



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:03 PM UTC

PDB ID : 3CX8 / pdb_00003cx8
Title : Crystal Structure of PDZRhGEF rgRGS Domain in a Complex with Galpha-13 Bound to GTP-gamma-S
Authors : Sprang, S.R.; Chen, Z.
Deposited on : 2008-04-23
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

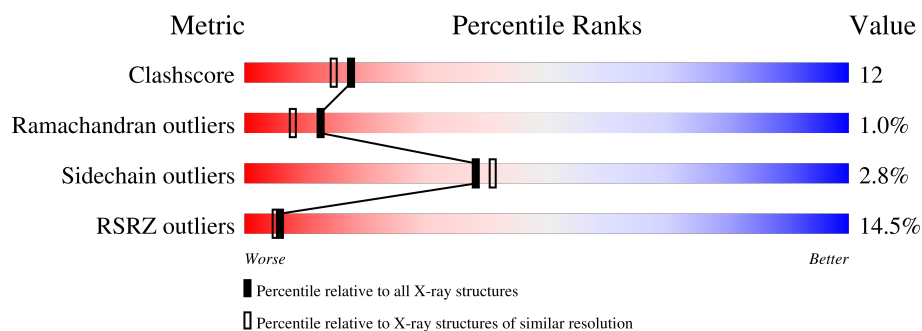
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	338	
2	B	203	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4513 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 alpha-13 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2635	1678	467	480	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLY	-	expression tag	UNP P27601

- Molecule 2 is a protein called Rho guanine nucleotide exchange factor 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1547	977	260	303	7			

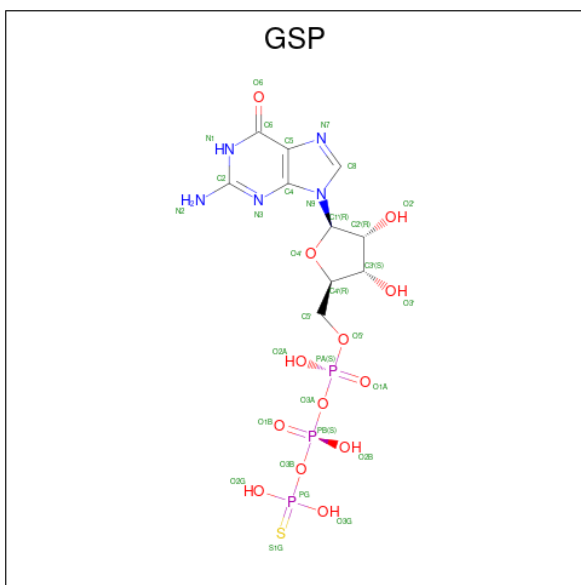
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	306	GLY	-	expression tag	UNP Q9ES67

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

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

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

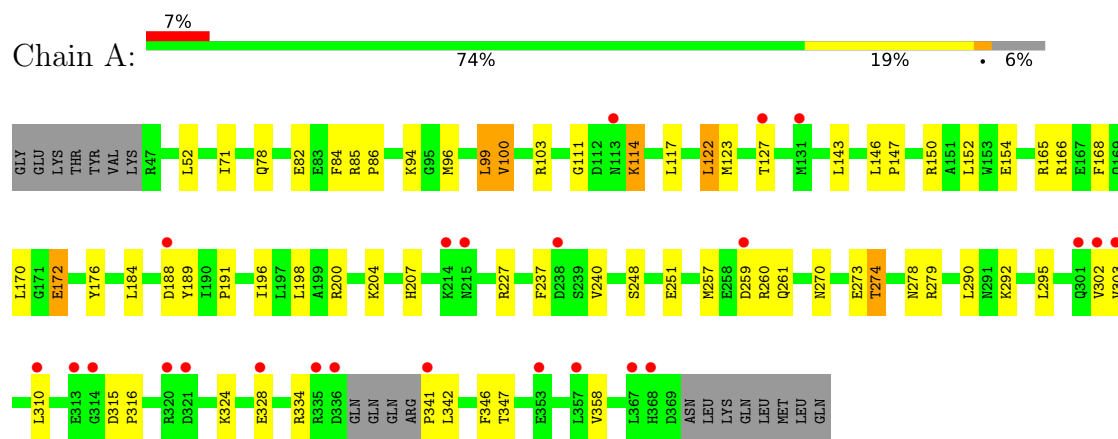
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	220	Total O 220 220	0	0
5	B	78	Total O 78 78	0	0

