



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:12 AM UTC

PDB ID : 5JCZ / pdb_00005jcz
Title : Rab11 bound to MyoVa-GTD
Authors : Pylypenko, O.; Attanda, W.; Gauquelin, C.; Malherbes, G.; Houdusse, A.
Deposited on : 2016-04-15
Resolution : 2.06 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:

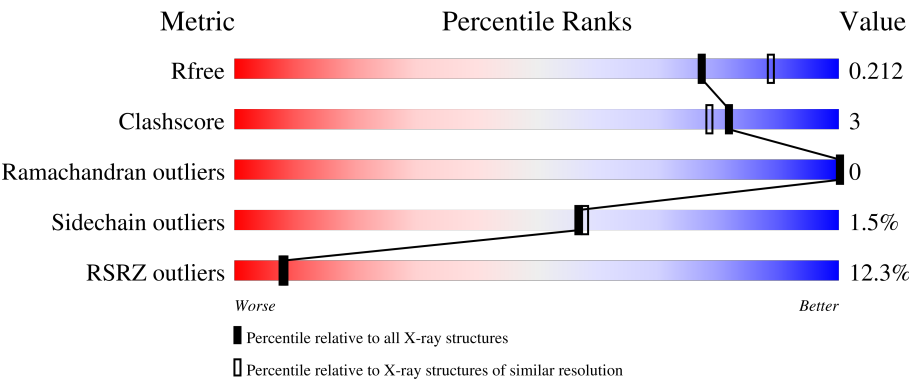
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	179	2% 89% 7% .
1	D	179	2% 92% . . .
1	I	179	71% 82% 18%
2	B	397	9% 84% 7% . 8%
2	C	397	3% 84% 7% . 8%

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Mol	Chain	Length	Quality of chain
2	E	397	4% 82% 8% • 9%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13842 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 Ras-related protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	6	0
			1391	883	236	271	1			
1	D	173	Total	C	N	O	S	0	3	0
			1386	880	239	266	1			
1	I	147	Total	C	N	O	S	0	0	0
			980	606	176	197	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P62491
A	0	ALA	-	expression tag	UNP P62491
D	-1	GLY	-	expression tag	UNP P62491
D	0	ALA	-	expression tag	UNP P62491
I	-1	GLY	-	expression tag	UNP P62491
I	0	ALA	-	expression tag	UNP P62491

- Molecule 2 is a protein called Unconventional myosin-Va.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	0	3	0
			2891	1852	490	526	23			
2	C	364	Total	C	N	O	S	0	8	0
			2948	1882	501	541	24			
2	E	361	Total	C	N	O	S	0	6	0
			2920	1861	500	537	22			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1457	GLY	-	expression tag	UNP Q9Y4I1
B	1458	ALA	-	expression tag	UNP Q9Y4I1

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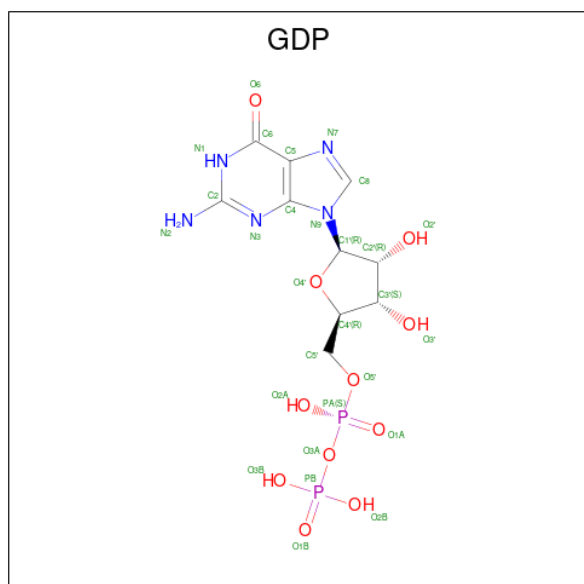
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1459	MET	-	expression tag	UNP Q9Y4I1
B	1460	GLY	-	expression tag	UNP Q9Y4I1
B	1461	SER	-	expression tag	UNP Q9Y4I1
C	1457	GLY	-	expression tag	UNP Q9Y4I1
C	1458	ALA	-	expression tag	UNP Q9Y4I1
C	1459	MET	-	expression tag	UNP Q9Y4I1
C	1460	GLY	-	expression tag	UNP Q9Y4I1
C	1461	SER	-	expression tag	UNP Q9Y4I1
E	1457	GLY	-	expression tag	UNP Q9Y4I1
E	1458	ALA	-	expression tag	UNP Q9Y4I1
E	1459	MET	-	expression tag	UNP Q9Y4I1
E	1460	GLY	-	expression tag	UNP Q9Y4I1
E	1461	SER	-	expression tag	UNP Q9Y4I1

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

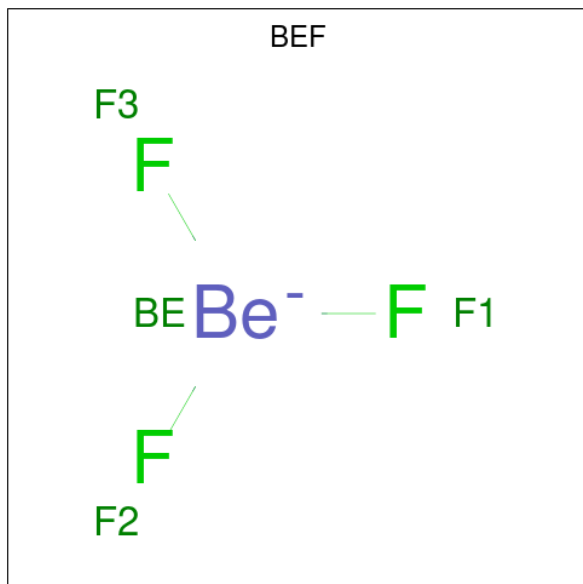
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	I	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Be	F	0	0
			4	1	3		
5	D	1	Total	Be	F	0	0
			4	1	3		
5	I	1	Total	Be	F	0	0
			4	1	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



