



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:01 pm BST

PDB ID : 3FMI
Title : Crystal structure of Mycobacterium tuberculosis dethiobiotin synthetase complexed with 7-Keto 8-aminopelargonic acid
Authors : Dey, S.; Sacchettini, J.C.
Deposited on : 2008-12-22
Resolution : 2.18 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 ⓘ 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

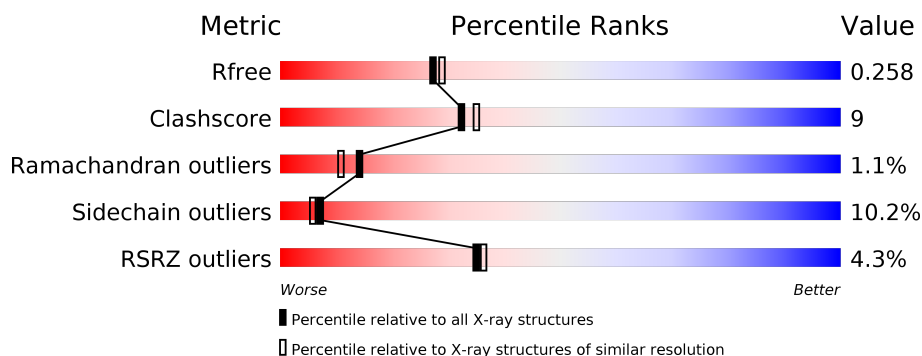
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 ≥ 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	251	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	251	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	251	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	251	<div> <div>8%</div> <div> <div></div> <div>64%</div> <div>20%</div> <div>•</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6599 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 Dethiobiotin synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1621	1014	292	307	8			
1	B	224	Total	C	N	O	S	0	1	0
			1563	976	282	297	8			
1	C	227	Total	C	N	O	S	0	0	0
			1585	989	287	301	8			
1	D	224	Total	C	N	O	S	0	0	0
			1561	975	282	297	7			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	EXPRESSION TAG	UNP O06620
A	-23	GLY	-	EXPRESSION TAG	UNP O06620
A	-22	SER	-	EXPRESSION TAG	UNP O06620
A	-21	SER	-	EXPRESSION TAG	UNP O06620
A	-20	HIS	-	EXPRESSION TAG	UNP O06620
A	-19	HIS	-	EXPRESSION TAG	UNP O06620
A	-18	HIS	-	EXPRESSION TAG	UNP O06620
A	-17	HIS	-	EXPRESSION TAG	UNP O06620
A	-16	HIS	-	EXPRESSION TAG	UNP O06620
A	-15	HIS	-	EXPRESSION TAG	UNP O06620
A	-14	SER	-	EXPRESSION TAG	UNP O06620
A	-13	SER	-	EXPRESSION TAG	UNP O06620
A	-12	GLY	-	EXPRESSION TAG	UNP O06620
A	-11	LEU	-	EXPRESSION TAG	UNP O06620
A	-10	GLN	-	EXPRESSION TAG	UNP O06620
A	-9	GLY	-	EXPRESSION TAG	UNP O06620
A	-8	THR	-	EXPRESSION TAG	UNP O06620
A	-7	GLU	-	EXPRESSION TAG	UNP O06620
A	-6	ASN	-	EXPRESSION TAG	UNP O06620
A	-5	LEU	-	EXPRESSION TAG	UNP O06620
A	-4	TYR	-	EXPRESSION TAG	UNP O06620

Continued on next page...

Continued from previous page...

