1:A:1404:ARG:HD3	2.21	0.41
1:B:256:SER:N	1:B:257:PRO:CD	2.83	0.41
1:B:204:THR:HG23	1:B:205:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:998:VAL:N	1:B:999:PRO:HD2	2.36	0.41
1:A:157:GLY:HA2	1:A:719:THR:HG21	2.03	0.41
1:A:191:SER:HB2	1:A:714:VAL:HG12	2.03	0.41
1:A:445:LEU:HD12	1:A:445:LEU:O	2.20	0.41
1:A:929:LEU:HD22	1:A:1006:VAL:HG13	2.01	0.41
1:A:1085:GLY:HA3	1:A:1513:GLY:O	2.21	0.41
1:B:246:HIS:O	1:B:248:GLU:OE2	2.39	0.41
1:B:742:ILE:HG12	1:B:776:TRP:CH2	2.56	0.41
1:B:929:LEU:HD22	1:B:1006:VAL:HG13	2.02	0.41
1:B:1397:ASP:OD2	1:B:1399:SER:OG	2.39	0.41
1:A:417:GLU:OE1	1:A:490:ARG:CZ	2.69	0.41
1:A:742:ILE:HG12	1:A:776:TRP:CH2	2.56	0.41
1:B:136:VAL:O	1:B:136:VAL:HG13	2.20	0.41
1:B:1418:THR:O	1:B:1419:SER:C	2.63	0.41
1:B:1429:GLU:HB2	1:B:1494:THR:CG2	2.50	0.41
1:A:792:LEU:HD12	1:A:793:PRO:HD2	2.03	0.40
1:A:1381:GLU:O	1:A:1384:ASP:HB3	2.21	0.40
1:B:164:GLU:HA	1:B:167:PHE:CD2	2.56	0.40
1:B:1514:CYS:HA	1:B:1517:ASP:OD2	2.21	0.40
1:A:154:LYS:HE3	1:A:190:ASN:O	2.20	0.40
1:A:196:TYR:HA	1:A:237:ALA:HB3	2.03	0.40
1:B:1117:ASP:C	1:B:1119:GLY:H	2.29	0.40
1:B:541:PRO:O	1:B:544:VAL:HG22	2.20	0.40
1:B:1085:GLY:HA3	1:B:1513:GLY:O	2.21	0.40
1:A:39:LYS:HG3	1:A:44:MET:HE2	2.03	0.40
1:A:1018:MET:HE2	1:A:1018:MET:HA	2.03	0.40
1:A:1093:TYR:CD1	1:A:1144:VAL:HG22	2.56	0.40
1:B:1131:TRP:CH2	1:B:1270:LEU:HD13	2.57	0.40
1:B:1222:ASP:O	1:B:1223:TRP:HB2	2.22	0.40
1:B:1225:THR:HG21	1:B:1227:LEU:HD12	2.04	0.40
1:A:143:LEU:O	1:A:696:ALA:HB2	2.22	0.40
1:A:960:VAL:HG13	1:A:987:MET:SD	2.61	0.40
1:A:1514:CYS:HA	1:A:1517:ASP:OD2	2.21	0.40
1:B:1357:ARG:HB3	1:B:1358:PRO:HD2	2.03	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	1522/1524 (100%)	1430 (94%)	89 (6%)	3 (0%)	43	72
1	B	1382/1524 (91%)	1269 (92%)	97 (7%)	16 (1%)	10	38
All	All	2904/3048 (95%)	2699 (93%)	186 (6%)	19 (1%)	18	50

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	SER
1	B	500	VAL
1	B	1334	ILE
1	B	1401	TYR
1	B	1496	LYS
1	A	1502	ASN
1	B	239	ASN
1	B	252	ASN
1	B	488	TYR
1	B	745	GLU
1	A	747	VAL
1	B	425	ARG
1	B	451	TYR
1	B	492	GLU
1	B	1200	ALA
1	A	358	PRO
1	B	248	GLU
1	B	747	VAL
1	B	1249	ALA

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	1343/1343 (100%)	1335 (99%)	8 (1%)	78	83
1	B	1225/1343 (91%)	1212 (99%)	13 (1%)	65	77
All	All	2568/2686 (96%)	2547 (99%)	21 (1%)	73	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	ILE
1	A	373	ILE
1	A	502	LEU
1	A	733	THR
1	A	905	GLU
1	A	1083	LEU
1	A	1166	ILE
1	A	1426	GLN
1	B	222	GLU
1	B	263	ILE
1	B	404	ASN
1	B	733	THR
1	B	824	GLU
1	B	1067	PHE
1	B	1073	ARG
1	B	1083	LEU
1	B	1161	LEU
1	B	1166	ILE
1	B	1217	VAL
1	B	1248	LYS
1	B	1394	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	275	GLN
1	A	369	ASN
1	A	390	ASN
1	A	421	GLN
1	A	715	GLN