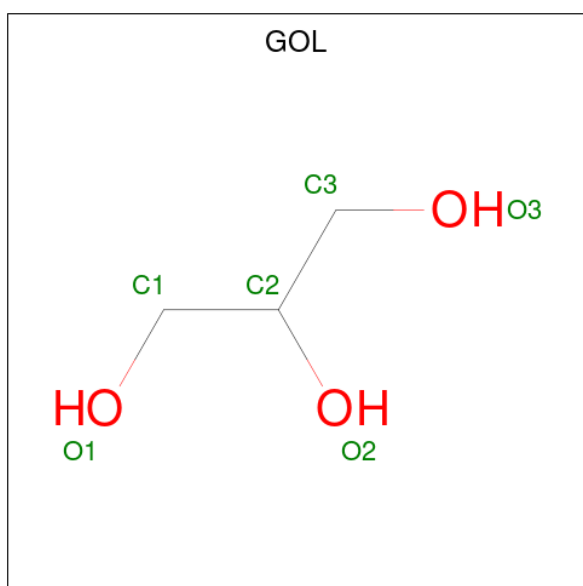
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

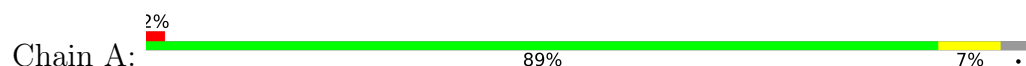
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	210	Total 210	O 210	0	0
9	B	163	Total 163	O 163	0	0
9	C	377	Total 377	O 377	0	0
9	D	146	Total 146	O 146	0	0
9	E	250	Total 250	O 250	0	0
9	I	8	Total 8	O 8	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.

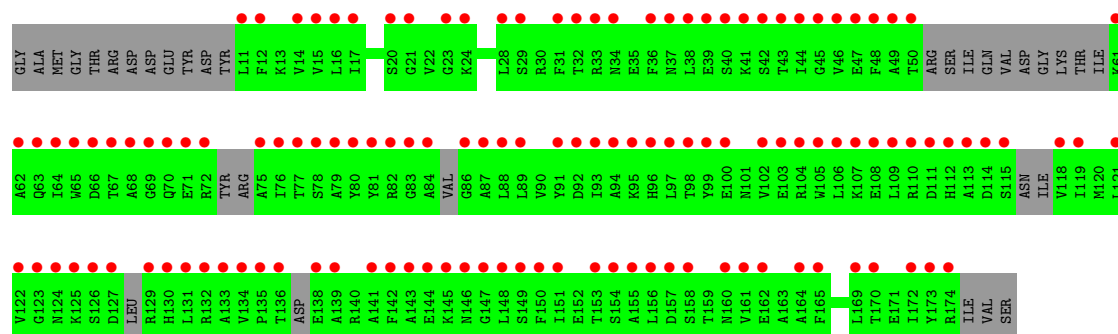
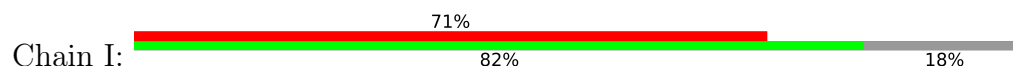
- Molecule 1: Ras-related protein Rab-11A



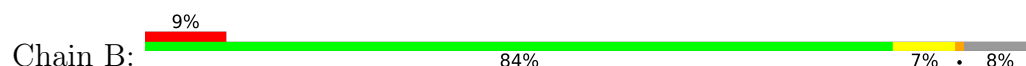
- Molecule 1: Ras-related protein Rab-11A

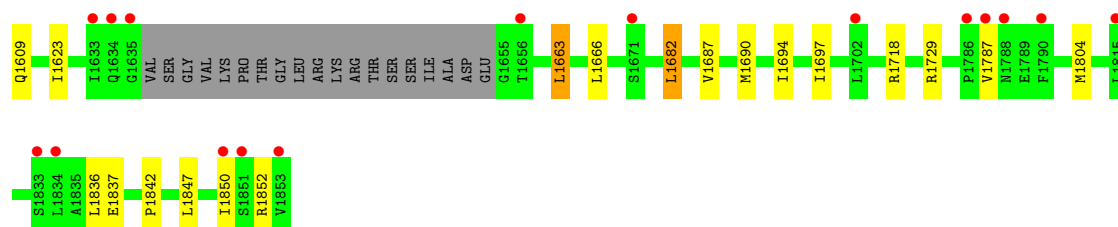


- Molecule 1: Ras-related protein Rab-11A

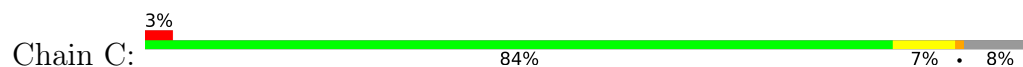


- Molecule 2: Unconventional myosin-Va

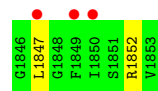
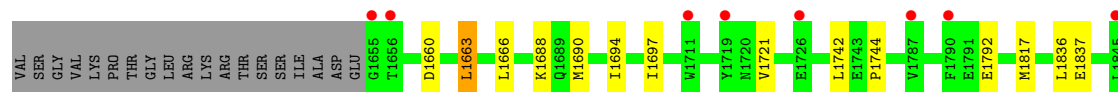
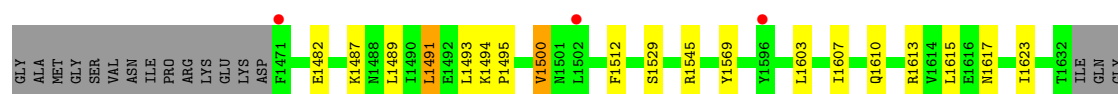
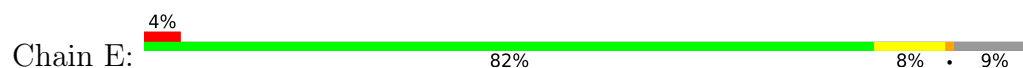




• Molecule 2: Unconventional myosin-Va



• Molecule 2: Unconventional myosin-Va



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.79Å 128.42Å 89.02Å 90.00° 98.27° 90.00°	Depositor
Resolution (Å)	48.88 – 2.06 48.88 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.88-2.06) 98.6 (48.88-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.180 , 0.208 0.185 , 0.212	Depositor DCC
R_{free} test set	7339 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13842	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, EDO, MG, GOL, GDP, ACT

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	0.26	0/1431	0.64	0/1934
1	D	0.26	0/1411	0.65	0/1908
1	I	0.27	0/986	0.65	0/1339
2	B	0.26	0/2949	0.69	0/3982
2	C	0.27	0/3021	0.68	1/4077 (0.0%)
2	E	0.26	0/2988	0.69	0/4034
All	All	0.26	0/12786	0.67	1/17274 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1623	ILE	N-CA-C	5.17	115.39	110.53

There are no chirality outliers.

