Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 01:32 PM EDT

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

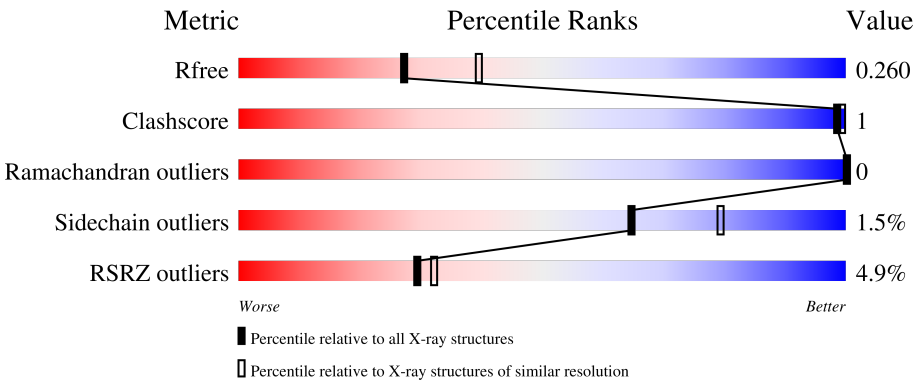
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2%, 92%, • 5%
1	B	481	5%, 90%, • • 6%
1	C	481	5%, 92%, • 6%
1	D	481	3%, 93%, • 5%
1	E	481	6%, 92%, • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	481	6% 93% 5%

2 Entry composition (i)

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 bisphosphate carboxylase.

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

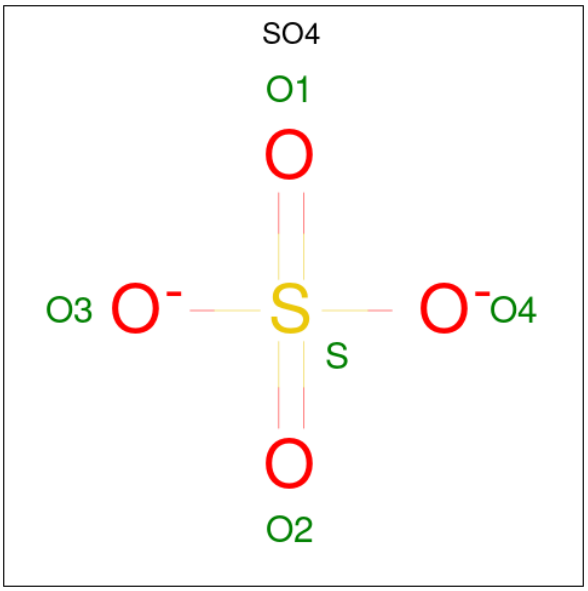
Continued from previous page...

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).

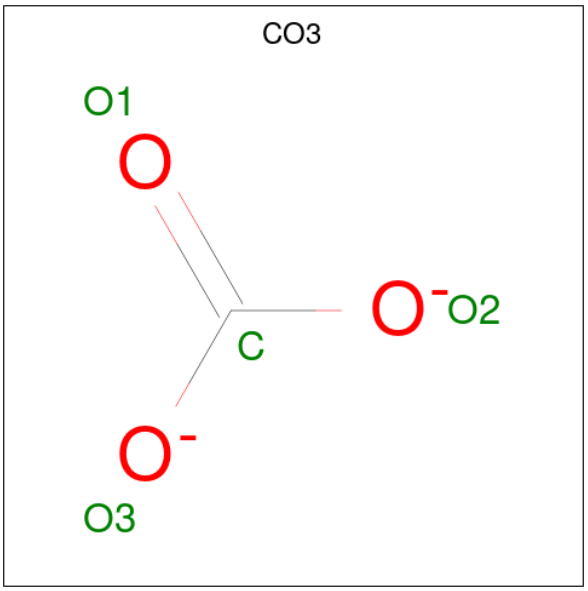
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

- Molecule 5 is water.

