Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 07:10 PM EDT

PDB ID	:	7SQ2 / pdb_00007sq2
Title	:	Reprocessed and refined structure of Phospholipase C-beta and Gq signaling complex
Authors	:	Endo-Streeter, S.T.; Sondek, J.; Harden, T.K.
Deposited on	:	2021-11-04
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

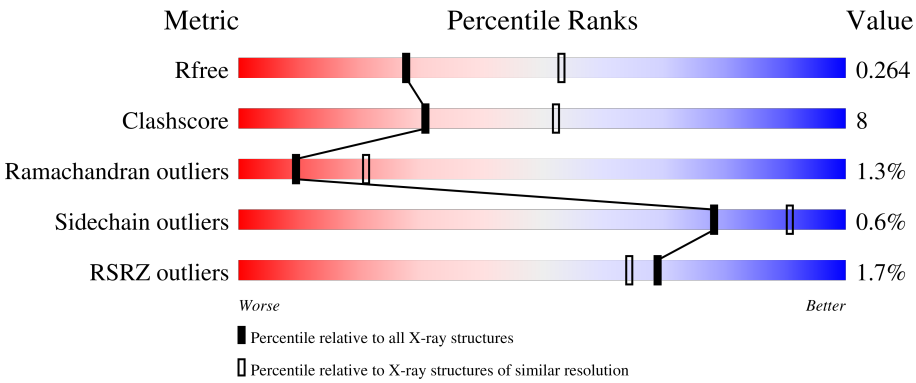
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	327	% 69% 25% • •
2	B	885	2% 65% 18% • 15%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8957 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 Guanine nucleotide-binding protein G(q) subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2616	1671	442	491	12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	expression tag	UNP P21279
A	34	ALA	-	expression tag	UNP P21279

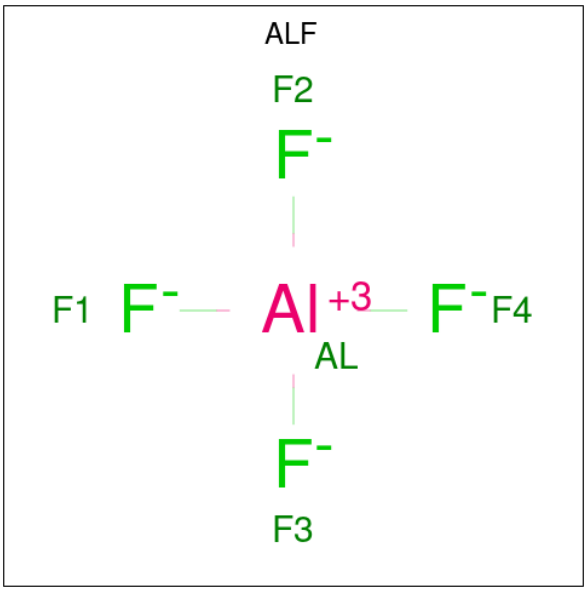
- Molecule 2 is a protein called 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	755	6062	3863	1034	1134	31	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	-	expression tag	UNP Q01970
B	3	ALA	-	expression tag	UNP Q01970
B	4	MET	-	expression tag	UNP Q01970
B	5	ASP	-	expression tag	UNP Q01970
B	6	PRO	-	expression tag	UNP Q01970
B	7	GLU	-	expression tag	UNP Q01970
B	8	PHE	-	expression tag	UNP Q01970
B	9	MET	-	expression tag	UNP Q01970

- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).

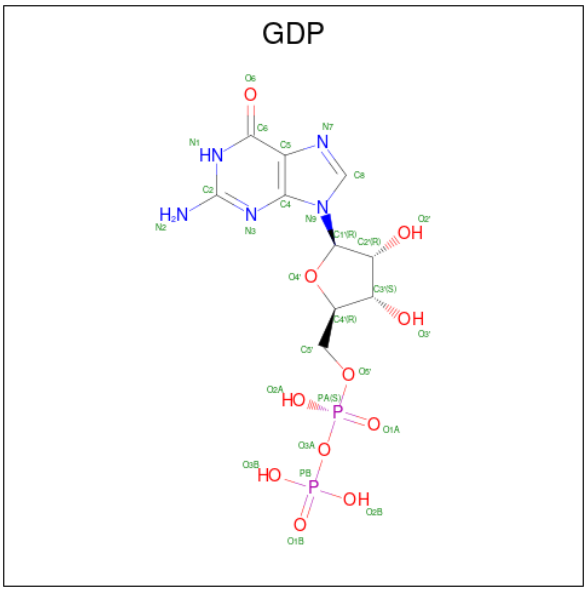


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
3	A	1	5	1	4	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

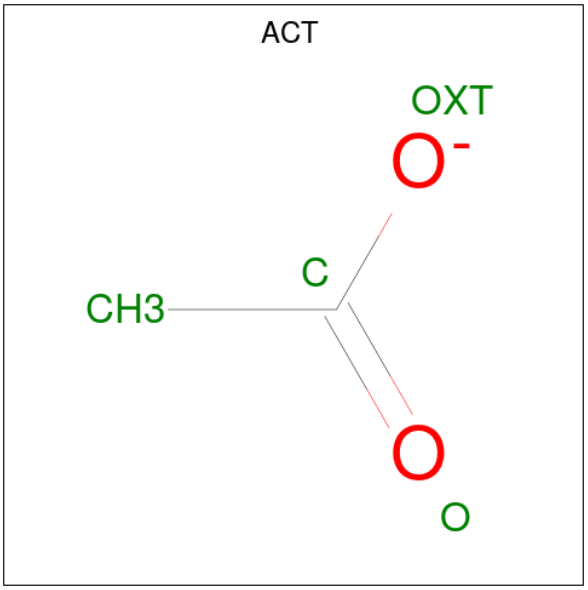
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	B	1	1	1	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	B	1	1	1	0	0

- Molecule 8 is water.

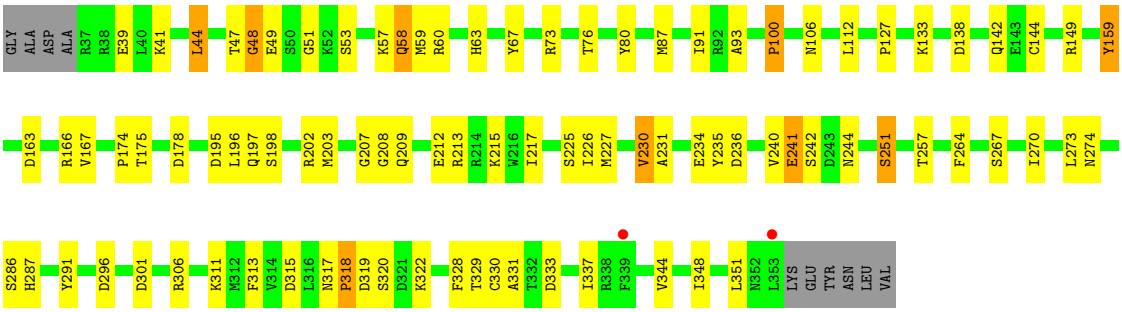
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	97	97	97	0	0
			Total	O		
8	B	118	118	118	0	0

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.