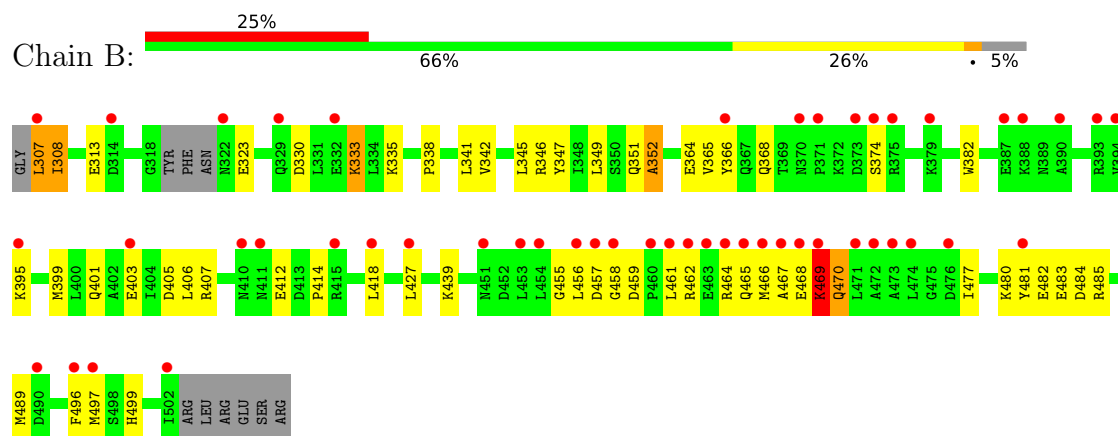
3 Residue-property plots

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

- Molecule 1: Guanine nucleotide-binding protein alpha-13 subunit



- Molecule 2: Rho guanine nucleotide exchange factor 11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.11Å 66.12Å 152.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-2.00) 98.2 (40.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.253 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.2	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	0.94	EDS
Total number of atoms	4513	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/2687	0.83	6/3618 (0.2%)
2	B	0.35	0/1574	0.87	2/2127 (0.1%)
All	All	0.39	0/4261	0.85	8/5745 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	470	GLN	N-CA-C	-7.37	102.21	112.45
2	B	352	ALA	N-CA-C	6.85	117.52	108.07
1	A	111	GLY	N-CA-C	-6.67	104.24	112.77
1	A	71	ILE	N-CA-C	5.73	117.25	111.00
1	A	257	MET	N-CA-C	-5.34	105.12	111.69
1	A	200	ARG	N-CA-C	5.24	117.50	109.07
1	A	114	LYS	N-CA-C	-5.18	106.22	112.54
1	A	227	ARG	N-CA-C	5.14	119.80	111.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2635	0	2631	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1547	0	1524	51	0
3	A	1	0	0	0	0
4	A	32	0	12	3	0
5	A	220	0	0	5	0
5	B	78	0	0	5	0
All	All	4513	0	4167	104	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 12.