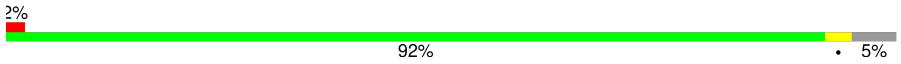
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	239	239	239	0	0
			Total	O		
5	B	243	243	243	0	0
			Total	O		
5	C	254	254	254	0	0
			Total	O		
5	D	245	245	245	0	0
			Total	O		
5	E	197	197	197	0	0
			Total	O		
5	F	184	184	184	0	0

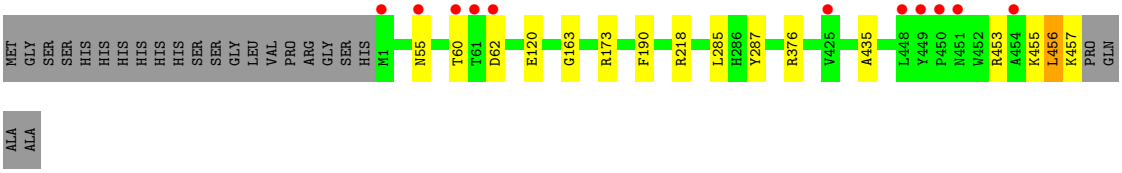
3 Residue-property plots (i)

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

• Molecule 1: Ribulose bisphosphate carboxylase

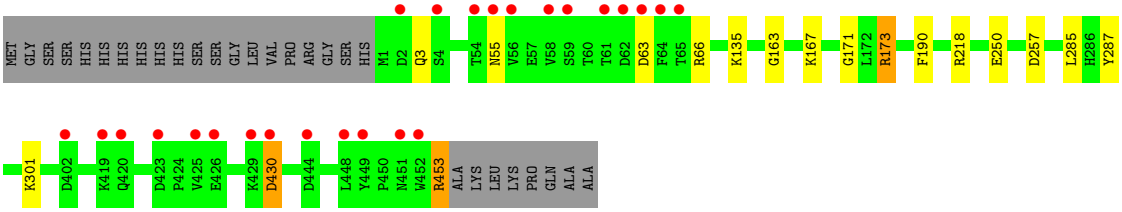
Chain A:





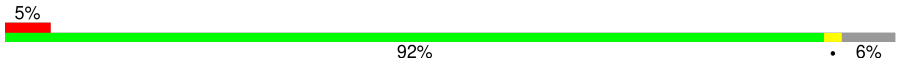
• Molecule 1: Ribulose bisphosphate carboxylase

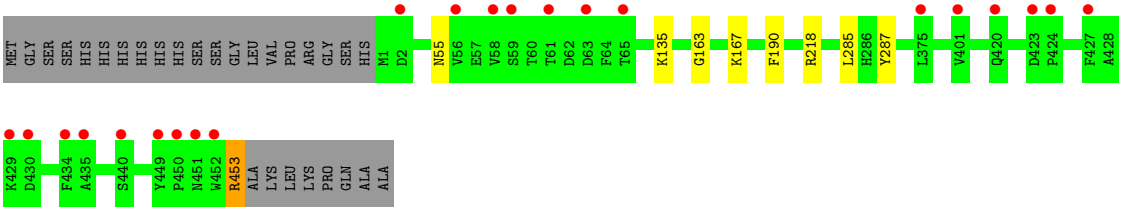
Chain B:



• Molecule 1: Ribulose bisphosphate carboxylase

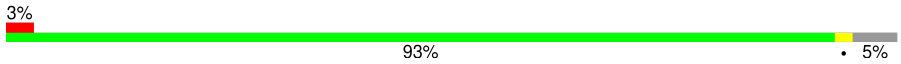
Chain C:

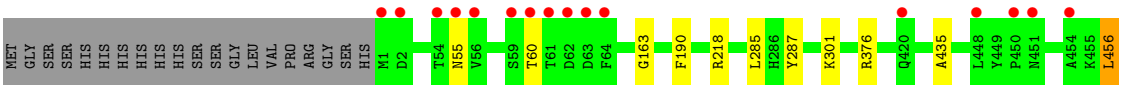




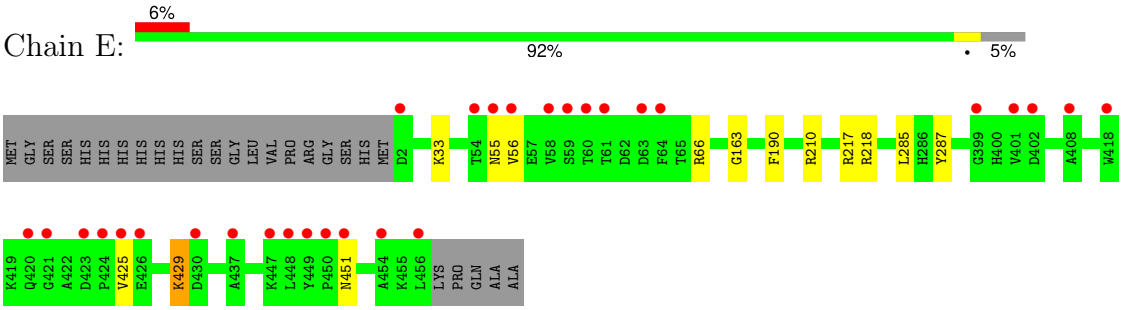
• Molecule 1: Ribulose bisphosphate carboxylase

Chain D:

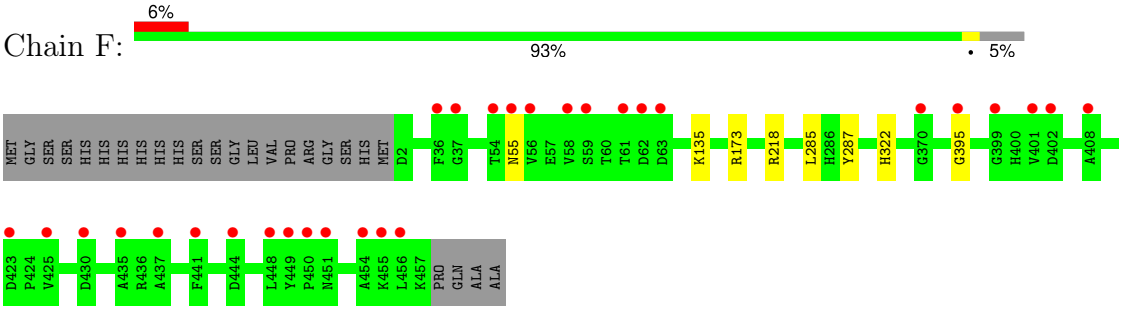




• Molecule 1: Ribulose bisphosphate carboxylase



• Molecule 1: Ribulose bisphosphate carboxylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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) 68.5 (87.28-1.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 1.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.258 0.207 , 0.260	Depositor DCC
R_{free} test set	7318 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, SO4, KCX, CO3

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.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	A	218	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	218	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	218	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	D	218	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	E	66	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	453	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	376	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	F	173	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	453	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	E	218	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	E	217	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	376	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	E	210	ARG	NE-CZ-NH1	5.08	122.84	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	453	ARG	CD-NE-CZ	5.02	130.63	123.60

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.

