Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 11:24 PM EDT

PDB ID	:	3TGS
Title	:	Crystal structure of HIV-1 clade C strain C1086 gp120 core in complex with NBD-556
Authors	:	Kwon, Y.D.; Kwong, P.D.
Deposited on	:	2011-08-17
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

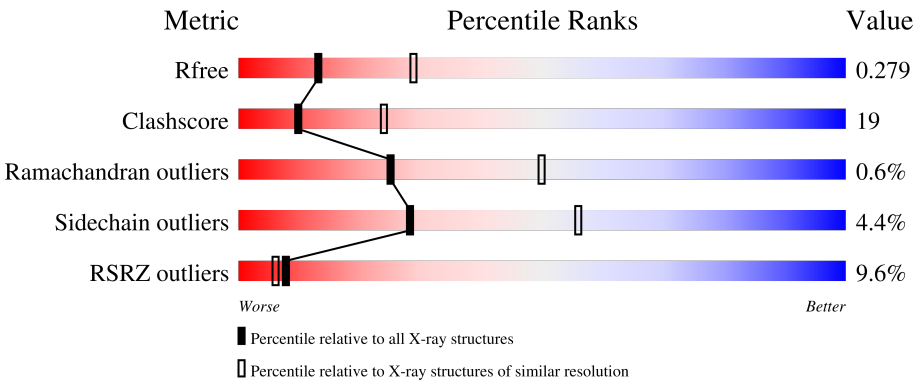
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	358	10% 62% 32%
1	B	358	9% 58% 36%

2 Entry composition (i)

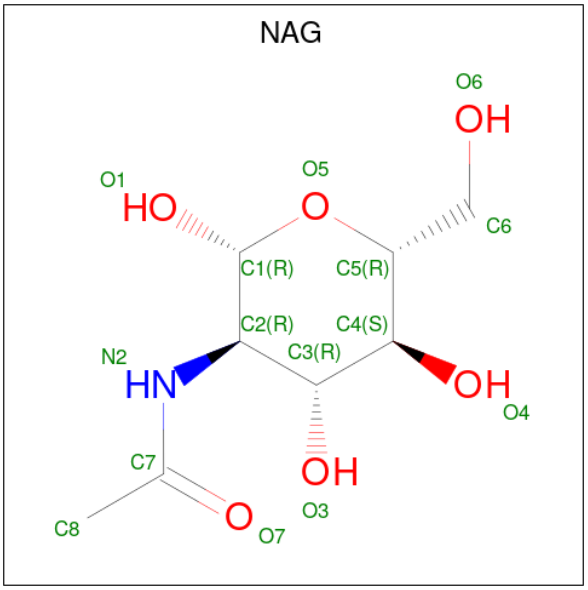
There are 4 unique types of molecules in this entry. The entry contains 5742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HIV-1 clade C1086 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	345	2705	1692	473	520	20	0	0	0
1	B	345	2705	1692	473	520	20	0	0	0

- 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
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

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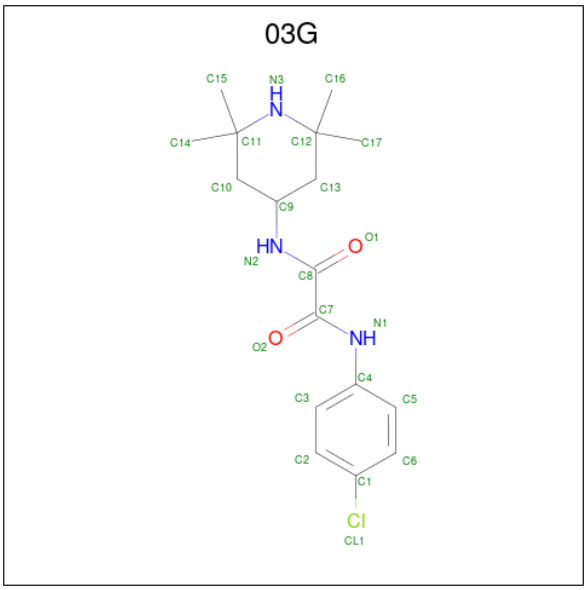
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0
2	B	1	14	8	1	5	0	0

- Molecule 3 is N-(4-chlorophenyl)-N'-(2,2,6,6-tetramethylpiperidin-4-yl)ethanediamide (three-letter code: 03G) (formula: $C_{17}H_{24}ClN_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	23	17	1	3	2	0	0
3	B	1	23	17	1	3	2	0	0

- Molecule 4 is water.

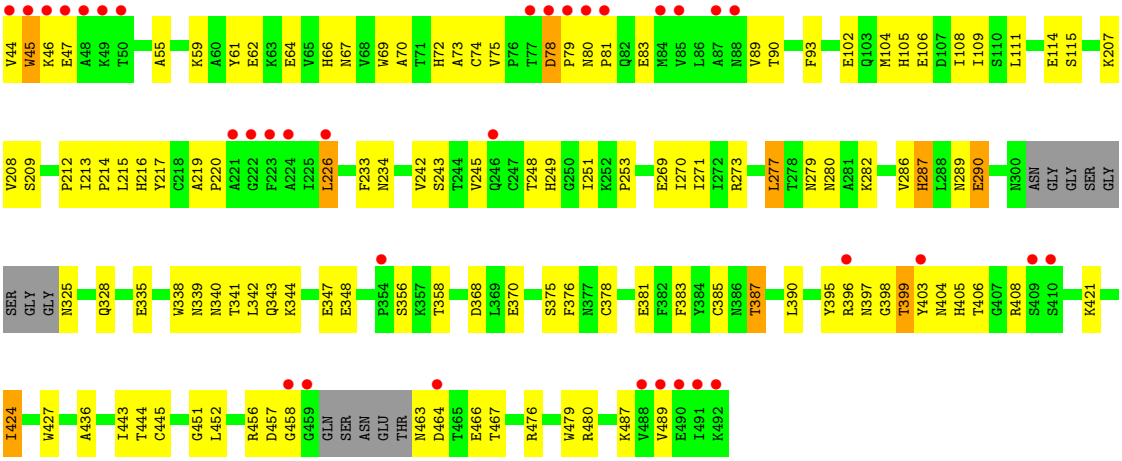
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	58	58	58	0	0
			Total	O		
4	B	46	46	46	0	0

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.