There are no planarity outliers.

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1391	0	1388	9	0
1	D	1386	0	1375	5	0
1	I	980	0	804	0	0
2	B	2891	0	2917	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2948	0	3012	18	0
2	E	2920	0	2965	18	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
4	A	28	0	12	1	0
4	D	28	0	12	1	0
4	I	28	0	12	0	0
5	A	4	0	0	0	0
5	D	4	0	0	0	0
5	I	4	0	0	0	0
6	A	12	0	18	2	0
6	B	8	0	12	0	0
6	C	16	0	24	2	0
6	D	8	0	12	0	0
6	E	8	0	12	0	0
7	A	4	0	3	0	0
7	C	4	0	3	0	0
8	A	6	0	8	0	0
8	B	6	0	8	1	0
9	A	210	0	0	0	0
9	B	163	0	0	0	0
9	C	377	0	0	2	0
9	D	146	0	0	0	0
9	E	250	0	0	2	0
9	I	8	0	0	0	0
All	All	13842	0	12597	64	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 3.

All (64) 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:28[B]:LEU:HD11	1:A:49:ALA:HB3	1.68	0.74
2:C:1623:ILE:HD12	2:C:1697:ILE:HD12	1.70	0.73
2:C:1491:LEU:HG	6:C:1903:EDO:H12	1.70	0.72
2:B:1623[A]:ILE:HD12	2:B:1697:ILE:HD12	1.73	0.71
1:D:28[B]:LEU:HD11	1:D:49:ALA:HB3	1.71	0.71
2:C:1623:ILE:HD13	2:C:1694:ILE:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1623[A]:ILE:HD13	2:B:1694:ILE:HA	1.80	0.63
2:E:1623:ILE:HD12	2:E:1697:ILE:HD12	1.83	0.60
2:C:1615:LEU:HD13	2:C:1690:MET:HG2	1.85	0.59
2:C:1487:LYS:HA	2:C:1491:LEU:HB2	1.85	0.57
2:E:1623:ILE:HD13	2:E:1694:ILE:HA	1.86	0.57
2:E:1615:LEU:HD13	2:E:1690:MET:HG2	1.86	0.56
2:E:1744:PRO:HG2	2:E:1817[A]:MET:HE1	1.89	0.55
2:E:1617[B]:ASN:ND2	9:E:2004:HOH:O	2.33	0.55
2:E:1491:LEU:O	2:E:1545:ARG:NH1	2.41	0.54
2:C:1540:LYS:HE2	6:C:1903:EDO:H11	1.90	0.53
2:E:1688:LYS:NZ	9:E:2003:HOH:O	2.32	0.53
2:B:1837:GLU:O	2:B:1852:ARG:NH1	2.41	0.53
2:B:1687:VAL:HA	2:B:1690:MET:HE2	1.91	0.51
2:E:1610[A]:GLN:OE1	2:E:1613:ARG:NH1	2.33	0.51
2:E:1603:LEU:O	2:E:1607:ILE:HG13	2.12	0.50
2:E:1837:GLU:O	2:E:1852:ARG:NH1	2.42	0.49
2:E:1487:LYS:HA	2:E:1491:LEU:HB2	1.94	0.49
1:A:17:ILE:HG22	6:A:204:EDO:H21	1.94	0.48
1:D:125:LYS:HG2	4:D:202:GDP:C6	2.48	0.48
2:C:1793:ARG:NH1	9:C:2015:HOH:O	2.46	0.48
2:E:1721:VAL:HG13	2:E:1742:LEU:HD23	1.96	0.48
1:A:125:LYS:HG2	4:A:202:GDP:C6	2.49	0.47
1:A:129:ARG:HB3	6:A:205:EDO:H12	1.97	0.47
2:B:1499:ALA:HB1	2:B:1842:PRO:HG2	1.96	0.47
2:C:1628:LEU:O	2:C:1713:LYS:NZ	2.36	0.47
2:C:1603:LEU:O	2:C:1607:ILE:HG13	2.15	0.46
2:B:1603:LEU:O	2:B:1607:ILE:HG13	2.14	0.46
2:C:1485:LEU:HG	2:C:1850:ILE:HD11	1.97	0.45
2:C:1512:PHE:CZ	2:C:1569:TYR:HB2	2.51	0.45
2:B:1512:PHE:CZ	2:B:1569:TYR:HB2	2.51	0.45
2:E:1489:LEU:HD13	2:E:1847:LEU:HD11	1.99	0.45
2:C:1482:GLU:OE2	2:C:1529:SER:OG	2.24	0.45
2:C:1687:VAL:HA	2:C:1690:MET:HE2	2.00	0.44
1:A:33:ARG:HD2	2:B:1729:ARG:NH2	2.33	0.44
2:C:1705:ARG:HB3	2:C:1707:ASP:OD1	2.18	0.44
2:E:1512:PHE:CZ	2:E:1569:TYR:HB2	2.53	0.44
2:C:1483:GLN:NE2	9:C:2008:HOH:O	2.36	0.43
2:E:1493:LEU:HD21	2:E:1500:VAL:HG21	2.00	0.43
1:A:120:MET:HE1	1:A:167:THR:HB	2.01	0.43
1:A:94:ALA:O	2:C:1833[B]:SER:OG	2.35	0.43
2:B:1491:LEU:HD11	2:B:1540:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:MET:HE1	1:D:167:THR:HB	2.01	0.42
2:B:1682:LEU:HD12	2:B:1682:LEU:HA	1.91	0.42
1:D:17:ILE:HD11	1:D:89:LEU:HG	2.02	0.42
1:A:12:PHE:CE1	1:A:60:ILE:HD13	2.55	0.41
1:D:170:THR:O	1:D:174:ARG:HG2	2.19	0.41
2:E:1482:GLU:OE2	2:E:1529:SER:OG	2.24	0.41
2:B:1663:LEU:HD12	2:B:1663:LEU:HA	1.83	0.41
1:A:145:LYS:HE3	1:A:145:LYS:HB2	1.83	0.41
2:B:1485:LEU:HD13	2:B:1850:ILE:HD11	2.01	0.41
2:C:1494:LYS:HA	2:C:1495:PRO:HD3	1.96	0.41
2:E:1494:LYS:HA	2:E:1495:PRO:HD3	1.88	0.41
2:B:1475:LEU:HG	2:B:1513:MET:HE2	2.03	0.41
2:B:1718:ARG:HA	2:B:1718:ARG:HD2	1.89	0.40
2:B:1847:LEU:HB3	2:B:1850:ILE:HD12	2.03	0.40
2:E:1663:LEU:HD12	2:E:1663:LEU:HA	1.89	0.40
2:C:1681:GLU:HB2	2:C:1828:PRO:HG3	2.02	0.40
2:B:1718:ARG:NH2	8:B:1903:GOL:H11	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	176/179 (98%)	175 (99%)	1 (1%)	0	100	100
1	D	174/179 (97%)	173 (99%)	1 (1%)	0	100	100
1	I	133/179 (74%)	130 (98%)	3 (2%)	0	100	100
2	B	363/397 (91%)	353 (97%)	10 (3%)	0	100	100
2	C	368/397 (93%)	359 (98%)	9 (2%)	0	100	100
2	E	363/397 (91%)	359 (99%)	4 (1%)	0	100	100
All	All	1577/1728 (91%)	1549 (98%)	28 (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	A	150/150 (100%)	150 (100%)	0	100	100
1	D	146/150 (97%)	145 (99%)	1 (1%)	76	79
1	I	77/150 (51%)	77 (100%)	0	100	100
2	B	316/360 (88%)	308 (98%)	8 (2%)	42	38
2	C	335/360 (93%)	331 (99%)	4 (1%)	63	65
2	E	328/360 (91%)	321 (98%)	7 (2%)	47	45
All	All	1352/1530 (88%)	1332 (98%)	20 (2%)	57	58