All (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:HE21	1:B:3[B]:GLN:HA	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
1:E:56:VAL:HG11	1:F:395:GLY:HA3	1.88	0.54
1:F:135:LYS:NZ	5:F:902:HOH:O	2.43	0.51
1:A:435:ALA:HB1	1:A:456:LEU:HD21	1.96	0.47
1:A:60:THR:OG1	1:B:167:LYS:O	2.22	0.46
1:C:167:LYS:O	1:D:60:THR:OG1	2.23	0.46
1:B:301:LYS:NZ	5:B:767:HOH:O	2.34	0.45
1:B:430:ASP:OD1	1:B:430:ASP:N	2.51	0.44
1:F:322:HIS:ND1	5:F:904:HOH:O	2.32	0.43
1:A:163:GLY:HA2	1:A:190:PHE:O	2.20	0.42
1:B:171:GLY:O	1:B:173:ARG:NH1	2.52	0.42
1:D:163:GLY:HA2	1:D:190:PHE:O	2.20	0.42
1:B:63:ASP:OD1	1:B:66:ARG:NH1	2.53	0.42
1:D:435:ALA:HB1	1:D:456:LEU:HD21	2.01	0.41
1:B:163:GLY:HA2	1:B:190:PHE:O	2.21	0.41
1:C:163:GLY:HA2	1:C:190:PHE:O	2.21	0.41
1:E:163:GLY:HA2	1:E:190:PHE:O	2.21	0.41
1:B:257:ASP:OD2	1:C:135:LYS:NZ	2.47	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	458/481 (95%)	447 (98%)	11 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (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	357/372 (96%)	350 (98%)	7 (2%)	55	72
1	B	352/372 (95%)	345 (98%)	7 (2%)	55	72
1	C	351/372 (94%)	347 (99%)	4 (1%)	73	86
1	D	353/372 (95%)	348 (99%)	5 (1%)	67	81
1	E	352/372 (95%)	346 (98%)	6 (2%)	60	76
1	F	354/372 (95%)	351 (99%)	3 (1%)	81	91
All	All	2119/2232 (95%)	2087 (98%)	32 (2%)	65	79

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	120	GLU
1	A	285	LEU
1	A	287	TYR
1	A	455	LYS
1	A	456	LEU
1	A	457	LYS
1	B	55	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	173	ARG
1	B	250	GLU
1	B	285	LEU
1	B	287	TYR
1	B	430	ASP
1	B	453	ARG
1	C	55	ASN
1	C	285	LEU
1	C	287	TYR
1	C	453	ARG
1	D	55	ASN
1	D	285	LEU
1	D	287	TYR
1	D	456	LEU
1	D	457	LYS
1	E	33	LYS
1	E	55	ASN
1	E	285	LEU
1	E	287	TYR
1	E	429	LYS
1	E	451	ASN
1	F	55	ASN
1	F	285	LEU
1	F	287	TYR

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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	E	192	1	10,11,12	0.52	0	6,12,14	0.51	0
1	KCX	A	192	2,1	10,11,12	0.56	0	6,12,14	0.50	0
1	KCX	C	192	1	10,11,12	0.51	0	6,12,14	0.48	0
1	KCX	B	192	2,1	10,11,12	0.51	0	6,12,14	0.53	0
1	KCX	D	192	2,1	10,11,12	0.56	0	6,12,14	0.49	0
1	KCX	F	192	1	10,11,12	0.61	0	6,12,14	0.46	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	E	192	1	-	0/9/10/12	-
1	KCX	A	192	2,1	-	0/9/10/12	-
1	KCX	C	192	1	-	0/9/10/12	-
1	KCX	B	192	2,1	-	0/9/10/12	-
1	KCX	D	192	2,1	-	0/9/10/12	-
1	KCX	F	192	1	-	0/9/10/12	-