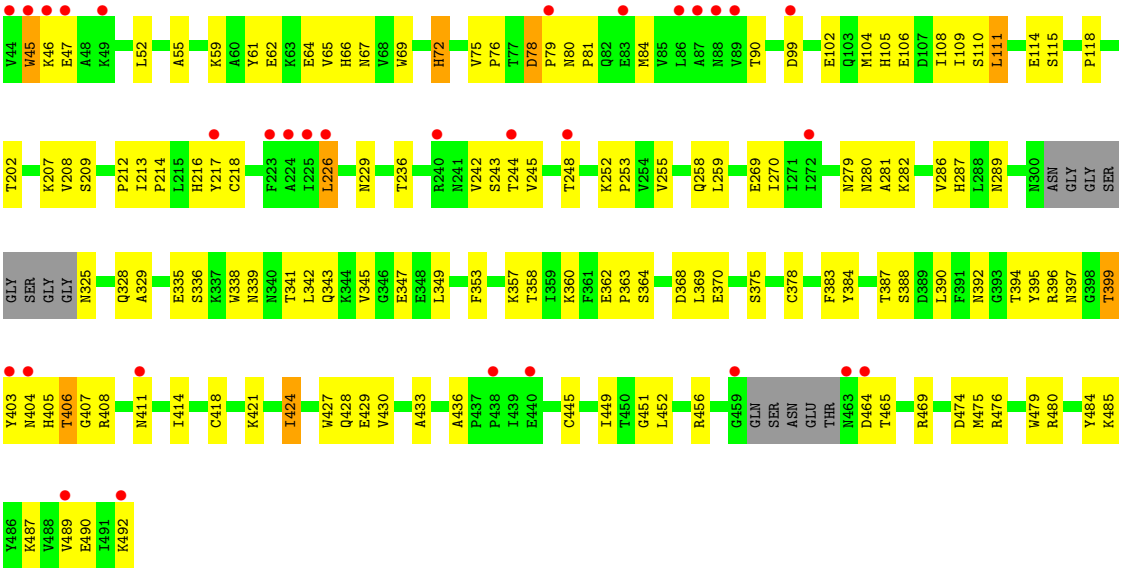
- Molecule 1: HIV-1 clade C1086 gp120 core

Chain A:



- Molecule 1: HIV-1 clade C1086 gp120 core

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	66.96Å 126.00Å 191.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.84 – 2.70 44.84 – 2.67	Depositor EDS
% Data completeness (in resolution range)	73.5 (44.84-2.70) 73.3 (44.84-2.67)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	8.62 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.239 , 0.295 0.229 , 0.279	Depositor DCC
R_{free} test set	861 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5742	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 03G

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	0.36	1/2762 (0.0%)	0.43	0/3746
1	B	0.23	0/2762	0.41	0/3746
All	All	0.30	1/5524 (0.0%)	0.42	0/7492

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	HIS	CG-ND1	-5.41	1.26	1.38

There are no bond angle outliers.

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	2705	0	2616	103	0
1	B	2705	0	2622	110	0
2	A	112	0	104	5	0
2	B	70	0	65	4	0
3	A	23	0	24	6	0
3	B	23	0	24	5	0
4	A	58	0	0	4	0
4	B	46	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5742	0	5455	213	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 19.

