



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:38 AM GMT

PDB ID : 2XTZ  
Title : CRYSTAL STRUCTURE OF THE G ALPHA PROTEIN ATGPA1 FROM ARABIDOPSIS THALIANA  
Authors : Jones, J.C.; Duffy, J.W.; Machius, M.; Temple, B.R.S.; Dohlman, H.G.; Jones, A.M.  
Deposited on : 2010-10-13  
Resolution : 2.34 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

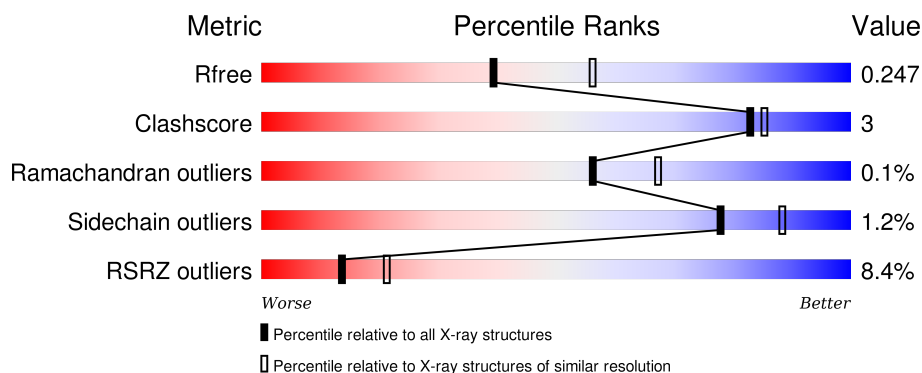
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	354	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>•</div> </div>
1	B	354	<div> <div>8%</div> <div>76%</div> <div>6%</div> <div>18%</div> </div>
1	C	354	<div> <div>12%</div> <div>70%</div> <div>5%</div> <div>•</div> <div>24%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7909 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-1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	3	0
			2838	1818	479	528	13			
1	B	291	Total	C	N	O	S	0	0	0
			2431	1573	405	444	9			
1	C	270	Total	C	N	O	S	0	0	0
			2263	1470	378	406	9			

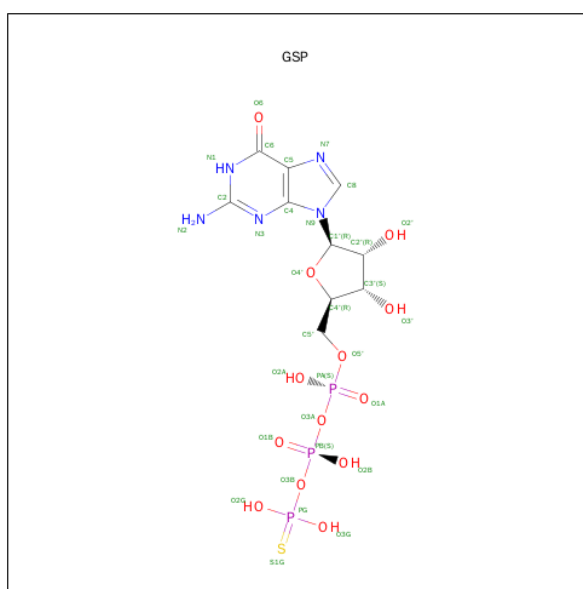
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	EXPRESSION TAG	UNP P18064
A	31	ALA	-	EXPRESSION TAG	UNP P18064
A	32	MET	-	EXPRESSION TAG	UNP P18064
A	33	GLY	-	EXPRESSION TAG	UNP P18064
A	34	SER	-	EXPRESSION TAG	UNP P18064
A	35	GLY	-	EXPRESSION TAG	UNP P18064
A	36	ILE	-	EXPRESSION TAG	UNP P18064
B	30	GLY	-	EXPRESSION TAG	UNP P18064
B	31	ALA	-	EXPRESSION TAG	UNP P18064
B	32	MET	-	EXPRESSION TAG	UNP P18064
B	33	GLY	-	EXPRESSION TAG	UNP P18064
B	34	SER	-	EXPRESSION TAG	UNP P18064
B	35	GLY	-	EXPRESSION TAG	UNP P18064
B	36	ILE	-	EXPRESSION TAG	UNP P18064
C	30	GLY	-	EXPRESSION TAG	UNP P18064
C	31	ALA	-	EXPRESSION TAG	UNP P18064
C	32	MET	-	EXPRESSION TAG	UNP P18064
C	33	GLY	-	EXPRESSION TAG	UNP P18064
C	34	SER	-	EXPRESSION TAG	UNP P18064
C	35	GLY	-	EXPRESSION TAG	UNP P18064
C	36	ILE	-	EXPRESSION TAG	UNP P18064