All (104) 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:307:LEU:HB2	5:B:274:HOH:O	1.83	0.79
2:B:395:LYS:HA	2:B:395:LYS:HE2	1.64	0.78
2:B:330:ASP:HB3	2:B:333:LYS:HD2	1.69	0.75
1:A:302:VAL:HG23	1:A:303:VAL:HG23	1.70	0.71
2:B:307:LEU:HB3	5:B:25:HOH:O	1.91	0.69
2:B:496:PHE:HD2	2:B:497:MET:HE2	1.59	0.67
1:A:259:ASP:O	1:A:261:GLN:N	2.30	0.65
2:B:330:ASP:HB3	2:B:333:LYS:CD	2.25	0.65
2:B:364:GLU:O	2:B:368:GLN:HG3	1.96	0.65
2:B:347:TYR:CE1	2:B:351:GLN:HG3	2.33	0.64
1:A:191:PRO:HB2	1:A:196:ILE:CD1	2.28	0.64
2:B:341:LEU:HD23	2:B:497:MET:HE1	1.82	0.62
1:A:191:PRO:HB2	1:A:196:ILE:HD11	1.83	0.61
2:B:307:LEU:HD12	2:B:307:LEU:N	2.14	0.61
1:A:146:LEU:HB3	1:A:147:PRO:HD3	1.82	0.61
1:A:188:ASP:HB2	5:A:948:HOH:O	2.00	0.60
1:A:278:ASN:HB2	2:B:351:GLN:HE22	1.68	0.58
1:A:100:VAL:CG2	1:A:123:MET:SD	2.92	0.58
2:B:466:MET:HG3	2:B:470:GLN:NE2	2.18	0.58
1:A:127:THR:HG22	5:A:767:HOH:O	2.03	0.58
1:A:117:LEU:HD12	1:A:117:LEU:N	2.20	0.57
1:A:172:GLU:H	1:A:172:GLU:CD	2.11	0.56
2:B:338:PRO:O	2:B:342:VAL:HG23	2.05	0.56
2:B:427:LEU:C	2:B:427:LEU:HD13	2.30	0.56
2:B:469:LYS:HE2	5:B:266:HOH:O	2.05	0.56
1:A:85:ARG:HB3	1:A:86:PRO:HD3	1.87	0.56
2:B:412:GLU:O	2:B:414:PRO:HD3	2.06	0.55
1:A:176:TYR:CD2	1:A:198:LEU:HD13	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:LYS:HE3	2:B:364:GLU:OE2	2.06	0.55
1:A:341:PRO:HD3	5:A:942:HOH:O	2.06	0.55
2:B:395:LYS:HE2	2:B:395:LYS:CA	2.36	0.55
1:A:96:MET:HG3	1:A:122:LEU:HD22	1.89	0.54
2:B:468:GLU:HG3	2:B:468:GLU:O	2.08	0.54
2:B:481:TYR:CD1	2:B:489:MET:HE1	2.43	0.54
2:B:352:ALA:HB1	5:B:90:HOH:O	2.08	0.53
2:B:482:GLU:HB2	2:B:484:ASP:OD1	2.08	0.53
1:A:176:TYR:CG	1:A:198:LEU:HD13	2.44	0.53
1:A:248:SER:O	1:A:251:GLU:HG2	2.08	0.53
1:A:204:LYS:O	1:A:207:HIS:HE1	1.93	0.52
1:A:117:LEU:HD12	1:A:117:LEU:H	1.74	0.51
1:A:143:LEU:HD11	5:A:951:HOH:O	2.10	0.51
2:B:346:ARG:HG3	2:B:477:ILE:CD1	2.40	0.51
2:B:481:TYR:CG	2:B:489:MET:HE1	2.46	0.51
1:A:270:ASN:O	1:A:274:THR:HG22	2.11	0.50
2:B:382:TRP:CH2	2:B:405:ASP:HB2	2.47	0.50
2:B:346:ARG:HG3	2:B:477:ILE:HD11	1.93	0.50
1:A:100:VAL:HG22	1:A:123:MET:SD	2.51	0.49
1:A:278:ASN:CB	2:B:351:GLN:HE22	2.26	0.49
1:A:292:LYS:HD3	1:A:295:LEU:HD12	1.95	0.49
2:B:466:MET:HG3	2:B:470:GLN:HE21	1.76	0.49
2:B:406:LEU:C	2:B:406:LEU:HD23	2.39	0.48
1:A:310:LEU:H	1:A:310:LEU:HD12	1.78	0.48
2:B:307:LEU:O	2:B:308:ILE:HB	2.14	0.47
1:A:166:ARG:HH21	1:A:303:VAL:HG21	1.80	0.47
2:B:466:MET:HE1	2:B:469:LYS:NZ	2.31	0.46
