



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:57 pm BST

PDB ID : 6AE3
Title : Crystal structure of GSK3beta complexed with Morin
Authors : Kim, K.L.; Cha, J.S.; Kim, J.S.; Ahn, J.S.; Ha, N.C.; Cho, H.S.
Deposited on : 2018-08-03
Resolution : 2.14 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

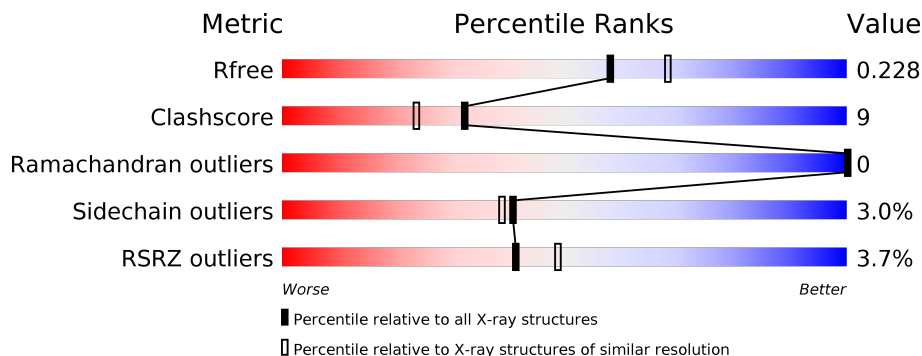
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 on 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	420	<p>2% 74% 8% 17%</p>
1	B	420	<p>2% 73% 8% 18%</p>
1	C	420	<p>3% 59% 19% 21%</p>
1	D	420	<p>5% 63% 14% 21%</p>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	502	-	-	X	-
3	GOL	C	501	-	-	X	-
3	GOL	D	501	-	-	X	-

2 Entry composition [i](#)

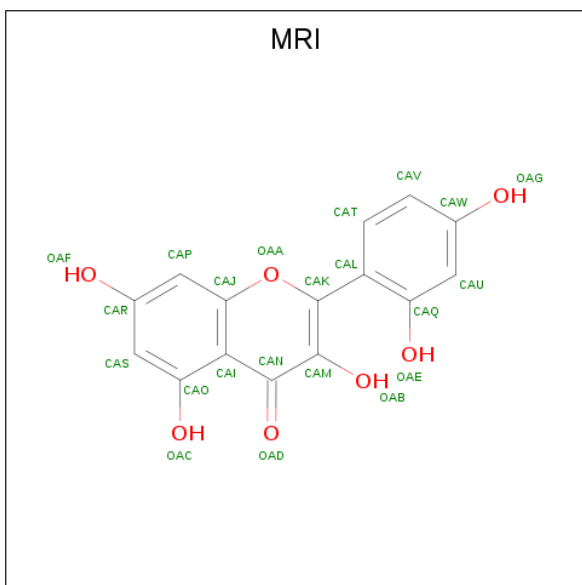
There are 4 unique types of molecules in this entry. The entry contains 10953 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 synthase kinase-3 beta.

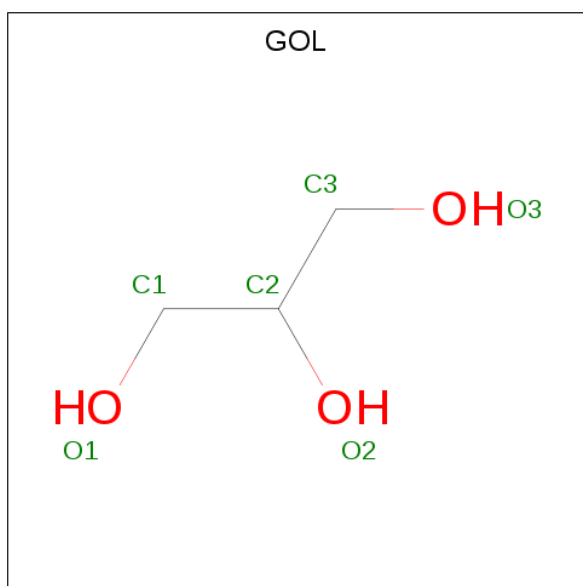
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	348	Total 2698	C 1736	N 455	O 495	P 1	S 11	0	0	0
1	B	344	Total 2666	C 1717	N 452	O 485	P 1	S 11	0	0	0
1	C	332	Total 2542	C 1640	N 425	O 465	P 1	S 11	0	0	0
1	D	333	Total 2557	C 1658	N 424	O 463	P 1	S 11	0	0	0

- Molecule 2 is 2-[2,4-bis(oxidanyl)phenyl]-3,5,7-tris(oxidanyl)chromen-4-one (three-letter code: MRI) (formula: C₁₅H₁₀O₇) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 22	C 15	O 7	0	0
2	B	1	Total 22	C 15	O 7	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

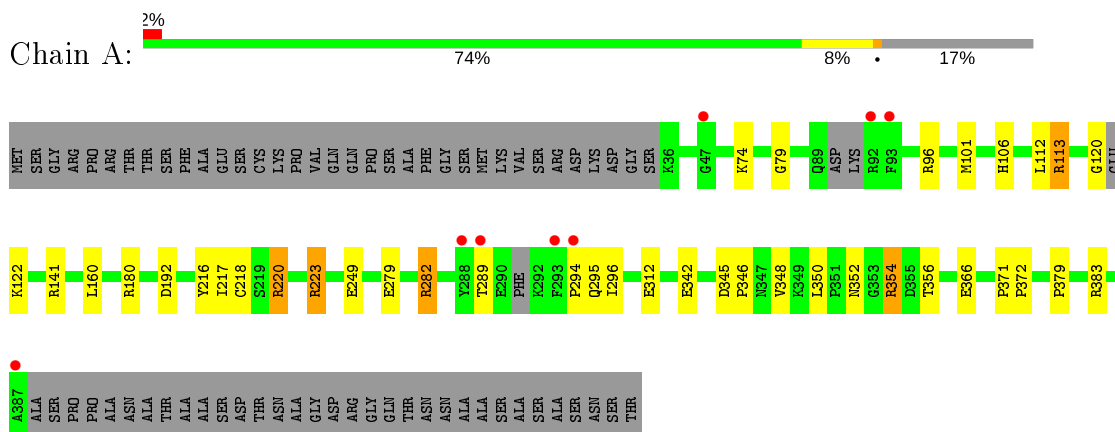
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	173	Total O 173 173	0	0
4	B	153	Total O 153 153	0	0
4	C	47	Total O 47 47	0	0
4	D	49	Total O 49 49	0	0