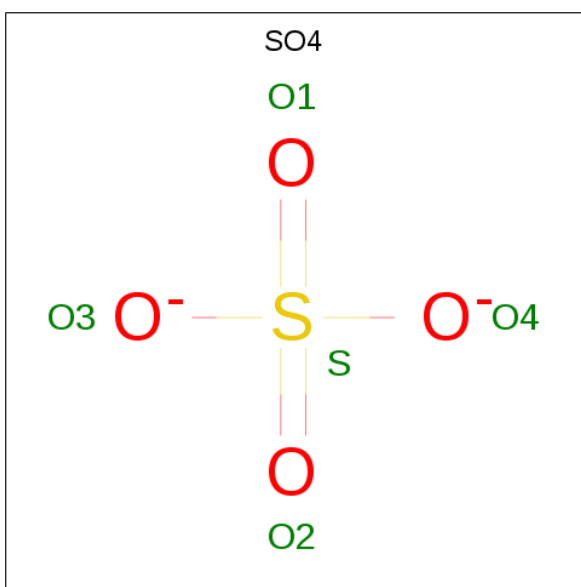
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	EXPRESSION TAG	UNP O06620
A	-2	GLN	-	EXPRESSION TAG	UNP O06620
A	-1	SER	-	EXPRESSION TAG	UNP O06620
A	0	HIS	-	EXPRESSION TAG	UNP O06620
B	-24	MET	-	EXPRESSION TAG	UNP O06620
B	-23	GLY	-	EXPRESSION TAG	UNP O06620
B	-22	SER	-	EXPRESSION TAG	UNP O06620
B	-21	SER	-	EXPRESSION TAG	UNP O06620
B	-20	HIS	-	EXPRESSION TAG	UNP O06620
B	-19	HIS	-	EXPRESSION TAG	UNP O06620
B	-18	HIS	-	EXPRESSION TAG	UNP O06620
B	-17	HIS	-	EXPRESSION TAG	UNP O06620
B	-16	HIS	-	EXPRESSION TAG	UNP O06620
B	-15	HIS	-	EXPRESSION TAG	UNP O06620
B	-14	SER	-	EXPRESSION TAG	UNP O06620
B	-13	SER	-	EXPRESSION TAG	UNP O06620
B	-12	GLY	-	EXPRESSION TAG	UNP O06620
B	-11	LEU	-	EXPRESSION TAG	UNP O06620
B	-10	GLN	-	EXPRESSION TAG	UNP O06620
B	-9	GLY	-	EXPRESSION TAG	UNP O06620
B	-8	THR	-	EXPRESSION TAG	UNP O06620
B	-7	GLU	-	EXPRESSION TAG	UNP O06620
B	-6	ASN	-	EXPRESSION TAG	UNP O06620
B	-5	LEU	-	EXPRESSION TAG	UNP O06620
B	-4	TYR	-	EXPRESSION TAG	UNP O06620
B	-3	PHE	-	EXPRESSION TAG	UNP O06620
B	-2	GLN	-	EXPRESSION TAG	UNP O06620
B	-1	SER	-	EXPRESSION TAG	UNP O06620
B	0	HIS	-	EXPRESSION TAG	UNP O06620
C	-24	MET	-	EXPRESSION TAG	UNP O06620
C	-23	GLY	-	EXPRESSION TAG	UNP O06620
C	-22	SER	-	EXPRESSION TAG	UNP O06620
C	-21	SER	-	EXPRESSION TAG	UNP O06620
C	-20	HIS	-	EXPRESSION TAG	UNP O06620
C	-19	HIS	-	EXPRESSION TAG	UNP O06620
C	-18	HIS	-	EXPRESSION TAG	UNP O06620
C	-17	HIS	-	EXPRESSION TAG	UNP O06620
C	-16	HIS	-	EXPRESSION TAG	UNP O06620
C	-15	HIS	-	EXPRESSION TAG	UNP O06620
C	-14	SER	-	EXPRESSION TAG	UNP O06620
C	-13	SER	-	EXPRESSION TAG	UNP O06620
C	-12	GLY	-	EXPRESSION TAG	UNP O06620

Continued on next page...

Continued from previous page...

