



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 03:50 pm BST

PDB ID : 1ND0
Title : CATIONIC CYCLIZATION ANTIBODY 4C6 COMPLEX WITH TRANSITION STATE ANALOG
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2002-12-05
Resolution : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

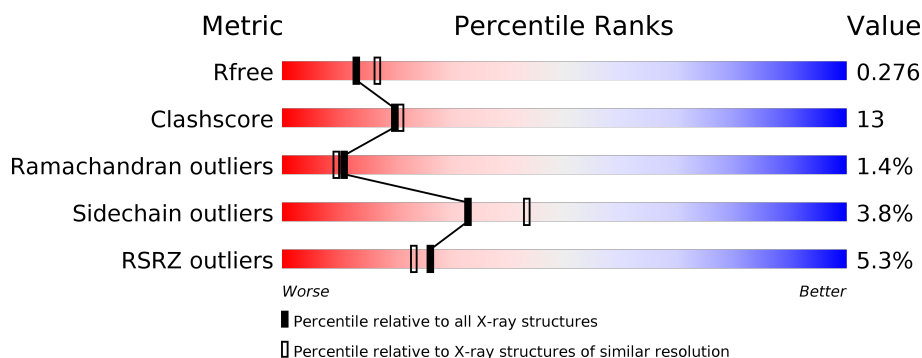
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 ≥ 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	219	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>
1	C	219	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>23%</div> </div> </div>
1	E	219	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>.</div> </div> </div>
1	G	219	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>23%</div> </div> </div>
2	B	222	<div> <div>7%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>.</div> </div> </div>
2	D	222	<div> <div>9%</div> <div> <div></div> <div>66%</div> <div>31%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	222	
2	H	222	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	503	-	X	-	-
4	SO4	D	504	-	X	-	-
4	SO4	F	501	-	X	-	-
4	SO4	H	502	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14002 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.

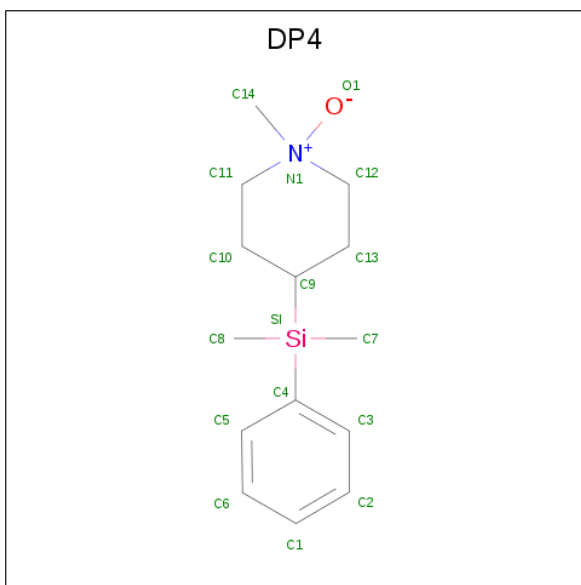
- Molecule 1 is a protein called IMMUNOGLOBULIN IGG2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1702	1064	291	340	7			
1	C	219	Total	C	N	O	S	0	0	0
			1702	1064	291	340	7			
1	E	219	Total	C	N	O	S	0	0	0
			1702	1064	291	340	7			
1	G	219	Total	C	N	O	S	0	0	0
			1702	1064	291	340	7			

- Molecule 2 is a protein called IMMUNOGLOBULIN IGG2A.

