Full wwPDB X-ray Structure Validation Report (i)

Apr 22, 2025 – 01:58 AM EDT

PDB ID	:	7LPP / pdb_00007lpp
Title	:	Crystal structure of Cryptococcus neoformans sterylglucosidase 1 with hit 1
Authors	:	Pereira de Sa, N.; Del Poeta, M.; Airola, M.V.
Deposited on	:	2021-02-12
Resolution	:	2.85 Å(reported)

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)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.85 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.
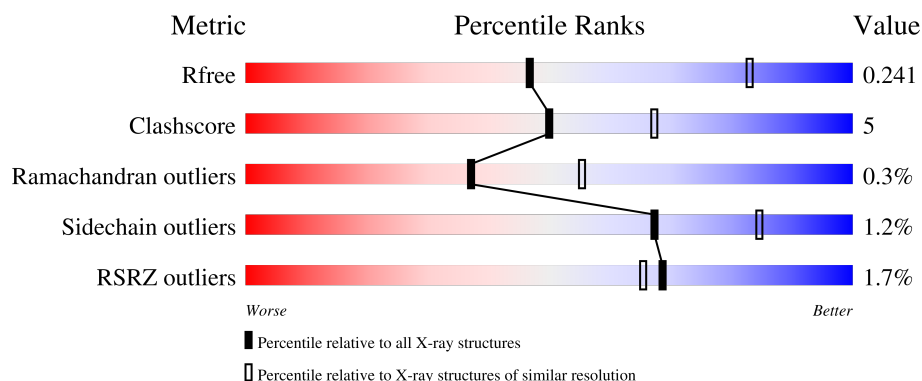
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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	797	82% 10% · 8%
1	B	797	79% 12% 9%
1	C	797	82% 10% 9%
1	D	797	70% 20% · 10%

2   Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23935 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 Cytoplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total 5815	C 3727	N 993	O 1072	S 23	0	1	0
1	B	727	Total 5782	C 3703	N 991	O 1065	S 23	0	1	0
1	C	729	Total 5795	C 3712	N 993	O 1067	S 23	0	1	0
1	D	719	Total 5716	C 3663	N 976	O 1054	S 23	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP J9W473
B	0	SER	-	expression tag	UNP J9W473
C	0	SER	-	expression tag	UNP J9W473
D	0	SER	-	expression tag	UNP J9W473

- Molecule 2 is 4-(hydroxymethyl)-1-[[2-(3-methoxyphenyl)-1,3-thiazol-5-yl]methyl]piperidin-4 -ol (CCD ID: YAG) (formula: $C_{17}H_{22}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).

WORLDWIDE PDB
PROTEIN DATA BANK
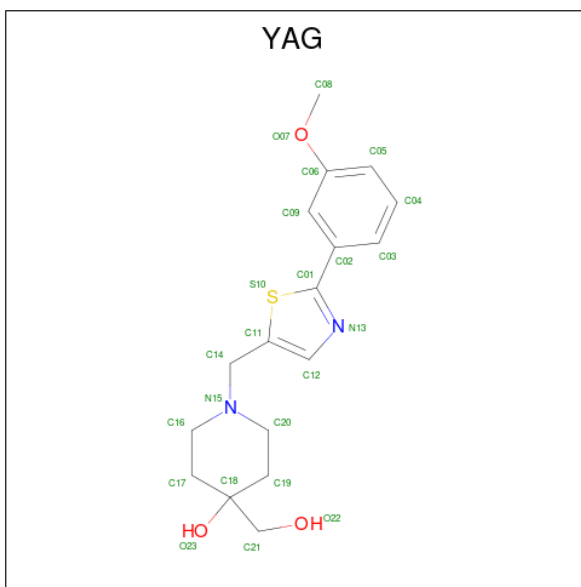
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	C	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	D	1	Total	C	N	O	S	0	0
			23	17	2	3	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).
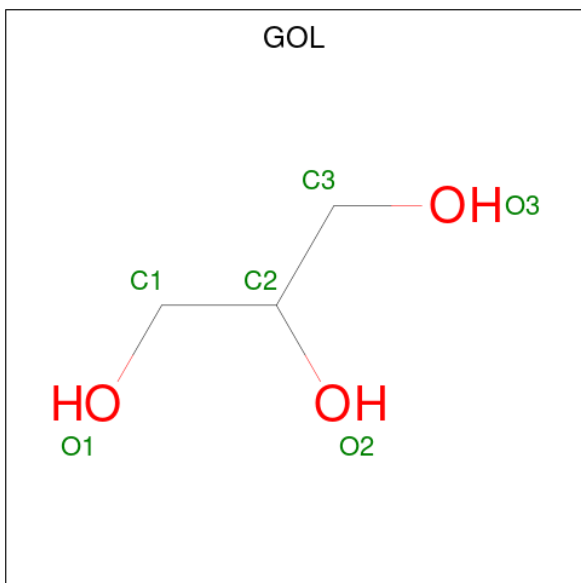
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	214	Total 214	O 214	0	0
5	B	177	Total 177	O 177	0	0
5	C	197	Total 197	O 197	0	0
5	D	122	Total 122	O 122	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Cytoplasmic protein

- Molecule 1: Cytoplasmic protein

• Molecule 1: Cytoplasmic protein

Chain C:

• Molecule 1: Cytoplasmic protein

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.10Å 133.16Å 129.59Å 90.00° 94.46° 90.00°	Depositor
Resolution (Å)	58.12 – 2.85 58.12 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.6 (58.12-2.85) 96.4 (58.12-2.85)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660	Depositor
R, R_{free}	0.191 , 0.242 0.191 , 0.241	Depositor DCC
R_{free} test set	3543 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	1.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.2	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	0.93	EDS
Total number of atoms	23935	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, YAG

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	0.25	0/6001	0.42	0/8182
1	B	0.25	0/5965	0.43	0/8130
1	C	0.30	0/5978	0.44	0/8149
1	D	0.29	0/5896	0.43	0/8035
All	All	0.28	0/23840	0.43	0/32496

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	311	ASP	Peptide

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5815	0	5551	46	1
1	B	5782	0	5531	53	0
1	C	5795	0	5546	44	0
1	D	5716	0	5461	93	0
2	A	23	0	0	0	0
2	B	23	0	0	1	0
2	C	23	0	0	1	0
2	D	23	0	0	0	0
3	A	6	0	8	0	0
3	B	12	0	16	1	0
3	D	6	0	8	1	0
4	B	1	0	0	0	0
5	A	214	0	0	2	0
5	B	177	0	0	2	0
5	C	197	0	0	2	0
5	D	122	0	0	1	0
All	All	23935	0	22121	235	1

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 5.

