



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:49 am GMT

PDB ID : 4LF2  
Title : Hexameric Form II RuBisCO from Rhodopseudomonas palustris, activated and complexed with sulfate and magnesium  
Authors : Chan, S.; Satagopan, S.; Sawaya, M.R.; Eisenberg, D.; Tabita, F.R.; Perry, L.J.  
Deposited on : 2013-06-26  
Resolution : 2.38 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](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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

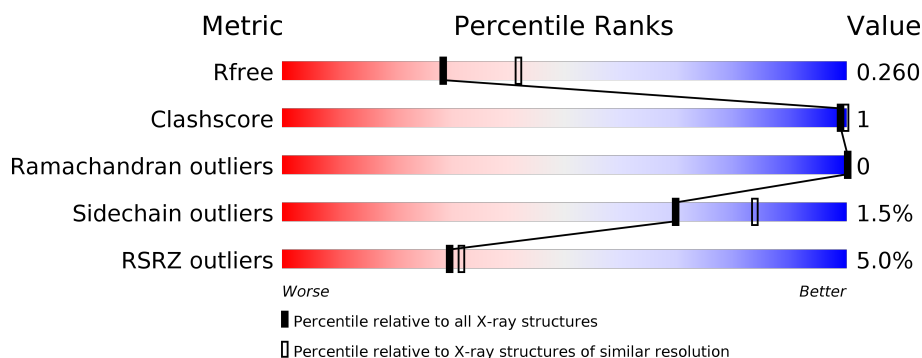
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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))
$R_{free}$	100719	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

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	481	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	B	481	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>
1	C	481	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
1	D	481	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	E	481	<div> <div>7%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	F	481	<div> <div>6%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22617 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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	5	4	0
			3557	2262	614	662	19			
1	B	453	Total	C	N	O	S	3	2	0
			3514	2232	608	655	19			
1	C	453	Total	C	N	O	S	5	1	0
			3513	2231	610	653	19			
1	D	457	Total	C	N	O	S	9	0	0
			3536	2247	613	657	19			
1	E	455	Total	C	N	O	S	6	1	0
			3522	2238	610	656	18			
1	F	456	Total	C	N	O	S	8	2	0
			3537	2249	613	657	18			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9
A	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
A	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
A	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
A	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
A	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
A	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
A	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
A	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
A	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
A	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
A	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
A	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9
A	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9
B	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
B	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
B	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
B	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
B	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
B	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
B	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
B	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
B	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
B	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
B	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9
B	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
B	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9
B	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9
C	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
C	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
C	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
C	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
C	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
C	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
C	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
C	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
C	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
C	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
C	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9
C	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
C	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9
D	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
D	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
D	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
D	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
D	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
D	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
D	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
D	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
D	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
D	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
D	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9
D	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
D	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9
D	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9
E	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
E	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
E	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
E	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
E	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
E	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
E	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
E	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
E	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
E	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
E	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9
E	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
E	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9
E	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-19	MET	-	INITIATING METHIONINE	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	EXPRESSION TAG	UNP Q6N0W9
F	-17	SER	-	EXPRESSION TAG	UNP Q6N0W9
F	-16	SER	-	EXPRESSION TAG	UNP Q6N0W9
F	-15	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-14	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-13	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-12	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-11	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-10	HIS	-	EXPRESSION TAG	UNP Q6N0W9
F	-9	SER	-	EXPRESSION TAG	UNP Q6N0W9
F	-8	SER	-	EXPRESSION TAG	UNP Q6N0W9
F	-7	GLY	-	EXPRESSION TAG	UNP Q6N0W9
F	-6	LEU	-	EXPRESSION TAG	UNP Q6N0W9
F	-5	VAL	-	EXPRESSION TAG	UNP Q6N0W9
F	-4	PRO	-	EXPRESSION TAG	UNP Q6N0W9
F	-3	ARG	-	EXPRESSION TAG	UNP Q6N0W9
F	-2	GLY	-	EXPRESSION TAG	UNP Q6N0W9
F	-1	SER	-	EXPRESSION TAG	UNP Q6N0W9
F	0	HIS	-	EXPRESSION TAG	UNP Q6N0W9