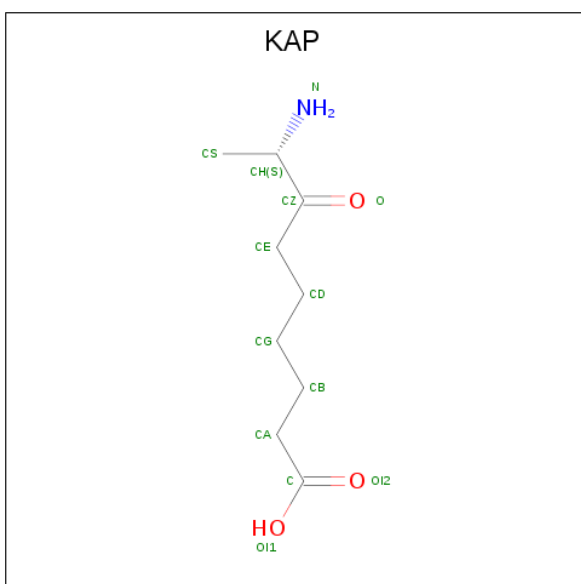
Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	LEU	-	EXPRESSION TAG	UNP O06620
C	-10	GLN	-	EXPRESSION TAG	UNP O06620
C	-9	GLY	-	EXPRESSION TAG	UNP O06620
C	-8	THR	-	EXPRESSION TAG	UNP O06620
C	-7	GLU	-	EXPRESSION TAG	UNP O06620
C	-6	ASN	-	EXPRESSION TAG	UNP O06620
C	-5	LEU	-	EXPRESSION TAG	UNP O06620
C	-4	TYR	-	EXPRESSION TAG	UNP O06620
C	-3	PHE	-	EXPRESSION TAG	UNP O06620
C	-2	GLN	-	EXPRESSION TAG	UNP O06620
C	-1	SER	-	EXPRESSION TAG	UNP O06620
C	0	HIS	-	EXPRESSION TAG	UNP O06620
D	-24	MET	-	EXPRESSION TAG	UNP O06620
D	-23	GLY	-	EXPRESSION TAG	UNP O06620
D	-22	SER	-	EXPRESSION TAG	UNP O06620
D	-21	SER	-	EXPRESSION TAG	UNP O06620
D	-20	HIS	-	EXPRESSION TAG	UNP O06620
D	-19	HIS	-	EXPRESSION TAG	UNP O06620
D	-18	HIS	-	EXPRESSION TAG	UNP O06620
D	-17	HIS	-	EXPRESSION TAG	UNP O06620
D	-16	HIS	-	EXPRESSION TAG	UNP O06620
D	-15	HIS	-	EXPRESSION TAG	UNP O06620
D	-14	SER	-	EXPRESSION TAG	UNP O06620
D	-13	SER	-	EXPRESSION TAG	UNP O06620
D	-12	GLY	-	EXPRESSION TAG	UNP O06620
D	-11	LEU	-	EXPRESSION TAG	UNP O06620
D	-10	GLN	-	EXPRESSION TAG	UNP O06620
D	-9	GLY	-	EXPRESSION TAG	UNP O06620
D	-8	THR	-	EXPRESSION TAG	UNP O06620
D	-7	GLU	-	EXPRESSION TAG	UNP O06620
D	-6	ASN	-	EXPRESSION TAG	UNP O06620
D	-5	LEU	-	EXPRESSION TAG	UNP O06620
D	-4	TYR	-	EXPRESSION TAG	UNP O06620
D	-3	PHE	-	EXPRESSION TAG	UNP O06620
D	-2	GLN	-	EXPRESSION TAG	UNP O06620
D	-1	SER	-	EXPRESSION TAG	UNP O06620
D	0	HIS	-	EXPRESSION TAG	UNP O06620

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is 7-KETO-8-AMINOPELARGONIC ACID (three-letter code: KAP) (formula: C₉H₁₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		
3	C	1	Total	C	N	O	0	0
			13	9	1	3		

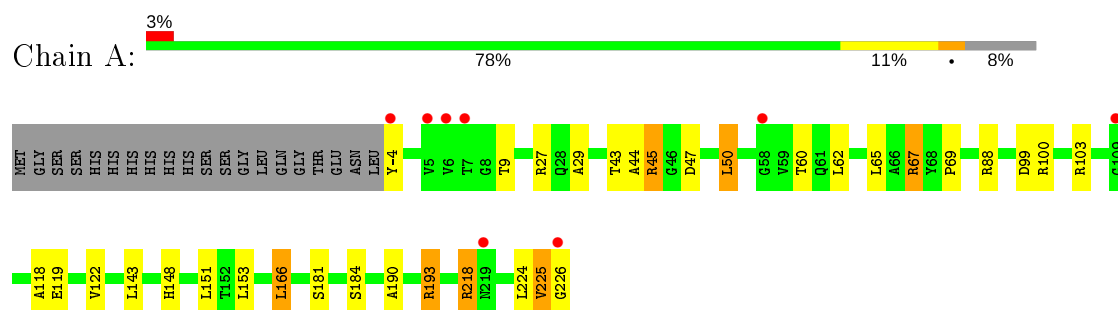
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	70	Total	O	0	0
			70	70		
4	C	55	Total	O	0	0
			55	55		
4	D	24	Total	O	0	0
			24	24		

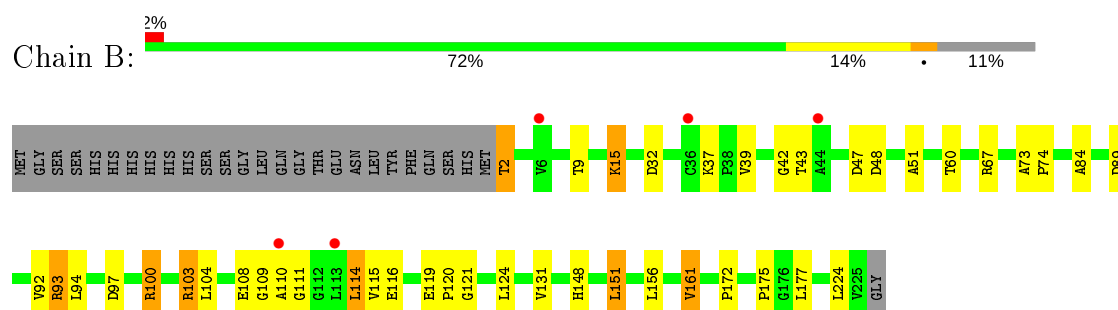
3 Residue-property plots [i](#)

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.

