



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:05 PM EDT

PDB ID : 6EKK / pdb_00006ekk
Title : Crystal structure of GEF domain of DENND 1A in complex with Rab GTPase Rab35-GDP bound state.
Authors : Srikannathasan, V.; Szykowska, A.; Tallant, C.; Strain-Damerell, C.; Kopec, J.; Kupinska, K.; Mukhopadhyay, S.; Gavin, M.; Wang, D.; Chalk, R.; Burgess-Brown, N.A.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; von Delft, F.; Huber, K.
Deposited on : 2017-09-26
Resolution : 1.82 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)

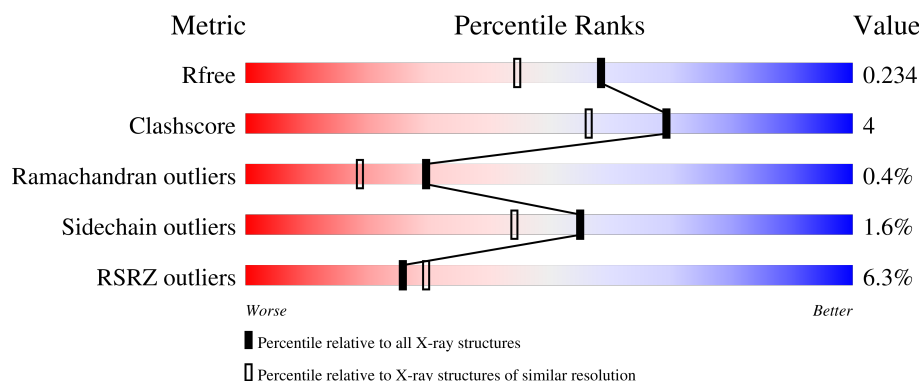
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	393	6% 87% 8% 5%
1	B	393	8% 88% 8% • •
2	C	176	5% 92% 8%

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	176	4% 90% 7% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9750 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.

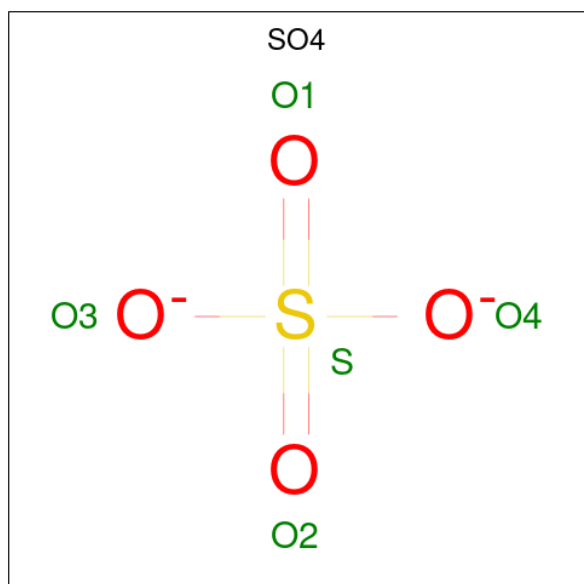
- Molecule 1 is a protein called DENN domain-containing protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	5	0
			2971	1919	483	552	17			
1	B	381	Total	C	N	O	S	0	6	0
			3052	1963	503	568	18			

- Molecule 2 is a protein called Ras-related protein Rab-35.

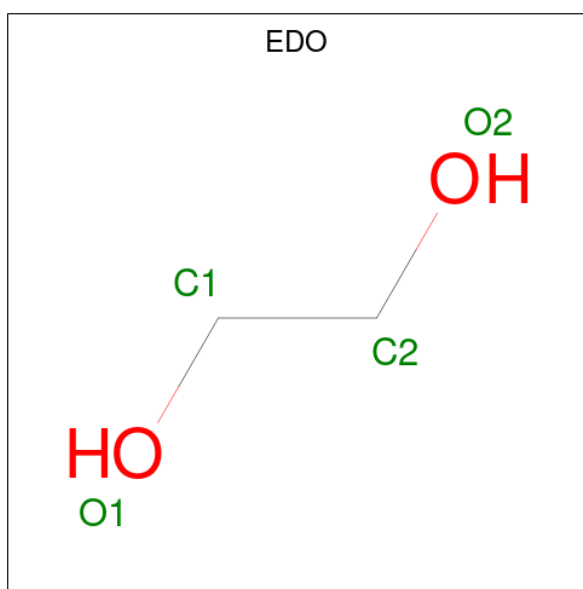
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	176	Total	C	N	O	S	0	1	0
			1376	872	233	266	5			
2	D	174	Total	C	N	O	S	0	0	0
			1358	861	228	264	5			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