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 monosaccharides 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	D	602	-	4,4,4	0.38	0	6,6,6	0.58	0
3	SO4	E	702	-	4,4,4	0.37	0	6,6,6	0.13	0
3	SO4	B	602	-	4,4,4	0.40	0	6,6,6	0.35	0
3	SO4	A	602	-	4,4,4	0.46	0	6,6,6	0.50	0
3	SO4	B	603	-	4,4,4	0.40	0	6,6,6	0.26	0
3	SO4	C	603	-	4,4,4	0.42	0	6,6,6	0.11	0
3	SO4	D	603	-	4,4,4	0.39	0	6,6,6	0.10	0
3	SO4	E	701	-	4,4,4	0.39	0	6,6,6	0.32	0
3	SO4	F	702	-	4,4,4	0.42	0	6,6,6	0.08	0
3	SO4	F	701	-	4,4,4	0.33	0	6,6,6	0.49	0
4	CO3	A	604	-	3,3,3	1.13	0	2,3,3	0.15	0
3	SO4	A	603	-	4,4,4	0.41	0	6,6,6	0.21	0
4	CO3	B	604	-	3,3,3	1.13	0	2,3,3	0.14	0
4	CO3	C	604	-	3,3,3	1.10	0	2,3,3	0.23	0
3	SO4	C	602	-	4,4,4	0.45	0	6,6,6	0.41	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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	456/481 (94%)	-0.28	11 (2%)	59	60	4, 17, 55, 90	2 (0%)
1	B	452/481 (93%)	-0.11	25 (5%)	25	27	5, 16, 61, 92	1 (0%)
1	C	452/481 (93%)	-0.11	22 (4%)	29	32	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	30 (6%)	18	20	4, 21, 75, 122	2 (0%)
1	F	455/481 (94%)	0.01	30 (6%)	18	20	5, 21, 69, 112	3 (0%)
All	All	2725/2886 (94%)	-0.12	134 (4%)	29	32	4, 18, 63, 130	16 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	450	PRO	7.2
1	F	401	VAL	6.2
1	E	63	ASP	5.9
1	F	449	TYR	5.8
1	E	61	THR	5.6
1	C	451	ASN	5.3
1	F	437	ALA	5.2
1	D	61	THR	5.0
1	E	54	THR	4.9
1	F	450	PRO	4.8
1	B	429	LYS	4.7
1	A	62	ASP	4.7
1	D	62	ASP	4.6
1	E	425	VAL	4.5
1	B	4	SER	4.4
1	F	448	LEU	4.4
1	E	448	LEU	4.3
1	E	59	SER	4.2
1	B	420	GLN	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	402	ASP	4.2
1	F	430	ASP	4.2
1	D	451	ASN	4.1
1	F	56	VAL	4.1
1	B	425	VAL	4.1
1	E	454	ALA	4.1
1	C	429	LYS	4.1
1	D	420	GLN	4.0
1	C	401	VAL	4.0
1	F	454	ALA	4.0
1	B	448	LEU	4.0
1	F	456	LEU	4.0
1	E	456	LEU	3.9
1	E	58	VAL	3.9
1	A	61	THR	3.9
1	F	425	VAL	3.8
1	E	418	TRP	3.8
1	B	55	ASN	3.8
1	E	60	THR	3.7
1	B	449	TYR	3.7
1	D	1	MET	3.7
1	F	58	VAL	3.6
1	E	56	VAL	3.6
1	E	420	GLN	3.6
1	F	370	GLY	3.5
1	B	61	THR	3.4
1	E	401	VAL	3.4
1	C	56	VAL	3.4
1	C	423	ASP	3.4
1	F	63	ASP	3.4
1	E	423	ASP	3.4
1	E	449	TYR	3.3
1	D	64	PHE	3.3
1	E	426	GLU	3.3
1	B	58	VAL	3.3
1	D	63	ASP	3.2
1	F	455	LYS	3.2
1	B	451	ASN	3.1
1	C	430	ASP	3.1
1	C	435	ALA	3.1
1	E	2	ASP	3.1
1	E	424	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	451	ASN	3.1
1	F	55	ASN	3.1
1	E	64	PHE	3.1
1	A	1	MET	3.0
1	D	56	VAL	3.0
1	A	451	ASN	3.0