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>S).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Cl 2 2	0	0
4	A	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

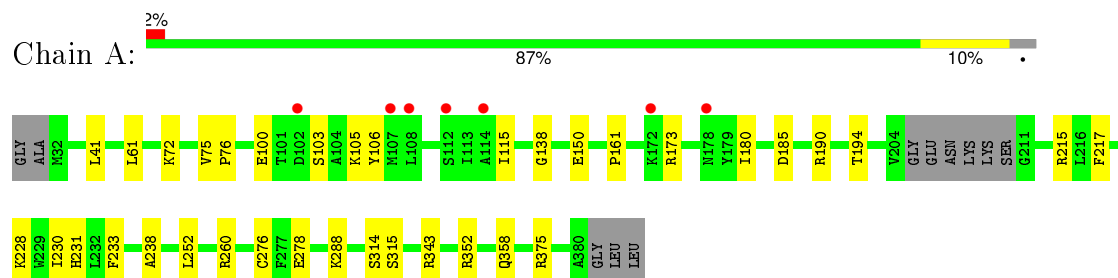
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	139	Total O 139 139	0	0
6	B	69	Total O 69 69	0	0
6	C	41	Total O 41 41	0	0

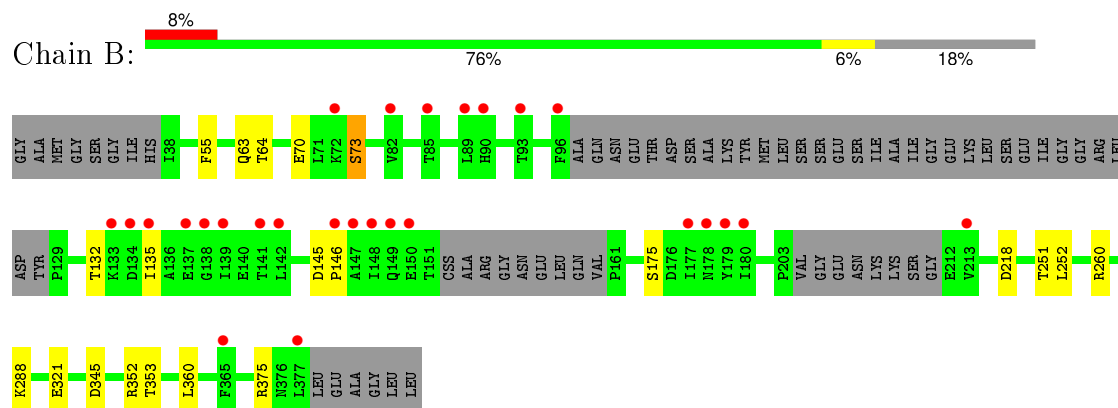
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