All (213) 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:64:GLU:HG2	1:A:209:SER:HB3	1.49	0.94
1:A:289:ASN:OD1	1:A:290:GLU:HB2	1.75	0.86
1:A:347:GLU:HG2	4:A:653:HOH:O	1.86	0.75
1:A:104:MET:O	1:A:108:ILE:HG12	1.87	0.73
1:A:335:GLU:OE2	1:A:408:ARG:HB3	1.88	0.72
1:B:405:HIS:CG	1:B:406:THR:H	2.04	0.72
1:B:104:MET:O	1:B:108:ILE:HG12	1.91	0.71
1:A:277:LEU:HD12	2:A:501:NAG:H81	1.74	0.70
1:A:405:HIS:CG	1:A:406:THR:H	2.11	0.69
1:A:325:ASN:HB3	1:A:328:GLN:HB2	1.73	0.69
1:B:411:ASN:HA	4:B:623:HOH:O	1.94	0.67
1:B:279:ASN:HD21	1:B:281:ALA:HB3	1.60	0.66
1:B:395:TYR:HD1	1:B:404:ASN:H	1.43	0.65
1:B:476:ARG:O	1:B:480:ARG:HG3	1.97	0.64
1:A:105:HIS:HD1	1:A:479:TRP:HZ3	1.45	0.64
1:A:456:ARG:NH1	1:A:458:GLY:HA2	2.12	0.64
1:B:395:TYR:CD1	1:B:403:TYR:HA	2.34	0.63
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.34	0.63
1:B:226:LEU:HD13	1:B:489:VAL:HG11	1.82	0.62
1:A:61:TYR:CE1	1:B:214:PRO:HG2	2.35	0.61
1:B:357:LYS:HG2	1:B:464:ASP:HA	1.81	0.61
1:B:46:LYS:O	1:B:489:VAL:HG23	2.01	0.61
1:A:395:TYR:CD1	1:A:403:TYR:HA	2.35	0.60
1:A:213:ILE:O	1:A:253:PRO:HD3	2.02	0.60
1:B:242:VAL:HG12	1:B:243:SER:H	1.66	0.60
1:A:59:LYS:HG2	1:A:61:TYR:OH	2.01	0.60
1:A:207:LYS:HE2	1:A:436:ALA:HB3	1.85	0.59
1:B:335:GLU:OE2	1:B:408:ARG:HB3	2.03	0.59
1:A:102:GLU:O	1:A:106:GLU:HG2	2.03	0.59
1:B:105:HIS:HD1	1:B:479:TRP:HZ3	1.50	0.59
1:A:279:ASN:HD22	1:A:282:LYS:HG2	1.68	0.58
1:A:424:ILE:HD12	3:A:507:03G:H3	1.85	0.58
1:A:46:LYS:O	1:A:489:VAL:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:TYR:HD1	1:B:403:TYR:HA	1.65	0.58
1:A:69:TRP:HA	1:A:72:HIS:CD2	2.37	0.58
1:B:207:LYS:HE2	1:B:436:ALA:HB3	1.86	0.58
1:B:406:THR:HG23	2:B:506:NAG:O6	2.03	0.58
1:B:405:HIS:CG	1:B:406:THR:N	2.72	0.58
1:B:286:VAL:HB	1:B:452:LEU:HB2	1.86	0.58
1:B:465:THR:HG23	1:B:465:THR:O	2.04	0.57
1:A:424:ILE:CD1	3:A:507:03G:H3	2.34	0.57
1:A:215:LEU:H	1:A:251:ILE:H	1.52	0.57
1:A:286:VAL:HB	1:A:452:LEU:HB2	1.86	0.57
1:B:358:THR:OG1	1:B:396:ARG:HD2	2.05	0.57
1:B:406:THR:HG21	2:B:506:NAG:C1	2.34	0.57
1:A:59:LYS:HG2	1:A:61:TYR:CZ	2.39	0.56
1:A:339:ASN:HA	1:A:403:TYR:CZ	2.40	0.56
1:B:339:ASN:HA	1:B:403:TYR:CZ	2.41	0.56
1:B:451:GLY:C	1:B:452:LEU:HD12	2.26	0.56
1:A:463:ASN:O	1:A:464:ASP:HB2	2.04	0.55
1:B:99:ASP:HA	1:B:102:GLU:OE1	2.07	0.55
1:A:476:ARG:O	1:A:480:ARG:HG3	2.07	0.54
1:B:484:TYR:CZ	1:B:485:LYS:HG3	2.43	0.54
1:B:78:ASP:HB2	1:B:81:PRO:HD3	1.89	0.54
1:B:370:GLU:HG3	1:B:384:TYR:CE2	2.42	0.54
1:A:342:LEU:HB2	1:A:403:TYR:HE2	1.73	0.54
1:A:280:ASN:ND2	1:A:457:ASP:O	2.37	0.54
1:A:105:HIS:ND1	1:A:479:TRP:HZ3	2.05	0.54
1:B:384:TYR:CE1	1:B:421:LYS:HB2	2.43	0.54
1:B:484:TYR:OH	1:B:485:LYS:HE3	2.08	0.53
1:A:69:TRP:HD1	1:A:114:GLU:OE1	1.91	0.53
1:A:78:ASP:N	1:A:79:PRO:HA	2.24	0.53
1:A:215:LEU:N	1:A:251:ILE:H	2.05	0.53
1:B:279:ASN:ND2	1:B:282:LYS:HG2	2.23	0.53
1:A:378:CYS:HB3	1:A:383:PHE:CE1	2.43	0.53
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.74	0.52
1:A:342:LEU:HB3	1:A:395:TYR:CE2	2.44	0.52
1:B:78:ASP:N	1:B:79:PRO:HA	2.24	0.52
1:A:226:LEU:HD13	1:A:489:VAL:HG11	1.90	0.52
1:B:335:GLU:HG2	1:B:414:ILE:HG13	1.91	0.52
1:B:102:GLU:O	1:B:106:GLU:HG2	2.10	0.52
1:B:279:ASN:HD22	1:B:282:LYS:HG2	1.74	0.51
1:A:358:THR:OG1	1:A:396:ARG:HD2	2.10	0.51
1:B:84:MET:HB2	1:B:244:THR:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:VAL:HG12	1:A:243:SER:H	1.75	0.51
1:A:72:HIS:CE1	1:A:73:ALA:HB2	2.46	0.51
1:A:269:GLU:O	1:A:271:ILE:HD12	2.11	0.51
1:B:64:GLU:HB2	1:B:67:ASN:HD22	1.74	0.51
1:A:456:ARG:HH12	1:A:458:GLY:HA2	1.76	0.51
1:A:47:GLU:HG2	1:A:487:LYS:HE3	1.93	0.50
1:A:405:HIS:CG	1:A:406:THR:N	2.79	0.50
1:A:398:GLY:HA2	4:A:653:HOH:O	2.11	0.50
1:A:451:GLY:C	1:A:452:LEU:HD12	2.32	0.50
1:A:89:VAL:HG13	4:A:624:HOH:O	2.11	0.50
1:B:105:HIS:O	1:B:109:ILE:HG13	2.11	0.50
1:B:370:GLU:HG3	1:B:384:TYR:HE2	1.77	0.50
1:B:378:CYS:HB3	1:B:383:PHE:CE1	2.46	0.50
1:B:343:GLN:O	1:B:347:GLU:HG3	2.12	0.49
1:B:64:GLU:HG2	1:B:209:SER:HB3	1.93	0.49
1:A:242:VAL:HG12	1:A:243:SER:N	2.28	0.49
1:A:273:ARG:NH2	1:A:287:HIS:ND1	2.50	0.49
1:A:67:ASN:ND2	1:A:213:ILE:HD11	2.28	0.49
1:B:242:VAL:HG12	1:B:243:SER:N	2.28	0.49
1:A:217:TYR:O	1:A:248:THR:HG23	2.13	0.48
1:A:368:ASP:HB3	1:A:370:GLU:OE1	2.13	0.48
1:A:395:TYR:HD1	1:A:404:ASN:H	1.59	0.48
1:B:338:TRP:CZ2	1:B:390:LEU:HG	2.48	0.48
1:B:216:HIS:HD2	1:B:248:THR:O	1.96	0.48
1:B:62:GLU:HG3	1:B:64:GLU:H	1.78	0.48
1:A:342:LEU:HB2	1:A:403:TYR:CE2	2.49	0.48
1:B:64:GLU:HB2	1:B:67:ASN:ND2	2.28	0.48
1:B:69:TRP:CB	1:B:111:LEU:HD13	2.43	0.48
1:B:339:ASN:HA	1:B:403:TYR:OH	2.13	0.47
1:A:340:ASN:O	1:A:344:LYS:HG3	2.14	0.47
1:A:375:SER:HA	1:A:383:PHE:O	2.14	0.47
1:B:280:ASN:HB2	1:B:456:ARG:O	2.14	0.47
1:A:270:ILE:HB	1:A:348:GLU:HG3	1.95	0.47
1:A:381:GLU:HG3	1:A:443:ILE:HD13	1.96	0.47
1:B:105:HIS:HA	1:B:479:TRP:CZ3	2.50	0.47