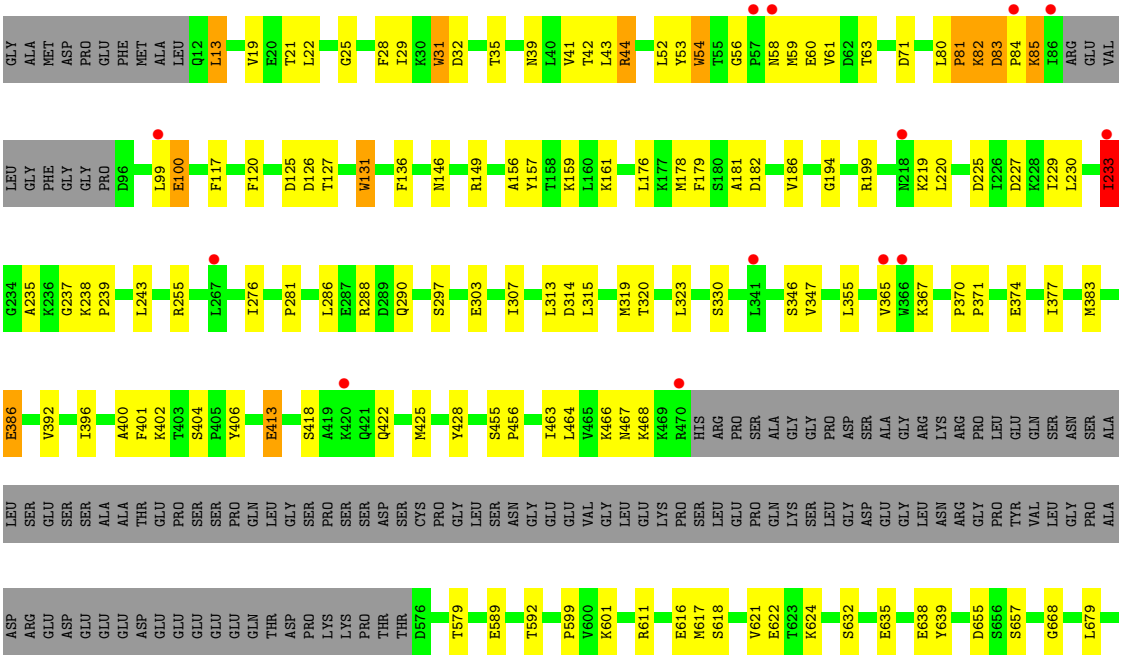
• Molecule 1: Guanine nucleotide-binding protein G(q) subunit alpha

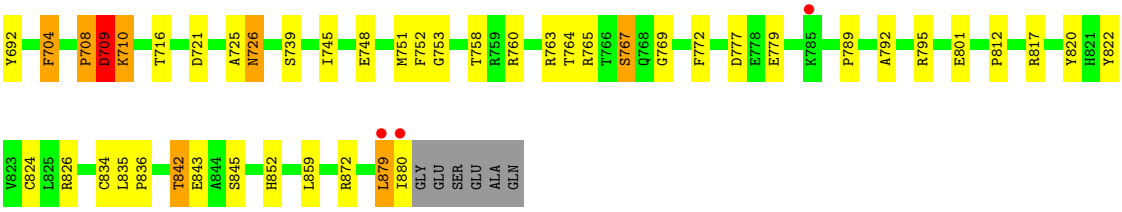
Chain A:



• Molecule 2: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase beta-3

Chain B:




Y692
F704
P708
D709
K710
T716
D721
A725
N726
S739
I745
E748
M751
F752
G753
T758
R759
R760
R763
T764
R765
T766
S767
Q768
G769
F772
D777
E778
E779
K785
P789
A792
R795
E801
P812
R817
Y820
H821
Y822
V823
C824
L825
R826
C834
L835
P836
T842
E843
A844
S845
H852
L859
R872
L879
I880
GLY
GLU
SER
GLU
ALA
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	202.84Å 90.82Å 93.14Å 90.00° 101.19° 90.00°	Depositor
Resolution (Å)	40.55 – 2.60 40.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.55-2.60) 99.6 (40.55-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.199 , 0.263 0.200 , 0.264	Depositor DCC
R_{free} test set	2571 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 66.6	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	0.96	EDS
Total number of atoms	8957	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.95	1/2672 (0.0%)	1.29	1/3612 (0.0%)
2	B	0.98	1/6193 (0.0%)	1.32	6/8383 (0.1%)
All	All	0.97	2/8865 (0.0%)	1.31	7/11995 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	31
2	B	0	60
All	All	0	91

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	668	GLY	C-O	11.41	1.39	1.24
1	A	291	TYR	C-O	5.09	1.31	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	25	GLY	CA-C-O	-6.98	117.68	122.22
2	B	753	GLY	CA-C-O	-6.95	116.11	120.91
2	B	406	TYR	CB-CA-C	6.40	118.08	108.86
1	A	100	PRO	CA-C-O	-5.22	115.22	121.48
2	B	709	ASP	CB-CA-C	-5.20	100.38	110.46
2	B	708	PRO	CA-C-N	5.12	127.85	120.38
2	B	708	PRO	C-N-CA	5.12	127.85	120.38

There are no chirality outliers.

All (91) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	PRO	Mainchain
1	A	133	LYS	Mainchain
1	A	142	GLN	Mainchain
1	A	149	ARG	Mainchain
1	A	159	TYR	Sidechain
1	A	166	ARG	Mainchain
1	A	167	VAL	Mainchain
1	A	174	PRO	Mainchain
1	A	195	ASP	Mainchain
1	A	213	ARG	Mainchain
1	A	215	LYS	Mainchain
1	A	225	SER	Mainchain
1	A	226	ILE	Mainchain
1	A	230	VAL	Mainchain
1	A	240	VAL	Mainchain
1	A	241	GLU	Mainchain
1	A	242	SER	Mainchain
1	A	244	ASN	Mainchain
1	A	251	SER	Mainchain
1	A	257	THR	Mainchain
1	A	273	LEU	Mainchain
1	A	287	HIS	Mainchain
1	A	301	ASP	Mainchain
1	A	330	CYS	Mainchain
1	A	39	GLU	Mainchain
1	A	44	LEU	Mainchain
1	A	48	GLY	Mainchain
1	A	51	GLY	Mainchain
1	A	60	ARG	Mainchain
1	A	63	HIS	Mainchain
1	A	73	ARG	Mainchain
2	B	100	GLU	Mainchain
2	B	117	PHE	Mainchain
2	B	120	PHE	Mainchain
2	B	13	LEU	Mainchain
2	B	131	TRP	Mainchain
2	B	156	ALA	Mainchain
2	B	194	GLY	Mainchain
2	B	219	LYS	Mainchain
2	B	227	ASP	Mainchain