All (235) 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:288:GLN:O	1:A:291:LYS:NZ	1.77	1.16
1:B:687:LYS:HG2	1:B:823:GLN:HG3	1.51	0.91
1:D:103:THR:HG23	1:D:106:SER:H	1.42	0.84
1:D:24:THR:HG22	1:D:26:HIS:H	1.45	0.82
1:D:128:ARG:HG2	1:D:257:LEU:HD21	1.63	0.81
1:A:43:SER:HB3	1:A:75:PRO:HB3	1.64	0.76
1:D:341:LYS:HG3	1:D:362:LEU:HB2	1.68	0.75
1:B:651:PRO:HG3	1:B:784:LEU:HD11	1.69	0.74
1:D:76:LEU:O	1:D:122:TYR:OH	2.04	0.74
1:D:480:SER:HB3	1:D:482:VAL:HG12	1.74	0.70
1:D:576:ASN:ND2	1:D:582:ASP:OD1	2.27	0.68
1:A:311:ASP:O	1:A:327:ARG:NH1	2.27	0.68
1:D:374:GLU:HB2	1:D:381:LEU:HD11	1.79	0.64
1:B:716:ALA:O	1:B:824:ARG:NH1	2.31	0.64
1:C:299:ILE:HD13	1:C:380:LEU:HD13	1.80	0.63
1:B:229:LYS:NZ	5:B:1003:HOH:O	2.32	0.62
1:D:121:ASP:HA	1:D:124:ILE:HD12	1.80	0.62
1:D:695:ARG:HG2	1:D:815:GLU:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:SER:HB3	1:D:75:PRO:HB3	1.83	0.61
1:B:576:ASN:ND2	1:B:582:ASP:OD1	2.33	0.61
1:C:638:ARG:NH1	1:D:252:GLU:OE2	2.33	0.61
1:D:117:TYR:HD1	1:D:249:ARG:HE	1.46	0.61
1:D:10:VAL:HG12	1:D:443:LYS:HB3	1.81	0.61
1:D:76:LEU:HD22	1:D:83:ALA:HA	1.82	0.60
1:C:436:LYS:NZ	5:C:1004:HOH:O	2.33	0.60
1:D:38:ARG:HG3	1:D:668:TYR:CE2	2.37	0.60
1:B:685:SER:HB2	1:B:687:LYS:HG3	1.83	0.58
1:D:268:ILE:HG23	1:D:271:PRO:HG3	1.85	0.58
1:C:521:ILE:HD11	1:C:555:SER:HB3	1.85	0.58
1:D:513:ASN:HB2	3:D:902:GOL:H12	1.85	0.58
1:A:22:SER:OG	1:A:446:ALA:O	2.21	0.58
1:C:269:ASN:HA	1:C:427:GLN:HE22	1.69	0.57
1:B:53:PRO:HG2	1:B:56:ILE:HG13	1.85	0.57
1:C:587:GLU:OE2	2:C:901:YAG:O23	2.22	0.57
1:D:59:GLY:O	1:D:63:THR:OG1	2.19	0.57
1:B:717:ALA:HA	1:B:824:ARG:HH12	1.69	0.57
1:D:113:LYS:NZ	5:D:1004:HOH:O	2.37	0.56
1:B:430:VAL:HG12	1:B:431:LEU:HG	1.85	0.56
1:D:281:LEU:HD12	1:D:383:PRO:HA	1.86	0.56
1:A:180:CYS:SG	1:A:181:GLU:HG3	2.46	0.56
1:B:122:TYR:O	1:B:126:VAL:HG23	2.07	0.56
1:D:103:THR:HG23	1:D:106:SER:N	2.18	0.56
1:B:559:CYS:HB3	1:B:565:LEU:HB2	1.88	0.55
1:D:717:ALA:O	1:D:824:ARG:NH2	2.38	0.55
1:C:59:GLY:O	1:C:63:THR:HG23	2.05	0.55
1:D:222:PRO:HD2	1:D:370:HIS:CD2	2.41	0.55
1:D:356:ARG:HD2	1:D:362:LEU:HD21	1.86	0.55
1:D:799:ILE:HA	1:D:804:LEU:HA	1.89	0.55
1:C:530:LYS:NZ	5:C:1006:HOH:O	2.38	0.55
1:C:673:VAL:HG11	1:C:700:ALA:HB2	1.90	0.54
1:A:52:GLN:NE2	1:A:58:GLU:O	2.41	0.54
1:C:655:LEU:HD11	1:C:719:LEU:HD13	1.89	0.54
1:D:789:THR:OG1	1:D:825:ASN:OD1	2.22	0.54
1:B:113:LYS:NZ	5:B:1005:HOH:O	2.37	0.53
1:C:42:LEU:HD12	1:C:43:SER:HB2	1.90	0.53
1:A:248:LYS:NZ	5:A:1006:HOH:O	2.41	0.53
1:A:42:LEU:HD12	1:A:43:SER:HB2	1.91	0.53
1:B:22:SER:OG	1:B:446:ALA:O	2.26	0.53
1:A:448:SER:HB3	1:A:516:THR:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:SER:OG	1:A:482:VAL:HG22	2.09	0.52
1:B:10:VAL:HA	1:B:443:LYS:HD2	1.91	0.52
1:A:576:ASN:ND2	1:A:582:ASP:OD1	2.42	0.52
1:D:531:LYS:NZ	1:D:537:ASP:OD2	2.42	0.52
1:B:208:GLN:O	1:B:212:THR:OG1	2.22	0.51
1:C:356:ARG:HD2	1:C:362:LEU:HD11	1.92	0.51
1:C:313:GLN:NE2	1:C:327:ARG:HG2	2.26	0.51
1:D:241:ASP:OD1	1:D:414:ARG:NH1	2.42	0.51
1:D:377:THR:HB	1:D:379:THR:OG1	2.11	0.51
1:A:789:THR:OG1	1:A:825:ASN:OD1	2.22	0.51
1:D:643:VAL:HG23	1:D:648:ASP:HB3	1.93	0.51
1:B:462[B]:HIS:ND1	1:B:528:ASP:OD1	2.42	0.50
1:B:669:PRO:HG3	1:B:690:TYR:CZ	2.46	0.50
1:C:307:GLY:HA2	1:C:332:PRO:HB2	1.93	0.50
1:D:507:THR:HG21	1:D:516:THR:OG1	2.11	0.50
1:D:578:HIS:NE2	1:D:596:ASP:OD1	2.43	0.50
1:B:349:SER:HB3	1:B:354:TRP:O	2.11	0.50
1:D:145:VAL:HG11	1:D:201:ASN:HB2	1.93	0.50
1:B:797:VAL:HG12	1:B:806:TRP:CD1	2.46	0.50
1:C:303:ARG:HB2	1:C:310:GLN:HG3	1.94	0.49
1:B:15:VAL:HB	1:B:19:TYR:CG	2.46	0.49
1:A:505:GLN:HA	1:A:508:ILE:HG22	1.94	0.49
1:C:338:TRP:HZ2	1:C:365:CYS:HG	1.60	0.49
1:C:145:VAL:O	1:C:150:THR:OG1	2.29	0.49
1:D:667:PRO:HB3	1:D:710:LEU:HD23	1.93	0.49
1:A:338:TRP:CE2	1:A:365:CYS:HA	2.48	0.49
1:D:22:SER:OG	1:D:446:ALA:O	2.30	0.49
1:D:281:LEU:HB2	1:D:380:LEU:HD21	1.94	0.49
1:A:442:LEU:HD22	1:A:446:ALA:HB2	1.95	0.48
1:B:229:LYS:HE2	1:B:234:PHE:HA	1.94	0.48
1:D:368:ALA:CB	1:D:375:ILE:HD11	2.43	0.48
1:D:795:GLY:HA3	1:D:808:TYR:HA	1.95	0.48
1:B:388:THR:HB	1:B:393:PRO:HA	1.95	0.48
1:D:339:LEU:O	1:D:363:GLY:N	2.46	0.48
1:A:500:LEU:HD23	1:A:558:ALA:HB1	1.96	0.48
1:D:476:LYS:N	1:D:476:LYS:HD2	2.28	0.48
1:B:68:LYS:N	1:B:68:LYS:HD2	2.29	0.48
1:B:505:GLN:HG3	1:B:509:ASP:OD1	2.14	0.48
1:C:576:ASN:ND2	1:C:582:ASP:OD1	2.46	0.48
1:A:695:ARG:HG2	1:A:815:GLU:HB3	1.95	0.48
1:A:129:LYS:O	1:A:133:TRP:HD1	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:GLU:OE2	2:B:901:YAG:O23	2.32	0.48
1:C:222:PRO:HD2	1:C:370:HIS:CD2	2.49	0.48
1:C:22:SER:OG	1:C:446:ALA:O	2.31	0.47
1:B:145:VAL:HG11	1:B:201:ASN:HB2	1.96	0.47
1:B:341:LYS:HG2	1:B:362:LEU:HB2	1.95	0.47
1:B:42:LEU:HD12	1:B:43:SER:HB2	1.96	0.47
1:C:311:ASP:OD1	1:C:329:THR:HA	2.15	0.47
1:C:42:LEU:HD21	1:C:76:LEU:HD11	1.97	0.47
1:B:713:VAL:O	1:B:831:ARG:NH1	2.48	0.47
1:D:50:ASN:ND2	1:D:72:ILE:O	2.40	0.47
1:B:384:ASP:HB2	1:B:387:SER:OG	2.15	0.47
1:D:556:MET:HB3	1:D:666:ARG:HD2	1.96	0.47
1:D:570:TRP:HD1	1:D:589:LEU:HD22	1.80	0.47
1:D:419:HIS:CG	1:D:422:SER:HB2	2.50	0.47
1:B:163:CYS:HB3	1:B:213:PHE:CE2	2.48	0.46
1:D:388:THR:OG1	1:D:389:LEU:N	2.47	0.46
1:C:313:GLN:OE1	1:C:325:GLY:N	2.48	0.46