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1491	LEU
2	B	1609	GLN
2	B	1663	LEU
2	B	1666	LEU
2	B	1682	LEU
2	B	1787	VAL
2	B	1804	MET
2	B	1836	LEU
2	C	1491	LEU
2	C	1521	LEU
2	C	1666	LEU
2	C	1845	LEU
1	D	89	LEU
2	E	1491	LEU
2	E	1500	VAL
2	E	1660	ASP
2	E	1663	LEU
2	E	1666	LEU
2	E	1792	GLU

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Mol	Chain	Res	Type
2	E	1836	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1586	HIS
2	C	1609	GLN
2	C	1670	HIS
2	C	1788	ASN
2	E	1598	GLN
2	E	1630	HIS
2	E	1670	HIS

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 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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	$\# Z > 2$
6	EDO	C	1902	-	3,3,3	0.42	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GDP	A	202	3,5	29,30,30	1.17	2 (6%)	45,47,47	1.69	6 (13%)
6	EDO	C	1904	-	3,3,3	0.41	0	2,2,2	0.40	0
8	GOL	B	1903	-	5,5,5	0.36	0	5,5,5	0.38	0
7	ACT	C	1906	-	3,3,3	0.81	0	3,3,3	1.33	0
6	EDO	E	1901	-	3,3,3	0.44	0	2,2,2	0.32	0
7	ACT	A	207	-	3,3,3	0.81	0	3,3,3	1.34	0
6	EDO	B	1902	-	3,3,3	0.43	0	2,2,2	0.37	0
6	EDO	B	1901	-	3,3,3	0.44	0	2,2,2	0.35	0
6	EDO	A	205	-	3,3,3	0.42	0	2,2,2	0.38	0
8	GOL	A	208	-	5,5,5	0.33	0	5,5,5	0.35	0
5	BEF	I	203	4	0,3,3	-	-	-	-	-
6	EDO	D	204	-	3,3,3	0.42	0	2,2,2	0.37	0
6	EDO	A	206	-	3,3,3	0.42	0	2,2,2	0.38	0
6	EDO	C	1903	-	3,3,3	0.42	0	2,2,2	0.37	0
6	EDO	A	204	-	3,3,3	0.44	0	2,2,2	0.35	0
5	BEF	D	203	4	0,3,3	-	-	-	-	-
6	EDO	C	1901	-	3,3,3	0.44	0	2,2,2	0.36	0
4	GDP	D	202	3,5	29,30,30	1.17	3 (10%)	45,47,47	1.72	6 (13%)
5	BEF	A	203	4	0,3,3	-	-	-	-	-
4	GDP	I	202	3,5	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
6	EDO	D	205	-	3,3,3	0.42	0	2,2,2	0.34	0
6	EDO	E	1902	-	3,3,3	0.43	0	2,2,2	0.32	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
6	EDO	C	1901	-	-	0/1/1/1	-
6	EDO	C	1902	-	-	0/1/1/1	-
6	EDO	E	1901	-	-	0/1/1/1	-
4	GDP	D	202	3,5	-	4/16/32/32	0/3/3/3
8	GOL	B	1903	-	-	2/4/4/4	-
6	EDO	B	1902	-	-	0/1/1/1	-
8	GOL	A	208	-	-	2/4/4/4	-
6	EDO	D	204	-	-	0/1/1/1	-
4	GDP	A	202	3,5	-	1/16/32/32	0/3/3/3
4	GDP	I	202	3,5	-	1/16/32/32	0/3/3/3
6	EDO	B	1901	-	-	0/1/1/1	-
6	EDO	A	205	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	206	-	-	0/1/1/1	-
6	EDO	C	1904	-	-	0/1/1/1	-
6	EDO	D	205	-	-	0/1/1/1	-
6	EDO	C	1903	-	-	0/1/1/1	-
6	EDO	A	204	-	-	0/1/1/1	-
6	EDO	E	1902	-	-	1/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	202	GDP	C5-C4	3.18	1.47	1.38
4	I	202	GDP	C5-C4	3.15	1.47	1.38
4	A	202	GDP	C5-C4	3.10	1.47	1.38
4	A	202	GDP	C6-N1	-2.38	1.34	1.38
4	I	202	GDP	C6-N1	-2.36	1.34	1.38
4	D	202	GDP	C6-N1	-2.29	1.34	1.38
4	D	202	GDP	C5-N7	-2.07	1.34	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	202	GDP	C5-C4-N3	-6.02	118.81	128.39
4	D	202	GDP	C5-C4-N3	-5.84	119.09	128.39
4	A	202	GDP	C5-C4-N3	-5.81	119.15	128.39
4	I	202	GDP	C2-N3-C4	4.99	120.89	112.30
4	D	202	GDP	C2-N3-C4	4.96	120.84	112.30
4	A	202	GDP	C2-N3-C4	4.82	120.60	112.30
4	I	202	GDP	N9-C4-N3	4.43	134.82	125.95
4	A	202	GDP	N9-C4-N3	4.27	134.50	125.95
4	D	202	GDP	N9-C4-N3	4.27	134.49	125.95
4	D	202	GDP	C6-C5-N7	3.46	136.59	130.29
4	A	202	GDP	C6-C5-N7	3.32	136.33	130.29
4	I	202	GDP	C6-C5-N7	3.29	136.27	130.29
4	D	202	GDP	C4-C5-N7	-2.60	106.54	110.67
4	I	202	GDP	C4-C5-N7	-2.58	106.58	110.67
4	A	202	GDP	C4-C5-N7	-2.55	106.63	110.67
4	A	202	GDP	O6-C6-C5	-2.12	120.92	126.53
4	D	202	GDP	O6-C6-C5	-2.11	120.96	126.53
4	I	202	GDP	C3'-C2'-C1'	2.11	105.45	101.46
4	I	202	GDP	O6-C6-C5	-2.06	121.10	126.53

There are no chirality outliers.