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Mol	Chain	Res	Type	Group
2	B	230	LEU	Mainchain
2	B	237	GLY	Peptide,Mainchain
2	B	276	ILE	Mainchain
2	B	28	PHE	Mainchain
2	B	29	ILE	Mainchain
2	B	297	SER	Mainchain
2	B	31	TRP	Mainchain
2	B	319	MET	Mainchain
2	B	330	SER	Mainchain
2	B	346	SER	Mainchain
2	B	347	VAL	Mainchain
2	B	365	VAL	Mainchain
2	B	367	LYS	Mainchain
2	B	383	MET	Mainchain
2	B	386	GLU	Mainchain
2	B	413	GLU	Mainchain
2	B	418	SER	Mainchain
2	B	42	THR	Mainchain
2	B	44	ARG	Mainchain
2	B	463	ILE	Mainchain
2	B	466	LYS	Mainchain
2	B	52	LEU	Mainchain
2	B	54	TRP	Mainchain
2	B	61	VAL	Mainchain
2	B	618	SER	Mainchain
2	B	621	VAL	Mainchain
2	B	624	LYS	Mainchain
2	B	63	THR	Mainchain
2	B	638	GLU	Mainchain
2	B	704	PHE	Mainchain
2	B	708	PRO	Mainchain
2	B	709	ASP	Mainchain
2	B	710	LYS	Mainchain
2	B	716	THR	Mainchain
2	B	726	ASN	Mainchain
2	B	739	SER	Mainchain
2	B	748	GLU	Mainchain
2	B	760	ARG	Mainchain
2	B	765	ARG	Mainchain
2	B	767	SER	Mainchain
2	B	777	ASP	Mainchain
2	B	789	PRO	Mainchain

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Mol	Chain	Res	Type	Group
2	B	801	GLU	Mainchain
2	B	820	TYR	Mainchain
2	B	822	TYR	Mainchain
2	B	824	CYS	Mainchain
2	B	842	THR	Mainchain
2	B	843	GLU	Mainchain
2	B	852	HIS	Mainchain
2	B	859	LEU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2616	0	2581	53	0
2	B	6062	0	6069	91	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	12	1	0
6	A	4	0	3	0	0
6	B	24	0	18	2	0
7	B	1	0	0	0	0
8	A	97	0	0	9	0
8	B	118	0	0	18	0
All	All	8957	0	8683	144	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 8.