1:D:24:THR:HG22	1:D:26:HIS:N	2.23	0.46
1:D:493:ARG:HG2	1:D:554:CYS:HB2	1.96	0.46
1:D:222:PRO:HD2	1:D:370:HIS:HD2	1.81	0.46
1:B:658:SER:HB2	1:B:661:VAL:HB	1.98	0.46
1:D:790:ILE:HG23	1:D:822:VAL:HG22	1.97	0.46
1:B:419:HIS:CG	1:B:422:SER:HB2	2.51	0.46
1:D:239:PHE:O	1:D:243:VAL:HG22	2.16	0.46
1:A:669:PRO:HG3	1:A:690:TYR:CZ	2.51	0.46
1:D:296:PRO:HB3	1:D:312:VAL:HG11	1.98	0.46
1:B:341:LYS:HE2	1:B:362:LEU:H	1.81	0.45
1:D:462[B]:HIS:ND1	1:D:528:ASP:OD1	2.48	0.45
1:D:525:TYR:O	1:D:548:GLN:NE2	2.45	0.45
1:A:800:GLN:HG2	1:A:805:ARG:HH12	1.81	0.45
1:B:797:VAL:HB	1:B:804:LEU:HD11	1.98	0.45
1:C:103:THR:HG22	1:C:142:HIS:O	2.16	0.45
1:A:65:GLU:OE1	1:A:351:LYS:NZ	2.49	0.45
1:A:86:HIS:ND1	1:A:572:TYR:OH	2.36	0.45
1:A:311:ASP:OD2	1:A:329:THR:OG1	2.34	0.45
1:A:531:LYS:HA	1:A:536:VAL:HG22	1.99	0.45
1:D:38:ARG:HD3	1:D:567:TYR:CZ	2.52	0.45
1:A:570:TRP:HA	1:A:571:ASN:HA	1.80	0.45
1:D:467:ASN:HB2	1:D:492:ILE:HD13	1.99	0.45
1:D:496:ILE:O	1:D:500:LEU:HD12	2.17	0.45
1:D:42:LEU:HB2	1:D:98:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:VAL:HG11	1:C:201:ASN:HB2	1.98	0.44
1:C:4:PRO:HG2	1:C:32:GLY:HA2	1.99	0.44
1:A:303:ARG:HD3	1:A:378:SER:HB3	1.99	0.44
1:B:42:LEU:HA	1:B:43:SER:HB2	2.00	0.44
1:B:59:GLY:O	1:B:63:THR:HG23	2.17	0.44
1:B:194:PRO:HB2	1:B:197:ILE:HB	2.00	0.44
1:C:39:GLY:HA3	1:C:97:LEU:O	2.18	0.44
1:D:10:VAL:HG12	1:D:443:LYS:CB	2.48	0.44
1:D:41:ASN:OD1	1:D:99:ARG:HD3	2.18	0.44
1:C:374:GLU:HB2	1:C:381:LEU:HD11	2.00	0.43
1:A:590:SER:O	1:A:659:ARG:NH2	2.48	0.43
1:B:556:MET:HB3	1:B:666:ARG:HD2	2.00	0.43
1:B:373:TRP:HA	1:B:381:LEU:HG	2.00	0.43
1:D:91:LYS:HD2	1:D:91:LYS:HA	1.83	0.43
1:D:173:THR:HG21	1:D:337:LEU:HB2	2.01	0.43
1:D:145:VAL:HB	1:D:207:ASN:ND2	2.33	0.43
1:D:797:VAL:HG12	1:D:806:TRP:CD1	2.52	0.43
1:C:66:ALA:HB3	1:C:68:LYS:HG2	2.00	0.43
1:C:338:TRP:CE2	1:C:365:CYS:HA	2.54	0.43
1:C:42:LEU:HA	1:C:43:SER:HB2	2.00	0.43
1:D:78:LEU:HD11	1:D:126:VAL:HG22	2.01	0.43
1:D:115:TYR:HB3	1:D:120:MET:HE1	2.00	0.43
1:C:339:LEU:O	1:C:362:LEU:HB3	2.18	0.43
1:D:121:ASP:OD2	1:D:249:ARG:NH1	2.52	0.43
1:D:449:SER:HA	1:D:517:LEU:O	2.18	0.43
1:D:692:VAL:O	1:D:817:VAL:HA	2.18	0.43
1:D:412:SER:HB2	1:D:424:HIS:NE2	2.33	0.43
1:B:338:TRP:NE1	1:B:365:CYS:HA	2.33	0.42
1:C:419:HIS:CG	1:C:422:SER:HB2	2.54	0.42
1:A:145:VAL:HG11	1:A:201:ASN:HB2	2.00	0.42
1:A:222:PRO:HD2	1:A:370:HIS:CD2	2.53	0.42
1:A:281:LEU:HD21	1:A:386:PHE:HD2	1.83	0.42
1:C:94:GLY:O	1:C:668:TYR:OH	2.28	0.42
1:D:786:LEU:HD12	1:D:799:ILE:HD13	2.00	0.42
1:C:161:TYR:HD1	1:C:339:LEU:HD11	1.85	0.42
1:C:478:TYR:HB3	1:C:480:SER:O	2.19	0.42
1:B:451:HIS:CG	1:B:520:GLU:HB2	2.55	0.42
1:B:577:VAL:O	1:B:581:GLY:N	2.49	0.42
1:C:115:TYR:CE2	1:C:245:GLU:HG3	2.54	0.42
1:A:229:LYS:NZ	5:A:1011:HOH:O	2.52	0.42
1:A:462[B]:HIS:HA	1:A:527:MET:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:SER:O	1:B:643:VAL:HG22	2.20	0.42
1:B:661:VAL:HA	1:B:664:PHE:CE2	2.55	0.42
1:C:661:VAL:HA	1:C:664:PHE:CE2	2.54	0.42
1:D:116:ASP:O	1:D:120:MET:HG3	2.20	0.42
1:D:649:PHE:O	1:D:784:LEU:HD22	2.20	0.42
1:A:85:LEU:HD12	1:A:85:LEU:HA	1.91	0.42
1:D:289:GLN:HG3	1:D:431:LEU:HD13	2.02	0.42
1:D:450:PRO:HG2	1:D:503:LEU:HD23	2.01	0.42
1:A:702:GLU:HA	1:A:807:TRP:CD1	2.55	0.42
1:D:273:GLU:HG2	1:D:399:PHE:CE2	2.55	0.42
1:D:333:LYS:HB2	1:D:333:LYS:HE3	1.72	0.42
1:D:368:ALA:HB2	1:D:373:TRP:CD1	2.55	0.42
1:D:667:PRO:HG3	1:D:715:TYR:OH	2.19	0.42
1:C:388:THR:OG1	1:C:395:HIS:O	2.22	0.42
1:B:94:GLY:HA3	1:B:709:TYR:CE2	2.55	0.41
1:A:419:HIS:ND1	1:A:422:SER:HB2	2.35	0.41
1:B:830:ARG:HD3	1:B:830:ARG:HA	1.78	0.41
1:C:47:LYS:HE2	1:C:142:HIS:NE2	2.35	0.41
1:D:119:TYR:CE2	1:D:123:ILE:HD11	2.55	0.41
1:B:299:ILE:HD12	1:B:299:ILE:HA	1.88	0.41
1:D:338:TRP:CE2	1:D:365:CYS:HA	2.56	0.41
1:B:690:TYR:CE2	1:B:692:VAL:HG22	2.55	0.41
1:B:513:ASN:H	3:B:903:GOL:H12	1.86	0.41
1:C:288:GLN:O	1:C:291:LYS:HE3	2.20	0.41
1:B:449:SER:HA	1:B:517:LEU:O	2.20	0.41
1:D:439:GLU:OE1	1:D:444:GLY:N	2.53	0.41
1:B:467:ASN:O	1:B:485:VAL:HA	2.21	0.41
1:D:577:VAL:HG23	1:D:580:TRP:H	1.84	0.41
1:D:591:LEU:HB3	1:D:664:PHE:CE2	2.56	0.41
1:A:710:LEU:HD22	1:A:822:VAL:HG11	2.02	0.41
1:B:573:VAL:H	1:B:590:SER:HB2	1.85	0.41
1:A:281:LEU:HD21	1:A:386:PHE:CD2	2.55	0.41
1:A:303:ARG:NH1	1:A:378:SER:O	2.54	0.41
1:A:527:MET:CE	1:A:547:SER:HB3	2.51	0.41
1:A:563:ASN:HB3	1:A:565:LEU:HG	2.03	0.41
1:A:800:GLN:HG3	1:A:803:THR:HB	2.03	0.41
1:C:374:GLU:O	1:C:378:SER:N	2.52	0.41
1:C:431:LEU:HD22	1:C:474:ILE:HD12	2.01	0.41
1:D:103:THR:HG1	1:D:105:GLU:H	1.69	0.41
1:D:406:LEU:HA	1:D:409:LEU:HD12	2.03	0.41
1:D:650:SER:OG	1:D:652:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HD22	1:A:446:ALA:CB	2.51	0.41
1:D:368:ALA:HB2	1:D:373:TRP:NE1	2.36	0.41
1:A:287:GLU:O	1:A:289:GLN:NE2	2.54	0.40
1:D:205:LEU:HD22	1:D:301:GLY:O	2.21	0.40
1:D:340:SER:HG	1:D:343:ASP:H	1.59	0.40
1:A:220:TYR:CE1	1:A:386:PHE:HA	2.57	0.40
1:C:43:SER:HB3	1:C:75:PRO:HB3	2.03	0.40
1:D:690:TYR:CZ	1:D:692:VAL:HG22	2.56	0.40
1:D:493:ARG:HA	1:D:554:CYS:SG	2.62	0.40
1:A:384:ASP:HB2	1:A:387:SER:OG	2.20	0.40
1:A:416:ARG:HA	1:A:419:HIS:O	2.21	0.40
1:D:120:MET:O	1:D:124:ILE:HG13	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ARG:NH1	1:A:783:GLN:OE1[2_546]	2.17	0.03

