



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2016 – 10:52 PM EST

PDB ID : 5TKB  
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 4D IN  
COMPLEX WITH A TETRAFLUORANILINE COMPOUND  
Authors : Sack, J.S.  
Deposited on : 2016-10-06  
Resolution : 2.16 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

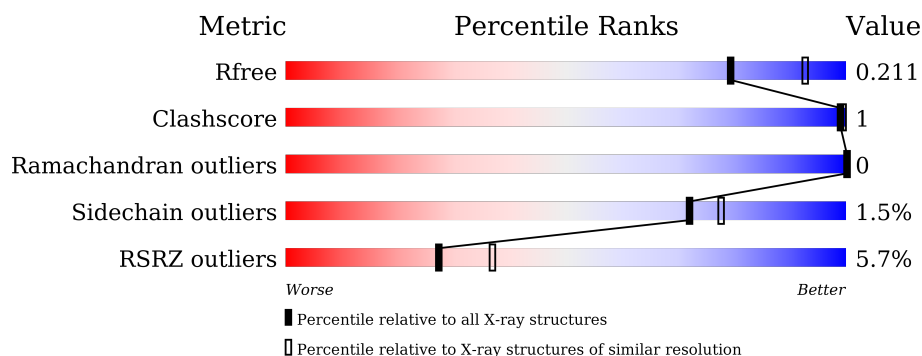
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	381	<div> <div>4%</div> <div>84%</div> <div>14%</div> </div>
1	B	381	<div> <div>6%</div> <div>81%</div> <div>15%</div> </div>
1	C	381	<div> <div>7%</div> <div>81%</div> <div>15%</div> </div>
1	D	381	<div> <div>3%</div> <div>83%</div> <div>15%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EOH	A	804	-	-	-	X
5	EOH	A	805	-	-	-	X
5	EOH	A	806	-	-	-	X
5	EOH	B	704	-	-	-	X
5	EOH	B	705	-	-	-	X
5	EOH	B	706	-	-	-	X
5	EOH	C	704	-	-	-	X
5	EOH	D	703	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11083 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2622	1662	446	500	14			
1	B	323	Total	C	N	O	S	0	0	0
			2593	1642	439	498	14			
1	C	323	Total	C	N	O	S	0	0	0
			2609	1649	445	501	14			
1	D	325	Total	C	N	O	S	0	0	0
			2617	1657	446	500	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	initiating methionine	UNP Q08499
A	579	ALA	SER	engineered mutation	UNP Q08499
A	581	ALA	SER	engineered mutation	UNP Q08499
A	618	HIS	-	expression tag	UNP Q08499
A	619	HIS	-	expression tag	UNP Q08499
A	620	HIS	-	expression tag	UNP Q08499
A	621	HIS	-	expression tag	UNP Q08499
A	622	HIS	-	expression tag	UNP Q08499
A	623	HIS	-	expression tag	UNP Q08499
B	243	MET	-	initiating methionine	UNP Q08499
B	579	ALA	SER	engineered mutation	UNP Q08499
B	581	ALA	SER	engineered mutation	UNP Q08499
B	618	HIS	-	expression tag	UNP Q08499
B	619	HIS	-	expression tag	UNP Q08499
B	620	HIS	-	expression tag	UNP Q08499
B	621	HIS	-	expression tag	UNP Q08499
B	622	HIS	-	expression tag	UNP Q08499
B	623	HIS	-	expression tag	UNP Q08499
C	243	MET	-	initiating methionine	UNP Q08499
C	579	ALA	SER	engineered mutation	UNP Q08499
C	581	ALA	SER	engineered mutation	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	HIS	-	expression tag	UNP Q08499
C	619	HIS	-	expression tag	UNP Q08499
C	620	HIS	-	expression tag	UNP Q08499
C	621	HIS	-	expression tag	UNP Q08499
C	622	HIS	-	expression tag	UNP Q08499
C	623	HIS	-	expression tag	UNP Q08499
D	243	MET	-	initiating methionine	UNP Q08499
D	579	ALA	SER	engineered mutation	UNP Q08499
D	581	ALA	SER	engineered mutation	UNP Q08499
D	618	HIS	-	expression tag	UNP Q08499
D	619	HIS	-	expression tag	UNP Q08499
D	620	HIS	-	expression tag	UNP Q08499
D	621	HIS	-	expression tag	UNP Q08499
D	622	HIS	-	expression tag	UNP Q08499
D	623	HIS	-	expression tag	UNP Q08499

