



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:59 AM UTC

PDB ID : 7UXZ / pdb_00007uxz
Title : Crystal structure of SARS-CoV-2 nucleocapsid protein C-terminal domain complexed with Chicoric acid
Authors : Bezerra, E.H.S.; Tonoli, C.C.C.; Soprano, A.S.; Franchini, K.G.; Trivella, D.B.B.; Benedetti, C.E.
Deposited on : 2022-05-06
Resolution : 1.73 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

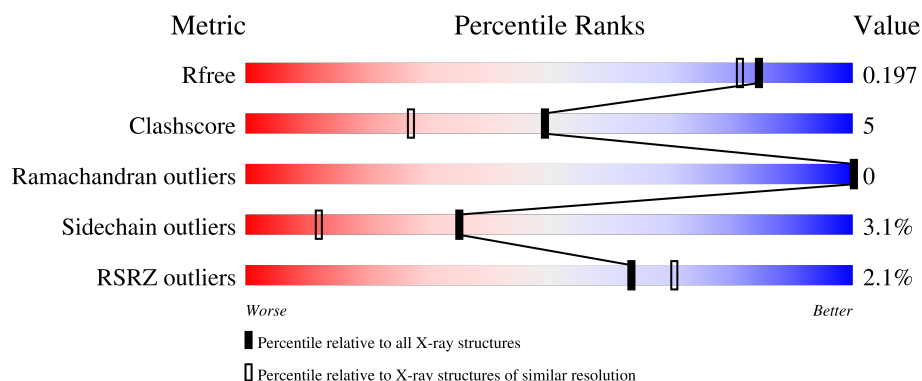
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	114	
1	BBB	114	
1	CCC	114	
1	DDD	114	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	EEE	114	 85% 11% •
1	FFF	114	 2% 80% 16% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	FFF	401	-	-	X	-

2 Entry composition [i](#)

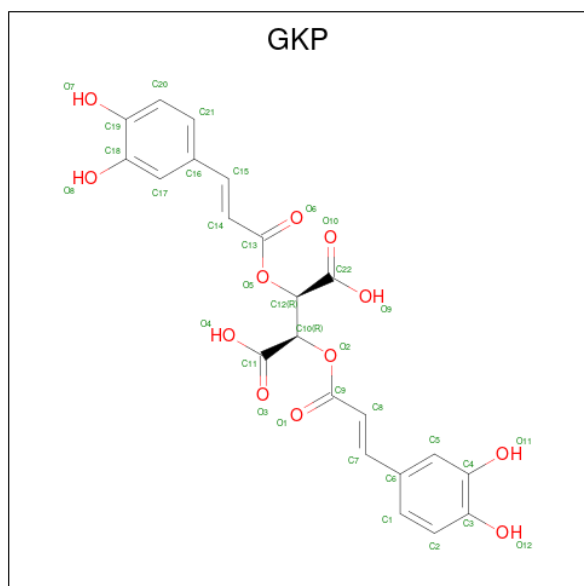
There are 7 unique types of molecules in this entry. The entry contains 6210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nucleoprotein.

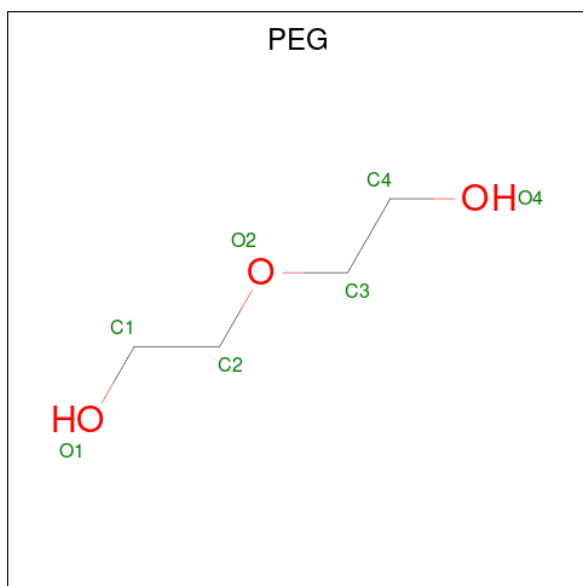
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	109	Total	C	N	O	S	0	3	0
			897	570	161	164	2			
1	BBB	109	Total	C	N	O	S	0	2	0
			890	565	158	164	3			
1	CCC	109	Total	C	N	O	S	0	2	0
			892	567	159	163	3			
1	DDD	109	Total	C	N	O	S	0	3	0
			901	571	162	165	3			
1	EEE	109	Total	C	N	O	S	0	2	0
			890	565	158	164	3			
1	FFF	109	Total	C	N	O	S	0	3	0
			898	570	159	165	4			