All (11) torsion outliers are listed below:

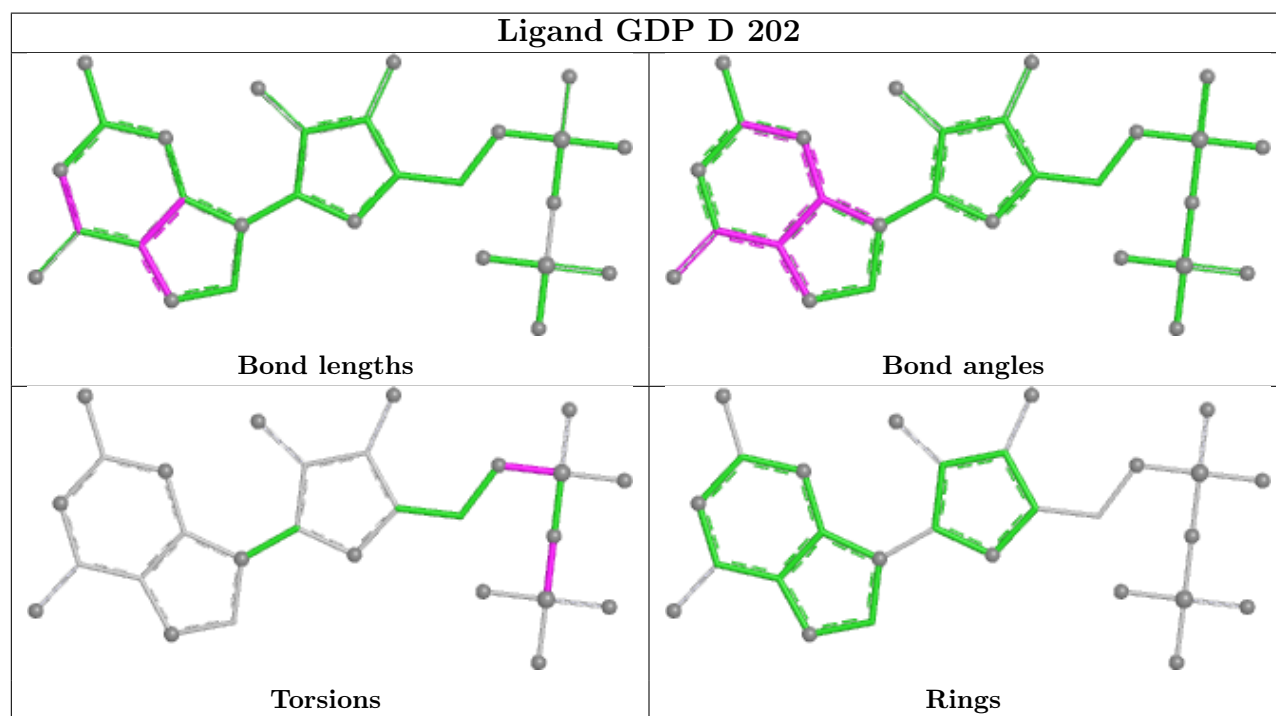
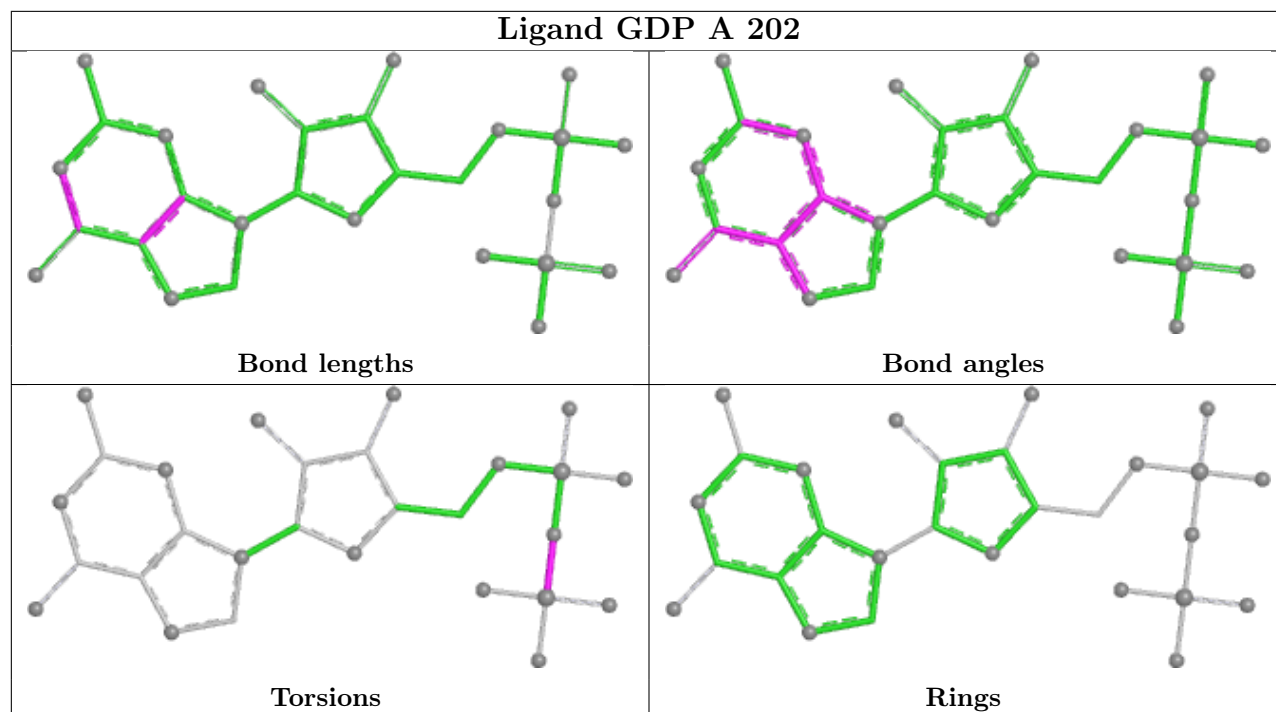
Mol	Chain	Res	Type	Atoms
4	A	202	GDP	PA-O3A-PB-O2B
4	D	202	GDP	PA-O3A-PB-O2B
4	D	202	GDP	PA-O3A-PB-O3B
4	I	202	GDP	PA-O3A-PB-O2B
8	A	208	GOL	O1-C1-C2-C3
8	B	1903	GOL	O1-C1-C2-C3
8	A	208	GOL	O1-C1-C2-O2
8	B	1903	GOL	O1-C1-C2-O2
4	D	202	GDP	C5'-O5'-PA-O1A
4	D	202	GDP	PA-O3A-PB-O1B
6	E	1902	EDO	O1-C1-C2-O2