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

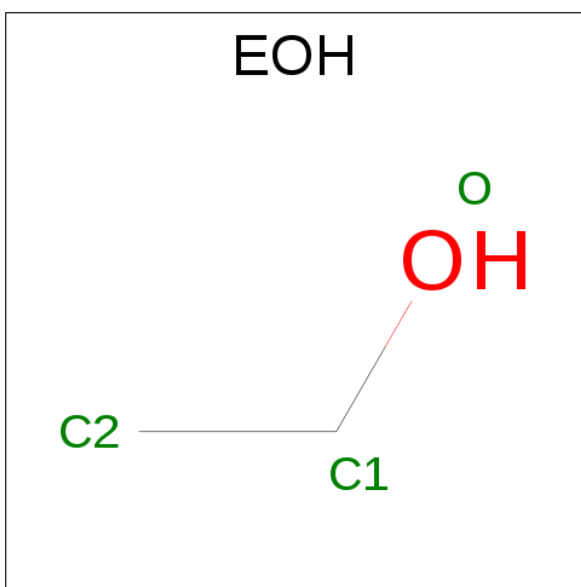
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

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



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

- Molecule 5 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



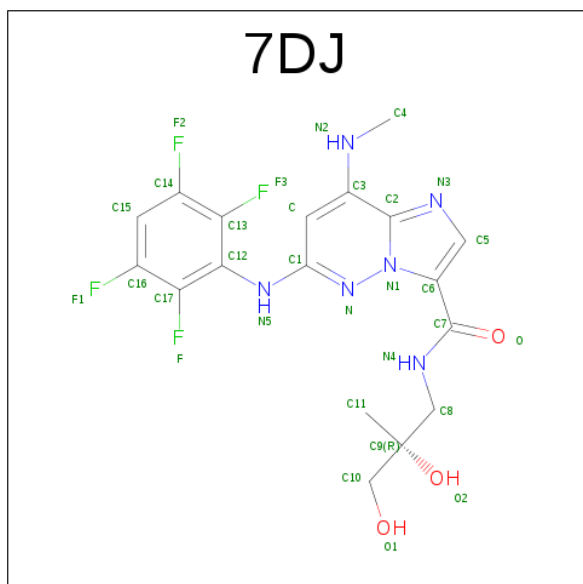
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	2	1		
5	A	1	Total	C	O	0	0
			3	2	1		
5	B	1	Total	C	O	0	0
			3	2	1		
5	B	1	Total	C	O	0	0
			3	2	1		
5	B	1	Total	C	O	0	0
			3	2	1		
5	C	1	Total	C	O	0	0
			3	2	1		
5	D	1	Total	C	O	0	0
			3	2	1		

- Molecule 6 is N-[(2R)-2,3-dihydroxy-2-methylpropyl]-8-(methylamino)-6-[(2,3,5,6-tetrafluorophenyl)amino]imidazo[1,2-b]pyridazine-3-carboxamide (three-letter code: 7DJ) (formula: C<sub>18</sub>H<sub>18</sub>F<sub>4</sub>N<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			31	18	4	6	3		
6	B	1	Total	C	F	N	O	0	0
			31	18	4	6	3		
6	C	1	Total	C	F	N	O	0	0
			31	18	4	6	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	F	N	O	0	0
			31	18	4	6	3		

- Molecule 7 is water.

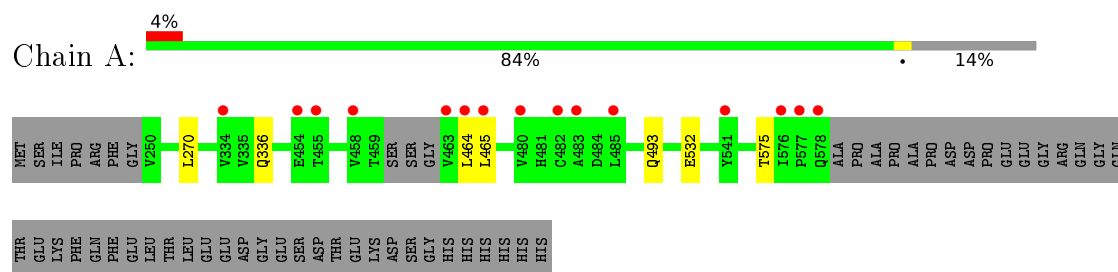
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	128	Total	O	0	0
			128	128		
7	B	90	Total	O	0	0
			90	90		
7	C	104	Total	O	0	0
			104	104		
7	D	149	Total	O	0	0
			149	149		