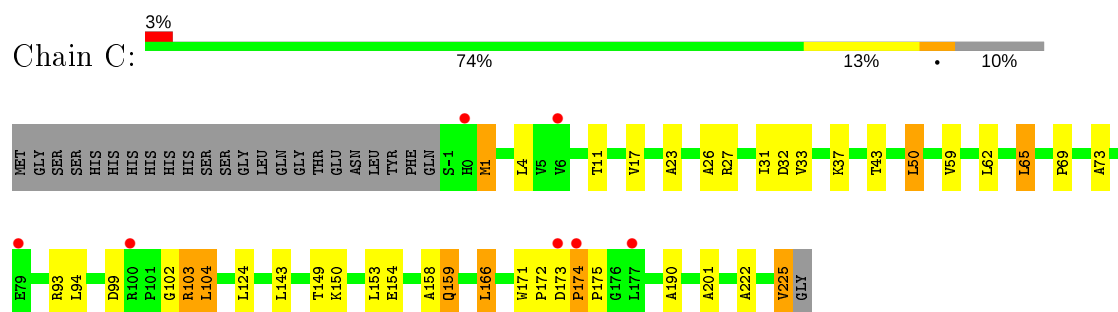
• Molecule 1: Dethiobiotin synthetase



• Molecule 1: Dethiobiotin synthetase

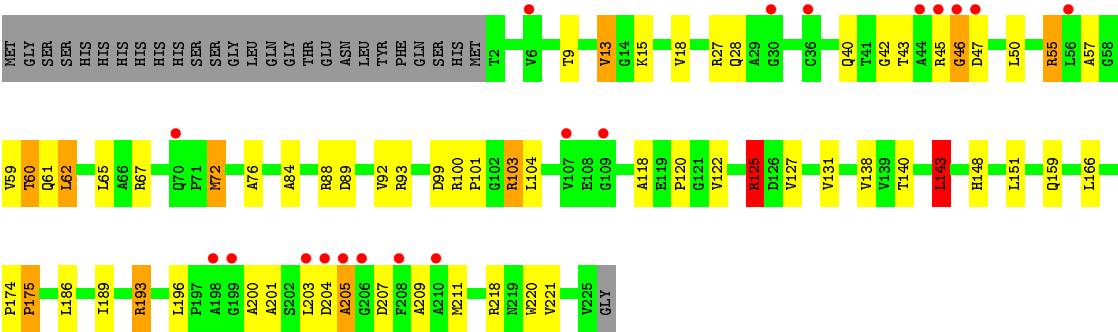


• Molecule 1: Dethiobiotin synthetase



• Molecule 1: Dethiobiotin synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.37Å 105.14Å 151.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.00 – 2.18 31.81 – 2.18	Depositor EDS
% Data completeness (in resolution range)	97.5 (32.00-2.18) 97.4 (31.81-2.18)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.264 0.207 , 0.258	Depositor DCC
R_{free} test set	2323 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6599	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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: KAP, SO4, CSX

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	0.57	0/1635	0.74	2/2234 (0.1%)
1	B	0.57	0/1578	0.72	1/2158 (0.0%)
1	C	0.49	0/1597	0.67	0/2183
1	D	0.50	0/1572	0.77	3/2150 (0.1%)
All	All	0.53	0/6382	0.72	6/8725 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	D	125	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	193	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	D	143	LEU	CA-CB-CG	5.36	127.62	115.30
1	D	125	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	151	LEU	CA-CB-CG	5.14	127.13	115.30

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	1621	0	1663	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1563	0	1611	35	0
1	C	1585	0	1634	29	0
1	D	1561	0	1610	39	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	13	0	16	4	0
3	B	13	0	16	0	0
3	C	13	0	16	4	0
4	A	61	0	0	0	0
4	B	70	0	0	2	0
4	C	55	0	0	0	0
4	D	24	0	0	2	0
All	All	6599	0	6566	114	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 9.