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

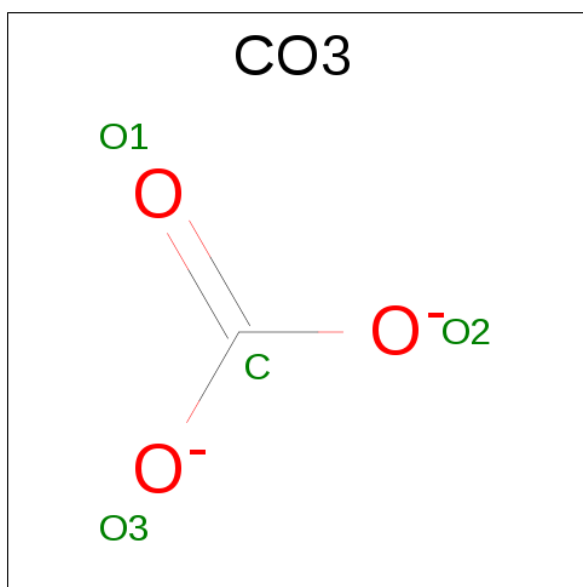
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		
4	C	1	Total	C	O	0	0
			4	1	3		

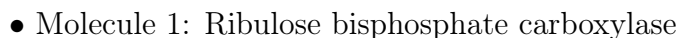
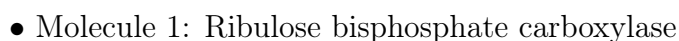
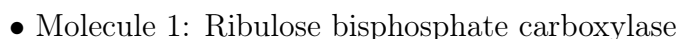
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total	O	0	0
			239	239		
5	B	243	Total	O	0	0
			243	243		
5	C	254	Total	O	0	0
			254	254		
5	D	245	Total	O	0	0
			245	245		
5	E	197	Total	O	0	0
			197	197		
5	F	184	Total	O	0	0
			184	184		





- Molecule 1: Ribulose biphosphate carboxylase



● A408 ● D423 ● P424 ● V425 ● K429 ● D430 ● A437 ● F441 ● D444 ● L448 ● Y449 ● P450 ● N451 ● A454 ● K455 ● L456 ● K457 PRO GLN ALA ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.22Å 99.78Å 100.00Å 67.30° 71.28° 86.63°	Depositor
Resolution (Å)	87.43 – 2.38 87.28 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.6 (87.43-2.38) 64.7 (87.28-1.85)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.203 , 0.258 0.207 , 0.260	Depositor DCC
$R_{free}$ test set	4851 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22617	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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 23.72 % 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 4.4135e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CO3, MG, KCX, 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	0.53	0/3645	0.78	5/4929 (0.1%)
1	B	0.54	0/3596	0.79	3/4866 (0.1%)
1	C	0.54	0/3592	0.79	3/4860 (0.1%)
1	D	0.52	0/3612	0.75	2/4886 (0.0%)
1	E	0.54	0/3601	0.78	4/4873 (0.1%)
1	F	0.54	0/3619	0.78	2/4895 (0.0%)
All	All	0.53	0/21665	0.78	19/29309 (0.1%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	453	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	B	453	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	453	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	A	173	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	F	218	ARG	NE-CZ-NH1	6.10	123.35	120.30

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	3557	0	3444	4	0
1	B	3514	0	3385	10	0
1	C	3513	0	3385	3	0
1	D	3536	0	3414	4	0
1	E	3522	0	3394	3	0
1	F	3537	0	3420	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	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
5	A	239	0	0	0	0
5	B	243	0	0	2	0
5	C	254	0	0	0	0
5	D	245	0	0	1	0
5	E	197	0	0	0	0
5	F	184	0	0	2	0
All	All	22617	0	20442	22	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.