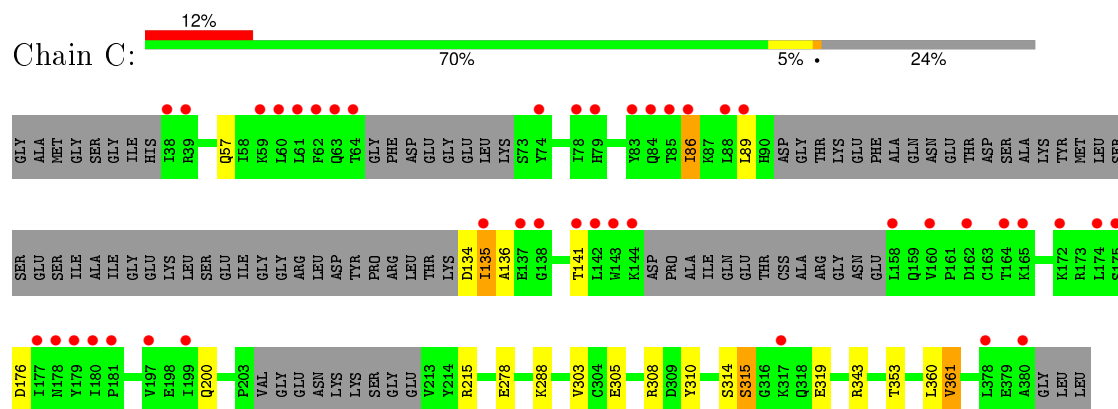
#### • Molecule 1: GUANINE NUCLEOTIDE-BINDING PROTEIN ALPHA-1 SUBUNIT



#### • Molecule 1: GUANINE NUCLEOTIDE-BINDING PROTEIN ALPHA-1 SUBUNIT



#### • Molecule 1: GUANINE NUCLEOTIDE-BINDING PROTEIN ALPHA-1 SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.13Å 119.35Å 161.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.03 – 2.34 44.60 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.9 (96.03-2.34) 94.0 (44.60-2.34)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.211 , 0.254 0.204 , 0.247	Depositor DCC
$R_{free}$ test set	1517 reflections (2.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 55736 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GSP, MG, SO4, CSS, CL

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	0.55	0/2878	0.63	0/3872
1	B	0.54	0/2473	0.60	0/3325
1	C	0.50	0/2300	0.60	0/3094
All	All	0.53	0/7651	0.61	0/10291

There are no bond length outliers.

There are no bond angle outliers.