- Molecule 2 is (2R,3R)-2,3-bis{[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy}butanedioic acid (CCD ID: GKP) (formula: C₂₂H₁₈O₁₂) (labeled as "Ligand of Interest" by depositor).



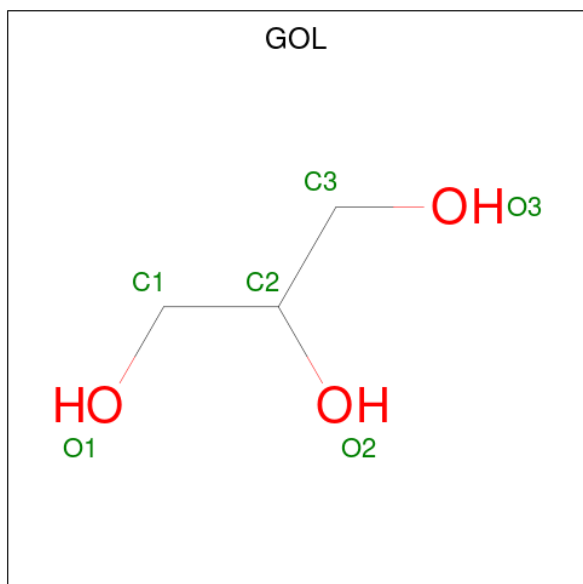
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			34	22	12		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			7	4	3		
3	FFF	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 6 3 3	0	0
4	DDD	1	Total C O 6 3 3	0	0
4	FFF	1	Total C O 6 3 3	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total Na 1 1	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	EEE	1	Total Cl 1 1	0	0

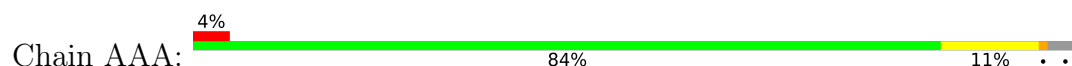
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	112	Total O 112 112	0	0
7	BBB	128	Total O 128 128	0	0
7	CCC	135	Total O 135 135	0	0
7	DDD	142	Total O 142 142	0	0
7	EEE	135	Total O 135 135	0	0
7	FFF	122	Total O 122 122	0	0

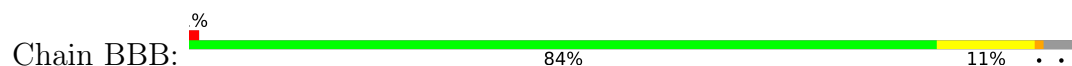
3 Residue-property plots [i](#)

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.

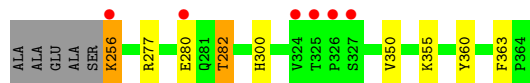
- Molecule 1: Nucleoprotein



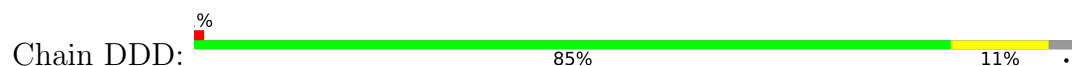
- Molecule 1: Nucleoprotein



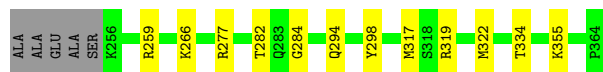
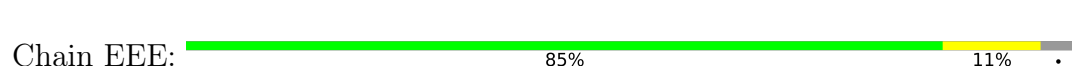
- Molecule 1: Nucleoprotein