All (144) 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)
2:B:834:CYS:O	8:B:1001:HOH:O	1.79	1.00
2:B:100:GLU:O	8:B:1002:HOH:O	1.81	0.98
2:B:83:ASP:HB2	2:B:84:PRO:HD3	1.45	0.95
1:A:231:ALA:O	1:A:234:GLU:HG2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLU:OE2	8:A:501:HOH:O	2.02	0.77
2:B:149:ARG:NH1	8:B:1001:HOH:O	2.07	0.76
1:A:159:TYR:OH	8:A:502:HOH:O	2.04	0.74
2:B:826:ARG:NH1	8:B:1003:HOH:O	2.22	0.72
2:B:795:ARG:NH2	8:B:1004:HOH:O	2.24	0.70
2:B:83:ASP:HB2	2:B:84:PRO:CD	2.20	0.69
1:A:306:ARG:HG2	1:A:328:PHE:CE1	2.28	0.69
1:A:58:GLN:HE21	1:A:58:GLN:HA	1.59	0.68
2:B:220:LEU:HG	2:B:772:PHE:CZ	2.30	0.67
6:B:906:ACT:H1	8:B:1010:HOH:O	1.96	0.65
2:B:704:PHE:CZ	2:B:710:LYS:HE2	2.32	0.64
2:B:763:ARG:NH1	2:B:764:THR:O	2.32	0.62
2:B:872:ARG:HG3	2:B:872:ARG:HH11	1.66	0.61
2:B:83:ASP:CB	2:B:84:PRO:HD3	2.28	0.60
1:A:320:SER:HB3	8:A:556:HOH:O	2.02	0.59
2:B:199:ARG:NH1	8:B:1008:HOH:O	2.36	0.59
2:B:243:LEU:C	2:B:243:LEU:HD23	2.28	0.58
2:B:13:LEU:N	2:B:13:LEU:HD23	2.18	0.58
2:B:39:ASN:HB2	8:B:1070:HOH:O	2.03	0.58
1:A:311:LYS:O	1:A:315:ASP:HB2	2.03	0.57
2:B:679:LEU:CD1	8:B:1027:HOH:O	2.53	0.57
2:B:879:LEU:O	2:B:880:ILE:C	2.46	0.57
1:A:196:LEU:O	1:A:198:SER:N	2.40	0.56
1:A:175:THR:O	1:A:178:ASP:HB2	2.05	0.55
1:A:317:ASN:C	1:A:319:ASP:N	2.62	0.55
1:A:44:LEU:HD11	1:A:227:MET:CE	2.36	0.55
2:B:35:THR:HG21	8:B:1070:HOH:O	2.07	0.55
2:B:374:GLU:OE2	2:B:428:TYR:OH	2.24	0.55
2:B:679:LEU:HD13	8:B:1027:HOH:O	2.07	0.55
2:B:255:ARG:HD3	8:B:1072:HOH:O	2.07	0.55
2:B:35:THR:CG2	8:B:1070:HOH:O	2.55	0.54
2:B:401:PHE:HA	2:B:404:SER:O	2.07	0.54
2:B:679:LEU:CD1	8:B:1074:HOH:O	2.55	0.54
2:B:377:ILE:HD12	2:B:392:VAL:HG21	1.90	0.53
2:B:233:ILE:O	2:B:233:ILE:HG22	2.06	0.53
2:B:146:ASN:ND2	2:B:313:LEU:HD22	2.24	0.53
2:B:19:VAL:HG12	2:B:21:THR:H	1.74	0.53
1:A:317:ASN:O	1:A:319:ASP:N	2.42	0.52
2:B:834:CYS:HB3	8:B:1028:HOH:O	2.09	0.52
2:B:396:ILE:O	2:B:400:ALA:HB2	2.09	0.52
2:B:58:ASN:O	2:B:59:MET:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:GLN:O	2:B:425:MET:HB3	2.09	0.51
2:B:467:ASN:OD1	2:B:468:LYS:N	2.37	0.51
1:A:317:ASN:O	1:A:320:SER:N	2.43	0.51
2:B:413:GLU:OE2	2:B:579:THR:OG1	2.24	0.51
2:B:370:PRO:HB2	2:B:371:PRO:HD3	1.92	0.50
1:A:93:ALA:CB	1:A:144:CYS:SG	3.00	0.50
1:A:106:ASN:ND2	1:A:138:ASP:HB2	2.26	0.50
2:B:288:ARG:O	2:B:290:GLN:HG3	2.11	0.50
1:A:87:MET:O	1:A:91:ILE:HG13	2.11	0.50
2:B:779:GLU:N	2:B:779:GLU:OE1	2.44	0.50
1:A:331:ALA:HA	1:A:337:ILE:HD11	1.94	0.49
1:A:236:ASP:OD2	1:A:286:SER:OG	2.29	0.49
1:A:202:ARG:HH22	2:B:709:ASP:HB3	1.77	0.49
1:A:49:GLU:HB2	8:A:512:HOH:O	2.12	0.49
2:B:826:ARG:NE	8:B:1005:HOH:O	2.30	0.48
1:A:209:GLN:HA	1:A:241:GLU:OE2	2.13	0.48
2:B:725:ALA:C	2:B:726:ASN:HD22	2.21	0.48
1:A:317:ASN:O	1:A:318:PRO:C	2.58	0.47
1:A:47:THR:O	1:A:208:GLY:O	2.33	0.47
2:B:315:LEU:O	2:B:315:LEU:HG	2.15	0.47
2:B:464:LEU:N	2:B:464:LEU:HD12	2.29	0.47
1:A:163:ASP:CG	8:A:507:HOH:O	2.58	0.47
2:B:745:ILE:O	2:B:767:SER:N	2.43	0.47
2:B:82:LYS:O	2:B:85:LYS:HG3	2.15	0.46
1:A:93:ALA:HB3	1:A:144:CYS:SG	2.55	0.46
2:B:692:TYR:CE2	2:B:812:PRO:HD3	2.49	0.46
2:B:632:SER:HB3	2:B:635:GLU:HB2	1.98	0.46
1:A:44:LEU:HD11	1:A:227:MET:HE3	1.96	0.46
2:B:601:LYS:O	2:B:601:LYS:HG3	2.16	0.46
1:A:317:ASN:C	1:A:319:ASP:H	2.24	0.46
1:A:264:PHE:HA	1:A:267:SER:OG	2.15	0.46
2:B:157:TYR:OH	2:B:161:LYS:HD2	2.15	0.46
1:A:264:PHE:O	1:A:322:LYS:NZ	2.48	0.46
1:A:274:ASN:HA	1:A:329:THR:O	2.15	0.46
1:A:207:GLY:HA3	1:A:212:GLU:HG3	1.97	0.45
2:B:220:LEU:HG	2:B:772:PHE:HZ	1.79	0.45
2:B:752:PHE:O	2:B:792:ALA:HA	2.16	0.45
1:A:264:PHE:O	1:A:322:LYS:HE3	2.17	0.45
2:B:58:ASN:OD1	2:B:58:ASN:N	2.48	0.45
1:A:230:VAL:HG21	1:A:313:PHE:CZ	2.52	0.45
2:B:182:ASP:O	2:B:186:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:LEU:CD2	2:B:772:PHE:HZ	2.30	0.45
1:A:41:LYS:NZ	2:B:721:ASP:OD2	2.46	0.45
1:A:264:PHE:O	1:A:322:LYS:CE	2.65	0.45
1:A:344:VAL:O	1:A:348:ILE:HG13	2.17	0.45
2:B:599:PRO:HA	2:B:617:MET:O	2.17	0.45
1:A:47:THR:HG23	1:A:48:GLY:N	2.32	0.44
1:A:320:SER:CB	8:A:556:HOH:O	2.63	0.44
2:B:71:ASP:HB2	2:B:355:LEU:HD13	1.99	0.44
2:B:81:PRO:O	2:B:82:LYS:CB	2.66	0.44
1:A:333:ASP:OD1	1:A:333:ASP:C	2.61	0.44
2:B:178:MET:HG2	2:B:179:PHE:CE2	2.53	0.44
2:B:58:ASN:ND2	2:B:60:GLU:HB3	2.33	0.44
2:B:639:TYR:CD1	2:B:639:TYR:C	2.96	0.44
1:A:93:ALA:HB1	1:A:144:CYS:SG	2.57	0.44
5:A:403:GDP:O1A	8:A:503:HOH:O	2.21	0.44
2:B:41:VAL:HG12	2:B:56:GLY:HA2	2.00	0.44
2:B:611:ARG:NH2	2:B:616:GLU:OE2	2.49	0.44
1:A:44:LEU:CD1	1:A:227:MET:HE3	2.48	0.43
1:A:57:LYS:HG2	1:A:67:TYR:OH	2.17	0.43
2:B:159:LYS:HD2	6:B:905:ACT:H2	2.00	0.43
2:B:43:LEU:HD12	2:B:54:TRP:HB3	2.00	0.43
1:A:296:ASP:OD1	1:A:296:ASP:N	2.51	0.43
2:B:22:LEU:HG	2:B:131:TRP:CZ3	2.54	0.43
2:B:136:PHE:CE1	2:B:402:LYS:HE2	2.53	0.43
2:B:286:LEU:HD23	2:B:286:LEU:C	2.43	0.43
2:B:307:ILE:HG13	2:B:307:ILE:O	2.19	0.42
1:A:47:THR:O	1:A:208:GLY:C	2.61	0.42
2:B:31:TRP:HE3	2:B:32:ASP:O	2.02	0.42
2:B:179:PHE:C	2:B:181:ALA:H	2.28	0.42
2:B:386:GLU:O	2:B:386:GLU:HG2	2.17	0.42
1:A:112:LEU:HD21	1:A:127:PRO:HG2	2.01	0.42
2:B:176:LEU:HD12	2:B:186:VAL:HG11	2.02	0.42
2:B:589:GLU:OE1	2:B:589:GLU:N	2.50	0.42
1:A:59:MET:SD	1:A:203:MET:HE1	2.59	0.42
1:A:217:ILE:HG13	8:A:505:HOH:O	2.19	0.42
2:B:817:ARG:O	2:B:842:THR:OG1	2.35	0.42
2:B:879:LEU:O	2:B:880:ILE:HD12	2.19	0.42
1:A:76:THR:HG22	1:A:80:TYR:CZ	2.54	0.42
2:B:323:LEU:HD12	2:B:456:PRO:HG3	2.01	0.42
1:A:53:SER:HB2	8:A:503:HOH:O	2.19	0.42
2:B:655:ASP:O	2:B:657:SER:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TYR:OH	1:A:286:SER:O	2.27	0.41
2:B:13:LEU:HD21	2:B:314:ASP:OD1	2.20	0.41
2:B:835:LEU:HB2	2:B:836:PRO:HD3	2.01	0.41
1:A:270:ILE:HD12	1:A:270:ILE:N	2.36	0.41
2:B:679:LEU:HD12	8:B:1027:HOH:O	2.18	0.41
1:A:47:THR:HB	1:A:251:SER:HB3	2.03	0.41
2:B:44:ARG:HG3	2:B:53:TYR:CZ	2.56	0.41
2:B:44:ARG:HA	2:B:131:TRP:HH2	1.85	0.41
2:B:238:LYS:O	2:B:239:PRO:C	2.59	0.41
2:B:225:ASP:O	2:B:229:ILE:HG13	2.21	0.40
1:A:58:GLN:HA	1:A:58:GLN:NE2	2.33	0.40
2:B:125:ASP:O	2:B:127:THR:N	2.44	0.40
2:B:320:THR:O	2:B:455:SER:OG	2.39	0.40
2:B:589:GLU:O	2:B:592:THR:HG22	2.21	0.40
2:B:751:MET:O	2:B:758:THR:HA	2.21	0.40
2:B:679:LEU:HD11	8:B:1074:HOH:O	2.17	0.40
2:B:679:LEU:HD12	2:B:679:LEU:N	2.37	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	315/327 (96%)	292 (93%)	20 (6%)	3 (1%)	12 28
2	B	749/885 (85%)	664 (89%)	74 (10%)	11 (2%)	8 18
All	All	1064/1212 (88%)	956 (90%)	94 (9%)	14 (1%)	9 21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	81	PRO