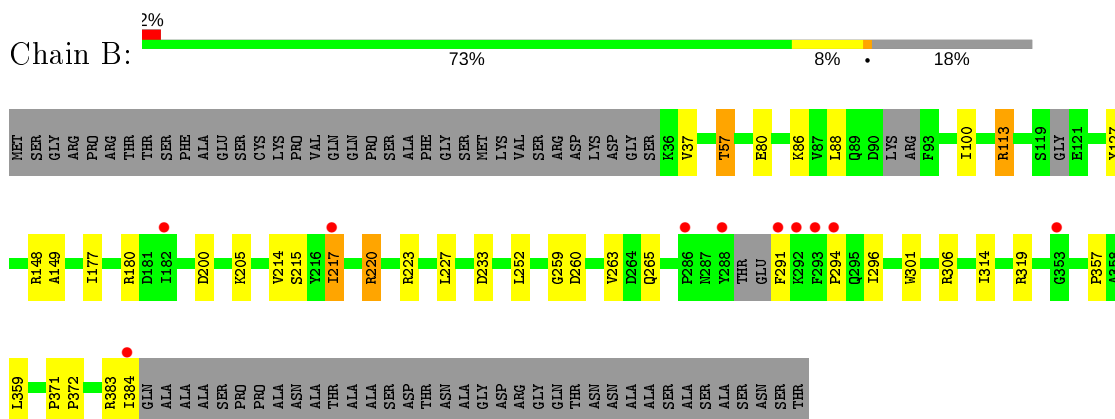
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

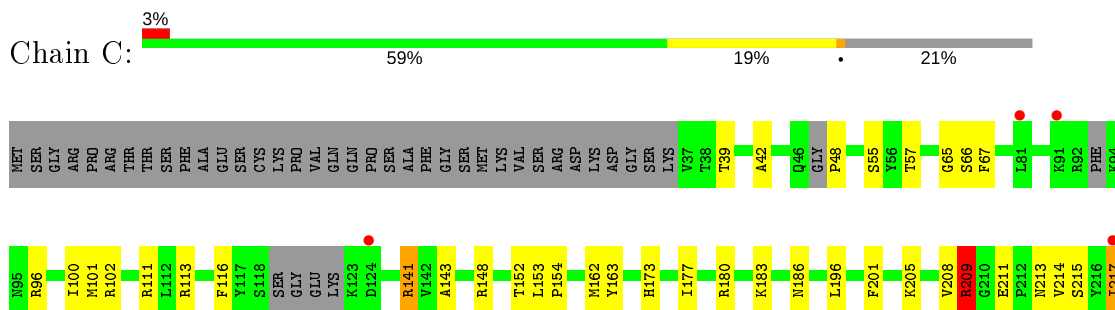
- Molecule 1: Glycogen synthase kinase-3 beta

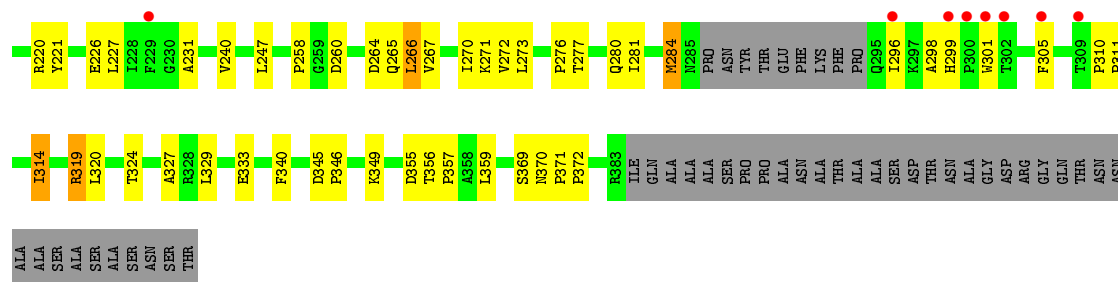


- Molecule 1: Glycogen synthase kinase-3 beta

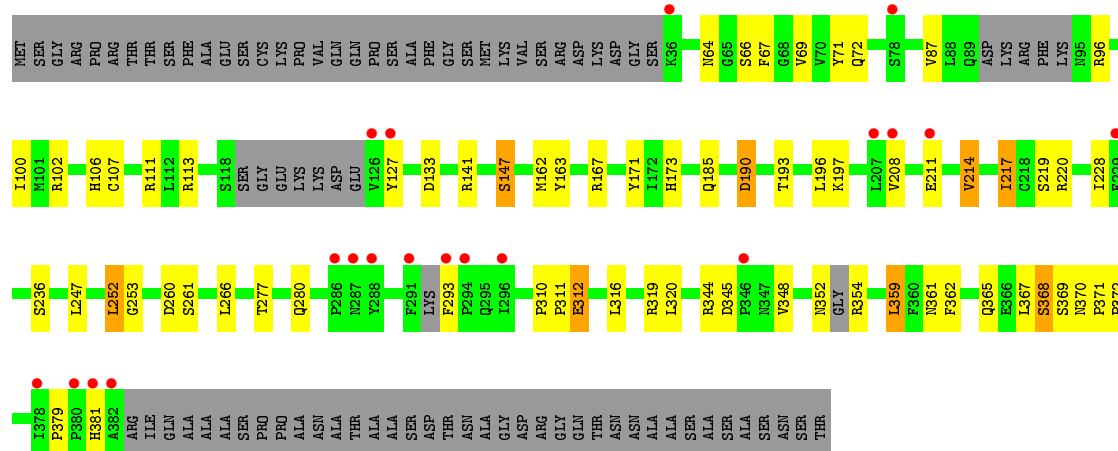


- Molecule 1: Glycogen synthase kinase-3 beta





- Molecule 1: Glycogen synthase kinase-3 beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.59Å 134.36Å 100.39Å 90.00° 103.80° 90.00°	Depositor
Resolution (Å)	40.00 – 2.14 37.00 – 2.14	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.00-2.14) 97.7 (37.00-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 2.14Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.191 , 0.226 0.194 , 0.228	Depositor DCC
R_{free} test set	4608 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10953	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: GOL, MRI, PTR