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Mol	Chain	Res	Type
1	A	1311	ASN
1	B	224	ASN
1	B	404	ASN
1	B	766	HIS
1	B	866	GLN
1	B	1359	ASN
1	B	1449	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 ⓘ

2 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	NBV	B	1601	-	15,15,15	0.29	0	19,20,20	0.75	0
2	NBV	A	1601	-	15,15,15	0.34	0	19,20,20	1.22	3 (15%)

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	NBV	B	1601	-	-	3/6/26/26	0/1/1/1
2	NBV	A	1601	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	NBV	C12-C11-N1	-2.48	107.47	112.51
2	A	1601	NBV	C7-C8-C9	-2.45	107.25	110.17
2	A	1601	NBV	C12-C11-C10	-2.04	109.85	112.93

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1601	NBV	C10-C11-C12-O9
2	B	1601	NBV	N1-C13-C14-C15
2	B	1601	NBV	C13-C14-C15-C16
2	A	1601	NBV	C14-C13-N1-C7
2	A	1601	NBV	C14-C13-N1-C11

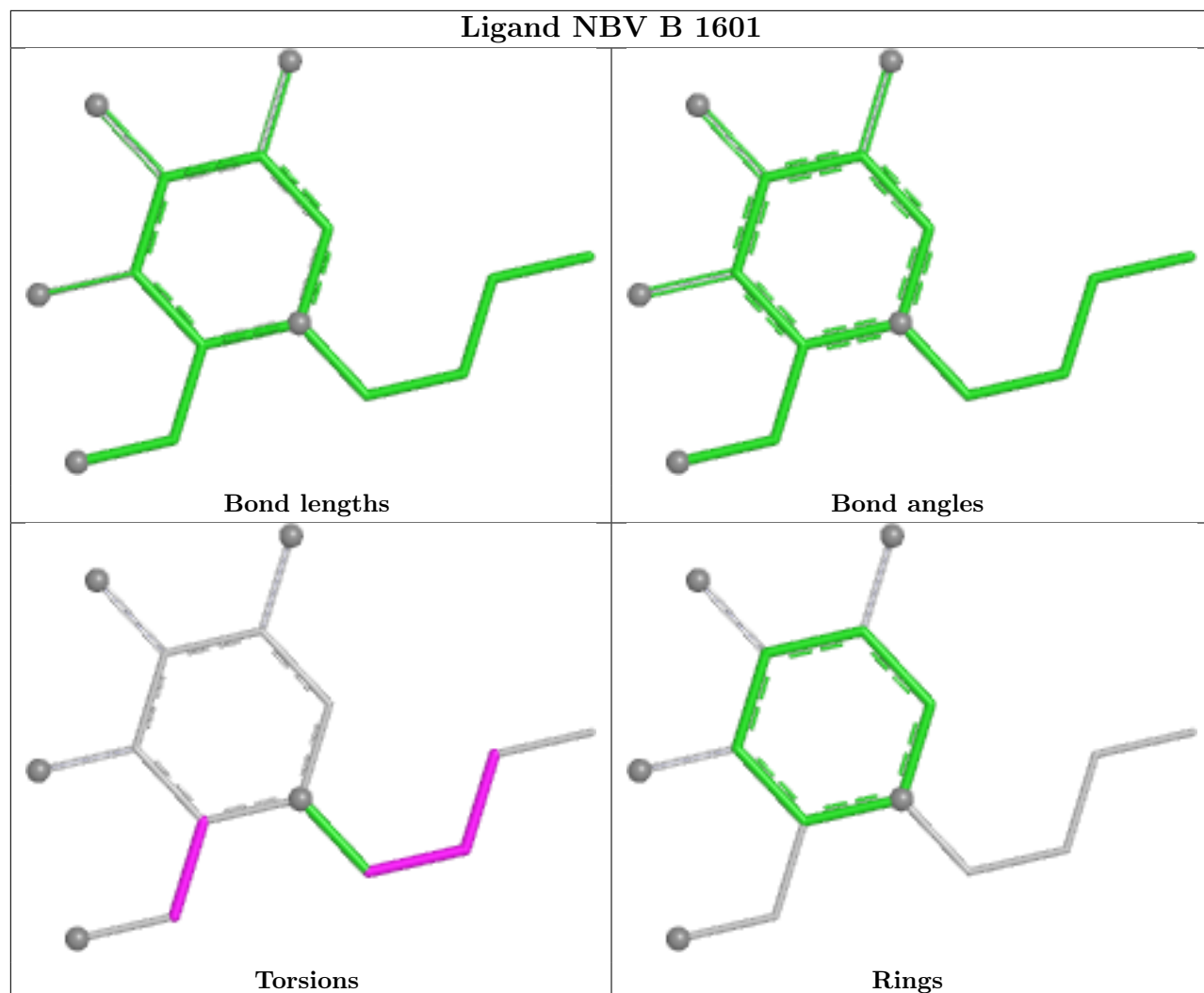
There are no ring outliers.