All (114) 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:C:159:GLN:HA	1:C:159:GLN:HE21	1.14	1.07
1:D:55:ARG:HG2	1:D:55:ARG:HH21	1.24	1.01
1:B:100:ARG:HH11	1:B:100:ARG:CG	1.88	0.87
1:C:174:PRO:HB2	1:C:175:PRO:HA	1.57	0.86
1:C:159:GLN:HA	1:C:159:GLN:NE2	1.94	0.81
1:D:118:ALA:HB3	1:D:122:VAL:HG22	1.64	0.80
1:D:72:MET:HE3	1:D:76:ALA:HB1	1.64	0.79
1:C:159:GLN:CA	1:C:159:GLN:HE21	1.96	0.79
3:A:430:KAP:HA1	1:B:73:ALA:HB2	1.65	0.76
3:A:430:KAP:CA	1:B:73:ALA:HB2	2.16	0.76
1:C:174:PRO:HB2	1:C:175:PRO:CA	2.17	0.74
1:D:55:ARG:HG2	1:D:55:ARG:NH2	2.01	0.72
1:A:166:LEU:HD22	1:A:190:ALA:HB3	1.71	0.72
3:C:430:KAP:HB1	1:D:143:LEU:HD22	1.72	0.71
1:D:13:VAL:HG13	1:D:138:VAL:HG12	1.74	0.69
1:C:1:MET:SD	1:C:99:ASP:HA	2.32	0.68
1:B:116:GLU:HG3	1:B:121:GLY:HA2	1.76	0.68
1:C:1:MET:HB2	1:C:99:ASP:OD2	1.94	0.68
1:B:100:ARG:HH11	1:B:100:ARG:HG3	1.57	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HD2	1:A:47:ASP:OD2	1.95	0.67
1:D:45:ARG:HG3	1:D:46:GLY:N	2.09	0.67
1:B:119:GLU:OE2	1:B:119:GLU:HA	1.95	0.67
1:B:100:ARG:HH11	1:B:100:ARG:HG2	1.60	0.66
1:D:72:MET:HE3	1:D:76:ALA:CB	2.28	0.64
1:B:15:LYS:HZ3	1:B:111:GLY:HA2	1.63	0.64
1:A:-4:TYR:HB3	1:A:226:GLY:O	1.99	0.63
3:A:430:KAP:HG2	1:B:73:ALA:HA	1.80	0.62
1:D:27:ARG:NH1	1:D:57:ALA:O	2.33	0.61
1:B:15:LYS:NZ	1:B:111:GLY:HA2	2.15	0.61
1:C:23:ALA:O	1:C:27:ARG:HG3	1.99	0.61
1:A:151:LEU:HD23	1:B:114:LEU:HD22	1.84	0.60
3:C:430:KAP:HS2	1:D:143:LEU:HD11	1.84	0.59
1:D:118:ALA:HB3	1:D:122:VAL:CG2	2.32	0.57
1:B:9:THR:HB	1:B:148:HIS:HB3	1.86	0.57
1:D:125:ARG:HD2	4:D:227:HOH:O	2.04	0.57
1:A:118:ALA:HB3	1:A:122:VAL:HB	1.87	0.56
1:C:65:LEU:HB2	1:C:94:LEU:HD22	1.87	0.55
1:D:174:PRO:O	1:D:175:PRO:O	2.24	0.55
1:C:17:VAL:HG21	1:C:201:ALA:HB2	1.89	0.55
1:B:109:GLY:HA3	1:B:124:LEU:HD22	1.87	0.55
3:A:430:KAP:HA2	1:B:73:ALA:HB2	1.88	0.54
1:D:55:ARG:HH21	1:D:55:ARG:CG	2.07	0.54
1:A:88:ARG:HG3	1:A:122:VAL:HG11	1.90	0.54
1:C:173:ASP:HA	1:C:174:PRO:C	2.27	0.54
1:D:60:THR:CG2	1:D:61:GLN:OE1	2.57	0.53
1:B:100:ARG:CG	1:B:100:ARG:NH1	2.57	0.53
1:C:26:ALA:HB3	1:C:33:VAL:HG21	1.89	0.53
1:D:9:THR:HB	1:D:148:HIS:HB3	1.90	0.53
1:A:9:THR:HB	1:A:148:HIS:HB3	1.92	0.52
1:A:44:ALA:HB2	1:A:69:PRO:HB3	1.92	0.52
1:D:13:VAL:HG13	1:D:138:VAL:CG1	2.39	0.52
1:A:50:LEU:HG	1:A:62:LEU:HB3	1.92	0.51
1:C:171:TRP:CZ2	1:C:175:PRO:HG3	2.46	0.51
1:B:32:ASP:OD1	1:B:103:ARG:HD3	2.11	0.51
1:B:92:VAL:HG13	1:B:131:VAL:CG1	2.41	0.51
1:D:55:ARG:CG	1:D:55:ARG:NH2	2.71	0.51
1:D:100:ARG:O	1:D:103:ARG:HB3	2.11	0.51
1:D:18:VAL:HG22	1:D:196:LEU:HD22	1.94	0.50
1:D:42:GLY:O	1:D:47:ASP:HB2	2.10	0.50
1:D:13:VAL:HG23	1:D:140:THR:HG23	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ARG:HG2	1:D:220:TRP:CH2	2.47	0.49
1:C:174:PRO:CB	1:C:175:PRO:CA	2.90	0.49