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	0.65	2/2745 (0.1%)	0.80	4/3747 (0.1%)
1	B	0.60	0/2714	0.75	2/3707 (0.1%)
1	C	0.50	0/2585	0.66	0/3533
1	D	0.52	0/2605	0.66	0/3563
All	All	0.58	2/10649 (0.0%)	0.72	6/14550 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	7
1	D	0	4
All	All	0	19

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	CYS	N-CA	5.58	1.57	1.46
1	A	249	GLU	CD-OE1	5.15	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ARG	NE-CZ-NH1	-11.06	114.77	120.30
1	B	220	ARG	NE-CZ-NH1	-10.01	115.29	120.30
1	A	220	ARG	NE-CZ-NH1	-9.61	115.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	B	223	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	180	ARG	NE-CZ-NH2	-5.33	117.63	120.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	223	ARG	Sidechain
1	A	282	ARG	Sidechain
1	A	96	ARG	Sidechain
1	B	113	ARG	Sidechain
1	B	148	ARG	Sidechain
1	B	220	ARG	Sidechain
1	B	383	ARG	Sidechain
1	C	102	ARG	Sidechain
1	C	113	ARG	Sidechain
1	C	141	ARG	Sidechain
1	C	148	ARG	Sidechain
1	C	209	ARG	Sidechain
1	C	319	ARG	Sidechain
1	C	96	ARG	Sidechain
1	D	102	ARG	Sidechain
1	D	141	ARG	Sidechain
1	D	319	ARG	Sidechain
1	D	344	ARG	Sidechain

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	2698	0	2651	33	0
1	B	2666	0	2607	34	0
1	C	2542	0	2471	73	0
1	D	2557	0	2474	46	0
2	A	22	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	22	0	8	0	0
3	A	6	0	8	0	0
3	B	6	0	8	11	0
3	C	6	0	8	6	0
3	D	6	0	8	5	0
4	A	173	0	0	4	0
4	B	153	0	0	4	0
4	C	47	0	0	4	0
4	D	49	0	0	2	0
All	All	10953	0	10251	183	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 9.