1	C	440	SER	3.0
1	F	54	THR	2.9
1	F	59	SER	2.9
1	B	54	THR	2.9
1	C	449	TYR	2.9
1	B	59	SER	2.8
1	F	61	THR	2.8
1	E	399	GLY	2.8
1	D	55	ASN	2.8
1	C	434	PHE	2.8
1	E	55	ASN	2.8
1	D	54	THR	2.7
1	D	454	ALA	2.7
1	A	60	THR	2.7
1	D	59	SER	2.7
1	C	427	PHE	2.6
1	B	64	PHE	2.6
1	B	423	ASP	2.6
1	F	423	ASP	2.6
1	F	37	GLY	2.6
1	F	451	ASN	2.6
1	F	399	GLY	2.6
1	A	450	PRO	2.5
1	F	36	PHE	2.5
1	A	55	ASN	2.5
1	F	408	ALA	2.5
1	B	56	VAL	2.5
1	E	450	PRO	2.5
1	B	2	ASP	2.5
1	C	424	PRO	2.4
1	D	448	LEU	2.4
1	C	63	ASP	2.4
1	F	62	ASP	2.4
1	C	58	VAL	2.4
1	E	408	ALA	2.4
1	B	430	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	420	GLN	2.4
1	E	437	ALA	2.3
1	B	452	TRP	2.3
1	D	60	THR	2.3
1	B	63	ASP	2.3
1	F	395	GLY	2.3
1	A	454	ALA	2.3
1	C	65	THR	2.3
1	E	402	ASP	2.2
1	C	452	TRP	2.2
1	C	2	ASP	2.2
1	F	441	PHE	2.2
1	B	62	ASP	2.2
1	B	444	ASP	2.2
1	A	448	LEU	2.1
1	C	375	LEU	2.1
1	F	444	ASP	2.1
1	B	419	LYS	2.1
1	E	421	GLY	2.1
1	B	426	GLU	2.1
1	D	2	ASP	2.1
1	A	449	TYR	2.1
1	D	450	PRO	2.1
1	C	61	THR	2.1
1	F	435	ALA	2.1
1	B	402	ASP	2.0
1	E	447	LYS	2.0
1	C	59	SER	2.0
1	A	425	VAL	2.0
1	B	65	THR	2.0
1	E	430	ASP	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. 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(Å^2)	Q<0.9
1	KCX	A	192	12/13	0.90	0.11	11,17,26,28	0
1	KCX	B	192	12/13	0.90	0.13	14,25,34,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	D	192	12/13	0.90	0.12	15,18,28,31	0
1	KCX	C	192	12/13	0.91	0.11	13,22,36,52	0
1	KCX	F	192	12/13	0.92	0.12	16,25,45,53	0
1	KCX	E	192	12/13	0.93	0.10	11,17,36,42	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
2	MG	B	601	1/1	0.68	0.14	62,62,62,62	0
2	MG	C	601	1/1	0.79	0.13	52,52,52,52	0
4	CO3	C	604	4/4	0.79	0.11	28,31,46,64	0
2	MG	D	601	1/1	0.85	0.13	44,44,44,44	0
4	CO3	B	604	4/4	0.87	0.09	37,38,40,70	0
4	CO3	A	604	4/4	0.89	0.11	29,43,50,57	0
3	SO4	B	602	5/5	0.89	0.12	18,29,42,53	0
3	SO4	C	602	5/5	0.89	0.11	15,31,34,44	0
3	SO4	E	701	5/5	0.93	0.17	25,37,47,72	0
3	SO4	A	602	5/5	0.93	0.12	15,19,39,44	0
3	SO4	F	701	5/5	0.94	0.17	35,38,45,63	0
2	MG	A	601	1/1	0.94	0.10	34,34,34,34	0
3	SO4	B	603	5/5	0.95	0.15	29,36,44,56	0
3	SO4	D	602	5/5	0.95	0.08	15,23,46,47	0
3	SO4	F	702	5/5	0.95	0.10	39,51,62,70	0
3	SO4	C	603	5/5	0.96	0.09	42,43,59,79	0
3	SO4	E	702	5/5	0.97	0.09	39,44,50,52	0
3	SO4	D	603	5/5	0.99	0.08	18,24,31,33	0
3	SO4	A	603	5/5	0.99	0.07	17,29,32,35	0

6.5 Other polymers (i)

There are no such residues in this entry.