1:B:105:HIS:ND1	1:B:479:TRP:HZ3	2.11	0.47
1:B:349:LEU:O	1:B:353:PHE:HD2	1.97	0.47
1:A:249:HIS:O	1:A:251:ILE:HG13	2.14	0.47
1:B:69:TRP:HA	1:B:72:HIS:CD2	2.50	0.47
1:B:490:GLU:HG2	1:B:492:LYS:H	1.80	0.47
1:A:342:LEU:CB	1:A:403:TYR:HE2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:SER:O	1:B:392:ASN:HB2	2.15	0.47
1:A:343:GLN:O	1:A:347:GLU:HG3	2.15	0.46
1:A:387:THR:HG23	1:A:387:THR:O	2.14	0.46
1:B:427:TRP:CE2	1:B:428:GLN:HG3	2.50	0.46
3:B:502:03G:H14	3:B:502:03G:H23	1.97	0.46
1:A:69:TRP:CD1	1:A:111:LEU:HA	2.50	0.46
1:A:104:MET:HA	1:A:217:TYR:OH	2.16	0.46
1:A:216:HIS:HD2	1:A:248:THR:O	1.98	0.46
1:B:45:TRP:HB3	1:B:489:VAL:HG21	1.98	0.46
1:B:384:TYR:OH	1:B:424:ILE:HB	2.16	0.46
1:A:69:TRP:CB	1:A:111:LEU:HD13	2.45	0.46
1:A:269:GLU:HB3	2:A:504:NAG:H61	1.98	0.46
1:B:269:GLU:HA	1:B:289:ASN:HD22	1.81	0.46
1:B:55:ALA:HA	1:B:75:VAL:O	2.16	0.45
1:B:395:TYR:HB2	4:B:619:HOH:O	2.17	0.45
1:A:213:ILE:HG23	1:A:214:PRO:HD2	1.98	0.45
1:A:338:TRP:CZ2	1:A:390:LEU:HG	2.52	0.45
1:A:456:ARG:HD2	1:A:466:GLU:OE1	2.17	0.45
1:B:259:LEU:HD13	1:B:449:ILE:HD13	1.98	0.45
1:A:55:ALA:HA	1:A:75:VAL:O	2.17	0.45
1:A:234:ASN:ND2	2:A:501:NAG:O7	2.50	0.45
1:B:67:ASN:ND2	1:B:213:ILE:HD11	2.31	0.45
1:A:427:TRP:HB3	3:A:507:03G:C7	2.46	0.44
1:B:375:SER:HA	1:B:383:PHE:O	2.16	0.44
1:B:255:VAL:HG13	1:B:475:MET:SD	2.56	0.44
1:B:363:PRO:HG3	1:B:388:SER:HA	1.99	0.44
1:B:364:SER:HB3	4:B:622:HOH:O	2.17	0.44
1:A:376:PHE:HE1	1:A:385:CYS:SG	2.40	0.44
1:B:69:TRP:HD1	1:B:114:GLU:OE1	2.00	0.44
1:B:424:ILE:HD12	3:B:502:03G:H4	1.99	0.44
1:B:329:ALA:HB3	1:B:418:CYS:HB2	1.98	0.44
1:A:62:GLU:HG3	1:A:64:GLU:H	1.82	0.44
1:B:104:MET:HA	1:B:217:TYR:OH	2.18	0.44
1:B:368:ASP:HB3	1:B:370:GLU:OE1	2.17	0.44
1:B:75:VAL:HG13	1:B:76:PRO:HD2	2.00	0.44
1:B:226:LEU:HD13	1:B:489:VAL:CG1	2.47	0.44
1:A:105:HIS:O	1:A:109:ILE:HG13	2.17	0.44
1:A:370:GLU:HG2	3:A:507:03G:H5	1.83	0.44
1:B:396:ARG:H	1:B:399:THR:HG22	1.83	0.44
1:A:396:ARG:O	1:A:399:THR:HG22	2.17	0.43
1:B:65:VAL:HG13	1:B:208:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASP:CB	1:B:81:PRO:HD3	2.47	0.43
1:B:258:GLN:OE1	1:B:387:THR:HG21	2.18	0.43
1:A:208:VAL:HG22	1:A:209:SER:N	2.33	0.43
1:B:406:THR:HG21	2:B:506:NAG:O5	2.18	0.43
1:A:399:THR:HG23	1:A:403:TYR:N	2.33	0.43
1:B:325:ASN:HB3	1:B:328:GLN:HB2	1.99	0.43
1:B:342:LEU:CB	1:B:403:TYR:HE1	2.32	0.43
1:B:362:GLU:O	1:B:469:ARG:HA	2.18	0.43
1:A:78:ASP:HB2	1:A:80:ASN:N	2.33	0.43
1:A:108:ILE:HD12	1:A:253:PRO:HB3	2.01	0.43
1:B:270:ILE:HG23	1:B:287:HIS:O	2.19	0.43
1:B:52:LEU:HG	1:B:218:CYS:O	2.18	0.43
1:A:61:TYR:CD1	1:B:214:PRO:HG2	2.53	0.43
1:A:69:TRP:CG	1:A:111:LEU:HD13	2.53	0.43
1:B:279:ASN:ND2	1:B:281:ALA:HB3	2.32	0.43
1:B:360:LYS:HG2	1:B:394:THR:HB	2.00	0.43
1:A:70:ALA:O	1:A:74:CYS:N	2.52	0.42
1:B:396:ARG:O	1:B:399:THR:HG22	2.19	0.42
1:B:430:VAL:HG22	3:B:502:03G:H20	2.00	0.42
1:A:421:LYS:HB3	1:A:421:LYS:HE2	1.79	0.42
1:B:66:HIS:CE1	1:B:212:PRO:HA	2.54	0.42
1:B:69:TRP:HB3	1:B:111:LEU:HD13	2.01	0.42
1:B:59:LYS:HB3	1:B:61:TYR:CE2	2.55	0.42
1:B:229:ASN:OD1	1:B:243:SER:HB2	2.20	0.42
1:B:445:CYS:SG	2:B:503:NAG:H83	2.59	0.42
1:B:217:TYR:O	1:B:248:THR:HG23	2.19	0.42
1:B:474:ASP:HB2	3:B:502:03G:H15	2.02	0.42
2:A:504:NAG:O3	2:A:504:NAG:C7	2.68	0.41
1:B:78:ASP:HB2	1:B:80:ASN:N	2.35	0.41
1:A:78:ASP:HB2	1:A:81:PRO:HD3	2.01	0.41
1:A:64:GLU:HB2	1:A:67:ASN:HD22	1.85	0.41
1:A:395:TYR:HD1	1:A:403:TYR:HA	1.81	0.41
1:B:111:LEU:HD12	1:B:115:SER:OG	2.21	0.41
1:B:252:LYS:HA	1:B:253:PRO:HD3	1.80	0.41
1:A:289:ASN:OD1	1:A:290:GLU:N	2.52	0.41
1:A:83:GLU:HG2	1:A:245:VAL:CG1	2.50	0.41
1:B:427:TRP:HB3	3:B:502:03G:C7	2.51	0.41
1:A:339:ASN:HA	1:A:403:TYR:OH	2.20	0.41
1:A:405:HIS:C	1:A:408:ARG:NH2	2.74	0.41
1:B:396:ARG:HG2	1:B:397:ASN:N	2.36	0.41
1:B:369:LEU:HB3	1:B:384:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:HA	1:A:220:PRO:HD3	1.94	0.41
1:B:118:PRO:HB3	1:B:433:ALA:HB1	2.03	0.41
1:B:212:PRO:HB3	1:B:253:PRO:HD2	2.03	0.41
1:B:341:THR:O	1:B:345:VAL:HG23	2.21	0.41
1:A:45:TRP:HB3	1:A:489:VAL:HG21	2.03	0.41
1:A:80:ASN:HB2	4:A:634:HOH:O	2.21	0.41
1:A:376:PHE:HA	3:A:507:03G:CL1	2.57	0.41
1:A:427:TRP:HA	3:A:507:03G:C13	2.51	0.41
1:A:66:HIS:CE1	1:A:212:PRO:HA	2.56	0.40
1:A:335:GLU:HB2	2:A:505:NAG:H62	2.04	0.40
1:B:429:GLU:HG2	1:B:430:VAL:N	2.35	0.40
1:A:396:ARG:HG2	1:A:397:ASN:N	2.35	0.40
1:B:47:GLU:HG2	1:B:487:LYS:HE3	2.03	0.40
1:B:476:ARG:HB2	1:B:480:ARG:NH1	2.37	0.40
1:A:105:HIS:HA	1:A:479:TRP:CZ3	2.57	0.40
1:B:421:LYS:HB3	1:B:421:LYS:HE2	1.82	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	339/358 (95%)	305 (90%)	31 (9%)	3 (1%)	17 40
1	B	339/358 (95%)	306 (90%)	32 (9%)	1 (0%)	41 66
All	All	678/716 (95%)	611 (90%)	63 (9%)	4 (1%)	25 50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	SER
1	A	115	SER