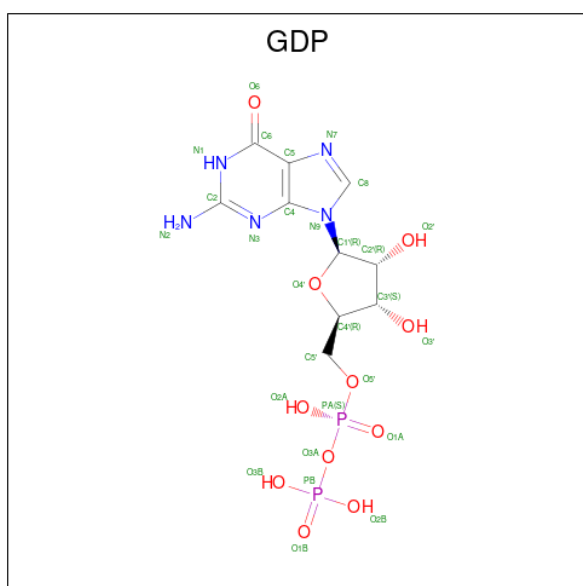
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

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

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	276	Total	O	0	0
			276	276		
6	B	287	Total	O	0	0
			287	287		

Continued on next page...

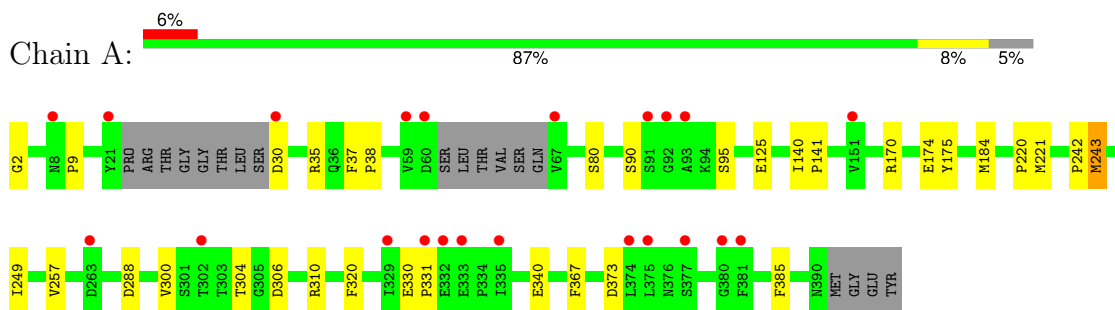
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	138	Total 138	O 138	0	0
6	D	159	Total 159	O 159	0	0

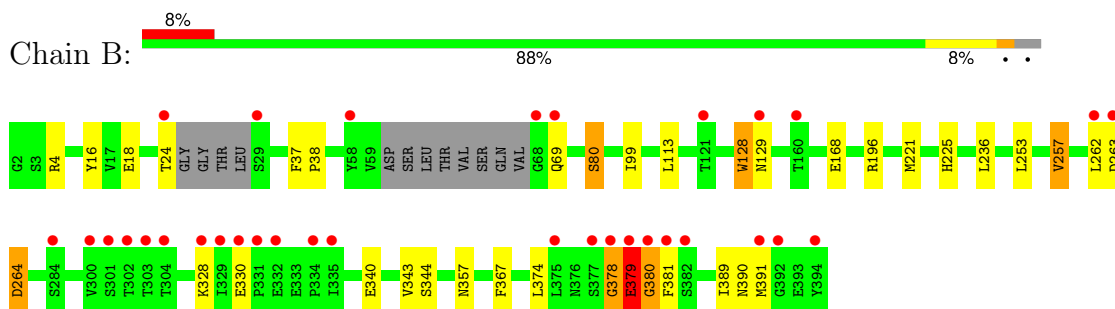
3 Residue-property plots [i](#)

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.

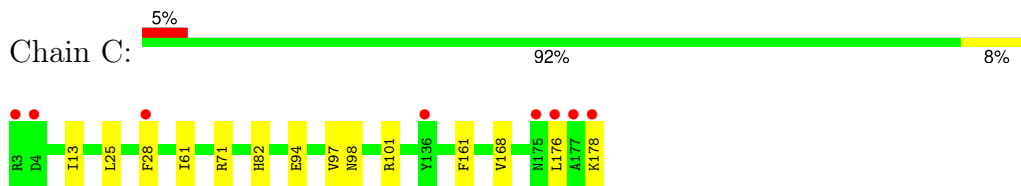
- Molecule 1: DENN domain-containing protein 1A