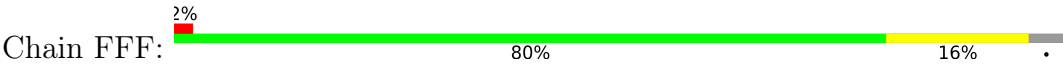
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.67Å 120.66Å 128.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.98 – 1.73 43.98 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.98-1.73) 99.9 (43.98-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.174 , 0.215 (Not available) , 0.197	Depositor DCC
R_{free} test set	3571 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6210	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% 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: CL, GOL, GKP, NA, PEG

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	AAA	1.01	0/926	1.11	0/1247
1	BBB	1.04	0/913	1.12	0/1231
1	CCC	1.02	0/915	1.10	0/1232
1	DDD	1.03	0/924	1.10	0/1245
1	EEE	1.01	1/913 (0.1%)	1.06	0/1231
1	FFF	1.00	0/921	1.11	0/1241
All	All	1.02	1/5512 (0.0%)	1.10	0/7427

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	284	GLY	C-O	5.16	1.30	1.23

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	AAA	897	0	888	10	0
1	BBB	890	0	873	11	0
1	CCC	892	0	878	7	0
1	DDD	901	0	885	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EEE	890	0	873	15	0
1	FFF	898	0	881	19	0
2	AAA	34	0	0	0	0
3	AAA	7	0	10	0	0
3	FFF	7	0	10	4	0
4	AAA	6	0	8	0	0
4	DDD	6	0	8	0	0
4	FFF	6	0	8	1	0
5	AAA	1	0	0	0	0
6	EEE	1	0	0	1	0
7	AAA	112	0	0	5	0
7	BBB	128	0	0	1	0
7	CCC	135	0	0	3	0
7	DDD	142	0	0	4	0
7	EEE	135	0	0	7	0
7	FFF	122	0	0	1	0
All	All	6210	0	5322	58	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 5.