1:A:84:PHE:CD1	1:A:196:ILE:HG13	2.51	0.46
2:B:345:LEU:O	2:B:349:LEU:HD13	2.15	0.46
2:B:457:ASP:O	2:B:459:ASP:N	2.49	0.46
1:A:84:PHE:CG	1:A:196:ILE:HG13	2.51	0.46
2:B:466:MET:CE	2:B:469:LYS:HB3	2.46	0.46
1:A:248:SER:OG	1:A:292:LYS:HD2	2.16	0.45
1:A:114:LYS:O	1:A:117:LEU:HD13	2.17	0.45
1:A:165:ARG:HA	1:A:168:PHE:CZ	2.51	0.45
1:A:198:LEU:HA	4:A:755:GSP:HO2'	1.79	0.45
1:A:310:LEU:HD12	1:A:310:LEU:N	2.31	0.45
2:B:462:ARG:O	2:B:465:GLN:HB3	2.17	0.45
2:B:485:ARG:HB3	2:B:489:MET:HE2	1.99	0.45
1:A:165:ARG:HA	1:A:168:PHE:CE2	2.52	0.44
1:A:273:GLU:OE1	2:B:439:LYS:NZ	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:HG22	1:A:358:VAL:HG21	2.00	0.44
1:A:117:LEU:H	1:A:117:LEU:CD1	2.30	0.44
1:A:292:LYS:HG2	4:A:755:GSP:C6	2.52	0.44
2:B:366:TYR:CE1	2:B:374:SER:HB2	2.53	0.44
1:A:334:ARG:HH22	1:A:341:PRO:N	2.16	0.44
1:A:94:LYS:HE2	1:A:127:THR:OG1	2.17	0.44
1:A:198:LEU:HA	4:A:755:GSP:O2'	2.18	0.44
1:A:122:LEU:HD13	1:A:152:LEU:CD1	2.48	0.43
1:A:237:PHE:HA	1:A:240:VAL:CG2	2.49	0.43
2:B:307:LEU:O	2:B:308:ILE:CB	2.66	0.43
2:B:462:ARG:O	2:B:462:ARG:HD2	2.18	0.43
1:A:146:LEU:HG	1:A:150:ARG:HH12	1.83	0.42
2:B:338:PRO:HB2	2:B:467:ALA:HB2	2.02	0.42
1:A:99:LEU:HD13	1:A:170:LEU:HD22	2.02	0.42
2:B:456:LEU:HD23	2:B:462:ARG:NE	2.34	0.42
1:A:78:GLN:O	1:A:82:GLU:HG3	2.20	0.42
1:A:127:THR:HG23	2:B:313:GLU:OE1	2.20	0.42
2:B:399:MET:O	2:B:403:GLU:HG3	2.19	0.42
2:B:308:ILE:N	5:B:274:HOH:O	2.33	0.41
2:B:406:LEU:HD23	2:B:406:LEU:O	2.20	0.41
1:A:324:LYS:O	1:A:328:GLU:HG3	2.20	0.41
1:A:114:LYS:HD2	1:A:114:LYS:C	2.45	0.41
1:A:184:LEU:HD22	1:A:189:TYR:CZ	2.56	0.41
1:A:237:PHE:HA	1:A:240:VAL:HG21	2.01	0.41
2:B:365:VAL:HG13	2:B:499:HIS:CD2	2.55	0.41
1:A:310:LEU:H	1:A:310:LEU:CD1	2.33	0.41
2:B:461:LEU:HA	2:B:464:ARG:HH11	1.85	0.41
1:A:103:ARG:NE	5:A:956:HOH:O	2.21	0.41
1:A:150:ARG:O	1:A:154:GLU:HG3	2.21	0.41
1:A:290:LEU:HD12	1:A:346:PHE:CE2	2.56	0.41
2:B:466:MET:HE2	2:B:470:GLN:HG3	2.03	0.40
1:A:279:ARG:O	2:B:480:LYS:HE2	2.21	0.40
2:B:403:GLU:O	2:B:407:ARG:HG3	2.21	0.40
1:A:315:ASP:HA	1:A:316:PRO:HD2	1.94	0.40
1:A:334:ARG:NH1	1:A:342:LEU:HB2	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	315/338 (93%)	306 (97%)	8 (2%)	1 (0%)	36	35
2	B	189/203 (93%)	180 (95%)	5 (3%)	4 (2%)	5	2
All	All	504/541 (93%)	486 (96%)	13 (3%)	5 (1%)	12	8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	ARG
2	B	469	LYS
2	B	308	ILE
2	B	455	GLY
2	B	458	GLY