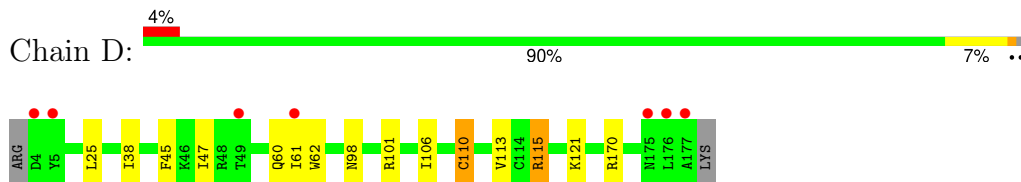
- Molecule 1: DENN domain-containing protein 1A



- Molecule 2: Ras-related protein Rab-35



- Molecule 2: Ras-related protein Rab-35



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.70Å 67.99Å 101.71Å 80.50° 76.80° 67.06°	Depositor
Resolution (Å)	50.45 – 1.82 50.45 – 1.82	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.45-1.82) 96.4 (50.45-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.194 , 0.232 0.198 , 0.234	Depositor DCC
R_{free} test set	5773 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9750	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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: GDP, EDO, SO4

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	0.47	1/3047 (0.0%)	0.76	1/4155 (0.0%)
1	B	0.46	0/3128	0.79	5/4258 (0.1%)
2	C	0.49	0/1398	0.74	0/1893
2	D	0.49	0/1380	0.77	0/1870
All	All	0.47	1/8953 (0.0%)	0.77	6/12176 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	MET	CG-SD	-5.04	1.68	1.80

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	GLY	N-CA-C	-10.82	94.87	110.88
1	A	243	MET	CA-CB-CG	-8.21	97.68	114.10
1	B	330	GLU	CA-C-N	-6.87	111.26	119.84
1	B	330	GLU	C-N-CA	-6.87	111.26	119.84
1	B	128	TRP	N-CA-C	-6.69	101.25	110.35
1	B	378	GLY	CA-C-O	-5.95	115.76	121.83

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	2971	0	2807	21	0
1	B	3052	0	2913	21	0
2	C	1376	0	1336	9	0
2	D	1358	0	1314	10	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
4	A	12	0	18	2	0
4	B	16	0	24	0	0
4	C	4	0	6	0	0
5	C	28	0	12	0	0
5	D	28	0	12	1	0
6	A	276	0	0	4	0
6	B	287	0	0	3	0
6	C	138	0	0	1	0
6	D	159	0	0	1	0
All	All	9750	0	8442	61	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 4.