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	729/797 (92%)	699 (96%)	28 (4%)	2 (0%)	37	55
1	B	722/797 (91%)	691 (96%)	29 (4%)	2 (0%)	37	55
1	C	724/797 (91%)	692 (96%)	32 (4%)	0	100	100
1	D	712/797 (89%)	677 (95%)	31 (4%)	4 (1%)	22	40
All	All	2887/3188 (91%)	2759 (96%)	120 (4%)	8 (0%)	37	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	800	GLN
1	A	454	ASP
1	D	454	ASP
1	D	799	ILE
1	B	560	ASP
1	D	801	GLY
1	A	69	GLY
1	B	69	GLY

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	610/670 (91%)	605 (99%)	5 (1%)	79	90
1	B	608/670 (91%)	601 (99%)	7 (1%)	67	84
1	C	609/670 (91%)	602 (99%)	7 (1%)	70	85
1	D	601/670 (90%)	590 (98%)	11 (2%)	54	76
All	All	2428/2680 (91%)	2398 (99%)	30 (1%)	67	84

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	291	LYS
1	A	422	SER
1	A	547	SER
1	A	659	ARG
1	B	191	GLN
1	B	422	SER
1	B	432	ARG
1	B	448	SER
1	B	640	SER
1	B	659	ARG
1	B	695	ARG
1	C	8	SER
1	C	267	SER

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Mol	Chain	Res	Type
1	C	467	ASN
1	C	637	LEU
1	C	650	SER
1	C	659	ARG
1	C	830	ARG
1	D	8	SER
1	D	38	ARG
1	D	91	LYS
1	D	260	GLU
1	D	311	ASP
1	D	346	LYS
1	D	517	LEU
1	D	540	ARG
1	D	640	SER
1	D	645	ASP
1	D	659	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	ASN
1	C	396	GLN
1	D	328	GLN