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Mol	Chain	Res	Type
2	B	82	LYS
1	A	197	GLN
2	B	85	LYS
2	B	99	LEU
2	B	126	ASP
1	A	351	LEU
2	B	235	ALA
2	B	622	GLU
2	B	769	GLY
2	B	83	ASP
1	A	318	PRO
2	B	281	PRO
2	B	233	ILE

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	289/297 (97%)	288 (100%)	1 (0%)	86 94
2	B	672/777 (86%)	667 (99%)	5 (1%)	76 89
All	All	961/1074 (90%)	955 (99%)	6 (1%)	78 91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
2	B	80	LEU
2	B	233	ILE
2	B	303	GLU
2	B	845	SER
2	B	879	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	63	HIS
1	A	81	GLN
2	B	290	GLN
2	B	321	GLN
2	B	333	ASN
2	B	340	GLN
2	B	643	GLN
2	B	662	GLN
2	B	808	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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	ACT	B	906	-	3,3,3	0.99	0	3,3,3	0.83	0
6	ACT	B	904	-	3,3,3	1.02	0	3,3,3	0.82	0
3	ALF	A	401	5	4,4,4	1.47	0	-		
6	ACT	A	404	-	3,3,3	1.03	0	3,3,3	0.80	0
6	ACT	B	903	-	3,3,3	1.03	0	3,3,3	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ACT	B	901	-	3,3,3	0.99	0	3,3,3	0.84	0
6	ACT	B	902	-	3,3,3	1.07	0	3,3,3	0.74	0
6	ACT	B	905	-	3,3,3	1.02	0	3,3,3	0.81	0
5	GDP	A	403	4,3	29,30,30	1.25	4 (13%)	45,47,47	1.91	10 (22%)

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
5	GDP	A	403	4,3	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	GDP	C5-C4	3.50	1.48	1.38
5	A	403	GDP	PA-O3A	2.67	1.62	1.59
5	A	403	GDP	C6-N1	-2.35	1.34	1.38
5	A	403	GDP	C5-N7	-2.19	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	403	GDP	C5-C4-N3	-6.08	118.71	128.39
5	A	403	GDP	C2-N3-C4	5.01	120.93	112.30
5	A	403	GDP	N9-C4-N3	4.31	134.57	125.95
5	A	403	GDP	C6-C5-N7	3.60	136.85	130.29
5	A	403	GDP	C4-C5-N7	-2.94	106.01	110.67
5	A	403	GDP	O3B-PB-O2B	2.63	117.65	107.80
5	A	403	GDP	O6-C6-C5	-2.57	119.75	126.53
5	A	403	GDP	O3A-PA-O1A	-2.51	103.14	110.70
5	A	403	GDP	O3B-PB-O3A	-2.19	97.29	104.64
5	A	403	GDP	C8-N7-C5	2.07	107.95	104.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	403	GDP	PA-O3A-PB-O2B
5	A	403	GDP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
5	A	403	GDP	PA-O3A-PB-O1B

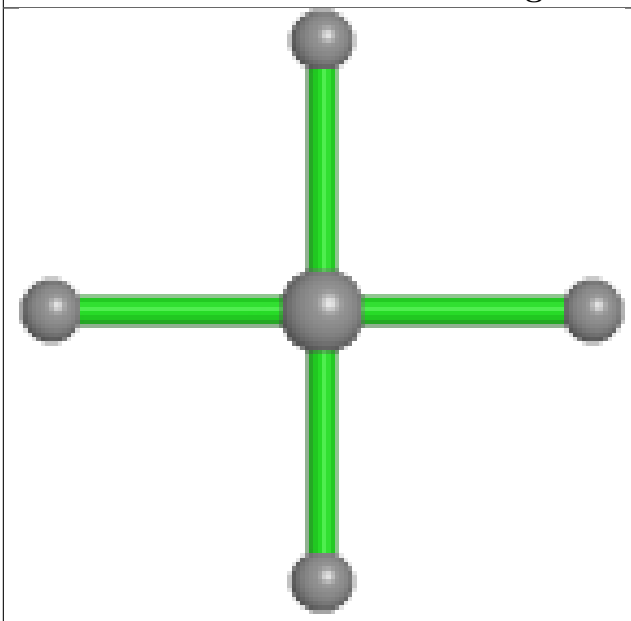
There are no ring outliers.

3 monomers are involved in 3 short contacts:

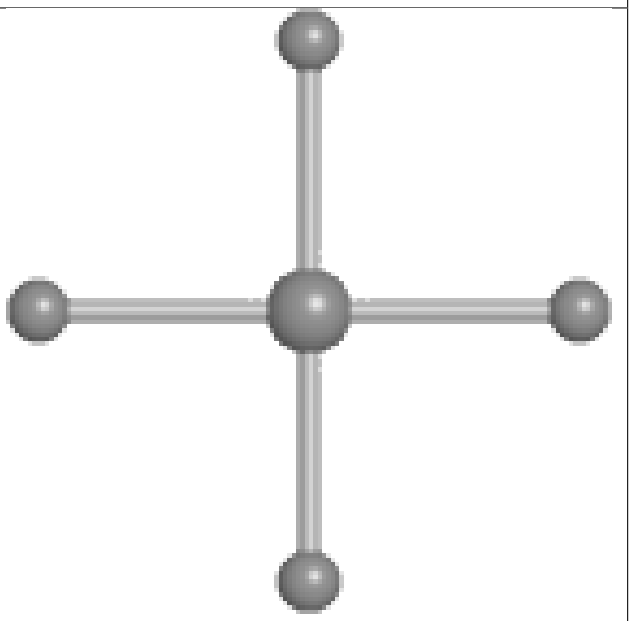
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	906	ACT	1	0
6	B	905	ACT	1	0
5	A	403	GDP	1	0

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 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.