All (61) 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:B:196[B]:ARG:NH2	1:B:263:ASP:O	1.99	0.94
1:A:2:GLY:N	6:A:501:HOH:O	2.19	0.73
1:B:129:ASN:ND2	6:B:502:HOH:O	2.20	0.66
1:B:4:ARG:NH2	1:B:225:HIS:O	2.31	0.64
1:A:174:GLU:HG3	6:A:628:HOH:O	2.04	0.58
1:B:99:ILE:HG13	1:B:113:LEU:HD21	1.86	0.57
1:A:242:PRO:HD2	1:A:243:MET:HE3	1.87	0.56
1:A:373:ASP:CG	2:C:71:ARG:HH22	2.14	0.56
2:C:82:HIS:HB3	2:C:168:VAL:CG2	2.38	0.54
1:B:257:VAL:HG13	1:B:262:LEU:HD11	1.90	0.54
2:D:98:ASN:OD1	2:D:101:ARG:NH2	2.39	0.53
1:B:4:ARG:HD2	1:B:80:SER:O	2.10	0.52
2:D:106:ILE:HG21	2:D:115:ARG:HD2	1.92	0.50
1:B:18:GLU:OE1	6:B:501:HOH:O	2.19	0.50
1:B:374:LEU:HG	1:B:379:GLU:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:GLY:C	1:B:379:GLU:HG3	2.37	0.49
1:B:263:ASP:O	1:B:264:ASP:C	2.55	0.49
1:A:300:VAL:O	1:A:304:THR:HG23	2.13	0.49
1:B:16:TYR:HD1	1:B:99:ILE:HG12	1.78	0.49
2:D:115:ARG:HG2	3:D:201:SO4:O1	2.13	0.49
1:A:249:ILE:HD13	1:A:257:VAL:HG21	1.95	0.48
1:A:35:ARG:NH2	1:A:125:GLU:OE1	2.47	0.48
2:C:13:ILE:HB	2:C:61:ILE:HD11	1.95	0.48
1:A:221:MET:HE1	1:A:320:PHE:CG	2.48	0.48
2:C:25:LEU:HD22	6:C:328:HOH:O	2.14	0.47
2:D:110:CYS:O	2:D:113:VAL:HG12	2.13	0.47
2:C:82:HIS:HB3	2:C:168:VAL:HG23	1.97	0.47
1:B:380:GLY:N	1:B:381:PHE:HA	2.31	0.46
2:C:25:LEU:HD11	2:C:61:ILE:HD13	1.99	0.44
1:A:288:ASP:OD1	1:A:288:ASP:N	2.51	0.44
1:B:389:ILE:C	1:B:391:MET:H	2.26	0.44
1:A:221:MET:HG2	1:A:367:PHE:HB2	1.98	0.44
2:D:170:ARG:HD2	6:D:428:HOH:O	2.19	0.43
1:A:170:ARG:HB3	4:A:404:EDO:H11	2.00	0.43
2:C:94:GLU:O	2:C:97:VAL:HG22	2.19	0.43
2:C:98:ASN:OD1	2:C:101:ARG:NH2	2.42	0.43
1:A:175:TYR:CE2	1:A:184:MET:HE3	2.54	0.43
1:A:140:ILE:HA	1:A:141:PRO:HD3	1.83	0.42
4:A:405:EDO:H21	6:A:658:HOH:O	2.19	0.42
2:C:28:PHE:HB2	2:C:161:PHE:CZ	2.54	0.42
2:D:47:ILE:CD1	2:D:60:GLN:HG2	2.49	0.42
1:A:330:GLU:HA	1:A:331:PRO:HD2	1.90	0.42
1:B:389:ILE:O	1:B:391:MET:N	2.52	0.42
1:B:389:ILE:C	1:B:391:MET:N	2.77	0.42
1:B:221:MET:HG2	1:B:367:PHE:HB2	2.01	0.42
1:A:9:PRO:HG2	1:A:140:ILE:HD13	2.02	0.42
2:D:25:LEU:HD21	2:D:61:ILE:HG12	2.02	0.42
1:A:30:ASP:N	6:A:515:HOH:O	2.52	0.42
1:A:90:SER:OG	1:A:95:SER:OG	2.35	0.42
1:A:306:ASP:O	1:A:310:ARG:HG2	2.19	0.42
2:D:121:LYS:HG2	5:D:203:GDP:C6	2.54	0.42
2:D:113:VAL:O	2:D:115:ARG:HD3	2.19	0.42
1:A:220:PRO:HG3	1:A:385:PHE:CG	2.55	0.41
1:B:128:TRP:O	1:B:129:ASN:CB	2.67	0.41
1:B:236:LEU:HD13	1:B:253:LEU:HD13	2.03	0.41
1:B:37:PHE:HA	1:B:38:PRO:C	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASN:HB3	6:B:608:HOH:O	2.21	0.41
2:D:45:PHE:HB3	2:D:62:TRP:CE3	2.55	0.41
1:A:220:PRO:HG3	1:A:385:PHE:CD2	2.56	0.40
1:A:37:PHE:HA	1:A:38:PRO:C	2.46	0.40
1:B:340:GLU:OE2	1:B:344[A]:SER:OG	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/393 (95%)	365 (98%)	9 (2%)	0	100	100
1	B	381/393 (97%)	363 (95%)	14 (4%)	4 (1%)	12	4
2	C	175/176 (99%)	173 (99%)	2 (1%)	0	100	100
2	D	172/176 (98%)	167 (97%)	5 (3%)	0	100	100
All	All	1102/1138 (97%)	1068 (97%)	30 (3%)	4 (0%)	30	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	380	GLY
1	B	390	ASN
1	B	264	ASP
1	B	379	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/357 (89%)	317 (99%)	2 (1%)	78	74
1	B	331/357 (93%)	323 (98%)	8 (2%)	43	27
2	C	148/156 (95%)	146 (99%)	2 (1%)	59	49
2	D	146/156 (94%)	143 (98%)	3 (2%)	47	32
All	All	944/1026 (92%)	929 (98%)	15 (2%)	55	44

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	340	GLU
1	B	24	THR
1	B	69	GLN
1	B	80	SER
1	B	168	GLU
1	B	257	VAL
1	B	328	LYS
1	B	343	VAL
1	B	379	GLU
2	C	176	LEU
2	C	178	LYS
2	D	38	ILE
2	D	110	CYS
2	D	115	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	44	GLN
1	A	82	GLN
1	A	316	GLN
1	B	36	GLN
1	B	356	GLN
2	D	104	HIS
2	D	109	ASN