1:D:60:THR:HG23	1:D:61:GLN:OE1	2.13	0.49
1:B:156:LEU:HD22	1:B:161:VAL:HG22	1.95	0.48
1:B:100:ARG:HG3	1:B:100:ARG:NH1	2.21	0.48
1:D:40:GLN:NE2	1:D:47:ASP:HB3	2.28	0.48
1:D:28:GLN:NE2	1:D:209:ALA:HB1	2.28	0.48
1:B:15:LYS:NZ	1:B:111:GLY:CA	2.77	0.48
1:C:154:GLU:CD	1:D:125:ARG:HH22	2.17	0.47
1:C:173:ASP:HA	1:C:174:PRO:O	2.14	0.47
1:D:203:LEU:HD22	1:D:207:ASP:HB3	1.97	0.47
1:B:172:PRO:HG2	1:B:175:PRO:HA	1.95	0.47
1:B:42:GLY:O	1:B:47:ASP:HB2	2.14	0.47
1:B:39:VAL:HG11	1:B:74:PRO:HB3	1.97	0.47
1:B:97:ASP:HB2	4:B:254:HOH:O	2.15	0.47
1:B:116:GLU:HG3	1:B:121:GLY:CA	2.44	0.47
1:A:99:ASP:O	1:A:100:ARG:HD3	2.15	0.46
1:D:211:MET:C	1:D:211:MET:SD	2.94	0.46
1:C:102:GLY:O	1:C:225:VAL:HG11	2.15	0.46
1:A:151:LEU:CD2	1:B:114:LEU:HD22	2.45	0.46
1:D:204:ASP:O	1:D:205:ALA:HB2	2.16	0.46
1:C:73:ALA:HA	3:C:430:KAP:HG2	1.98	0.45
1:C:73:ALA:HB2	3:C:430:KAP:HA2	1.99	0.45
1:D:59:VAL:HG12	1:D:62:LEU:HD13	1.98	0.45
1:C:103:ARG:HG3	1:C:104:LEU:N	2.32	0.45
1:C:37:LYS:HB3	1:C:50:LEU:HD22	1.98	0.45
1:C:43:THR:OG1	1:C:69:PRO:HA	2.17	0.45
1:A:29:ALA:HB2	1:A:218:ARG:HE	1.82	0.44
1:D:100:ARG:HA	1:D:101:PRO:HD2	1.83	0.44
1:C:32:ASP:OD1	1:C:103:ARG:HD3	2.17	0.44
1:D:89:ASP:O	1:D:93:ARG:HG3	2.17	0.44
1:B:43:THR:HG21	1:B:67:ARG:HB3	2.00	0.44
1:B:37:LYS:HD2	1:B:108:GLU:HG2	1.98	0.43
1:C:50:LEU:HG	1:C:62:LEU:HB3	1.98	0.43
1:D:88:ARG:O	1:D:92:VAL:HG13	2.17	0.43
1:D:43:THR:HG21	1:D:67:ARG:HB3	2.00	0.43
1:B:2:THR:CG2	1:B:224:LEU:O	2.67	0.43
1:C:166:LEU:HD22	1:C:190:ALA:HB3	2.01	0.43
1:C:172:PRO:HG2	1:C:175:PRO:HB3	2.00	0.43
1:B:89:ASP:O	1:B:93:ARG:HB2	2.19	0.42
1:D:125:ARG:CD	4:D:227:HOH:O	2.65	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ALA:O	1:B:115:VAL:HG11	2.19	0.42
1:D:193:ARG:HG2	1:D:220:TRP:CZ2	2.54	0.42
1:C:158:ALA:O	1:C:159:GLN:NE2	2.53	0.42
1:B:119:GLU:HA	1:B:120:PRO:HA	1.94	0.41
1:C:31:ILE:HD11	1:C:222:ALA:HA	2.03	0.41
1:B:92:VAL:HG13	1:B:131:VAL:HG12	2.02	0.41
1:B:15:LYS:HE3	4:B:234:HOH:O	2.20	0.41
1:D:186:LEU:HD23	1:D:189:ILE:HD11	2.03	0.41
1:A:43:THR:HG21	1:A:67:ARG:HB3	2.02	0.41
1:B:48:ASP:OD1	1:B:51:ALA:HB2	2.20	0.41
1:A:225:VAL:HG23	1:A:225:VAL:O	2.21	0.41
1:D:127:VAL:O	1:D:131:VAL:HG22	2.21	0.41
1:C:149:THR:O	1:C:153:LEU:HG	2.22	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	228/251 (91%)	224 (98%)	4 (2%)	0	100	100
1	B	222/251 (88%)	217 (98%)	4 (2%)	1 (0%)	29	28
1	C	224/251 (89%)	216 (96%)	6 (3%)	2 (1%)	17	15
1	D	221/251 (88%)	211 (96%)	3 (1%)	7 (3%)	4	1
All	All	895/1004 (89%)	868 (97%)	17 (2%)	10 (1%)	14	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	174	PRO
1	D	175	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	205	ALA
1	B	84	ALA
1	C	1	MET
1	D	200	ALA
1	D	84	ALA
1	D	201	ALA
1	D	46	GLY
1	D	120	PRO