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	2838	0	2837	20	0
1	B	2431	0	2450	14	0
1	C	2263	0	2296	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	32	0	12	1	0
3	B	32	0	12	1	0
3	C	32	0	12	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	C	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	15	0	0	0	0
6	A	139	0	0	2	0
6	B	69	0	0	0	0
6	C	41	0	0	0	0
All	All	7909	0	7619	47	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 (47) 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:63:GLN:HG3	1:B:64:THR:H	1.23	1.03
1:C:305:GLU:O	1:C:308:ARG:HG3	1.73	0.87
1:B:63:GLN:HG3	1:B:64:THR:N	2.03	0.70
1:A:105:LYS:HG2	1:A:150:GLU:HG2	1.73	0.69
1:B:251:THR:O	1:B:260:ARG:HD2	1.95	0.66
1:A:215[A]:ARG:HG2	1:A:217:PHE:CE2	2.41	0.55
1:A:288:LYS:HG2	3:A:1382:GSP:C6	2.45	0.51
1:A:115:ILE:HG21	1:A:138:GLY:O	2.10	0.51
1:A:100:GLU:HG3	1:A:106:TYR:CE1	2.45	0.51
1:C:278:GLU:HA	1:C:343:ARG:HG2	1.92	0.51
1:C:134:ASP:C	1:C:136:ALA:H	2.13	0.51
1:C:134:ASP:CG	1:C:135:ILE:N	2.65	0.51
1:C:57:GLN:HB3	1:C:361:VAL:HG21	1.92	0.51
1:B:132:THR:H	1:B:135:ILE:HG22	1.76	0.50
1:A:278:GLU:HA	1:A:343:ARG:HG2	1.94	0.49
1:B:288:LYS:HG2	3:B:1379:GSP:C6	2.48	0.49
1:A:230:ILE:HG13	6:A:2056:HOH:O	2.13	0.49
1:A:375:ARG:NH2	6:A:2134:HOH:O	2.47	0.48
1:A:103:SER:OG	1:A:105:LYS:HB2	2.13	0.48
1:B:321:GLU:OE2	1:B:352:ARG:NH2	2.35	0.48
1:C:86:ILE:HA	1:C:89:LEU:HD12	1.97	0.47
1:B:375:ARG:O	1:B:375:ARG:HD3	2.15	0.47
1:A:100:GLU:HG3	1:A:106:TYR:HE1	1.80	0.47
1:C:314:SER:OG	1:C:315:SER:N	2.48	0.46
1:A:161:PRO:HB3	1:A:190:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:THR:O	1:A:228:LYS:NZ	2.48	0.46
1:B:63:GLN:CG	1:B:64:THR:H	2.08	0.46
1:C:86:ILE:HG13	1:C:86:ILE:H	1.39	0.45
1:B:353:THR:HA	1:B:360:LEU:HD21	1.97	0.45
1:A:252:LEU:HD23	1:A:260:ARG:HG2	1.98	0.45
1:C:353:THR:HA	1:C:360:LEU:HD21	1.98	0.45
1:C:57:GLN:CB	1:C:361:VAL:HG21	2.47	0.44
1:A:314:SER:OG	1:A:315:SER:N	2.49	0.44
1:C:200:GLN:OE1	1:C:215:ARG:NH1	2.51	0.43
1:A:41:LEU:HD22	1:A:238:ALA:HB3	2.00	0.43
1:A:72:LYS:HE2	1:A:180:ILE:HG12	2.00	0.43
1:A:173:ARG:NH1	1:A:185:ASP:OD1	2.40	0.42
1:B:70:GLU:O	1:B:73:SER:HB3	2.19	0.42
1:B:252:LEU:HD23	1:B:260:ARG:HG2	2.01	0.42
1:B:345:ASP:O	1:B:375:ARG:NH2	2.53	0.42
1:B:55:PHE:CD1	1:B:218:ASP:HB2	2.55	0.42
1:C:310:TYR:OH	1:C:319:GLU:OE2	2.31	0.41
1:C:288:LYS:HG2	3:C:1382:GSP:C6	2.55	0.41
1:A:233:PHE:HB3	1:A:276[A]:CYS:SG	2.61	0.41
1:B:145:ASP:HA	1:B:146:PRO:HD3	1.94	0.41
1:A:75:VAL:N	1:A:76:PRO:HD2	2.36	0.41
1:A:61:LEU:HD12	1:A:358:GLN:HE21	1.85	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	340/354 (96%)	335 (98%)	5 (2%)	0	100	100
1	B	282/354 (80%)	278 (99%)	4 (1%)	0	100	100
1	C	259/354 (73%)	250 (96%)	8 (3%)	1 (0%)	39	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	881/1062 (83%)	863 (98%)	17 (2%)	1 (0%)	56 67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	135	ILE

### 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	308/313 (98%)	306 (99%)	2 (1%)	90 96
1	B	267/313 (85%)	265 (99%)	2 (1%)	88 95
1	C	249/313 (80%)	243 (98%)	6 (2%)	57 69
All	All	824/939 (88%)	814 (99%)	10 (1%)	78 88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	A	352	ARG
1	B	73	SER
1	B	175	SER
1	C	86	ILE
1	C	141	THR
1	C	176	ASP
1	C	303	VAL
1	C	315	SER
1	C	361	VAL