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 ⓘ

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	A	405	-	3,3,3	0.52	0	2,2,2	0.16	0
3	SO4	C	201	-	4,4,4	0.23	0	6,6,6	0.09	0
4	EDO	B	404	-	3,3,3	0.53	0	2,2,2	0.25	0
5	GDP	D	203	-	29,30,30	1.15	4 (13%)	45,47,47	1.72	7 (15%)
3	SO4	A	401	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	C	202	-	4,4,4	0.26	0	6,6,6	0.13	0
4	EDO	C	203	-	3,3,3	0.42	0	2,2,2	0.41	0
4	EDO	B	405	-	3,3,3	0.46	0	2,2,2	0.21	0
4	EDO	B	407	-	3,3,3	0.42	0	2,2,2	0.31	0
3	SO4	B	403	-	4,4,4	0.22	0	6,6,6	0.13	0
4	EDO	A	404	-	3,3,3	0.40	0	2,2,2	0.42	0
5	GDP	C	204	-	29,30,30	1.27	4 (13%)	45,47,47	1.78	10 (22%)
4	EDO	A	403	-	3,3,3	0.48	0	2,2,2	0.26	0
3	SO4	A	402	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	D	201	-	4,4,4	0.15	0	6,6,6	0.11	0
4	EDO	B	406	-	3,3,3	0.56	0	2,2,2	0.27	0
3	SO4	B	401	-	4,4,4	0.24	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	202	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	B	402	-	4,4,4	0.27	0	6,6,6	0.22	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	EDO	B	405	-	-	0/1/1/1	-
4	EDO	A	405	-	-	0/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
5	GDP	D	203	-	-	3/16/32/32	0/3/3/3
4	EDO	B	407	-	-	0/1/1/1	-
4	EDO	B	406	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	C	203	-	-	0/1/1/1	-
5	GDP	C	204	-	-	3/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	204	GDP	PA-O3A	3.53	1.63	1.59
5	D	203	GDP	C5-C4	3.09	1.47	1.38
5	C	204	GDP	C5-C4	3.02	1.47	1.38
5	D	203	GDP	PA-O3A	2.42	1.62	1.59
5	C	204	GDP	C6-N1	-2.18	1.34	1.38
5	D	203	GDP	C6-N1	-2.14	1.34	1.38
5	C	204	GDP	C4-N9	-2.07	1.32	1.38
5	D	203	GDP	C4-N9	-2.03	1.32	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	203	GDP	C5-C4-N3	-5.28	119.99	128.39
5	C	204	GDP	C5-C4-N3	-5.01	120.41	128.39
5	C	204	GDP	C2-N3-C4	4.83	120.62	112.30
5	D	203	GDP	C2-N3-C4	4.50	120.05	112.30
5	D	203	GDP	N9-C4-N3	4.16	134.27	125.95
5	C	204	GDP	C6-C5-N7	4.00	137.57	130.29
5	C	204	GDP	N9-C4-N3	3.89	133.74	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	203	GDP	C6-C5-N7	3.43	136.53	130.29
5	D	203	GDP	O2A-PA-O3A	2.97	115.31	107.27
5	C	204	GDP	O2B-PB-O3A	2.58	113.28	104.64
5	D	203	GDP	C4-C5-N7	-2.46	106.77	110.67
5	C	204	GDP	O2A-PA-O3A	2.41	113.78	107.27
5	D	203	GDP	O6-C6-C5	-2.40	120.20	126.53
5	C	204	GDP	C4-C5-N7	-2.40	106.87	110.67
5	C	204	GDP	C6-C5-C4	-2.18	115.56	118.83
5	C	204	GDP	O6-C6-C5	-2.07	121.07	126.53
5	C	204	GDP	C8-N9-C4	2.07	109.90	106.03

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	204	GDP	PA-O3A-PB-O2B
5	C	204	GDP	PA-O3A-PB-O3B
5	D	203	GDP	PA-O3A-PB-O1B
5	C	204	GDP	PA-O3A-PB-O1B
5	D	203	GDP	PA-O3A-PB-O2B
5	D	203	GDP	PA-O3A-PB-O3B