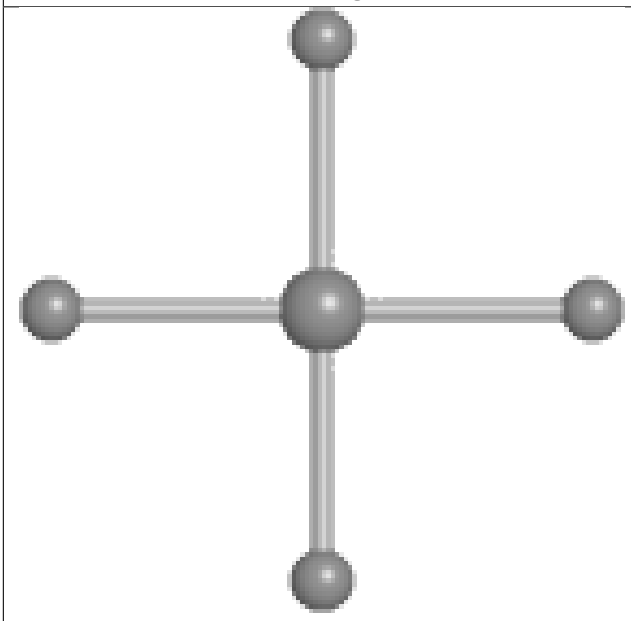
Ligand ALF A 401



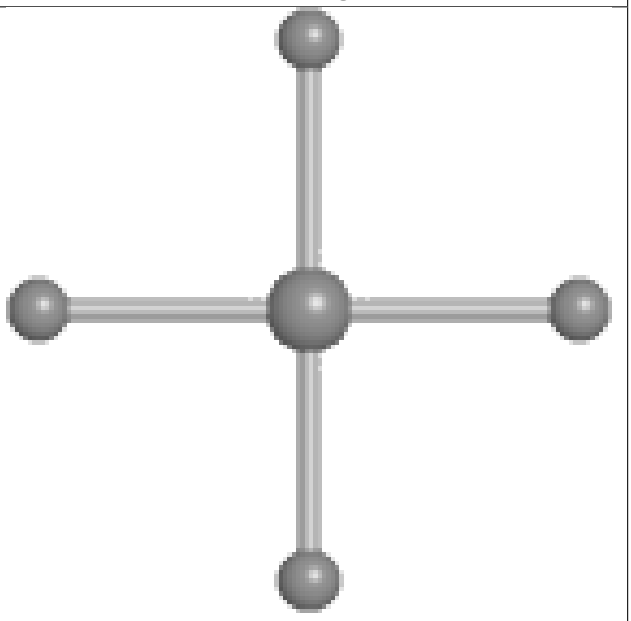
Bond lengths



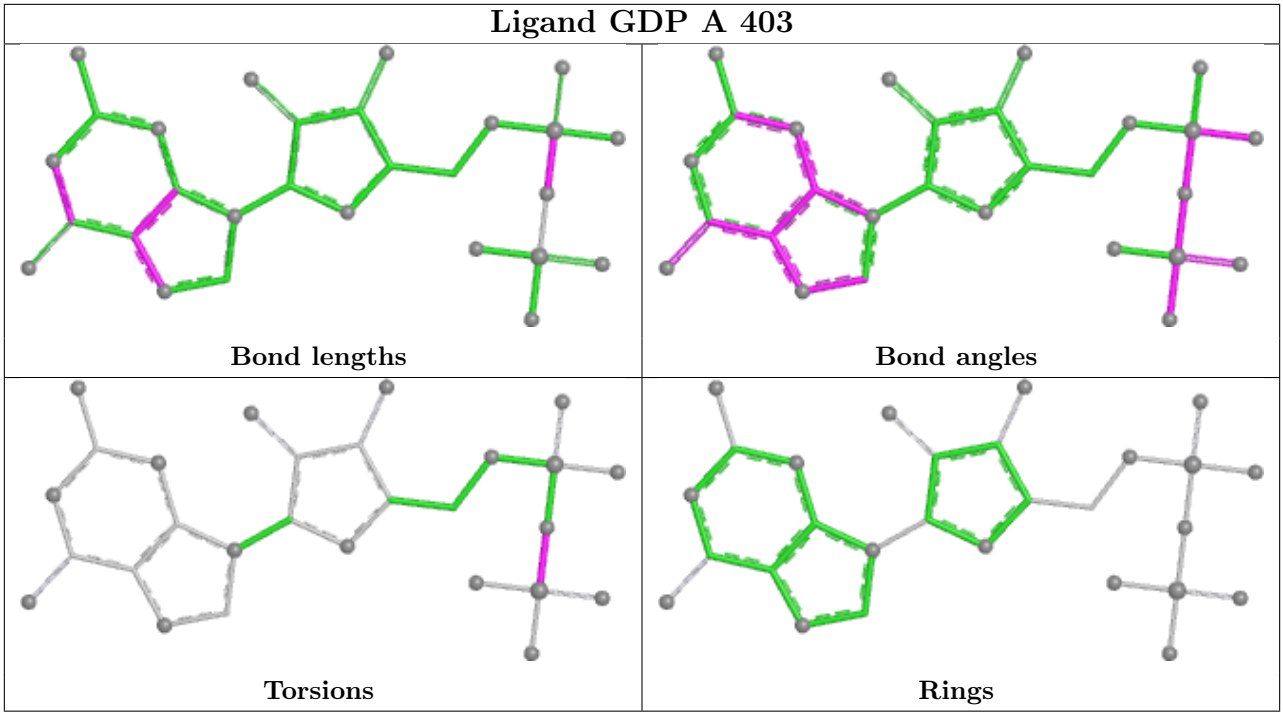
Bond angles



Torsions



Rings



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	317/327 (96%)	-0.19	2 (0%)	85	83	58, 81, 118, 171	0
2	B	755/885 (85%)	0.09	16 (2%)	63	58	63, 99, 157, 208	0
All	All	1072/1212 (88%)	0.01	18 (1%)	69	64	58, 92, 153, 208	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	880	ILE	4.7
2	B	86	ILE	4.4
2	B	233	ILE	4.2
2	B	99	LEU	3.4
1	A	353	LEU	3.0
2	B	267	LEU	2.9
2	B	366	TRP	2.9
2	B	420	LYS	2.6
2	B	84	PRO	2.6
2	B	57	PRO	2.6
2	B	341	LEU	2.4
2	B	470	ARG	2.2
2	B	218	ASN	2.2
2	B	365	VAL	2.2
2	B	879	LEU	2.1
2	B	785	LYS	2.1
1	A	339	PHE	2.1
2	B	58	ASN	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)

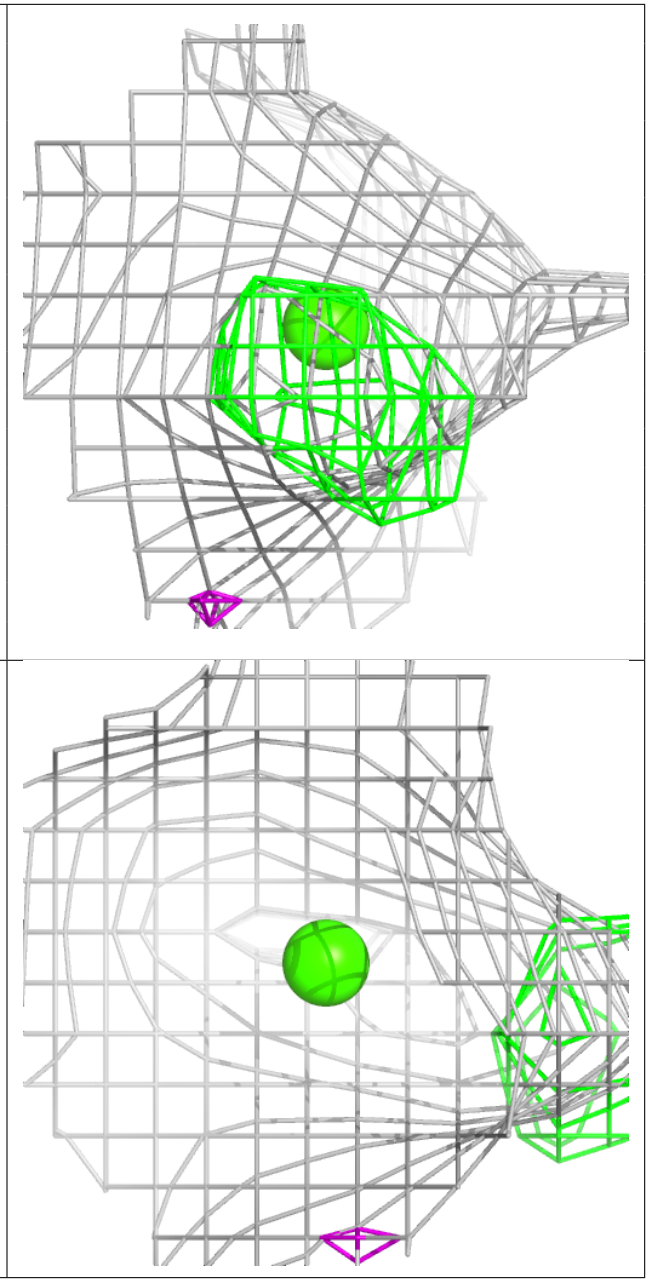
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	B	906	4/4	0.64	0.35	86,102,115,117	0
6	ACT	B	905	4/4	0.70	0.34	95,111,121,131	0
7	CA	B	907	1/1	0.74	0.13	126,126,126,126	0
6	ACT	B	901	4/4	0.79	0.20	83,91,96,102	0
6	ACT	B	902	4/4	0.81	0.16	53,60,63,78	0
6	ACT	A	404	4/4	0.81	0.32	103,121,122,148	0
4	MG	B	908	1/1	0.83	0.29	90,90,90,90	0
6	ACT	B	903	4/4	0.85	0.13	87,87,96,103	0
6	ACT	B	904	4/4	0.92	0.23	100,116,118,122	0
4	MG	A	402	1/1	0.94	0.17	59,59,59,59	0
3	ALF	A	401	5/5	0.96	0.11	67,75,103,129	0
5	GDP	A	403	28/28	0.97	0.07	35,51,70,88	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.