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 ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	GOL	B	903	-	5,5,5	0.96	0	5,5,5	1.04	0
2	YAG	A	901	-	24,25,25	4.75	8 (33%)	22,35,35	1.62	7 (31%)
3	GOL	D	902	-	5,5,5	0.92	0	5,5,5	1.11	0
2	YAG	B	901	-	24,25,25	4.80	8 (33%)	22,35,35	2.62	8 (36%)
2	YAG	D	901	-	24,25,25	4.81	8 (33%)	22,35,35	2.64	9 (40%)
3	GOL	A	902	-	5,5,5	0.99	0	5,5,5	1.05	0
2	YAG	C	901	-	24,25,25	4.75	8 (33%)	22,35,35	1.76	7 (31%)
3	GOL	B	902	-	5,5,5	0.90	0	5,5,5	1.04	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
3	GOL	B	903	-	-	3/4/4/4	-
2	YAG	A	901	-	-	2/12/25/25	1/3/3/3
3	GOL	D	902	-	-	1/4/4/4	-
2	YAG	B	901	-	-	2/12/25/25	0/3/3/3
2	YAG	D	901	-	-	2/12/25/25	0/3/3/3
3	GOL	A	902	-	-	0/4/4/4	-
2	YAG	C	901	-	-	2/12/25/25	1/3/3/3
3	GOL	B	902	-	-	2/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	YAG	C14-N15	-14.23	1.20	1.47
2	A	901	YAG	C14-N15	-14.21	1.20	1.47
2	D	901	YAG	C14-N15	-14.12	1.20	1.47
2	B	901	YAG	C14-N15	-14.05	1.20	1.47
2	B	901	YAG	C19-C18	-9.54	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	YAG	C19-C18	-9.19	1.44	1.52
2	A	901	YAG	C19-C18	-8.71	1.44	1.52
2	C	901	YAG	C19-C18	-8.55	1.44	1.52
2	D	901	YAG	C12-N13	8.26	1.48	1.36
2	A	901	YAG	C12-N13	8.20	1.48	1.36
2	C	901	YAG	C12-N13	8.20	1.48	1.36
2	D	901	YAG	C01-S10	-8.10	1.62	1.73
2	B	901	YAG	C12-N13	8.10	1.48	1.36
2	A	901	YAG	C01-S10	-8.00	1.62	1.73
2	C	901	YAG	C01-S10	-7.97	1.62	1.73
2	B	901	YAG	C01-S10	-7.78	1.62	1.73
2	D	901	YAG	C11-S10	-6.66	1.59	1.73
2	C	901	YAG	C11-S10	-6.60	1.60	1.73
2	A	901	YAG	C11-S10	-6.56	1.60	1.73
2	B	901	YAG	C11-S10	-6.52	1.60	1.73
2	B	901	YAG	C17-C18	-6.46	1.46	1.52
2	D	901	YAG	C17-C18	-6.33	1.46	1.52
2	C	901	YAG	C17-C18	-6.24	1.47	1.52
2	A	901	YAG	C17-C18	-6.06	1.47	1.52
2	B	901	YAG	C01-N13	5.91	1.40	1.31
2	A	901	YAG	C01-N13	5.90	1.40	1.31
2	D	901	YAG	C01-N13	5.86	1.39	1.31
2	C	901	YAG	C01-N13	5.82	1.39	1.31
2	D	901	YAG	O23-C18	2.90	1.50	1.44
2	A	901	YAG	O23-C18	2.73	1.49	1.44
2	B	901	YAG	O23-C18	2.73	1.49	1.44
2	C	901	YAG	O23-C18	2.59	1.49	1.44

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	YAG	C19-C18-C17	7.99	118.99	109.68
2	B	901	YAG	C19-C18-C17	7.57	118.50	109.68
2	B	901	YAG	O23-C18-C17	5.53	121.48	108.25
2	D	901	YAG	O23-C18-C17	5.27	120.85	108.25
2	D	901	YAG	O23-C18-C19	4.73	119.57	108.25
2	B	901	YAG	O23-C18-C19	4.71	119.53	108.25
2	C	901	YAG	C19-C20-N15	3.80	115.03	111.16
2	C	901	YAG	C19-C18-C17	3.73	114.03	109.68
2	A	901	YAG	C19-C18-C17	3.67	113.96	109.68
2	A	901	YAG	C19-C20-N15	3.53	114.76	111.16
2	C	901	YAG	C20-C19-C18	2.72	115.94	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	901	YAG	C12-C11-S10	-2.69	109.33	112.00
2	B	901	YAG	C19-C20-N15	2.66	113.87	111.16
2	D	901	YAG	C19-C20-N15	2.63	113.84	111.16
2	C	901	YAG	O22-C21-C18	-2.60	107.78	112.47
2	C	901	YAG	C16-N15-C20	2.54	114.31	108.84
2	A	901	YAG	O22-C21-C18	-2.47	108.02	112.47
2	B	901	YAG	C17-C16-N15	2.44	113.65	111.16
2	A	901	YAG	C12-C11-S10	-2.44	109.58	112.00
2	C	901	YAG	C17-C16-N15	2.37	113.57	111.16
2	B	901	YAG	C16-C17-C18	-2.36	108.62	112.02
2	D	901	YAG	C12-C11-S10	-2.32	109.70	112.00
2	A	901	YAG	C17-C16-N15	2.27	113.47	111.16
2	D	901	YAG	C16-C17-C18	-2.19	108.86	112.02
2	D	901	YAG	C17-C16-N15	2.14	113.34	111.16
2	A	901	YAG	C20-C19-C18	2.13	115.09	112.02
2	A	901	YAG	C16-N15-C20	2.11	113.39	108.84
2	B	901	YAG	C16-N15-C20	2.07	113.31	108.84
2	B	901	YAG	C12-C11-S10	-2.04	109.97	112.00
2	D	901	YAG	C16-N15-C20	2.03	113.21	108.84
2	D	901	YAG	O22-C21-C18	-2.02	108.81	112.47

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	901	YAG	C17-C18-C21-O22
3	B	902	GOL	O1-C1-C2-C3
3	B	903	GOL	O1-C1-C2-C3
3	B	902	GOL	O1-C1-C2-O2
2	B	901	YAG	C09-C06-O07-C08
2	B	901	YAG	C05-C06-O07-C08
2	C	901	YAG	C09-C06-O07-C08
2	C	901	YAG	C05-C06-O07-C08
3	B	903	GOL	O2-C2-C3-O3
2	A	901	YAG	C09-C06-O07-C08
2	A	901	YAG	C05-C06-O07-C08
2	D	901	YAG	O23-C18-C21-O22
3	B	903	GOL	O1-C1-C2-O2
3	D	902	GOL	O2-C2-C3-O3

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	YAG	C16-C17-C18-C19-C20-N15
2	A	901	YAG	C16-C17-C18-C19-C20-N15