All (183) 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:C:266:LEU:HD22	1:C:270:ILE:HD11	1.47	0.95
1:C:305:PHE:CD2	1:C:314:ILE:HD11	2.02	0.94
1:B:217:ILE:O	4:B:602:HOH:O	1.86	0.91
1:C:39:THR:OG1	1:C:55:SER:OG	1.87	0.90
1:C:260:ASP:N	1:C:264:ASP:OD2	2.04	0.90
1:B:306:ARG:NH2	4:B:601:HOH:O	1.82	0.89
1:C:273:LEU:O	1:C:298:ALA:HB2	1.74	0.88
1:D:214:VAL:HG22	3:D:501:GOL:H12	1.56	0.87
1:A:295:GLN:C	1:A:296:ILE:HD12	1.94	0.87
1:A:120:GLY:C	1:A:122:LYS:N	2.28	0.86
1:C:270:ILE:H	1:C:270:ILE:HD12	1.44	0.82
1:A:192:ASP:OD1	4:A:601:HOH:O	1.98	0.81
1:D:190:ASP:OD2	1:D:193:THR:OG1	1.98	0.80
1:A:294:PRO:HB2	1:A:296:ILE:HD11	1.63	0.79
1:C:267:VAL:HA	1:C:270:ILE:HD13	1.65	0.77
1:D:277:THR:HG23	1:D:280:GLN:H	1.51	0.76
1:A:342:GLU:O	1:A:348:VAL:HG11	1.86	0.75
1:C:270:ILE:N	1:C:270:ILE:HD12	2.03	0.73
1:C:305:PHE:CD2	1:C:314:ILE:CD1	2.72	0.72
1:A:279:GLU:OE2	1:A:282:ARG:NH2	2.23	0.72
1:C:209:ARG:NH2	1:C:209:ARG:HG2	2.03	0.72
1:C:271:LYS:O	1:C:299:HIS:HE1	1.74	0.71
1:C:267:VAL:CA	1:C:270:ILE:HD13	2.21	0.70
1:A:345:ASP:O	1:A:348:VAL:HG13	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:LEU:CD2	1:C:270:ILE:HD11	2.21	0.70
1:D:87:VAL:O	1:D:127:TYR:HD1	1.74	0.69
1:A:279:GLU:OE1	1:A:282:ARG:NH2	2.22	0.68
1:C:180:ARG:HH12	3:C:501:GOL:H12	1.59	0.67
1:C:141:ARG:NH2	1:D:260:ASP:OD2	2.28	0.66
1:D:163:TYR:CE2	1:D:359:LEU:HG	2.30	0.66
1:D:217:ILE:O	4:D:601:HOH:O	2.13	0.66
1:B:180:ARG:HH12	3:B:502:GOL:H32	1.62	0.65
1:A:279:GLU:CD	1:A:282:ARG:NH2	2.50	0.65
1:B:263:VAL:HG12	1:B:291:PHE:CE1	2.32	0.65
1:D:371:PRO:HD2	1:D:372:PRO:HD3	1.79	0.65
1:A:216:PTR:O3P	1:A:220:ARG:HD3	1.98	0.64
1:A:160:LEU:HD11	1:A:350:LEU:HD21	1.79	0.64
1:C:277:THR:HG23	1:C:280:GLN:H	1.63	0.64
1:C:277:THR:O	1:C:281:ILE:HD12	1.98	0.63
1:D:214:VAL:H	3:D:501:GOL:H12	1.63	0.63
1:D:185:GLN:OE1	1:D:185:GLN:N	2.29	0.62
1:C:296:ILE:N	1:C:296:ILE:HD13	2.14	0.62
1:C:273:LEU:C	1:C:298:ALA:HB2	2.18	0.62
1:A:279:GLU:CD	1:A:282:ARG:HH22	2.03	0.62
1:C:305:PHE:HD2	1:C:314:ILE:HD11	1.63	0.61
1:A:296:ILE:N	1:A:296:ILE:HD12	2.16	0.60
1:C:305:PHE:CE2	1:C:314:ILE:HG13	2.36	0.60
1:B:214:VAL:N	3:B:502:GOL:O3	2.29	0.60
1:C:205:LYS:NZ	1:C:213:ASN:OD1	2.28	0.60
1:D:190:ASP:OD2	1:D:193:THR:N	2.31	0.60
1:C:143:ALA:O	4:C:601:HOH:O	2.16	0.60
1:C:209:ARG:NH2	4:C:605:HOH:O	2.34	0.60
1:A:74:LYS:HE3	1:A:79:GLY:O	2.01	0.60
1:B:180:ARG:HH22	3:B:502:GOL:H32	1.66	0.59
1:C:371:PRO:N	1:C:372:PRO:CD	2.66	0.59
1:C:356:THR:HB	1:C:357:PRO:HD2	1.85	0.59
1:C:270:ILE:H	1:C:270:ILE:CD1	2.14	0.59
1:A:101:MET:HG2	1:A:112:LEU:HB2	1.85	0.58
1:C:264:ASP:O	1:C:267:VAL:HG13	2.03	0.58
1:A:113:ARG:HD2	4:A:613:HOH:O	2.02	0.58
1:C:214:VAL:HG22	3:C:501:GOL:H12	1.84	0.58
1:C:65:GLY:HA3	1:C:67:PHE:CE1	2.37	0.58
1:D:67:PHE:HB2	1:D:87:VAL:HG12	1.85	0.58
1:B:100:ILE:HG23	1:B:177:ILE:HD13	1.85	0.58
1:D:214:VAL:HG22	3:D:501:GOL:C1	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:HB3	1:A:348:VAL:CG1	2.33	0.58
1:C:277:THR:HG22	1:C:280:GLN:CG	2.34	0.57
1:A:279:GLU:OE2	1:A:279:GLU:HA	2.05	0.57
1:B:149:ALA:HB2	1:C:209:ARG:HD2	1.87	0.56
1:D:173:HIS:CE1	1:D:236:SER:HB3	2.40	0.56
1:D:196:LEU:C	1:D:196:LEU:HD23	2.27	0.56
1:C:101:MET:HE1	1:C:201:PHE:CD1	2.41	0.56
1:D:147:SER:OG	1:D:253:GLY:O	2.24	0.55
1:D:107:CYS:O	1:D:197:LYS:NZ	2.40	0.54
1:C:214:VAL:HG22	3:C:501:GOL:C1	2.38	0.54
1:C:215:SER:HB3	1:C:231:ALA:O	2.07	0.54
1:D:362:PHE:CD2	1:D:367:LEU:HD21	2.43	0.54
1:B:86:LYS:HE3	1:B:127:TYR:CG	2.42	0.53
1:C:153:LEU:HD12	1:C:154:PRO:HD2	1.90	0.53
1:C:208:VAL:CG2	1:C:211:GLU:CB	2.86	0.53
1:B:200:ASP:OD2	4:B:603:HOH:O	2.19	0.53
1:C:349:LYS:HE2	1:C:355:ASP:OD1	2.09	0.52
1:C:272:VAL:HA	1:C:299:HIS:CE1	2.45	0.52
1:C:214:VAL:H	3:C:501:GOL:H11	1.75	0.51
1:D:277:THR:HG22	1:D:280:GLN:OE1	2.10	0.51
1:C:66:SER:N	4:C:603:HOH:O	2.26	0.51
1:D:371:PRO:N	1:D:372:PRO:CD	2.74	0.51
1:C:370:ASN:C	1:C:372:PRO:HD2	2.31	0.50
1:D:277:THR:HG23	1:D:280:GLN:N	2.24	0.50
1:D:312:GLU:H	1:D:312:GLU:CD	2.11	0.50
1:C:305:PHE:CD2	1:C:314:ILE:CG1	2.94	0.50
1:C:162:MET:HG3	1:C:247:LEU:HD13	1.94	0.49
1:C:277:THR:HG22	1:C:280:GLN:CD	2.32	0.49
1:B:205:LYS:HZ2	3:B:502:GOL:H31	1.77	0.49
1:D:214:VAL:H	3:D:501:GOL:C1	2.25	0.49
1:D:345:ASP:O	1:D:348:VAL:HG12	2.13	0.49
1:D:371:PRO:CD	1:D:372:PRO:HD3	2.43	0.49