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	156/173 (90%)	139 (89%)	17 (11%)	6	5
1	B	151/173 (87%)	139 (92%)	12 (8%)	12	11
1	C	153/173 (88%)	139 (91%)	14 (9%)	9	8
1	D	150/173 (87%)	131 (87%)	19 (13%)	4	3
All	All	610/692 (88%)	548 (90%)	62 (10%)	7	6

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	45	ARG
1	A	50	LEU
1	A	60	THR
1	A	65	LEU
1	A	67	ARG
1	A	103	ARG
1	A	119	GLU
1	A	143	LEU
1	A	153	LEU
1	A	166	LEU
1	A	181	SER
1	A	184	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	193	ARG
1	A	218	ARG
1	A	224	LEU
1	A	225	VAL
1	B	2	THR
1	B	15	LYS
1	B	60	THR
1	B	93	ARG
1	B	94	LEU
1	B	100	ARG
1	B	103	ARG
1	B	104	LEU
1	B	114	LEU
1	B	151	LEU
1	B	161	VAL
1	B	177	LEU
1	C	4	LEU
1	C	11	THR
1	C	50	LEU
1	C	59	VAL
1	C	65	LEU
1	C	93	ARG
1	C	103	ARG
1	C	104	LEU
1	C	124	LEU
1	C	143	LEU
1	C	150	LYS
1	C	159	GLN
1	C	166	LEU
1	C	225	VAL
1	D	13	VAL
1	D	15	LYS
1	D	50	LEU
1	D	55	ARG
1	D	60	THR
1	D	62	LEU
1	D	65	LEU
1	D	72	MET
1	D	99	ASP
1	D	103	ARG
1	D	104	LEU
1	D	125	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	143	LEU
1	D	151	LEU
1	D	159	GLN
1	D	166	LEU
1	D	193	ARG
1	D	218	ARG
1	D	221	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	C	159	GLN
1	D	80	HIS
1	D	160	GLN
1	D	219	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSX	C	163	1	3,6,7	0.57	0	1,6,8	0.88	0
1	CSX	A	163	1	3,6,7	1.05	0	1,6,8	0.46	0
1	CSX	D	163	1	3,6,7	0.55	0	1,6,8	0.68	0
1	CSX	B	163	1	3,6,7	4.21	1 (33%)	1,6,8	2.43	1 (100%)

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	CSX	C	163	1	-	0/1/5/7	-
1	CSX	A	163	1	-	0/1/5/7	-
1	CSX	D	163	1	-	0/1/5/7	-
1	CSX	B	163	1	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	CSX	O-C	7.12	1.48	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	CSX	CA-CB-SG	-2.43	108.05	113.36

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](#)