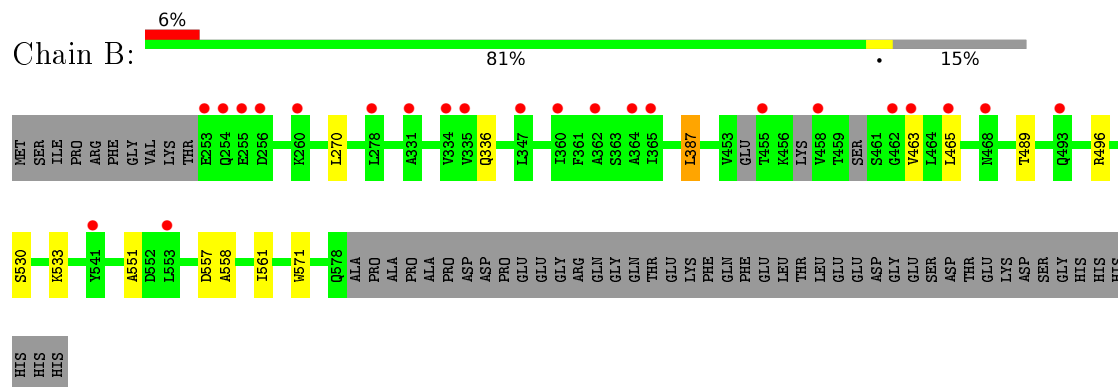
### 3 Residue-property plots

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.

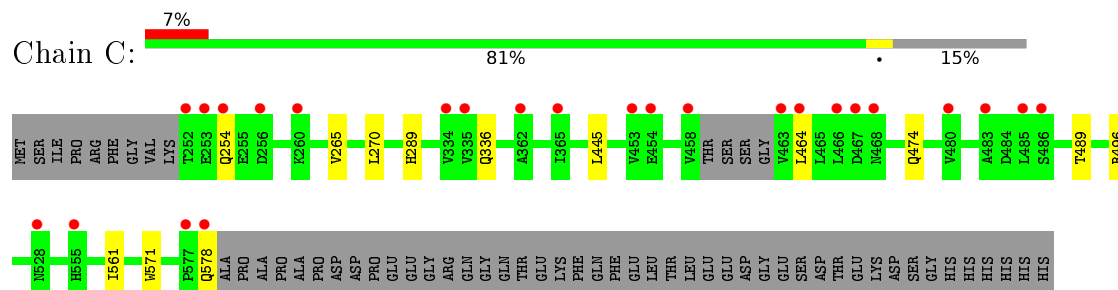
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



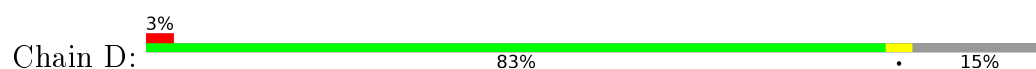
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.00Å 112.70Å 159.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.62 – 2.16 31.10 – 2.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.62-2.16) 100.0 (31.10-2.16)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.188 , 0.209 0.190 , 0.211	Depositor DCC
$R_{free}$ test set	4770 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, 0.333 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: ZN, MG, EOH, 7DJ, 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	0.50	0/2675	0.57	0/3638
1	B	0.49	0/2644	0.59	0/3594
1	C	0.49	0/2662	0.58	0/3620
1	D	0.51	0/2671	0.57	0/3631
All	All	0.50	0/10652	0.58	0/14483

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 [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	2622	0	2562	3	0
1	B	2593	0	2519	6	0
1	C	2609	0	2536	3	0
1	D	2617	0	2565	3	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	9	0	18	0	0
5	B	9	0	18	0	0
5	C	3	0	6	0	0
5	D	3	0	6	0	0
6	A	31	0	0	0	0
6	B	31	0	0	0	0
6	C	31	0	0	0	0
6	D	31	0	0	0	0
7	A	128	0	0	1	0
7	B	90	0	0	1	0
7	C	104	0	0	0	0
7	D	149	0	0	0	0
All	All	11083	0	10230	15	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 1.