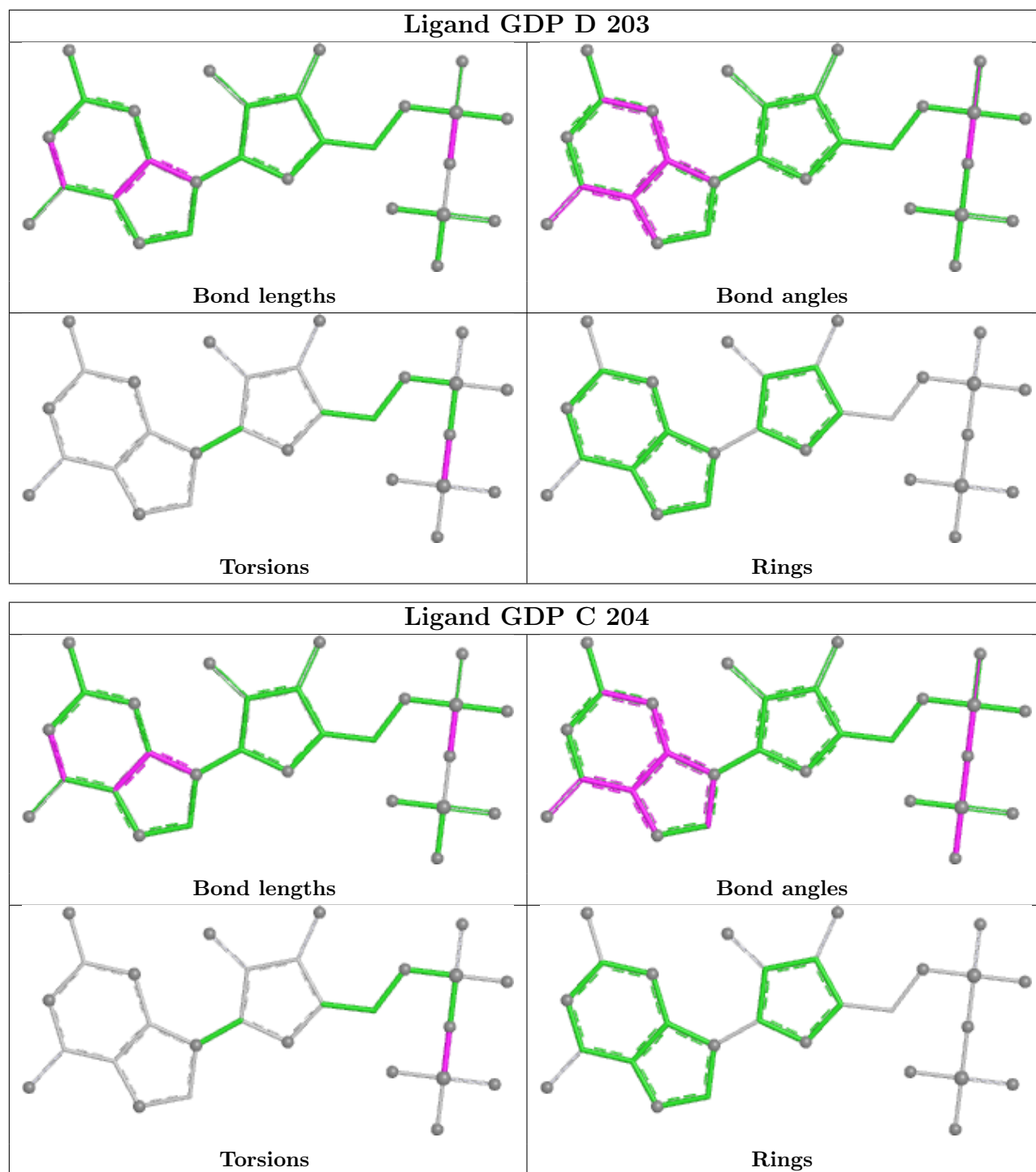
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	EDO	1	0
5	D	203	GDP	1	0
4	A	404	EDO	1	0
3	D	201	SO4	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 ⓘ

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	375/393 (95%)	0.35	22 (5%)	28 32	12, 32, 60, 112	5 (1%)
1	B	381/393 (96%)	0.29	33 (8%)	16 18	13, 33, 64, 130	6 (1%)
2	C	176/176 (100%)	0.05	8 (4%)	38 44	13, 31, 53, 94	1 (0%)
2	D	174/176 (98%)	0.07	7 (4%)	42 48	21, 30, 51, 117	0
All	All	1106/1138 (97%)	0.24	70 (6%)	26 30	12, 32, 59, 130	12 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	ASP	6.5
2	D	4	ASP	5.5
2	D	177	ALA	5.5
1	A	21	TYR	4.9
1	A	302	THR	4.6
1	B	304	THR	4.6
1	B	381	PHE	4.5
1	B	380	GLY	4.3
1	A	331	PRO	4.3
1	A	60	ASP	4.2
1	A	67	VAL	4.0
1	B	303	THR	4.0
1	A	333	GLU	4.0
2	C	178	LYS	3.9
1	A	329	ILE	3.9
1	A	381	PHE	3.9
2	C	3	ARG	3.8
1	B	24	THR	3.8
1	B	331	PRO	3.7
1	B	302	THR	3.6
1	B	391	MET	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	91	SER	3.5
2	D	176	LEU	3.5
1	B	301	SER	3.4
1	A	374	LEU	3.2
2	C	175	ASN	3.2
1	A	93	ALA	3.1
2	C	177	ALA	3.1
1	B	68	GLY	3.1
1	B	58	TYR	3.1
1	B	375	LEU	3.1
1	B	378	GLY	3.0
2	C	28	PHE	3.0
1	A	59	VAL	3.0
1	A	92	GLY	2.9
1	A	377	SER	2.9
1	A	375	LEU	2.9
1	A	263	ASP	2.8
1	B	160	THR	2.8
1	A	380	GLY	2.7
1	B	382	SER	2.7
2	D	175	ASN	2.7
2	D	61	ILE	2.7
1	B	329	ILE	2.6
1	B	379	GLU	2.6
1	A	151	VAL	2.5
1	A	332	GLU	2.5
1	B	262	LEU	2.4
1	A	30	ASP	2.4
1	B	69	GLN	2.4
1	B	392	GLY	2.4
1	A	8	ASN	2.3
1	B	377	SER	2.3
2	C	176	LEU	2.3
1	B	394	TYR	2.3
1	B	330	GLU	2.2
2	D	5	TYR	2.2
1	B	129	ASN	2.2
1	B	121	THR	2.2
2	C	4	ASP	2.2
2	C	136	TYR	2.1
2	D	49	THR	2.1
1	B	284	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	335	ILE	2.1
1	B	300	VAL	2.1
1	B	29	SER	2.1
1	B	332	GLU	2.0
1	B	328	LYS	2.0
1	A	335	ILE	2.0
1	B	334	PRO	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.