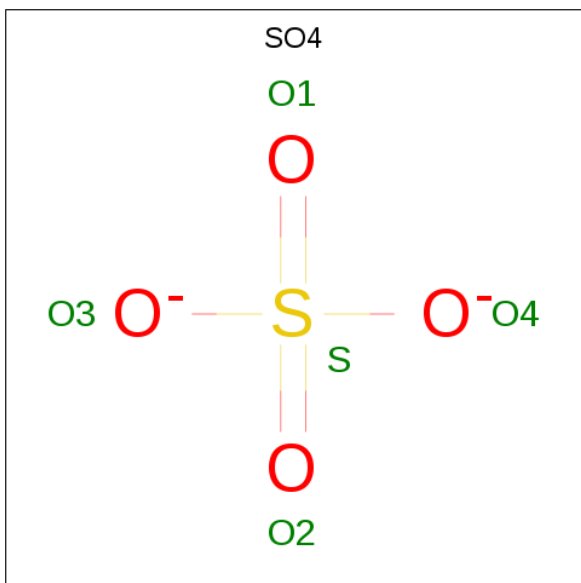
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	222	Total	C	N	O	S	0	0	0
			1678	1063	277	332	6			
2	D	222	Total	C	N	O	S	0	0	0
			1678	1063	277	332	6			
2	F	222	Total	C	N	O	S	0	0	0
			1678	1063	277	332	6			
2	H	222	Total	C	N	O	S	0	0	0
			1678	1063	277	332	6			

- Molecule 3 is (1s,4s)-4-[dimethyl(phenyl)silyl]-1-methylpiperidine 1-oxide (three-letter code: DP4) (formula: C₁₄H₂₃NOSi).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	Si	0	0
			17	14	1	1	1		
3	C	1	Total	C	N	O	Si	0	0
			17	14	1	1	1		
3	E	1	Total	C	N	O	Si	0	0
			17	14	1	1	1		
3	G	1	Total	C	N	O	Si	0	0
			17	14	1	1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

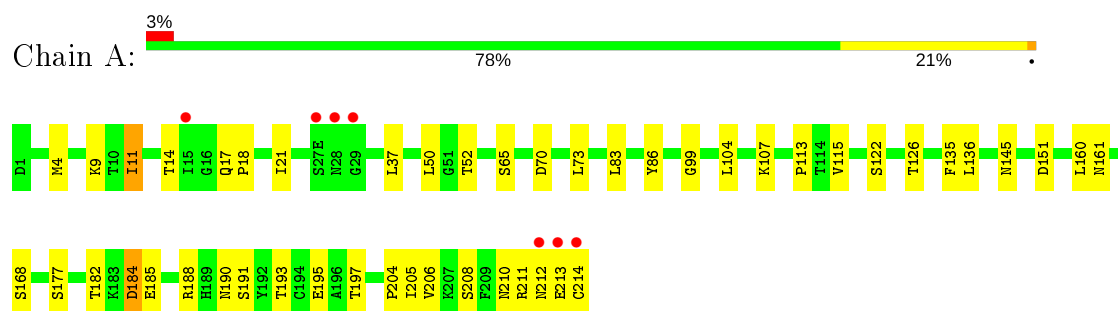
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	53	Total O 53 53	0	0
5	B	48	Total O 48 48	0	0
5	C	41	Total O 41 41	0	0
5	D	49	Total O 49 49	0	0
5	E	56	Total O 56 56	0	0
5	F	52	Total O 52 52	0	0
5	G	59	Total O 59 59	0	0
5	H	36	Total O 36 36	0	0

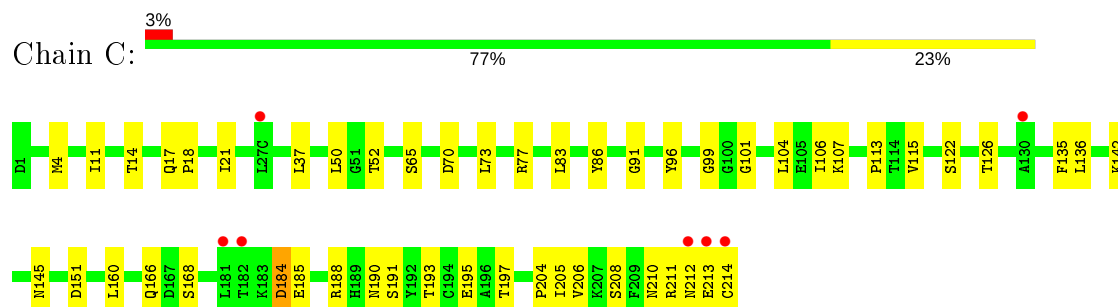
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