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Mol	Chain	Res	Type
1	A	341	THR
1	B	407	GLY

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	304/312 (97%)	291 (96%)	13 (4%)	29	57
1	B	304/312 (97%)	290 (95%)	14 (5%)	27	54
All	All	608/624 (97%)	581 (96%)	27 (4%)	28	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	45	TRP
1	A	78	ASP
1	A	90	THR
1	A	226	LEU
1	A	277	LEU
1	A	290	GLU
1	A	387	THR
1	A	399	THR
1	A	424	ILE
1	A	444	THR
1	A	445	CYS
1	A	467	THR
1	B	45	TRP
1	B	72	HIS
1	B	78	ASP
1	B	90	THR
1	B	110	SER
1	B	111	LEU
1	B	202	THR
1	B	226	LEU

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Mol	Chain	Res	Type
1	B	236	THR
1	B	245	VAL
1	B	336	SER
1	B	399	THR
1	B	406	THR
1	B	424	ILE

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

Mol	Chain	Res	Type
1	A	67	ASN
1	A	203	GLN
1	A	216	HIS
1	A	229	ASN
1	A	230	ASN
1	A	279	ASN
1	A	417	GLN
1	B	67	ASN
1	B	216	HIS
1	B	279	ASN
1	B	300	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	B	503	1	14,14,15	0.28	0	17,19,21	0.56	0
2	NAG	A	501	-	14,14,15	0.28	0	17,19,21	0.57	0
2	NAG	B	506	1	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	A	502	1	14,14,15	0.30	0	17,19,21	0.76	0
3	03G	A	507	-	24,24,24	2.79	7 (29%)	36,36,36	2.27	15 (41%)
2	NAG	A	508	1	14,14,15	0.26	0	17,19,21	0.50	0
2	NAG	A	506	1	14,14,15	0.37	0	17,19,21	1.02	1 (5%)
2	NAG	A	504	1	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	A	509	1	14,14,15	0.27	0	17,19,21	0.84	1 (5%)
2	NAG	A	503	1	14,14,15	0.34	0	17,19,21	0.57	0
2	NAG	B	505	1	14,14,15	0.29	0	17,19,21	0.64	0
3	03G	B	502	-	24,24,24	2.72	7 (29%)	36,36,36	1.97	11 (30%)
2	NAG	B	501	1	14,14,15	0.33	0	17,19,21	0.51	0
2	NAG	B	504	1	14,14,15	0.30	0	17,19,21	0.62	0
2	NAG	A	505	1	14,14,15	0.29	0	17,19,21	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	503	1	-	2/6/23/26	0/1/1/1
2	NAG	A	501	-	-	4/6/23/26	0/1/1/1
2	NAG	B	506	1	-	3/6/23/26	0/1/1/1
2	NAG	A	502	1	-	2/6/23/26	0/1/1/1
3	03G	A	507	-	-	1/12/28/28	0/2/2/2
2	NAG	A	508	1	-	3/6/23/26	0/1/1/1
2	NAG	A	506	1	-	2/6/23/26	0/1/1/1
2	NAG	A	504	1	-	5/6/23/26	0/1/1/1
2	NAG	A	509	1	-	2/6/23/26	0/1/1/1
2	NAG	A	503	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	505	1	-	3/6/23/26	0/1/1/1
3	03G	B	502	-	-	2/12/28/28	0/2/2/2
2	NAG	B	501	1	-	2/6/23/26	0/1/1/1
2	NAG	B	504	1	-	3/6/23/26	0/1/1/1
2	NAG	A	505	1	-	4/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	507	03G	C1-CL1	-10.75	1.49	1.74
3	B	502	03G	C1-CL1	-9.98	1.51	1.74
3	B	502	03G	C7-N1	4.00	1.43	1.35
3	A	507	03G	C7-N1	3.77	1.43	1.35
3	B	502	03G	C8-C7	3.76	1.61	1.53
3	A	507	03G	C13-C12	3.42	1.57	1.53
3	A	507	03G	C8-C7	3.21	1.60	1.53
3	B	502	03G	C8-N2	2.95	1.40	1.34
3	A	507	03G	C8-N2	2.85	1.40	1.34
3	B	502	03G	C4-N1	2.80	1.47	1.41
3	B	502	03G	C10-C11	2.66	1.56	1.53
3	A	507	03G	C4-N1	2.45	1.46	1.41
3	B	502	03G	O2-C7	-2.18	1.19	1.23
3	A	507	03G	O2-C7	-2.17	1.19	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	507	03G	C12-C13-C9	5.17	116.43	112.41
3	A	507	03G	C6-C1-C2	-5.07	114.96	121.24
3	B	502	03G	C6-C1-C2	-4.94	115.12	121.24
3	B	502	03G	C8-C7-N1	4.13	119.23	112.25
3	B	502	03G	C5-C6-C1	4.04	123.31	119.24
3	A	507	03G	C8-C7-N1	4.02	119.04	112.25
3	A	507	03G	C5-C6-C1	3.73	122.99	119.24
3	A	507	03G	C3-C2-C1	3.49	122.76	119.24
3	A	507	03G	C13-C12-N3	3.26	116.40	110.42
3	A	507	03G	C5-C4-C3	-3.21	114.78	119.04
3	A	507	03G	C6-C1-CL1	3.00	123.78	119.36
3	B	502	03G	C3-C2-C1	2.99	122.25	119.24
3	B	502	03G	O2-C7-C8	-2.94	116.45	121.24
3	B	502	03G	C5-C4-C3	-2.93	115.15	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	507	03G	O2-C7-C8	-2.83	116.63	121.24
3	B	502	03G	C15-C11-C10	-2.80	106.97	110.06
3	A	507	03G	C17-C12-C13	-2.79	106.98	110.06
3	B	502	03G	C6-C1-CL1	2.61	123.21	119.36
2	A	506	NAG	O5-C1-C2	-2.54	107.36	111.29
3	A	507	03G	C11-C10-C9	-2.48	110.49	112.41
3	B	502	03G	C10-C11-N3	2.42	114.85	110.42
2	A	509	NAG	O5-C1-C2	-2.41	107.57	111.29
3	A	507	03G	C4-N1-C7	-2.33	123.31	127.45
3	B	502	03G	C2-C3-C4	2.30	122.95	120.30
3	B	502	03G	C12-N3-C11	-2.26	116.14	118.98
3	A	507	03G	C12-N3-C11	-2.25	116.14	118.98
3	A	507	03G	C15-C11-C10	-2.22	107.60	110.06
3	A	507	03G	C2-C3-C4	2.17	122.80	120.30