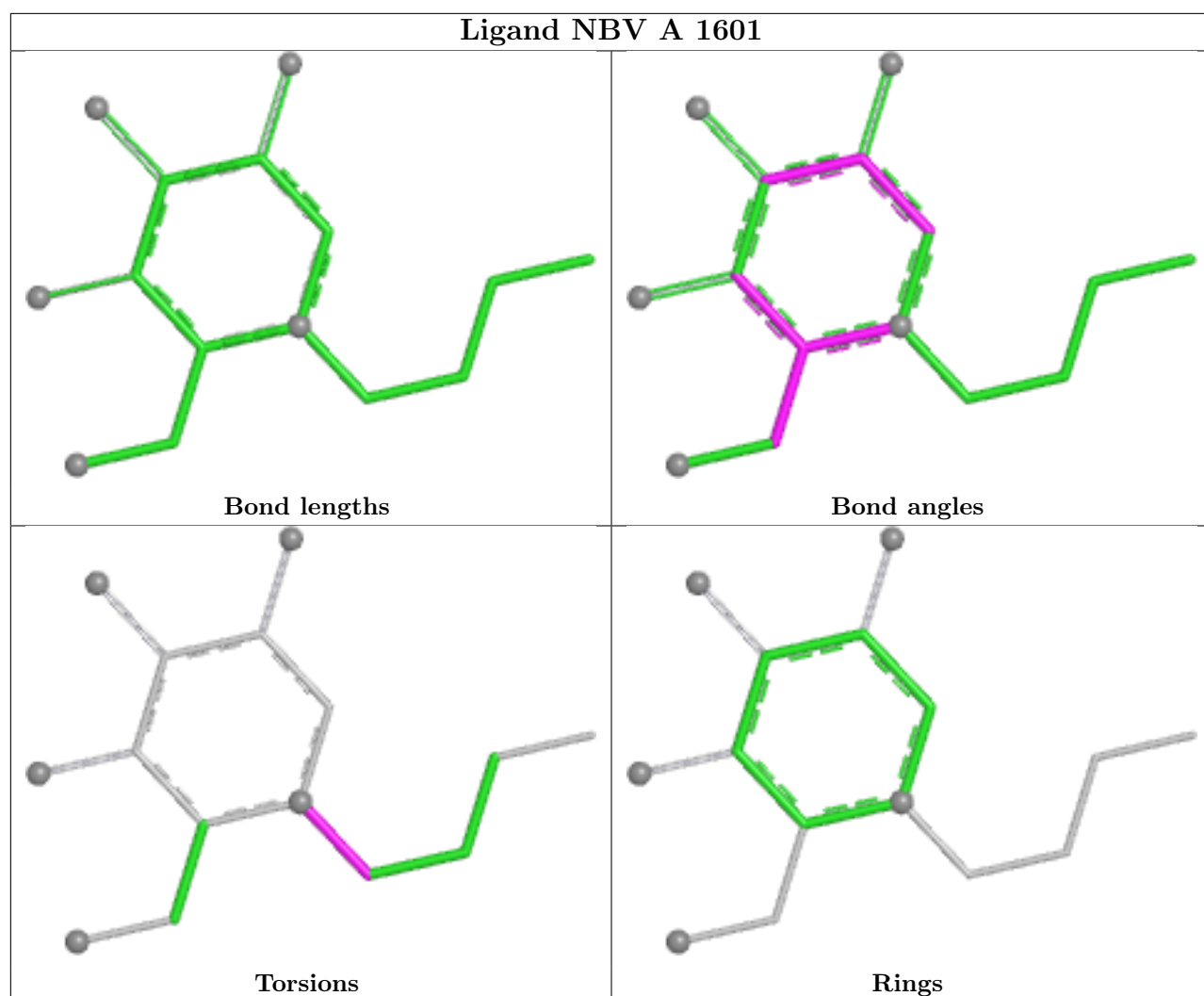
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	NBV	4	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.