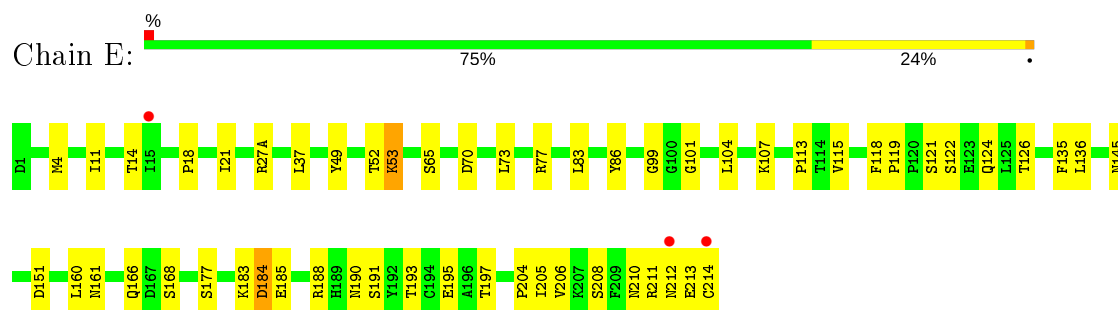
• Molecule 1: IMMUNOGLOBULIN IGG2A



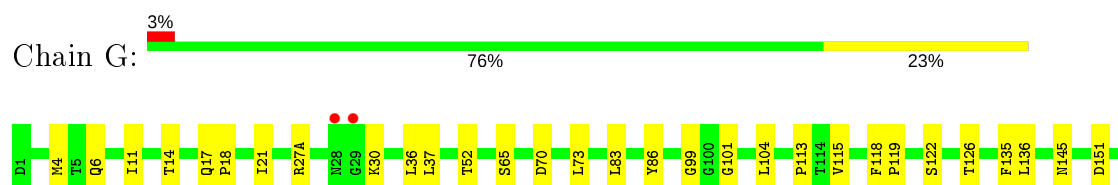
• Molecule 1: IMMUNOGLOBULIN IGG2A



• Molecule 1: IMMUNOGLOBULIN IGG2A

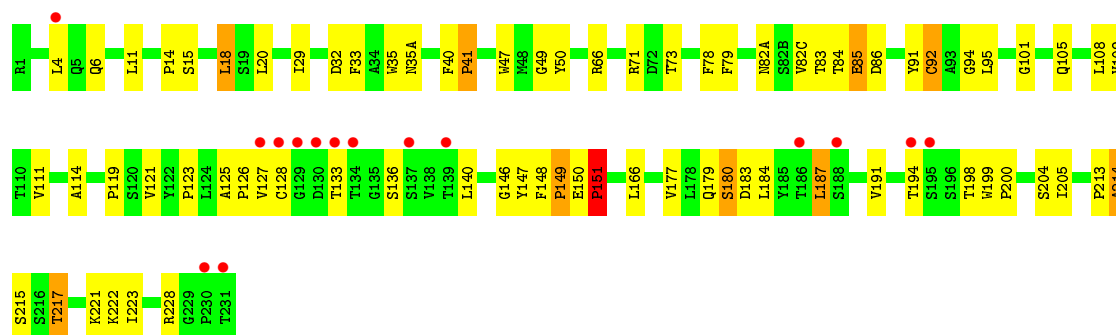


• Molecule 1: IMMUNOGLOBULIN IGG2A

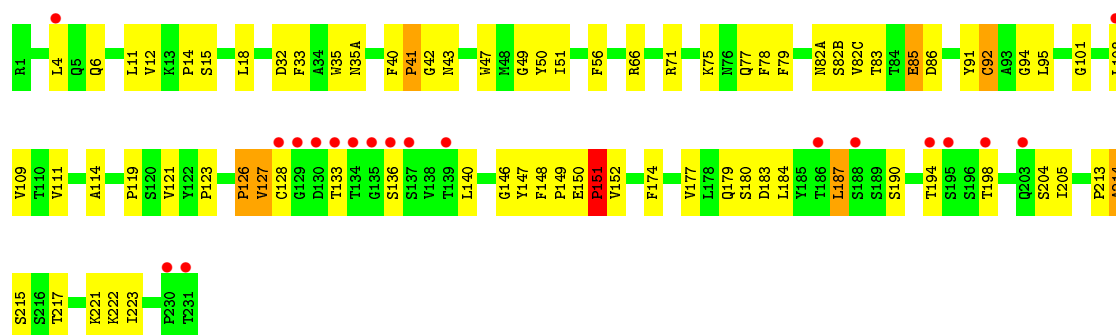




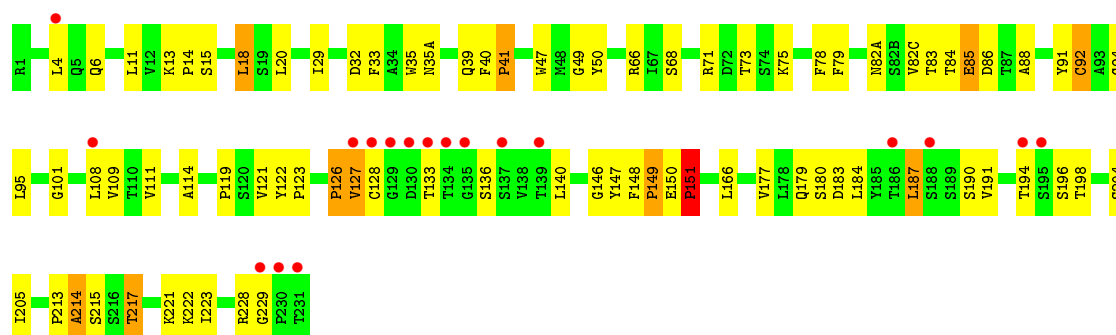
• Molecule 2: IMMUNOGLOBULIN IGG2A



• Molecule 2: IMMUNOGLOBULIN IGG2A

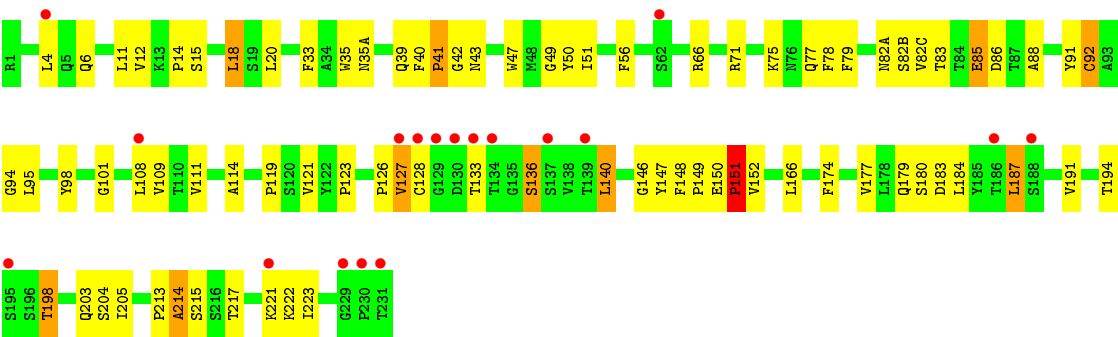


• Molecule 2: IMMUNOGLOBULIN IGG2A



• Molecule 2: IMMUNOGLOBULIN IGG2A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	36.57Å 95.16Å 141.06Å 75.51° 88.64° 89.28°	Depositor
Resolution (Å)	50.00 – 2.45 36.56 – 2.45	Depositor EDS
% Data completeness (in resolution range)	72.9 (50.00-2.45) 72.9 (36.56-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.286 0.238 , 0.276	Depositor DCC
R_{free} test set	2539 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14002	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0687e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DP4, 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	0.36	0/1740	0.62	0/2358
1	C	0.37	0/1740	0.62	0/2358
1	E	0.37	0/1740	0.63	0/2358