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAG	O7-C7-N2-C2
2	A	502	NAG	C8-C7-N2-C2
2	A	502	NAG	O7-C7-N2-C2
2	A	504	NAG	C3-C2-N2-C7
2	A	504	NAG	C8-C7-N2-C2
2	A	504	NAG	O7-C7-N2-C2
2	A	505	NAG	C8-C7-N2-C2
2	A	508	NAG	C8-C7-N2-C2
2	A	508	NAG	O7-C7-N2-C2
2	A	509	NAG	C8-C7-N2-C2
2	A	509	NAG	O7-C7-N2-C2
2	B	501	NAG	C8-C7-N2-C2
2	B	501	NAG	O7-C7-N2-C2
2	B	503	NAG	C8-C7-N2-C2
2	B	503	NAG	O7-C7-N2-C2
2	B	505	NAG	C8-C7-N2-C2
2	B	505	NAG	O7-C7-N2-C2
2	B	506	NAG	C8-C7-N2-C2
2	B	506	NAG	O7-C7-N2-C2
2	A	501	NAG	C8-C7-N2-C2
2	A	501	NAG	O5-C5-C6-O6
2	A	505	NAG	O7-C7-N2-C2
2	A	505	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	501	NAG	C4-C5-C6-O6
2	A	505	NAG	C4-C5-C6-O6
2	A	503	NAG	C8-C7-N2-C2
2	A	503	NAG	O7-C7-N2-C2
2	A	506	NAG	C8-C7-N2-C2
2	B	504	NAG	C8-C7-N2-C2
2	B	504	NAG	O7-C7-N2-C2
2	A	506	NAG	O7-C7-N2-C2
2	A	504	NAG	O5-C5-C6-O6
3	A	507	03G	O1-C8-N2-C9
3	B	502	03G	C10-C9-N2-C8
2	B	504	NAG	O5-C5-C6-O6
2	B	505	NAG	C3-C2-N2-C7
2	A	508	NAG	O5-C5-C6-O6
2	B	506	NAG	C1-C2-N2-C7
2	A	504	NAG	C4-C5-C6-O6
3	B	502	03G	C13-C9-N2-C8

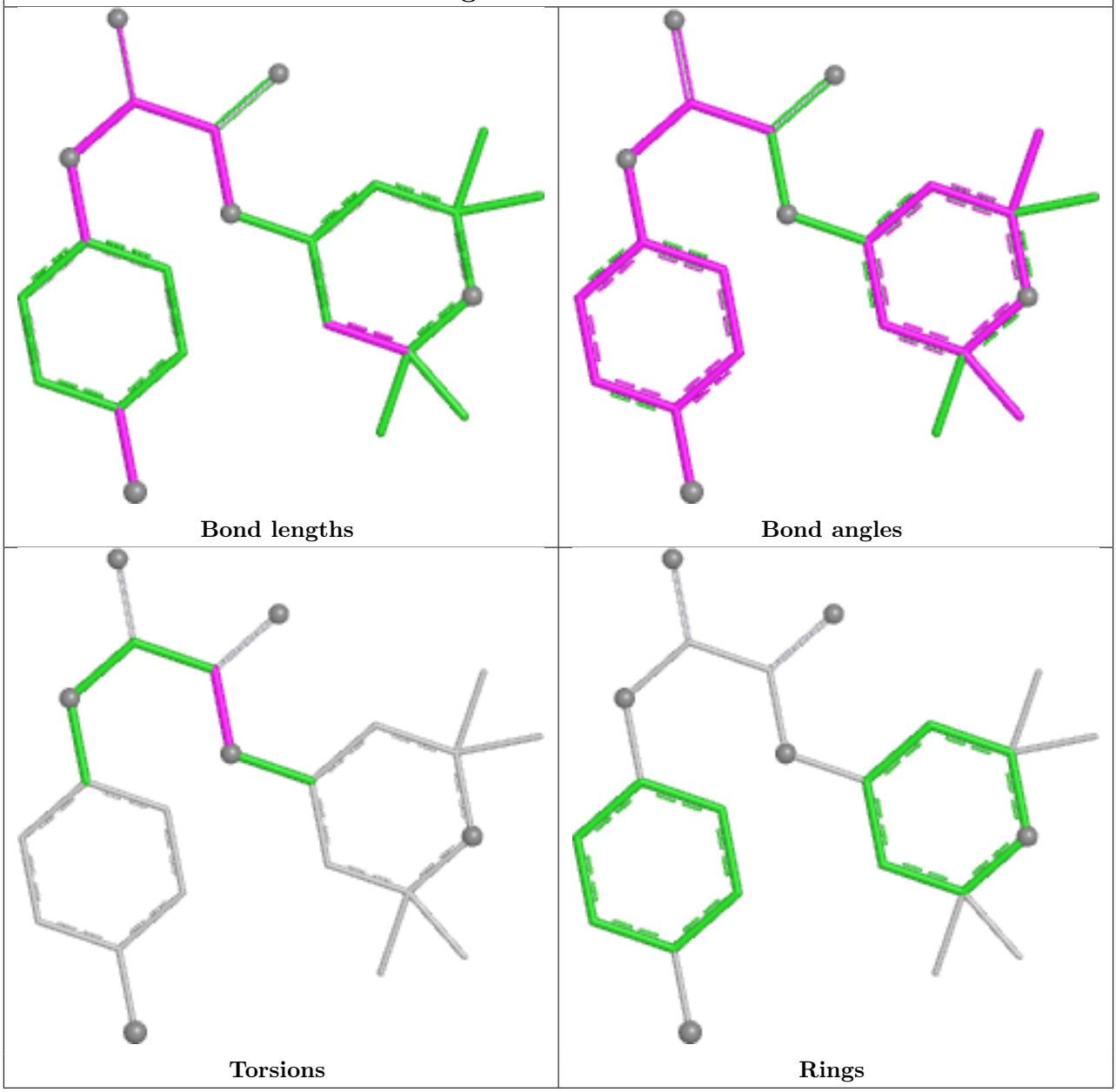
There are no ring outliers.

7 monomers are involved in 20 short contacts:

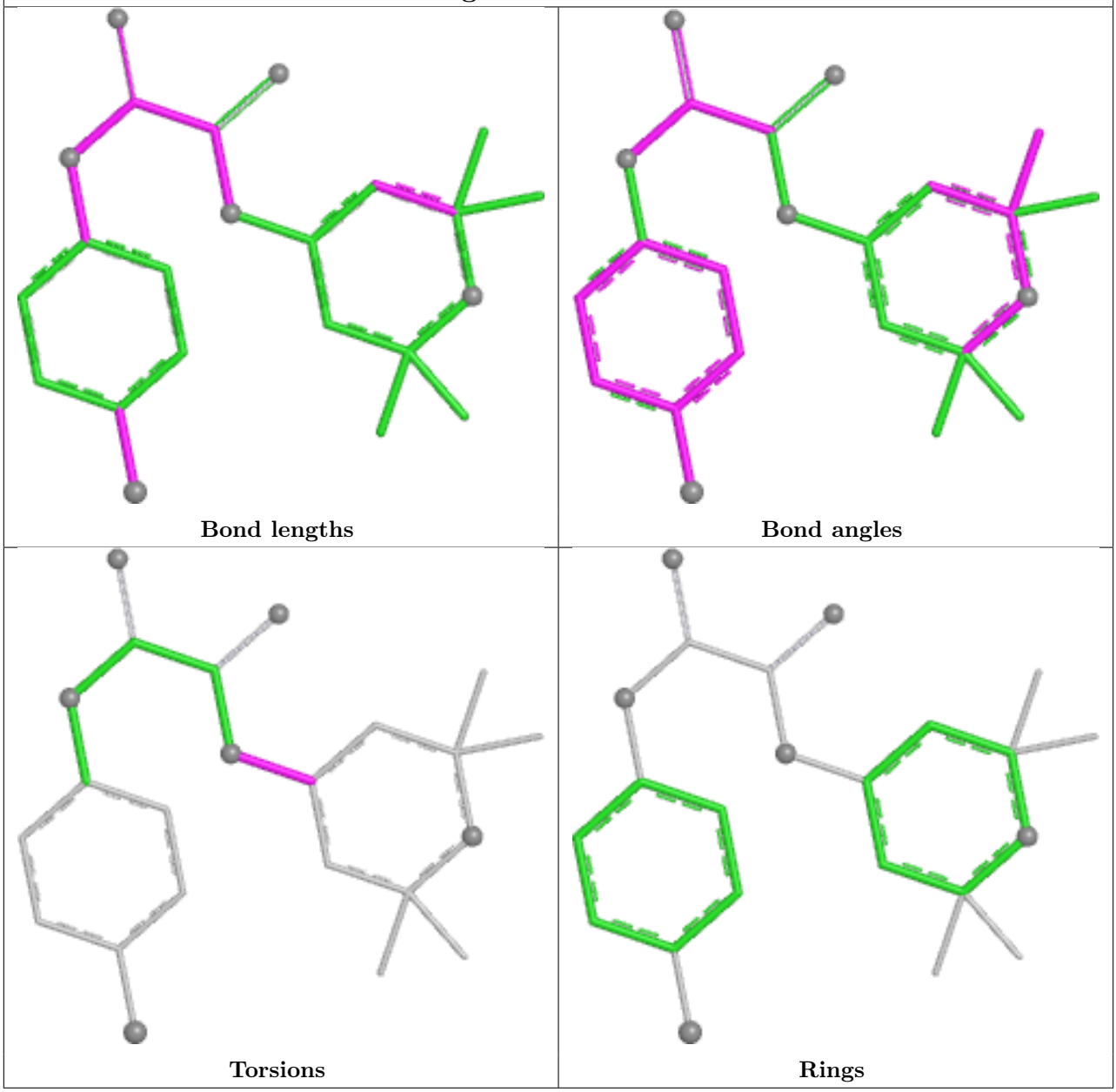
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	NAG	1	0
2	A	501	NAG	2	0
2	B	506	NAG	3	0
3	A	507	03G	6	0
2	A	504	NAG	2	0
3	B	502	03G	5	0
2	A	505	NAG	1	0

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 03G A 507



Ligand 03G B 502



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	345/358 (96%)	0.41	35 (10%)	7	5	20, 56, 148, 235	0
1	B	345/358 (96%)	0.57	31 (8%)	9	7	34, 73, 146, 252	0
All	All	690/716 (96%)	0.49	66 (9%)	8	6	20, 65, 148, 252	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	VAL	22.8
1	B	45	TRP	15.3
1	A	48	ALA	12.3
1	B	46	LYS	9.5
1	A	44	VAL	9.4
1	A	87	ALA	8.0
1	A	492	LYS	7.2
1	A	46	LYS	6.2
1	A	403	TYR	5.7
1	A	489	VAL	5.3
1	A	458	GLY	5.2
1	B	459	GLY	5.1
1	B	224	ALA	4.8
1	B	492	LYS	4.8
1	A	491	ILE	4.7
1	B	47	GLU	4.5
1	A	488	VAL	4.5
1	A	45	TRP	4.3
1	B	403	TYR	4.2
1	B	87	ALA	4.2
1	B	86	LEU	4.1
1	A	410	SER	4.1
1	A	78	ASP	4.1
1	A	464	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	225	ILE	3.8
1	A	88	ASN	3.7
1	B	464	ASP	3.6
1	A	354	PRO	3.5
1	B	411	ASN	3.4
1	B	244	THR	3.3
1	B	404	ASN	3.3
1	B	88	ASN	3.3
1	A	224	ALA	3.3
1	A	47	GLU	3.1
1	A	77	THR	3.1
1	B	226	LEU	3.1
1	A	490	GLU	3.1
1	A	80	ASN	3.0
1	B	489	VAL	3.0
1	A	459	GLY	3.0
1	B	79	PRO	2.9
1	A	222	GLY	2.9
1	A	226	LEU	2.8
1	B	89	VAL	2.8
1	A	223	PHE	2.7
1	B	49	LYS	2.7
1	B	272	ILE	2.7
1	B	463	ASN	2.6
1	B	83	GLU	2.6
1	A	396	ARG	2.6
1	A	221	ALA	2.5
1	B	217	TYR	2.5
1	A	50	THR	2.5
1	B	99	ASP	2.5
1	A	49	LYS	2.4
1	A	84	MET	2.4
1	B	248	THR	2.3
1	B	438	PRO	2.2
1	B	240	ARG	2.2
1	A	79	PRO	2.2
1	A	85	VAL	2.2
1	A	81	PRO	2.2
1	A	409	SER	2.1
1	B	223	PHE	2.1
1	B	440	GLU	2.1
1	A	246	GLN	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