All (15) 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:A:532:GLU:HG2	1:A:575:THR:HG22	1.73	0.68
1:B:387:LEU:HG	7:B:879:HOH:O	2.00	0.61
1:B:489:THR:HB	1:B:561:ILE:HG23	1.89	0.54
1:C:496:ARG:HD3	1:C:571:TRP:CH2	2.48	0.48
1:D:496:ARG:HD3	1:D:571:TRP:CH2	2.49	0.47
1:B:496:ARG:HD3	1:B:571:TRP:CH2	2.50	0.47
1:A:270:LEU:HD22	1:A:336:GLN:HG3	1.97	0.46
1:B:270:LEU:HD22	1:B:336:GLN:HG3	1.98	0.46
1:C:270:LEU:HD22	1:C:336:GLN:HG3	1.99	0.43
1:D:489:THR:HB	1:D:561:ILE:HG23	2.00	0.43
1:B:551:ALA:HA	1:B:558:ALA:HB3	1.99	0.43
1:B:530:SER:HB3	1:B:533:LYS:HB2	2.01	0.42
1:C:489:THR:HB	1:C:561:ILE:HG23	2.00	0.42
1:D:270:LEU:HD22	1:D:336:GLN:HG3	2.00	0.42
1:A:493:GLN:HG3	7:A:961:HOH:O	2.21	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	322/381 (84%)	316 (98%)	6 (2%)	0	100	100
1	B	315/381 (83%)	310 (98%)	5 (2%)	0	100	100
1	C	319/381 (84%)	314 (98%)	5 (2%)	0	100	100
1	D	323/381 (85%)	318 (98%)	5 (2%)	0	100	100
All	All	1279/1524 (84%)	1258 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	293/345 (85%)	291 (99%)	2 (1%)	88	93
1	B	290/345 (84%)	286 (99%)	4 (1%)	74	80
1	C	292/345 (85%)	285 (98%)	7 (2%)	57	60
1	D	294/345 (85%)	290 (99%)	4 (1%)	74	80
All	All	1169/1380 (85%)	1152 (98%)	17 (2%)	72	78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	LEU
1	A	465	LEU
1	B	387	LEU
1	B	463	VAL
1	B	465	LEU
1	B	557	ASP
1	C	254	GLN
1	C	265	VAL
1	C	289	HIS
1	C	445	LEU
1	C	464	LEU
1	C	474	GLN
1	C	578	GLN
1	D	344	THR
1	D	445	LEU
1	D	474	GLN
1	D	569	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	A	535	GLN
1	B	293	GLN
1	B	474	GLN
1	B	535	GLN
1	C	424	GLN
1	C	478	ASN
1	C	535	GLN
1	D	289	HIS
1	D	293	GLN
1	D	474	GLN
1	D	478	ASN
1	D	535	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 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	SO4	A	803	-	4,4,4	0.72	0	6,6,6	0.31	0
5	EOH	A	804	-	2,2,2	0.50	0	1,1,1	0.76	0
5	EOH	A	805	-	2,2,2	0.60	0	1,1,1	0.62	0
5	EOH	A	806	-	2,2,2	0.37	0	1,1,1	0.96	0
6	7DJ	A	807	-	27,33,33	1.20	2 (7%)	31,49,49	1.12	4 (12%)
4	SO4	B	703	-	4,4,4	0.25	0	6,6,6	0.15	0
5	EOH	B	704	-	2,2,2	0.67	0	1,1,1	0.64	0
5	EOH	B	705	-	2,2,2	0.47	0	1,1,1	0.67	0
5	EOH	B	706	-	2,2,2	0.49	0	1,1,1	0.78	0
6	7DJ	B	707	-	27,33,33	1.16	4 (14%)	31,49,49	1.07	4 (12%)
4	SO4	C	703	-	4,4,4	0.31	0	6,6,6	0.31	0
5	EOH	C	704	-	2,2,2	0.50	0	1,1,1	0.73	0
6	7DJ	C	705	-	27,33,33	1.22	3 (11%)	31,49,49	1.07	3 (9%)
5	EOH	D	703	-	2,2,2	0.51	0	1,1,1	0.74	0
6	7DJ	D	704	-	27,33,33	1.20	4 (14%)	31,49,49	0.85	1 (3%)