1	G	0.38	0/1740	0.63	0/2358
2	B	0.39	0/1724	0.70	2/2361 (0.1%)
2	D	0.41	0/1724	0.70	2/2361 (0.1%)
2	F	0.42	0/1724	0.71	2/2361 (0.1%)
2	H	0.42	0/1724	0.71	1/2361 (0.0%)
All	All	0.39	0/13856	0.67	7/18876 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	92	CYS	CA-CB-SG	5.47	123.85	114.00
2	B	92	CYS	CA-CB-SG	5.46	123.83	114.00
2	D	32	ASP	N-CA-C	5.15	124.92	111.00
2	F	32	ASP	N-CA-C	5.13	124.86	111.00
2	H	92	CYS	CA-CB-SG	5.07	123.13	114.00

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	1702	0	1657	32	0
1	C	1702	0	1657	36	0
1	E	1702	0	1657	40	0
1	G	1702	0	1657	33	0
2	B	1678	0	1633	49	0
2	D	1678	0	1633	51	0
2	F	1678	0	1633	63	0
2	H	1678	0	1633	54	0
3	A	17	0	16	0	0
3	C	17	0	16	0	0
3	E	17	0	16	0	0
3	G	17	0	16	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	F	5	0	0	0	0
4	H	5	0	0	0	0
5	A	53	0	0	3	0
5	B	48	0	0	3	0
5	C	41	0	0	2	0
5	D	49	0	0	3	0
5	E	56	0	0	4	0
5	F	52	0	0	7	0
5	G	59	0	0	4	0
5	H	36	0	0	2	0
All	All	14002	0	13224	339	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 13.

The worst 5 of 339 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:G:160:LEU:HD11	2:H:179:GLN:HG3	1.46	0.98
2:D:204:SER:HB2	2:D:222:LYS:HE3	1.51	0.91