1:C:319:ARG:HG3	1:C:319:ARG:HH11	1.78	0.49
1:A:294:PRO:CB	1:A:296:ILE:HD11	2.39	0.49
1:C:370:ASN:OD1	1:C:372:PRO:HD2	2.13	0.49
1:D:266:LEU:HD23	1:D:293:PHE:HE2	1.79	0.48
1:D:96:ARG:HH22	3:D:501:GOL:HO3	1.62	0.48
1:B:88:LEU:HD13	1:B:127:TYR:CZ	2.49	0.48
1:C:305:PHE:CD2	1:C:314:ILE:HG13	2.49	0.48
1:D:316:LEU:O	1:D:320:LEU:HG	2.14	0.48
1:B:214:VAL:H	3:B:502:GOL:HO3	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:TYR:CD1	1:C:258:PRO:HA	2.49	0.47
1:A:217:ILE:O	4:A:602:HOH:O	2.19	0.47
1:C:264:ASP:HA	1:C:267:VAL:HG13	1.97	0.47
1:A:160:LEU:HD11	1:A:350:LEU:CD2	2.45	0.47
1:C:276:PRO:HA	1:C:280:GLN:OE1	2.14	0.47
1:B:180:ARG:NH1	3:B:502:GOL:H32	2.28	0.47
1:D:228:ILE:HG21	1:D:266:LEU:HB2	1.96	0.47
1:C:180:ARG:HH12	3:C:501:GOL:C1	2.27	0.47
1:B:263:VAL:CG1	1:B:291:PHE:CE1	2.96	0.46
1:A:295:GLN:CA	1:A:296:ILE:HD12	2.45	0.46
1:D:370:ASN:OD1	1:D:372:PRO:HD2	2.14	0.46
1:C:217:ILE:HD12	1:C:227:LEU:HD13	1.98	0.46
1:A:352:ASN:ND2	1:A:354:ARG:HB2	2.31	0.46
1:D:113:ARG:NE	1:D:133:ASP:OD1	2.33	0.46
1:B:180:ARG:HH12	3:B:502:GOL:C3	2.28	0.45
1:C:209:ARG:CG	1:C:209:ARG:NH2	2.77	0.45
1:A:294:PRO:C	1:A:296:ILE:CD1	2.85	0.45
1:C:196:LEU:C	1:C:196:LEU:HD23	2.37	0.45
1:A:352:ASN:HD21	1:A:354:ARG:HB2	1.82	0.45
1:C:217:ILE:CD1	1:C:227:LEU:HD13	2.47	0.45
1:D:106:HIS:CD2	1:D:171:TYR:CG	3.05	0.45
1:B:214:VAL:HG12	3:B:502:GOL:O3	2.17	0.44
1:B:180:ARG:NH2	3:B:502:GOL:H32	2.31	0.44
1:C:324:THR:O	1:C:327:ALA:HB3	2.16	0.44
1:D:379:PRO:HB2	1:D:381:HIS:ND1	2.32	0.44
1:A:295:GLN:N	1:A:296:ILE:HD12	2.32	0.44
1:A:141:ARG:HG3	1:B:260:ASP:OD2	2.18	0.44
1:C:163:TYR:HB2	1:C:340:PHE:CD1	2.52	0.44
1:D:208:VAL:HB	1:D:211:GLU:HG3	1.99	0.44
1:A:371:PRO:N	1:A:372:PRO:CD	2.81	0.44
1:B:37:VAL:HG22	1:B:57:THR:HG22	1.99	0.44
1:B:80:GLU:OE1	1:B:113:ARG:NH1	2.46	0.44
1:C:329:LEU:HD22	1:C:333:GLU:HB3	1.99	0.44
1:B:217:ILE:HD12	1:B:227:LEU:HD13	2.00	0.44
1:B:319:ARG:NH1	4:B:618:HOH:O	2.51	0.44
1:B:86:LYS:HE3	1:B:127:TYR:CB	2.48	0.44
1:C:100:ILE:HG23	1:C:177:ILE:HD13	2.00	0.44
1:C:371:PRO:N	1:C:372:PRO:HD2	2.32	0.43
1:C:273:LEU:O	1:C:298:ALA:CB	2.56	0.43
1:A:312:GLU:CD	1:A:312:GLU:H	2.21	0.43
1:C:240:VAL:HG13	1:C:320:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ASP:OD1	1:C:346:PRO:HD2	2.18	0.43
1:D:352:ASN:C	1:D:354:ARG:N	2.72	0.43
1:B:259:GLY:HA3	1:B:265:GLN:OE1	2.19	0.43
1:C:220:ARG:HG2	1:C:265:GLN:HE21	1.83	0.43
1:D:220:ARG:HD2	1:D:261:SER:C	2.38	0.43
1:D:361:ASN:ND2	4:D:605:HOH:O	2.43	0.42
1:D:111:ARG:HG2	1:D:133:ASP:OD2	2.19	0.42
1:C:163:TYR:CE1	1:C:359:LEU:HB3	2.55	0.42
1:A:74:LYS:HG3	1:A:79:GLY:O	2.19	0.42
1:B:233:ASP:O	1:B:233:ASP:CG	2.58	0.42
1:C:65:GLY:CA	4:C:603:HOH:O	2.67	0.42
1:A:379:PRO:O	1:A:383:ARG:HG3	2.20	0.42
1:B:301:TRP:HB3	1:B:314:ILE:HG23	2.02	0.42
1:B:205:LYS:HD2	3:B:502:GOL:H31	2.01	0.42
1:A:346:PRO:O	4:A:603:HOH:O	2.22	0.41
1:B:371:PRO:N	1:B:372:PRO:CD	2.83	0.41
1:D:96:ARG:HG2	1:D:100:ILE:HD12	2.02	0.41
1:D:162:MET:CE	1:D:247:LEU:HB2	2.50	0.41
1:B:252:LEU:HA	1:B:252:LEU:HD23	1.92	0.41
1:B:294:PRO:HG2	1:B:296:ILE:HD11	2.03	0.41
1:B:263:VAL:CG1	1:B:291:PHE:CD1	3.03	0.41
1:C:42:ALA:HB2	1:C:116:PHE:HB3	2.02	0.41
1:C:214:VAL:H	3:C:501:GOL:C1	2.34	0.41
1:C:310:PRO:HA	1:C:311:PRO:HD3	1.93	0.41
1:D:69:VAL:HG13	1:D:71:TYR:CE1	2.55	0.41
1:B:205:LYS:NZ	3:B:502:GOL:H31	2.35	0.41
1:D:163:TYR:CD2	1:D:359:LEU:HG	2.55	0.41
1:A:106:HIS:HE2	1:A:366:GLU:CD	2.25	0.40
1:C:371:PRO:HD2	1:C:372:PRO:HD3	2.03	0.40
1:D:106:HIS:HD2	1:D:171:TYR:CG	2.38	0.40
1:B:357:PRO:O	1:B:359:LEU:HG	2.21	0.40
1:C:183:LYS:HE2	1:C:186:ASN:ND2	2.36	0.40
1:C:226:GLU:HB3	1:C:284:MET:HG2	2.03	0.40
1:D:310:PRO:HA	1:D:311:PRO:HD2	2.00	0.40
1:D:365:GLN:O	1:D:368:SER:HB3	2.22	0.40
1:D:252:LEU:HD23	1:D:252:LEU:HA	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	339/420 (81%)	335 (99%)	4 (1%)	0	100	100
1	B	335/420 (80%)	329 (98%)	6 (2%)	0	100	100
1	C	321/420 (76%)	313 (98%)	8 (2%)	0	100	100
1	D	322/420 (77%)	313 (97%)	9 (3%)	0	100	100
All	All	1317/1680 (78%)	1290 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	288/362 (80%)	285 (99%)	3 (1%)	76	79
1	B	284/362 (78%)	280 (99%)	4 (1%)	67	70
1	C	268/362 (74%)	256 (96%)	12 (4%)	27	23
1	D	268/362 (74%)	254 (95%)	14 (5%)	23	18
All	All	1108/1448 (76%)	1075 (97%)	33 (3%)	41	39