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	SO4	A	803	-	-	0/0/0/0	0/0/0/0
5	EOH	A	804	-	-	0/0/0/0	0/0/0/0
5	EOH	A	805	-	-	0/0/0/0	0/0/0/0
5	EOH	A	806	-	-	0/0/0/0	0/0/0/0
6	7DJ	A	807	-	-	0/15/19/19	0/3/3/3
4	SO4	B	703	-	-	0/0/0/0	0/0/0/0
5	EOH	B	704	-	-	0/0/0/0	0/0/0/0
5	EOH	B	705	-	-	0/0/0/0	0/0/0/0
5	EOH	B	706	-	-	0/0/0/0	0/0/0/0
6	7DJ	B	707	-	-	0/15/19/19	0/3/3/3
4	SO4	C	703	-	-	0/0/0/0	0/0/0/0
5	EOH	C	704	-	-	0/0/0/0	0/0/0/0
6	7DJ	C	705	-	-	0/15/19/19	0/3/3/3
5	EOH	D	703	-	-	0/0/0/0	0/0/0/0
6	7DJ	D	704	-	-	0/15/19/19	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	704	7DJ	C10-C9	2.03	1.56	1.51
6	B	707	7DJ	C1-N5	2.06	1.42	1.38
6	C	705	7DJ	C10-C9	2.08	1.56	1.51
6	B	707	7DJ	C10-C9	2.42	1.57	1.51
6	D	704	7DJ	C1-N5	2.50	1.43	1.38
6	B	707	7DJ	C3-C2	3.28	1.49	1.42
6	C	705	7DJ	C-C1	3.31	1.47	1.39
6	D	704	7DJ	C-C1	3.32	1.47	1.39
6	B	707	7DJ	C-C1	3.57	1.48	1.39
6	A	807	7DJ	C3-C2	3.72	1.50	1.42
6	D	704	7DJ	C3-C2	3.88	1.50	1.42
6	A	807	7DJ	C-C1	4.07	1.49	1.39
6	C	705	7DJ	C3-C2	4.36	1.51	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	807	7DJ	O1-C10-C9	-2.71	106.98	111.96
6	B	707	7DJ	C2-C3-N2	-2.41	115.22	116.78
6	C	705	7DJ	C2-C3-N2	-2.31	115.29	116.78
6	A	807	7DJ	C2-C3-N2	-2.08	115.44	116.78
6	B	707	7DJ	C11-C9-C8	2.06	114.81	109.91
6	A	807	7DJ	C11-C9-C8	2.14	115.00	109.91
6	B	707	7DJ	C4-N2-C3	2.32	126.57	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	705	7DJ	C4-N2-C3	2.64	127.14	122.49
6	D	704	7DJ	C-C3-N2	2.74	126.63	122.04
6	C	705	7DJ	C-C3-N2	2.99	127.05	122.04
6	A	807	7DJ	C-C3-N2	3.35	127.65	122.04
6	B	707	7DJ	C-C3-N2	3.46	127.83	122.04

There are no chirality outliers.

There are no torsion outliers.