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	291/309 (94%)	285 (98%)	6 (2%)	47	52
2	B	170/179 (95%)	163 (96%)	7 (4%)	27	26
All	All	461/488 (94%)	448 (97%)	13 (3%)	38	41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	100	VAL
1	A	122	LEU
1	A	172	GLU
1	A	274	THR
2	B	307	LEU
2	B	323	GLU
2	B	333	LYS
2	B	401	GLN
2	B	418	LEU
2	B	469	LYS
2	B	483	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	78	GLN
1	A	160	ASN
1	A	207	HIS
1	A	368	HIS
2	B	329	GLN
2	B	351	GLN
2	B	368	GLN
2	B	383	ASN
2	B	416	ASN
2	B	430	GLN
2	B	434	ASN
2	B	465	GLN
2	B	470	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GSP	A	755	3	33,34,34	1.39	7 (21%)	47,54,54	1.72	12 (25%)

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	GSP	A	755	3	-	2/21/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	755	GSP	PA-O3A	3.09	1.62	1.59
4	A	755	GSP	PG-S1G	-2.94	1.84	1.90
4	A	755	GSP	PB-O3B	2.72	1.62	1.59
4	A	755	GSP	PG-O2G	-2.43	1.46	1.54
4	A	755	GSP	C2-N3	2.33	1.38	1.33
4	A	755	GSP	PB-O2B	-2.15	1.45	1.55
4	A	755	GSP	O4'-C1'	2.08	1.46	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	755	GSP	C2-N3-C4	4.37	119.83	112.30
4	A	755	GSP	C5-C4-N3	-3.56	122.72	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	755	GSP	C6-C5-N7	3.47	136.61	130.29
4	A	755	GSP	C8-N7-C5	3.07	109.72	104.26
4	A	755	GSP	N9-C8-N7	-2.90	108.03	113.40
4	A	755	GSP	O4'-C1'-N9	-2.67	102.32	108.36
4	A	755	GSP	C5-C6-N1	2.58	119.81	113.25
4	A	755	GSP	C4-C5-N7	-2.47	106.76	110.67
4	A	755	GSP	O6-C6-N1	-2.23	115.93	120.11
4	A	755	GSP	N9-C4-N3	2.18	130.32	125.95
4	A	755	GSP	N1-C2-N3	-2.14	119.40	123.32
4	A	755	GSP	O3G-PG-O3B	2.14	111.78	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