The worst 5 of 22 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:3[B]:GLN:HA	1:B:3[B]:GLN:HE21	1.62	0.64
1:A:62:ASP:OD2	1:B:173:ARG:NH2	2.30	0.64
1:B:135:LYS:NZ	5:B:784:HOH:O	2.33	0.62
1:D:301:LYS:NZ	5:D:935:HOH:O	2.33	0.59
1:E:425:VAL:O	1:E:429:LYS:NZ	2.38	0.56

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	458/481 (95%)	447 (98%)	11 (2%)	0	100	100
1	B	452/481 (94%)	442 (98%)	10 (2%)	0	100	100
1	C	451/481 (94%)	442 (98%)	9 (2%)	0	100	100
1	D	454/481 (94%)	444 (98%)	10 (2%)	0	100	100
1	E	453/481 (94%)	441 (97%)	12 (3%)	0	100	100
1	F	455/481 (95%)	443 (97%)	12 (3%)	0	100	100
All	All	2723/2886 (94%)	2659 (98%)	64 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	357/372 (96%)	350 (98%)	7 (2%)	60	77
1	B	352/372 (95%)	345 (98%)	7 (2%)	60	77
1	C	351/372 (94%)	347 (99%)	4 (1%)	78	89
1	D	353/372 (95%)	348 (99%)	5 (1%)	71	85
1	E	352/372 (95%)	346 (98%)	6 (2%)	66	81
1	F	354/372 (95%)	351 (99%)	3 (1%)	85	93
All	All	2119/2232 (95%)	2087 (98%)	32 (2%)	70	84

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	55	ASN
1	C	453	ARG
1	F	55	ASN
1	C	287	TYR
1	D	55	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	ASN
1	F	55	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	KCX	A	192	1,2	8,11,12	0.45	0	6,12,14	1.07	0
1	KCX	B	192	1,2	8,11,12	0.31	0	6,12,14	1.03	0
1	KCX	C	192	1	8,11,12	0.40	0	6,12,14	1.03	0
1	KCX	D	192	1,2	8,11,12	0.49	0	6,12,14	1.10	0
1	KCX	E	192	1	8,11,12	0.36	0	6,12,14	1.11	0
1	KCX	F	192	1	8,11,12	0.56	0	6,12,14	1.09	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	KCX	A	192	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	192	1,2	-	0/6/10/12	0/0/0/0
1	KCX	C	192	1	-	0/6/10/12	0/0/0/0
1	KCX	D	192	1,2	-	0/6/10/12	0/0/0/0
1	KCX	E	192	1	-	0/6/10/12	0/0/0/0
1	KCX	F	192	1	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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 19 ligands modelled in this entry, 4 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	$\# Z  > 2$
3	SO4	A	602	-	4,4,4	0.43	0	6,6,6	0.46	0
3	SO4	A	603	-	4,4,4	0.40	0	6,6,6	0.21	0
4	CO3	A	604	-	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	B	602	-	4,4,4	0.39	0	6,6,6	0.33	0
3	SO4	B	603	-	4,4,4	0.37	0	6,6,6	0.22	0
4	CO3	B	604	-	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	C	602	-	4,4,4	0.42	0	6,6,6	0.37	0
3	SO4	C	603	-	4,4,4	0.40	0	6,6,6	0.07	0
4	CO3	C	604	-	0,3,3	0.00	-	0,3,3	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	D	602	-	4,4,4	0.36	0	6,6,6	0.57	0
3	SO4	D	603	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	E	701	-	4,4,4	0.37	0	6,6,6	0.32	0
3	SO4	E	702	-	4,4,4	0.35	0	6,6,6	0.13	0
3	SO4	F	701	-	4,4,4	0.29	0	6,6,6	0.46	0
3	SO4	F	702	-	4,4,4	0.40	0	6,6,6	0.12	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	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
4	CO3	A	604	-	-	0/0/0/0	0/0/0/0
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
4	CO3	B	604	-	-	0/0/0/0	0/0/0/0
3	SO4	C	602	-	-	0/0/0/0	0/0/0/0
3	SO4	C	603	-	-	0/0/0/0	0/0/0/0
4	CO3	C	604	-	-	0/0/0/0	0/0/0/0
3	SO4	D	602	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	SO4	E	701	-	-	0/0/0/0	0/0/0/0
3	SO4	E	702	-	-	0/0/0/0	0/0/0/0
3	SO4	F	701	-	-	0/0/0/0	0/0/0/0
3	SO4	F	702	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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	456/481 (94%)	-0.29	10 (2%) 62 63	4, 17, 55, 90	2 (0%)
1	B	452/481 (93%)	-0.11	24 (5%) 27 29	5, 16, 61, 92	1 (0%)
1	C	452/481 (93%)	-0.10	22 (4%) 30 33	4, 16, 61, 102	2 (0%)
1	D	456/481 (94%)	-0.27	16 (3%) 44 47	4, 16, 50, 130	6 (1%)
1	E	454/481 (94%)	0.05	32 (7%) 17 18	4, 21, 75, 122	2 (0%)
1	F	455/481 (94%)	0.01	31 (6%) 18 19	5, 21, 69, 112	3 (0%)
All	All	2725/2886 (94%)	-0.12	135 (4%) 30 32	4, 18, 63, 130	16 (0%)