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSS	A	152	1	4,6,7	0.62	0	3,6,8	1.18	0
1	CSS	A	163	1	4,6,7	0.84	0	3,6,8	2.26	1 (33%)
1	CSS	B	163	1	4,6,7	0.90	0	3,6,8	1.56	0
1	CSS	C	163	1	4,6,7	0.80	0	3,6,8	1.35	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
1	CSS	A	152	1	-	0/1/5/7	0/0/0/0
1	CSS	A	163	1	-	0/1/5/7	0/0/0/0
1	CSS	B	163	1	-	0/1/5/7	0/0/0/0
1	CSS	C	163	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	CSS	CB-SG-SD	3.00	109.82	103.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	$\# Z  > 2$
3	GSP	A	1382	2	25,34,34	1.60	2 (8%)	31,54,54	1.60	4 (12%)
5	SO4	A	1384	-	4,4,4	0.30	0	6,6,6	0.32	0
3	GSP	B	1379	2	25,34,34	1.77	2 (8%)	31,54,54	1.76	6 (19%)
5	SO4	B	1381	-	4,4,4	0.13	0	6,6,6	0.09	0
3	GSP	C	1382	2	25,34,34	2.12	2 (8%)	31,54,54	1.59	4 (12%)
5	SO4	C	1383	-	4,4,4	0.16	0	6,6,6	0.25	0
5	SO4	C	1384	-	4,4,4	0.13	0	6,6,6	0.17	0
5	SO4	C	1385	-	4,4,4	0.17	0	6,6,6	0.48	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
3	GSP	A	1382	2	-	0/15/38/38	0/3/3/3
5	SO4	A	1384	-	-	0/0/0/0	0/0/0/0
3	GSP	B	1379	2	-	0/15/38/38	0/3/3/3
5	SO4	B	1381	-	-	0/0/0/0	0/0/0/0
3	GSP	C	1382	2	-	0/15/38/38	0/3/3/3
5	SO4	C	1383	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1384	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1385	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1382	GSP	PG-S1G	-9.29	1.72	1.90
3	B	1379	GSP	PG-S1G	-7.10	1.76	1.90
3	A	1382	GSP	PG-S1G	-6.20	1.78	1.90
3	A	1382	GSP	C6-N1	2.64	1.38	1.33
3	C	1382	GSP	C6-N1	3.00	1.38	1.33
3	B	1379	GSP	C6-N1	3.47	1.39	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1379	GSP	N3-C2-N1	-5.03	119.78	127.44
3	C	1382	GSP	N3-C2-N1	-4.96	119.88	127.44
3	A	1382	GSP	N3-C2-N1	-4.93	119.93	127.44
3	A	1382	GSP	PA-O3A-PB	-3.57	122.70	132.73
3	B	1379	GSP	C5-C6-N1	-3.38	118.97	123.59
3	B	1379	GSP	PA-O3A-PB	-3.03	124.23	132.73
3	C	1382	GSP	PA-O3A-PB	-2.67	125.24	132.73
3	C	1382	GSP	C5-C6-N1	-2.30	120.44	123.59
3	B	1379	GSP	C1'-N9-C4	-2.29	123.48	126.94
3	B	1379	GSP	O3'-C3'-C4'	-2.14	104.64	111.05
3	A	1382	GSP	C5-C6-N1	-2.10	120.71	123.59
3	C	1382	GSP	C6-N1-C2	2.47	119.36	115.94
3	A	1382	GSP	C6-N1-C2	2.61	119.56	115.94
3	B	1379	GSP	C6-N1-C2	3.44	120.72	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1382	GSP	1	0
3	B	1379	GSP	1	0
3	C	1382	GSP	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	341/354 (96%)	0.06	7 (2%) 67 78	15, 31, 68, 86	0
1	B	290/354 (81%)	0.32	27 (9%) 11 17	18, 36, 88, 105	0