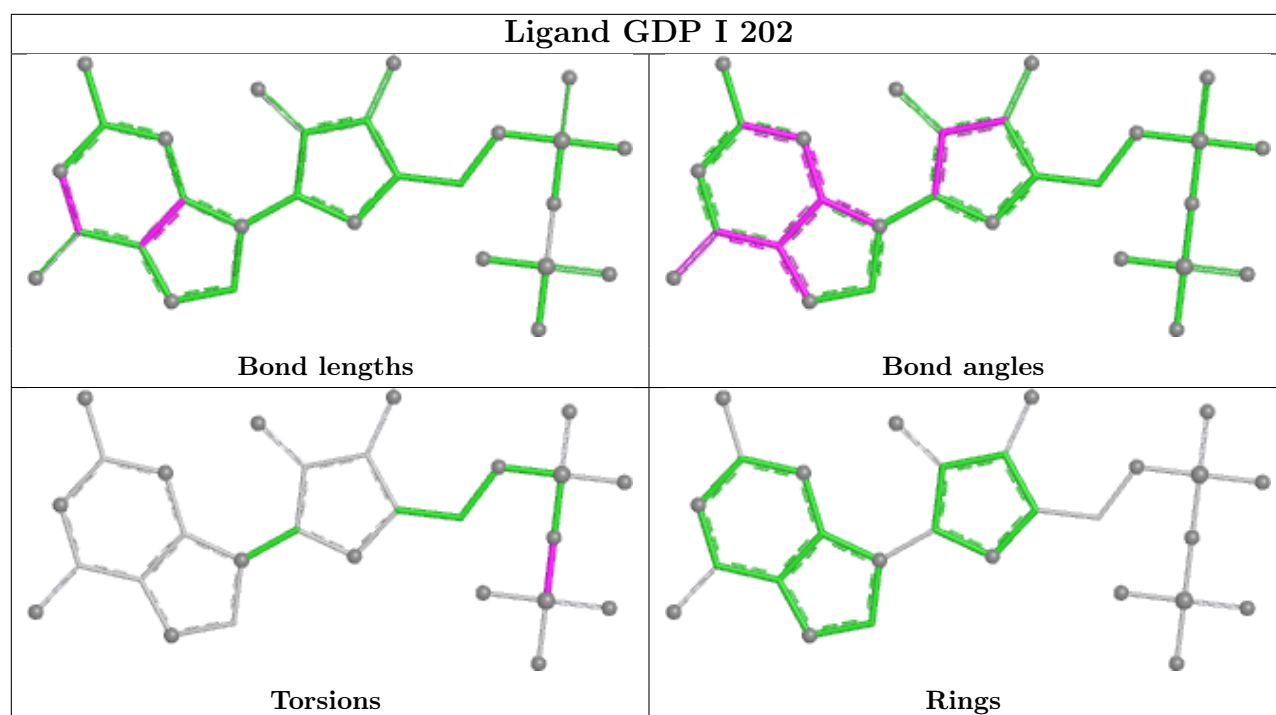
There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	202	GDP	1	0
8	B	1903	GOL	1	0
6	A	205	EDO	1	0
6	C	1903	EDO	2	0
6	A	204	EDO	1	0
4	D	202	GDP	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 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	A	172/179 (96%)	-0.05	4 (2%) 61 63	24, 44, 66, 107	6 (3%)
1	D	173/179 (96%)	0.24	4 (2%) 61 63	22, 56, 84, 125	3 (1%)
1	I	147/179 (82%)	3.59	127 (86%) 0 0	12, 15, 19, 22	147 (100%)
2	B	364/397 (91%)	0.82	36 (9%) 13 13	34, 72, 110, 131	3 (0%)
2	C	364/397 (91%)	0.06	10 (2%) 56 58	24, 49, 74, 120	9 (2%)
2	E	361/397 (90%)	0.36	14 (3%) 43 44	29, 57, 98, 120	7 (1%)
All	All	1581/1728 (91%)	0.64	195 (12%) 8 8	12, 54, 98, 131	175 (11%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	79	ALA	9.0
1	I	31	PHE	8.9
1	I	44	ILE	8.8
1	I	76	ILE	8.6
1	I	46	VAL	7.4
1	I	131	LEU	6.6
1	I	99	TYR	6.6
1	I	75	ALA	6.6
1	I	72	ARG	6.4
1	I	12	PHE	6.2
1	I	102	VAL	6.2
1	I	67	THR	6.0
1	I	115	SER	5.9
1	I	84	ALA	5.8
1	I	135	PRO	5.8
1	I	156	LEU	5.6
1	I	11	LEU	5.5
1	I	71	GLU	5.3
1	I	169	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	I	91	TYR	5.2
1	I	173	TYR	5.2
1	I	129	ARG	5.2
1	I	149	SER	5.2
1	I	64	ILE	5.0
1	I	50	THR	5.0
1	I	113	ALA	4.8
1	I	23	GLY	4.8
1	I	111	ASP	4.8
1	I	97	LEU	4.7
1	I	65	TRP	4.7
1	I	45	GLY	4.6
1	I	83	GLY	4.6
1	I	148	LEU	4.6
1	I	78	SER	4.6
1	I	141	ALA	4.5
1	I	160	ASN	4.5
1	I	144	GLU	4.5
1	I	48	PHE	4.4
2	E	1790	PHE	4.4
2	B	1787	VAL	4.4
1	I	142	PHE	4.3
2	E	1787	VAL	4.3
1	I	114	ASP	4.3
1	I	103	GLU	4.3
1	I	105	TRP	4.2
1	I	110	ARG	4.2
1	I	15	VAL	4.2
1	I	96	HIS	4.2
1	I	17	ILE	4.1
1	I	100	GLU	4.1
1	I	81	TYR	4.0
1	I	172	ILE	4.0
1	I	157	ASP	4.0
1	I	106	LEU	3.9
1	I	147	GLY	3.9
1	I	69	GLY	3.9
1	I	130	HIS	3.8
1	I	89	LEU	3.8
1	I	82	ARG	3.8
1	I	136	THR	3.8
1	I	62	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	68	ALA	3.7
1	I	165	PHE	3.7
1	I	133	ALA	3.7
1	I	155	ALA	3.7
1	I	63	GLN	3.7
1	I	121	LEU	3.6
1	I	40	SER	3.6
1	I	112	HIS	3.6
1	I	108	GLU	3.6
1	I	143	ALA	3.6
2	B	1472	GLN	3.6
1	I	122	VAL	3.6
1	I	33	ARG	3.6
1	I	174	ARG	3.6
1	I	109	LEU	3.5
1	I	139	ALA	3.5
2	B	1788	ASN	3.4
1	I	77	THR	3.4
1	I	70	GLN	3.4
2	B	1545	ARG	3.3
1	I	80	TYR	3.3
1	I	86	GLY	3.3
2	B	1633	ILE	3.3
2	B	1596	TYR	3.2
1	I	95	LYS	3.2
2	B	1790	PHE	3.2
1	I	20	SER	3.2
1	I	170	THR	3.2
1	I	38	LEU	3.1
2	C	1634	GLN	3.1
1	I	104	ARG	3.1
1	I	127	ASP	3.1
2	B	1656	THR	3.0
2	B	1591	PHE	3.0
1	I	29	SER	3.0
1	I	164	ALA	3.0
1	I	118	VAL	3.0
2	B	1635	GLY	2.9
1	I	151	ILE	2.9
1	I	92	ASP	2.9
2	B	1589	THR	2.9
2	E	1711[A]	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	134	VAL	2.8
1	D	73	TYR	2.8
1	I	47	GLU	2.8
2	B	1595	GLU	2.8
2	B	1477	TYR	2.8
1	I	94	ALA	2.8
1	I	14	VAL	2.8
2	B	1486	VAL	2.8
1	I	93	ILE	2.8
1	I	107	LYS	2.8
1	I	125	LYS	2.8
1	I	132	ARG	2.8
1	A	6	ASP	2.8
2	B	1853	VAL	2.8
2	B	1471	PHE	2.7
2	C	1790	PHE	2.7
1	I	66	ASP	2.7
1	I	145	LYS	2.7
1	A	158	SER	2.7
2	B	1524	ASP	2.7
1	I	61	LYS	2.7
2	E	1656	THR	2.7
1	I	138	GLU	2.6
1	I	32	THR	2.6
1	I	124	ASN	2.6
2	B	1588	LEU	2.6
2	B	1592	ASP	2.6
1	I	36	PHE	2.6
1	I	87	ALA	2.6
2	E	1850	ILE	2.5
1	I	119	ILE	2.5
1	I	123	GLY	2.5
1	I	39	GLU	2.4
2	E	1719	TYR	2.4
2	B	1786	PRO	2.4
1	I	49	ALA	2.4
2	E	1655	GLY	2.4
2	C	1470	ASP	2.4
2	C	1596	TYR	2.4
2	E	1849	PHE	2.4
1	D	6	ASP	2.4
2	B	1500	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	42	SER	2.4
2	C	1469	LYS	2.4
2	B	1702	LEU	2.3
1	I	41	LYS	2.3
1	I	154	SER	2.3
2	B	1851	SER	2.3
2	C	1656	THR	2.3
2	E	1596	TYR	2.3
1	I	16	LEU	2.3
1	D	5	ASP	2.3
1	I	126	SER	2.3
2	B	1850	ILE	2.3
1	I	98	THR	2.3
2	C	1788	ASN	2.3
1	I	162	GLU	2.3
1	A	175	ILE	2.3
2	B	1527	VAL	2.3
1	I	146	ASN	2.3
2	B	1815	LEU	2.3
2	E	1847	LEU	2.3
1	I	158	SER	2.2
2	C	1853	VAL	2.2
1	I	21	GLY	2.2
1	D	109	LEU	2.2
1	I	150	PHE	2.2
1	I	28	LEU	2.2
1	I	37	ASN	2.2
1	I	161	VAL	2.2
2	B	1475	LEU	2.2
2	B	1511	LEU	2.2
2	B	1833	SER	2.2
1	I	34	ASN	2.2
1	I	153	THR	2.2
2	B	1593	LEU	2.1
2	C	1793	ARG	2.1
2	B	1671	SER	2.1
1	A	111	ASP	2.1
1	I	24	LYS	2.1
2	E	1502	LEU	2.1
1	I	43	THR	2.1
2	B	1834	LEU	2.1
2	B	1634	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	1471	PHE	2.1
2	E	1726	GLU	2.0
1	I	88	LEU	2.0
2	B	1519	ASP	2.0
2	B	1478	LYS	2.0
2	B	1476	GLU	2.0
2	E	1845	LEU	2.0
2	C	1602	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	C	1902	4/4	0.76	0.28	74,82,86,89	0
5	BEF	I	203	4/4	0.78	0.15	40,40,40,41	4
8	GOL	B	1903	6/6	0.80	0.16	64,74,77,83	0
8	GOL	A	208	6/6	0.84	0.13	59,78,84,87	0
4	GDP	I	202	28/28	0.84	0.15	31,45,54,66	28
7	ACT	A	207	4/4	0.89	0.22	47,64,69,71	0
6	EDO	E	1901	4/4	0.90	0.19	45,57,60,67	0
6	EDO	E	1902	4/4	0.90	0.11	48,51,57,57	0
3	MG	C	1905	1/1	0.90	0.11	85,85,85,85	0
6	EDO	C	1903	4/4	0.90	0.13	56,57,65,71	0
6	EDO	C	1904	4/4	0.90	0.21	34,48,65,69	0
6	EDO	B	1901	4/4	0.91	0.19	56,59,62,63	0
7	ACT	C	1906	4/4	0.92	0.14	59,61,65,69	0
6	EDO	D	204	4/4	0.92	0.11	67,68,71,80	0
6	EDO	A	206	4/4	0.92	0.12	48,49,51,66	0