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	903	GOL	1	0
3	D	902	GOL	1	0
2	B	901	YAG	1	0
2	C	901	YAG	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.
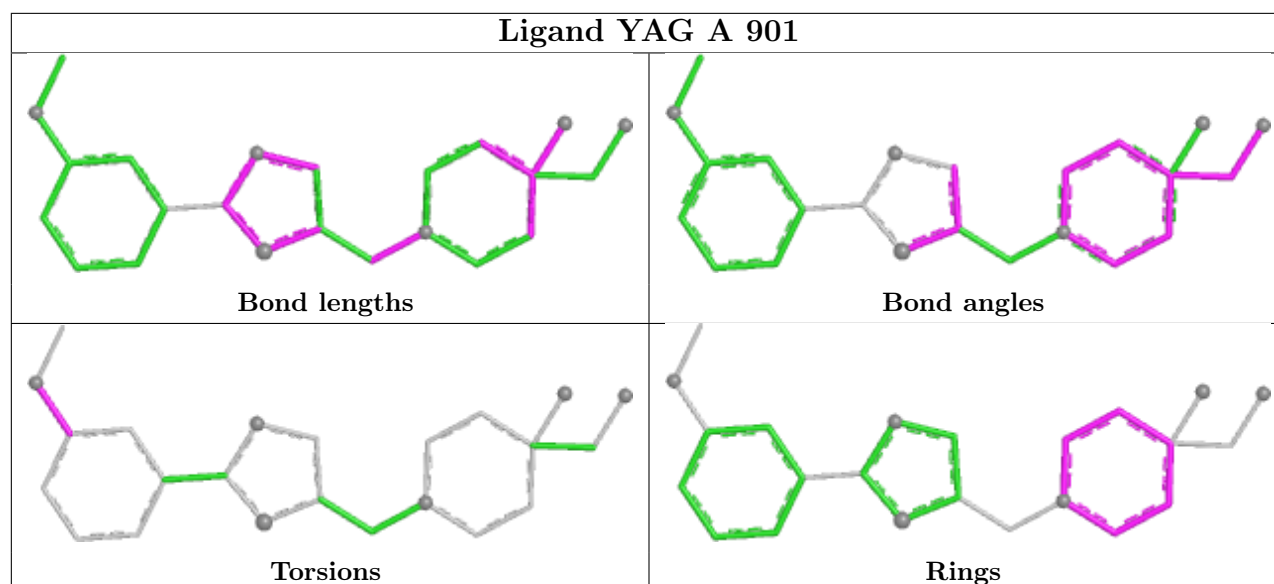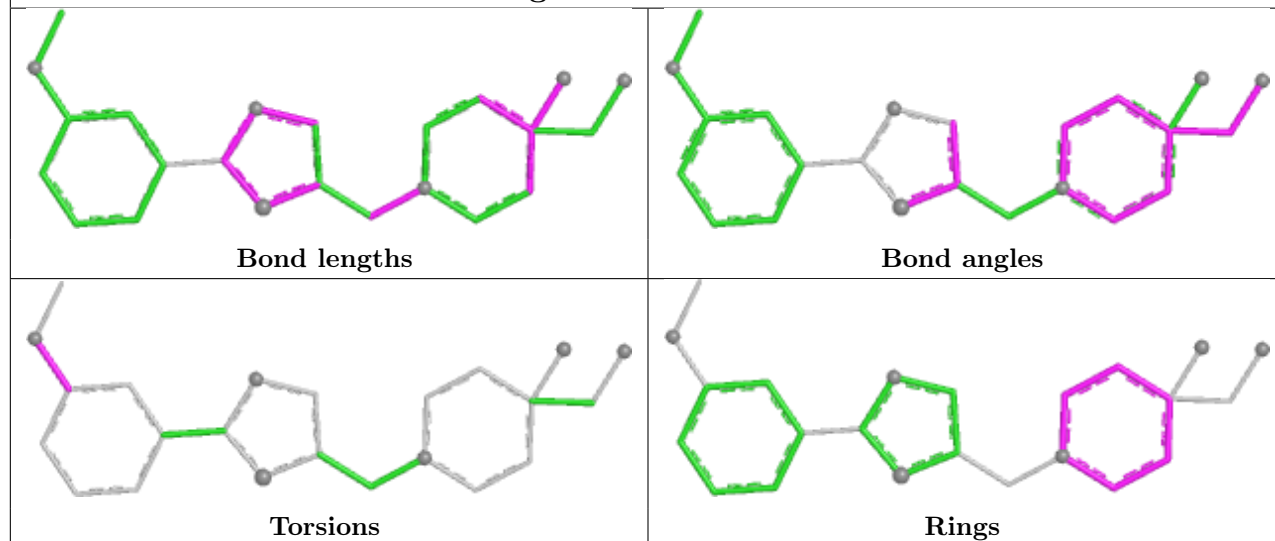