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	450	PRO	7.5
1	E	63	ASP	6.8
1	F	401	VAL	6.2
1	E	61	THR	5.7
1	C	451	ASN	5.6

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

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	KCX	D	192	12/13	0.90	0.12	-	15,18,28,31	0
1	KCX	F	192	12/13	0.92	0.12	-	16,25,45,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KCX	B	192	12/13	0.90	0.13	-	14,25,34,48	0
1	KCX	E	192	12/13	0.92	0.11	-	11,17,36,42	0
1	KCX	C	192	12/13	0.91	0.11	-	13,22,36,52	0
1	KCX	A	192	12/13	0.90	0.11	-	11,17,26,28	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	SO4	E	701	5/5	0.93	0.15	1.73	25,37,47,72	0
4	CO3	C	604	4/4	0.77	0.11	0.78	28,31,46,64	0
3	SO4	F	701	5/5	0.94	0.17	0.70	35,38,45,63	0
3	SO4	A	602	5/5	0.93	0.11	0.22	15,19,39,44	0
3	SO4	B	602	5/5	0.89	0.12	0.13	18,29,42,53	0
3	SO4	B	603	5/5	0.95	0.15	-0.10	29,36,44,56	0
4	CO3	A	604	4/4	0.89	0.11	-0.11	29,43,50,57	0
2	MG	D	601	1/1	0.88	0.11	-0.56	44,44,44,44	0
3	SO4	C	602	5/5	0.89	0.11	-0.59	15,31,34,44	0
2	MG	C	601	1/1	0.86	0.13	-0.73	52,52,52,52	0
3	SO4	C	603	5/5	0.96	0.10	-0.94	42,43,59,79	0
3	SO4	F	702	5/5	0.95	0.10	-0.97	39,51,62,70	0
3	SO4	D	602	5/5	0.94	0.09	-1.05	15,23,46,47	0
3	SO4	A	603	5/5	0.99	0.07	-1.05	17,29,32,35	0
2	MG	B	601	1/1	0.76	0.11	-1.11	62,62,62,62	0
3	SO4	D	603	5/5	0.99	0.07	-1.12	18,24,31,33	0
3	SO4	E	702	5/5	0.96	0.09	-1.15	39,44,50,52	0
4	CO3	B	604	4/4	0.86	0.09	-1.16	37,38,40,70	0
2	MG	A	601	1/1	0.92	0.07	-1.20	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.