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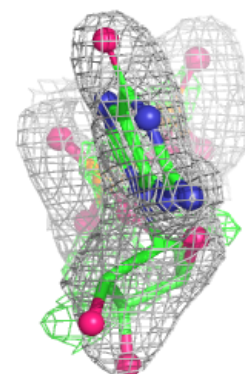
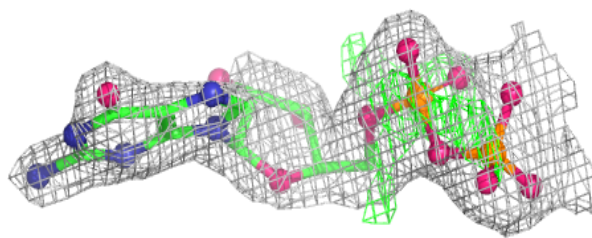
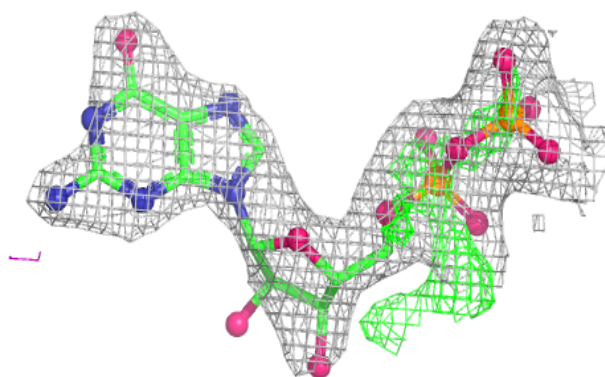
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	A	205	4/4	0.93	0.16	47,63,67,73	0
6	EDO	B	1902	4/4	0.94	0.12	56,57,58,65	0
6	EDO	D	205	4/4	0.94	0.13	56,58,60,61	0
5	BEF	D	203	4/4	0.95	0.08	46,46,49,49	0
6	EDO	C	1901	4/4	0.97	0.14	44,45,53,60	0
5	BEF	A	203	4/4	0.97	0.07	38,40,40,43	0
6	EDO	A	204	4/4	0.97	0.07	42,44,45,46	0
3	MG	I	201	1/1	0.98	0.06	42,42,42,42	1
4	GDP	A	202	28/28	0.98	0.05	35,39,43,44	0
4	GDP	D	202	28/28	0.98	0.06	41,47,51,53	0
3	MG	A	201	1/1	0.99	0.04	43,43,43,43	0
3	MG	D	201	1/1	0.99	0.05	47,47,47,47	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.