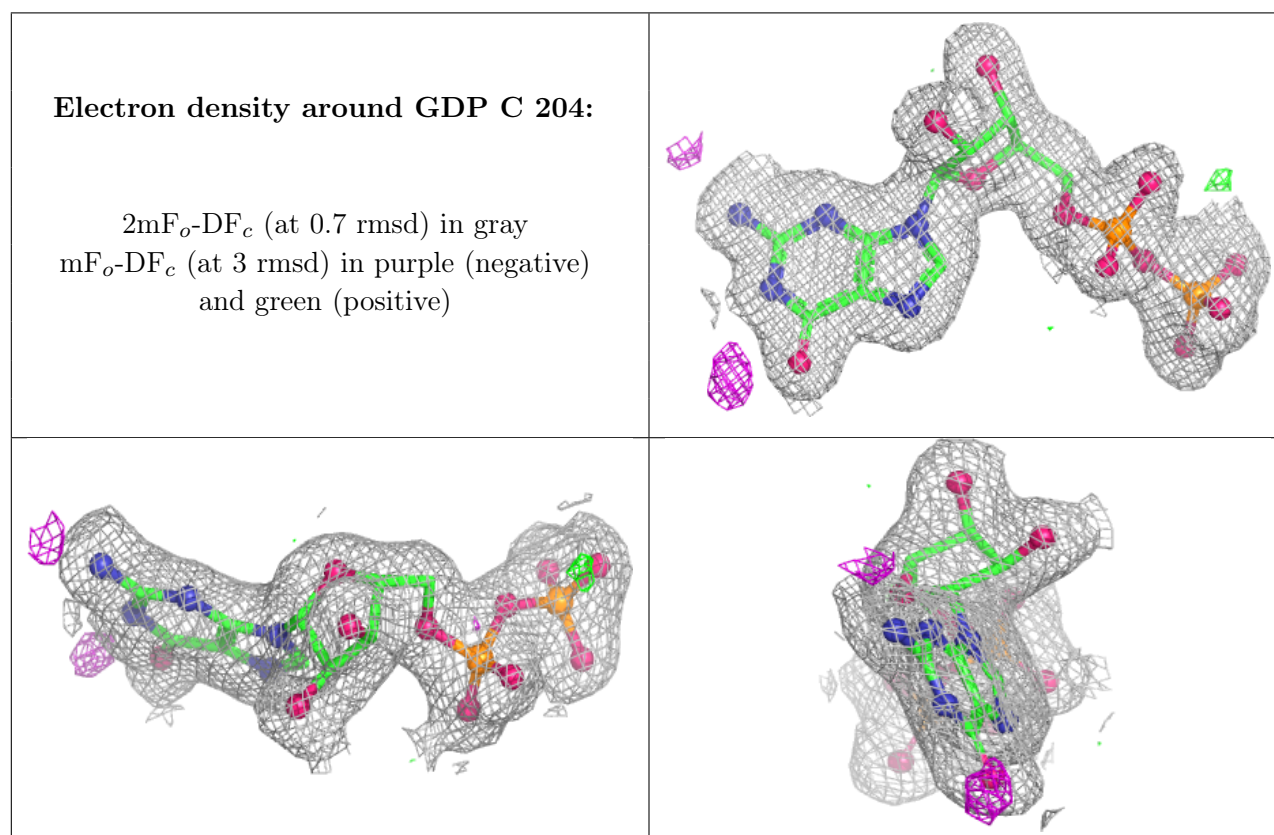
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	401	5/5	0.69	0.17	86,86,87,88	0
3	SO4	C	201	5/5	0.69	0.13	92,92,92,93	0
4	EDO	B	405	4/4	0.77	0.20	62,62,62,62	0
3	SO4	C	202	5/5	0.78	0.12	77,77,79,79	0
3	SO4	B	403	5/5	0.78	0.19	99,99,100,100	0
4	EDO	A	405	4/4	0.79	0.18	47,48,49,51	0
3	SO4	A	402	5/5	0.82	0.14	66,66,67,68	0
3	SO4	D	202	5/5	0.86	0.13	80,80,80,81	0
4	EDO	B	407	4/4	0.86	0.16	56,57,58,59	0
4	EDO	A	403	4/4	0.88	0.12	31,33,33,33	0
3	SO4	D	201	5/5	0.88	0.12	58,62,63,65	0
4	EDO	B	404	4/4	0.89	0.12	35,37,37,37	0
3	SO4	A	401	5/5	0.90	0.09	53,54,55,57	0
3	SO4	B	402	5/5	0.90	0.10	51,55,56,56	0
4	EDO	C	203	4/4	0.91	0.11	46,47,49,52	0
4	EDO	A	404	4/4	0.96	0.08	39,39,40,40	0