All (58) 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:BBB:319:ARG:HB2	1:BBB:334[B]:THR:HG22	1.63	0.79
1:FFF:288:ASP:H	1:FFF:356:HIS:HD2	1.32	0.77
1:AAA:293[B]:ARG:NH2	7:AAA:601:HOH:O	2.21	0.73
1:EEE:259:ARG:NH1	1:FFF:317[A]:MET:HE3	2.02	0.72
1:EEE:322:MET:CE	1:FFF:353:LEU:HB2	2.19	0.72
7:EEE:504:HOH:O	1:FFF:334[B]:THR:HG21	1.89	0.71
1:BBB:276:ARG:NH1	7:BBB:402:HOH:O	2.23	0.71
1:BBB:288:ASP:H	1:BBB:356:HIS:HD2	1.37	0.70
1:BBB:319:ARG:HB2	1:BBB:334[B]:THR:CG2	2.24	0.68
7:AAA:644:HOH:O	1:BBB:334[B]:THR:HG21	1.95	0.67
1:FFF:348:ASP:HB3	4:FFF:402:GOL:H2	1.77	0.66
1:DDD:334[B]:THR:HG21	7:DDD:676:HOH:O	1.98	0.64
1:FFF:325:THR:HG22	3:FFF:401:PEG:H12	1.84	0.59
1:FFF:281:GLN:O	1:FFF:282:THR:HB	2.03	0.59
1:FFF:323:GLU:HA	3:FFF:401:PEG:H42	1.85	0.57
6:EEE:401:CL:CL	7:EEE:551:HOH:O	2.55	0.56
1:CCC:355:LYS:HE2	7:CCC:516:HOH:O	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:327:SER:O	1:BBB:338:LYS:NZ	2.40	0.54
1:EEE:294:GLN:HE21	1:EEE:298:TYR:HA	1.73	0.53
1:FFF:354:ASN:ND2	7:FFF:503:HOH:O	2.41	0.53
1:EEE:259:ARG:HH11	1:FFF:317[A]:MET:HE3	1.70	0.53
1:FFF:360:TYR:HA	1:FFF:363:PHE:CZ	2.45	0.51
1:FFF:324:VAL:O	3:FFF:401:PEG:H31	2.10	0.51
1:AAA:272:GLN:NE2	7:AAA:605:HOH:O	2.40	0.50
1:FFF:324:VAL:H	3:FFF:401:PEG:H42	1.75	0.50
1:AAA:353:LEU:HB2	1:BBB:322[A]:MET:HE1	1.94	0.49
1:EEE:334:THR:OG1	1:FFF:334[A]:THR:HG22	2.12	0.49
1:AAA:281:GLN:HA	1:BBB:319:ARG:HD2	1.93	0.49
1:EEE:319:ARG:HB2	1:EEE:334:THR:HG22	1.95	0.48
1:DDD:281:GLN:HG3	7:DDD:738:HOH:O	2.14	0.47
1:BBB:276:ARG:HH11	1:BBB:276:ARG:HB3	1.80	0.47
1:EEE:266:LYS:CE	7:EEE:506:HOH:O	2.63	0.46
1:CCC:280:GLU:OE1	1:CCC:282:THR:HG22	2.16	0.46
1:CCC:300:HIS:HD2	7:CCC:499:HOH:O	1.98	0.45
1:CCC:350:VAL:HG13	1:DDD:322[B]:MET:HE1	1.98	0.45
1:AAA:293[A]:ARG:NH1	1:AAA:294:GLN:HE21	2.14	0.45
1:BBB:299:LYS:HD3	1:BBB:299:LYS:HA	1.84	0.44
1:EEE:294:GLN:NE2	7:EEE:501:HOH:O	2.23	0.44
1:DDD:360:TYR:HA	1:DDD:363:PHE:CZ	2.53	0.44
1:BBB:360:TYR:HA	1:BBB:363:PHE:CZ	2.53	0.43
1:EEE:322:MET:HE1	1:FFF:350:VAL:HA	2.00	0.43
1:EEE:322:MET:HE3	1:FFF:353:LEU:HB2	1.99	0.43
1:DDD:340:ASP:OD2	7:DDD:601:HOH:O	2.21	0.43
1:AAA:355:LYS:HB2	1:AAA:355:LYS:HE2	1.81	0.43
1:DDD:345:ASN:ND2	7:DDD:608:HOH:O	2.51	0.42
1:EEE:266:LYS:NZ	7:EEE:506:HOH:O	2.52	0.42
1:EEE:322:MET:CE	1:FFF:353:LEU:CB	2.94	0.42
1:AAA:300:HIS:HD2	7:AAA:690:HOH:O	2.01	0.42
1:EEE:317[A]:MET:HE3	1:FFF:259:ARG:NH1	2.34	0.42
1:AAA:259:ARG:NH1	7:AAA:609:HOH:O	2.48	0.41
1:FFF:299:LYS:HA	1:FFF:299:LYS:HD3	1.83	0.41
1:CCC:360:TYR:HA	1:CCC:363:PHE:CE2	2.55	0.41
7:CCC:446:HOH:O	1:DDD:338:LYS:HE2	2.20	0.41
1:AAA:360:TYR:HA	1:AAA:363:PHE:CE2	2.55	0.41
1:CCC:280:GLU:OE1	1:CCC:282:THR:CG2	2.69	0.41
1:EEE:282[A]:THR:HG21	7:EEE:603:HOH:O	2.21	0.41
1:EEE:282[A]:THR:CG2	7:EEE:603:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	110/114 (96%)	108 (98%)	2 (2%)	0	100	100
1	BBB	109/114 (96%)	108 (99%)	1 (1%)	0	100	100
1	CCC	108/114 (95%)	106 (98%)	2 (2%)	0	100	100
1	DDD	110/114 (96%)	109 (99%)	1 (1%)	0	100	100
1	EEE	109/114 (96%)	107 (98%)	2 (2%)	0	100	100
1	FFF	110/114 (96%)	108 (98%)	2 (2%)	0	100	100
All	All	656/684 (96%)	646 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	94/93 (101%)	91 (97%)	3 (3%)	34	11
1	BBB	93/93 (100%)	89 (96%)	4 (4%)	26	6
1	CCC	93/93 (100%)	89 (96%)	4 (4%)	26	6
1	DDD	94/93 (101%)	90 (96%)	4 (4%)	26	6
1	EEE	93/93 (100%)	91 (98%)	2 (2%)	45	22
1	FFF	94/93 (101%)	93 (99%)	1 (1%)	65	50
All	All	561/558 (100%)	543 (97%)	18 (3%)	35	11