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	THR
1	A	354	ARG

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Mol	Chain	Res	Type
1	A	356	THR
1	B	57	THR
1	B	215	SER
1	B	217	ILE
1	B	384	ILE
1	C	48	PRO
1	C	57	THR
1	C	111	ARG
1	C	152	THR
1	C	173	HIS
1	C	209	ARG
1	C	217	ILE
1	C	266	LEU
1	C	284	MET
1	C	301	TRP
1	C	314	ILE
1	C	369	SER
1	D	64	ASN
1	D	66	SER
1	D	72	GLN
1	D	147	SER
1	D	167	ARG
1	D	190	ASP
1	D	214	VAL
1	D	217	ILE
1	D	219	SER
1	D	252	LEU
1	D	312	GLU
1	D	359	LEU
1	D	368	SER
1	D	369	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	99	GLN
1	C	64	ASN
1	C	265	GLN
1	C	299	HIS
1	D	72	GLN
1	D	352	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](#)

4 non-standard protein/DNA/RNA residues 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
1	PTR	A	216	1	15,16,17	1.02	0	19,22,24	0.78	0
1	PTR	B	216	1	15,16,17	1.43	2 (13%)	19,22,24	1.11	1 (5%)
1	PTR	C	216	1	15,16,17	0.98	1 (6%)	19,22,24	1.27	3 (15%)
1	PTR	D	216	1	15,16,17	0.87	1 (6%)	19,22,24	1.07	1 (5%)

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
1	PTR	A	216	1	-	0/10/11/13	0/1/1/1
1	PTR	B	216	1	-	0/10/11/13	0/1/1/1
1	PTR	C	216	1	-	0/10/11/13	0/1/1/1
1	PTR	D	216	1	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	PTR	OH-CZ	-3.25	1.33	1.40
1	B	216	PTR	P-O2P	-2.84	1.43	1.54
1	D	216	PTR	OH-CZ	-2.19	1.35	1.40
1	C	216	PTR	OH-CZ	-2.02	1.36	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	216	PTR	O3P-P-O2P	3.40	120.62	107.64
1	C	216	PTR	O2P-P-OH	-2.68	96.87	105.24
1	B	216	PTR	CB-CA-C	2.38	115.93	111.47
1	D	216	PTR	O3P-P-O2P	2.26	116.28	107.64
1	C	216	PTR	O3P-P-O1P	2.04	118.67	110.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	216	PTR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	GOL	B	502	-	5,5,5	1.20	0	5,5,5	1.47	1 (20%)
3	GOL	D	501	-	5,5,5	0.64	0	5,5,5	1.45	1 (20%)
3	GOL	C	501	-	5,5,5	0.67	0	5,5,5	0.96	0
3	GOL	A	502	-	5,5,5	0.63	0	5,5,5	1.64	0
2	MRI	B	501	-	20,24,24	1.73	5 (25%)	28,36,36	1.92	9 (32%)
2	MRI	A	501	-	20,24,24	1.35	2 (10%)	28,36,36	1.34	3 (10%)

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
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	D	501	-	-	4/4/4/4	-
3	GOL	C	501	-	-	4/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
2	MRI	B	501	-	-	2/3/4/4	0/3/3/3
2	MRI	A	501	-	-	2/3/4/4	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MRI	CAO-CAI	-4.42	1.34	1.43
2	B	501	MRI	CAI-CAJ	-2.79	1.37	1.41
2	A	501	MRI	CAO-CAI	-2.69	1.38	1.43
2	B	501	MRI	OAD-CAN	2.64	1.27	1.23
2	A	501	MRI	OAD-CAN	2.53	1.27	1.23
2	B	501	MRI	CAN-CAM	2.32	1.49	1.41
2	B	501	MRI	CAU-CAQ	2.15	1.42	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MRI	CAT-CAL-CAK	-4.78	112.70	120.09
2	A	501	MRI	CAT-CAL-CAK	-3.65	114.44	120.09
2	B	501	MRI	OAA-CAJ-CAP	3.42	120.12	116.11
2	B	501	MRI	CAQ-CAL-CAK	3.17	127.66	121.91
2	A	501	MRI	CAM-CAN-CAI	-3.05	117.12	121.38
2	B	501	MRI	OAC-CAO-CAI	-2.95	114.33	121.10
2	B	501	MRI	CAM-CAN-CAI	-2.76	117.51	121.38
3	B	502	GOL	O2-C2-C3	-2.65	97.45	109.12
2	A	501	MRI	CAQ-CAL-CAK	2.62	126.66	121.91
2	B	501	MRI	CAP-CAR-CAS	-2.32	119.07	120.94
3	D	501	GOL	C3-C2-C1	-2.29	102.81	111.70
2	B	501	MRI	CAU-CAQ-CAL	-2.24	118.73	120.83
2	B	501	MRI	OAA-CAJ-CAI	-2.20	118.87	121.03
2	B	501	MRI	CAN-CAI-CAO	-2.18	118.12	121.85

There are no chirality outliers.

All (16) torsion outliers are listed below:

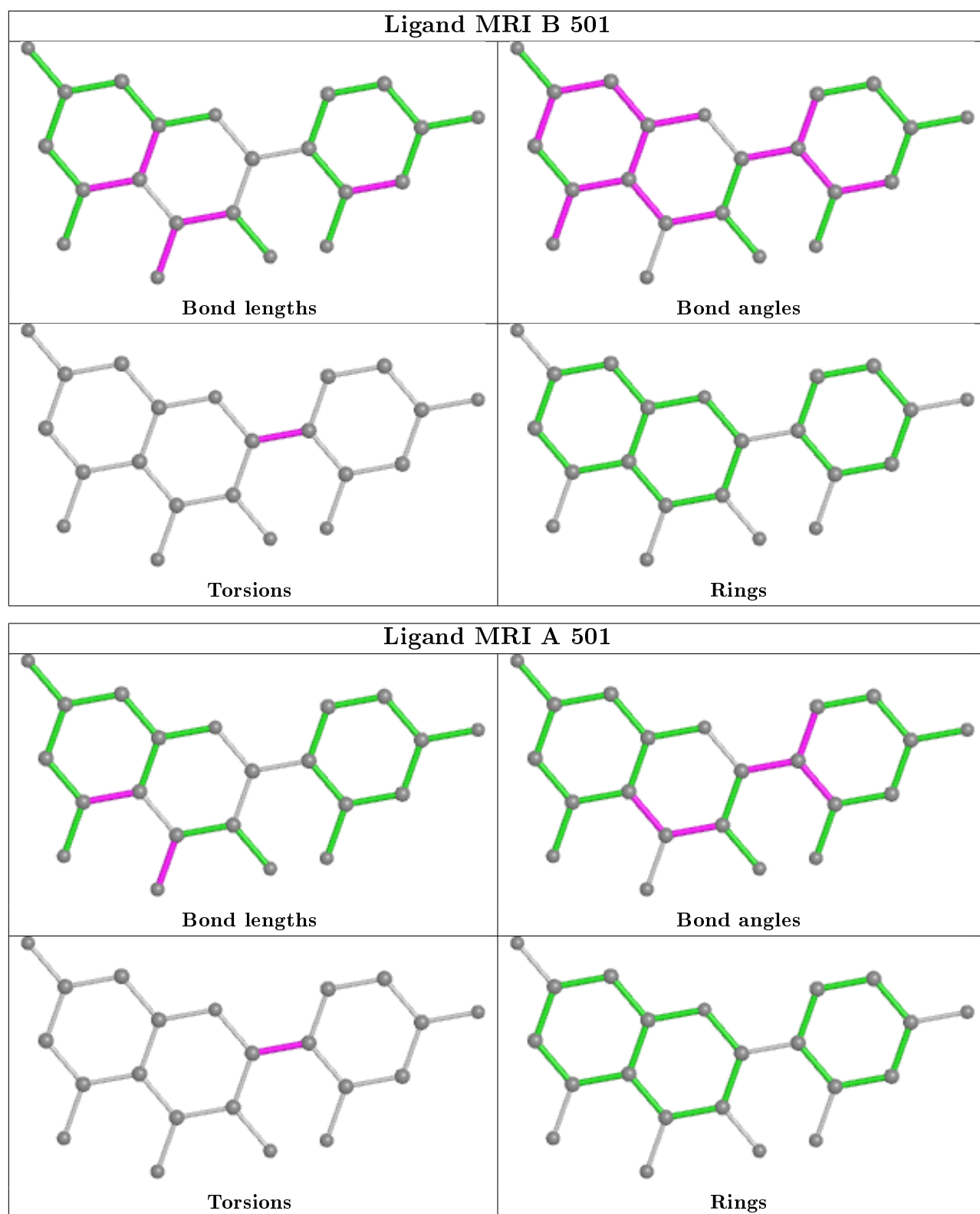
Mol	Chain	Res	Type	Atoms
3	D	501	GOL	C1-C2-C3-O3
3	C	501	GOL	C1-C2-C3-O3
2	B	501	MRI	CAM-CAK-CAL-CAT
2	B	501	MRI	CAM-CAK-CAL-CAQ
2	A	501	MRI	CAM-CAK-CAL-CAT
2	A	501	MRI	CAM-CAK-CAL-CAQ
3	C	501	GOL	O1-C1-C2-O2
3	B	502	GOL	C1-C2-C3-O3
3	D	501	GOL	O1-C1-C2-C3
3	C	501	GOL	O1-C1-C2-C3
3	A	502	GOL	C1-C2-C3-O3
3	D	501	GOL	O1-C1-C2-O2
3	D	501	GOL	O2-C2-C3-O3
3	C	501	GOL	O2-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
3	B	502	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	GOL	11	0
3	D	501	GOL	5	0
3	C	501	GOL	6	0

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



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	347/420 (82%)	-0.07	8 (2%) 60 67	21, 37, 68, 93	0
1	B	343/420 (81%)	0.07	10 (2%) 51 59	20, 38, 71, 102	0
1	C	331/420 (78%)	0.13	12 (3%) 42 50	35, 56, 86, 123	0
1	D	332/420 (79%)	0.26	20 (6%) 21 27	32, 56, 88, 110	0
All	All	1353/1680 (80%)	0.09	50 (3%) 41 49	20, 48, 82, 123	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	293	PHE	6.2
1	D	127	TYR	5.6
1	D	288	TYR	5.5
1	A	294	PRO	5.3
1	D	294	PRO	4.8
1	B	294	PRO	4.6
1	D	378	ILE	4.3
1	C	301	TRP	4.2
1	D	380	PRO	4.2
1	D	382	ALA	4.0
1	C	305	PHE	3.8
1	D	287	ASN	3.7
1	B	293	PHE	3.7
1	C	296	ILE	3.7
1	B	291	PHE	3.4
1	A	387	ALA	3.3
1	D	36	LYS	2.9
1	D	296	ILE	2.9
1	B	288	TYR	2.8
1	D	381	HIS	2.8
1	D	78	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	292	LYS	2.8
1	D	291	PHE	2.7
1	D	126	VAL	2.7
1	C	302	THR	2.7
1	A	288	TYR	2.6
1	A	289	THR	2.6
1	C	81	LEU	2.5
1	D	208	VAL	2.5
1	A	93	PHE	2.5
1	B	286	PRO	2.4
1	B	217	ILE	2.4
1	A	293	PHE	2.4
1	B	384	ILE	2.4
1	C	300	PRO	2.4
1	C	217	ILE	2.3
1	C	299	HIS	2.3
1	A	92	ARG	2.3
1	D	229	PHE	2.2
1	D	346	PRO	2.2
1	B	353	GLY	2.1
1	C	229	PHE	2.1
1	D	207	LEU	2.1
1	D	211	GLU	2.1
1	D	286	PRO	2.1
1	C	124	ASP	2.0
1	C	91	LYS	2.0
1	C	309	THR	2.0
1	B	182	ILE	2.0
1	A	47	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	C	216	16/17	0.95	0.09	46,53,65,65	0
1	PTR	D	216	16/17	0.97	0.10	36,41,46,47	0
1	PTR	A	216	16/17	0.99	0.12	25,29,33,34	0
1	PTR	B	216	16/17	0.99	0.13	29,33,37,40	0