1	C	269/354 (75%)	0.62	42 (15%) 3 5	21, 51, 105, 122	0
All	All	900/1062 (84%)	0.31	76 (8%) 14 21	15, 38, 92, 122	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	LEU	6.2
1	C	178	ASN	5.7
1	C	180	ILE	5.7
1	C	141	THR	5.5
1	B	148	ILE	5.5
1	C	74	TYR	5.3
1	B	177	ILE	5.2
1	C	174	LEU	5.0
1	C	143	TRP	5.0
1	A	114	ALA	4.9
1	C	158	LEU	4.2
1	B	180	ILE	4.2
1	C	86	ILE	4.2
1	C	89	LEU	4.2
1	C	165	LYS	4.1
1	B	146	PRO	4.1
1	C	164	THR	3.9
1	B	96	PHE	3.8
1	B	90	HIS	3.8
1	A	112	SER	3.8
1	B	377	LEU	3.7
1	C	142	LEU	3.7
1	C	38	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	178	ASN	3.6
1	C	63	GLN	3.3
1	B	89	LEU	3.3
1	C	181	PRO	3.2
1	B	138	GLY	3.2
1	B	147	ALA	3.2
1	C	179	TYR	3.2
1	B	141	THR	3.1
1	C	135	ILE	3.1
1	C	84	GLN	3.1
1	C	62	PHE	3.1
1	C	160	VAL	3.1
1	C	177	ILE	3.0
1	B	134	ASP	3.0
1	A	108	LEU	3.0
1	B	150	GLU	3.0
1	B	179	TYR	3.0
1	C	175	SER	3.0
1	C	172	LYS	2.9
1	C	78	ILE	2.9
1	B	137	GLU	2.8
1	B	135	ILE	2.8
1	C	378	LEU	2.8
1	B	142	LEU	2.7
1	C	39	ARG	2.7
1	C	138	GLY	2.7
1	B	82	VAL	2.7
1	B	139	ILE	2.6
1	C	60	LEU	2.5
1	C	137	GLU	2.5
1	C	317	LYS	2.5
1	C	162	ASP	2.5
1	C	61	LEU	2.5
1	A	102	ASP	2.5
1	A	107	MET	2.4
1	C	380	ALA	2.4
1	C	85	THR	2.3
1	C	144	LYS	2.3
1	C	59	LYS	2.3
1	C	197	VAL	2.2
1	A	172	LYS	2.2
1	B	213	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	93	THR	2.2
1	B	133	LYS	2.2
1	C	64	THR	2.2
1	B	149	GLN	2.1
1	B	365	PHE	2.1
1	A	178	ASN	2.1
1	B	85	THR	2.1
1	C	83	TYR	2.1
1	B	72	LYS	2.0
1	C	199	ILE	2.0
1	C	79	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSS	B	163	7/8	0.89	0.10	-	59,61,63,63	0
1	CSS	A	163	7/8	0.95	0.09	-	34,35,36,37	0
1	CSS	C	163	7/8	0.83	0.13	-	82,84,87,87	0
1	CSS	A	152	7/8	0.90	0.11	-	42,43,46,48	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GSP	A	1382	32/32	0.99	0.15	1.08	20,26,35,38	0
2	MG	A	1381	1/1	0.96	0.14	0.33	18,18,18,18	0
5	SO4	C	1385	5/5	0.90	0.19	-0.04	71,72,72,72	0
3	GSP	B	1379	32/32	0.99	0.12	-0.45	20,23,31,34	0
2	MG	B	1378	1/1	0.97	0.10	-0.67	25,25,25,25	0
3	GSP	C	1382	32/32	0.98	0.09	-0.76	34,38,44,48	0
2	MG	C	1381	1/1	0.93	0.06	-1.56	44,44,44,44	0
4	CL	B	1382	1/1	0.94	0.14	-	68,68,68,68	0
5	SO4	C	1383	5/5	0.93	0.10	-	81,82,82,83	0
4	CL	A	1383	1/1	0.96	0.19	-	49,49,49,49	0
5	SO4	C	1384	5/5	0.96	0.15	-	65,66,67,67	0
4	CL	C	1386	1/1	0.93	0.08	-	85,85,85,85	0
5	SO4	A	1384	5/5	0.98	0.09	-	45,45,46,46	0
4	CL	B	1380	1/1	0.94	0.09	-	76,76,76,76	0
5	SO4	B	1381	5/5	0.94	0.16	-	79,79,79,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.