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	266	LYS
1	AAA	277	ARG
1	AAA	355	LYS
1	BBB	256	LYS
1	BBB	276	ARG
1	BBB	277	ARG
1	BBB	347	LYS
1	CCC	256[A]	LYS
1	CCC	256[B]	LYS
1	CCC	277	ARG
1	CCC	282	THR
1	DDD	256	LYS
1	DDD	277	ARG
1	DDD	282	THR
1	DDD	342	LYS
1	EEE	277	ARG
1	EEE	355	LYS
1	FFF	277	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	FFF	402	-	5,5,5	0.29	0	5,5,5	0.70	0
3	PEG	AAA	502	-	6,6,6	0.16	0	5,5,5	0.21	0
4	GOL	AAA	503	-	5,5,5	0.13	0	5,5,5	0.37	0
3	PEG	FFF	401	-	6,6,6	0.23	0	5,5,5	0.17	0
2	GKP	AAA	501	-	35,35,35	1.51	8 (22%)	46,48,48	2.94	20 (43%)
4	GOL	DDD	501	-	5,5,5	0.23	0	5,5,5	0.63	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
4	GOL	FFF	402	-	-	2/4/4/4	-
3	PEG	AAA	502	-	-	3/4/4/4	-
4	GOL	AAA	503	-	-	3/4/4/4	-
3	PEG	FFF	401	-	-	1/4/4/4	-
2	GKP	AAA	501	-	-	12/30/30/30	0/2/2/2
4	GOL	DDD	501	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	501	GKP	O2-C9	3.05	1.41	1.34
2	AAA	501	GKP	O8-C18	2.92	1.42	1.36
2	AAA	501	GKP	C8-C9	2.74	1.54	1.48
2	AAA	501	GKP	O5-C13	2.58	1.40	1.34
2	AAA	501	GKP	C14-C13	2.39	1.53	1.48
2	AAA	501	GKP	O12-C3	2.32	1.41	1.36
2	AAA	501	GKP	C16-C15	2.29	1.54	1.47
2	AAA	501	GKP	O11-C4	2.18	1.40	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	501	GKP	C12-C10-C11	10.15	131.06	110.72
2	AAA	501	GKP	C16-C15-C14	8.05	144.51	126.92
2	AAA	501	GKP	O5-C12-C10	-7.53	94.90	107.13
2	AAA	501	GKP	O5-C12-C22	-4.26	102.54	111.24
2	AAA	501	GKP	O2-C9-C8	4.24	120.62	111.39
2	AAA	501	GKP	O2-C10-C12	3.96	113.57	107.13
2	AAA	501	GKP	C10-C12-C22	3.82	118.37	110.72
2	AAA	501	GKP	O9-C22-C12	3.15	125.01	113.64
2	AAA	501	GKP	O4-C11-O3	-3.12	117.00	124.08
2	AAA	501	GKP	C1-C6-C5	2.88	122.35	118.72
2	AAA	501	GKP	C17-C16-C15	-2.72	112.48	120.61
2	AAA	501	GKP	O4-C11-C10	2.62	123.09	113.64
2	AAA	501	GKP	C5-C6-C7	-2.32	113.69	120.61
2	AAA	501	GKP	C2-C1-C6	-2.30	118.25	121.22
2	AAA	501	GKP	C21-C16-C17	2.23	121.53	118.72
2	AAA	501	GKP	O9-C22-O10	-2.17	119.15	124.08
2	AAA	501	GKP	O1-C9-C8	-2.17	116.31	123.69
2	AAA	501	GKP	C6-C5-C4	-2.14	119.28	120.79
2	AAA	501	GKP	C20-C21-C16	-2.12	118.48	121.22
2	AAA	501	GKP	O5-C13-O6	2.12	126.74	123.34