Ligand YAG A 901
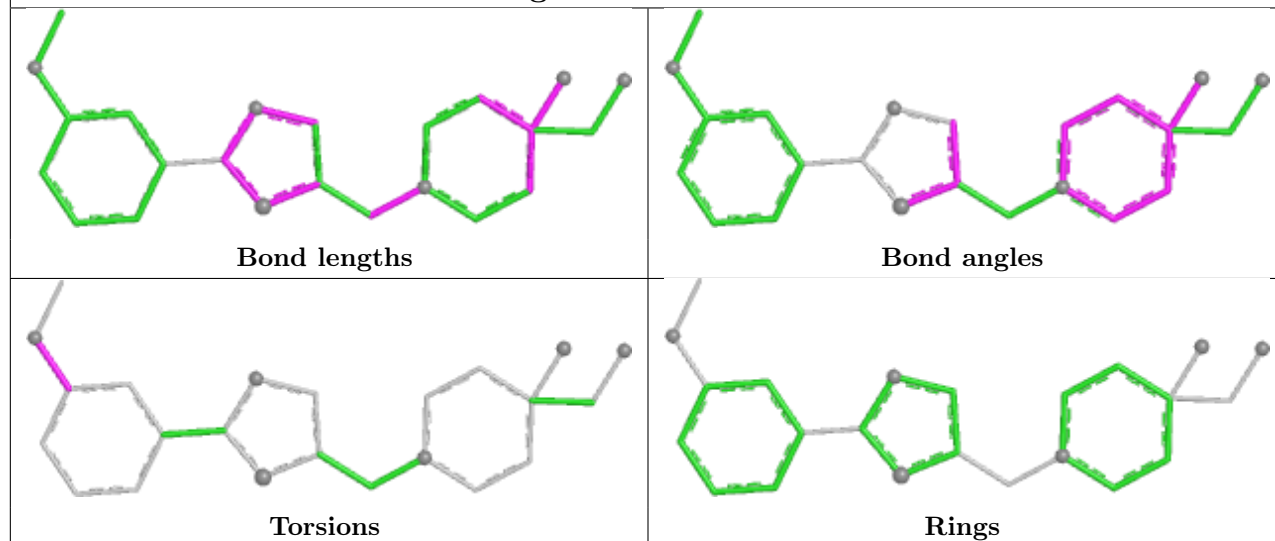
Bond lengths

Bond angles

Torsions

Rings

Ligand YAG B 901

Bond lengths

Bond angles

Torsions

Rings

Ligand YAG D 901

Bond lengths

Bond angles

Torsions

Rings

Ligand YAG C 901

Bond lengths

Bond angles

Torsions

Rings
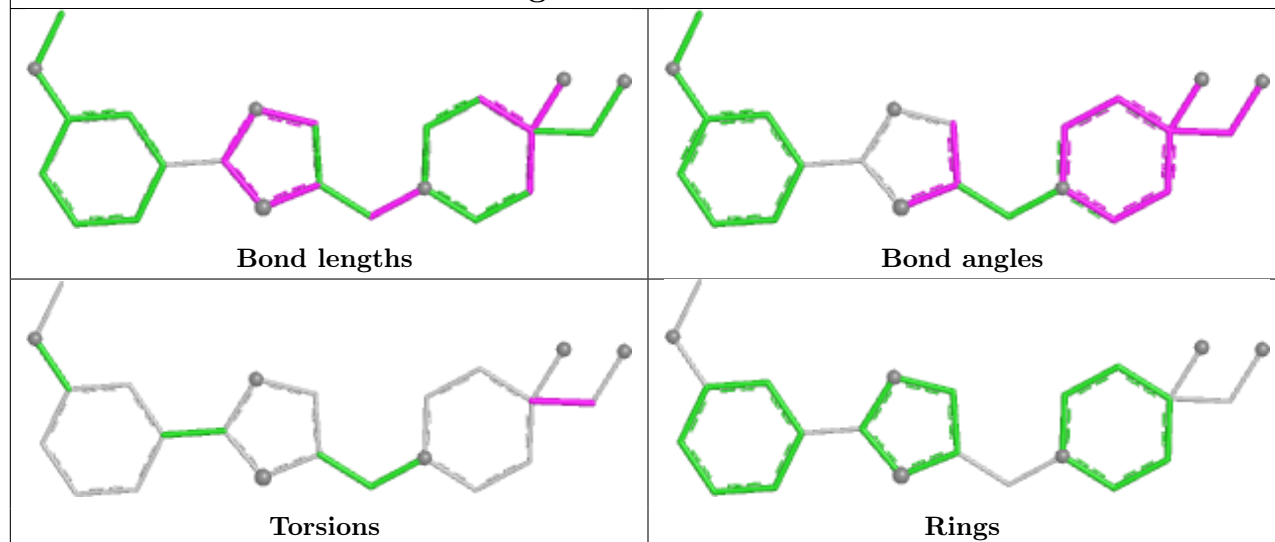
5.7 Other polymers ⓘ

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	732/797 (91%)	-0.20	11 (1%)	71	68	13, 36, 68, 127	1 (0%)
1	B	727/797 (91%)	-0.11	10 (1%)	73	70	12, 36, 69, 110	1 (0%)
1	C	729/797 (91%)	-0.20	13 (1%)	67	64	11, 35, 67, 114	1 (0%)
1	D	719/797 (90%)	0.24	15 (2%)	63	60	14, 49, 82, 116	1 (0%)
All	All	2907/3188 (91%)	-0.07	49 (1%)	69	65	11, 39, 73, 127	4 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	544	ASP	5.1
1	A	647	GLY	4.0
1	D	799	ILE	3.7
1	C	782	ALA	3.4
1	A	4	PRO	3.2
1	C	311	ASP	3.2
1	A	5	PRO	3.2
1	A	639	PRO	3.1
1	C	5	PRO	3.0
1	D	810	VAL	3.0
1	C	481	ILE	2.9
1	D	656	ASP	2.8
1	A	648	ASP	2.7
1	B	639	PRO	2.7
1	B	813	THR	2.7
1	D	721	ALA	2.7
1	B	31	ASN	2.7
1	A	780	SER	2.7
1	C	479	TRP	2.6
1	B	5	PRO	2.6
1	C	313	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	719	LEU	2.6
1	A	180	CYS	2.5
1	B	480	SER	2.5
1	D	784	LEU	2.5
1	D	696	ALA	2.5
1	D	5	PRO	2.4
1	C	637	LEU	2.4
1	D	801	GLY	2.4
1	D	812	GLY	2.4
1	B	696	ALA	2.3
1	A	781	PHE	2.3
1	C	480	SER	2.3
1	A	479	TRP	2.3
1	D	479	TRP	2.2
1	D	642	SER	2.2
1	D	388	THR	2.2
1	B	479	TRP	2.2
1	C	312	VAL	2.2
1	B	642	SER	2.2
1	A	778	TYR	2.1
1	C	721	ALA	2.1
1	D	786	LEU	2.1
1	B	814	GLY	2.1
1	D	507	THR	2.1
1	C	639	PRO	2.1
1	C	289	GLN	2.1
1	A	696	ALA	2.0
1	B	289	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	B	902	6/6	0.80	0.17	50,51,53,54	0
2	YAG	D	901	23/23	0.89	0.14	63,67,73,77	0
2	YAG	C	901	23/23	0.89	0.15	36,62,67,68	0
3	GOL	D	902	6/6	0.89	0.12	45,48,53,58	0
3	GOL	B	903	6/6	0.90	0.11	32,54,57,61	0
3	GOL	A	902	6/6	0.90	0.15	46,52,55,60	0
2	YAG	A	901	23/23	0.91	0.12	34,57,60,60	0
2	YAG	B	901	23/23	0.91	0.12	37,47,50,54	0
4	MG	B	904	1/1	0.97	0.12	31,31,31,31	0