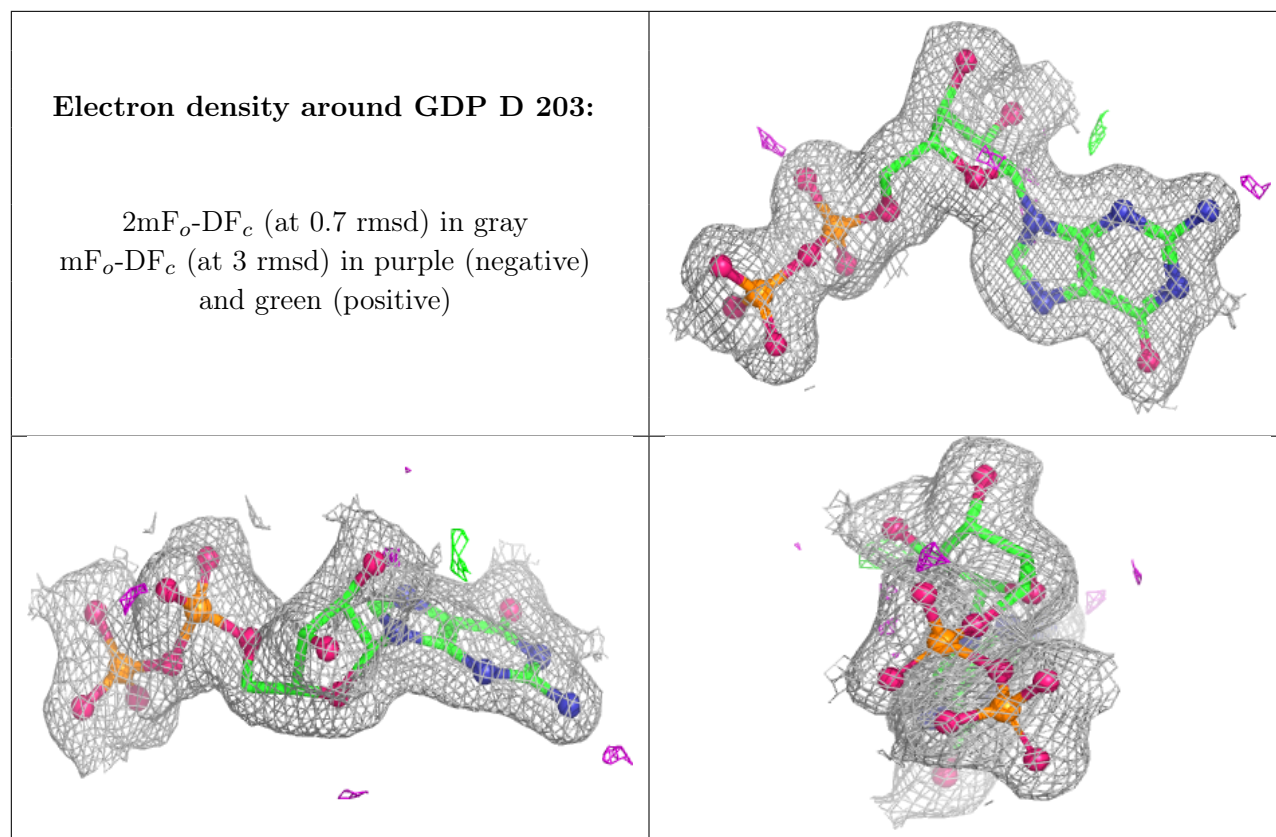
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	406	4/4	0.97	0.08	28,29,30,30	0
5	GDP	C	204	28/28	0.97	0.06	28,32,34,36	0
5	GDP	D	203	28/28	0.98	0.05	25,30,32,33	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.