2:F:83:THR:OG1	2:F:85:GLU:HG2	1.72	0.89
2:D:83:THR:OG1	2:D:85:GLU:HG2	1.75	0.85
2:H:83:THR:OG1	2:H:85:GLU:HG2	1.77	0.85

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	217/219 (99%)	205 (94%)	11 (5%)	1 (0%)	29	34
1	C	217/219 (99%)	206 (95%)	10 (5%)	1 (0%)	29	34
1	E	217/219 (99%)	206 (95%)	10 (5%)	1 (0%)	29	34
1	G	217/219 (99%)	205 (94%)	11 (5%)	1 (0%)	29	34
2	B	220/222 (99%)	203 (92%)	12 (6%)	5 (2%)	6	4
2	D	220/222 (99%)	203 (92%)	12 (6%)	5 (2%)	6	4
2	F	220/222 (99%)	202 (92%)	13 (6%)	5 (2%)	6	4
2	H	220/222 (99%)	202 (92%)	13 (6%)	5 (2%)	6	4
All	All	1748/1764 (99%)	1632 (93%)	92 (5%)	24 (1%)	11	9

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
1	C	213	GLU
1	E	213	GLU
1	G	213	GLU
2	B	126	PRO

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	195/195 (100%)	192 (98%)	3 (2%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	195/195 (100%)	193 (99%)	2 (1%)	76	84
1	E	195/195 (100%)	192 (98%)	3 (2%)	65	76
1	G	195/195 (100%)	193 (99%)	2 (1%)	76	84
2	B	192/192 (100%)	180 (94%)	12 (6%)	18	22
2	D	192/192 (100%)	180 (94%)	12 (6%)	18	22
2	F	192/192 (100%)	180 (94%)	12 (6%)	18	22
2	H	192/192 (100%)	179 (93%)	13 (7%)	16	19
All	All	1548/1548 (100%)	1489 (96%)	59 (4%)	33	43