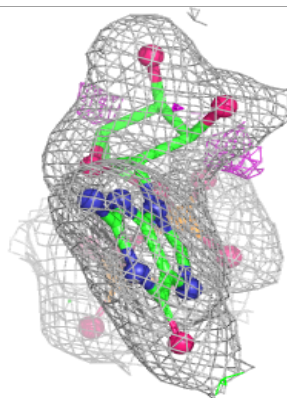
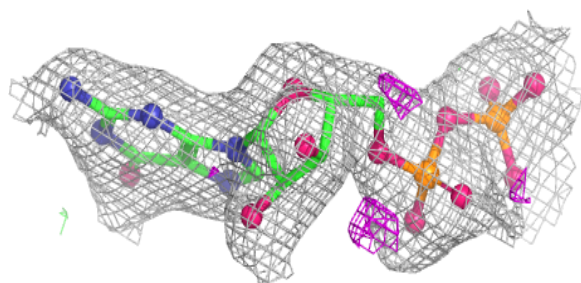
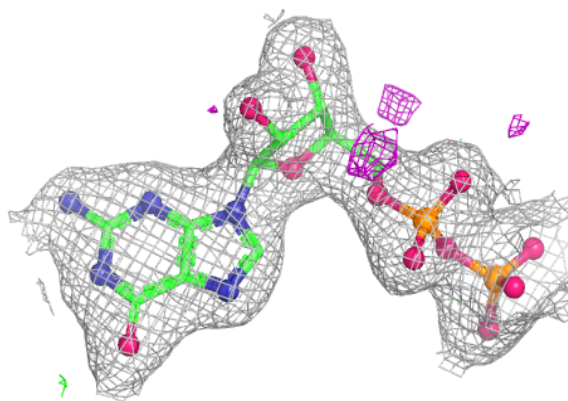
Electron density around GDP I 202:

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

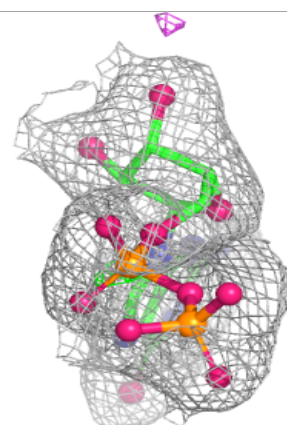
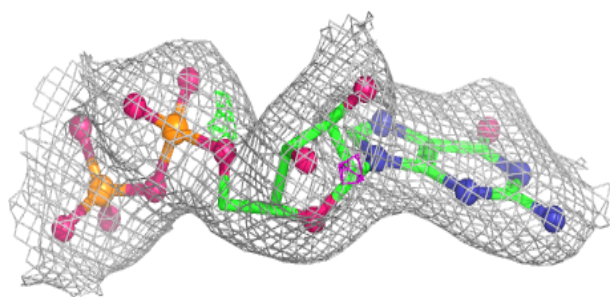
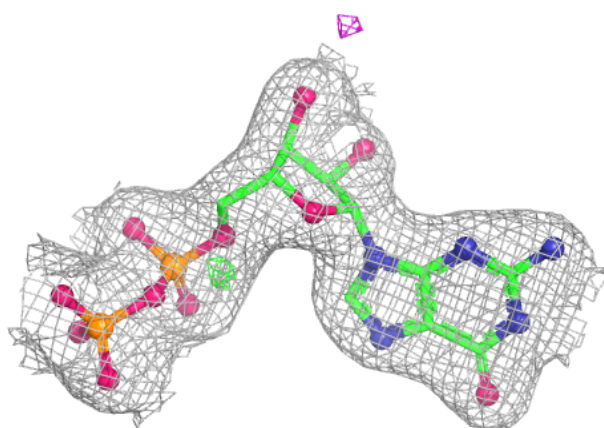


Electron density around GDP A 202:

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

**Electron density around GDP D 202:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.