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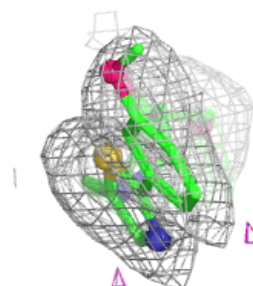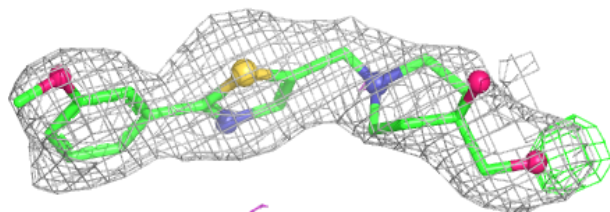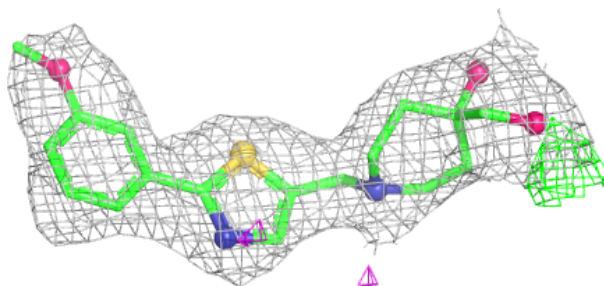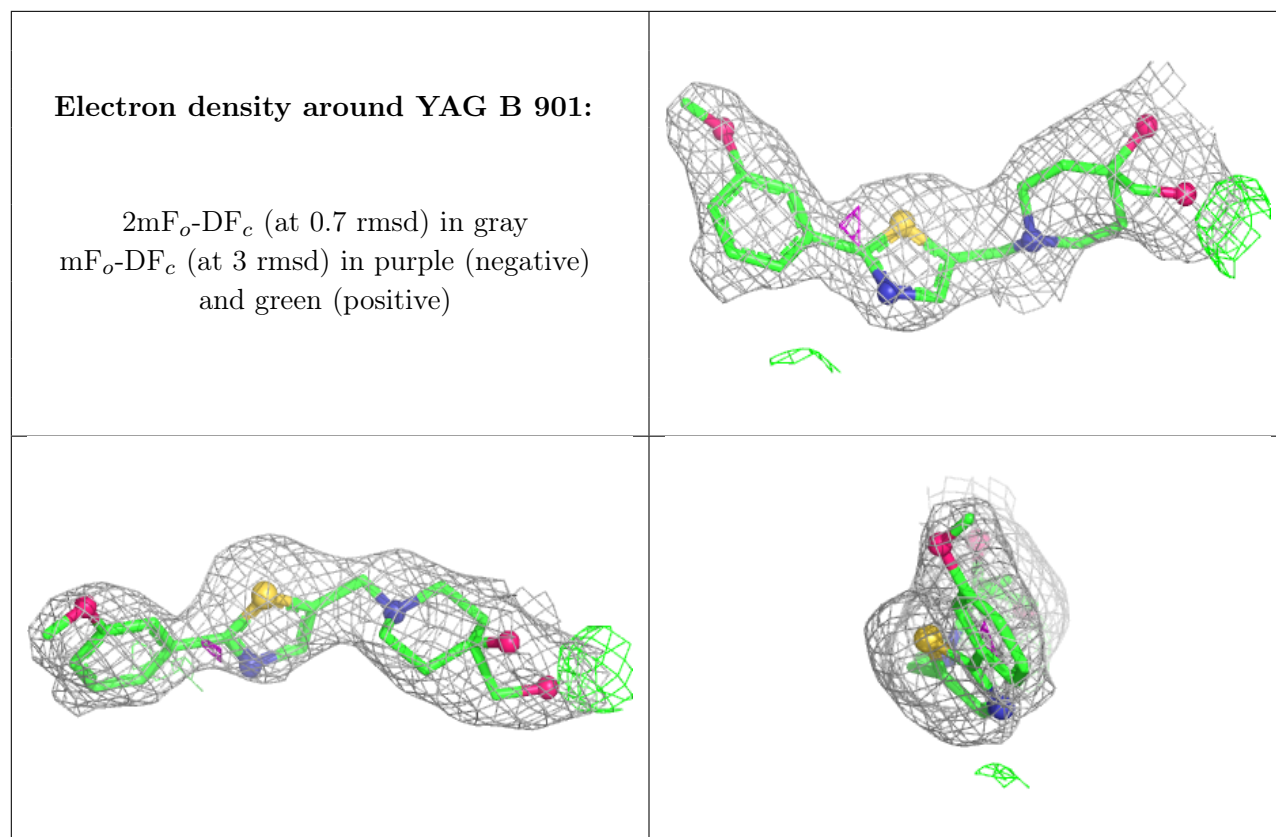

Electron density around YAG D 901:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
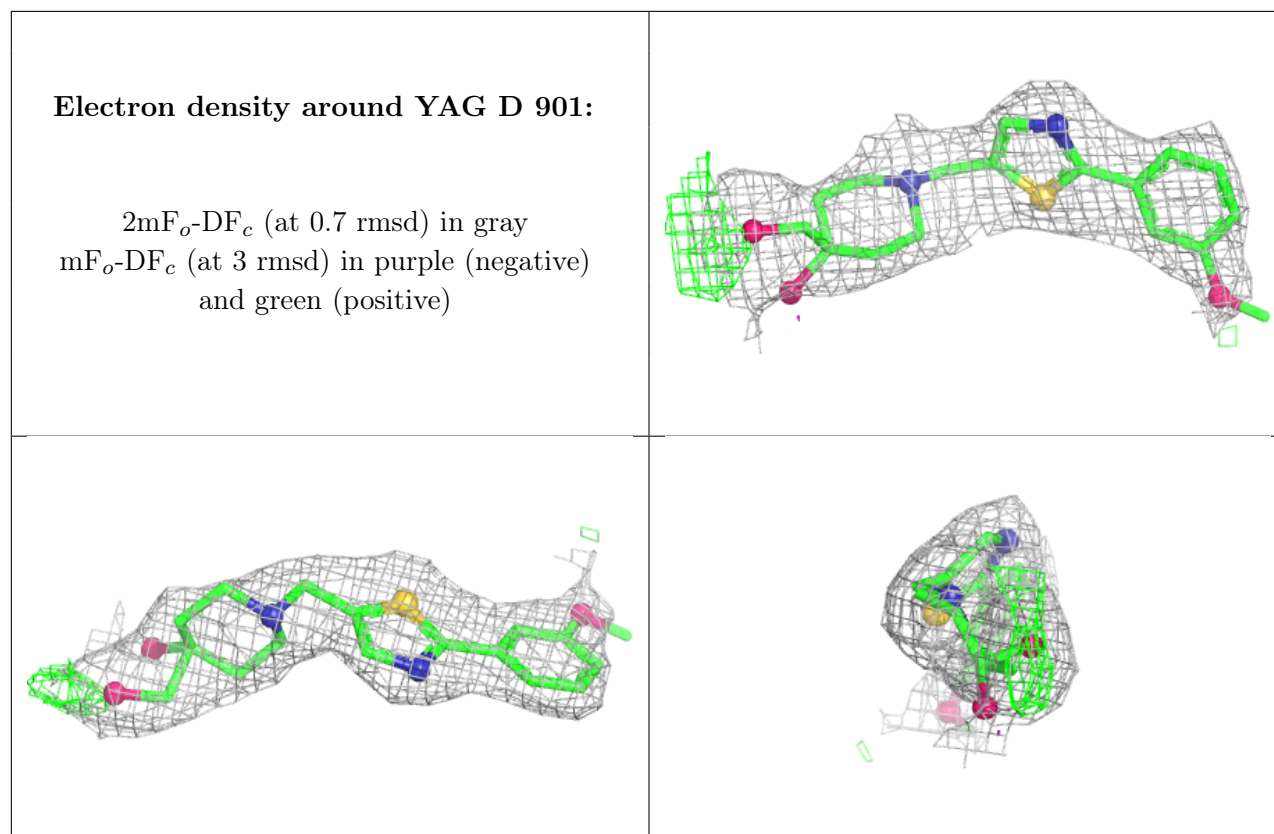
Electron density around YAG C 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
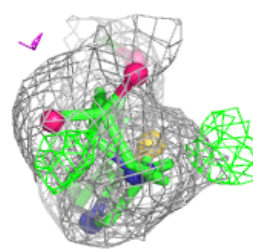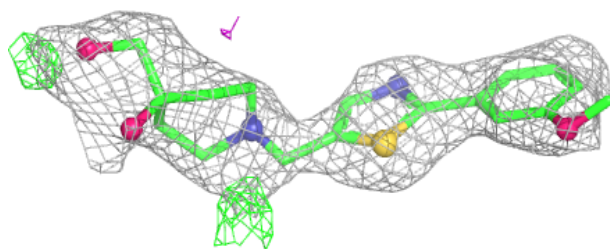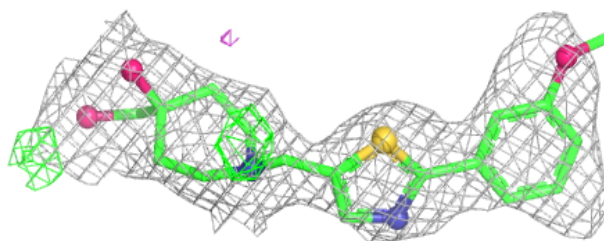
Electron density around YAG A 901:

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

Electron density around YAG B 901:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.