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	501	GKP	C11-C10-C12-O5
2	AAA	501	GKP	C12-C10-O2-C9
2	AAA	501	GKP	O1-C9-O2-C10
2	AAA	501	GKP	C7-C8-C9-O2
3	AAA	502	PEG	C4-C3-O2-C2
3	AAA	502	PEG	O1-C1-C2-O2
2	AAA	501	GKP	C8-C9-O2-C10
2	AAA	501	GKP	C7-C8-C9-O1
2	AAA	501	GKP	O2-C10-C11-O3
4	DDD	501	GOL	C1-C2-C3-O3
4	FFF	402	GOL	C1-C2-C3-O3
4	DDD	501	GOL	O2-C2-C3-O3
2	AAA	501	GKP	O2-C10-C11-O4
3	FFF	401	PEG	O1-C1-C2-O2
2	AAA	501	GKP	O5-C13-C14-C15
4	FFF	402	GOL	O2-C2-C3-O3
2	AAA	501	GKP	C11-C10-C12-C22
2	AAA	501	GKP	O6-C13-C14-C15

Continued on next page...

Continued from previous page...

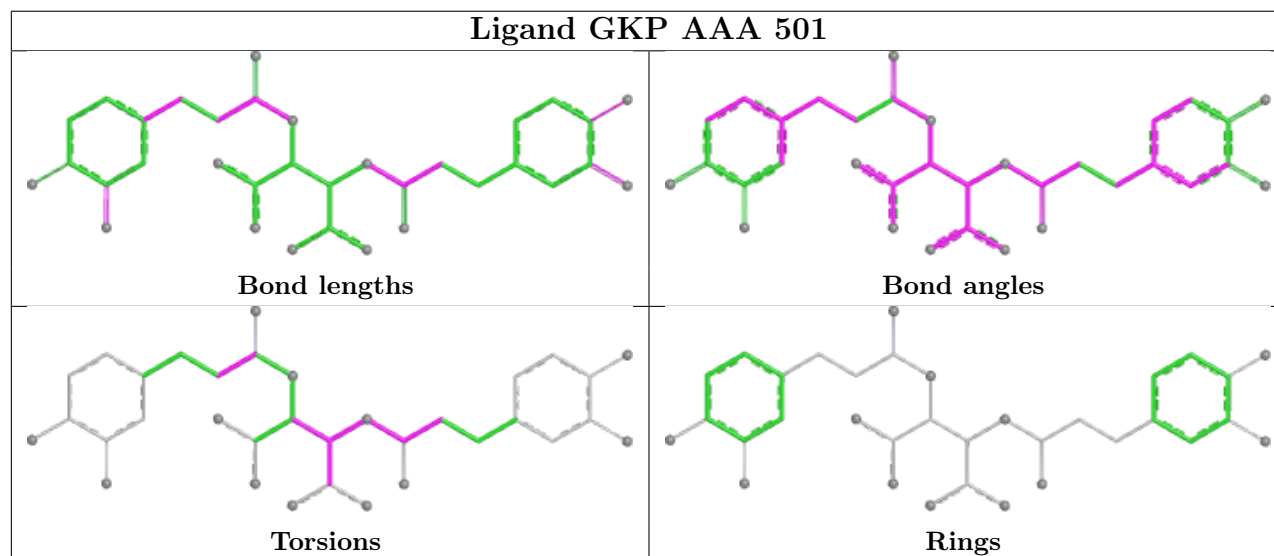
Mol	Chain	Res	Type	Atoms
4	AAA	503	GOL	O2-C2-C3-O3
2	AAA	501	GKP	O2-C10-C12-C22
4	AAA	503	GOL	O1-C1-C2-C3
3	AAA	502	PEG	O2-C3-C4-O4
4	AAA	503	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	FFF	402	GOL	1	0
3	FFF	401	PEG	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	AAA	109/114 (95%)	0.08	4 (3%)	45 54	10, 21, 40, 65	3 (2%)
1	BBB	109/114 (95%)	-0.07	1 (0%)	81 87	7, 19, 38, 53	2 (1%)
1	CCC	109/114 (95%)	-0.07	6 (5%)	30 37	11, 16, 44, 53	2 (1%)
1	DDD	109/114 (95%)	-0.35	1 (0%)	81 87	7, 15, 29, 42	3 (2%)
1	EEE	109/114 (95%)	-0.32	0	100 100	8, 15, 33, 47	2 (1%)
1	FFF	109/114 (95%)	-0.28	2 (1%)	67 74	6, 17, 32, 57	3 (2%)
All	All	654/684 (95%)	-0.17	14 (2%)	63 70	6, 17, 38, 65	15 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	324	VAL	4.0
1	CCC	327	SER	3.7
1	CCC	325	THR	3.5
1	AAA	256	LYS	3.3
1	FFF	256	LYS	3.3
1	CCC	326	PRO	3.0
1	FFF	282	THR	2.6
1	CCC	256[A]	LYS	2.5
1	BBB	256	LYS	2.5
1	DDD	256	LYS	2.4
1	AAA	267	ALA	2.3
1	AAA	364	PRO	2.2
1	AAA	294	GLN	2.1
1	CCC	280	GLU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