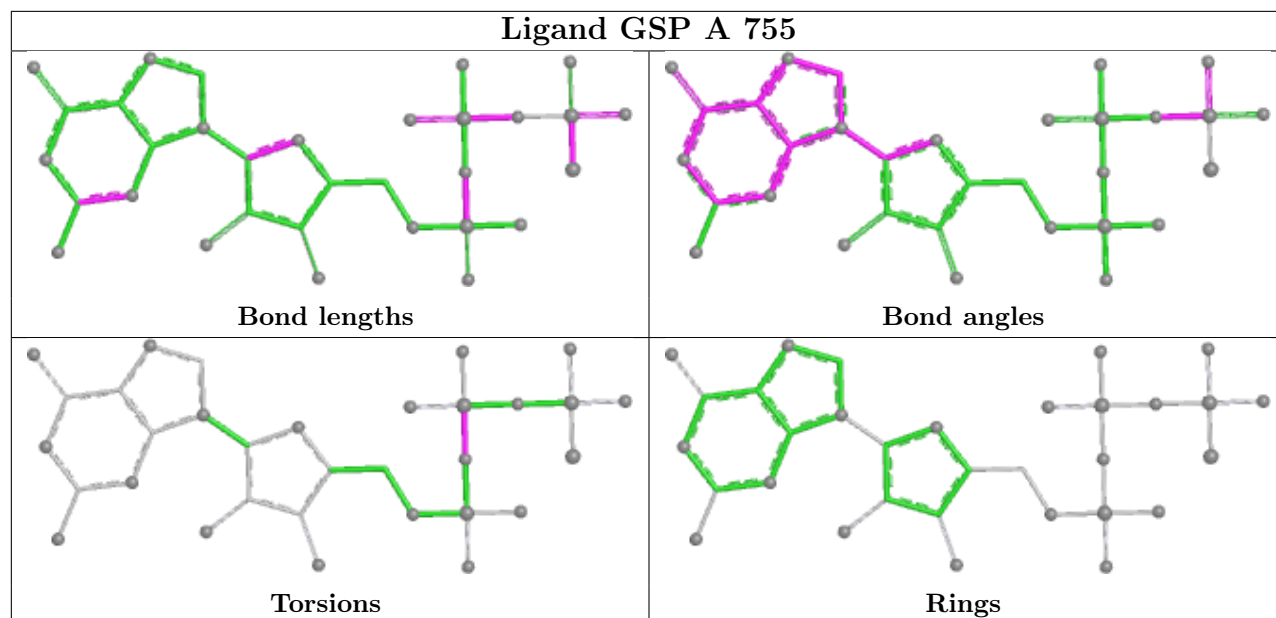
Mol	Chain	Res	Type	Atoms
4	A	755	GSP	PA-O3A-PB-O1B
4	A	755	GSP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	755	GSP	3	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	319/338 (94%)	0.41	24 (7%) 20 19	10, 25, 45, 60	0
2	B	193/203 (95%)	1.39	50 (25%) 1 1	20, 40, 60, 66	0
All	All	512/541 (94%)	0.78	74 (14%) 6 5	10, 29, 58, 66	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	307	LEU	5.8
2	B	458	GLY	5.4
2	B	502	ILE	4.7
2	B	465	GLN	4.5
1	A	336	ASP	4.5
2	B	370	ASN	4.1
1	A	368	HIS	4.1
1	A	259	ASP	3.9
2	B	457	ASP	3.8
2	B	462	ARG	3.7
2	B	332	GLU	3.6
1	A	188	ASP	3.5
2	B	466	MET	3.4
2	B	322	ASN	3.3
2	B	393	ARG	3.3
2	B	471	LEU	3.2
2	B	472	ALA	3.1
2	B	461	LEU	3.1
2	B	463	GLU	3.0
1	A	341	PRO	3.0
1	A	301	GLN	2.9
2	B	481	TYR	2.9
1	A	313	GLU	2.9
2	B	473	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	388	LYS	2.9
2	B	467	ALA	2.9
2	B	415	ARG	2.8
2	B	469	LYS	2.8
2	B	464	ARG	2.8
2	B	394	VAL	2.8
1	A	314	GLY	2.7
1	A	320	ARG	2.7
1	A	357	LEU	2.6
2	B	375	ARG	2.6
2	B	476	ASP	2.6
1	A	215	ASN	2.5
2	B	371	PRO	2.5
2	B	468	GLU	2.5
1	A	335	ARG	2.5
2	B	374	SER	2.5
2	B	390	ALA	2.5
2	B	366	TYR	2.4
2	B	395	LYS	2.4
1	A	238	ASP	2.4
2	B	490	ASP	2.4
2	B	456	LEU	2.3
2	B	496	PHE	2.3
1	A	113	ASN	2.3
2	B	474	LEU	2.3
1	A	310	LEU	2.2
2	B	453	LEU	2.2
1	A	303	VAL	2.2
2	B	314	ASP	2.2
2	B	387	GLU	2.2
2	B	451	ASN	2.2
2	B	403	GLU	2.2
2	B	418	LEU	2.2
2	B	427	LEU	2.2
2	B	379	LYS	2.2
2	B	410	ASN	2.2
2	B	454	LEU	2.1
2	B	497	MET	2.1
2	B	373	ASP	2.1
1	A	353	GLU	2.1
2	B	460	PRO	2.1
1	A	302	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	328	GLU	2.1
1	A	214	LYS	2.1
1	A	367	LEU	2.0
2	B	329	GLN	2.0
1	A	127	THR	2.0
1	A	131	MET	2.0
2	B	411	ASN	2.0
1	A	321	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](#)