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, 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	326/381 (85%)	-0.02	15 (4%)	36 47	24, 34, 59, 117	0
1	B	323/381 (84%)	0.32	23 (7%)	19 26	25, 43, 68, 112	0
1	C	323/381 (84%)	0.16	25 (7%)	16 22	22, 38, 70, 115	0
1	D	325/381 (85%)	-0.07	11 (3%)	49 59	20, 33, 54, 92	0
All	All	1297/1524 (85%)	0.10	74 (5%)	27 37	20, 37, 66, 117	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	GLU	5.6
1	A	578	GLN	5.6
1	C	458	VAL	5.4
1	B	462	GLY	5.1
1	A	577	PRO	4.7
1	B	254	GLN	4.6
1	C	253	GLU	4.1
1	C	463	VAL	3.8
1	C	467	ASP	3.8
1	B	334	VAL	3.7
1	C	334	VAL	3.6
1	D	256	ASP	3.6
1	A	458	VAL	3.6
1	B	255	GLU	3.5
1	D	260	LYS	3.5
1	D	254	GLN	3.4
1	B	458	VAL	3.4
1	A	483	ALA	3.3
1	B	455	THR	3.2
1	A	334	VAL	3.2
1	C	252	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	335	VAL	3.1
1	B	335	VAL	3.0
1	B	256	ASP	3.0
1	B	362	ALA	3.0
1	C	528	ASN	2.9
1	C	555	HIS	2.9
1	B	365	ILE	2.9
1	C	577	PRO	2.8
1	C	254	GLN	2.8
1	C	464	LEU	2.8
1	B	553	LEU	2.7
1	C	480	VAL	2.7
1	C	578	GLN	2.7
1	A	485	LEU	2.7
1	D	362	ALA	2.7
1	B	463	VAL	2.7
1	B	541	TYR	2.6
1	A	463	VAL	2.6
1	D	334	VAL	2.6
1	B	260	LYS	2.6
1	B	465	LEU	2.6
1	C	454	GLU	2.6
1	A	576	ILE	2.6
1	A	464	LEU	2.6
1	D	467	ASP	2.5
1	D	364	ALA	2.5
1	C	365	ILE	2.5
1	C	260	LYS	2.5
1	D	257	VAL	2.4
1	C	468	ASN	2.4
1	C	485	LEU	2.4
1	A	480	VAL	2.4
1	A	482	CYS	2.4
1	D	255	GLU	2.4
1	C	362	ALA	2.4
1	B	360	ILE	2.3
1	C	256	ASP	2.3
1	C	453	VAL	2.3
1	C	483	ALA	2.3
1	A	455	THR	2.3
1	A	541	TYR	2.3
1	A	465	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	347	LEU	2.3
1	A	454	GLU	2.3
1	B	278	LEU	2.2
1	B	331	ALA	2.2
1	B	493	GLN	2.2
1	D	335	VAL	2.1
1	B	468	ASN	2.1
1	D	363	SER	2.1
1	C	486	SER	2.1
1	B	364	ALA	2.0
1	C	466	LEU	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 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(Å <sup>2</sup> )	Q<0.9
5	EOH	A	806	3/3	0.92	0.24	16.87	38,38,39,41	0
5	EOH	B	705	3/3	0.95	0.20	12.30	43,43,43,44	0
5	EOH	A	805	3/3	0.84	0.20	10.67	45,45,48,51	0
5	EOH	D	703	3/3	0.88	0.27	6.33	27,27,33,37	0
5	EOH	B	704	3/3	0.86	0.17	6.29	37,37,39,39	0
5	EOH	C	704	3/3	0.80	0.14	4.68	31,31,35,37	0
5	EOH	A	804	3/3	0.92	0.11	2.81	30,30,37,42	0
5	EOH	B	706	3/3	0.92	0.13	2.80	35,35,39,41	0
4	SO4	C	703	5/5	0.90	0.17	1.35	65,75,77,79	0
6	7DJ	D	704	31/31	0.90	0.14	1.25	44,54,65,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	703	5/5	0.84	0.23	0.99	93,96,97,98	0
6	7DJ	A	807	31/31	0.87	0.17	0.88	44,53,62,67	0
6	7DJ	B	707	31/31	0.90	0.14	0.74	50,63,73,75	0
6	7DJ	C	705	31/31	0.86	0.16	0.68	49,60,70,70	0
4	SO4	A	803	5/5	0.96	0.14	0.40	49,59,63,64	0
3	MG	D	702	1/1	0.99	0.13	0.33	24,24,24,24	0
3	MG	A	802	1/1	0.99	0.11	-0.30	25,25,25,25	0
3	MG	C	702	1/1	0.98	0.12	-0.43	25,25,25,25	0
2	ZN	D	701	1/1	1.00	0.11	-0.66	28,28,28,28	0
2	ZN	C	701	1/1	1.00	0.10	-1.24	32,32,32,32	0
2	ZN	A	801	1/1	1.00	0.10	-1.43	29,29,29,29	0
2	ZN	B	701	1/1	0.99	0.09	-1.50	35,35,35,35	0
3	MG	B	702	1/1	0.99	0.09	-1.65	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.