7 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
2	SO4	D	252	-	4,4,4	0.20	0	6,6,6	0.29	0
3	KAP	B	430	-	8,12,12	0.97	1 (12%)	7,14,14	1.55	2 (28%)
2	SO4	A	250	-	4,4,4	0.28	0	6,6,6	0.20	0
2	SO4	B	251	-	4,4,4	0.20	0	6,6,6	0.30	0
3	KAP	A	430	-	8,12,12	0.90	1 (12%)	7,14,14	2.19	3 (42%)
3	KAP	C	430	-	8,12,12	0.75	0	7,14,14	1.74	2 (28%)
2	SO4	C	253	-	4,4,4	0.16	0	6,6,6	0.42	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	KAP	A	430	-	-	3/8/12/12	-
3	KAP	B	430	-	-	2/8/12/12	-
3	KAP	C	430	-	-	3/8/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	430	KAP	CE-CZ	2.26	1.54	1.51
3	A	430	KAP	CE-CZ	2.04	1.54	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	430	KAP	CD-CE-CZ	-4.27	107.19	114.60
3	C	430	KAP	CD-CE-CZ	-3.31	108.86	114.60
3	A	430	KAP	CE-CZ-CH	2.98	122.68	116.94
3	B	430	KAP	CD-CE-CZ	-2.65	110.00	114.60
3	C	430	KAP	CE-CZ-CH	2.56	121.88	116.94
3	B	430	KAP	CE-CZ-CH	2.53	121.81	116.94
3	A	430	KAP	O-CZ-CE	-2.12	117.93	121.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	430	KAP	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	430	KAP	CE-CD-CG-CB
3	B	430	KAP	CS-CH-CZ-O
3	C	430	KAP	CS-CH-CZ-O
3	B	430	KAP	CS-CH-CZ-CE
3	C	430	KAP	CS-CH-CZ-CE
3	A	430	KAP	CS-CH-CZ-O
3	A	430	KAP	CS-CH-CZ-CE

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	430	KAP	4	0
3	C	430	KAP	4	0

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	230/251 (91%)	0.12	8 (3%)	44	44	17, 29, 45, 62	2 (0%)
1	B	223/251 (88%)	0.04	5 (2%)	62	62	21, 33, 52, 73	4 (1%)
1	C	226/251 (90%)	-0.03	7 (3%)	49	50	26, 36, 53, 75	2 (0%)
1	D	223/251 (88%)	0.40	19 (8%)	10	11	25, 40, 62, 74	2 (0%)
All	All	902/1004 (89%)	0.13	39 (4%)	35	36	17, 34, 56, 75	10 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-4	TYR	6.3
1	C	177	LEU	4.3
1	D	203	LEU	4.0
1	D	6	VAL	4.0
1	C	174	PRO	3.6
1	D	44	ALA	3.5
1	A	6	VAL	3.3
1	D	45	ARG	3.3
1	D	47	ASP	3.1
1	D	56	LEU	3.1
1	D	107	VAL	3.1
1	D	206	GLY	3.0
1	D	46	GLY	3.0
1	D	199	GLY	2.9
1	C	0	HIS	2.9
1	D	204	ASP	2.7
1	A	58	GLY	2.6
1	A	5	VAL	2.5
1	C	6	VAL	2.4
1	A	226	GLY	2.4
1	B	110	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	173	ASP	2.4
1	C	100	ARG	2.3
1	B	6	VAL	2.3
1	C	79	GLU	2.3
1	A	7	THR	2.2
1	B	44	ALA	2.2
1	A	219	ASN	2.1
1	D	36	CYS	2.1
1	D	109	GLY	2.1
1	D	210	ALA	2.1
1	B	113	LEU	2.1
1	D	198	ALA	2.1
1	D	208	PHE	2.1
1	A	109	GLY	2.1
1	D	30	GLY	2.1
1	D	205	ALA	2.1
1	D	70	GLN	2.0
1	B	36	CYS	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	CSX	B	163	7/8	0.90	0.16	32,34,36,54	0
1	CSX	A	163	7/8	0.94	0.14	26,31,33,35	0
1	CSX	C	163	7/8	0.94	0.06	27,30,34,37	0
1	CSX	D	163	7/8	0.95	0.10	36,39,43,47	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. 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
3	KAP	C	430	13/13	0.82	0.36	20,30,38,42	9
3	KAP	A	430	13/13	0.89	0.28	26,35,46,47	9
3	KAP	B	430	13/13	0.93	0.14	21,33,43,48	0
2	SO4	D	252	5/5	0.98	0.09	42,50,52,59	0
2	SO4	C	253	5/5	0.99	0.16	43,47,52,52	0
2	SO4	B	251	5/5	1.00	0.09	23,28,31,32	0
2	SO4	A	250	5/5	1.00	0.05	26,29,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.