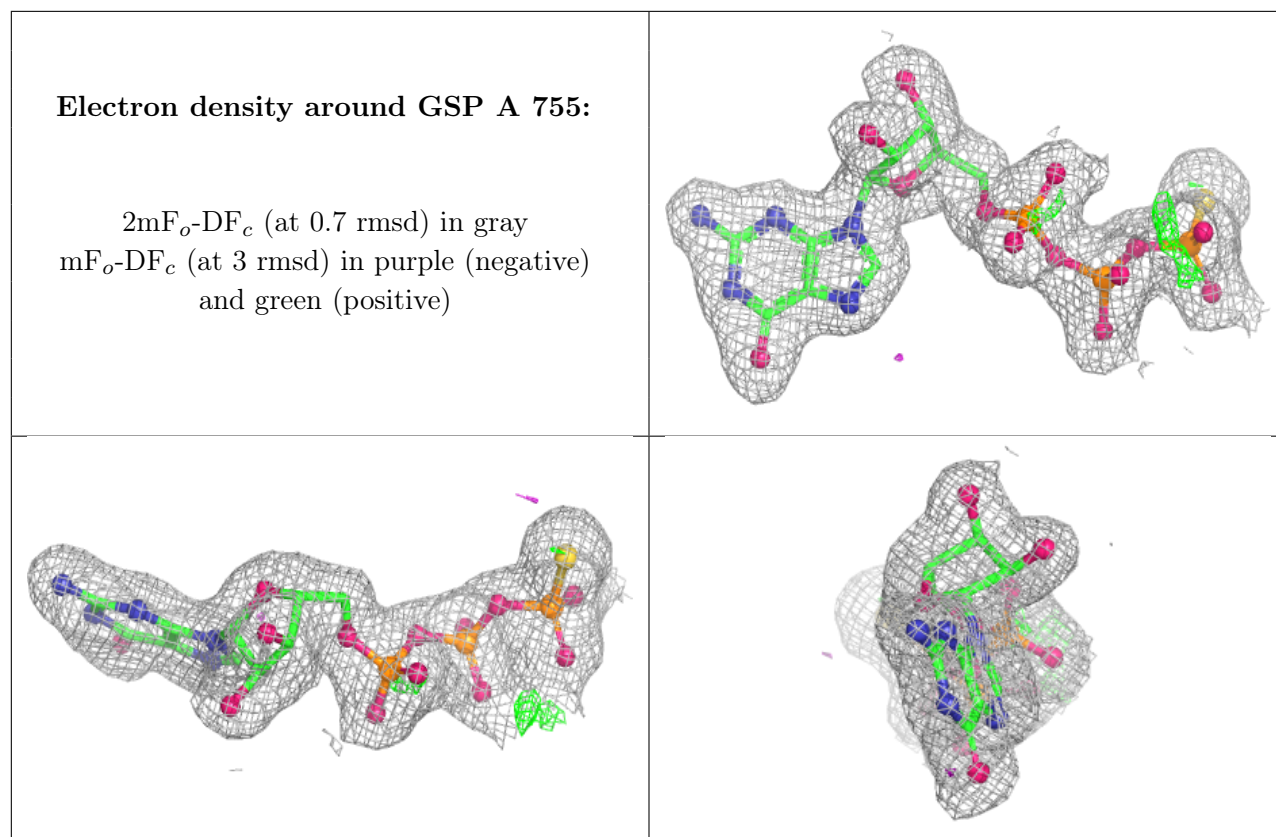
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	MG	A	378	1/1	0.95	0.12	22,22,22,22	0
4	GSP	A	755	32/32	0.98	0.05	14,17,19,21	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.