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	194	THR
2	F	41	PRO
2	H	183	ASP
2	D	198	THR
1	E	53	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	3	GLN
1	E	28	ASN
1	G	145	ASN
1	C	161	ASN
1	G	161	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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
3	DP4	E	403	-	16,18,18	3.89	12 (75%)	19,27,27	1.28	3 (15%)
4	SO4	H	502	-	4,4,4	3.30	4 (100%)	6,6,6	0.08	0
4	SO4	F	501	-	4,4,4	3.20	4 (100%)	6,6,6	0.23	0
4	SO4	B	503	-	4,4,4	3.22	4 (100%)	6,6,6	0.10	0
3	DP4	C	402	-	16,18,18	3.94	12 (75%)	19,27,27	1.30	3 (15%)
3	DP4	A	401	-	16,18,18	4.02	12 (75%)	19,27,27	1.29	3 (15%)
4	SO4	D	504	-	4,4,4	3.25	4 (100%)	6,6,6	0.10	0
3	DP4	G	404	-	16,18,18	3.89	12 (75%)	19,27,27	1.31	3 (15%)

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	DP4	E	403	-	-	1/12/24/24	0/2/2/2
3	DP4	C	402	-	-	1/12/24/24	0/2/2/2
3	DP4	A	401	-	-	1/12/24/24	0/2/2/2
3	DP4	G	404	-	-	1/12/24/24	0/2/2/2

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	DP4	SI-C9	-9.77	1.82	1.89
3	C	402	DP4	SI-C9	-9.42	1.82	1.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	404	DP4	SI-C9	-8.70	1.83	1.89
3	E	403	DP4	SI-C9	-8.65	1.83	1.89
3	G	404	DP4	SI-C4	-7.58	1.80	1.88

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	DP4	O1-N1-C11	-3.32	105.50	109.65
3	G	404	DP4	O1-N1-C11	-3.31	105.50	109.65
3	C	402	DP4	O1-N1-C11	-3.23	105.60	109.65
3	E	403	DP4	O1-N1-C11	-3.22	105.62	109.65
3	C	402	DP4	C8-SI-C7	-2.54	104.89	109.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	403	DP4	C5-C4-SI-C7
3	C	402	DP4	C5-C4-SI-C7
3	A	401	DP4	C5-C4-SI-C7
3	G	404	DP4	C5-C4-SI-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	219/219 (100%)	0.06	7 (3%) 47 44	14, 32, 54, 94	0
1	C	219/219 (100%)	0.16	7 (3%) 47 44	16, 33, 54, 95	0
1	E	219/219 (100%)	0.04	3 (1%) 75 74	15, 32, 52, 93	0
1	G	219/219 (100%)	0.13	7 (3%) 47 44	16, 33, 53, 94	0
2	B	222/222 (100%)	0.20	15 (6%) 17 13	10, 29, 66, 100	9 (4%)
2	D	222/222 (100%)	0.35	19 (8%) 10 7	12, 30, 67, 100	9 (4%)
2	F	222/222 (100%)	0.26	18 (8%) 12 9	14, 29, 64, 100	9 (4%)
2	H	222/222 (100%)	0.44	18 (8%) 12 9	11, 30, 68, 100	9 (4%)
All	All	1764/1764 (100%)	0.21	94 (5%) 26 23	10, 31, 59, 100	36 (2%)

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	231	THR	14.1
2	F	231	THR	9.2
2	D	231	THR	8.5
2	H	127	VAL	7.7
2	B	231	THR	7.3

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

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

6.3 Carbohydrates ⓘ

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. 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(\AA^2)	Q<0.9
4	SO4	H	502	5/5	0.88	0.26	90,90,91,91	0
4	SO4	D	504	5/5	0.90	0.17	72,73,74,74	0
3	DP4	E	403	17/17	0.91	0.25	49,55,70,76	0
3	DP4	G	404	17/17	0.91	0.26	48,54,71,75	0
3	DP4	C	402	17/17	0.92	0.22	48,55,70,75	0
3	DP4	A	401	17/17	0.92	0.26	48,55,72,77	0
4	SO4	F	501	5/5	0.97	0.15	32,33,35,36	0
4	SO4	B	503	5/5	0.98	0.11	22,25,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.