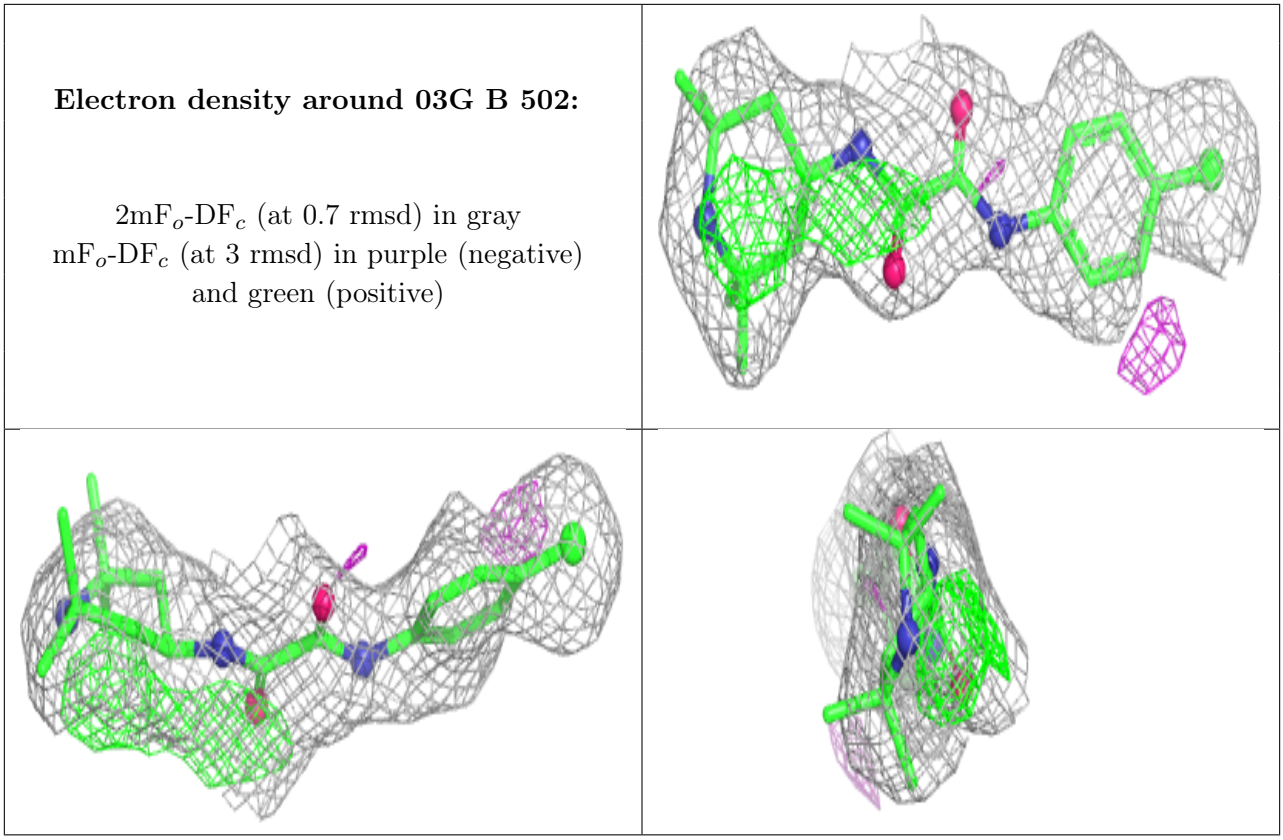
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	509	14/15	0.69	0.37	105,113,126,126	0
2	NAG	A	504	14/15	0.70	0.32	63,73,85,85	0
2	NAG	A	505	14/15	0.74	0.39	37,68,88,100	0
2	NAG	B	501	14/15	0.76	0.29	57,100,109,110	0
2	NAG	B	505	14/15	0.80	0.24	54,80,85,89	0
2	NAG	A	501	14/15	0.83	0.25	93,99,107,108	0
2	NAG	B	506	14/15	0.85	0.19	67,78,88,88	0
2	NAG	B	504	14/15	0.89	0.17	57,67,85,88	0
2	NAG	A	506	14/15	0.90	0.16	47,55,71,72	0
2	NAG	A	503	14/15	0.90	0.15	60,62,66,68	0
3	03G	B	502	23/23	0.91	0.21	30,50,77,112	0
2	NAG	B	503	14/15	0.92	0.20	57,62,71,73	0
2	NAG	A	508	14/15	0.94	0.17	32,39,54,56	0
3	03G	A	507	23/23	0.95	0.16	5,26,39,96	0
2	NAG	A	502	14/15	0.97	0.18	31,40,54,56	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.

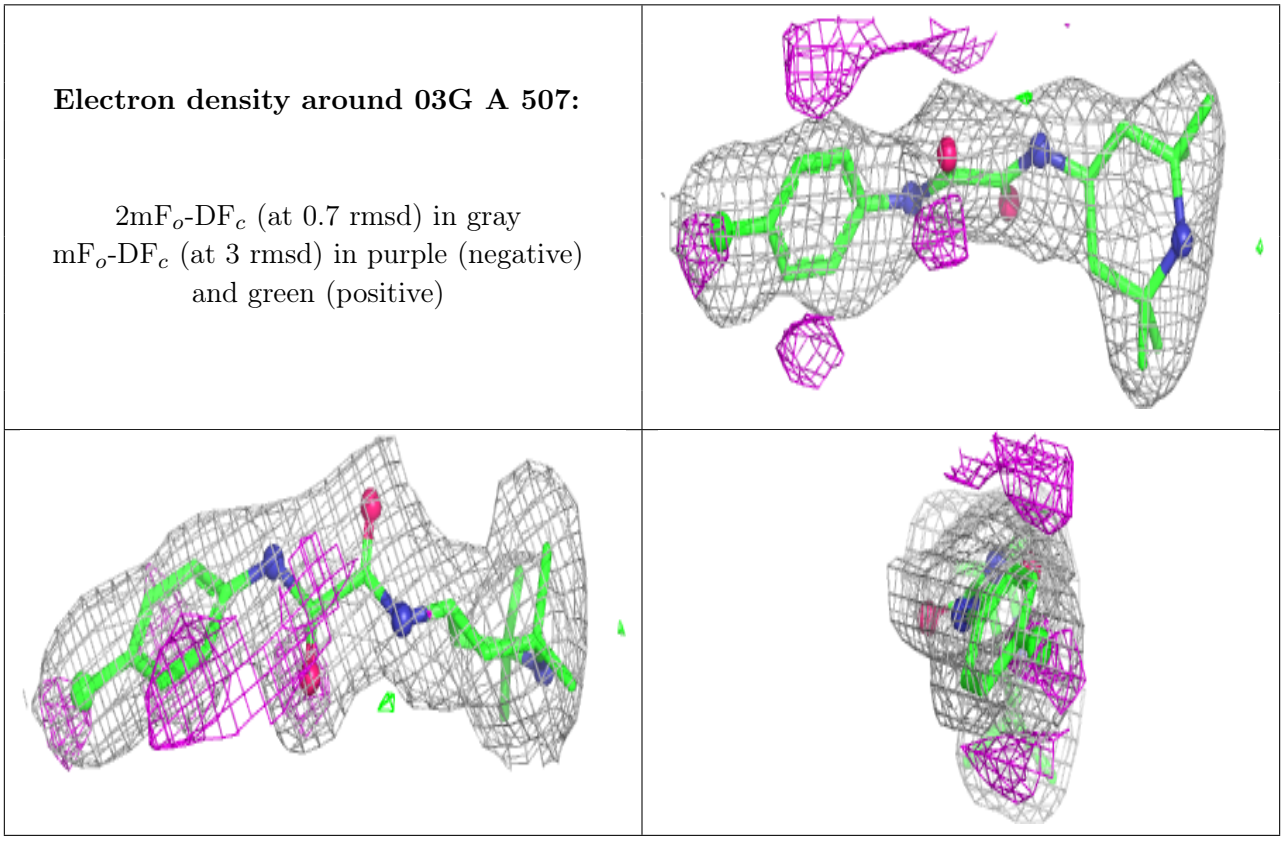
Electron density around 03G B 502:

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



Electron density around 03G A 507:

$2mF_o$-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.