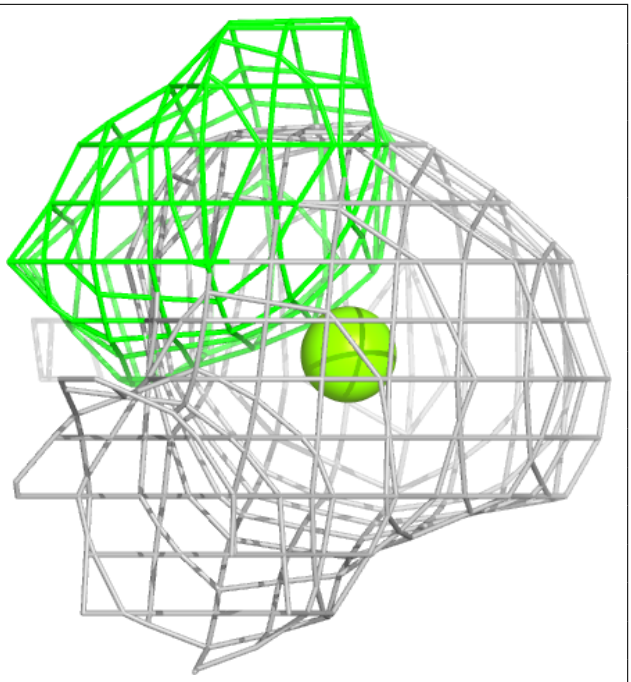
Electron density around CA B 907:

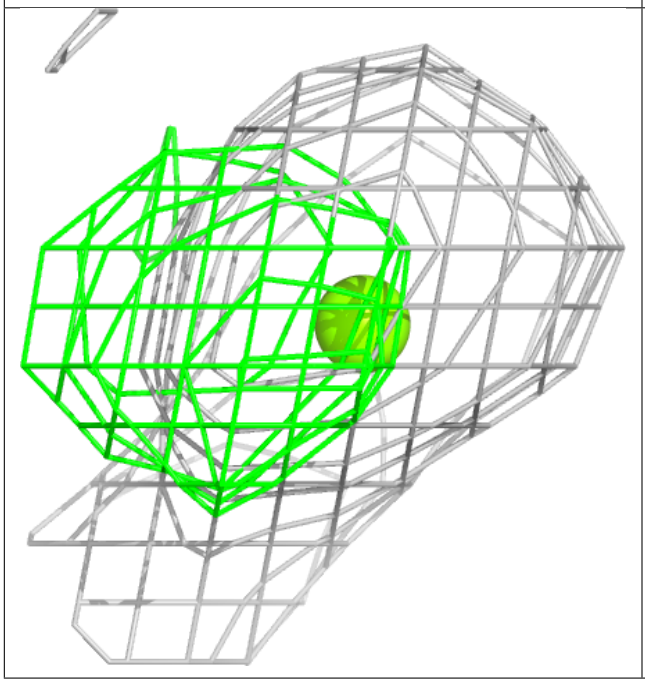
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

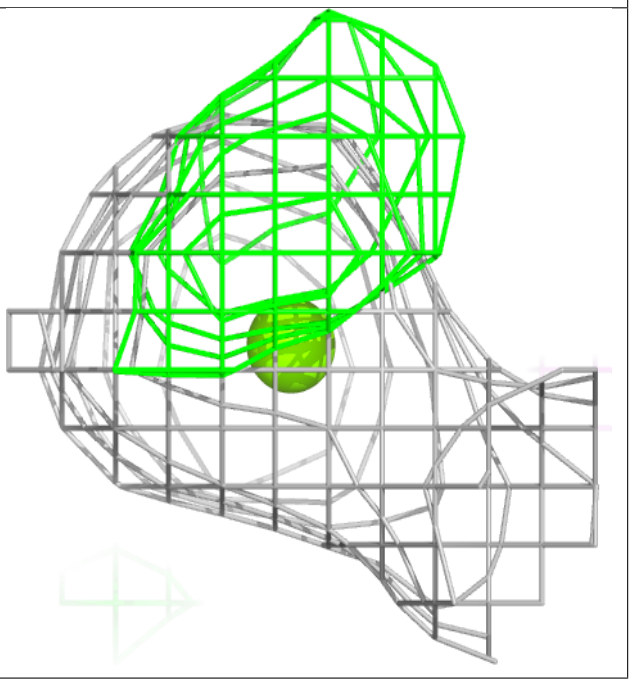


Electron density around MG B 908:

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

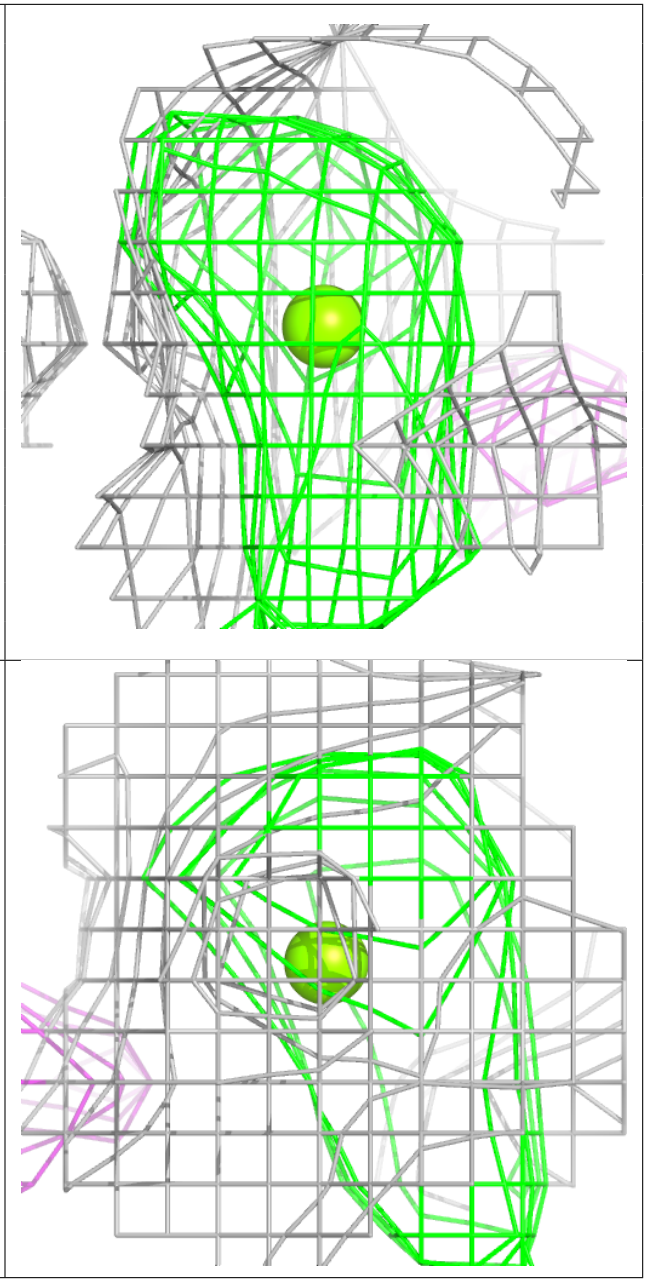






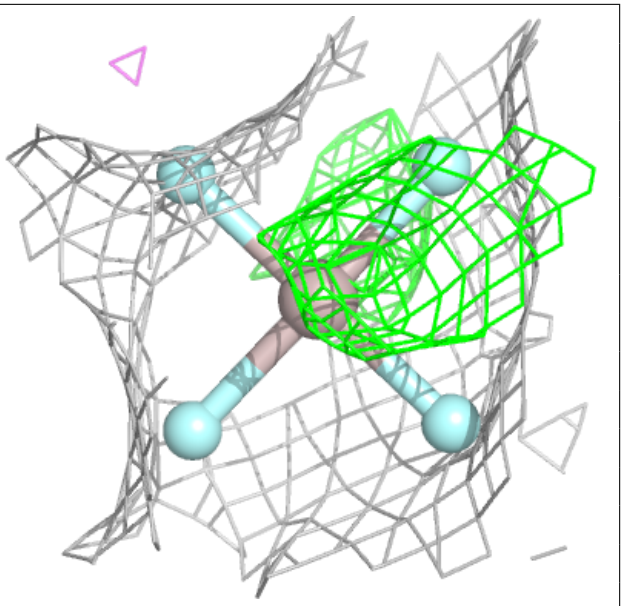
Electron density around MG A 402:

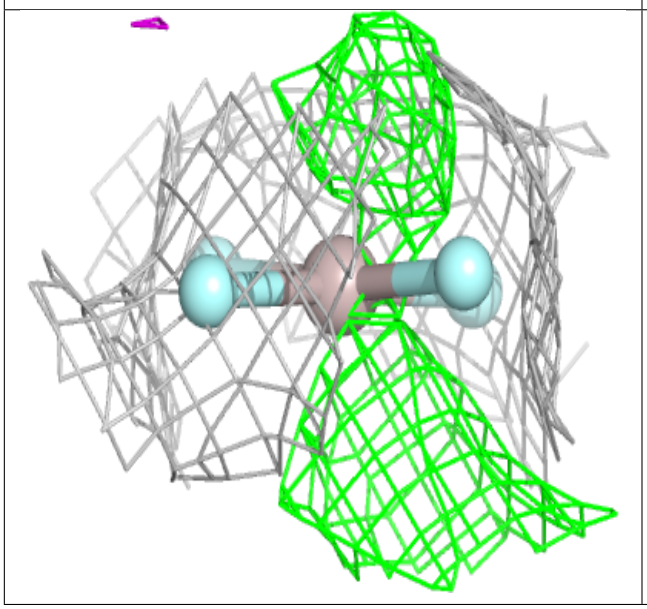
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

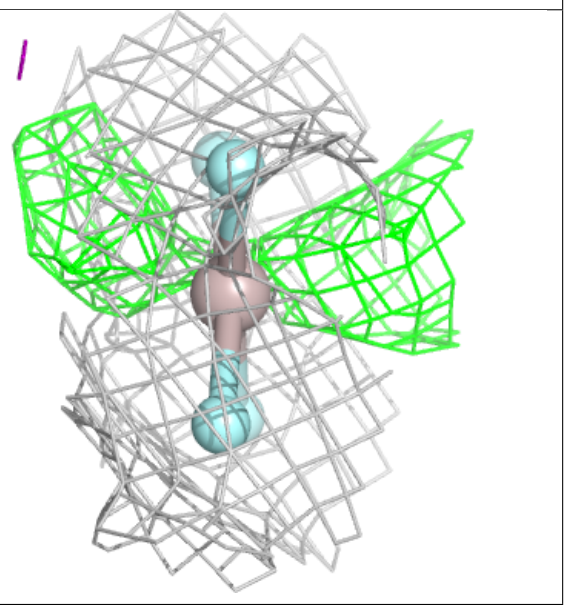


Electron density around ALF A 401:

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

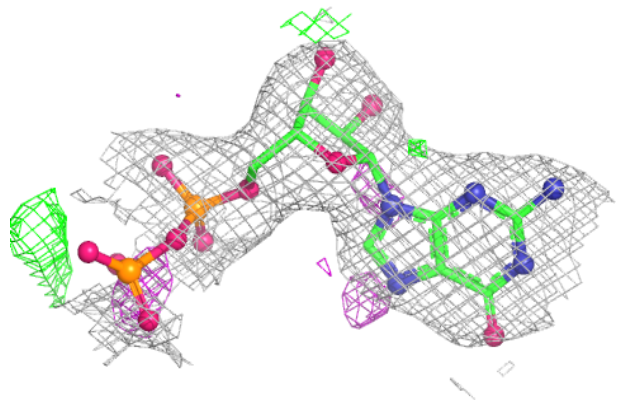


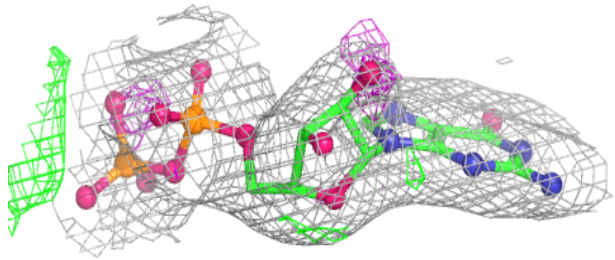


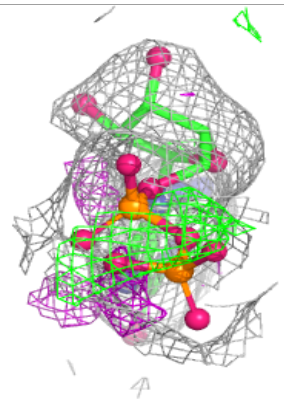


Electron density around GDP A 403:

$2mF_o$-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.