Ligand NBV B 1601





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	1524/1524 (100%)	-0.10	13 (0%) 81 64	46, 92, 158, 204	0
1	B	1388/1524 (91%)	-0.09	17 (1%) 76 58	37, 75, 113, 167	0
All	All	2912/3048 (95%)	-0.09	30 (1%) 79 63	37, 82, 148, 204	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1075	TRP	3.3
1	B	1240	MET	3.3
1	B	1071	TYR	3.2
1	B	1239	TRP	3.2
1	B	388	TYR	3.2
1	A	1129	ALA	3.0
1	A	1387	LEU	3.0
1	A	1076	GLY	2.9
1	A	1239	TRP	2.7
1	B	500	VAL	2.7
1	A	193	TYR	2.6
1	B	1128	ASP	2.4
1	B	664	PHE	2.4
1	A	1071	TYR	2.3
1	A	285	LEU	2.3
1	B	457	ALA	2.2
1	B	436	PRO	2.2
1	B	1509	ALA	2.2
1	B	1074	CYS	2.2
1	A	1115	LEU	2.2
1	A	1241	ASP	2.2
1	A	355	ALA	2.1
1	A	150	SER	2.1
1	B	1432	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	426	ILE	2.1
1	B	928	GLY	2.1
1	B	1358	PRO	2.1
1	B	495	VAL	2.0
1	B	193	TYR	2.0
1	A	1360	PHE	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](#)

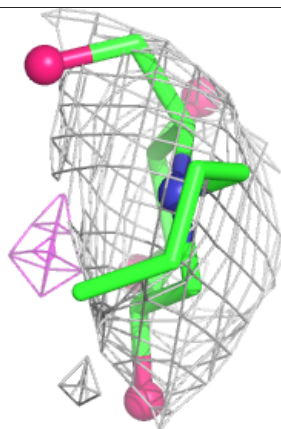
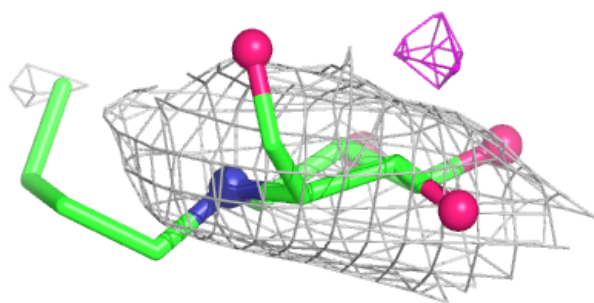
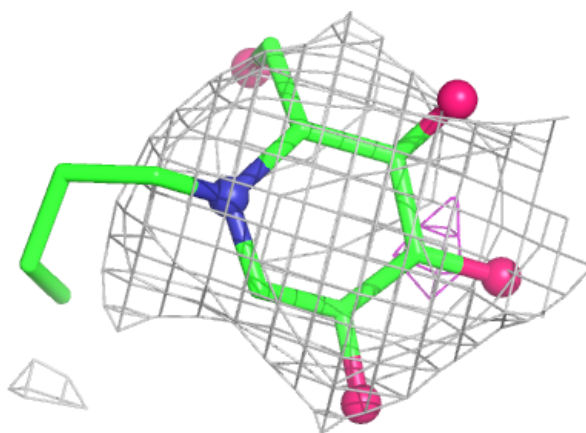
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NBV	A	1601	15/15	0.89	0.12	83,89,91,92	0
2	NBV	B	1601	15/15	0.96	0.11	75,82,86,88	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.

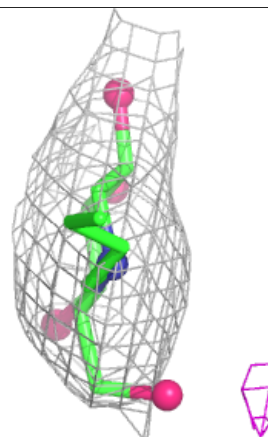
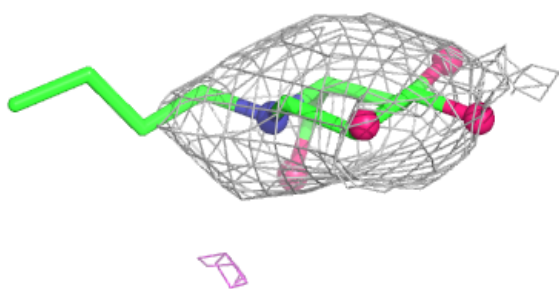
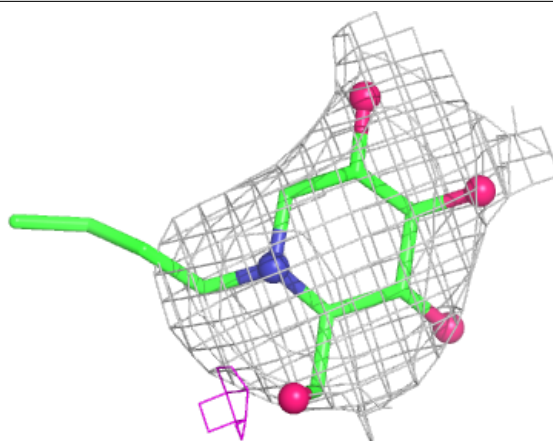
Electron density around NBV A 1601:

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



Electron density around NBV B 1601:

$2mF_o-DF_c$ (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.