6.3 Carbohydrates [i](#)

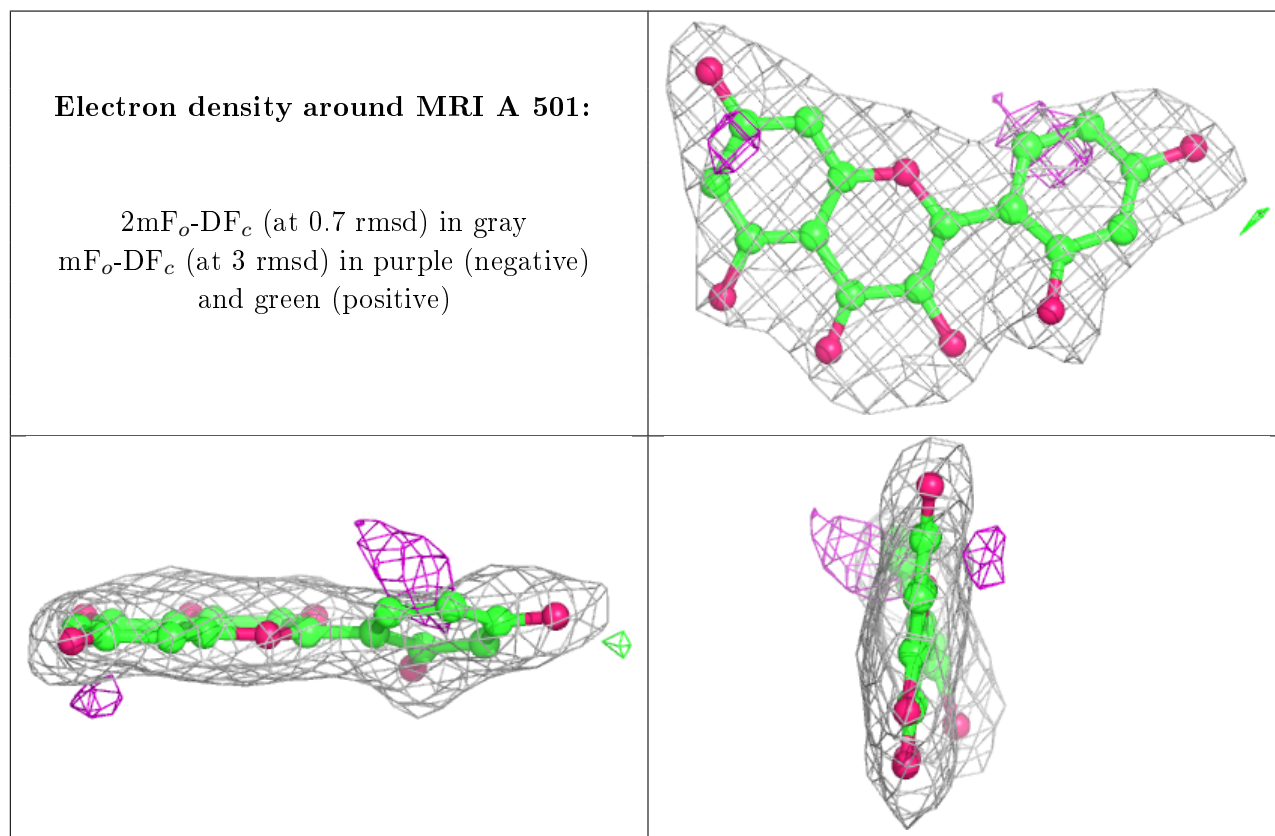
There are no carbohydrates in this entry.

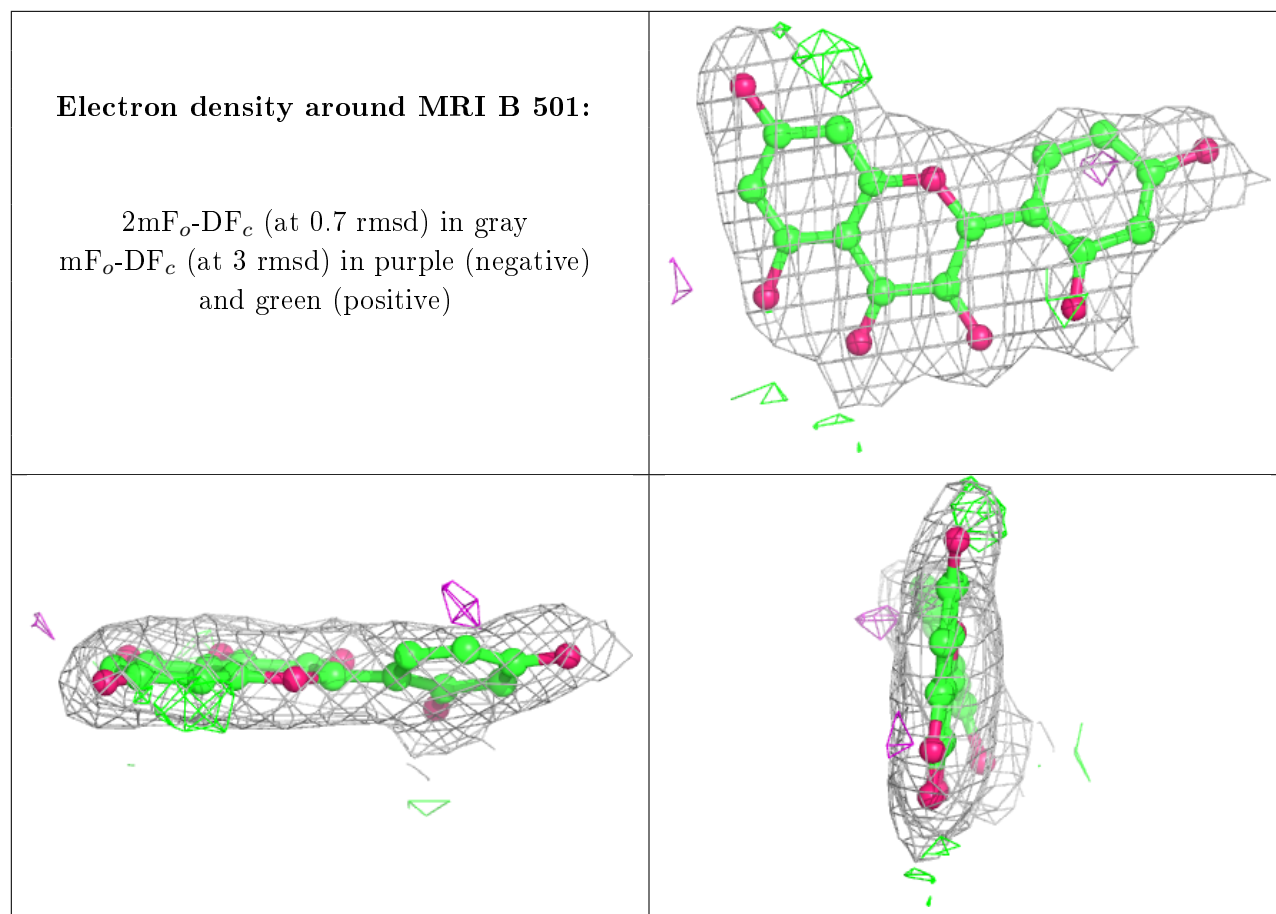
6.4 Ligands [i](#)

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
3	GOL	C	501	6/6	0.79	0.22	49,60,65,67	0
3	GOL	B	502	6/6	0.80	0.16	34,43,49,53	0
3	GOL	D	501	6/6	0.82	0.18	52,57,65,67	0
3	GOL	A	502	6/6	0.90	0.12	36,49,54,55	0
2	MRI	A	501	22/22	0.92	0.13	41,48,52,57	0
2	MRI	B	501	22/22	0.94	0.11	36,46,53,54	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.