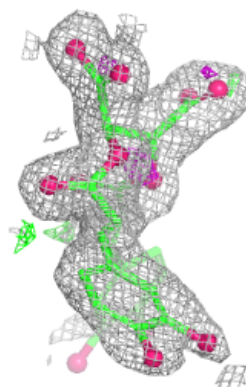
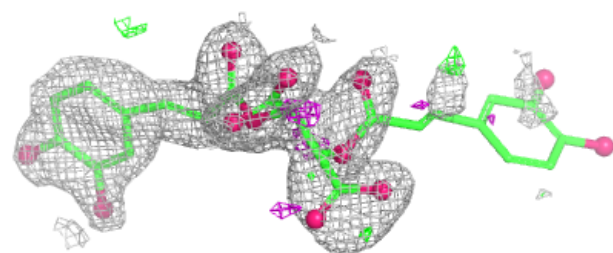
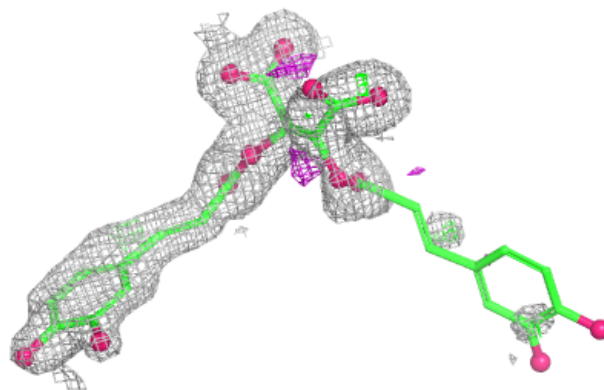
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	FFF	401	7/7	0.72	0.19	38,45,54,58	0
3	PEG	AAA	502	7/7	0.75	0.19	53,54,59,64	0
4	GOL	AAA	503	6/6	0.79	0.16	46,50,51,52	0
4	GOL	DDD	501	6/6	0.81	0.14	26,31,35,39	0
4	GOL	FFF	402	6/6	0.81	0.15	29,36,38,38	0
2	GKP	AAA	501	34/34	0.86	0.14	28,43,100,106	0
6	CL	EEE	401	1/1	0.91	0.10	60,60,60,60	0
5	NA	AAA	504	1/1	0.93	0.07	36,36,36,36	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 GKP AAA 501:

$2mF_o-DF_c$ (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.